Roberto Battiti · Mauro Brunato

The LION Way

Machine Learning *plus* Intelligent Optimization

Version 3.0 — December 2017

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Chapter 1

Introduction

Fatti non foste a viver come bruti ma per seguir virtute e canoscenza
You were not made to live like beasts, but to follow virtue and knowledge.
(Dante Alighieri)

QVI COELVM CECINIT MEDIVMQVE IMVMQVE TRIBVNAL LVSTRAVITQVE ANIMO CVNCTA POETA SVO DOCTVS ADEST DANTES SVA QVEM FLORENTIA SAEPE
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1.1 Learning and Intelligent Optimization: a prairie fire

Almost by definition, **optimization, the automated search for improving solutions, is a tireless power** for continually improving processes, decisions, products and services. This is related to decision making but goes far beyond that. Decision making picks the best among a set of possible solutions which is given, optimization actively **creates new solutions**.

Optimization fuels **automated creativity and innovation**. It looks like a manifest contradiction, because creativity is usually *not* related to automation. This is why the message you will find in this book is disruptive, far from trivial, even irritating and provoking for people believing that machines are only for shallow mechanical and repetitive tasks.

Starting from Galileo Galilei (1564-1642), to change the world with science, not only to interpret it with philosophy, one needs **measurements and experiments**. “Measure what is measurable, and make measurable what is not so.” Measurements start shy and humble but permit a gradual and pragmatic conquering of the world as far as production means and quality of life are concerned.

Almost all business problems can be formulated as **finding an optimal decision x by maximizing a measure** *goodness*$(\boldsymbol{x})$. For a concrete mental image, think of $\boldsymbol{x}$ as a collective variable $\boldsymbol{x} = (x_1, \ldots, x_n)$ describing the settings of one or more knobs to be rotated, choices to be made, parameters to be fixed. In marketing, $\boldsymbol{x}$ can be a vector of values specifying the budget allocation to different campaigns (TV, newspaper, web, social), and *goodness*$(\boldsymbol{x})$ can be a count of the new customers generated by the campaign. In website optimization, $\boldsymbol{x}$ can be related to using images, links, topics, text of different size, and *goodness*$(\boldsymbol{x})$ can be the conversion rate from a casual visitor to a customer. In engineering, $\boldsymbol{x}$ can be the set of all design choices of a car motor, *goodness*$(\boldsymbol{x})$ can be the miles per gallon traveled.

Formulating a problem as “optimize a goodness function” also **encourages decision makers to use quantitative goals, to understand intents in a measurable manner, to focus on policies more than on implementation details**. Getting stuck in implementations, to the point of forgetting goals, is a plague infecting businesses and limiting their speed of movement when external conditions change.

Automation is the key: after formulating the problem, deliver the goodness model to a computer which will create and search for one or more optimal choices. And when conditions or priorities change, just revise the goals quantified by the goodness measure, restart the optimization process, *et voilà*. To be sure, CPU time is an issue and globally-optimal solutions are not always guaranteed, but for sure the speed and latitude of the search by computers surpass human capabilities by a huge and growing factor.

But the awesome power of optimization is still largely stifled in most real-world contexts. The main reason blocking its widespread adoption is that **standard mathematical optimization assumes the existence of a function** to be maximized, in other words, an explicitly defined model *goodness*$(\boldsymbol{x})$ associating a result to each input configuration $\boldsymbol{x}$. Now, in most real-world business contexts this function does not exist or is extremely difficult and costly to build by hand. Try asking a CEO “Can you please tell me the mathematical formula that your business is optimizing?”, probably this is not the best way to start a conversation for a consultancy job. For sure, a manager has *some* ideas about objectives and tradeoffs, but these objectives are not specified as a mathematical model, they are dynamic, changing in time, fuzzy and subject to estimation errors and human learning processes. *Gut feelings* and intuition are assumed to substitute clearly specified, quantitative and data-driven decision processes.

If optimization is fuel, the match to light the fire is **machine learning**. Machine learning comes to the rescue by renouncing to a clearly specified goal *goodness*$(\boldsymbol{x})$: **the goodness model can be built by machine learning from abundant data**.

Learning and Intelligent Optimization (LION) is the combination of learning from data and optimization to solve complex and dynamic problems. The LION way is about increasing the automation level and connecting data directly to decisions and actions. **Prescriptive analytics** is the third and final phase, beyond descriptive and predictive analytics. With support of the right software, more **power is directly in the hands of decision makers in a self-service manner**, without resorting to intermediate layers of data scientists. LION is a complex array of mechanisms, like the engine in a car, but the user (driver) does not need to know the inner workings of the engine in order to realize its tremendous benefits. LION’s adoption will create a prairie fire of innovation which will reach most businesses in the next decades. Businesses, like plants in wildfire-prone ecosystems, will survive and prosper by adapting and embracing LION techniques, or they risk being transformed from giant trees to ashes by the spreading competition.

The questions to be asked in the LION paradigm are not about mathematical goodness models but about abundant data, expert judgment of concrete options (examples of success cases), interactive definition of success criteria, at a level which makes a human person at ease with his mental models. For example, in marketing, relevant data can describe the money allocation and success of previous campaigns, in engineering they can describe experiments about motor designs (real or simulated) and corresponding measurements of fuel consumption.

1.2 Searching for gold and for partners

Machine learning for optimization needs data. Data can be created by **the previous history of the optimization process** or by **feedback by decision makers**.

Figure 1.1: Danie Gerhardus Krige, the inventor of *Kriging*.

To understand the two contexts, let's start with two concrete examples. Danie G. Krige, a South African mining engineer, had a problem to solve: how to identify the best coordinates $\boldsymbol{x}$ on a geographical map where to dig gold mines [242]. Around 1951 he began his pioneering work on applying insights in statistics to the valuation of new gold mines by using a limited number of boreholes. The function to be optimized was a glittering *Gold*$(\boldsymbol{x})$, the quantity of gold extracted from a mine at position $\boldsymbol{x}$. For sure, evaluating *Gold*$(\boldsymbol{x})$ at a new position $\boldsymbol{x}$ is very costly. As you can imagine, digging a new mine is not a quick and simple job. But after digging some exploratory mines, engineers accumulate **knowledge in the form of examples** relating coordinates $\boldsymbol{x}_1$, $\boldsymbol{x}_2$, $\boldsymbol{x}_3$... to the corresponding gold quantities *Gold*$(\boldsymbol{x}_1)$, *Gold*$(\boldsymbol{x}_2)$, *Gold*$(\boldsymbol{x}_3)$. Krige's intuition was to use these examples (**data about the previous history of the optimization process**) to build a model of the function *Gold*$(\boldsymbol{x})$, let's call it *GoldModel*$(\boldsymbol{x})$, which could generalize the experimental results by predicting output values for each position $\boldsymbol{x}$. The model could be used by an optimizer to identify the next point to dig, by finding the position $\boldsymbol{x}_{best}$ maximizing the estimated gold output of *GoldModel*$(\boldsymbol{x})$.

Think of this model as starting from "training" information given by pins at the boreholes locations, with height proportional to the gold content found, and building a complete surface over the geographical area, with height at a given position proportional to the estimated gold content (Fig. 1.2). Optimizing means identifying the highest point on this model surface, and the corresponding position where to dig the next mine.

This technique is now called *Kriging* and it is based on the idea that the output value at an unknown point should be the average of the known values at its neighbors, weighted by the neighbors' distance to the unknown point. *Gaussian processes, Bayesian inference, splines* refer to related modeling techniques.

For the second example about getting **feedback by decision makers**, let's imagine a dating service: you pay and you are delivered a contact with the best possible partner from millions of waiting candidates. In Kriging the function to be optimized exists, it is only extremely difficult to evaluate. In this case, it is difficult to assume that a function *IdealMate*$(\boldsymbol{x})$ exists, relating individual characteristics $\boldsymbol{x}$ like beauty, intelligence, etc. to your individual preference. If you are not convinced and you think that this function does exist, as homework you are invited to define in precise mathematical terms the *IdealMate* function for your ideal partner. Even assuming that you can identify some building

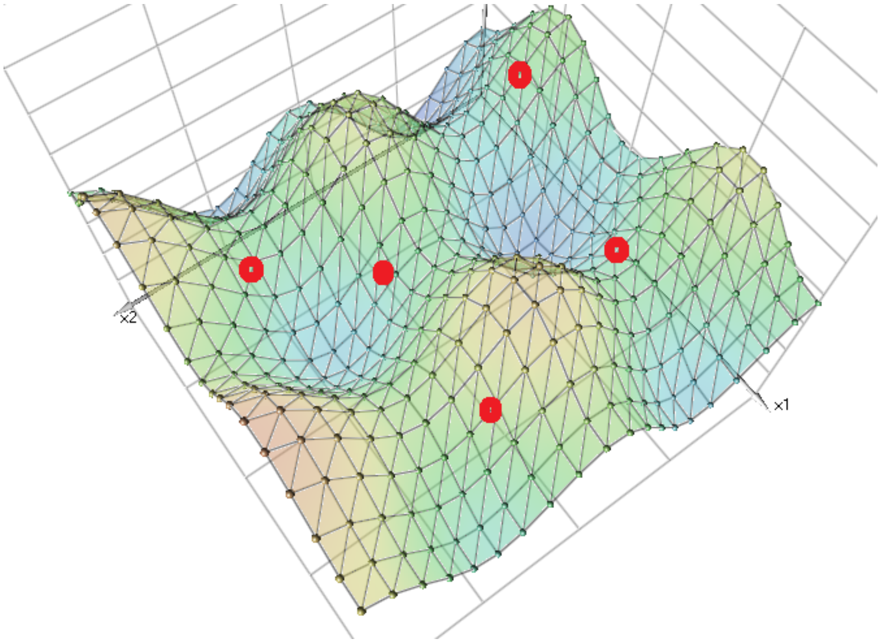


Figure 1.2: *Kriging* method constructing a model from samples. Some samples are shown as dots. Height and color of the surface depend on gold content.

blocks and make them precise, like *Beauty*$(\boldsymbol{x})$ and *Intelligence*$(\boldsymbol{x})$, you will have difficulties in combining the two objectives *a priori*, before starting the search for the optimal candidate. Questions like: "How many IQ points are you willing to sacrifice for one less beauty point?" or "Is beauty more important than intelligence for you? By how much?" will be difficult to answer. Even if you are tortured and deliver an initial answer, for sure you will not trust the optimization and you will probably like to give a look at the real candidate before paying the matching service and be satisfied. You will want to know the $\boldsymbol{x}$ and not only the value of the provisional function *IdealMate*$(\boldsymbol{x})$ that the system will optimize. Only after considering different candidates and giving feedback to the matching service you may hope to identify your best significant other.

In other words, some information about the function to be optimized is missing at the beginning, and only the decision maker will be able to fine-tune the search process. **Solving many if not most real-world problems requires iterative processes with learning involved**. The user will learn and adjust his preferences after knowing more and more cases, the system will build models of the user preferences from his feedback. The steps will continue until the user is satisfied or the time allocated for the decision is finished.

1.3 All you need is data

Let's continue with some motivation for business users. If this is not your case you can safely skip this part and continue with Section 1.7.

Enterprises are flooded with data in digital form. Big data is a popular term to refer to abundant and partially structured data. By the way, data used to be much bigger *with respect to available storage* in the seventies and eighties so that the term "big data" now is more related to marketing hype than to reality: a single PC will easily deal with all data produced by all apart from the biggest companies.

With the explosion in social network usage, rapidly expanding e-commerce, and the rise of the internet of things, the web is creating a tsunami of structured and unstructured data, driving billions in spending on information technology. Recent evidence also indicates a decline in the use of standard business intelligence platforms as enterprises are forced to consider a mass of unstructured data that has uncertain real-world value. For example, social networks create vast amounts of data, most of which resists classification and the rigid hierarchies of traditional data. How do you measure the value of a Facebook *Like*? Moreover, unstructured data requires an adaptive approach to analysis. How does the value of a *Like* change over time? These questions are driving the adoption of advanced methodologies for data modeling, adaptive learning, and optimization.

LION tools deal with software capable of self-improvement and rapid adaptation to new data and revised business objectives. The strength in this approach lies in abilities that are often associated with the human brain: learning from past experiences, **learning on the job**, coping with incomplete information, and quickly adapting to new situations.

This inherent flexibility is critical where decisions depend on factors and priorities that are not identifiable before starting the solution process. For example, what factors should be used and to what degree do they matter in scoring the value of a marketing lead? With the LION approach, the answer is: “It doesn’t matter.” The system will begin to train itself, and successive data plus feedback by the final user will rapidly improve performance. Experts —in this case marketing managers— can further refine the output by contributing their points of view.

1.4 Beyond traditional business intelligence

Every business has three fundamental needs from their data:

1. to **understand** the current business processes and to review past performance;
2. to **predict** the effect of business decisions;
3. to **improve** profitability by identifying and implementing informed and rational decisions about critical business factors.

Traditional **descriptive** business intelligence excels at recording and visualizing historical performance. Building these maps meant hiring a top-level consultancy or on-boarding of personnel specifically trained in statistics, analysis, and databases. Experts had to design data extraction and manipulation processes and hand them over to programmers for the actual execution. This is a slow and cumbersome process when you consider the dynamic environment of most businesses.

As a result, enterprises relying heavily on BI are using snapshots of performance to try to understand and react to conditions and trends. Like driving a car by looking into the rear view mirror, it’s most likely that you’re going to hit something. For the enterprise, it appears that they already have hit a wall of rigidity and lack of quick adaptation.

Predictive analytics does better in trying to anticipate the effect of decisions, but the real power comes from the **integration of data-driven models with optimization**, the automated creation of improving solutions. **Prescriptive analytics** leads from the data directly to the best improving plan, **from data, to actionable insight, to actions**!

1.5 Implementing LION

The steps for fully adopting LION as a business practice vary depending on the current business state, and most importantly, on the state of the underlying data. It goes without saying that it is easier and less costly to introduce the paradigm if data capture has already been established. For some enterprises, legacy systems can prove quite costly to migrate, as there is extensive cleaning involved. This is where skilled service providers can play a valuable role.

Beyond cleaning and defining the structure of the underlying data, the most important factor is to establish a collaboration between the data analytics team and their business end-user customers. By its nature, LION presents a way to collectively discover the hidden potential of structured and semi-structured data stores. The key in having the data analytics team work effectively alongside the business end-user is to enable changing business objectives to quickly reflect into the models. The introduction of LION methods can help analytics teams generate radical changes in the value-creation chain, revealing hidden opportunities and increasing the speed by which their business counterparts can respond to customer requests and to changes in the market.

The job market will also be disrupted. Software learning from human examples will infer the rules we tacitly apply but do not explicitly understand. This will eliminate barriers to further automation and substitute machines for workers in many tasks requiring adaptability, common sense and creativity, possibly putting the middle class at risk[367].

The LION way is a radically disruptive **intelligent approach to uncover hidden value, quickly adapt to changes and improve businesses**. Through proper planning and implementation, LION will help enterprises to lead the competition and avoid being burned by wild prairie fires, and will help individuals to remain competitive in the high-skill job market.

1.6 Teaching and learning in Internet times

Figure 1.3: A professor teaching “ex cathedra” in a University.

Books were made by hand in the middle ages, carefully written by *amanuensis* on parchment made from animal skins. In addition to hundreds of killed animals, a total of some man years were required for a single illustrated copy. The University institution, *universitas magistrorum et scholarium* – “community of teachers and scholars”, the first one founded in 1088 in Bologna, was created to make knowledge cheaper and accessible to more people, and, by the way, more free . A professor used to stay in front of an audience to read a book “*ex cathedra*” to the students for subsequent discussion and deepening. For most of them, this was the only way to get knowledge.

We think that books still have a role is this era of information-at-your-fingertips, but a different one with respect to the ages before internet and the web. Nobody needs books to get detailed knowledge, demonstration of theorems, pieces of software, original research papers. But human people need a **global vision and connected ideas** to solve problems in a professional manner. A book is like a mental map to orient our steps in a foreign territory. In a tourism analogy one needs to know the whole "meaning" of Trentino-South Tirol, its peaks (cathedrals in the Alps), its abundance of public mountain huts, the pleasure of dining together with people hiking and climbing from all over the world, in order to be motivated to spend a vacation here. Then the dots can be easily connected with web reservations, train schedules, getting the proper boots, etc.

Our goal is to give a clear map of machine learning and intelligent optimization, **some concrete and connected ideas that will stick to your mind** and that will guide you in the search for details and software when they are needed. On the contrary, if too much effort is spent on details, they will be easily forgotten some days after your university exam is passed. As an example, one can easily find software for realizing a specific ML model from examples, but the lack of a global vision about how to proceed can lead to catastrophic mistakes like confusing training error with generalization error, or putting the random ID of a customer in the inputs to derive some marketing measure, or picking a sub-symbolic neural-network model when a human explanation of a diagnosis is required.

Needless to say, the definition of what is basic and what is detail is personal and subject to discussion. Our choice is based on tens of courses on the subject but we take the full responsibility for the lack of completeness in this huge territory covering machine learning and optimization.

If one does not know to which port one is sailing, no wind is favorable (*Ignoranti quem portum petat, nullus suus ventus est* - Seneca).

1.7 A "hands on" community approach

Because this book is about (machine) learning from examples we need to be coherent: most of the content follows the learning from examples and **learning-by-doing** principle. The different techniques are introduced by presenting the basic theory, and concluded by giving the "gist to take home." Experimentation on real-world cases is encouraged with the examples and software in the book website. This is the best way to avoid the impression that LION techniques are only for experts and not for practitioners in different positions, interested in quick and measurable results.

Some of the theoretical parts can be skipped for a first adoption. But some knowledge of the theory is critical both for developing new and more advanced LION tools and for a more competent use of the technology.

We tried to keep both developers and final users in mind in our effort.

Accompanying data, instructions and short tutorial movies by us and by our community of readers will be posted on the book's website:

`http://intelligent-optimization.org/LIONbook/.`

A sign of gratitude goes to the many contributors to our effort. Let's start from photos and drawings. Venice photo by Carlo Nicolini for LION4@VENICE 2010. Dante's painting in the Introduction by Domenico di Michelino, Florence, 1465. Mushroom basket image by George Chernilevsky. Brain drawing in the Neural Networks chapter by Leonardo da Vinci (1452 − 1519). Deep network for clustering figure by Geoffrey Hinton. Photo of prof. Vapnik in

the SVM chapter from Yann LeCun. Extreme Learning Machine image by Guangbin Huang. Reservoir architecture image by Herbert Jaeger. Venice painting in the Democracy chapter by Canaletto, 1730. Painting in the Clustering chapter by Michelangelo Buonarroti (Sistine Chapel), 1541. Wikipedia has been mined for some explanatory images, while the authors and their sons contributed to the wikipedia project with additional images and definitions. Hopfield network figure by Gorayni, energy landscape by Mrazvan22. Lagrange multipliers figure from Nexcis (wikipedia). Reschensee photo in reservoir chapter by Markus Bernet. Frog image by André Karwath. Hopfield network images by Alejandro Cartas Ayala. Viterbis' algoritm figure by Luz Abril Torres-Méndez. Fig. 24.10 from Randall Munroe *xkcd* webcomic. Dart photo in Chapter 25 by Harris Morgan. Initial figure of Satisfiability chapter from Squidsoup art group installation.

Last but not least, we are happy to acknowledge the growing contribution of our readers to the quality of this book including Patrizia Nardon, Fabian Pedregosa, Fred Glover, Alberto Todeschini, Yaser Abu-Mostafa, Marco Dallariva, Enrico Sartori, Danilo Tomasoni, Nick Maravich, Marco Zugliani, Dinara Mukhlisullina, Rohit Jain, Jon Lehto, George Hart, Markus Dreyer, Yuyi Wang, Gianluca Bortoli, Davide Pedranz, Stefano Fioravanzo. Cartoons are courtesy of Marco Dianti. We are always pleased to communicate with our readers. Please email us with comments, suggestions or *errata* and we will be glad to add your name in the next edition. You find a contact form and email addresses in our LIONlab website:

`http://intelligent-optimization.org/.`

Addendum to Version 3.0

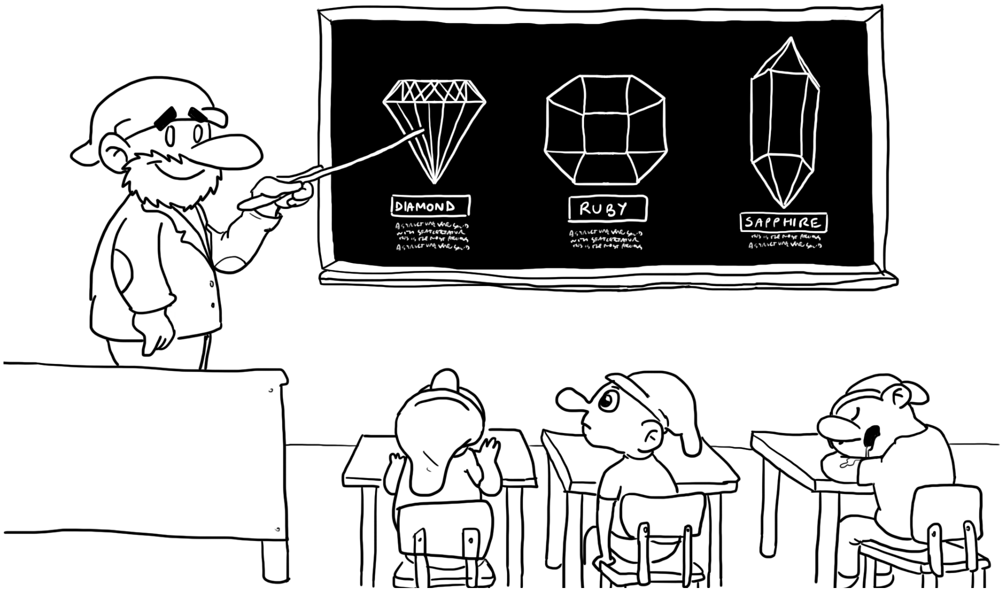
You are now reading version 3.0 of this book: the main changes with respect to the previous version are:

- A new section on **hashing** (Sec. 2.2) and locality-sensitive Hashing (LSH) and approximated nearest neighbors (Sec. 2.3). Hashing is one of the most useful tricks in computer science, but not widely known to ML users.
- The addition of more details related to entropy and mutual information (Sec. 7.6), including generalization to continous variables.
- The addition of a new section about **projection pursuit** (Sec. 20.6) in Chapter 20 dedicated to linear projections.
- The addition of a new Chapter about Feature extraction and Independent Component Analysis (ICA) (Chapter 21)

Chapter 2

Lazy learning: nearest neighbors

Natura non facit saltus
Nature does not make jumps



If you still remember how you learned to read, you have everything it takes to understand **learning from examples**, in particular supervised learning. Your parents and your teachers presented you with examples of written characters (“a”, “b”, “c”, ...) and told you: This is an “a”, this is a “b”, ...

For sure, they did not specify mathematical formulas or precise rules for the geometry of “a” “b” “c”... They just presented **labeled examples**, in many different styles, forms, sizes, colors. From those examples, after some effort and some mistakes, your brain managed not only to recognize the examples in a correct manner, which you can do via memorization, but to extract the underlying patterns and regularities, to filter out irrelevant “noise” (like the color) and to **generalize by recognizing new cases**, not seen during the training phase. A natural but remarkable result indeed. It did not require advanced theory, it did not require a PhD. Wouldn’t it be nice if you could solve business problems in the same natural and effortless way? The LION unification of learning from data and optimization is the way and we will start from this familiar context.

Figure 2.1: Mushroom hunting requires classifying edible and poisonous species.

In **supervised learning** a system is trained by a supervisor (teacher) giving **labeled examples**. Each example is an array, a *vector* of input parameters $\boldsymbol{x}$ called **features** with an associated output label y.

The authors live in an area of mountains and forests and a very popular pastime is mushroom hunting. Popular and fun, but deadly if the wrong kind of mushroom is eaten. Kids are trained early to distinguish between edible and poisonous mushrooms. Tourists can buy books showing photos and characteristics of both classes, or they can bring mushrooms to the local Police and have them checked by experts for free.

Let's consider a simplified example, and assume that two parameters, like the height and width of the mushrooms are sufficient to discriminate them, as in Fig. 2.2. In general, imagine many more input parameters, like color, geometrical characteristics, smell, etc., and a much more confused distribution of positive (edible) and negative cases.

Lazy beginners in mushroom picking follow a simple pattern. They do not study anything before picking; after all, they are in awesome Trentino for vacation, not for work. When they spot a mushroom they search in the book for images of similar ones and then double-check for similar characteristics listed in the details. This is a practical usage of the **lazy "nearest neighbor" method of machine learning**.

Why does this simple method work? The explanation is in the *Natura non facit saltus* (Latin for "nature does not make jumps") principle. Natural things and properties change gradually, rather than suddenly. If you consider a prototype edible mushroom in your book, and the one you are picking has very similar characteristics, you may assume that it is edible too.

Disclaimer: do not use this toy example to classify real mushrooms, every classifier has a probability of making mistakes and *false positive* classifications of mushrooms (classifying it as non-poisonous when in fact it is) can be very harmful to your health.

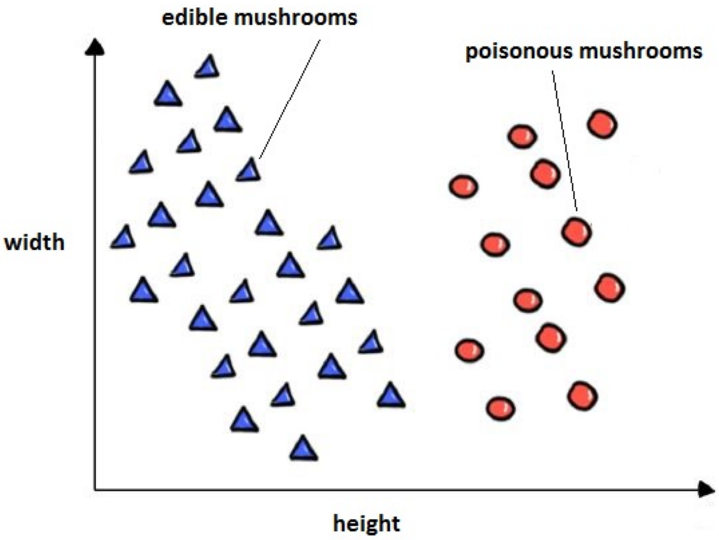


Figure 2.2: A toy example: two features (width and height) to classify edible and poisonous mushrooms.

2.1 Nearest Neighbors Methods

The **nearest-neighbors** basic form of learning, also related to **instance-based learning**, **case-based** or **memory-based**, works as follows. The labeled examples (inputs and corresponding output labels) are stored and no action is taken until a new input pattern demands an output value. The system is a **lazy learner**: it does nothing but store labelled examples until the user interrogates them. When a new input pattern arrives, the memory is searched for examples which are *near* the new pattern, and the output is determined by retrieving the stored outputs of the close patterns, as shown in Fig. 2.3. Over a century old, this form of data mining is still being used very intensively by statisticians and machine learners alike, both for classification and for regression problems.

A simple version is that the output for the new input is simply that of the *closest* example in memory. If the task is to classify mushrooms as edible or poisonous, a new mushroom is classified in the same class as the most similar mushrooms in the memorized set.

Although simple, surprisingly this technique is effective in many cases. It pays to be lazy! Unfortunately, the time to recognize a new case can grow in a manner proportional to the number of stored examples unless less lazy methods are used. Think about a student who is just collecting books, and then reading them only when confronted with a problem to solve.

A more robust and flexible technique considers a set of k nearest neighbors instead of one, not surprisingly it is called **k-nearest-neighbors (KNN)**. The flexibility is given by different possible classification techniques. For example, the output can be that of the **majority** of the k neighbors outputs. If one wants to be on the safer side, one may decide to classify the new case only if all k outputs agree (**unanimity rule**), and to report “unknown” in the other cases. This can be suggested for classifying edible mushrooms: if “unknown” contact the local mushroom police for guidance.

If one considers **regression** (the prediction of a real number, like the content of poison in a mushroom), the output can be obtained as a simple average of the outputs corresponding to the k closest examples.

Of course, the vicinity of the k examples to the new case can be very different and in some cases it is reasonable

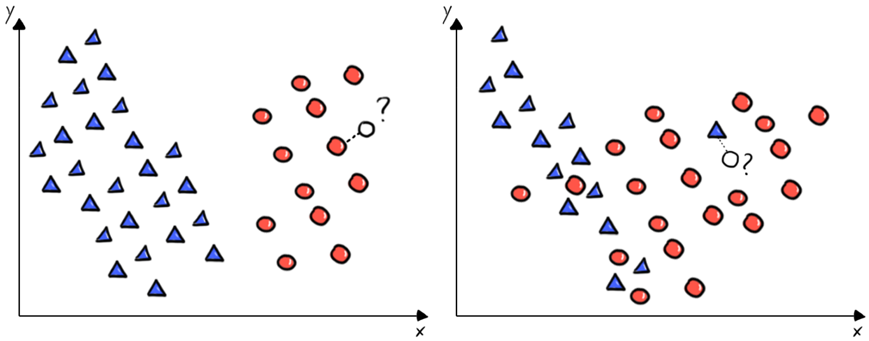


Figure 2.3: Nearest neighbor classification: a clear situation (left), a more confusing situation (right). In the second case the nearest neighbor to the query point with the question mark belongs to the wrong class although most other close neighbors belong to the right class.

that closer neighbors should have a bigger influence on the output. In the **weighted k-nearest-neighbors** technique (WKNN), the weights depend on the distance.

Let ℓ be the number of labeled examples and $k \leq \ell$ be a fixed positive integer, and consider a feature vector $\boldsymbol{x}$. A simple algorithm to estimate its corresponding outcome y consists of two steps:

1. Find within the training set the k indices $i_1, \ldots, i_k$ whose feature vectors $\boldsymbol{x}_{i_1}, \ldots, \boldsymbol{x}_{i_k}$ are nearest (according to a given feature-space metric) to the given $\boldsymbol{x}$ vector.

2. Calculate the estimated outcome y by the following average, weighted with the inverse of the distance between $\boldsymbol{x}$ and the stored feature vectors:

$$y = \frac{\displaystyle\sum_{j=1}^{k} \frac{y_{i_j}}{d(\boldsymbol{x}_{i_j}, \boldsymbol{x}) + d_0}}{\displaystyle\sum_{j=1}^{k} \frac{1}{d(\boldsymbol{x}_{i_j}, \boldsymbol{x}) + d_0}}; \tag{2.1}$$

   where $d(\boldsymbol{x}_i, \boldsymbol{x})$ is the distance between the two vectors in the feature space (for example the Euclidean distance), and d_0 is a small constant offset used to avoid division by zero. The larger d_0, the larger the relative contribution of far away points to the estimated output. If d_0 goes to infinity, the predicted output tends to the *mean* output over all training examples.

The WKNN algorithm is simple to implement, and often achieving low estimation errors. Unfortunately it requires massive amount of memory, and lots of computation in the prediction phase. To reduce memory consumption one can *cluster* the examples, by grouping similar cases together. Only the prototypes (*centroids*) of the identified clusters are then stored. More details in the chapter about clustering.

As we will see in the following part of this book the idea of considering distances between the current case and the cases stored in memory can be generalized. **Kernel methods and locally-weighted regression** generalize the nearest-neighbors idea in a flexible and smooth manner; the distant points are not brutally excluded, all points contribute to the output but with a significance ("weight") related to their distance from the query point.

2.2 From brute-force to smarter lookups: Hashing

Up to now, the topic of nearest neighbors looked simple. But we did not consider CPU time, in particular when the number of stored items ℓ and/or the input dimensionality d become large. A **brute-force** method to find a nearest neighbor calculates all possible distances to identify the smallest one, in time $O(\ell\ d)$, i.e., growing linearly in $\ell\ d$.

If you are not familiar with the asymptotic notation, the letter O (also referred to as *order* of the function) denotes the "growth rate" and determines how a function value grows for very large inputs and apart from a constant multiplicative term. In detail, $f(x) \in O(g(x))$ if there exists $c > 0$ and x_0 such that $f(x) \leq cg(x)$ whenever $x \geq x_0$.

Worst-case situations, corresponding to malicious counter-examples, are loved by theoreticians but can be very rare in most practical situations. Worst-cases situations can be like small flies on an elephant of highly probable well-behaved cases. Can we develop faster methods, at least **on average** if not in the worst case?

The answer is yes, provided that we invest in supporting data structures, or if we tolerate **approximated results**. The topic is rapidly getting complex, so that you may want to skip this Section at a first reading. On the other hand, finding closest neighbors is so central in machine learning that we cannot resist mentioning some basic tricks and results.

Examples of applications in **very large databases** include finding duplicate pages on the Web (for more efficient search engines), image retrieval (from multi-dimensional image descriptors), music retrieval, computational biology and drug design, computational linguistics, etc.

Let's start from a radical simplification: imagine that the potential query points are picked only from the set of ℓ stored examples. Why should one search for items which are already known? Well, one may want to retrieve information *associated* with the items, like output labels, or values. For example, imagine to set up a telephone directory which associates names with telephone numbers. A generalization is the so-called **dictionary data structure** in computer science, storing *key-value* pairs (k, v) so that, when a key k is given, the corresponding value v is returned. "Brute-force" means comparing all possible stored keys with the query k and returning the corresponding v as soon as the correct key is found.

To understand how hard this search can be, imagine a telephone directory with randomly placed names, where the only effective strategy to search a name is to scan the whole directory from the beginning until a match is found.

Now, if names are alphabetically ordered, one can open the directory at an approximated good starting point, to then proceed gradually to search before or after the opening page depending on what one finds there. This is much faster than searching through all pages, on average (the worst case can be in a town with most citizens sharing the same family name).

A better supporting data structure (like an alphabetically ordered index) means more work at the beginning, but a faster lookup. **Binary search** can be used for the lookup: the content at the middle position in the index is retrieved: if the key comes before (in alphabetical order), the search is recursively executed on the first half of the list, if the key comes later, the search is recursively executed on the second half of the list.

For a uniform distribution of keys, binary search in an ℓ-entry directory passes from $O(\ell)$ to $O(\log \ell)$ lookup time[1], on average. This is already a huge improvement for large numbers of stored keys. An index in a database (like in most SQL databases) is built precisely with this purpose. Can we do better? Can we search for a key, out of a set of ℓ, in a time which is approximately constant, on average?

Yes, we can: by using **hashing**, one can retrieve stored items in almost constant time, a very surprising result at first. To "hash" means to chop into small pieces, mince, mix up, from Latin *ascia* (ax). The idea is surprisingly simple: take your key k and "chop it" in a brutal (but deterministic!) manner to obtain an integer number. Consider the integer as an *index*, or an *address*, and store the corresponding value v at that address in memory. If one uses a function hash(k) which is fast to compute, lookup is fast: **hash the key to get the address, retrieve the stored key** at the calculated address.

Are we done? Almost. If you got your coffee this morning you may notice that *hashing* could produce, by chance, the *same* integer address for two different keys (Fig. 2.4). These *collisions* need to be dealt with, otherwise some values get lost. The solution is to have, at the obtained address, not only the space for a single value, but for a **bucket**

[1] If you know enough about logarithms, you may ask: "what base?" But remember, the asymptotic notation discards multiplicative constants

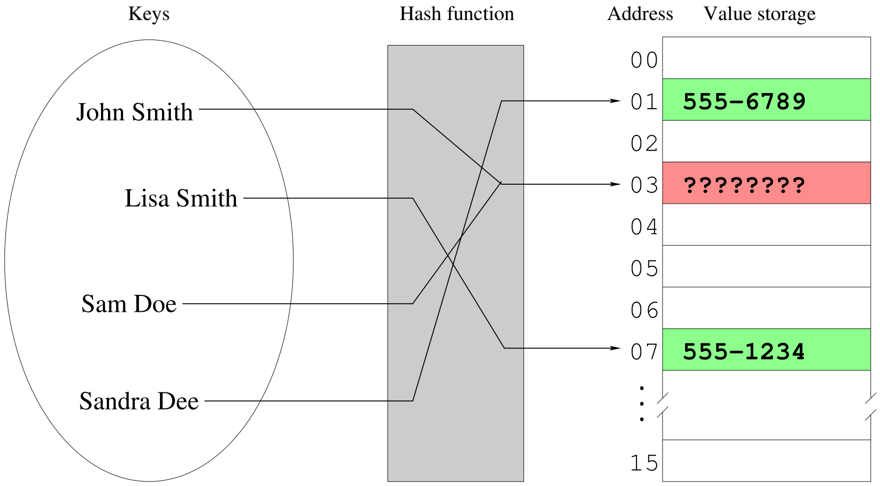


Figure 2.4: A collision when hashing names.

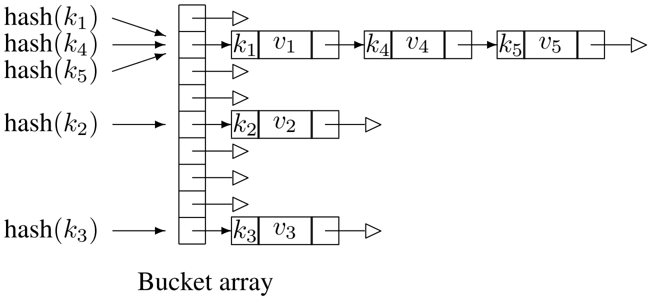


Figure 2.5: Open hashing scheme: items (configuration, or compressed hashed value, etc.) are stored in "buckets." The index of the bucket array is calculated from the configuration.

containing all *key-value* pairs for the keys hashed there, so that one can still identify the correct value in spite of the collision.

In the telephone directory example, hash(name) could give the number of a directory page (our physical *bucket*), which is big enough to contain all name-telno pairs to be stored there.

Hashing should be designed to make collisions rare and to spread the stored keys approximately in a uniform manner onto a given range of integers. This is why it is called hashing after all, the "ax" will scatter keys in a pseudo-random way onto a range of integers. To avoid wasting memory, the range of integers should be a small multiple of the total number ℓ of stored items.

The storage of labeled examples through a **hash table** requires CPU time for lookup that is approximately constant with respect to the number of items to store.

An example of a memory configuration for the hashing scheme is shown in Fig. 27.5. From the key k one obtains an index into a "bucket array." The items (k_i with associated information v_i etc.) are then stored in linked lists starting from the indexed array entry. Each cell contains the address of the next one (or *null* if it is the last cell), this is called **chaining**. Both storage and retrieval require an approximately constant amount of time if: i) the number of stored items is not much larger than the size of the bucket array, and ii) the hashing function scatters the items with a uniform probability over the different array indices. More precisely, given a hash table with m slots that stores ℓ elements, a load factor $\alpha = \ell/m$ is defined. If collisions are resolved by chaining, searches take $O(1+\alpha)$ time, on average.

2.3 Locality-sensitive Hashing (LSH) and approximated nearest neighbors

When hashing is used to map from a set of keys to the corresponding values, one is dealing with memorization and **databases**, not with machine learning and generalizing.

Returning to the nearest-neighbors for ML context just considered in Sec. 2.1, imagine now that the query $\boldsymbol{q}$ is a point placed in the d-dimensional space $\mathbb{R}^d$, and not necessarily equal to one of the stored points. Standard hash tables fail: remember that a hash function is intentionally meant to randomize things, and the new point $\boldsymbol{q}$ will be hashed to an index without any clear relationship with the index of nearby points in $\mathbb{R}^d$.

Locality-Sensitive Hashing (LSH) considers specialized versions of hashing, designed to **preferentially map close items to the same bucket**, with a probability which is higher for nearby points than for distant ones [336].

LSH is the first example of a **randomized algorithm**. A randomized algorithm contains calls to a random number generator, and its output is studied with probability and statistics. LSH does not guarantee an exact answer to a nearest-neighbor query but it provides **a high-probability guarantee that it returns the correct answer** or one close to it. By investing more computational effort, the probability can be pushed as high as desired. Because a small probability of failure in identifying the exact nearest neighbors is acceptable for most ML applications, LSH is becoming a widely used tool for very-large-scale applications.

Let's assume that one wants to guarantee with a probability equal to $1-\delta$ that the nearest neighbor will be retrieved for any query point, in a large database.

A possibility is to consider **randomized linear projections** of points in $\mathbb{R}^d$ as hashing functions. If you are not familiar with projections, consider points in 3 dimensions, projected onto a plane by a torch. Rendering a multidimensional sphere onto a two-dimensional page is a good example (Fig.2.6). Or read Chapter 20 for more details.

The motivation for LSH is based on the idea that, if two points are close together, they will remain close together after a "projection" operation. On the contrary, if two points are far apart, for most random projections they will remain distant: they will be mapped to close positions only for rare choices of the orientation of the projection. LSH therefore differs from conventional and cryptographic hash functions because it aims at **maximizing the probability of a "collision" for similar items**.

One creates **projections from a number of different random directions**, keeps track of the nearby projected points, those falling in the same buckets and notes the points that appear close to each other in more than one projection. Finally, one scans the remaining candidate list to identify the closest point. To limit the probability of failure (of returning a wrong nearest neighbor), one can adjust the number of randomized projections.

The starting point and intuition is simple, the technical details and analysis are complex and can be found in [109]. We just sketch a random projection algorithm to understand the main building blocks.

If $\boldsymbol{q}$ is a query point, a randomized scalar projection is obtained by a scalar product:

$$\text{hash}(\boldsymbol{q}) = \boldsymbol{p} \cdot \boldsymbol{q}$$

in which $\boldsymbol{p}$ is a vector with components that are selected at random from a Gaussian distribution, for example $\mathcal{N}(0,1)$.

This scalar projection is then *quantized* into a set of hash bins, with the intention that nearby items in the original space will tend fall into the same bin. The resulting full hash function is given by:

$$\text{hash}_{\boldsymbol{p},b}(\boldsymbol{q}) = \left\lfloor \frac{\boldsymbol{p} \cdot \boldsymbol{q} + b}{w} \right\rfloor,$$

where w is the width of each quantization bin, b is a random value uniformly distributed between 0 and w, and the "floor" operator $\lfloor \cdot \rfloor$ maps a positive real value to an integer by eliminating the digits after the dot (e.g., $\lfloor 2.34 \rfloor = 2$). Note that quantizing a set of real values still means that nearby points *can* end up in different bins if by chance they are

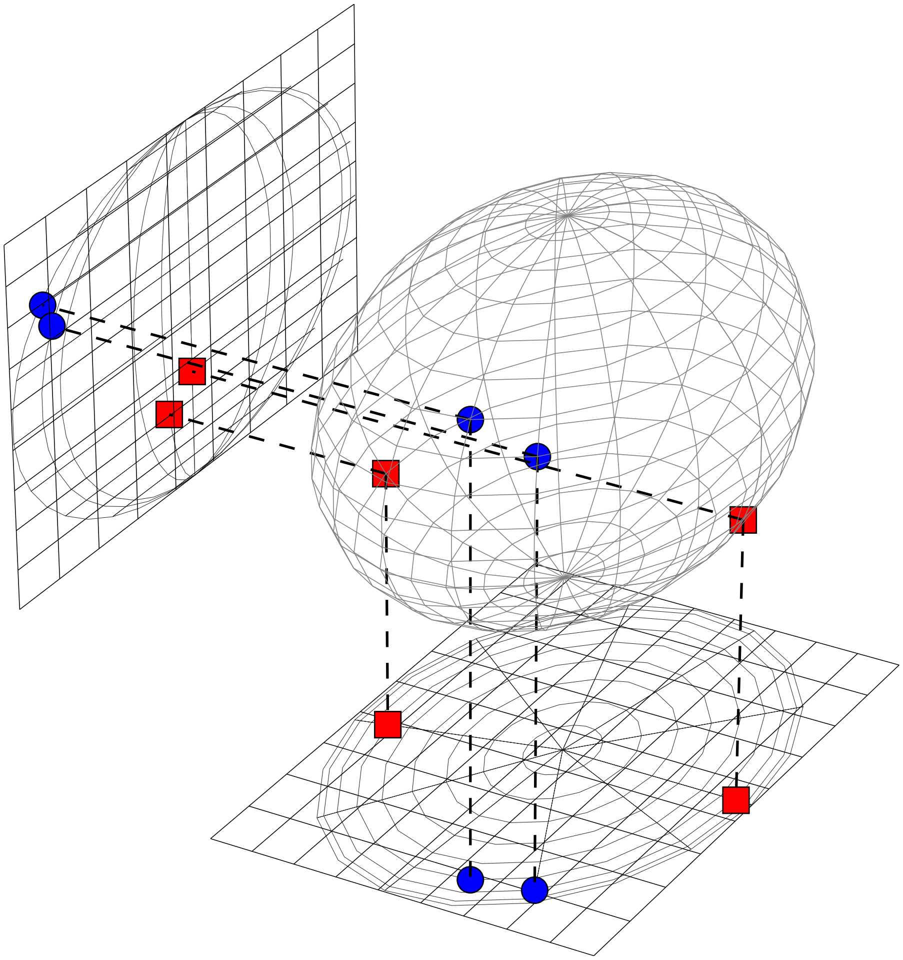


Figure 2.6: Locality-sensitive hashing by projections: points that are close to each other in the high-dimensional space are guaranteed to be close in the projection; the opposite is not always true.

on different sides of a boundary between bins (e.g., one is mapped to $2.99999w$, the other one to $3.00001w$). Adding a random value b ensures that if two such points are unlucky and sit on the opposite side of a boundary for one hash function, they can be more lucky and end up in the *same* bin for a different choice of b.

The two starting facts are that:

- close points will have a large probability of falling into the same bucket:

$$\Pr(\text{hash}(\boldsymbol{p}) = \text{hash}(\boldsymbol{q})) \geq P_1 \quad \text{for} \quad \|\boldsymbol{p} - \boldsymbol{q}\| \leq R_1;$$

- points $\boldsymbol{p}$ and $\boldsymbol{q}$ that are far apart have a low probability $P_2 < P_1$ to fall into the same bucket:

$$\Pr(\text{hash}(\boldsymbol{p}) = \text{hash}(\boldsymbol{q})) \leq P_2 \quad \text{for} \quad \|\boldsymbol{p} - \boldsymbol{q}\| \geq R_2,$$

  where $R_2 > R_1$.

Due to the linearity of the dot product, the difference between two image points $\|\,\text{hash}(\boldsymbol{p}) - \text{hash}(\boldsymbol{q})\|$ has a magnitude whose distribution is proportional to $\|\boldsymbol{p} - \boldsymbol{q}\|$ and therefore, $P_1 > P_2$.

Since the gap between the probabilities P_1 and P_2 could be quite small, an **amplification** process is needed in order to achieve the desired probabilities of collision, by performing k independent dot products in parallel. A far point could end up in the same bucket for an unlucky projection, but being unlucky k times has a much smaller probability.

Within each set of k dot products, one achieves success if the query and the nearest neighbor are in the same bin in *all* k dot products. This occurs with probability P_1^k, which decreases as we include more dot products. To reduce the impact of an "unlucky" quantization in any one projection, we form L independent projections and pool the neighbors from all of these. A true near neighbor will be unlikely to be unlucky in all the L projections.

A large k (AND-ing more projections) will filter out bad (distant) points, while a large L (OR-ing the contents of all L retrieved buckets) will ensure that we do not throw away the baby (the closest neighbors) with the dirty water.

Let's assume that one wants to retrieve R-neighbors of a query point $\boldsymbol{q}$ (neighbors at distance less than R). The query algorithm is:

- For each $j = 1, 2, \ldots, L$:
  1. Retrieve the points from the bucket obtained by concatenating the k integers in the j-th hash table.
  2. For each retrieved point, compute the distance from $\boldsymbol{q}$ to it, and report the point if it is a correct answer (an R-near neighbor).
  3. (optional) Stop as soon as the number of reported points is more than L'.

As an additional optimization, because many bins can be empty in a k-dimensional space, one can use standard hashing to efficiently store and retrieve only the non-empty bins.

After running the math so that the desired probability of success is guaranteed by a proper choice of k and L, the time needed to calculate and hash the projections is $O(dkL)$, a huge improvement with respect to the linear scan of all points, provided that the time to deal with collisions is limited. A practical approach to choosing k is introduced in the E2LSH package [10], by starting from estimates of CPU time obtained over a small set of sample queries.

The research in this area is still active, some of the best results have been encouraged by the need to analyze huge amounts of data, and obtained in the last five-ten years [245, 109].

2.4 Space-partitioning data structure: k-d trees

LSH is not the only possibility to speed up search in **computational geometry**. Other **space-partitioning data structures** have been proposed for organizing points in a d-dimensional space. Trees of boxes in $\mathbb{R}^n$ are a standard way to go from a linear CPU time to one logarithmic in the number of stored points. ***k*-d trees** are a special case of binary space partitioning trees. The root of the tree corresponds to the entire $\mathbb{R}^d$ space, at each node a left and right

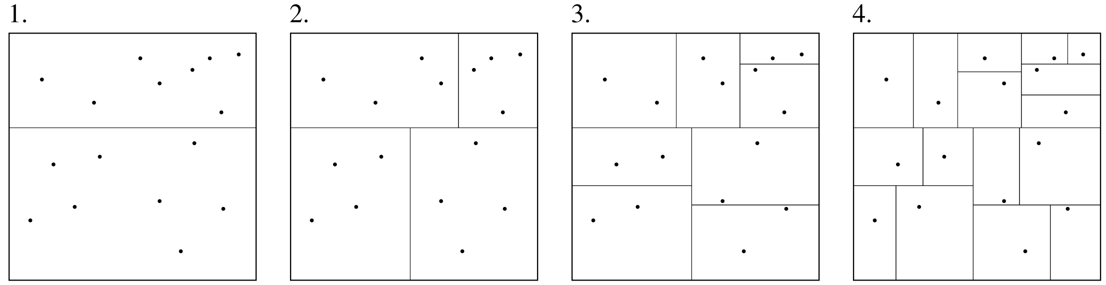


Figure 2.7: A k-d tree data structure.

subtrees are defined by a test on a single coordinate. If the coordinate c and threshold x_c are chosen for a particular split, all points whose c-th coordinate is less than x_c will appear in the left subtree, the other points in the right subtree. Imagine a sequence of hyperplanes perpendicular to coordinate axes leading to boxes containing two boxes, containing two boxes... untile a single point remains. If each split divides the points approximately into two equal parts, a **logarithmic time for searching** is obtained. The initial N points are divided by two, then again, ..., until $N/2^s \approx 1$ which means $s \approx \log_2 N$.

A logarithmic time for searching exact matches is not particularly relevant since $O(1)$ time can be obtained by hashing. But k-d trees become interesting for nearest-neighbor searches.

Searching for a nearest neighbour in a k-d tree proceeds as follows: Starting with the root node, the algorithm moves down the tree recursively, in the same way that it would if the search point were being inserted (i.e., it goes left or right depending on whether the point is lesser than or greater than the current node in the split dimension). Once the algorithm reaches a leaf node, it saves that node point as the "current best." After having this bound on the minimum distance the algorithm unwinds the recursion of the tree to check if more promising candidate subtrees exist. A decision whether subtrees need to be examined is made by intersecting the splitting hyperplane with a hypersphere around the search point that has a radius equal to the current nearest distance. Details vary for different implementations and assumptions, building a static k-d tree from N points can be done in $O(N \log N)$ time, finding one nearest neighbour in a balanced k-d tree with randomly distributed points takes $O(\log N)$ time on average, [51, 137]

Appropriate data structures can bring huge improvements with respect to brute-force techniques, but have to be chosen and used with great care. In particular k-d trees maintain logarithmic search times only in small dimensions. The **curse of dimensionality** strikes: as soon as the number of dimension d grows so that the number of points is not sufficiently large (approximately $N \gg 2^k$), most of the points in the tree will be evaluated during the search and the efficiency becomes worse than exhaustive search (given the added overhead in building the structure). Approximate nearest-neighbour methods like LSH should be used instead.

Never use a data structure without considering if the assumptions for its range of validity hold in your case, or you may be greatly disappointed.

Gist

KNN (K Nearest Neighbors) is a primitive and lazy form of machine learning: just store all training examples into memory (inputs and associated output label).

When a new input to be evaluated appears, search in memory for the K closest examples stored. Read their outputs and derive the new output by majority or averaging. Laziness during training causes long response times when many examples are stored.

KNN works in many real-world cases because similar inputs are usually related to similar outputs, a basic hypothesis in *machine learning*. It is similar to some "case-based" human reasoning processes. Although simple and brutal, it can be surprisingly effective in many cases.

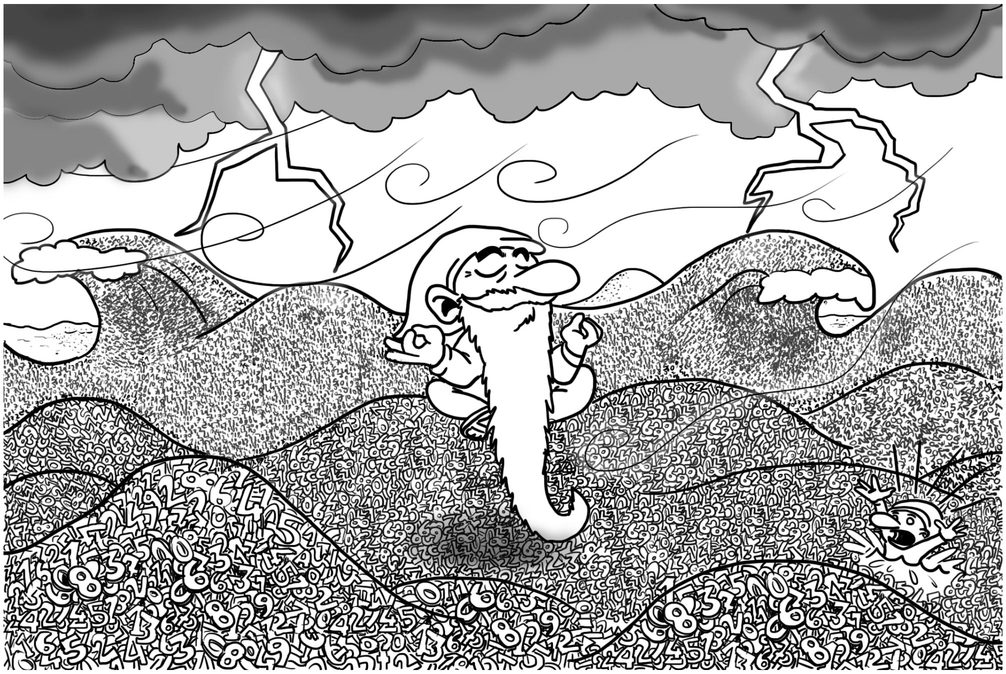
Investing in smart data-structures is critical to obtain fast exact or approximated nearest-neighbors searches. **Hashing** is a key trick, and now you can see a deeper meaning of the "hashtag" term popular in social networks, related to searching for keys and retrieving . . . tweets. **LSH (locality-sensitive hashing)** is not to be confused with psychedelic LSD, its advantages are very real in a context of big data.

Now, do not sleep motivated by this lazy-learning topic but go ahead and digest additional chapters of this book.

Chapter 3

Learning requires a method

Data Mining, noun 1. Torturing the data until it confesses...
and if you torture it long enough, you can get it to confess to anything.



Learning, both human and machine-based, is a powerful but subtle instrument. Real learning is associated with extracting the deep and basic relationships in a phenomenon, with summarizing a wide range of events through compact models, with **unifying different cases by discovering the underlying explanatory laws**.

Above all, learning from examples is only a means to reach the real end: **generalization, the capability of explaining new cases**, of predicting new outputs, in the same application area but not already encountered during the learning phase. On the contrary, learning by heart or memorizing are considered very poor forms of learning, useful for beginners but not for real experts. If the goal is generalization, **estimating the performance has to be done with extreme care**. Observing the behavior of the model on the learning examples does not guarantee a proper generalization and may lead to unjustified optimism. After all, a student who is good at learning by heart and repeating the exact words of the teacher will not always end up being the most successful individual in life!

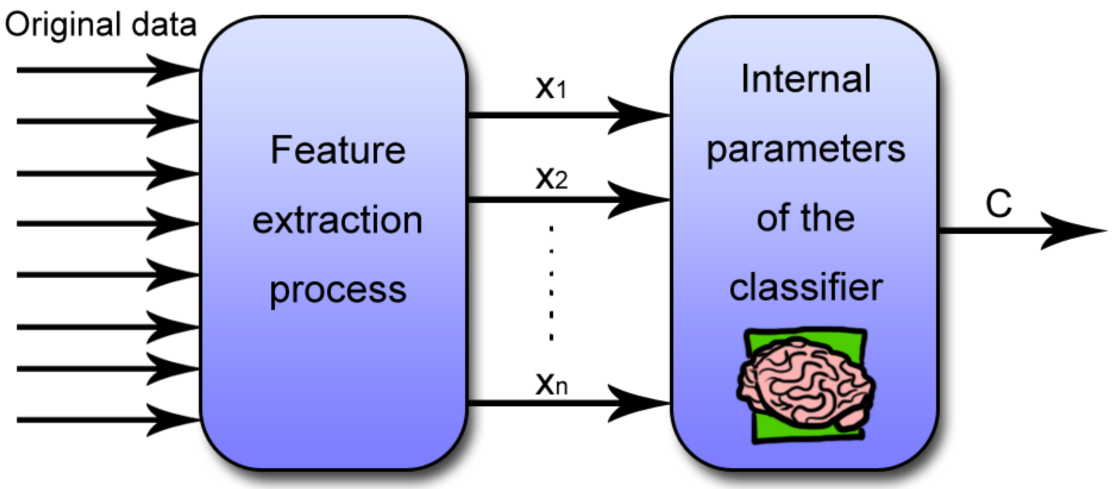

Original data
Feature extraction process
x1
x2
xn
Internal parameters of the classifier
C

Figure 3.1: Supervised learning architecture: feature extraction and classification.

Let's now define the machine learning context (ML for short) so that its high voltage can be switched on without electric shock injuries caused by improper usage and over-optimism. Furthermore, switching on ML does not imply switching off our brain.

In fact, before starting the machine learning process, it is useful to clean and extract an informative subset or a combination of the original data by using intuition and intelligence. Features (or attributes) are individual measurable properties of the phenomena being observed with useful information to derive the output value. **Feature selection** (for a subset) and **feature extraction** (for a combination) are the names of this preparatory phase (Fig. 3.1).

An input example can be the image of a letter of the alphabet, with the output corresponding to the letter symbol. Automated reading of zip codes for routing mail, or automated conversion of images of old book pages into the corresponding text are relevant applications, called optical character recognition. Intuition tells us that the absolute image brightness is not an informative feature (digits remain the same under more or less light). In this case, suitable features can be related to edges in the image, to histograms of gray values collected along rows and columns of an image, etc. More sophisticated techniques try to ensure that a translated or enlarged image is recognized as the original one, for example by extracting features measured with respect to the barycenter of the image (considering a gray value in a pixel as a mass value), or scaled with respect to the maximum extension of the black part of the image, etc. Extracting useful features often requires concentration, insight and knowledge about the problem, but doing so greatly simplifies the subsequent automated learning phase. The analogy is with a competent professor filtering and preparing teaching material for an effective lesson.

To fix the notation, a training set of ℓ *tuples* (ordered lists of elements) is considered, where each tuple is of the form $(\boldsymbol{x}_i, y_i)$, $i = 1, \dots, \ell$; $\boldsymbol{x}_i$ being a vector (array) of input parameter values in d dimensions ($\boldsymbol{x}_i \in \mathbb{R}^d$); y_i being the measured outcome to be learned by the algorithm. As mentioned before, we consider two possible problems: *regression*, where y_i is a real numeric value; and *classification*, where y_i belongs to a finite set.

In **classification** (recognition of the class of a specific object described by features $\boldsymbol{x}$), the output is a suitable code for the class. The output y belongs to a finite set, e.g., $y_i = \pm 1$ or $y_i \in \{1, \dots, N\}$. For example, think about classifying a mushroom as edible or poisonous.

In **regression**, the output is a real number, and the objective is to model the relationship between a dependent variable (the output y) and one or more independent variables (the input features $\boldsymbol{x}$). For example, think about predicting the poison content of a mushroom from its characteristics.

In some applications, the classification is not always crisp and there are confused boundaries between the different classes. Think about classifying bald versus hairy people: no clear-cut distinction exists as anxious people and sellers of hair loss cures know very well.

In these cases there is a natural way to transform a "crisp" classification into a regression problem. To take care of indecision, the output can be a real value ranging between zero and one, and it can be interpreted as the **posterior probability for a given class**, given the input values, or as a **fuzzy membership** when probabilities cannot be used. For example, if a person has a few hair left, it makes little sense to talk about a probability of 0.2 of being hairy, in this case *fuzzy membership* of 0.2 in the class of hairy persons can be more appropriate. Probability is used properly when there are experiments with uncertain outcome which can be repeated.

Having a continuous output value, for example from 0 to 1, gives additional **flexibility** for the practical usage of classification systems. Depending on a threshold, a human person or a more sophisticated system can be consulted in the more confused cases (for example the cases with output falling in the range from 0.4 to 0.6). The clear cases are handled automatically, the most difficult cases can be handled by a human person. In optical character recognition, consider an image which may correspond to the digit 0 (zero) or the letter O (like in Old). It may be preferable to output 0.5 for each case instead of forcing a hard classification. A subsequent step may consider adjacent characters or semantic information to disambiguate the two possibilities.

3.1 Learning from labeled examples: minimization and generalization

Supervised learning uses the examples to build an association (a function) $y = \hat{f}(\boldsymbol{x})$ between input $\boldsymbol{x}$ and output y. The association is selected within a **flexible model** $\hat{f}(\boldsymbol{x};\boldsymbol{w})$, where the flexibility is given by some **tunable parameters** (or **weights**) $\boldsymbol{w}$.

For a concrete image, think about a mincer transforming inputs into outputs, with tunable gears and levers to regulate it. Or think about a "multi-purpose box" waiting for input and producing the corresponding output depending on operations influenced by internal parameters. The information to be used for "customizing" the box is extracted from the training examples. The magic of ML is that the gears are not fixed by hand but automatically, through optimization, by showing examples of correct input-output pairs.

A scheme of the architecture is shown in Fig. 3.1, the two parts of feature extraction and identification of optimal internal weights of the classifier are distinguished. In many cases feature extraction requires some human insight, while the **determination of the best parameters is fully automated**, this is why the method is called *machine* learning after all. The free parameters are fixed by **demanding that the learned model works correctly on the examples** in the *training set*.

As a true believer in the power of optimization one defines an *error measure* to be minimized[1], and runs (automated) optimization to determine the optimal parameters. A suitable *error measure* is the sum of the errors between the correct answer (given by the example label) and the outcome predicted by the model (the output ejected by the multi-purpose box). The errors are considered as absolute values and often squared. The "**sum of squared errors**" is possibly the most widely used error measure in ML. If the error is zero, the model works correctly on the given examples. The smaller the error, the better the average behavior on the examples.

Supervised learning therefore becomes **minimization of a specific error function**, depending on parameters $\boldsymbol{w}$. If you only care about the final result you may take the optimization part as a **"big red button"** to push on the multi-purpose box, to have it customized for your specific problem after feeding it with a set of labeled examples.

If you are interested in developing new LION tools, you will get more details about optimization techniques in the following chapters. The gist is the following: if the function is smooth (think about pleasant grassy California hills) one can discover points of low altitude (lakes?) by being blindfolded and parachuted to a random initial point,

[1] Minimization becomes maximization after multiplying the function to be optimized by minus one, this is why one often talks about "optimization", without specifying the direction min or max.

by sampling neighboring points with his feet, and by moving always in the direction of steepest descent. No "human vision" is available to the computer to "see" the lakes, only the possibility to sample one point at a time. By repeating the two steps of sampling in the neighborhood of the current point – in $\boldsymbol{w}$ space – and moving to a neighbor that decreases the error, one builds a trajectory leading to smaller and smaller values. Amazingly, this simple process is sufficient to reach an appropriate $\boldsymbol{w}^*$ value for many applications.

Let's speak mathematics. If the function to be optimized is differentiable, a simple approach consists of using **gradient descent**. One iterates by calculating the gradient of the function with respect to the weights and by taking a small step in the direction of the negative gradient. This is in fact the popular technique in neural networks known as learning by **backpropagation** of the error [383, 384, 311].

Assuming a smooth function is not artificial: There is a basic **smoothness assumption** underlying supervised learning: if two input points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ are close, the corresponding outputs y_1 and y_2 should also be close[2]. If the assumption is not true, it would be impossible to generalize from a finite set of examples to a set of possibly infinite new and unseen test cases. Let's note that the physical reality of signals and interactions in our brain tends to naturally satisfy the smoothness assumption. The activity of a neuron in our neural network tends to depend smoothly on the neuron inputs, in turn caused by chemical and electrical interactions in their dendritic trees.

Up to now, you may think that machine learning equals optimization of a performance measure on the training examples, but one ingredient is still missing. Minimization of an error function is a first critical component, but not the only one. If the **model complexity** (the flexibility, the number of tunable parameters) is too large, learning the examples with zero errors becomes trivial, but predicting outputs for new data may fail brutally. In the human metaphor, if learning becomes rigid memorization of the examples without grasping the underlying model, students have difficulties in generalizing to new cases. This is related to the *bias-variance* dilemma, and requires care in model selection, or minimization of a weighted combination of model error on the examples plus model complexity.

The **bias-variance dilemma** can be stated as follows.

- Models with too few parameters are inaccurate because of a large bias: they lack flexibility.
- Models with too many parameters are inaccurate because of a large variance: they are too sensitive to the sample details (changes in the details will produce huge variations).
- Identifying the best model requires controlling the "model complexity", i.e., the proper architecture and number of parameters, to reach an appropriate compromise between bias and variance.

The issue goes back to problems related to measuring physical systems. When measuring a system one encounters two kinds of possible errors: *systematic errors* (bias) and *random errors* (variance), as shown in Fig.3.2. Systematic errors, leading to *inaccuracy*, refer to deviations that are not due to chance alone. An example occurs with a measuring device that is improperly calibrated so that it consistently overestimates (or underestimates) the measurements. Random error has no preferred direction, so we expect that averaging over a large number of observations will yield a net effect of zero. The impact of random error, *imprecision*, can be minimized with large sample sizes. The precision related to the number of significant figures in digits: it refers to the *stability* of that measurement when repeated many times. If you measure height of a person with a mater stick (say 182 centimeters), it is useless to use more than 3-4 digits, nobody would answer 182.368638 cm). Bias, on the other hand, has a net direction and magnitude, so that averaging over a large number of observations does not eliminate its effect.

Let's now focus on machine learning and introduce the **bias–variance decomposition of squared error**[212]. The context is that the output is obtained by a true functional, but noisy relation of the input: $y_i = f(x_i) + \epsilon$, where the noise ϵ has zero mean and variance σ^2.

The objective of ML is to find a function $\hat{f}(x)$, that approximates the true function $y = f(x)$ as well as possible, in particular by minimizing the squared error $(y - \hat{f}(x))^2$. Given the noise ϵ in the true function one must be prepared to accept an *irreducible error* in any function $\hat{f}(x)$. If one samples from the same distribution and averages over the

[2] In some cases the closeness between points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ can be measured by the standard Euclidean distance, in other cases more problem-specific distance measures are needed.

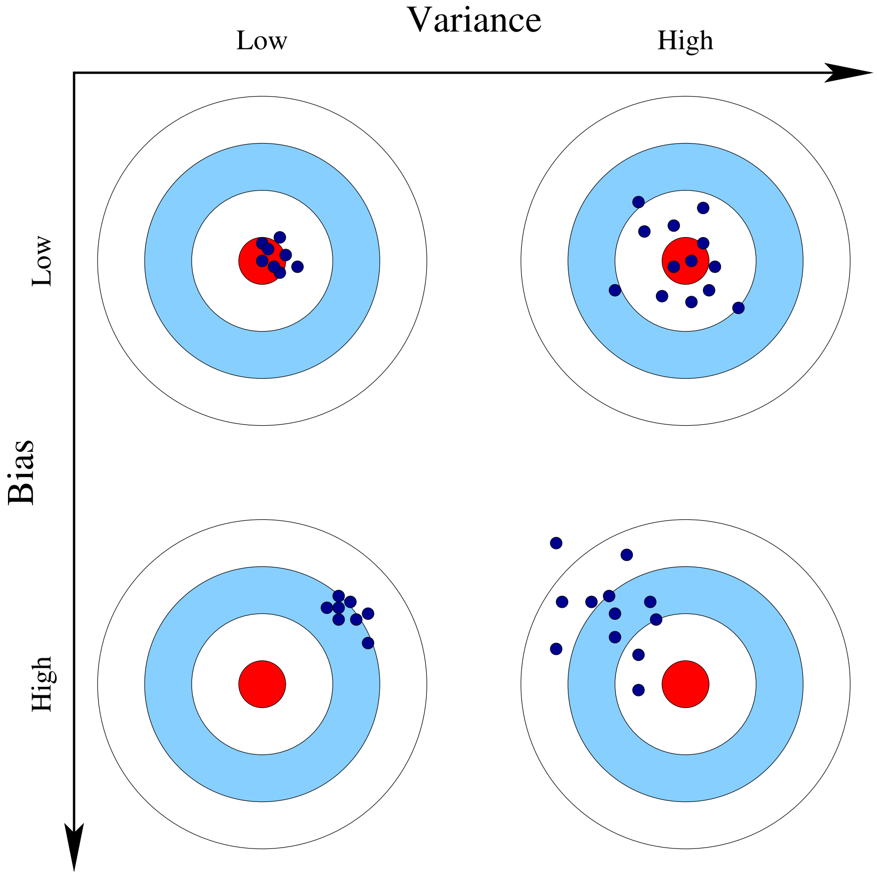


Figure 3.2: Difference between bias (systematic errors) and variance (random errors) when playing darts.

different choices of $x_1, \ldots, x_n, y_1, \ldots, y_n$, one can decompose the expected error on an unseen sample x as follows:

$$\mathrm{E}\Big[\big(y - \hat{f}(x)\big)^2\Big] = \mathrm{Bias}\big[\hat{f}(x)\big]^2 + \mathrm{Var}\big[\hat{f}(x)\big] + \sigma^2$$

Where Bias measures how the expected model output differs from the “true” $f(x)$ value:

$$\mathrm{Bias}\big[\hat{f}(x)\big] = \mathrm{E}\big[\hat{f}(x)\big] - f(x)$$

and Var measures the scatter in the distribution of $\hat{f}(x)$ values around its mean:

$$\mathrm{Var}\big[\hat{f}(x)\big] = \mathrm{E}\Big[\big(\hat{f}(x) - \mathrm{E}[\hat{f}(x)]\big)^2\Big]$$

The irreducible error σ^2 gives a lower bound on the expected error on unseen examples. The more complex and flexible the model $\hat{f}(x)$ is, the lower the bias will be. However, flexibility will make the model details “move” more when the training examples change, and hence its variance will be larger.

The preference of simple models to avoid over-complicated models has been given a fancy name: **Occam’s razor**, referring to “shaving away” unnecessary complications in theories[3]. Optimization is still used, but the error measure needs an integration, to take model complexity into account.

[3] Occam’s razor is attributed to the 14th-century theologian and Franciscan friar Father William of Ockham who wrote “entities must not be

It is also useful to distinguish between two families of methods for supervised classification. In one case one is interested in deriving a “constructive model” of how the output is generated from the input, in the other case one cares about the bottom line: obtaining a correct classification. The first case is more concerned with explaining the underlying mechanisms, the second with crude performance.

Among examples of the first class, **generative methods** try to model the process by which the measured data $\boldsymbol{x}$ are generated for the different classes y. Given a certain class, for example of a poisonous mushroom, what is the probability of obtaining real mushrooms of different geometrical forms? In mathematical terms, one learns a class-conditional density $p(\boldsymbol{x}|y)$, the probability of $\boldsymbol{x}$ given y. Then, given a fresh measurements $\boldsymbol{x}$, one assigns a class y by maximizing the posterior probability of a class given the measurement, obtained by Bayes’ theorem:

$$p(y|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|y)p(y)}{\sum_y p(\boldsymbol{x}|y)p(y)}; \tag{3.1}$$

where $p(\boldsymbol{x}|y)$ is known as the likelihood of the data, and $p(y)$ is the prior probability, which reflects the probability of the outcome before any measure is performed. The term at the denominator is the usual normalization term to make sure that probabilities sum up to one. A mnemonic way to remember Bayes’ rule is: “posterior = prior times likelihood.”

Discriminative algorithms do not attempt at modeling the data generation process, they just aim at directly estimating $p(y|\boldsymbol{x})$, a problem which is in some cases simpler than the two-steps process (first model $p(\boldsymbol{x}|y)$ and then derive $p(y|\boldsymbol{x})$) implied by generative methods. Multilayer perceptron neural networks, as well as Support Vector Machines (SVM), are examples of discriminative methods described in the following chapters.

The shortcut implied by the second option is profound, **accurate classifiers can be built without knowing or building a detailed model** of the process by which a certain class generates input examples. You do not need to be an expert mycologist in order to pick mushroom without risking death, you just need an abundant and representative set of example mushrooms, with correct classifications.

Understanding that one does not need to be a domain expert to bring a measurable contribution is a small step for a man, but one giant leap along the LION way. Needless to say, successful businesses complement expertise with humble but powerful data- and optimization-driven tools.

3.2 Learn, validate, test!

When learning from labeled examples we need to follow **careful experimental procedures** to measure the effectiveness of the learning process. In particular, it is a shameful and unforgivable mistake to evaluate the performance of the learning systems on the same examples used for training. The objective of machine learning is to obtain a system capable of **generalizing** to new and previously unseen data. Otherwise the system is not learning, it is merely memorizing a set of known patterns. This is why questions at university exams change from time to time…

Let’s assume we have a supervisor (a software program or an experimental process) who can generate labeled examples with a given probability distribution. We should ask the supervisor for some examples during training, and then test the performance by asking for some fresh examples. Ideally, the number of examples used for training should be sufficiently large to permit convergence, and the number used for testing should be very large to ensure a statistically sound estimation. We strongly suggest you not to conclude that a machine learning system to identify edible from poisonous mushrooms is working, after testing it on seven mushrooms.

This ideal situation may be far from reality. In some cases the set of examples is rather small, and has to be used in the best possible way *both* for training *and* for measuring performance. In this case the set has to be clearly partitioned between a **training set** and a **validation set**, the first used to train, the second to measure performance, as illustrated in Fig. 3.3. A typical performance measure is the **root mean square (abbreviated RMS)** error between the output of

multiplied beyond necessity” (*entia non sunt multiplicanda praeter necessitatem*). To quote Isaac Newton, “We are to admit no more causes of natural things than such as are both true and sufficient to explain their appearances. Therefore, to the same natural effects we must, so far as possible, assign the same causes.”

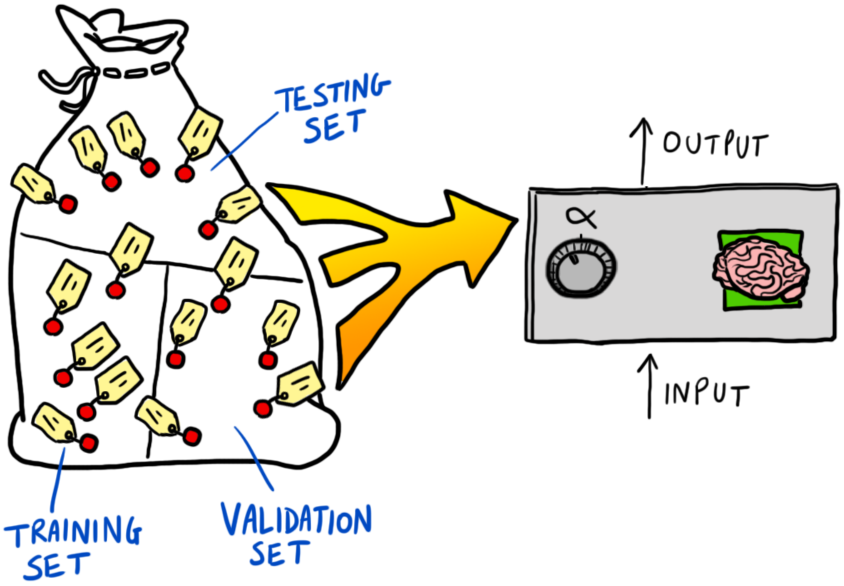


Figure 3.3: Labeled examples need to be split into training, validation and test sets.

the system and the correct output given by the supervisor. The RMS value of a set of values is the *square root* of the arithmetic *mean* (average) of the *squares* of the original values. If e_i is the error on the i-th example, the RMS value is given by:

$$RMS = \sqrt{\frac{e_1^2 + e_2^2 + \cdots + e_\ell^2}{\ell}}$$

.

In general, the learning process optimizes the model parameters to make the model *reproduce* the output of the training data as well as possible. If we then take an independent sample of validation data from the same population as the training data, it will generally turn out that the error on the validation set will be larger than the error on the training set. This discrepancy is likely to become severe if training is excessive, leading to **over-fitting** (**overtraining**), likely to happen when the number of training examples is small, or when the number of parameters in the model is large.

If the examples are limited, we now face a problem: do we use more of them for training and risk a poor and noisy measurement of the performance, or to have a more robust measure at the price of reducing the training examples? In concrete terms: if you have 50 mushroom examples, do you use 45 for training and 5 for testing, 30 for training and 20 for testing? . . . Luckily, there is a way to jump over this embarrassing situation, just use **cross-validation**. Cross-validation is a generally applicable way to predict the performance of a model on a validation set by using repeated experiments instead of mathematical analysis.

The idea is to **repeat** many train-and-test experiments, by using different partitions of the original set of examples into two sets, one for training one for testing, and then averaging the test results. This general idea can be implemented as K**-fold cross-validation**: the original sample is randomly partitioned into K subsamples. $K-1$ subsamples are used for training, a single subsample is used for validation. The process is then repeated K times (the folds), with each of the K subsamples used exactly once for validation. The results from the folds are then averaged to produce a single estimation. The advantage is that all observations are used for both training and validation, and each observation is used for validation exactly once. If the example set is really small one can use the extreme case of **leave-one-out cross-validation**, using a single observation from the original sample as the validation data, and the remaining observations as the training data (in this case K equals the number of examples).

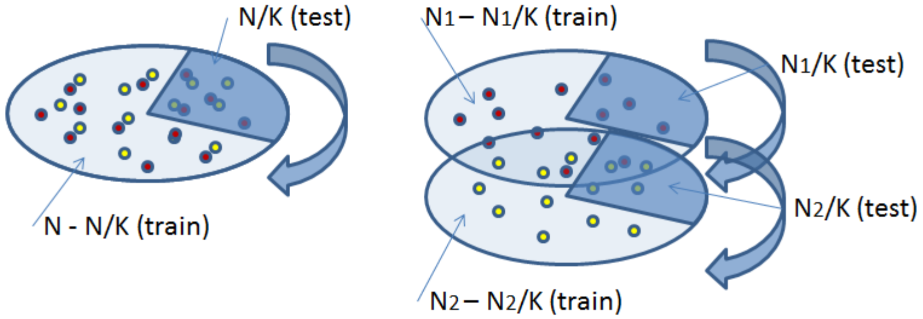


Figure 3.4: Stratified cross-validation, examples of two classes. In normal cross-validation $1/K$ of the examples are kept for testing, the slice is then “rotated” K times. In stratification, a separate slice is kept for each class to maintain the relative proportion of cases of the two classes.

Stratified cross-validation is an improvement to avoid different class balances in the training and validation set. It avoids that, by chance, a class is more present in the training examples and therefore less present in validation (with respect to its average presence among all examples). With stratification, the ℓ/K testing patterns are extracted separately for examples of each class, to ensure a fair balance among the different classes (Fig. 3.4).

If the machine learning method itself has some **parameters to be tuned**, this creates an additional problem. Let’s call them **meta-parameters** in order to distinguish them from the basic parameters of the model, the weights of the “multi-purpose box” to be customized. Think for example about deciding the termination criterion for an iterative minimization technique (when to stop training), or the number of hidden neurons in a multilayer perceptron, or appropriate values for the crucial parameters of Support Vector Machine (SVM). Finding optimal values for the meta-parameters implies **reusing** the validation set many times. Reusing validation examples means that they also *become part of the training process*. We are in fact dealing with a kind of meta-learning, learning the best way to learn. The more one reuses the validation set, the more the danger that the measured performance will be optimistic, not corresponding to the real performance on new data. One is in practice “torturing the data until it confesses. . . and if you torture it long enough, you can get it to confess to anything.”

In the previous context of a limited set of examples to be used for all needs, to proceed in a sound manner one has to split the data into **three sets: a training, a validation and a (final) testing one**. The test set is *used only once for a final measure of performance*.

Let’s note that, to increase the confusion, in the standard case of a single train-validation cycle, the terms validation and testing are often used as synonyms.

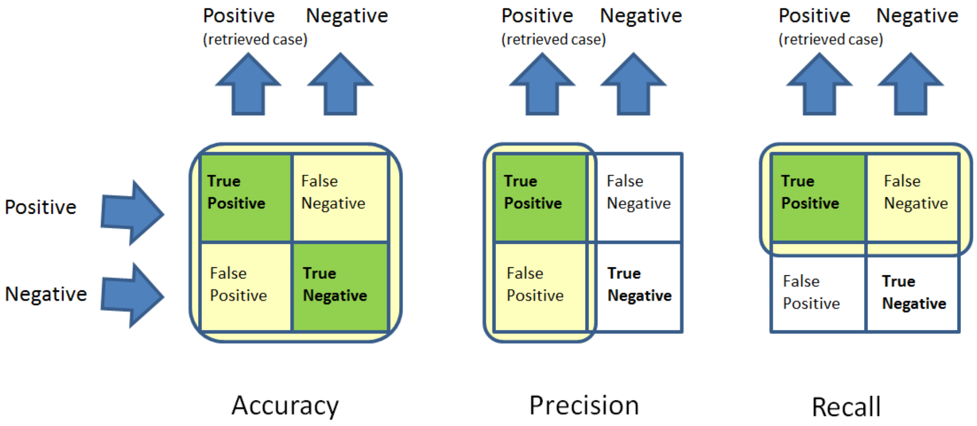


Figure 3.5: Each line in the matrix reports the different classifications for cases of a class. You can visualize cases entering at the left and being sorted out by the different columns to exit at the top. Accuracy is defined as the fraction of correct answers over the total, precision as the fraction of correct answers over the number of retrieved cases and recall is computed as the fraction of correct answers over the number of relevant cases. In the plot: divide the cases in the dark gray part by the cases in the light gray area.

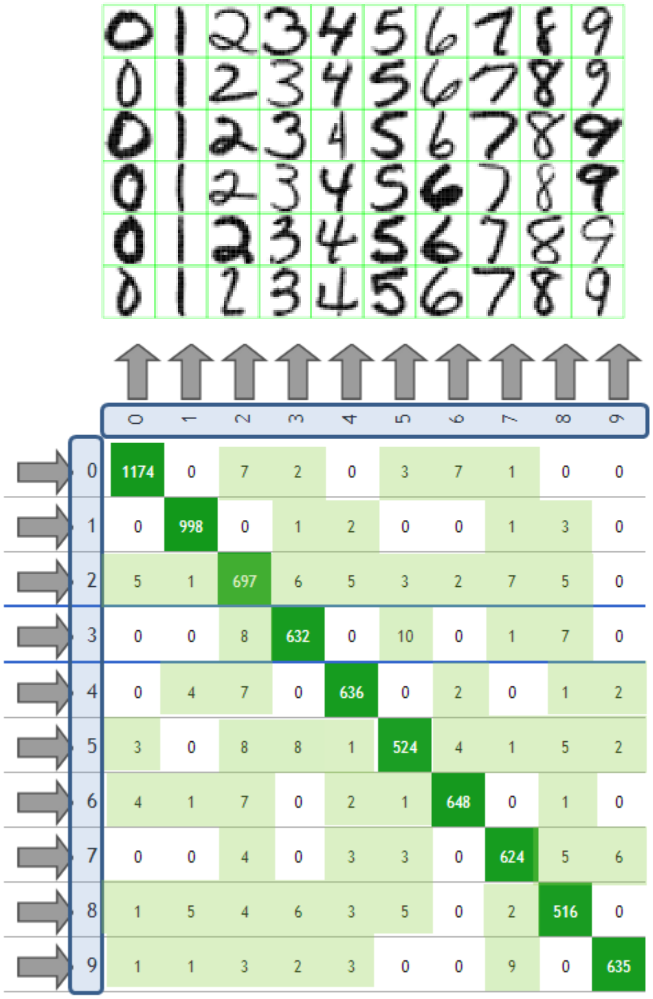
3.3 Errors of different kinds

When measuring the performance of a model, mistakes are not born to be equal. If you classify a poisonous mushroom as edible you are going to die, if you classify an edible mushroom as poisonous you are wasting a little time. Depending on the problem, the criterion for deciding the best classification changes. Let's consider a binary classification (with "yes" or "no" output). Some possible criteria are: **accuracy, precision, and recall**. The definitions are simple but require some concentration to avoid confusions (Fig. 3.5).

The **accuracy** is the proportion of true results given by the classifier (both true positives and true negatives). The other measures focus on the cases which are labeled as belonging to the class (the "positives"). The **precision** is the number of true positives (the items *correctly* labeled as belonging to the positive class) divided by the total number of elements labeled as positive (the sum of true positives and false positives, incorrectly labeled as belonging to the class). The **recall** is the number of true positives divided by the total number of elements that actually belong to the positive class (i.e., the sum of true positives and false negatives, which are not labeled as belonging to the positive class but should have been). Precision answers the question: "How many of the cases labeled as positive are correct?" Recall answers the question: "How many of the truly positive cases are retrieved as positive?" Now, if you are picking mushrooms, are you more interested in high precision or high recall?

A **confusion matrix** explains how cases of the different classes are correctly classified or confused as members of wrong classes (Fig. 3.6).

Each row tells the story for a single class: the total number of cases considered and how the various cases are recognized as belonging to the correct class (cell on the diagonal) or confused as members of the other classes (cells corresponding to different columns).



	0	1	2	3	4	5	6	7	8	9
0	1174	0	7	2	0	3	7	1	0	0
1	0	998	0	1	2	0	0	1	3	0
2	5	1	697	6	5	3	2	7	5	0
3	0	0	8	632	0	10	0	1	7	0
4	0	4	7	0	636	0	2	0	1	2
5	3	0	8	8	1	524	4	1	5	2
6	4	1	7	0	2	1	648	0	1	0
7	0	0	4	0	3	3	0	624	5	6
8	1	5	4	6	3	5	0	2	516	0
9	1	1	3	2	3	0	0	9	0	635

Figure 3.6: Confusion matrix for optical character recognition (handwritten ZIP code digits). The various confusions make sense. For example the digit “3” is recognized correctly in 632 cases, confused with “2” in 8 cases, with “5” in 10 cases, with “8” in 7 cases. “3” is never confused as “1” or “4”, digits with a very different shape.

Gist

The goal of machine learning is to exploit a set of training examples to realize a system which will correctly generalize to new cases, in the same context but not seen during learning.

ML learns, i.e., determines appropriate values for the free parameters of a flexible model, by **automatically minimizing a measure of the error** on the example set, possibly corrected to discourage overly complex models, and therefore to improve the chances of correct generalization.

The output value of the system can be a class (classification), or a number (regression). In some cases having as output the probability for a class increases flexibility of usage.

Accurate classifiers can be built without any knowledge elicitation phase, just starting from an abundant and representative set of example data. This is a dramatic paradigm change with respect to systems designed by hand from domain knowledge.

ML is very powerful but requires a strict method (a kind of "pedagogy" of ML). For sure, **never estimate performance on the training set**, this is a mortal sin, and be aware that re-using validation data will create optimistic estimates. If examples are scarce, use **cross-validation** to show off that you are an expert ML user.

To be on the safe side and enter the ML paradise, set away some test examples and use them only once at the end to estimate performance.

There is no single way to measure the performance of a model, different kinds of mistakes can have very different costs. **Accuracy, precision and recall** are some possibilities for binary classification, a **confusion matrix** is giving the complete picture for more classes.

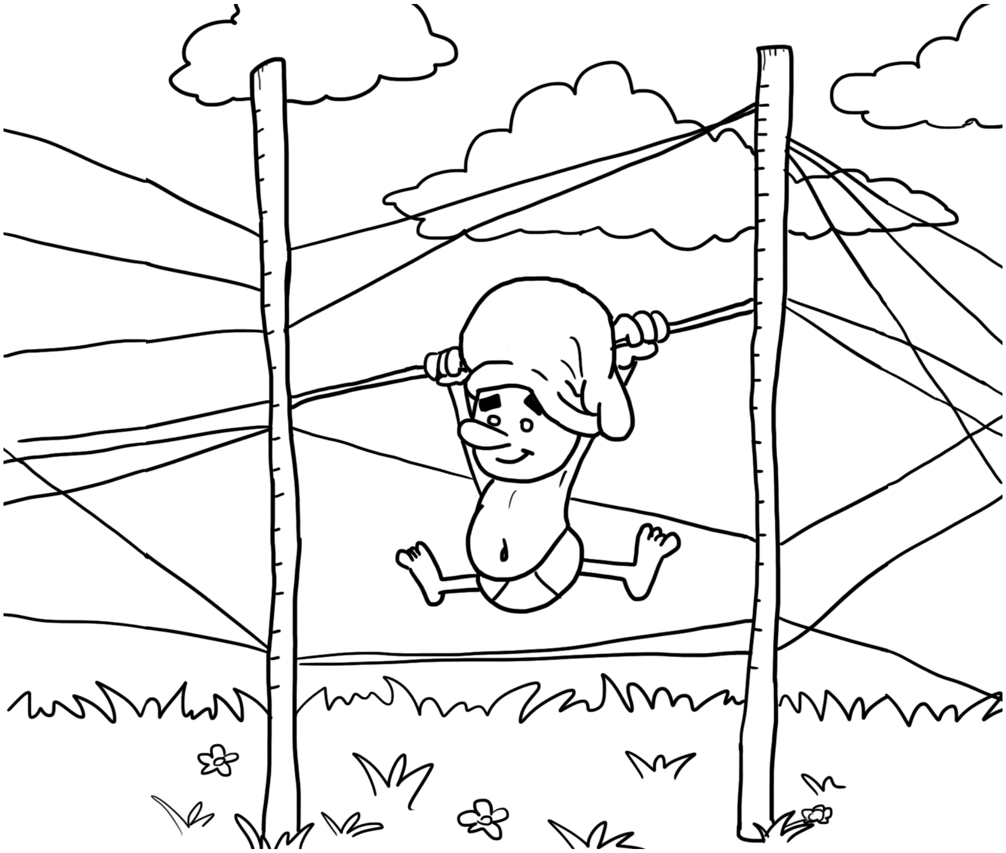
Part I

Supervised learning

Chapter 4

Linear models

Most right-handed people are linear thinking, think inside the box.
(our readers are free to disbelieve our openings)



Just below the mighty power of optimization lies the awesome power of linear algebra. Do you remember your teacher at school: “Study linear algebra, you will need it in life”? Well, with more years on your shoulders you know he was right. Linear algebra is a “math survival kit.” When confronted with a difficult problem, try with linear equations first. In many cases you will either solve it or at least come up with a workable approximation. Not surprisingly, this is true also for models to explain data.

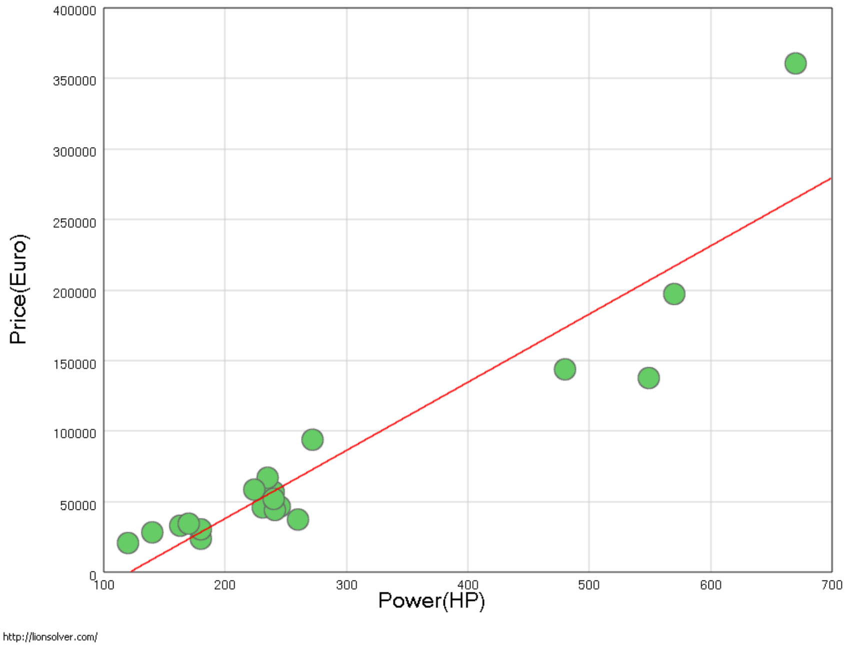


Figure 4.1: Data about price and power of different car models. A linear model is shown as a line.

Fig. 4.1 plots the price of different car models as a function of their horse power. As you can expect, the bigger the power the bigger the price, car dealers are honest, and there is an approximate linear relationship between the two quantities. If we summarize the data with the linear model (the line) we lose some details but most of the trend is preserved. We are *fitting* the data with a line.

Of course, defining what we mean by "best fit" will immediately lead us to *optimizing* the corresponding goodness function.

4.1 Linear regression

A linear dependence of the output from the input features is a widely used model. The model is simple, it can be easily trained, and the computed *weights* in the linear summation provide a direct explanation of the *importance* of the various attributes: the bigger the absolute value of the weight, the bigger the effect of the corresponding attribute. Therefore, do not complicate your life and consider nonlinear models unless you are strongly motivated by your application.

Math people do not want to waste trees and paper[1], arrays of numbers (*vectors*) are denoted with a single variable, like $\boldsymbol{w}$. The vector $\boldsymbol{w}$ contains its components $(w_1, w_2, ..., w_d)$, d being the number of input attributes or *dimension*. Vectors "stand up" like columns, to make them lie down you can transpose them, getting $\boldsymbol{w}^T$. The scalar product between vector $\boldsymbol{w}$ and vector $\boldsymbol{x}$ is therefore $\boldsymbol{w}^T \cdot \boldsymbol{x}$, with the usual matrix-multiplication definition, equal to $w_1 x_1 + w_2 x_2 + \cdots + w_d x_d$.

The hypothesis of a linear dependence of the outcomes on the input parameters can be expressed as

$$y_i = \boldsymbol{w}^T \cdot \boldsymbol{x}_i + \epsilon_i,$$

[1] We cannot go very deep into linear algebra in our book: we will give the basic definitions and motivations, it will be very easy for you to find more extended presentations in dedicated books or websites.

where $\boldsymbol{w} = (w_1, \ldots, w_d)$ is the vector of *weights* to be determined and ϵ_i is the error. In some cases the error ϵ_i is assumed to have a Gaussian distribution. Even if a linear model correctly explains the phenomenon, errors arise during measurements: **every physical quantity can be measured only with a finite precision**. Approximations are not needed because of negligence but because measurements are imperfect.

One is now looking for the weight vector $\boldsymbol{w}$ so that the linear function

$$\hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \cdot \boldsymbol{x} \tag{4.1}$$

approximates the experimental data as closely as possible. This goal can be achieved by finding the vector $\boldsymbol{w}^*$ that minimizes the sum of the squared errors (**least squares** approximation):

$$\text{ModelError}(\boldsymbol{w}) = \sum_{i=1}^{\ell} (\boldsymbol{w}^T \cdot \boldsymbol{x}_i - y_i)^2. \tag{4.2}$$

In the unrealistic case of zero measurement errors and a perfect linear model, one is left with a set of **linear equations** $\boldsymbol{w}^T \cdot \boldsymbol{x}_i = y_i$, one for each measurement, which can be solved by standard linear algebra if the system of linear equations is properly defined (d non-redundant equations in d unknowns). In all real-world cases, measurements have errors, and the number of measurements $(\boldsymbol{x}_i, y_i)$ can be much larger than the input dimension. Therefore one needs to search for an approximated solution, for weights $\boldsymbol{w}$ obtaining the lowest possible value of the above equation (4.2), low but typically larger than zero.

To use a linear model, you do not need to know *how* the equation is minimized. True believers in optimization can safely trust its magic problem-solving hand for linear models. But if you are curious, masochistic, or dealing with very large and problematic cases you may consider reading Sections 4.6 and 4.7.

4.2 A trick for nonlinear dependencies

Your appetite as a true believer in the awesome power of linear algebra is now huge but unfortunately not every case can be solved with a linear model. In most cases, a function in the form $f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$ is too restrictive to be useful. In particular, it assumes that $f(0) = 0$. One can change from a *linear* to an *affine* model by inserting a constant term w_0, obtaining: $f(\boldsymbol{x}) = w_0 + \boldsymbol{w}^T \cdot \boldsymbol{x}$. The constant term can be incorporated into the dot product through the simple creation of an additional dummy input fixed to 1. One defines $\boldsymbol{x} = (1, x_1, \ldots, x_d)$, so that equation (4.1) remains valid also for affine models.

The insertion of a constant term is a special case of a more general technique to model nonlinear dependencies while remaining in the easier context of linear least squares approximations. This apparent contradiction is solved by a trick: the model remains linear but it is applied to *nonlinear features* calculated from the raw input data instead of the original input $\boldsymbol{x}$. It is possible to define a set of functions:

$$\phi_1, \ldots, \phi_n : \mathbb{R}^d \to \mathbb{R}^n$$

that map the input space into some more complex space, in order to apply the linear regression to the vector $\boldsymbol{\varphi}(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \ldots, \phi_n(\boldsymbol{x}))$ rather than to $\boldsymbol{x}$ directly.

For example if $d = 2$ and $\boldsymbol{x} = (x_1, x_2)$ is an input vector, a quadratic dependence of the outcome can be obtained by defining the following *basis functions*:

$$\phi_1(\boldsymbol{x}) = 1, \quad \phi_2(\boldsymbol{x}) = x_1, \quad \phi_3(\boldsymbol{x}) = x_2,$$

$$\phi_4(\boldsymbol{x}) = x_1 x_2, \quad \phi_5(\boldsymbol{x}) = x_1^2, \quad \phi_6(\boldsymbol{x}) = x_2^2.$$

Note that $\phi_1(\boldsymbol{x})$ is defined in order to allow for a constant term in the dependence. The linear regression technique described above is then applied to the 6-dimensional vectors obtained by applying the basis functions, and not to the original 2-dimensional parameter vector.

More precisely, we look for a dependence given by a scalar product between a vector of weights $\boldsymbol{w}$ and a vector of features $\boldsymbol{\varphi}(\boldsymbol{x})$, as follows:

$$\hat{f}(\boldsymbol{x}) = \boldsymbol{w}^T \cdot \boldsymbol{\varphi}(\boldsymbol{x}).$$

The output is a weighted sum of the derived features.

4.3 Linear models for classification

Section 4.1 considers a linear function that fits the observed data, by minimizing the sum of squared errors. Some tasks, however, allow for a small set of possible outcomes. One is faced with a *classification* problem.

Let the outcome variable be two-valued (e.g., ± 1). In this case, linear functions can be used as **discriminants**, the idea is to have an hyperplane perpendicular to the vector $\boldsymbol{w}$ separating the two classes. A plane generalizes a line, and a hyperplane generalizes a plane when the number of dimensions is more than three.

The goal of the training procedure is to find the best hyperplane so that the examples of one class are on a side of the hyperplane, examples of the other class are on the other side. Mathematically one finds the best coefficient vector $\boldsymbol{w}$ so that the decision procedure:

$$y = \begin{cases} +1 & \text{if } \boldsymbol{w}^T \cdot \boldsymbol{x} \geq 0 \\ -1 & \text{otherwise} \end{cases} \tag{4.3}$$

performs the classification. The method for determining the **best separating linear function** (geometrically a hyperplane) depends on the chosen classification criteria and error measures.

For what we know from this chapter about regression, we can ask that points of the first class are mapped to $+1$, and points of the second classed are mapped to -1. This is a stronger requirement than separability but permits us to use a technique for regression, like gradient descent or pseudo-inverse. Furthermore, least squares not only achieves separation of the two classes (if separation is possible), but **robust separation, with a boundary which is far from the examples**, a *leitmotif* we will encounter in the following chapters. By forcing the outputs to be far (+1 and -1) and penalizing squared errors, the fragility caused by accepting any separating hyperplane disappears. A generic separating hyperplane may cause some examples of the two classes to have outputs very close to zero (like 0.000001 for the "$+1$" class, -0.000001 for the "-1" class), a small noise or measurement error on new cases will suffice to ruin the correct classification, and have them cross the boundary to the wrong side (see also Fig 12.1).

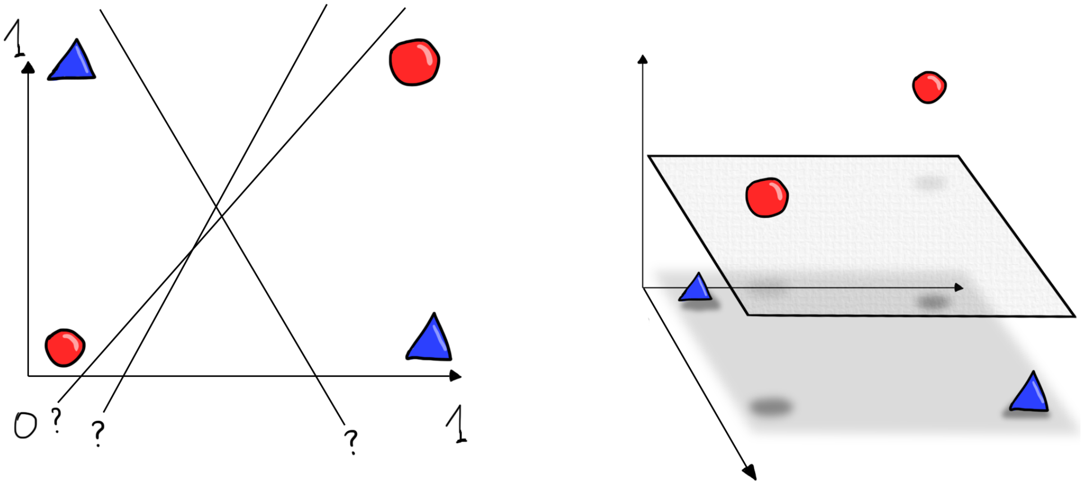


Figure 4.2: A case where a linear separation is impossible (XOR function, left). A linear separability with a hyperplane can be obtained by mapping the point in a nonlinear way to a higher-dimensional space.

If the examples are not separable with a hyperplane, one can either live with some error rate, or try the trick suggested before and calculate some *nonlinear features* from the raw input data to see if the transformed inputs are now separable. An example is shown in Fig. 4.2, the two inputs have 0-1 coordinates, the output is the *exclusive OR* function (XOR) of the two inputs (one or the other, but not both equal to 1).

The two classes (with output 1 or 0) cannot be separated by a line — a hyperplane of dimension one — in the original two-dimensional input space. But they can be separated by a plane in a three-dimensional transformed input space.

4.4 How does the brain work?

Our brains are a mess, at least those of the authors. For sure the system at work when summing two large numbers is very different from that active while playing "shoot'em up" action games. The system at work when calculating or reasoning in logical terms is different from the system at work when recognizing the face of your mother. The first system is iterative, it works by a sequence of steps, it requires conscious effort and attention. The second system works in parallel, is very fast, often effortless, sub-symbolic (not using symbols and logic).

Different mechanisms in machine learning resemble the two systems. Linear discrimination, with iterative *gradient-descent* learning techniques for gradual improvements, resembles more our sub-symbolic system, while classification trees based on a sequence of "if-then-else" rules (we will encounter them in the following chapters) resemble more our logical part.

Linear functions for classification have been known under many names, the historic one being *perceptron*, a name that stresses the analogy with biological neurons. Neurons communicate via chemical synapses (Fig. 4.3). Synapses [2]

[2] The term *synapse* has been coined from the Greek "syn-" ("together") and "haptein" ("to clasp").

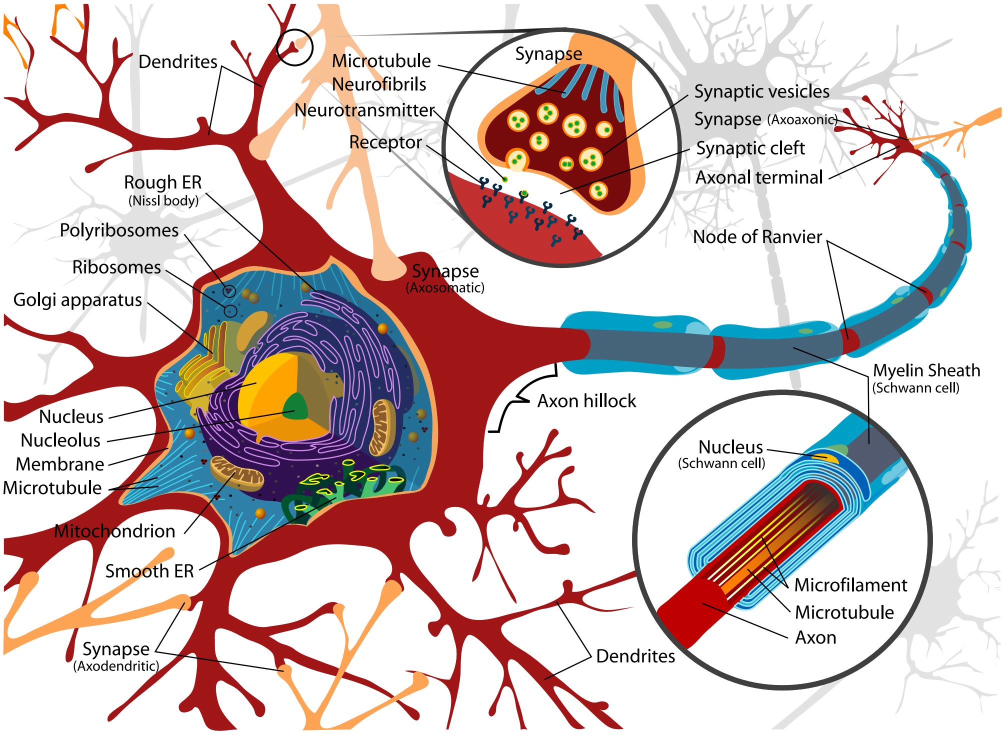


Figure 4.3: Neurons and synapses in the human brain.

are essential to neuronal function: neurons are cells that are specialized to pass signals to individual target cells, and synapses are the means by which they do so.

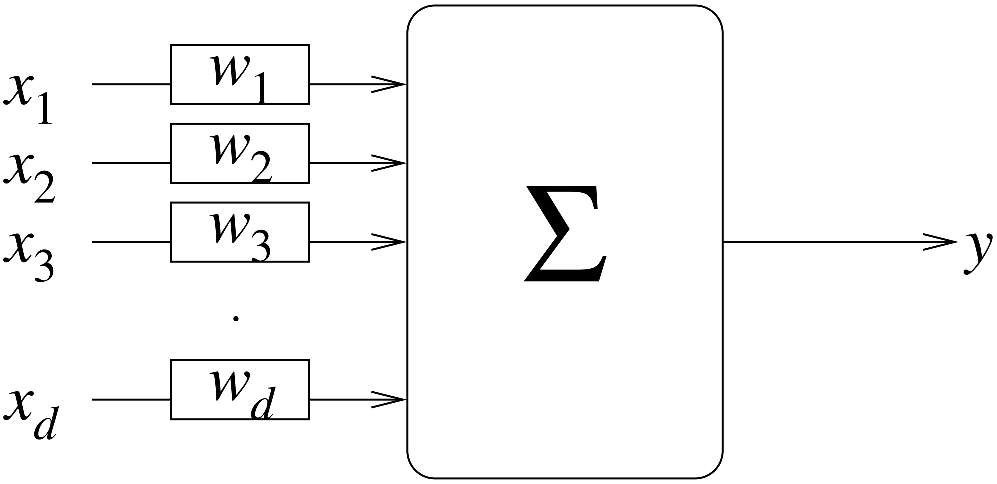


Figure 4.4: The Perceptron: the output is obtained by a weighted sum of the inputs passed through a final threshold function.

The fundamental process that triggers synaptic transmission is a propagating electrical signal that is generated by exploiting the electrically excitable membrane of the neuron. This signal is generated (the neuron output *fires*) if and only if the result of incoming signals combined with excitatory and inhibitory synapses and integrated surpasses a given threshold. Fig. 4.4 can be seen as the abstract and functional representation of a single nerve cell.

4.5 Why are linear models popular and successful?

The deep reason why linear models are so popular is the **smoothness** underlying many if not most of the physical phenomena ("Nature does not make jumps"). An example is in Fig. 4.5, the average stature of kids grows gradually, without jumps, to slowly reach a saturating stature after adolescence.

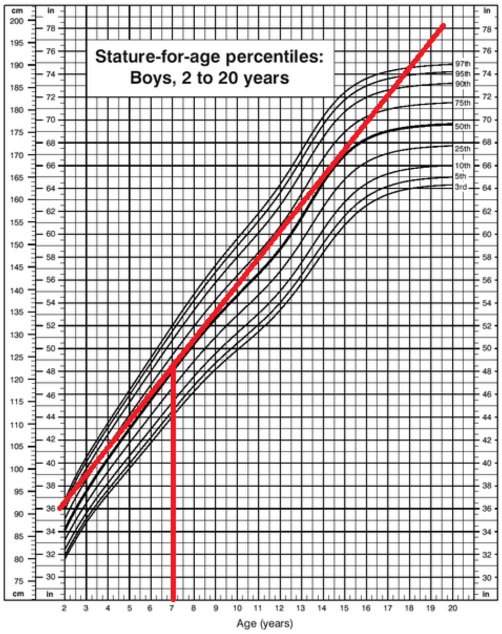


Figure 4.5: Functions describing physical phenomena tend to be *smooth*. The stature-for-age curve can be approximated well by a tangent line (dark) from 2 to about 15 years.

Now, if you remember calculus, every smooth (differentiable) function can be approximated around an operating point x_c with its **Taylor series approximation**. The second term of the series is linear, given by a scalar product between the gradient $\nabla f(x_c)$ and the displacement vector, the additional terms go to zero in a quadratic manner:

$$f(x) = f(x_c) + \nabla f(x_c) \cdot (x - x_c) + O(\|x - x_c\|^2). \tag{4.4}$$

Therefore, if the operating point of the smooth systems is close to a specific point x_c, a linear approximation is a reasonable place to start.

In general, the local model will work reasonably well only in the neighborhood of a given operating point. A linear model for stature growth of children obtained by a tangent at the 7 years stature point will stop working at about 15 years, luckily for the size of our houses.

4.6 Minimizing the sum of squared errors

Linear models are identified by minimizing the sum of squared errors of equation (4.2). If you are not satisfied with a "proof in the pudding" approach but want to go deeper into the matter, read on.

As mentioned, in the unrealistic case of zero measurement errors and of a perfect linear model, one is left with a set of **linear equations** $\boldsymbol{w}^T \cdot \boldsymbol{x}_i = y_i$, one for each measurement. If the system of linear equations is properly defined (d non-redundant equations in d unknowns) one can solve them by *inverting the matrix* containing the coefficients.

In practice, in real-world cases, reaching zero for the ModelError is impossible, errors are present and the number of data points can be much larger than the number of parameters d. Furthermore, let's remember that the goal of learning is generalization. We are interested in reducing the *future* prediction errors. We do not need to stress the system too much to reduce the error on the training examples. Reaching very small or zero training error can be counterproductive.

We need to **generalize the solution of a system of linear equations by allowing for errors**, and to generalize matrix inversion. We are lucky that equation (4.2) is quadratic, minimizing it leads again to a system of linear equations. Actually, one may suspect that the success of the quadratic model is related precisely to the fact that, after calculating derivatives, one is left with a linear expression.

If you are familiar with analysis, finding the minimum is straightforward: calculate the gradient and demand that it is equal to zero. If you are not familiar, think that the bottom of the valleys (the points of minimum) are characterized by the fact that small movements keep you at the same altitude.

The following equation determines the optimal value for w:

$$\boldsymbol{w}^* = (X^T X)^{-1} X^T \boldsymbol{y}; \tag{4.5}$$

where $\boldsymbol{y} = (y_1, \ldots, y_\ell)$ and X is the matrix whose rows are the $\boldsymbol{x}_i$ vectors.

The matrix $(X^T X)^{-1} X^T$ is the **pseudo-inverse** and it is a natural generalization of a matrix inverse to the case in which the matrix is non-square. If the matrix is invertible and the problem can be solved with zero error, the pseudo-inverse is equal to the inverse, but in general, e.g., if the number of examples is larger than the number of weights, aiming at a *least-square* solution avoids the embarrassment of not having an exact solution and provides a statistically sound least-squares "compromise" solution. In the real world, exact models are not compatible with the noisy characteristics of nature and of physical measurements and it is not surprising that the *least-square* and *pseudo-inverse* beasts are among the most popular tools.

The solution in equation (4.5) is "one shot:" calculate the pseudo-inverse from the experimental data and multiply to get the optimal weights. In some cases, if the number of examples is huge, **an iterative technique based on gradient descent** can be preferable: start from initial weights and keep moving them by executing small steps along the direction of the negative gradient, until the gradient becomes zero and the iterations reach a stable point. By the way, as you may anticipate, real neural systems like our brain do not work in a "one shot" manner with linear algebra but more in an iterative manner by gradually modifying synaptic weights. Maybe this is why linear algebra is not so popular at school?

Let us note that the minimization of squared errors has a physical analogy to the spring model presented in Fig. 4.6. Imagine that every sample point is connected by a vertical spring to a rigid bar, the physical realization of the best fit line. All springs have equal elastic constants and zero extension at rest. In this case, the potential energy of each spring is proportional to the square of its length, so that equation (4.2) describes the overall potential energy of the system up to a multiplicative constant. If one starts and lets the physical system oscillate until equilibrium is reached, with some friction to damp the oscillations, the final position of the rigid bar can be read out to obtain the least square fit parameters; an analog computer for line fitting!

For sure you will forget the pseudo-inverse but you will never forget this physical system of damped oscillating springs connecting the best-fit line to the experimental data.

If features are transformed by some φ function (as a trick to deal with nonlinear relationships), the solution is very similar. Let $\boldsymbol{x}'_i = \varphi(\boldsymbol{x}_i)$, $i = 1, \ldots, \ell$, be the transformations of the training input tuples $\boldsymbol{x}_i$. If X' is the matrix whose rows are the $\boldsymbol{x}'_i$ vectors, then the optimal weights with respect to the least squares approximation are computed as:

$$\boldsymbol{w}^* = (X'^T X')^{-1} X'^T y. \tag{4.6}$$

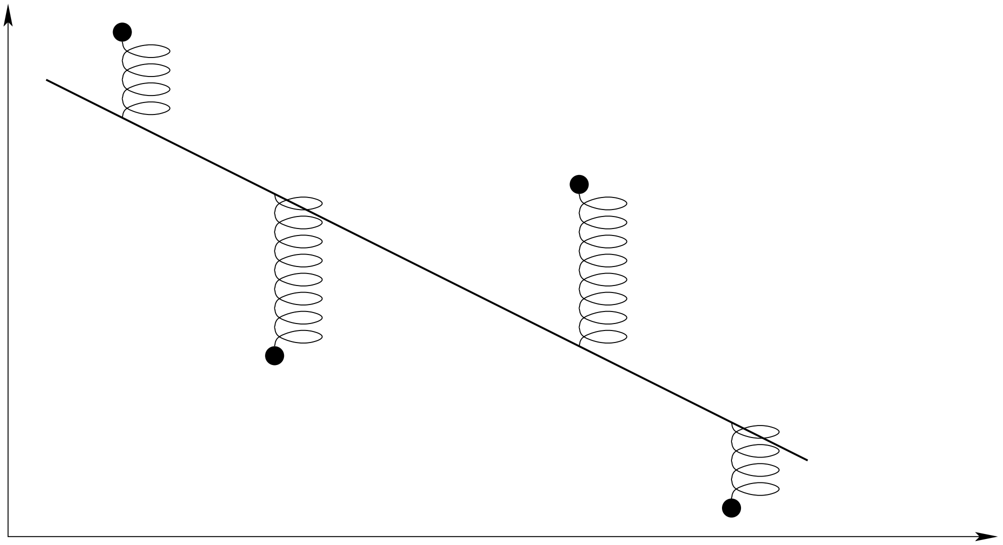


Figure 4.6: Physics gives an intuitive spring analogy for least squares fits. The best fit is the line that minimizes the overall potential energy of the system (proportional to the sum of the squares of the spring length).

4.7 Numerical instabilities and ridge regression

Real numbers (like π and "most" numbers) cannot be represented in a digital computer, they are "faked". Each number is assigned a *fixed and limited* number of bits, no way to represent an infinite number of digits like in 3.14159265... Therefore real numbers represented in a computer are "fake," they can and most often will have mistakes. Mistakes will propagate during mathematical operations, in certain cases the results of a sequence of operations can be very different from the mathematical results. Get a matrix, find its inverse and multiply the two. You are assumed to get the identity but you end up with something different. Maybe you should check which precision your bank is using.

When the number of examples is large, equation (4.6) is the solution of a linear system in the over-determined case (more linear equations than variables). In particular, matrix X^TX must be non-singular, and this can only happen if the training set points $x_1, \ldots, x_\ell$ do not lie in a proper subspace of $\mathbb{R}^d$, i.e., they are not "aligned." In many cases, even though X^TX *is* invertible, the distribution of the training points is not generic enough to make it *stable*. **Stability** here means that small perturbations of the sample points lead to small changes in the results. An example is given in Fig. 4.7, where a bad choice of sample points (in the right plot, x_1 and x_2 are not independent) makes the system much more dependent on noise, or even to rounding errors.

If there is no way to modify the choice of the training points, the standard mathematical tool to ensure numerical stability when sample points cannot be distributed at will is known as **ridge regression**. It consists of the addition of a **regularization** term to the (least squares) error function to be minimized:

$$\text{error}(\boldsymbol{w}; \lambda) = \sum_{i=1}^{\ell} (\boldsymbol{w}^T \cdot \boldsymbol{x}_i - y_i)^2 + \lambda \boldsymbol{w}^T \cdot \boldsymbol{w}. \tag{4.7}$$

The minimization with respect to $\boldsymbol{w}$ leads to the following:

$$\boldsymbol{w}^* = (\lambda I + X^TX)^{-1} X^T \boldsymbol{y}.$$

The insertion of a small diagonal term makes the inversion more robust. Moreover, one is actually demanding that the solution takes the size of the weight vector into account, to avoid steep interpolating planes such as the one in

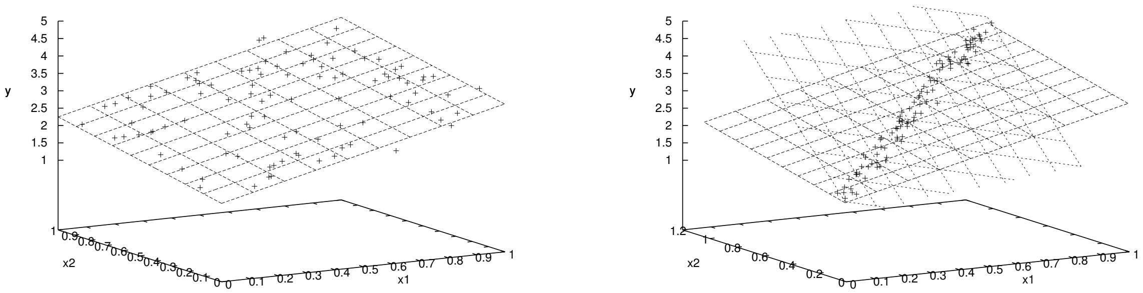


Figure 4.7: A well-spread training set (left) provides a stable numerical model, whereas a bad choice of sample points (right) may result in wildly changing planes, including very steep ones (adapted from [27]).

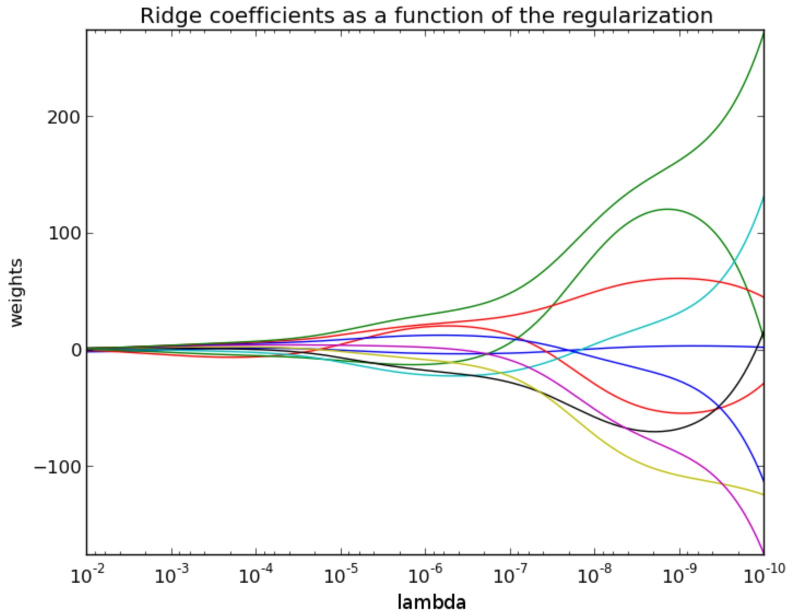


Figure 4.8: A "ridge" plot showing how weights tend to be contracted for large values of λ.

the right plot of Fig. 4.7. The term "ridge" refers to the graphical ridge pattern created when the optimal weights are plotted as a function of λ. As you can imagine, larger λ values causes an overall shrinkage of the weights (Fig. 4.8).

If you are interested, the theory justifying the approach is based on *Tichonov regularization*, which is the most commonly used method for curing *ill-posed* problems. A problem is ill-posed if no unique solution exists because there is not enough information specified in the problem, for example because the number of examples is limited. It is necessary to supply extra information or smoothness assumptions. By jointly minimizing the empirical error and penalty, one seeks a model that not only fits well but is also simple to avoid large variation which occurs in estimating complex models.

You do not need to know the theory to use machine learning but you need to be aware of the problem, this will raise your debugging capability if complex operations do not lead to the expected result. Avoiding very large or very small numbers is a pragmatic way to cure most problems, for example by scaling your input data before starting with machine learning.

Gist

Traditional linear models for regression (linear approximation of a set of input-output pairs) identify the best possible linear fit of experimental data by **minimizing a sum the squared errors** between the values predicted by the linear model and the output values of the training examples. Minimization can be "one shot" by generalizing matrix inversion in linear algebra (**pseudo-inverse**), or iteratively, by gradually modifying the model parameters to lower the error. The pseudo-inverse method is possibly the most used technique for fitting experimental data.

In classification, linear models aim at separating examples with lines, planes and hyper-planes. To identify a separating plane one can require a mapping of the inputs to two distinct output values (like $+1$ and -1) and use regression. More advanced techniques to find robust separating hyper-planes when considering generalization will be the Support Vector Machines described in the future chapters.

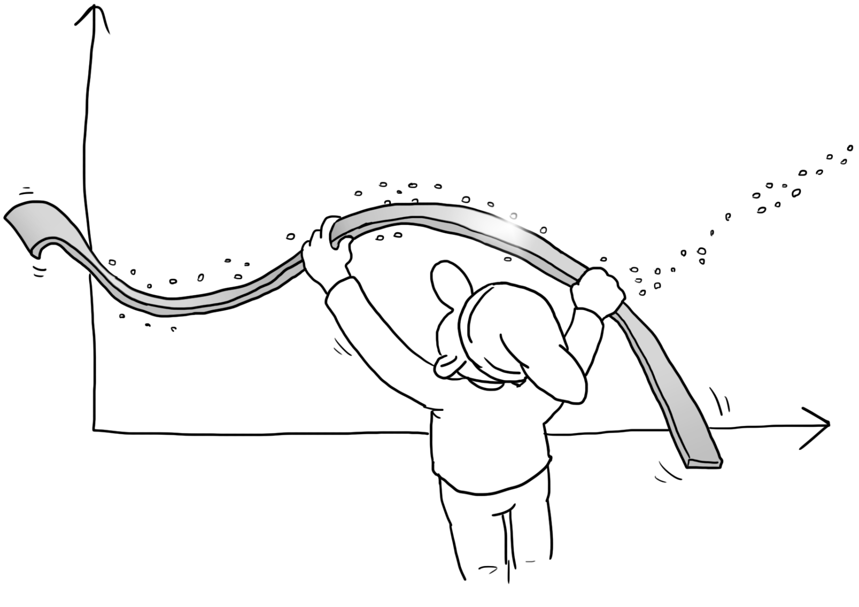
Real numbers do not live in a computer and their approximation by limited-size binary numbers is a possible cause of mistakes and instability (small perturbations of the sample points leading to large changes in the results).

Some machine learning methods are loosely related to the way in which biological brains learn from experience and function. Learning to drive a bicycle is not a matter of symbolic logic and equations but a matter of gradual tuning and ... rapidly recovering from initial accidents.

Chapter 5

Mastering generalized linear least-squares

Entia non sunt multiplicanda praeter necessitatem.
Entities must not be multiplied beyond necessity.
(William of Ockham c. 1285 – 1349)



Some issues were left open in the previous chapter about linear models, models with the coefficients appearing in a linear manner (a.k.a. linear-in-the-coefficients). The output of a serious effort is not only a single "take it or leave it" model. Usually one deals with multiple modeling architectures, with **judging the quality of a model** (the goodness-of-fit in our case) and **selecting the best possible architecture**, with **determining confidence regions** (e.g., error bars) for the estimated model parameters, etc. After reading this chapter you are supposed to raise from the status of casual user to that of professional least-squares guru.

In the previous chapter we mentioned a trick to take care of some nonlinearities: mapping the original input by some nonlinear function φ and then considering a linear model in the transformed input space (see Section 4.2). While the topics discussed in this Chapter are valid in the general case, your intuition will be helped if you keep in mind the special case of **polynomial fits** in one input variable, in which the nonlinear functions consist of powers of the original inputs, like

$$\phi_0(x) = x^0 = 1, \quad \phi_1(x) = x^1 = x, \quad \phi_2(x) = x^2, \ldots$$

The case is of particular interest and widely used in practice to deserve being studied.

Given raw data in the form of pairs of values:

$$(x_i, y_i), \qquad i \in 1, 2, \ldots, N,$$

the aim is to derive a function $f(x)$ which appropriately models the dependence of Y on X, so that one can evaluate the function on new and unknown x values.

Identifying significant patterns and relationships implies eliminating insignificant details like measurement *noise*, stochastic errors cause by the finite-precision physical measurements. Think about modeling how the height of a person changes with age. If you repeat measuring with a high precision instrument, you will get different values for each measurement. A reflection of these noisy measurements is the simple fact that you are giving a limited number of digits to describe your height, no mentally sane person would answer 1823477 micrometers when asked about his height.

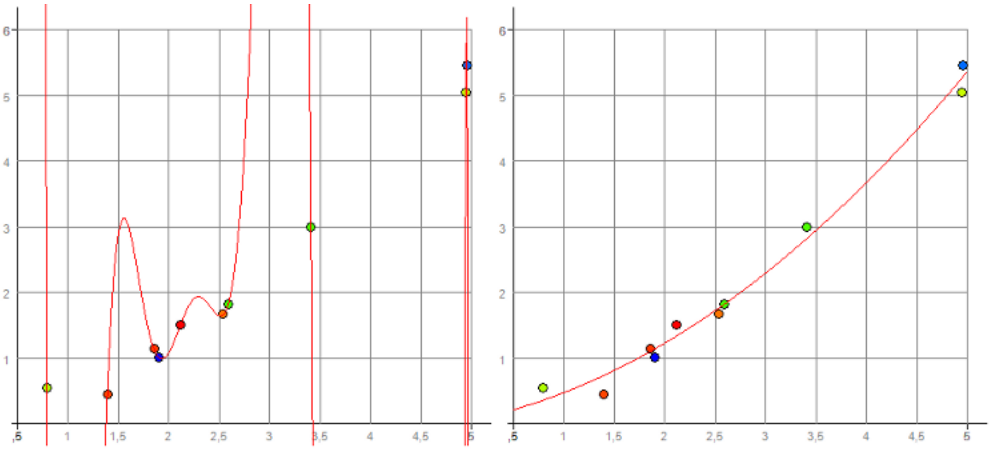


Figure 5.1: Comparison between interpolation and fitting. The number of free parameters of the polynomial (equal to its degree minus one) changes from the number of data points (left), to three (right).

Coming back to the model, we do *not* demand that the function models also the noise and that the plot passes exactly through the sample values. I.e., we don't require that $y_i = f(x_i)$ for all points. We do not deal with **interpolation** but with **fitting** (being compatible, similar or consistent). Losing absolute fidelity is not a weakness but a strength, providing an opportunity to simplifying the analysis, create more powerful models and permit reasoning that isn't bogged down by trivia. A comparison between a function interpolating all the examples, and a much simpler one, like in Fig. 5.1, shows the obvious difference. *Occam's razor* illustrates this basic principle that simpler models should be preferred over unnecessarily complicated ones.

The freedom to choose among different models, e.g., by picking polynomials of different degrees, is accompanied by the responsibility of judging the goodness of the different models. A standard way for polynomial fits is by statistics from the resulting sum-of-squared-errors.

5.1 Goodness of fit and and chi-square

Let's start with a polynomial of degree $M - 1$, where M is defined as the *degree bound*, equal to the degree plus one. M is also the number of free parameters (the constant term in the polynomial also counts). One searches for the polynomial of a suitable degree that best describes the data distribution:

$$f(x, \boldsymbol{c}) = c_0 + c_1 x + c_2 x^2 + \cdots + c_{M-1} x^{M-1} = \sum_{k=0}^{M-1} c_k x^k. \tag{5.1}$$

When the dependence on parameters $\boldsymbol{c}$ is taken for granted, we will just use $f(x)$ for brevity. Because a polynomial is determined by its M parameters (collected in vector $\boldsymbol{c}$), we search for *optimal values* of these parameters. This is an example of what we call the *power of optimization*. The general recipe is: formulate the problem as one of minimizing a function and then resort to optimization.

For reasons having roots in statistics and maximum-likelihood estimation, described in the following Section 5.2, a widely used merit function to estimate the **goodness-of-fit** is given by the **chi-squared**, a term derived from the Greek letter used to identify a connected statistical distribution, χ^2:

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{y_i - f(x_i)}{\sigma_i} \right)^2 . \tag{5.2}$$

The explanation is simple if the parameters σ_i are all equal to one: in this case, χ^2 measures the sum of squared errors between the actual value y_i and the value obtained by the model $f(x_i)$, and it is precisely the ModelError($\boldsymbol{w}$) function described in the previous Chapter.

In some cases, however, the measurement processes may be different for different points and one has an estimate of the measurement error σ_i, assumed to be the standard deviation. Think about measurements done with instruments characterized by different degrees of precision, like a meter stick and a high-precision caliper.

The chi-square definition is a precise, mathematical method of expressing the obvious fact that an error of one millimeter is acceptable with a meter stick, much less so with a caliper: when computing χ^2, the errors have to be compared to the standard deviation (i.e., *normalized*), therefore the error is divided by σ_i. The result is a number that is independent from the actual error size, and whose meaning is standardized.

Now that you have a precise way of measuring the quality of a polynomial model by the normalized *chi-square*, your problem becomes that of finding polynomial coefficients *minimizing* this error. An inspiring physical interpretation is illustrated in Fig. 5.2. Luckily, this problem is solvable with standard linear algebra techniques, as already explained in the previous chapter.

Here we complete the details of the analysis exercise as follows: take partial derivatives $\partial\chi^2/\partial c_k$ and require that they are equal to zero. Because the *chi-square* is quadratic in the coefficients c_k, we get a set of M linear equations to be solved:

$$0 = \frac{\partial \chi^2}{\partial c_k} = 2 \sum_{i=1}^{N} \frac{1}{{\sigma_i}^2} \left(y_i - \sum_{j=0}^{M-1} c_j {x_i}^j \right) {x_i}^k, \qquad \text{for } k = 0, 1, \ldots, M-1 \tag{5.3}$$

To shorten the math it is convenient to introduce the $N \times M$ matrix $A = (a_{ij})$ such that $a_{ij} = {x_i}^j/\sigma_i$, containing powers of the x_i coordinates normalized by σ_i, the vector $\boldsymbol{c}$ of the unknown coefficients, and the vector $\boldsymbol{b}$ such that $b_i = y_i/\sigma_i$.

It is easy to check that the linear system in equation (5.3) can be rewritten in a more compact form as:

$$(A^T \cdot A) \cdot \boldsymbol{c} = A^T \cdot \boldsymbol{b}, \tag{5.4}$$

which is called the *normal equation* of the least-squares problem.

The coefficients can be obtained by deriving the inverse matrix $C = (A^T \cdot A)^{-1}$, and using it to obtain $\boldsymbol{c} = C \cdot A^T \cdot \boldsymbol{b}$. Interestingly, C is the covariance matrix of the coefficients' vector $\boldsymbol{c}$ seen as a random variable: the diagonal elements of C are the variances (squared uncertainties) of the fitted parameters $c_{ii} = \sigma^2(c_i)$, and the off-diagonal elements are the covariances between pairs of parameters.

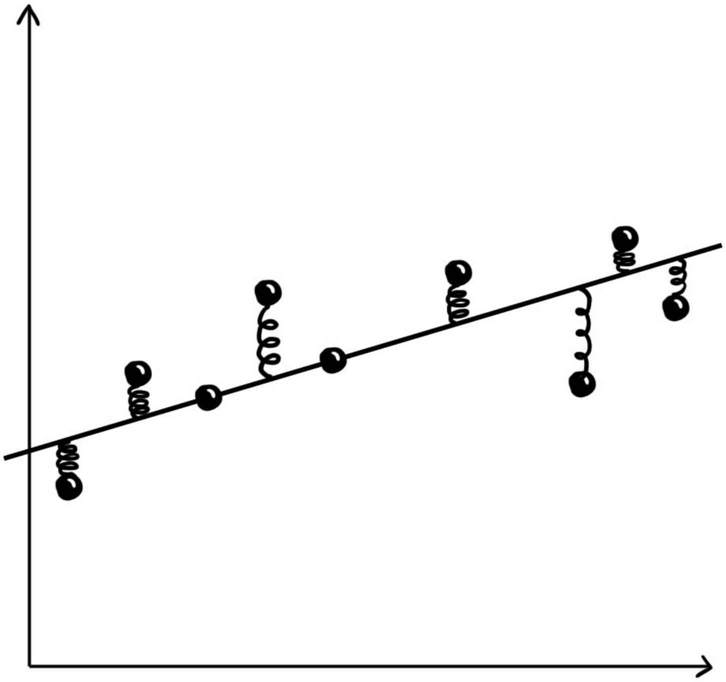


Figure 5.2: A fit by a line with a physical analogy: each data point is connected by a spring to the fitting line. The strength of the spring is proportional to $1/{\sigma_i}^2$. The minimum energy configuration corresponds to the minimum *chi-square*.

The matrix $(A^T \cdot A)^{-1} A^T$ is the **pseudo-inverse** already encountered in the previous chapter, generalizing the solutions of a system of linear equations in the **least-squared-errors** sense:

$$\min_{\boldsymbol{c} \in \mathbb{R}^M} \chi^2 = \|A \cdot \boldsymbol{c} - \boldsymbol{b}\|^2. \tag{5.5}$$

If an exact solution of equation (5.5) is possible the resulting *chi-squared* value is zero, and the line of fit passes exactly through all data points. This occurs if we have M parameters and M distinct pairs of points (x_i, y_i), leading to an invertible system of M linear equations in M unknowns. In this case we are not dealing with an approximated fit but with interpolation. If no exact solution is possible, as in the standard case of more pairs of points than parameters, the pseudo-inverse gives us the vector $\boldsymbol{c}$ such that $A \cdot \boldsymbol{c}$ is as close as possible to $\boldsymbol{b}$ in the Euclidean norm, a very intuitive way to interpret the approximated solution. Remember that good models of noisy data need to *summarize* the observed data, not to reproduce them exactly, so that the number of parameters has to be (much) less than the number of data points.

The above derivations are not limited to fitting a polynomial, we can now easily fit many other functions. In particular, if the function is given by a linear combination of basis functions $\phi_k(\boldsymbol{x})$, as

$$f(x) = \sum_{k=0}^{M-1} c_k \phi_k(\boldsymbol{x})$$

most of the work is already done. In fact, it is sufficient to substitute the basis function values in the matrix A, which now become $a_{ij} = \phi_j(\boldsymbol{x}_i)/\sigma_i$. We have therefore a powerful mechanism to fit more complex functions like, for example,

$$f(x) = c_0 + c_1 \cos x + c_2 \log x + c_3 \tanh x^3.$$

Let's only note that the unknown parameters must appear *linearly*, they cannot appear in the arguments of functions. For example, by this method we cannot fit directly $f(x) = \exp(-cx)$, or $f(x) = \tanh(x^3/c)$. At most, we can try to transform the problem to recover the case of a linear combination of basis functions. In the first case, we can for example fit the values $\hat{y}_i = \log y_i$ with a linear function $f(\hat{y}) = -cx$, but this trick will not be possible in the general case.

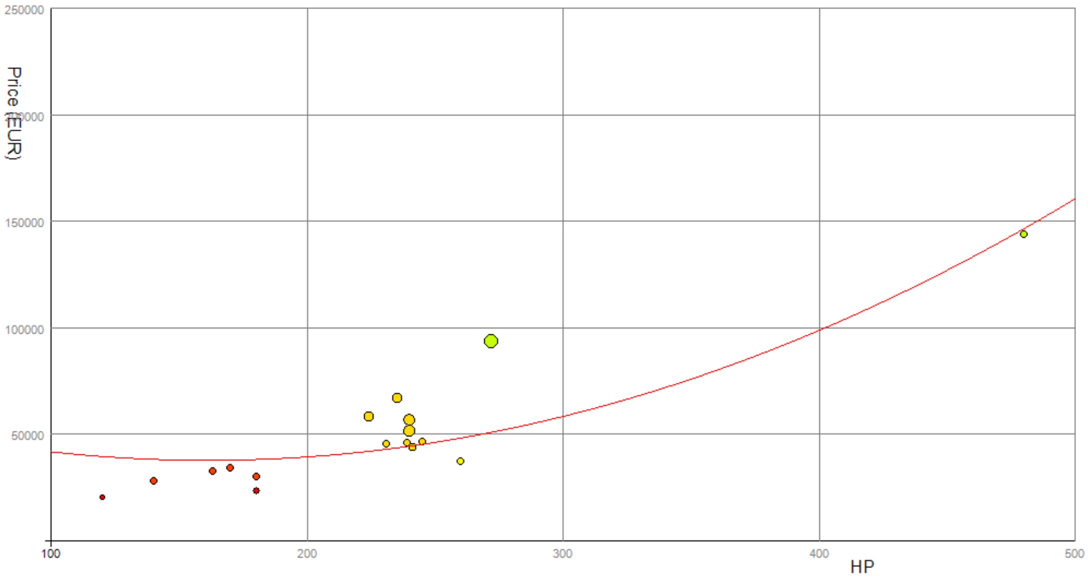


Figure 5.3: A polynomial fit: price of cars as a function of engine power.

A polynomial fit is shown as a curve in the scatterplot of Fig. 5.3, which shows a fit with a polynomial of degree 2 (a parabola). A visual comparison of the line against the data points can already give a visual feedback about the goodness-of-fit (the *chi-squared* value). This 'chi-by-eye" approach consists of looking at the plot and judging it to look nice or bad with respect to the scatterplot of the original measurements.

When the experimental data do not follow a polynomial law, fitting a polynomial is not very useful and can be misleading. As explained above, a low value of the *chi-squared* can still be reached by increasing the degree of the polynomial: this will give it a larger freedom of movement to pass closer and closer to the experimental data. The polynomial will actually *interpolate* the points with zero error if the number of parameters of the polynomial equals the number of points. But this reduction in the error will be paid by wild oscillations of the curve *between* the original points, as shown in Fig. 5.1 (left). The model is not summarizing the data and it has serious *difficulties in generalizing*. It fails to predict y values for x values which are different from the ones used for building the polynomial.

In statistics, **overfitting** occurs when a model tends to describe random error or noise instead of the underlying relationship. Overfitting occurs when a model is too complex, such as having too many degrees of freedom, in relation to the amount of data available (too many coefficients in the polynomial in our case).

An overfitted model will generally have a poor predictive performance. An analogy in human behavior can be found in teaching: if a student concentrates and memorizes only the details of the teacher's presentation (for example the details of a specific exercise in mathematics) without extracting and understanding the underlying rules and meaning, he will only be able to vacuously repeat the teacher's words by heart, but not to generalize his knowledge to new cases.

5.2 Least squares and maximum likelihood estimation

Now that the basic technology for generalized least-squares fitting is known, let's consider additional motivations from statistics. Given the freedom of selecting different models, for example different degrees for a fitting polynomial, instructions to identify the best model architecture are precious to go beyond the superficial "chi-by-eye" method.

The least-squares fitting process is as follows:

1. Assume that Mother Nature and the experimental procedure (including measurements) are generating independent experimental samples (x_i, y_i). Assume that the y_i values are affected by errors distributed according to a normal (i.e., Gaussian) distribution.

2. If the model parameters $\boldsymbol{c}$ are known, one can estimate the probability of our measured data, given the parameters. In statistical terms this is called **likelihood** of the data.

3. Least-squares fitting is equivalent to searching for the parameters which are maximizing the likelihood of our data. Least-squares is a **maximum likelihood estimator**. Intuitively, this maximizes the "agreement" of the selected model with the observed data.

The demonstration is straightforward. You may want to refresh Gaussian distributions in Section 5.3 before proceeding. The probability for a single data point to be in an interval of width $\mathrm{d}y$ around its measure value y_i is proportional to

$$\exp\left(-\frac{1}{2}\left(\frac{y_i - f(x_i,\boldsymbol{c})}{\sigma_i}\right)^2\right)\ \mathrm{d}y. \tag{5.6}$$

Because points are generated independently, the same probability for the entire experimental sequence (its *likelihood*) is obtained by multiplying individual probabilities:

$$\mathrm{d}P \propto \prod_{i=1}^{N} \exp\left(-\frac{1}{2}\left(\frac{y_i - f(x_i,\boldsymbol{c})}{\sigma_i}\right)^2\right)\ \mathrm{d}y. \tag{5.7}$$

One is maximizing over $\boldsymbol{c}$ and therefore constant factors like $(\ \mathrm{d}y)^N$ can be omitted. In addition, maximizing the likelihood is equivalent to maximizing its logarithm (the logarithm is in fact an increasing function of its argument). Well, because of basic properties of logarithms (namely they transform products into sums, powers into products, etc.), the logarithm of equation (5.7), when constant terms are omitted, is precisely the definition of *chi-squared* in equation (5.2). The connection between least-squares fitting and maximum likelihood estimation is now clear.

5.2.1 Hypothesis testing

Statistical hypothesis testing can be used to **judge the quality** of a model. The fundamental question to ask is: considering the N experimental points and the estimated M parameters, what is the probability that, by chance, values equal to or larger than the measured *chi-squared* are obtained? The above question translates the obvious question about our data ("**what is the likelihood of measuring the data that one actually did measure?**") into a more precise statistical form, i.e.: "**what's the probability that another set of sample data fits the model even worse than our current set does?**" If this probability is high, the obtained discrepancies between y_i and $f(x_i, \boldsymbol{c})$ make sense from a statistical point of view. If this probability is very low, either you have been very unlucky, or something does not work in your model: errors are too large with respect to what can be expected by Mother Nature plus the measurement generation process.

Fisher introduced the concept of **null hypothesis** by an example[127], the now famous "lady tasting tea" experiment. A lady claimed the ability to determine the means of tea preparation by taste. Fisher proposed an experiment and an analysis to test her claim. She was to be offered 8 cups of tea, 4 prepared by each method, for determination. He proposed the null hypothesis that she possessed no such ability, so she was just guessing. With this assumption, the number of correct guesses (the test statistic) formed a binomial distribution. Fisher calculated that her chance of guessing all cups correctly was 1/70. Fisher commented: "…the null hypothesis is never proved or established, but is possibly disproved, in the course of experimentation. Every experiment may be said to exist only in order to give the facts a chance of disproving the null hypothesis."

Let $\hat{\chi}^2$ be the *chi-squared* computed on your chosen model for a given set of inputs and outputs. This value follows a probability distribution called, again, *chi-squared with ν degrees of freedom* (χ^2_ν), where the number of degrees of freedom ν determines how much the dataset is "larger" than the model. If we assume that errors are normally distributed with null mean and unit variance (remember, we already normalized them), then $\nu = N - M$. In the general case, the correct number of degrees of freedom also depends on the number of parameters needed to express the error distribution (e.g., skewness). Our desired goodness-of-fit measure is therefore expressed by the parameter Q as follows:

$$Q = Q_{\hat{\chi}^2,\nu} = \Pr(\chi^2_\nu \geq \hat{\chi}^2).$$

The value of Q for a given empirical value of $\hat{\chi}^2$ and the given number of degrees of freedom can be calculated or read from tables[1].

The **reduced chi-square** statistic χ^2_{red} is simply the chi-squared divided by the number of degrees of freedom, in our example $\nu = N - M$. The advantage of the reduced chi-squared is that it already normalizes for the number of data points and model complexity. Some rules of thumb follow.

- A value $\chi^2_{\text{red}} \approx 1$ is what we would expect if the σ_i are good estimates of the measurement noise and the model is good.

- Values of χ^2_{red} that are too large mean that either you underestimated your source of errors, or that the model does not fit very well. If you trust your σ_i's, maybe increasing the polynomial degree will improve the result.

- Finally, if χ^2_{red} is too small, then the agreement between the model $f(x)$ and the data (x_i, y_i) is suspiciously good; we are possibly in the situation shown in the left-hand side of Fig. 5.1. The model is 'over-fitting' the data: either the model is improperly fitting noise, or the error variance has been overestimated. We should try reducing the polynomial degree[2].

The importance of the **number of degrees of freedom** ν, which decreases when the number of parameters in the model increases, becomes apparent when models with different numbers of parameters are compared. As we mentioned, it is easy to get a low *chi-square* value by increasing the number of parameters. Using Q to measure the goodness-of-fit takes this effect into account. A model with a larger *chi-square* value (larger errors) can produce a higher Q value (i.e., be better) with respect to one with smaller errors but a larger number of parameters.

By using the goodness-of-fit Q measure one can rank different models and pick the most appropriate one. The process sounds now clear and quantitative. If you are fitting a polynomial, you can now repeat the process with different degrees, measure Q and select the best model architecture (the best polynomial degree).

But the devil is in the details: the machinery works *provided that the assumptions are correct*, provided that errors follow the correct distribution, that the σ_i are known and appropriate, that the measurements are independent. By the way, asking for σ_i values can be a puzzling question for non-sophisticated users. You need to proceed with caution: **statistics is a minefield if assumptions are wrong** and a single wrong assumption makes the entire chain of arguments explode.

[1] The exact formula is

$$Q_{\hat{\chi}^2,\nu} = \Pr(\chi^2_\nu \geq \hat{\chi}^2) = \left(2^{\frac{\nu}{2}}\Gamma\left(\frac{\nu}{2}\right)\right)^{-1} \int_{\hat{\chi}^2}^{+\infty} t^{\frac{\nu}{2}-1} e^{-\frac{t}{2}}\ \mathrm{d}t,$$

which can be easily calculated in this era of cheap CPU power.

[2] Pearson's $chi - squared$ test provides objective thresholds for assessing the goodness-of-fit based on the value of χ^2, on the number of parameters and of data points, and on a desired confidence level, as explained in Section 5.2.

5.2.2 Cross-validation

Up to now we presented "historical" results, statistics was born well before the advent of computers, when calculations were very costly. Luckily, the current abundance of computational power permits robust techniques to estimate error bars and gauge the confidence in your models and their predictions. These methods do not require advanced mathematics, they are normally easy to understand, and they tend to be robust with respect to different distributions of errors.

In particular the **cross-validation** method of Section 3.2 can be used to select the best model. As usual the basic idea is to keep some measurements in the pocket, use the other ones to identify the model, take them out of the pocket to estimate errors on new examples, repeat and average the results. These estimates of generalization can be used to identify the best model architecture in a robust manner, provided that data is abundant. The distribution of results by the different folds of cross-validation gives information about the stability of the estimates, and permits to assert that, with a given probability (confidence), expected generalization results will be in a given performance range. The issue of deriving **error bars** for performance estimates, or, in general, for quantities estimated from the data, is explored in the next section.

5.3 Bootstrapping your confidence (error bars)

Let's imagine that Mother Nature is producing data (input-output pairs) from a true polynomial characterized by parameters $\boldsymbol{c}$. Mother Nature picks all x_i's randomly, independently and from the same distribution and produces $y_i = f(x_i, \boldsymbol{c}) + \epsilon_i$, according to equation (5.1) plus error ϵ_i.

By using generalized linear least squares you determine the maximum likelihood value $\boldsymbol{c}^{(0)}$ for the (x_i, y_i) pairs that you have been provided. If the above generation by Mother Nature and the above estimation process are repeated, there is no guarantee that you will get the same value $\boldsymbol{c}^{(0)}$ again. On the contrary, most probably you will get a different $\boldsymbol{c}^{(1)}$, then $\boldsymbol{c}^{(2)}$, etc.

It is unfair to run the estimation once and just use the first $\boldsymbol{c}^{(0)}$ that you get. If you could run many processes you could find average values for the coefficients, estimate **error bars**, maybe even use many different models and average their results (*ensemble* or *democratic* methods will be considered in later chapters). Error bars allow quantifying your confidence level in the estimation, so that you can say: with probability 90% (or whatever confidence value you decide), the coefficient c_i will have a value between $c - B$ and $c + B$, B being the estimated error bar[3]. Or, "We are 99% confident that the true value of the parameter is in our confidence interval." When the model is used, similar error bars can be obtained on the predicted y values. For data generated by simulators, this kind of repeated and randomized process is called a **Monte Carlo experiment**. Monte Carlo methods are a class of computational algorithms that rely on repeated random sampling to obtain numerical results; i.e., by running simulations many times over just like actually playing and recording your results in a real casino situation: hence the name from the town of Monte Carlo in the Principality of Monaco, the European version of Las Vegas.

On the other hand, Mother Nature, i.e. the process generating your data, can deliver just a single set of measurements, and repeated interrogations can be too costly to afford. How can you get the advantages of repeating different and randomized estimates by using just *one* series of measurements? At first, it looks like an absurdly impossible action. Similar absurdities occur in the "Surprising Adventures," when Baron Munchausen pulls himself and his horse out of a swamp by his hair (Fig. 5.4), and to imitate him one could try to "pull oneself over a fence by one's bootstraps," hence the modern meaning of the term *bootstrapping* as a description of a self-sustaining process.

Well, it turns out that there is indeed a way to use a single series of measurements to imitate a real Monte Carlo method. This can be implemented by constructing a number of *resamples* of the observed dataset (and of equal size). Each new sample is obtained by *random sampling with replacement*, so that the same case can be taken more than once (Fig. 5.5). By simple math and for large numbers N of examples, about 37% of the examples (actually approximately

[3] As a side observation, if you know that an error bar is 0.1, you will avoid putting too many digits after the decimal point. If you estimate your height, please do not write "182.326548435054cm": stopping at 182.3cm (plus or minus 0.1cm) will be fine.

Figure 5.4: Baron Munchausen pulls himself out of a swamp by his hair.

$1/e$) are not present in a sample, because they are replaced by multiple copies of the original cases[4].

For each new i-th resample the fit procedure is repeated, obtaining many estimates $\boldsymbol{c}_i$ of the model parameters. One can then analyze how the various estimates are distributed, using observed frequencies to estimate a probability distribution, and summarizing the distribution with confidence intervals. For example, after fixing a confidence level of 90% one can determine the region around the median value of $\boldsymbol{c}$ where an estimated $\boldsymbol{c}$ will fall with probability 0.9. Depending on the sophistication level, the confidence region in more than one dimension can be given by rectangular intervals or by more flexible regions, like ellipses. An example of a confidence interval in one dimension (a single parameter c to be estimated) is given in Fig. 5.6. Note that confidence intervals can be obtained for arbitrary distributions, not necessarily normal, and confidence intervals do not need to be symmetric around the median.

Appendix: Plotting confidence regions (percentiles and box plots)

A quick-and-dirty way to analyze the distribution of estimated parameters is by histograms (counting frequencies for values occurring in a set of intervals). In some cases the histogram contains more information than what is needed, and the information is not easily interpreted. A very compact way to represent a distribution of values is by its **average**

[4] In spite of its "brute force" quick-and-dirty look, bootstrapping enjoys a growing reputation also among statisticians. The basic idea is that the actual data set, viewed as a probability distribution consisting of a sum of *Dirac delta* functions on the measured values, is in most cases the best available estimator of the underlying probability distribution [300].

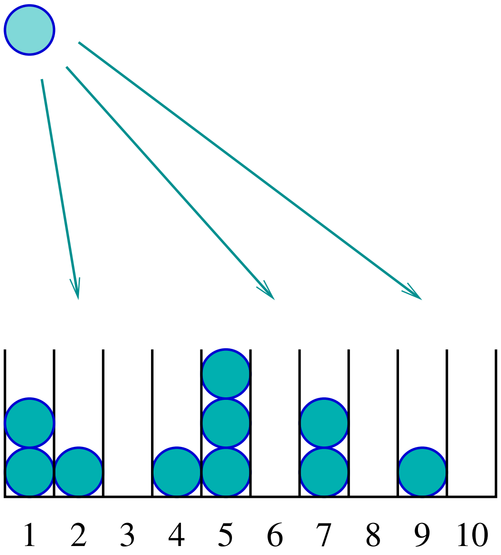


Figure 5.5: Bootstrapping: 10 balls are thrown with uniform probability to end up in the 10 boxes. They decide which cases and how many copies are present in the bootstrap sample (two copies of case 1, one copy of case 2, zero copies of case 3,. . .

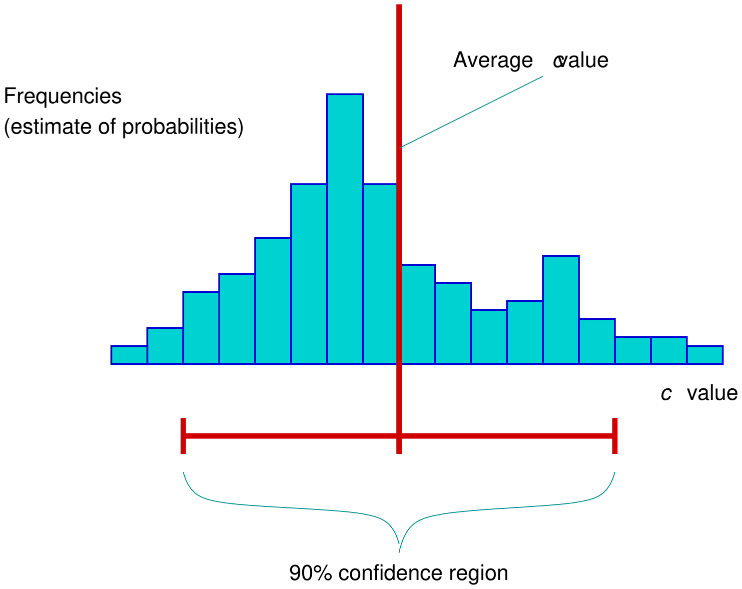


Figure 5.6: Confidence interval: from the histogram characterizing the distribution of the estimated c values one derives the region around the average value collecting 90% of the cases. Other confidence levels can be used, like 68.3%, 95.4%. etc. (the historical probability values corresponding to σ and 2σ in the case of normal distributions).

value μ. Given a set $\mathcal{X}$ of N values x_i, the average is

$$\mu(\mathcal{X}) = (\sum_{i=1}^{N} x_i)/N, \qquad x_{i,\dots,N} \in \mathcal{X}. \tag{5.8}$$

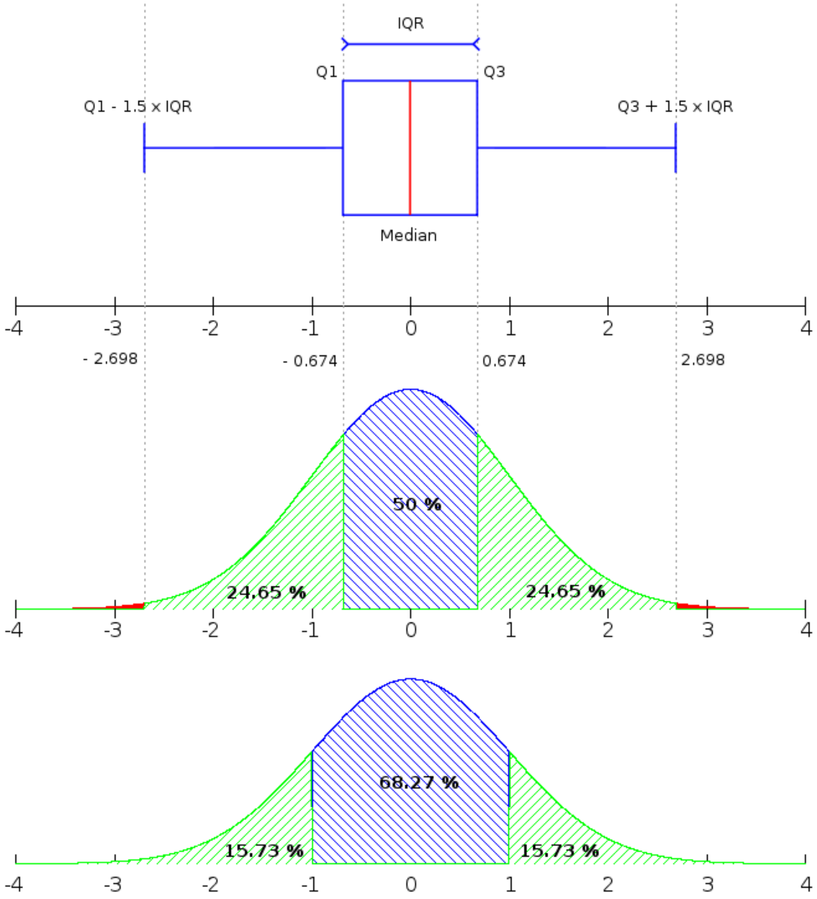


Figure 5.7: Comparison between box plot (above) and a normal distribution. The X axis shows positions in terms of the standard deviation σ. For example, in the bottom plot, 68.27% of the points fall within plus or minus one σ from the mean value.

The average value is also called the expected value, or mathematical expectation, or mean, or first moment, and denoted in different ways, for example as $\overline{x}$ or $E(x)$.

A related but different value is the **median**, defined as the value separating the higher half of a sample from the lower half. Given a finite list of values, it can be found by sorting all the observations from the lowest to the highest value and picking the middle one. If some **outliers** are present (data which are far from most of the other values), the median is a more robust measure than the average, which can be heavily influenced by outliers. On the contrary, if the data are clustered, like when they are produced by a normal distribution, the average tends to coincide with the median. The median can be generalized by considering the **percentile**, the value of a variable below which a certain percentage of observations fall. So the 10th percentile is the value below which 10 percent of the observations are found. **Quartiles** are a specific case, they are the lower quartile (25th percentile), the median, and the upper quartile (75th percentile). The interquartile range (IQR), also called the midspread or middle fifty, is a measure of statistical dispersion, being equal to the difference between the third and first quartiles.

A **box plot**, also known as a **box-and-whisker plot**, shows five-number summaries of the set of values: the smallest observation (sample minimum), the lower quartile (Q1), the median (Q2), the upper quartile (Q3), and the largest observation (sample maximum). A box plot may also indicate which observations, if any, might be considered outliers, usually shown by circles. In a box plot, the bottom and top of the box are always the lower and upper quartiles, and the band near the middle of the box is always the median. The ends of the whiskers can represent several possible alternative values, for example:

- the minimum and maximum of all the data;
- one standard deviation above and below the mean of the data;
- the 9th percentile and the 91st percentile;
- ...

Fig. 5.7 presents a box plot with 1.5 IQR whiskers, which is the usual (default) value, corresponding to about plus or minus 2.7σ and 99.3 coverage, if the data are normally distributed. In other words, for a Gaussian distribution, on average less than 1 percent of the data fall outside the box-plus-whiskers range, a useful indication to identify possible outliers. As mentioned, an outlier is one observation that appears to deviate markedly from other members of the sample in which it occurs. Outliers can occur by chance in any distribution, but they often indicate either measurement errors or that the population has a *heavy-tailed distribution*. In the former case one should discard them or use statistics that are *robust* to outliers, while in the latter case one should be cautious in relying on tools or intuitions that assume a normal distribution.

Gist

Polynomial fits are a specific way to use **linear-in-the-coefficients models** to deal with nonlinear problems. The model consists of a linear sum of coefficients (to be determined) multiplying products of original input variables. The same technology works if products are substituted with arbitrary functions of the input variables, provided that the functions are fixed (no free parameters in the functions, only as multiplicative coefficients). Optimal coefficients are determined by minimizing a sum of squared errors, which leads to solving a set of linear equations. If the number of coefficients is large with respect to the number of input-output examples, **over-fitting** appears and it is dangerous to use the model to derive outputs for novel input values.

The **goodness of a polynomial fit** can be judged by evaluating the probability of getting the observed discrepancy between predicted and measured data (the likelihood of the data given the model parameters). If this probability is very low we should not trust the model too much. But wrong assumptions about how the errors are generated may easily lead us to overly optimistic or overly pessimistic conclusions. Statistics builds solid scientific constructions starting from assumptions. **Even the most solid statistics construction will be shattered if built on the sand of invalid assumptions**. Luckily, approaches based on easily affordable massive computation like cross-validation are easy to understand and robust.

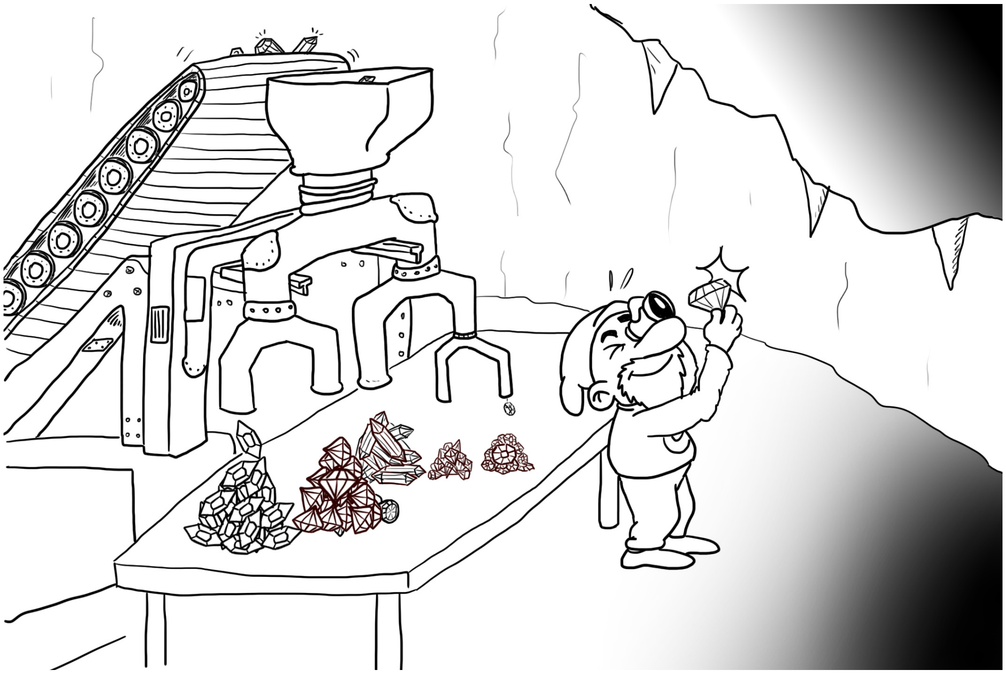
“Absurdities” like **bootstrapping** (re-sampling the same data with replacement, and repeating the estimation process in a Monte Carlo fashion) can be used to obtain confidence intervals around estimated parameter values.

You just maximized the likelihood of being recognized as linear least-squares guru.

Chapter 6

Rules, decision trees, and forests

If a tree falls in the forest and there's no one there to hear it, does it make a sound?



Rules are a way to **condense nuggets of knowledge in a way amenable to human understanding**. If "customer is wealthy" then "he will buy my product." If "body temperature greater than 37 degrees Celsius" then "patient is sick." Decision rules are commonly used in the medical field, in banking and insurance, in specifying processes to deal with customers, etc.

In a rule one distinguishes the **antecedent, or precondition** (a series of tests), and the **consequent, or conclusion**. The conclusion gives the output class corresponding to inputs which make the precondition true, or a probability distribution over the classes if the class is not 100% clear. Usually, the preconditions are *AND*-ed together: all tests must succeed if the rule is to "fire," i.e., to lead to the conclusion. If "distance less than 2 miles" AND "sunny" then "walk." A test can be on the value of a categorical variable ("sunny"), or on the result of a simple calculation on numerical variables ("distance less than 2 miles"). The calculation has to be simple if a human has to understand. A practical improvement is to unite in one statement also the classification when the antecedent is false. If "distance less than 3 kilometers" AND "no car" then "walk" else "take the bus".

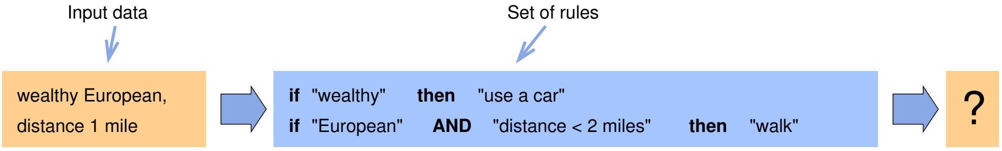

Input data
Set of rules
wealthy European, distance 1 mile
if "wealthy" then "use a car"
if "European" AND "distance < 2 miles" then "walk"
?

Figure 6.1: A set of unstructured rules can lead to contradictory classifications.

Extracting knowledge nuggets as a set of simple rules is enticing. But **designing and maintaining rules by hand is expensive** and difficult. When the set of rules gets large, complexities can appear, like rules leading to different and contradictory classifications (Fig. 6.1). In these cases, the classification may depend on the order with which the different rules are tested on the data and fire. **Automated ways to extract non-contradictory rules** from data are precious.

Instead of dealing with very long preconditions with many tests, breaking rules into a chain of simple questions has value. In a greedy manner, the most informative questions are better placed at the beginning of the sequence, leading to **a hierarchy of questions**, from the most informative to the least informative. The above motivations lead in a natural way to consider **decision trees**, an organized hierarchical arrangement of decision rules, without contradictions (Fig. 6.2, top).

Decision trees have been popular since the beginning of machine learning (ML). Now, it is true that only small and shallow trees can be "understood" by a human, but the popularity of decision trees is recently growing with the abundance of computing power and memory. Many, in some cases hundreds of trees, can be jointly used as **decision forests** to obtain robust classifiers. When considering forests, the care for human understanding falls in the background, the pragmatic search for robust top-quality performance without the risk of overtraining comes to the foreground.

6.1 Building decision trees

A decision tree is a set of questions organized in a hierarchical manner which can be represented graphically as a tree. Historically, trees in ML, as in all of Computer Science, tend to be drawn with their root upwards — imagine trees in Australia if you are in the Northern hemisphere. For a given input object, a decision tree estimates an unknown property of the object by asking successive questions about its known properties. Which question to ask next depends on the answer to the previous questions and this relationship is represented graphically as a path through the tree which the object follows, the orange thick path in the bottom part of Fig. 6.2. The decision is then made based on the terminal node on the path. Terminal nodes are called leaves. A decision tree can also be thought of as a technique for splitting complex problems into a set of simpler ones, until the problem is so simple (the leaf) that the answer is ready.

A basic way to build a decision tree from labeled examples proceeds in a greedy manner: the most informative questions are asked as soon as possible in the hierarchy. Imagine that one considers the initial set of labeled examples. A question with two possible outputs ("YES" or "NO") will divide this set into two subsets, containing the examples with answer "YES", and those with answer "NO", respectively. The initial situation is usually confused, and examples of different classes are present. When the leaves are reached after the chain of questions descending from the root, the final remaining set in the leaf should be almost "pure", consisting of examples of the same class. This class is returned as classification output for all cases trickling down to reach that leaf.

We need to transition from an initial confused set to a final family of (nearly) pure sets. A **greedy** way to aim at this goal is to start with the "most informative" question. This will split the initial set into two subsets, corresponding to the "YES" or "NO" answer, the children sets of the initial root node (Fig. 6.3). A greedy algorithm will take a first step leading as close as possible to the final goal. In a greedy algorithm, the first question is designed in order to get the two children subsets as pure as possible. After the first subdivision is done, one proceeds in a **recursive** manner (Fig. 6.4), by using the *same* method for the left and right children sets, designing the appropriate questions, and so on

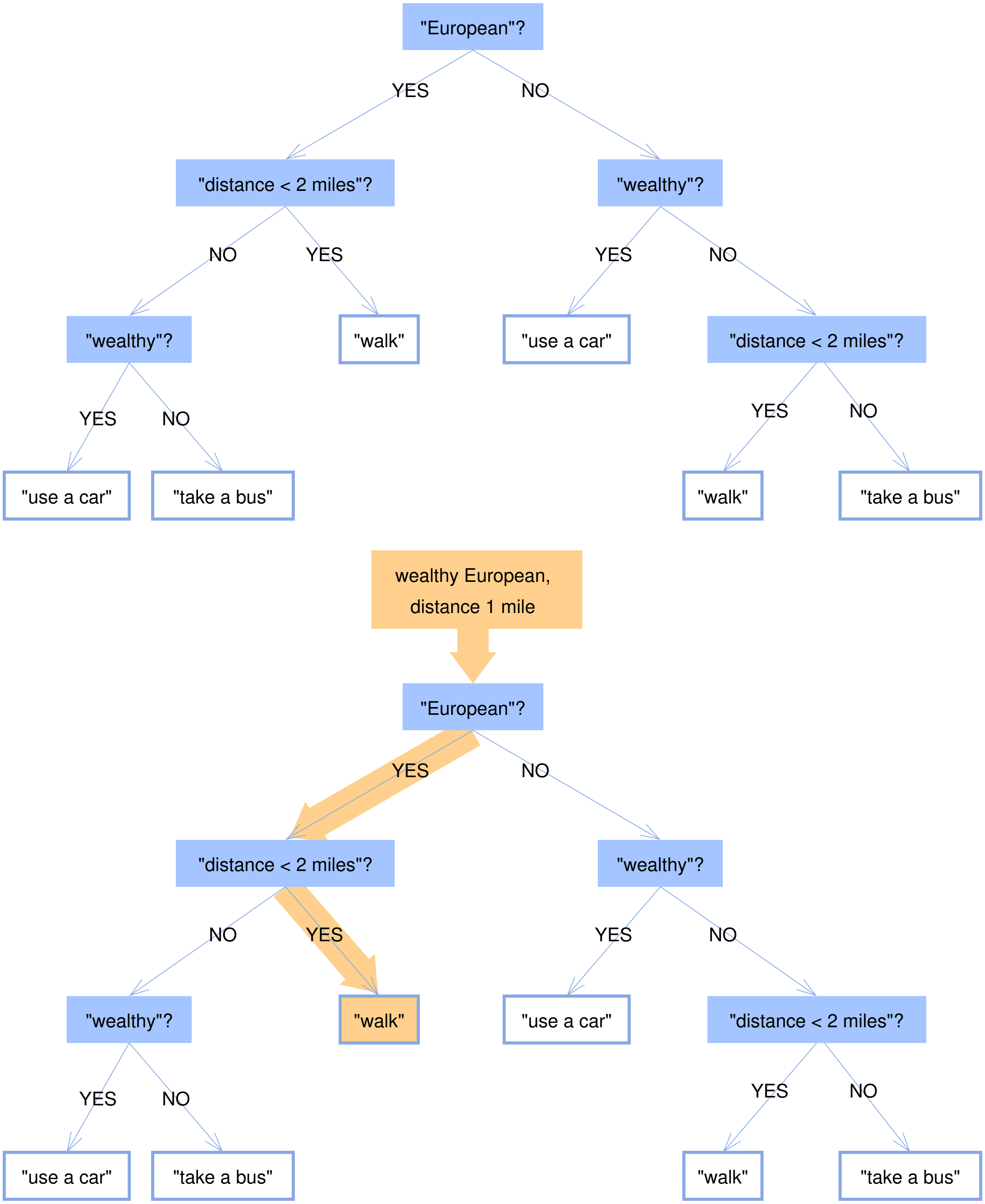


Figure 6.2: A decision tree (top), and the same tree working to reach a classification (bottom). The data point arriving at the split node is sent to its left or right child node according to the result of the test function.

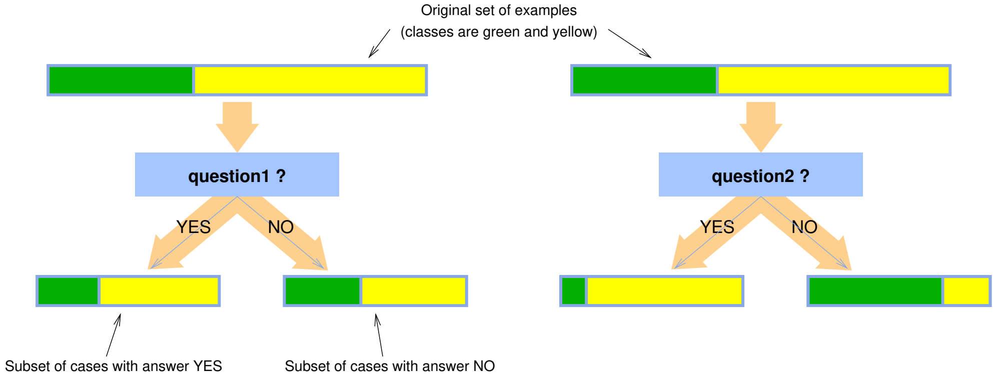

Original set of examples
(classes are green and yellow)
question1 ?
YES
NO
question2 ?
YES
NO
Subset of cases with answer YES
Subset of cases with answer NO

Figure 6.3: Purification of sets (examples of two classes): question2 produces purer subsets of examples at the children nodes.

and so forth until the remaining sets are sufficiently pure to stop the recursion. The complete decision tree is induced in a top-down process guided by the relative proportions of cases remaining in the created subsets.

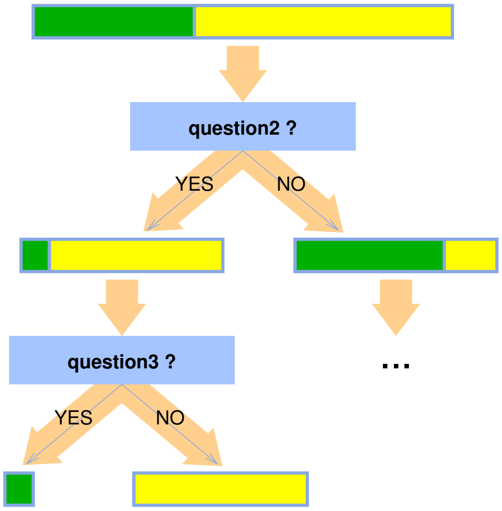


Figure 6.4: Recursive step in tree building: after the initial purification by *question2*, the same method is applied on the left and right example subsets. In this case *question3* is sufficient to completely purify the subsets. No additional recursive call is executed on the pure subsets.

The two main ingredients are a quantitative measure of purity and the kind of questions to ask at each node. We all agree that maximum purity is for subsets with cases of one class only, the different measures deal with measuring impure combinations. Additional spices have to do with termination criteria: let's remember that we aim at generalization so that we want to discourage very large trees with only one or two examples left in the leaves. In some cases one stops with slightly impure subsets, and an output probability for the different classes when cases reach a given leaf node.

For the following description, let's assume that all variables involved are categorical (names, like the "European" in the above example). The two widely used measures of purity of a subset are the *information gain* and the *Gini impurity*. Note that we are dealing with supervised classification, so that we know the correct output classification for the training examples.

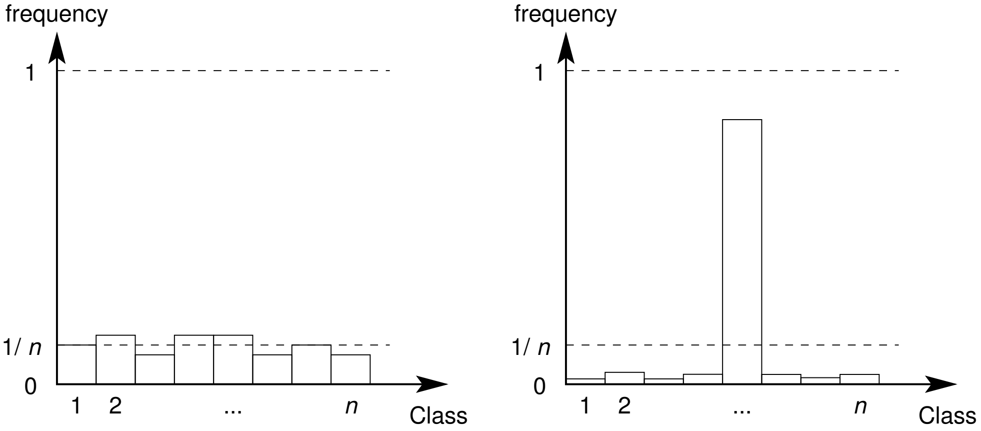


Figure 6.5: Two distributions with widely different entropy. High entropy (left): events have similar probabilities, the uncertainty is close to the maximum one $(\log n)$. Low entropy (right): events have very different probabilities, the uncertainty is small and close to zero because one event collects most probability.

Information gain Suppose that we sample from a set associated to an internal node or to a leaf of the tree. We are going to get examples of a class y with a probability $\Pr(y)$ proportional to the fraction of cases of the class present in the set. The statistical uncertainty in the obtained class is measured by Shannon's **entropy** of the label probability distribution:

$$H(Y) = -\sum_{y \in Y} \Pr(y) \log \Pr(y). \tag{6.1}$$

In information theory, entropy quantifies the average information needed to specify which event occurred (Fig. 6.5). If the logarithm's base is 2, information (hence entropy) is measured in bits. Entropy is maximum, $H(Y) = \log n$, when all n classes have the same share of a set, while it is minimum, $H(Y) = 0$, when all cases belong to the same class (no information is needed in this case, we already know which class we are going to get).

In the information gain method **the impurity of a set is measured by the entropy** of the class probability distribution. Knowledge of the answer to a question will decrease the entropy, or leave it equal only if the answer does not depend on the class. Let $\mathcal{S}$ be the current set of examples, and let $\mathcal{S} = \mathcal{S}_{\text{YES}} \cup \mathcal{S}_{\text{NO}}$ be the splitting obtained after answering a question about an attribute. The ideal question leaves no indecision: all elements in $\mathcal{S}_{\text{YES}}$ are cases of one class, while elements of $\mathcal{S}_{\text{NO}}$ belong to another class, therefore the entropy of the two resulting subsets is zero.

The average reduction in entropy after knowing the answer, also known as the "information gain", is the mutual information (MI) between the answer and the class variable. With this notation, the information gain (mutual information) is:

$$\text{IG} = H(\mathcal{S}) - \frac{|\mathcal{S}_{\text{YES}}|}{|\mathcal{S}|} H(\mathcal{S}_{\text{YES}}) - \frac{|\mathcal{S}_{\text{NO}}|}{|\mathcal{S}|} H(\mathcal{S}_{\text{NO}}). \tag{6.2}$$

Probabilities needed to compute entropies can be approximated with the corresponding frequencies of each class value within the sample subsets.

Information gain is used by the ID3, C4.5 and C5.0 methods pioneered by Quinlan [301]. Let's note that, because we are interested in generalization, the information gain is useful but not perfect. Suppose that we are building a decision tree for some data describing the customers of a business and that each node can have more than two children. One of the input attributes might be the customer's credit card number. This attribute has a high mutual information with respect to any classification, because it uniquely identifies each customer, but we do not want to include it in the decision tree: deciding how to treat a customer based on their credit card number is unlikely to generalize to customers we haven't seen before (we are over-fitting).

Gini impurity Imagine that we extract a random element from a set and label it randomly, with probability proportional to the shares of the different classes in the set. Primitive as it looks, this quick and dirty method produces zero errors if the set is pure, and a small error rate if a single class gets the largest share of the set.
In general, the Gini impurity (GI for short) measures how often a randomly chosen element from the set would be incorrectly labeled if it were randomly labeled according to the distribution of labels in the subset [1] . It is computed as the expected value of the mistake probability. For each class, one adds the probability of mistaking the classification of an item in that class (i.e., the probability of assigning it to any class but the correct one: $1-p_i$) times the probability for an item to be in that class (p_i). Suppose that there are m classes, and let f_i be the fraction of items labeled with value i in the set. Then, by estimating probabilities with frequencies ($p_i \approx f_i$):

$$\text{GI}(f) = \sum_{i=1}^{m} f_i(1-f_i) = \sum_{i=1}^{m}(f_i - {f_i}^2) = \sum_{i=1}^{m} f_i - \sum_{i=1}^{m} {f_i}^2 = 1 - \sum_{i=1}^{m} {f_i}^2. \tag{6.3}$$

GI reaches its minimum (zero) when all cases in the node fall into a single target category. GI is used by the CART algorithm (Classification And Regression Tree) proposed by Breiman [66].

When one considers the kind of questions asked at each node, considering **questions with a binary output** is sufficient in practice. For a categorical variable, the test can be based on the variable having a subset of the possible values (for example, if day is "Saturday or Sunday" YES, otherwise NO). For real-valued variables, the tests at each node can be on a single variable (like: *distance* $<$ *2 miles*) or on simple combinations, like a linear function of a subset of variables compared with a threshold (like: *average of customer's spending on cars and motorbikes greater than 20K dollars*). The above concepts can be generalized for a numeric variable to be predicted, leading to **regression trees** [66]. Each leaf can contain either the average numeric output value for cases reaching the leaf, or a simple model derived from the contained cases, like a linear fit (in this last case one talks about **model trees**).

In real-world data, **missing values** are abundant like snowflakes in winter. A missing value can have two possible meanings. In some cases the fact that a value *is* missing provides useful information —e.g., in marketing if a customer *does* not answer a question, we can assume that he is not very interested,— and "missing" can be treated as another value for a categorical variable. In other cases there is no significant information in the fact that a value is missing (e.g., if a sloppy salesman forgets to record some data about a customer). Decision trees provide a natural way to deal also with the second case. If an instance reaches a node and the question cannot be answered because data is lacking, one can ideally "split the instance into pieces", and send part of it down each branch in proportion to the number of training instances going down that branch. As Fig. 6.6 suggests, if 30% of training instances go left, an instance with a missing value at a decision node will be virtually split so that a portion of 0.3 will go left, and a portion of 0.7 will go right. When the different pieces of the instance eventually reach the leaves, the corresponding leaf output values can be averaged, or a distribution can be computed. The weights in the weighted average are proportional to the weights of the pieces reaching the leaves. In the example, the output value will be 0.3 times the output obtained by going left plus 0.7 times the output obtained by going right. Needless to say, a recursive call of the same routine with the left and right subtrees as argument is a way to obtain a very compact software implementation.

As a final remark, do not confuse the construction of the decision trees (using the labeled examples, the purity measures, the choice of appropriate questions) with the usage of a built tree. When used, a input case is rapidly tested with a single chain of questions leading from the root to the final assigned leaf.

6.2 Democracy and decision forests

In the nineties, researchers discovered how using **democratic ensembles of learners** (e.g., generic "weak" classifiers with a performance slightly better than random guessing) yields greater accuracy and generalization[315, 29]. The analogy is with human society: in many cases setting up a **committee of experts** is a way to reach a decision with

[1] For curiosity, a more general version, known as Gini Index, Coefficient, or Ratio, is widely used in econometrics to describe inequalities in resource distribution within a population; newspapers periodically publish rankings of countries based on their Gini index with respect to socioeconomical variables — without any explanation for the layperson, of course.

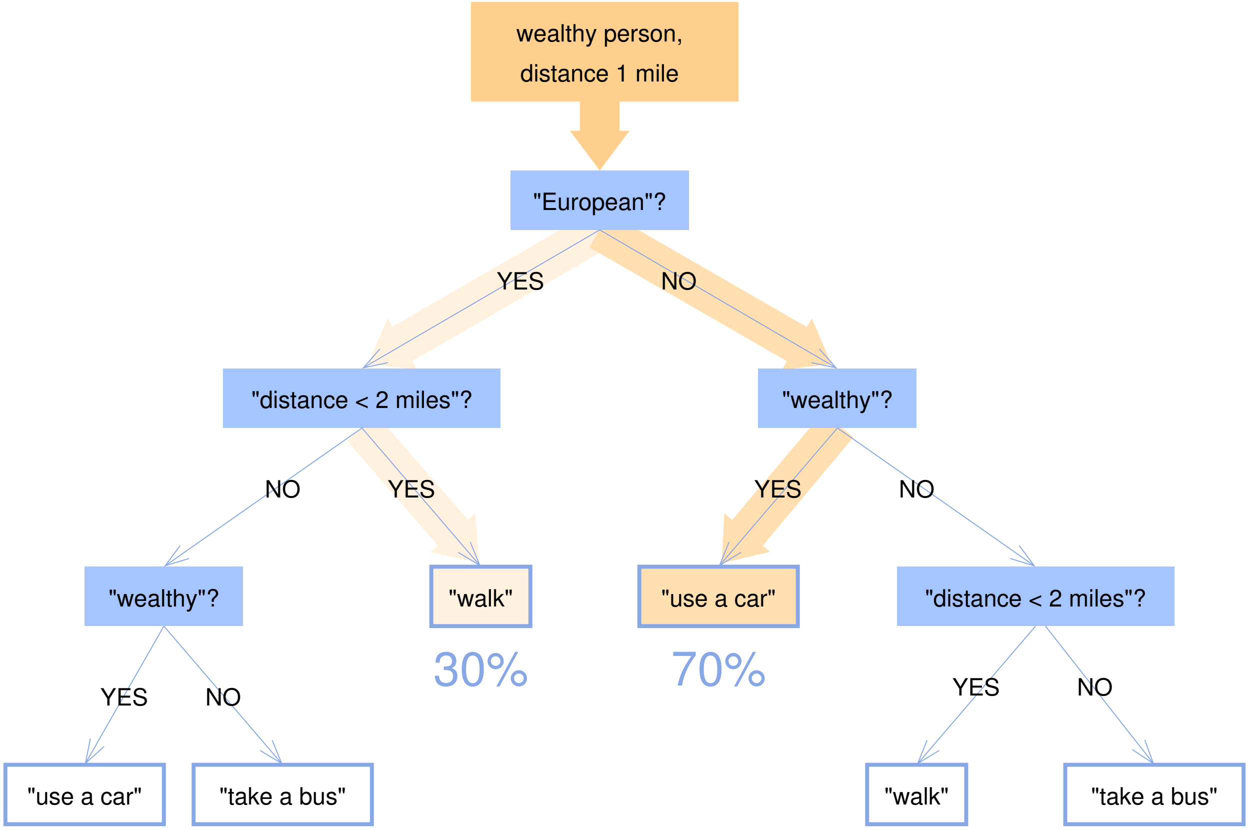


Figure 6.6: Missing nationality information. The data point arriving at the top node is sent both to its left and right child nodes with different weights depending on the frequency of “YES” and “NO” answers in the training set.

a better quality by either reaching consensus or by coming up with different proposals and voting (in other cases it is a way of postponing a decision, all analogies have their weaknesses). “Wisdom of crowds” [353] is a recent term to underline the positive effect of democratic decisions. For machine learning, outputs are combined by majority (in classification) or by averaging (in regression).

Democratic ensembles seem particularly effective for high-dimensional data, with many irrelevant attributes, as often encountered in real-world applications. The topic is not as abstract as it looks: many relevant applications have been created, ranging from Optical Character Recognition with neural networks [29] to using ensembles of trees in input devices for game consoles[2] [105].

In order for a committee of experts to produce superior decisions you need them to be different (no *groupthink* effect, experts thinking in the same manner are useless) and of reasonable quality. Ways to obtain different trees are, for example, training them on different sets of examples, or training them with different randomized choices (in the human case, think about students following different courses on the same subject):

- Creating **different sets of training examples** from an initial set can be done with **bootstrap samples** (Section 5.3): given a standard training set D of size ℓ, bootstrap sampling generates new training sets by sampling from D uniformly and with replacement (some cases can be repeated). After ℓ samples, a training set is expected to have $1 - 1/e \approx 63.2\%$ of the unique examples of D, the rest being duplicates. Think about randomly throwing ℓ balls into ℓ boxes (recall Fig. 5.5): for large ℓ, only about 63.2% of the boxes will contain one or more balls. For each ball in the box, pick one version of the corresponding example. In each bootstrap training set, about one-third of the instances are left out. The application of bootstrapping to the creation of different sample sets is called **bagging** (“bootstrap aggregation”): different trees are built by using different random bootstrap samples and combined by averaging the output (for regression) or voting (for classification).

- **Different randomized choices** during training can be executed by limiting the choices when picking the optimal question at a node.

As an example of the differentiating methods just described, here’s how they are implemented in **random decision forests** [183, 65]:

- each tree is trained on a bootstrap sample (i.e., with replacement) of the original data set;

- each time a leaf must be split, only a randomly chosen subset of the dimensions is considered for splitting. In the extreme case, only one random attribute (one dimension) is considered.

To be more precise, if d is the total number of input variables, each tree is constructed as follows: a small number d' of input variables, usually much smaller than d (in the extreme case just one), are used to determine the decision at a node. A bootstrap sample (“bag”) is guiding the tree construction, while the cases which are not in the bag can be used to estimate the error of the tree. For each node of the tree, d' variables are randomly chosen on which to base the decision at that node. The best split based on these d' variables is calculated (“best” according to the chosen purity criterion, IG or GI). Each time a categorical variable is selected to split on at a node, one can select a random subset of the categories of the variable, and define a substitute variable equal to 1 when the categorical value of the variable is in the subset, and 0 outside. Each tree is fully grown and not pruned (as may be done in constructing a normal tree classifier).

By the above procedure we have actually populated a committee (“forest”) where every expert (“tree”) has received a different training, because they have seen a different set of examples (by bagging) and because they look at the problem from different points of view (they use different, randomly chosen criteria at each node). No expert is guaranteed to be very good at its job: the order at which each expert looks at the variables is far from being the greedy criterion that favors the most informative questions, thus an isolated tree is rather weak; however, as long as most experts are better than random classifiers, the majority (or weighted average) rule will provide reasonable answers.

[2] Decision forests are used for human body tracking in the Microsoft Kinect sensor for the Xbox gaming console.

Estimates of generalization when using bootstrap sampling can be obtained in a natural way during the training process: the **out-of-bag error** (error for cases not in the bootstrap sample) for each data point is recorded and averaged over the forest.

The relevance of the different variables (**feature or attribute ranking**) in decision forests can also be estimated in a simple manner. The idea is: if a categorical feature is important, randomly permuting its values should decrease the performance in a significant manner. After fitting a decision forest to the data, to derive the importance of the i-th feature after training, the values of the i-th feature are randomly permuted and the out-of-bag error is again computed on this perturbed data set. The difference in out-of-bag error before and after the permutation is averaged over all trees. The score is the percent increase in misclassification rate as compared to the out-of-bag rate with all variables intact. Features which produce large increase are ranked as more important than features which produce small increases.

The fact that many trees can be used (thousands are not unusual) implies that, for each instance to be classified or predicted, a very large number of output values of the individual trees are available. By collecting and analyzing the entire distribution of outputs of the many trees one can derive confidence bars for the regression or probabilities for classification. For example, if 300 trees predict "sun" and 700 trees predict "rain" we can come up with an estimate of a 70% probability of "rain."

Gist

Simple "if-then" rules condense nuggets of information in a way which can be understood by human people. A simple way to avoid a confusing mess of possibly contradictory rules is to proceed with a hierarchy of questions (the most informative first) leading to an organized structure of simple successive questions called a **decision tree**.

Trees can be learned in a greedy and recursive manner, starting from the complete set of examples, picking a test to split it into two subsets which are as pure as possible, and repeating the procedure for the produced subsets. The recursive process terminates when the remaining subsets are sufficiently pure to conclude with a classification or an output value, associated with the leaf of the tree.

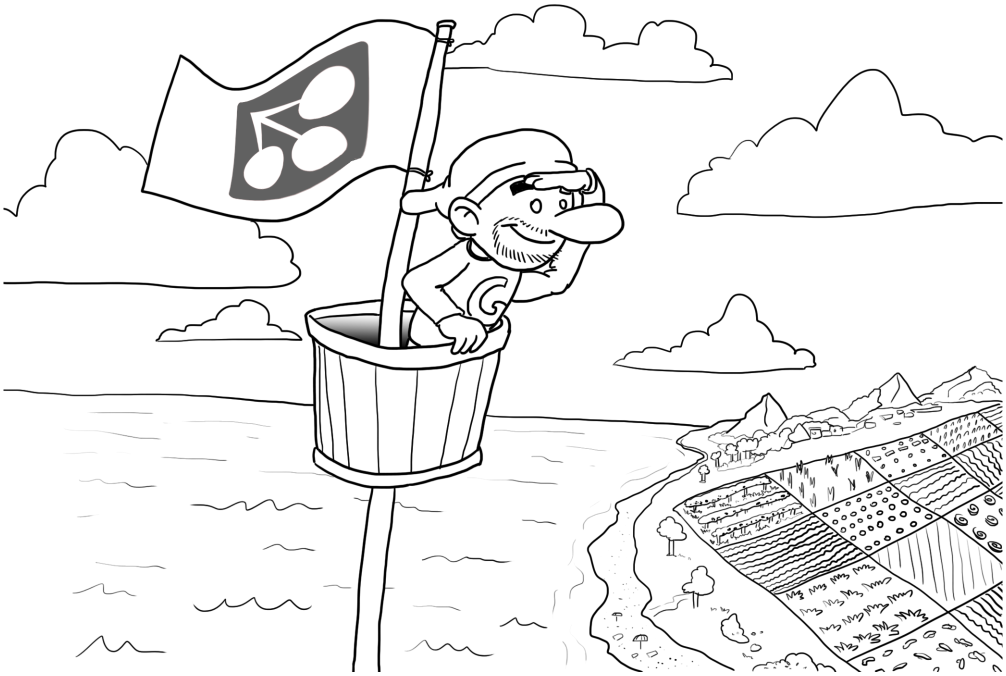
The abundance of memory and computing power permits training very large numbers of different trees. They can be fruitfully used as **decision forests** by collecting all outputs and averaging (regression) or voting (classification). Decision forests have various positive features: like all trees they naturally handle problems with more than two classes and with missing attributes, they provide a probabilistic output, probabilities and error bars, they generalize well to previously unseen data without risking over-training, they are fast and efficient thanks to their parallelism and reduced set of tests per data point.

A single tree casts a small shadow, hundreds of them can cool even the most torrid machine learning applications.

Chapter 7

Ranking and selecting features

I don't mind my eyebrows. They add... something to me. I wouldn't say they were my best feature, though. People tell me they like my eyes. They distract from the eyebrows.
(Nicholas Hoult)



Before starting to learn a model from the examples, one must be sure that the input data (input **attributes or features**) have sufficient information to predict the outputs. And after a model is built, one would like to get **insight** by identifying attributes which are influencing the output in a significant manner. If a bank investigates which customers are reliable enough to give them credit, knowing which factors are influencing the credit-worthiness in a positive or negative manner is of sure interest.

Feature selection, also known as attribute selection or variable subset selection, is the process of selecting a subset of relevant features to be used in model construction. Feature selection is different from **feature extraction**, which considers the creation of new features as functions of the original features.

The issue of selecting and ranking features is far from trivial. Let's assume that a linear model is built:

$$y = w_1 x_1 + w_2 x_2 + ... + w_d x_d.$$

If a weight, say w_j, is zero you can easily conclude that the corresponding feature x_j does not influence the output. But let's remember that numbers are not exact in computers and that examples are "noisy" (affected by measurement errors) so that getting zero is a very low-probability event indeed. Considering the non-zero weights, can you conclude that the largest weights (in magnitude) are related to the most informative and significant features?

Unfortunately you cannot. This has to do with how inputs are "scaled". If weight w_j is very large when feature x_j is measured in kilometers, it will jump to a very small value when measuring the same feature in millimeters (if we want the same result, the multiplication $w_j \times x_j$ has to remain constant when units are changed). An aesthetic change of units for our measurements immediately changes the weights. The value of a feature cannot depend on your choice of units, and therefore we cannot use the weight magnitude to assess its importance.

Nonetheless, the weights of a linear model can give *some* robust information if the inputs are *normalized*, pre-multiplied by constant factors so that the range of typical values is the same, for example the approximate range is from 0 to 1 for all input variables. If selecting features is already complicated for linear models, expect an even bigger complication for nonlinear ones.

7.1 Selecting features: the context

Let's now come to some definitions for the case of a classification task (Fig. 3.1 on page 22) where the output variable c identifies one among N_c classes and the input variable $\boldsymbol{x}$ has a finite set of possible values. For example, think about predicting whether a mushroom is edible (class 1) or poisonous (class 0). Among the possible features extracted from the data one would like to obtain a highly informative set, so that the classification problem starts from sufficient information, and only the actual construction of the classifier is left.

At this point you may ask why one is not using the entire set of inputs instead of a subset of features. After all, some information *shall* be lost if we eliminate some input data. True, but the **curse of dimensionality** holds here: if the dimension of the input is too large, the learning task becomes unmanageable. Think for example about the difficulty of estimating probability distributions from samples in very high-dimensional spaces. This is the standard case in "big data" text and web mining applications, in which each document can be characterized by tens of thousands dimensions (a dimension for each possible word in the vocabulary), so that vectors corresponding to the documents can be very sparse in the vector space.

Heuristically, one aims at **a small subset of features, possibly close to the smallest possible, which contains sufficient information to predict the output**, with redundancy eliminated. In this way not only memory usage is reduced but generalization can be improved because irrelevant features and irrelevant parameters are eliminated. Last but not least, your human understanding becomes easier if the model is small.

Think about recognizing digits from written text. If the text is written on colored paper, maintaining the color of the paper as a feature will make the learning task more difficult and worsen generalization if paper of different color is used to test the system.

Feature selection is a problem with many possible solutions and without formal guarantees of optimality. No simple recipe exists.

First, the **designer intuition and existing knowledge** should be applied. For example, if your problem is to recognize handwritten digits, images should be scaled and normalized (a "five" is still a five even if enlarged, reduced, stretched, more or less illuminated. . .), and clearly irrelevant features like the color should be eliminated from the beginning.

Second, one needs a way to **estimate the relevance or discrimination power of the individual features** and then one can proceed in a bottom-up or top-down manner, in some cases by directly testing the tentative feature set through repeated runs of the considered training model. The value of a feature is related to a model-construction method, and some evaluation techniques depend on the method. One identifies three classes of methods.

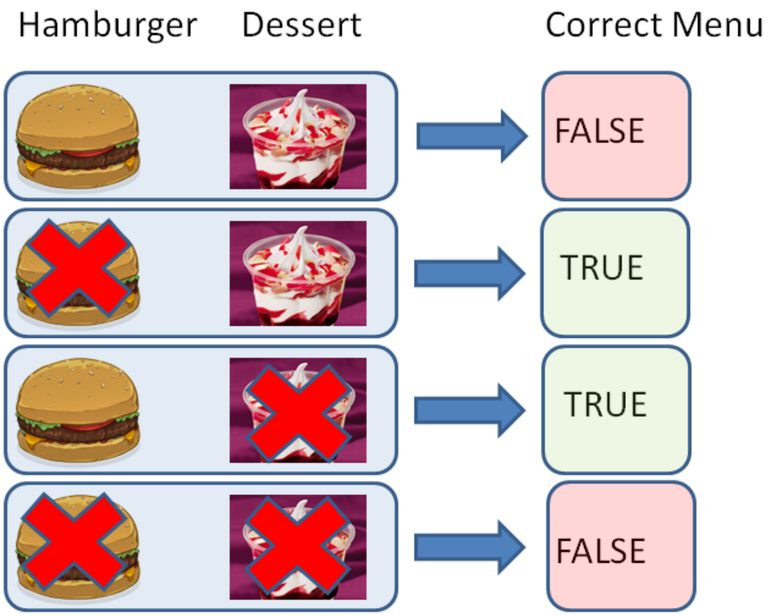


Figure 7.1: A classifier with two binary inputs and one output. Single features in isolation are not informative, both input features are needed and sufficient for a correct classification.

- **Wrapper methods** are built “around” a specific predictive model. Each feature subset is used to train a model. The generalization performance of the trained model gives the score for that subset. Wrapper methods are computationally intensive, but usually provide the best performing feature set for the specific model.
- **Filter methods** use a proxy measure instead of the error rate to score a feature subset. Common measures include the Mutual Information and the correlation coefficient. Many filters provide a feature ranking rather than an explicit best feature subset.
- **Embedded methods** perform feature selection as part of the model construction process. An example of this approach is the LASSO method for constructing a linear model, which penalizes the regression coefficients, shrinking many of them to zero, so that the corresponding features can be eliminated. Another approach is Recursive Feature Elimination, commonly used with Support Vector Machines to repeatedly construct a model and remove features with low weights.

By combining filtering with a wrapper method one can proceed in a bottom-up or top-down manner. In a **bottom-up method of greedy inclusion** one gradually inserts the ranked features in the order of their individual discrimination power and checks the effect on output error reduction through a validation set. The heuristically optimal number of features is determined when the output error measured on the validation set stops decreasing. In fact, if many more features are added beyond this point, the error may remain stable, or even gradually increase because of *over-fitting*.

In a **top-down truncation** method one starts with the complete set of features and progressively eliminates features while searching for the optimal performance point (always checking the error on a suitable validation set).

A word of caution for filter methods. Let’s note that **measuring individual features in isolation will discard mutual relationships** and therefore the result will be approximated. It can happen that two features in isolation have no relevant information and are discarded, even if their *combination* would allow perfect prediction of the output, think about realizing an *exclusive OR* function of two inputs.

As a example of the exclusive OR, imagine that the class to recognize is *CorrectMenu(hamburger, dessert)*, where the two variables *hamburger* and *dessert* have value 1 if present in a menu, 0 otherwise (Fig. 7.1). To get a proper amount of calories in a fast food you need to get either a hamburger or a dessert but not both. The individual presence or absence of a hamburger (or of a dessert) in a menu will not be related to classifying a menu as correct or not. But it would not be wise to eliminate one or both inputs because their *individual* information is not related to the output classification. You need to keep and read both attributes to correctly classify your meal! The toy example can be generalized: any diet expert will tell you that what matters are not individual quantities but an overall balanced combination.

Now that the context is clear, let's consider some example **proxy measures of the discrimination power of individual features**.

7.2 Correlation coefficient

Let Y be the random variable associated with the output classification, let $\Pr(y)$ ($y \in Y$) be the probability of y being its outcome; X_i is the random variable associated with the input variable x_i, and X is the input vector random variable, whose values are x.

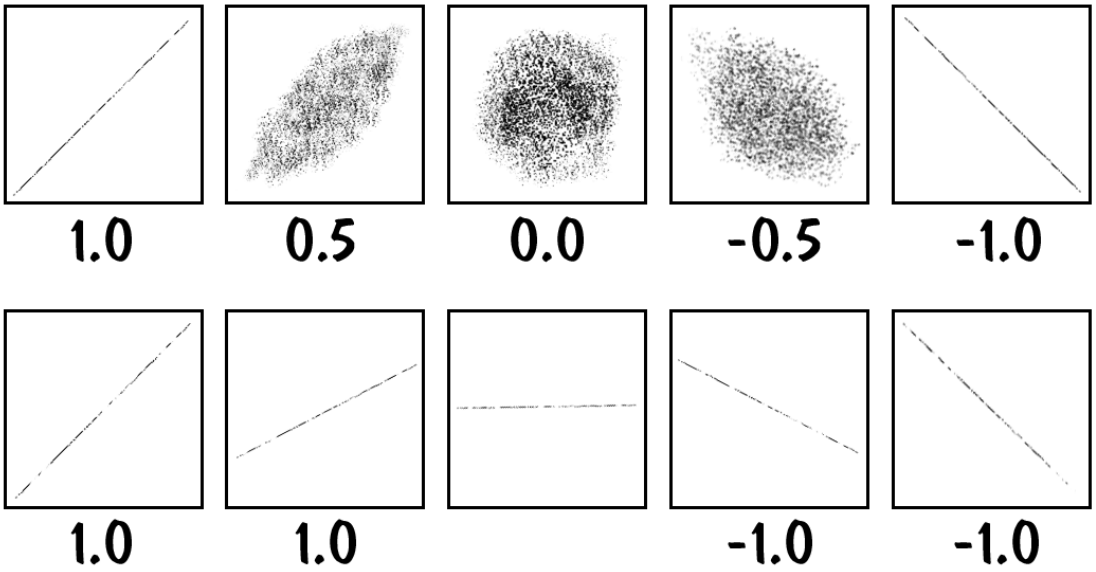


Figure 7.2: Examples of data distributions and corresponding correlation values. Remember that values are divided by the standard deviation, this is why the linear distributions of the bottom plots all have the same maximum correlation coefficient (positive 1 or negative -1). Also, note the sudden jump from +1 to -1 in the bottom plots: the correlation coefficient can be fragile in some cases.

The most widely used measure of **linear relationship between numeric variables** is the Pearson product-moment **correlation coefficient**, which is obtained by dividing the covariance of the two variables by the product of their standard deviations. In the above notation, the correlation coefficient $\rho_{X_i,Y}$ between the i-th input feature X_i and the classifier's outcome Y, with expected values μ_{X_i} and μ_Y and standard deviations σ_{X_i} and σ_Y, is defined as:

$$\rho_{X_i,Y} = \frac{\mathrm{cov}[X_i, Y]}{\sigma_{X_i}\sigma_Y} = \frac{E[(X_i - \mu_{X_i})(Y - \mu_Y)]}{\sigma_{X_i}\sigma_Y}; \tag{7.1}$$

where E is the expected value of the variable and cov is the covariance. After simple transformations one obtains the equivalent formula:

$$\rho_{X_i,Y} = \frac{E[X_i Y] - E[X_i]E[Y]}{\sqrt{E[X_i^2] - E^2[X_i]}\,\sqrt{E[Y^2] - E^2[Y]}}. \tag{7.2}$$

The division by the standard deviations makes the correlation coefficient independent of units (e.g., measuring in kilometers or millimeters will produce the same result). The correlation value varies from -1 to 1. Correlation close to 1 means increasing linear relationship (an increase of the feature value x_i relative to the mean is usually accompanied by an increase of the outcome y), close to -1 means a decreasing linear relationship. The closer the coefficient is to zero, the weaker the correlation between the variables, for example the plot of (x_i, y) points looks like an isotropic cloud around the expected values, without an evident direction, as shown in Fig. 37.1.

As mentioned before, statistically independent variables have zero correlation, but zero correlation does *not* imply that the variables are independent. The correlation coefficient detects only *linear* dependencies between two variables: it may well be that a variable has full information and actually determines the value of the second, as in the case that $y = f(x_i)$, while still having zero correlation.

The normal suggestion for this and other feature ranking criteria is not to use them blindly, but supported by experimental results on classification performance on test (validation) data, as in wrapper techniques.

7.3 Correlation ratio

In many cases, the desired outcome of our learning algorithm is categorical (a “yes/no” answer or a limited set of choices). The correlation coefficient assumes that the output is numeric, thus it is not applicable to the categorical case. In order to sort out general dependencies, the *correlation ratio* method measures a **relationship between a numeric input and a categorical output**.

The basic idea behind the correlation ratio is to partition the sample feature vectors into classes according to the observed outcome. If a feature is significant, then it should be possible to identify at least one outcome class where the feature’s average value is significantly different from the average on all classes, otherwise that component would not be useful to discriminate any outcome.

Suppose that one has a set of ℓ sample feature vectors, possibly collected during previous stages of the algorithm that one is trying to measure. Let ℓ_y be the number of times that outcome $y \in Y$ appears, so that one can partition the sample feature vectors by their outcome:

$$\forall y \in Y \qquad S_y = \big((x_{jy}^{(1)}, \dots, x_{jy}^{(n)}); j = 1, \dots, \ell_y\big).$$

In other words, the element $x_{jy}^{(i)}$ is the i-th component (feature) of the j-th sample vector among the ℓ_y samples having outcome y. Let us concentrate on the i-th feature from all sample vectors, and compute its average within each outcome class:

$$\forall y \in Y \qquad \bar{x}_y^{(i)} = \frac{1}{\ell_y} \sum_{j=1}^{\ell_y} x_{jy}^{(i)},$$

and the overall average:

$$\bar{x}^{(i)} = \frac{1}{\ell} \sum_{y \in Y} \sum_{j=1}^{\ell_y} x_{jy}^{(i)} = \frac{1}{\ell} \sum_{y \in Y} \ell_y \bar{x}_y^{(i)}.$$

Finally, the **correlation ratio** between the i-th component of the feature vector and the outcome is given by

$$\eta_{X_i,Y}^2 = \frac{\sum_{y \in Y} \ell_y (\bar{x}_y^{(i)} - \bar{x}^{(i)})^2}{\sum_{y \in Y} \sum_{j=1}^{\ell_y} (x_{jy}^{(i)} - \bar{x}^{(i)})^2}.$$

If the relationship between values of the i-th feature component and values of the outcome is linear, then both the correlation coefficient and the correlation ratio are equal to the slope of the dependence:

$$\eta^2_{X_i,Y} = \rho^2_{X_i,C}.$$

In all other cases, the correlation ratio can capture nonlinear dependencies.

7.4 Chi-square test to deny statistical independence

Let's again consider a two-way classification problem and a single feature with a binary value. For example, in text mining, the feature can express the presence/absence of a specific term (keyword) t in a document and the output can indicate if a document is about programming languages or not. We are therefore evaluating a **relationship between two categorical features**.

One can start by deriving four counters $\text{count}_{c,t}$, counting in how many cases one has (has not) the term t in a document which belongs (does not belong) to the given class. For example $\text{count}_{0,1}$ counts for class=0 and presence of term t, $\text{count}_{0,0}$ counts for class=0 and absence of term t... Then one can estimate probabilities by dividing the counts by the total number of cases n.

In the *null hypothesis* that the two events "occurrence of term t" and "document of class c" are independent, the expected value of the above counts for joint events are obtained by *multiplying* probabilities of individual events. For example $E(\text{count}_{0,1}) = n \cdot \Pr(\text{class} = 0) \cdot \Pr(\text{term } t \text{ is present})$.

If the count deviates from the one expected for two independent events, one can conclude that the two events are *dependent*, and that therefore the feature *is* significant to predict the output. All one has to do is to check if the *deviation is sufficiently large that it cannot happen by chance*. A statistically sound manner to test is by **statistical hypothesis testing**.

A statistical hypothesis test is a method of making statistical decisions by using experimental data. In statistics, a result is called **statistically significant if it is unlikely to have occurred by chance**. The phrase "test of significance" was coined around 1925 by Ronald Fisher, a genius who created the foundations for modern statistical science.

Hypothesis testing is sometimes called **confirmatory data analysis**, in contrast to exploratory data analysis. Decisions are almost always made by using *null-hypothesis tests*; that is, ones that answer the question: Assuming that the null hypothesis is true, what is the probability of observing a value for the test statistic that is at least as extreme as the value that was actually observed?

In our case one measures the χ^2 value:

$$\chi^2 = \sum_{c,t} \frac{[\text{count}_{c,t} - n \cdot \Pr(\text{class} = c) \cdot \Pr(\text{term} = t)]^2}{n \cdot \Pr(\text{class} = c) \cdot \Pr(\text{term} = t)}. \tag{7.3}$$

The larger the χ^2 value, the lower the belief that the independence assumption is supported by the observed data. The probability of a specific value happening by chance can be calculated by standard statistical formulas if one desires a quantitative value.

For feature ranking no additional calculation is needed and one is satisfied with the crude value: the best features according to this criterion are the ones with larger χ^2 values. They are deviating more from the independence assumption and therefore probably dependent.

7.5 Heuristic relevance based on nearest neighbors: Relief

There are multivariate relevance criteria to rank individual features according to their relevance *in the context of others*. To illustrate this concept, the Relief algorithm [233] derives a ranking index for classification problems based on the K-nearest neighbors algorithm. To evaluate the index, one first identifies for each example, in the original feature space, the K closest examples of the same class (nearest hits) and the K closest examples of a different class (nearest misses.). Then, in projection on feature j, the sum of the distances between the examples and their **nearest misses** is compared to the sum of distances to their **nearest hits**.

The idea is that a feature is good if neighbors (in the original space) of the same class tend to have close values of that feature, while neighbors of different classes tend to have different values. The radical approximation is caused by considering only a certain number of nearest neighbors instead of the entire set of examples, and a simple discrimination based on the similarity of features in the projected space (in the subset of selected features).

In a variation fo Relief in [167], one first identifies in the original feature space, for each example $\mathbf{x}_i$, the K closest examples of the same class $\mathbf{x}_{H_k}(i), k = 1, ..., K$ (nearest hits) and the K closest examples of a different class $\mathbf{x}_{M_k}(i)$ (nearest misses). Then, considering the individual feature j, the sum of the distances between the examples and their nearest misses is compared to the sum of distances to their nearest hits. In equation (7.4), the ratio of these two quantities is used to create an index of relevance $Rel(j)$ independent of feature scale variations.

$$Rel(j) = \frac{\sum_{i=1}^{m} \sum_{k=1}^{K} |x_{i,j} - x_{M_k(i),j}|}{\sum_{i=1}^{m} \sum_{k=1}^{K} |x_{i,j} - x_{H_k(i),j}|} \tag{7.4}$$

The larger $Rel(j)$ the better the j-th feature is separating near misses from near hits. A randomized set of examples can be considered to speedup the evaluation.

Relief does not discriminate between redundant features, and it can be fooled by low numbers of training instances. Updates to the algorithm in order to improve the reliability, make it robust to incomplete data, and generalising it to multi-class problems are presented in [237].

7.6 Entropy and mutual information (MIFS)

The qualitative criterion of "informative feature" can be made precise in a statistical way with the notion of **mutual information** (MI).

An output distribution is characterized by an *uncertainty* which can be measured from the probability distribution of the outputs. The theoretically sound way to measure the uncertainty is with the **entropy**, see below for the precise definition. Now, knowing a specific input value x, the uncertainty in the output can decrease. The amount by which the uncertainty in the output decreases after the input is known is termed **mutual information**.

If the mutual information between a feature and the output is zero, knowledge of the input does not reduce the uncertainty in the output. In other words, the selected feature cannot be used (in isolation) to predict the output - no matter how sophisticated our model is. The MI measure between a vector of input features and the output (the desired prediction) is therefore very relevant to identify promising (informative) features. Its use in feature selection is pioneered in [21].

In information theory **entropy**, measuring the statistical uncertainty in the output class (a random variable), is defined as:

$$H(Y) = -\sum_{y \in Y} \Pr(y) \log \Pr(y). \tag{7.5}$$

Entropy quantifies the average information, measured in bits, used to specify which event occurred (Fig. 6.5). It is also used to quantify how much a message can be compressed without losing information[1].

Let us now evaluate the impact that the i-th input feature x_i has on the classifier's outcome y. The entropy of Y after knowing the input feature value ($X_i = x_i$) is:

$$H(Y|x_i) = -\sum_{y \in Y} \Pr(y|x_i) \log \Pr(y|x_i),$$

[1] Shannon's source coding theorem shows that, in the limit, the average length of the shortest possible representation to encode the messages in a binary alphabet is their entropy. If events have the same probability, no compression is possible. If the probabilities are different one can *assign shorter codes to the most probable events*, therefore reducing the overall message length. This is why "zip" tools successfully compress meaningful texts with different probabilities for words and phrases, but have difficulties to compress quasi-random sequences of digits like JPEG or other efficiently encoded image files.

where $\Pr(y|x_i)$ is the conditional probability of being in class y given that the i-th feature has value x_i.

Finally, the *conditional entropy* of the variable Y is defined as the expected value of $H(Y|x_i)$ over all values $x_i \in X_i$ that the i-th feature can have:

$$H(Y|X_i) = E_{x_i \in X_i}\big[H(Y|x_i)\big] = \sum_{x_i \in X_i} \Pr(x_i) H(Y|x_i). \tag{7.6}$$

The conditional entropy $H(Y|X_i)$ is always less than or equal to the entropy $H(Y)$. It is equal if and only if the i-th input feature and the output class are *statistically independent*, i.e., the joint probability $\Pr(y, x_i)$ is equal to $\Pr(y)\Pr(x_i)$ for every $y \in Y$ and $x_i \in X_i$ (note: this definition does not talk about linear dependencies). The amount by which the uncertainty decreases is by definition the *mutual information* $I(X_i; Y)$ between variables X_i and Y:

$$I(X_i; Y) = I(Y; X_i) = H(Y) - H(Y|X_i). \tag{7.7}$$

An equivalent expression which makes the symmetry between X_i and Y evident is:

$$I(X_i; Y) = \sum_{y, x_i} \Pr(y, x_i) \log \frac{\Pr(y, x_i)}{\Pr(y)\Pr(x_i)}. \tag{7.8}$$

In classification, Mutual Information is related to upper and lower bounds on the optimal **Bayes error rate**.

The Bayes error rate is the lowest possible error rate that a classifier can achieve. If we knew the true probability $\Pr(y|\boldsymbol{x})$ of every outcome $y = C_1, \dots, C_\ell$ for any input pattern $\boldsymbol{x}$, then our best choice for a given pattern $\bar{\boldsymbol{x}}$ would be class C_i maximizing $\Pr(C_i|\bar{\boldsymbol{x}})$ or, equivalently, $p(\bar{\boldsymbol{x}}|C_i)\Pr(C_i)$, which is proportional to the former (by Bayes' rule "posterior equals prior times likelihood ratio"), $p(\boldsymbol{x}|y)$ being the probability density of $\boldsymbol{x}$ given the class y.

The probability of error for a given pattern $\bar{\boldsymbol{x}}$ is the sum of the other, non-winning probabilities, and the Bayes error rate is obtained by integrating the error probability over the whole input space:

$$\begin{aligned} E_{\text{Bayes}} = \Pr(\text{error}) &= \sum_{i=1}^{\ell} \int_{H_i} \left(\sum_{j \neq i} \Pr(C_j|\boldsymbol{x}) \right) p(\boldsymbol{x})\, d\boldsymbol{x} \\ &= \sum_{i=1}^{\ell} \sum_{j \neq i} \int_{H_i} p(\boldsymbol{x}|C_j) \Pr(C_j)\, d\boldsymbol{x}, \end{aligned} \tag{7.9}$$

where the input space has been partitioned into areas $H_1, \dots, H_\ell$: H_i is the area of the feature space associated by the optimal classifier to output classes C_i, with ties broken in any way. Note the fact that no classifier can escape this error, which is caused by the intrinsic randomness of the outcome.

In the case of $\ell = 2$ classes, Eq. (7.9) reduces to

$$E_{\text{Bayes}} = \overbrace{\int_{H_1} p(\boldsymbol{x}|C_2)\Pr(C_2)\, d\boldsymbol{x}}^{E_1} + \overbrace{\int_{H_2} p(\boldsymbol{x}|C_1)\Pr(C_1)\, d\boldsymbol{x}}^{E_2},$$

and the two integrals correspond to the two grey areas in Fig. 7.3, where the feature space is optimally divided into regions H_1 and H_2 depending on the error distributions. This error is clearly irreducible: any classifier that operates differently is bound to have a larger error. For instance, refer to Fig. 7.3: if patterns in E' are attributed to C_1 (i.e., features $\boldsymbol{x} \in H'$ are classified as C_2 instead of the more likely C_1), then the additional term E' (dashed area) is added to the error.

In particular, an upper bound containing the Mutual Information is [63]

$$E_{\text{Bayes}} \leq \frac{1}{2} H(Y|X) = \frac{1}{2}\big(H(Y) - I(Y, X)\big),$$

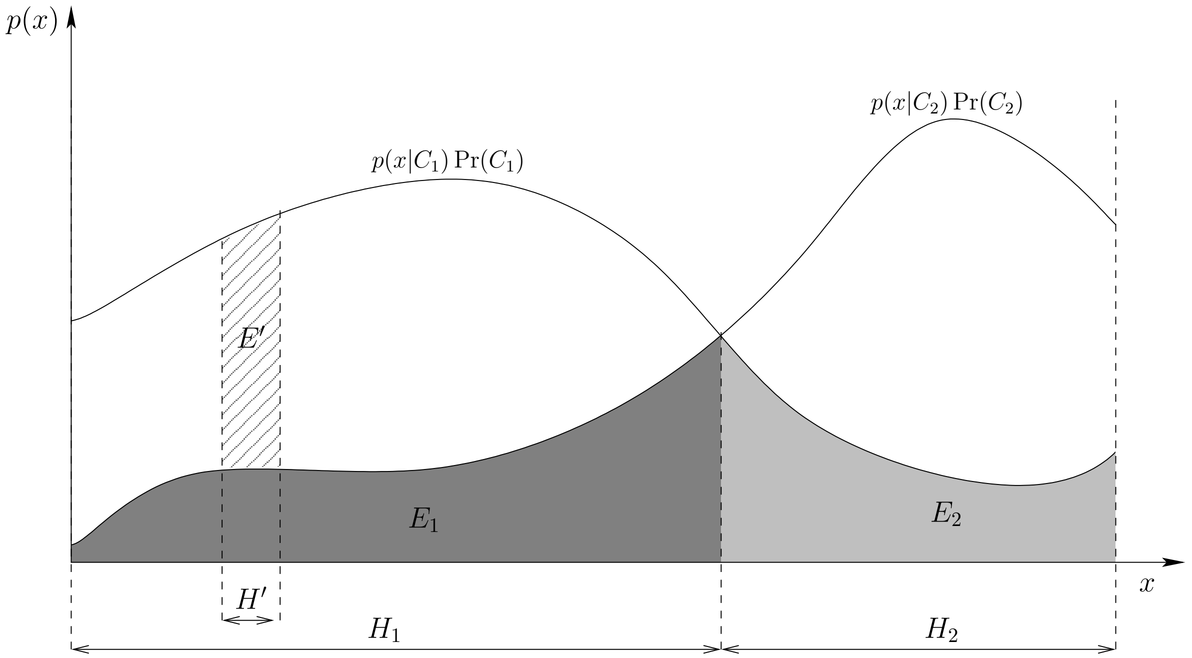


Figure 7.3: Optimal classification and Bayes error rate. Dashed area E' corresponds to additional error term for a suboptimal algorithm that misclassifies patterns in H'.

where X is a feature vector. Because the output class entropy cannot be changed, the upper bound is minimized when the Mutual Information $I(Y, X)$ is maximized.

Let's stress that the **mutual information is qualitatively different from the linear correlation**. A feature can be informative even if not linearly correlated with the output; a feature can provide useful information even if it is correlated with a second already-selected feature (linear correlation between two features does not imply redundancy!). The mutual information measure does not even require the two variables to be quantitative. Remember that a nominal categorical variable is one that has two or more categories, but there is no intrinsic ordering to the categories. For example, gender is a nominal variable with two categories (male and female) and no intrinsic ordering. Provided that you have sufficiently abundant data to estimate it, there is not a better way to measure information content than by Mutual Information.

But be advised: **having information is necessary to predict the output, but not sufficient**. The information has to be extracted by "learnable" techniques. A pseudo-random function linking a seed x to the generated value y gives the entire information to predict y from x, but identifying the function from examples can be demanding, if not impossible. Is this example too academic? Well, consider the case of an ID (like a randomized social security number). All details about a citizen can be predicted (actually, derived without ambiguity) after knowing the ID, but that does not mean that an ID is a useful feature to be used for generalization. When using MI for feature selection do not be fooled by IDs! **IDs (if randomized) should never be chosen as input features**.

Although very powerful in theory, estimating mutual information for vectors with large dimension after starting from labeled samples is not a trivial task. Discretization (quantization) of continuos variables into a discrete set of values, and substitution of probability density functions with counts of occurrences in **histogram bins** is s standard techniques, but large errors are present if most bins are empty or with very few events. In particular, estimation in very large-dimensional spaces is daunting because the number of bins can explode.

In some cases, estimates of the probability densities are derived before calculating MI, by using Parzen windows, kernel methods, or the assumption of a specific form of the densities (like Gaussian). In contrast to conventional estimators based on hitograms and binnings, entropy estimates taken directly from k-nearest neighbor distances are presented in [240]: they are data efficient, adaptive (the resolution is higher where data are more numerous), and have minimal bias. A seminal definition of the MIFS strategy (Mutual Information for Feature Selection) and heuristic methods which use only mutual information between individual features and the output and between couples of features is presented in [21], aiming at selecting a set of relevant but non-redundant features.

7.6.1 Entropy and Mutual Information for continuous variables

Let X be a random variable with a probability density function $p(\boldsymbol{x})$ whose support is a set $\mathbb{X}$. The **differential entropy** $H(X)$, or $H(p)$, is defined as

$$H(X) = -\int_{\mathbb{X}} p(\boldsymbol{x}) \log p(\boldsymbol{x})\, d\boldsymbol{x}. \tag{7.10}$$

One must take care in applying properties of discrete entropy to differential entropy, since probability density functions can be greater than 1, so that the differential entropy can be negative.

The chain rule for differential entropy holds as in the discrete case:

$$H(X_1, \ldots, X_n) = \sum_{i=1}^{n} H(X_i | X_1, \ldots, X_{i-1}) \leq \sum H(X_i). \tag{7.11}$$

Differential entropy is translation invariant, i.e., $H(X + c) = H(X)$ for a constant c, but in general not invariant under arbitrary invertible maps. In particular, for a constant a, $H(aX) = H(X) + \log |a|$. This is why maximization only makes sense with additional contraints: for example, the maximum differential entropy distribution under constraint of a given variance is the Gaussian. Gaussian is the "least interesting" (least structured) distribution according to the entropic criterion, a fact which will be used in Projection Pursuit (Sec 20.6) and Independent Component Analysis (Sec. 21.2).

For a vector-valued random variable $\mathbf{X}$ and a matrix A, $H(A\mathbf{X}) = H(\mathbf{X}) + \log |\det A|$, $\det A$ being the determinant of the matrix.

In general, for a bijective map from a random vector to another random vector with same dimension $\mathbf{Y} = m(\mathbf{X})$, the corresponding entropies are related via [289]:

$$H(\mathbf{Y}) = H(\mathbf{X}) + \int f(\boldsymbol{x}) \log \left| \frac{\partial m}{\partial \boldsymbol{x}} \right| d\boldsymbol{x} \tag{7.12}$$

where $|\partial m / \partial \boldsymbol{x}|$ is the *Jacobian determinant of the transformation* m. The Jacobian matrix $\partial m / \partial \boldsymbol{x}$, containing partial derivatives $\partial m_i / \partial x_j$, defines a linear map which is the best linear approximation of the function m near the point $\boldsymbol{x}$. This linear map is thus the generalization of the usual notion of derivative. The absolute value of the **Jacobian determinant** of a square matrix at $\boldsymbol{x}$ gives us the factor by which the mapping m **expands or shrinks volumes** near $\boldsymbol{x}$. As a special case, when m is a rigid rotation, translation, or combination thereof, the Jacobian determinant is always 1, and therefore $H(Y) = H(X)$.

For the Mutual Information in the case of continuous random variables, summation is replaced by a definite double integral:

$$I(X;Y) = \int_Y \int_X p(\boldsymbol{x}, \boldsymbol{y}) \log \left(\frac{p(\boldsymbol{x}, \boldsymbol{y})}{p(\boldsymbol{x})\, p(\boldsymbol{y})} \right) d\boldsymbol{x}\, d\boldsymbol{y}, \tag{7.13}$$

where $p(\boldsymbol{x}, \boldsymbol{y})$ is now the joint probability density function of X and Y, and $p(\boldsymbol{x})$ and $p(\boldsymbol{y})$ are the marginal probability density functions.

The continuous mutual information $I(X;Y)$ has the distinction of retaining its fundamental significance as a measure of discrete information since it is actually the limit of the discrete mutual information of partitions of X and

Y as these partitions become finer and finer. Thus it is invariant under non-linear homeomorphisms (continuous and uniquely invertible maps), including linear transformations of X and Y.

Gist

Reducing the number of input attributes used by a model, while keeping roughly equivalent performance, has many advantages: smaller model size and better human understandability, faster training and running times, possible higher generalization.

It is difficult to rank individual features without considering the specific modeling method and their mutual relationships. Think about a detective (in this case the classification to reach is between "guilty" and "innocent") intelligently combining multiple clues and avoiding confusing evidence. Ranking and filtering is only a first heuristic step and needs to be validated by trying different feature sets with the chosen method, "wrapping" the method with a feature selection scheme.

A short recipe is: trust the **correlation** coefficient only if you have reasons to suspect *linear* relationships, otherwise other correlation measures are possible, in particular the correlation ratio can be computed even if the outcome is not quantitative. Use **chi-square** to identify possible dependencies between inputs and outputs by estimating probabilities of individual and joint events. Finally, use the powerful **mutual information** to estimate arbitrary dependencies between qualitative or quantitative features, but be aware of possible overestimates when few examples are present, and never pick randomized IDs as input features (convince yourself that the useful information in the feature can actually be *extracted* by ML techniques).

As an exercise, pick your favorite Sherlock Holmes story and identify which feature (clue, evidence) selection technique he used to capture and expose a culprit and to impress his friend Watson.

Chapter 8

Models based on matrix factorization

La calunnia è un venticello / Un'auretta assai gentile
Che insensibile sottile / Leggermente dolcemente
Incomincia a sussurrar.
(Rossini — Il Barbiere di Siviglia)
Calumny is a little breeze, /a gentle zephyr,
which insensibly, subtly, / lightly and sweetly,
commences to whisper.

In this section we consider applications of linear algebra transformation to determine "factors of variations", in particular matrix factorization.

To make the presentation concrete, the guiding application is **collaborative filtering and recommendation**. Word of mouth has always been a powerful and effective technique to spread information and opinions from person to person, in a viral manner. It is a distributed and human way to **mine the data implicitly contained in many human minds**. It is effective because we naturally tend to speak with people similar to us, who share our habits, opinions,

	Movie 1	Movie 2	Movie 3	Movie 4
User 1	1	4	2	1
User 2	1	5	1	0
User 3	1	0	0	0

Table 8.1: A rating matrix.

way of life. By choosing to interact with a selected and small number of similar people we effectively **filter** the data. It is then up to us to integrate and weigh the information that we receive, to reach our final decisions. A similar process can be simulated through data mining and modeling methods. Starting from the raw data (potentially huge quantities, ranging from thousands to billions of items) one extracts information bits which are relevant for the specific final user, based on models of his explicit or implicit preferences, and on similarities with other people.

An interesting application is in the marketing sector: data collected about users and products, either bought or at least evaluated, can be used to estimate how a customer would evaluate a product he did not see before. The final purpose of predicting evaluations is to encourage the user to buy, for example by recommending a list of items corresponding to the highest predicted evaluations. Advertising is more effective if the presented products are filtered based on the user preferences. Other applications are in web mining, where the objective is to identify pages which the user may be interested in, while searching for information. The purpose is therefore to **imitate word of mouth** diffusion of information, for positive (fame) as well as for negative opinions (defamation).

Collaborative filtering and recommendation is a method of predicting the interests of a person by collecting taste information from many other collaborating people. The underlying assumption is that **those who agreed in the past tend to agree again in the future**. For example, a collaborative recommendation system for movies could make **personal predictions** about which movie a user should like, given some knowledge of the user's tastes and the information gathered from many other users.

Consider a user-item matrix R where the value of each entry r_{ui} is the rating of user u for item i as in Table 8.1. Every user u can vote for item i with a rating in the interval $[\text{min\_rating}, \text{max\_rating}]$. Let's get more concrete and assume that $\text{min\_rating} = 1$ and $\text{max\_rating} = 5$ and that value 0 is used to denote the unknown ratings. One wants to predict the unknown ratings in the matrix, either by some direct manner or by finding a more compact way to represent the data and by using the compact representation for prediction.

8.1 Combining ratings by similar users

A simple method to predict an unknown rating r_{ui} considers the ratings of other users on the same item i, and the *similarity* between user u and other users. A generic unknown rating r_{ui} is calculated by the following equation:

$$r_{ui} = \frac{\sum_{\text{known } r_{ki}} \text{similarity}(u,k) \cdot r_{ki}}{\sum_{\text{known } r_{ki}} \text{similarity}(u,k)}. \tag{8.1}$$

The vote is predicted with a weighted average of the other users' votes, with weights given by similarities, as shown in Fig. 8.1. The motivation is that similar users tend to give similar votes. If the denominator of the above equation is 0, then r_{ui} is calculated by default as the average value of all known ratings r_{ki}. If nobody rates item i, then r_{ui} is 0.

In a similar way, one could average the votes given by the same user on *different items*, with a weight proportional to the similarity between items, as explained in the bottom part of Fig. 8.1 (similar items tend to be judged in a similar manner).

The crucial issue is how to measure similarities. In this simplified context, the only knowledge about a user must be derived from his past evaluations of the different products. Therefore, in the above equation (8.1), the similarity between two users (u, k) is obtained by measuring the similarity between two vectors $(\mathbf{v}_u, \mathbf{v}_k)$, the u^{th}, k^{th} rows of the rating matrix R.

The usual cosine similarity between two vectors can be used in a standard implementation, but different and problem-specific metrics can be tested, as explained in Sec.17.2.

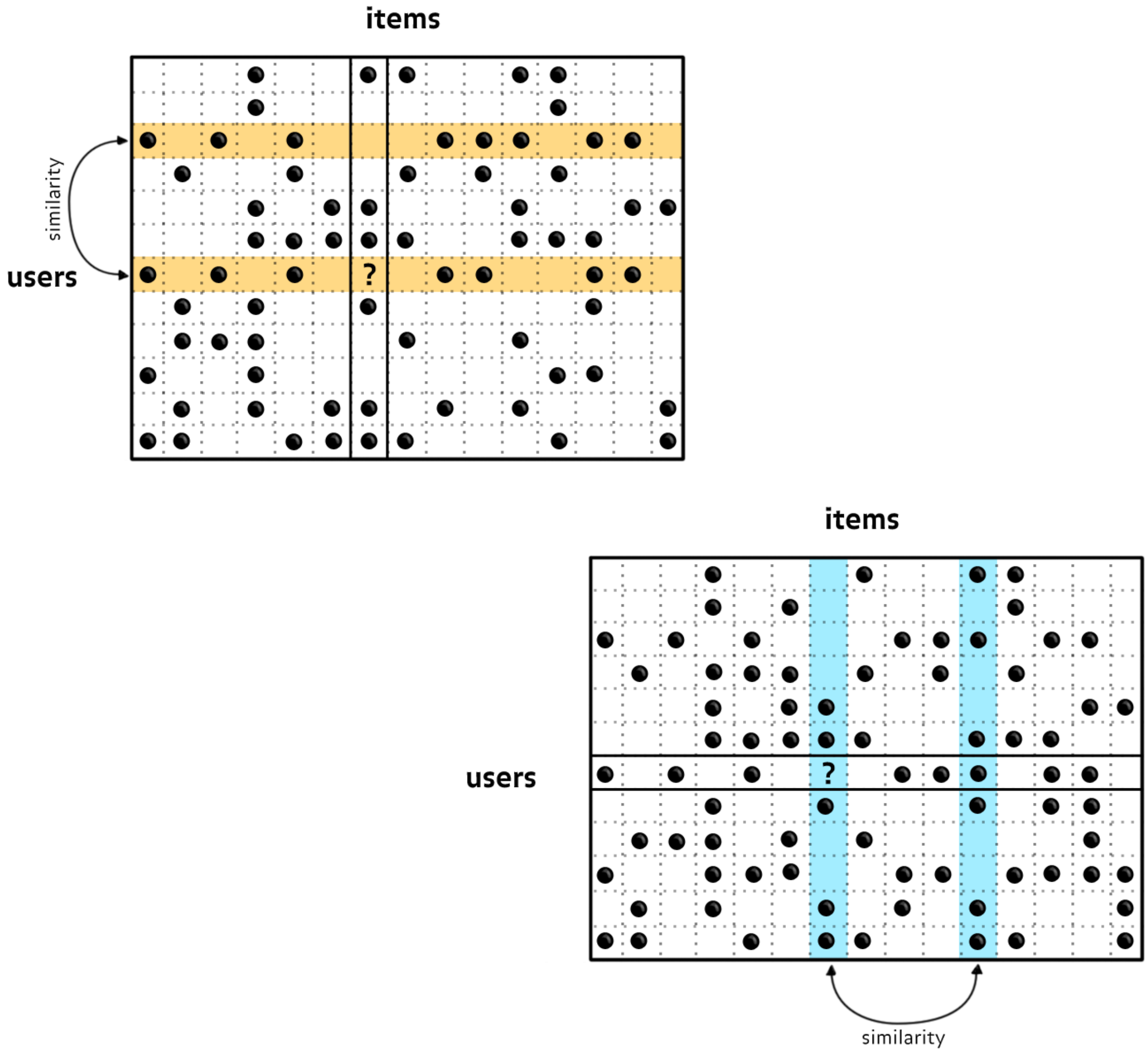


Figure 8.1: Collaborative recommendation. In order to predict unknown values, one computes a weighted average of known votes, weighted by the similarity either between users (rows) or between items (columns).

To be honest, people have very different ways of expressing opinions. A movie recommended as acceptable by an understating English reviewer may end up being a fantastic movie for a hyperbolizing Italian one. If you go by what a hypercritical reviewer says, you are going to end up seeing very few movies, and it can be useful to **discount individual evaluations** before using them to measure similarities and obtain predictions.

Let r_{uj} be the rating of user u for item j. Let I_u be the set of items that user u has rated. The mean rating for user

u is $\bar{r}_u = \frac{1}{|I_u|}\sum_{j \in I_u} r_{uj}$. Let the active user be denoted by subscript a. The goal is to predict the preference for an item i, or p_{ai}.

Because the votes may not be centered around zero, the system may have difficulties in reproducing the votes by scalar products. To help the system it can be useful to *center* the data by subtracting the average values. In detail, the prediction can be done by using the formula:

$$p_{ai} = \bar{r}_a + \frac{\sum_u w_{au}(r_{ui} - \bar{r}_u)}{\sum_u |w_{au}|}. \tag{8.2}$$

where the summation over u is over the set of users who have rated item i, and w_{au} is the weight between the active user a and user u. This weight can be defined as the Pearson correlation coefficient,

$$w_{au} = \frac{\sum_i (r_{ai} - \bar{r}_a)(r_{ui} - \bar{r}_u)}{\sqrt{\sum_i (r_{ai} - \bar{r}_a)^2}\sqrt{\sum_i (r_{ui} - \bar{r}_u)^2}}. \tag{8.3}$$

The summations over i are over the set $I_u \cap I_a$.

8.2 Models based on matrix factorization

The **sparsity** of the raw user-item evaluation matrix can be a problem. Each user evaluates only a very small subset of items and most entries are unknown. By **compressing and summarizing the user characteristics** into a much smaller vector, one hopes to reach better generalization results, and possibly a better understanding of the model, as explained by the Occam's razor principle.

A possible way to determine the interest or the vote of a user for an item is to associate a small **vector of characteristics with each user and with each item** and then deriving votes by observing the similarity between the user and item characteristic vectors. This operation can be done by hand, but it may be very time-consuming and it may not identify some characteristics which are crucial for the prediction. Let's see how the process can be automated.

Let us use vector $\boldsymbol{q}_i \in \Re^f$ to contain the characteristics (factors) of item i, and vector $\boldsymbol{p}_u \in \Re^f$ to denote the extent of interest that user u has in each item factor. One would like to obtain the rating of a user u for an item i by a simple scalar product of the corresponding vectors:

$$\hat{r} = \boldsymbol{q}_i^T \boldsymbol{p}_u. \tag{8.4}$$

For example, if the factors are built by hand, the aspect weights of movie *Terminator* can be exemplified as $(\text{action} = 5, \text{romance} = 1)$, and the interest of user *Patricia* in the movie aspects is $(\text{action} = 2, \text{romance} = 5)$, therefore the rating of user *Patricia* for movie *Terminator* is $5 \cdot 2 + 1 \cdot 5 = 15$.

Among automated ways to build effective factors to predict ratings, the traditional Singular Value Decomposition (SVD) can be used to find informative $\boldsymbol{q}_i$'s and $\boldsymbol{p}_u$'s. By using SVD, one decomposes a matrix R containing *all* ratings as $R = U\Sigma M^T$, where the rows of matrix U and M are the set of $\boldsymbol{p}_u$ and $\boldsymbol{q}_i$, scaled by the diagonal matrix Σ. By considering the size of the diagonal values in Σ one can then reduce the dimension of the vectors, and keep only the most relevant components. Unfortunately, in most cases one does *not* have the value of all cells in the rating matrix.

More flexible and robust learning algorithms based on optimization can be used to find effective approximations of the factor vectors $\boldsymbol{q}_i$ and $\boldsymbol{p}_u$. As usual, examples of expressed votes guide the learning process: to learn the factor vectors $\boldsymbol{q}_i$ and $\boldsymbol{p}_u$, one aims at minimizing the *regularized squared error (RSE)* on the set of *known* ratings:

$$\text{RSE} = \frac{1}{|K|}\sum_{(u,i)\in K} (r_{ui} - \boldsymbol{q}_i^T \boldsymbol{p}_u)^2 + \lambda(\|\boldsymbol{q}_i\|^2 + \|\boldsymbol{p}_u\|^2). \tag{8.5}$$

Here, K is the set of the (u, i) pairs for which r_{ui} is known (the training set). Let us know that the first term in the summation is the squared error between the model $\boldsymbol{q}_i^T \boldsymbol{p}_u$ and the known result r_{ui}. To facilitate *generalization* (prediction of novel ratings) it is useful to penalize the magnitudes of the factor vectors in a manner proportional to a constant λ. This term is called a **regularizing term**. When example ratings abound, most of the contribution to RSE derives from errors in reconstructing the expressed votes. On the other hand, when ratings are scarce, the regularizing term becomes crucial and it acts to discourage very large vectors with potentially dramatic (and wrong) effects on the predictions.

The problem is now one of minimizing a continuous function of the free parameters $\boldsymbol{p}_u$ and $\boldsymbol{q}_i$, for which methods illustrated in Chapter 26 can be used, for example the traditional gradient descent. The gradient of RSE is calculated as follows:

$$\frac{\partial \text{RSE}}{\partial \boldsymbol{q}_i} = \frac{2}{|K|} \sum_{(u,i)\in K} ((r_{ui} - \boldsymbol{q}_i^T \boldsymbol{p}_u)(-\boldsymbol{p}_u) + \lambda \boldsymbol{q}_i);$$
$$\frac{\partial \text{RSE}}{\partial \boldsymbol{p}_u} = \frac{2}{|K|} \sum_{(u,i)\in K} ((r_{ui} - \boldsymbol{q}_i^T \boldsymbol{p}_u)(-\boldsymbol{q}_i) + \lambda \boldsymbol{p}_u).$$

The term $\frac{1}{|K|}$ is a constant and therefore not influencing the minimization. One can start with random initial values for $\boldsymbol{q}_i$ and $\boldsymbol{p}_u$ and then iterate: at each step a small change in the direction of the negative gradient is executed to reduce the RSE error.

8.2.1 A more refined model: adding biases

As illustrated for the case of the simpler methods in Sec. 8.1, the rating of user u for item i does not only depend on the interaction $\boldsymbol{q}_i^T \boldsymbol{p}_u$ between two vectors $\boldsymbol{p}_u$ and $\boldsymbol{q}_i$, but also on the bias of a user or item. In other words, some people usually give higher ratings, and some items often receive higher ratings than others. The bias involved in rating r_{ui} can be described as: $b_{ui} = \mu + b_i + b_u$, where μ is the overall average, b_i and b_u are the observed deviation of user u and item i from the average, respectively. For example, assume that one wants to estimate the rating of user *Joe* for movie *Titanic*. Assume that the average rating over all movies, μ, is 3.7 stars. Furthermore, *Titanic* is better than an average movie, so it tends to be rated 0.5 stars above the average. On the other hand, *Joe* is a critical user, who tends to rate 0.3 stars lower than the average. Thus, the baseline estimate for *Titanic* rating by *Joe* would be 3.9 stars $(3.7 + 0.5 - 0.3)$.

According to this refined model, the estimated rating $\hat{r}_{ui}$ of user u and item i is calculated as:

$$\hat{r}_{ui} = \mu + b_i + b_u + \boldsymbol{q}_i^T \boldsymbol{p}_u. \tag{8.6}$$

The observed rating is broken down into its four components: *global average*, *item bias*, *user bias*, and *user-item interaction*. This allows each component to explain only the part of a rating relevant to it. The learning algorithm learns by minimizing the following regularized squared error function considering also bias factors (RSEB):

$$\text{RSEB} = \frac{1}{|K|} \sum_{u,i\in K} (r_{ui} - \mu - b_i - b_u - \boldsymbol{q}_i^T \boldsymbol{p}_u)^2 + \lambda(\|\boldsymbol{p}_u\|^2 + \|\boldsymbol{q}_i\|^2 + b_i^2 + b_u^2). \tag{8.7}$$

The usual default procedure starts by deriving the gradient and using steepest descent. A factorization process using steepest descent in action can be seen in Fig. 8.2: as the number of gradient descent iterations increases, the error (root mean squared error) over the training set decreases as expected. The error over the test set (votes not used during training) first decreases, but then reaches a plateau and eventually gradually increases. This is an instance of **over-training**: the system is trying to accurately reproduce the training examples but generalization worsens. Think about a student learning "by heart," without digesting the learning material to extract the relevant relationships.

Let us note **the power and flexibility of optimization**: if additional terms are added to the model, the best parameters can then be immediately identified by calculating the new partial derivatives and plugging them into the minimization algorithm. If one knows how to optimize, one can focus on the problem definition, then *rapidly* try many alternative models and test the obtained generalization results on validation data.

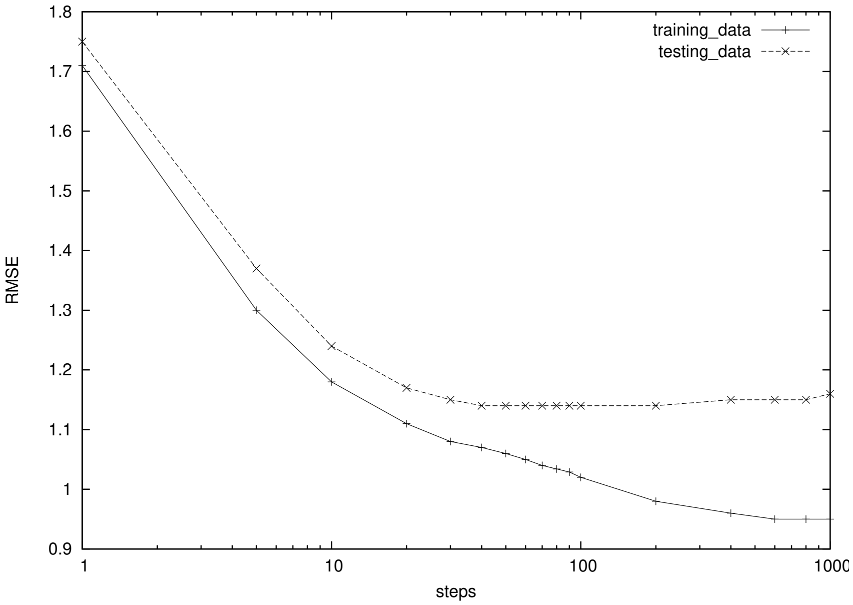


Figure 8.2: A factorization in action: training and testing performance as a function of gradient descent iterations.

Gist

When a potential customer visits your e-commerce web portal, he'll look at some items, put others in his cart, purchase them, write a comment and a score, leaving a trail, a scent that a well trained "nose" can follow.

All this information is there for you to improve your service: just like a good shopkeeper, who greets his patrons by name and proactively shows them what they'll like most, your website will lure customers with a personalized choice of items.

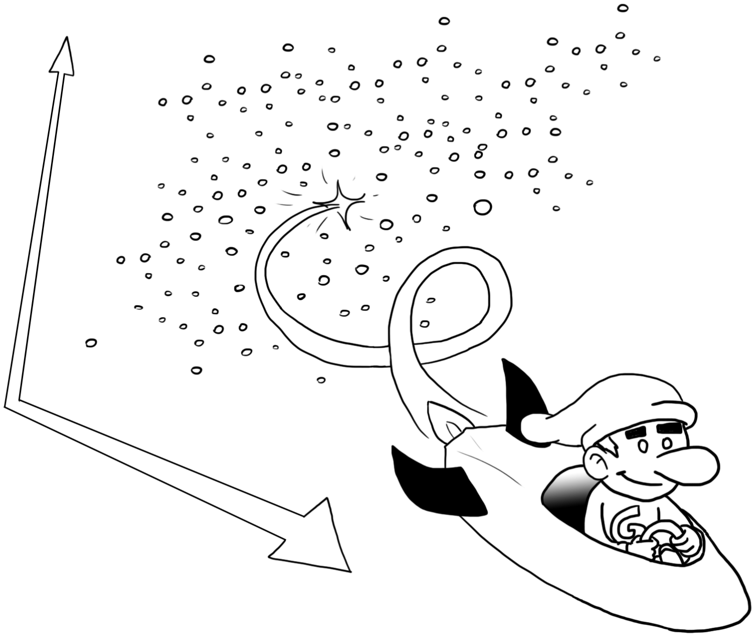
Collaborative filtering precisely does this: by memorizing and analyzing the behavior of customers, it simultaneously profiles visitors and items, grouping people by similar purchase habits, and **predicting what item a customer might like most**. This personalization is done without specific domain knowledge, by just mining the collective behaviour of customers. This is why a nerdy professor can end up consulting for a sophisticated fashion business.

Now think twice before clicking on a gossip title in your favorite online newspaper. If you do, more and more gossip-related news will appear on your personalized frontpage (and maybe also in different websites that you will visit, thanks to sharing of marketing data and *behavioral retargeting* strategies).

Chapter 9

Specific nonlinear models

He who would learn to fly one day must first learn to stand and walk and run and climb and dance; one cannot fly into flying.
(Friedrich Nietzsche)



In this chapter we continue along our path from linear to nonlinear models. In order to avoid the vertigo caused by an abrupt introduction of the most general and powerful models, we start by gradual modifications of the linear model, first to make it suitable for predicting probabilities (**logistic regression**), then by making the linear models *local* and giving more emphasis to the closest examples, in a kind of smoothed version of K nearest neighbors (**locally-weighted linear regression**), finally by selecting a subset of inputs via appropriate constraints on the weights (**LASSO**).

After this preparatory phase, in the next chapters we will be ready to enter the holy of holies of flexible nonlinear models for arbitrary smooth input-output relationships like Multi-Layer Perceptrons (MLP) and Support Vector Machines (SVM).

9.1 Logistic regression

In statistics, logistic regression is used for **predicting the probability of the outcome of a categorical variable** from a set of recorded past events. For example, one starts from data about patients which can have a heart disease (disease "yes" or "no" is the categorical output variable) and wants to predict the probability that a new patient has the heart disease. The name is somewhat misleading, it really is a technique for classification, not regression. But classification is obtained through an estimate of the probability, henceforth the term "regression." Frequently the output is binary, that is, the number of available categories is two.

The problem with using a linear model is that the output value is not bounded: we need to bound it to be between zero and one. In logistic regression most of the work is done by a linear model, but a **logistic function** (Fig. 9.1) is used to transform the output of a linear predictor to obtain a value between zero and one, which can be interpreted as a probability. The probability can then be compared with a threshold to reach a classification (e.g., classification "yes" if output probability greater than 0.5).

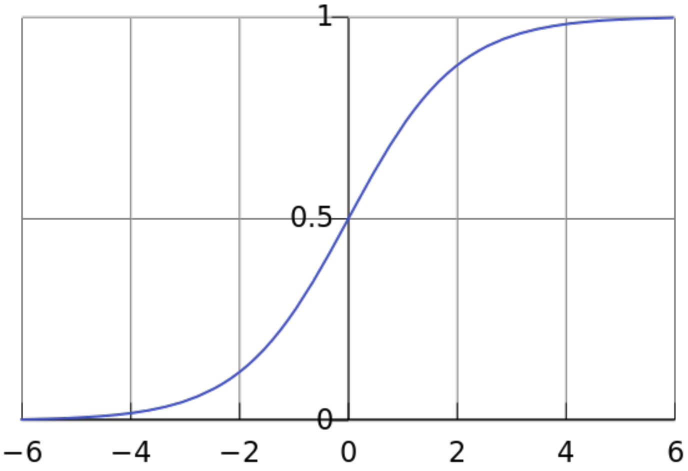


Figure 9.1: A logistic function transforms input values into an output value in the range 0-1, in a smooth manner. The output of the function can be interpreted as a probability.

A logistic curve is a common *sigmoid function*. The term "logistic" was given when this function was introduced to study population growth. In a population, the rate of reproduction is proportional to both the existing population and the amount of available resources. The available resources decrease when the population grows and become zero when the population reaches the "carrying capacity" of the system. The initial stage of growth is approximately exponential; then, as saturation begins, the growth slows, and at maturity, growth stops.

A standard logistic function is defined as:

$$P(t) = \frac{1}{1 + e^{-t}},$$

where e is Euler's number and the variable t might be thought of as time or, in our case, the output of the linear model, remember equation (4.1) at page 37:

$$P(\boldsymbol{x}) = \frac{1}{1 + e^{-(\boldsymbol{w}^T \boldsymbol{x})}}.$$

Remember that a constant value w_0 can also be included in the linear model $\boldsymbol{w}$, provided that an artificial input x_0 always equal to 1 is added to the list of input values.

Let's see which function is to be maximized in this case. The best values for the weights of the linear transformation are determined by **maximum likelihood estimation**, i.e., by maximizing the probability of getting the output values which were actually *obtained* on the given labeled examples. The probabilities of individual independent cases are multiplied. Let y_i be the observed output (1 or 0) for the corresponding input $\boldsymbol{x}_i$. If $\Pr(y = 1|\boldsymbol{x}_i)$ is the probability obtained by the model, the probability of obtaining the measured output value y_i is $\Pr(y = 1|\boldsymbol{x}_i)$ if the correct label is 1, $\Pr(y = 0|\boldsymbol{x}_i) = 1 - \Pr(y = 1|\boldsymbol{x}_i)$ if the correct label is 0. All factors need to be multiplied to get the overall probability of obtaining the complete series of examples. It is customary to work with logarithms, so that the multiplication of the factors (one per example) becomes a summation:

$$\text{LogLikelihood}(\boldsymbol{w}) = \sum_{i=1}^{\ell} \Big\{ y_i \ln \Pr(y_i|\boldsymbol{x}_i, \boldsymbol{w}) + (1 - y_i) \ln(1 - \Pr(y_i|\boldsymbol{x}_i, \boldsymbol{w})) \Big\}.$$

The dependence of $\Pr$ on the coefficients (weights) $\boldsymbol{w}$ has been made explicit.

Given the nonlinearities in the above expression, it is not possible to find a closed-form expression for the weight values that maximize the likelihood function: an iterative process must be used instead, for example gradient descent. This process begins with a tentative solution $\boldsymbol{w}_{\text{start}}$, revises it slightly by moving in the direction of the negative gradient to see if it can be improved, and repeats this revision until improvement is minute, at which point the process is said to have converged.

As usual, in ML one is interested in maximizing the generalization. The above minimization process can - and should - be stopped early, when the estimated generalization results measured by a validation set are maximal.

9.2 Locally-Weighted Regression

In Section 4.1 we have seen how to determine the coefficients of a linear dependence, fixed coefficients for the entire input range. The K Nearest Neighbors method in Chapter 2 predicts the output for a new input by comparing the new input with the closest old (and labeled) ones, giving as output either the one of the closest stored input, or some simple combination of the outputs of a selected set of closest neighbors.

This section considers a similar approach to obtain the output from a *linear* combination of the outputs of the closest neighbors. But one is less cruel in eliminating all but the K closest neighbors. The situation is smoothed out: instead of selecting a set of K winners one **gradually reduces the role of examples on the prediction based on their distance** from the case to predict.

Through weighting, the overall global dependence can be quite complex. When the model is evaluated at different points, one still uses linear regression, but the training points *near* the evaluation point are considered "more important" than distant ones. We encounter a very general principle here: in learning (natural or automated) similar cases are usually deemed more relevant than very distant ones.

Locally Weighted Regression is a *lazy* memory-based technique, meaning that all points and evaluations are stored and a specific model is built *on-demand* only when a specified query point demands an output.

To predict the outcome of an evaluation at a point $\boldsymbol{q}$ (named a *query point*), linear regression is applied to the training points. To enforce locality in the determination of the regression parameters (near points are more relevant), each sample point is assigned a *weight* that decreases with its distance from the query point. Note that, in the neural networks community, the term "weight" refers to the parameters of the model being computed by the training algorithm, while, in this case, it measures the importance of each training example. To avoid confusion let's use the term *significance* and the symbol s_i (and S for the diagonal matrix used below) for this different purpose.

In the following we assume, as explained in Section 4.1, that a constant 1 is attached as entry 0 to all input vectors $\boldsymbol{x}_i$ to include a constant term in the regression, so that the dimensionality of all equations is actually $d + 1$.

The weighted version of *least squares* fit aims at minimizing the following weighted error (compare with equa-

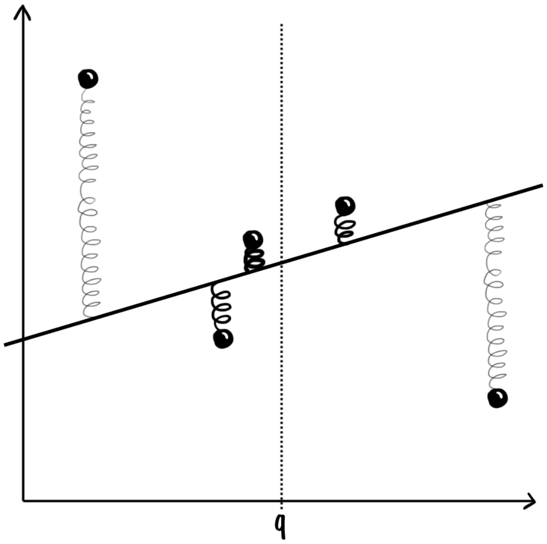


Figure 9.2: The spring analogy for the weighted least squares fit (compare with Fig. 4.6). Now springs have different elastic constants, thicker meaning harder, so that their contribution to the overall potential energy is weighted. In the above case, harder springs are for points closer to the query point $\boldsymbol{q}$.

tion (4.2), where weights are implicitly uniform):

$$\text{error}(\boldsymbol{w}; s_1, \dots, s_n) = \sum_{i=1}^{\ell} s_i(\boldsymbol{w}^T \cdot \boldsymbol{x}_i - y_i)^2. \tag{9.1}$$

From the viewpoint of the spring analogy discussed in Section 4.1, the distribution of different weights to sample points corresponds to using springs with a different elastic constant (strength), as shown in Fig. 9.2. Minimization of equation (9.1) is obtained by requiring its gradient with respect to $\boldsymbol{w}$ to be equal to zero, and we obtain the following solution:

$$\boldsymbol{w}^* = (X^T S^2 X)^{-1} X^T S^2 \boldsymbol{y}; \tag{9.2}$$

where $S = \text{diag}(s_1, \dots, s_d)$, while X and $\boldsymbol{y}$ are defined as in equation 4.5, page 42. Note that equation (9.2) reduces to equation (4.5) when all weights are equal.

A possible function used to assign significance values to the stored examples according to their distance from the query point is

$$s_i = \exp\left(-\frac{\|\boldsymbol{x}_i - \boldsymbol{q}\|^2}{W_K}\right);$$

where W_K is a parameter measuring the "kernel width," i.e. the sensitivity to distant sample points; if the distance is much larger than W_K the significance rapidly goes to zero.

An example is given in Fig. 9.3 (top), where the model must be evaluated at query point $\boldsymbol{q}$. Sample points x_i are plotted as circles, and their significance s_i decreases with the distance from $\boldsymbol{q}$ and is represented by the interior shade, black meaning highest significance. The linear fit (solid line) is computed by considering the significance of the various points and is evaluated at $\boldsymbol{q}$ to provide the model's value at that point. The significance of each sample point and the subsequent linear fit are recomputed for each query point, providing the curve shown in Fig. 9.3 (bottom).

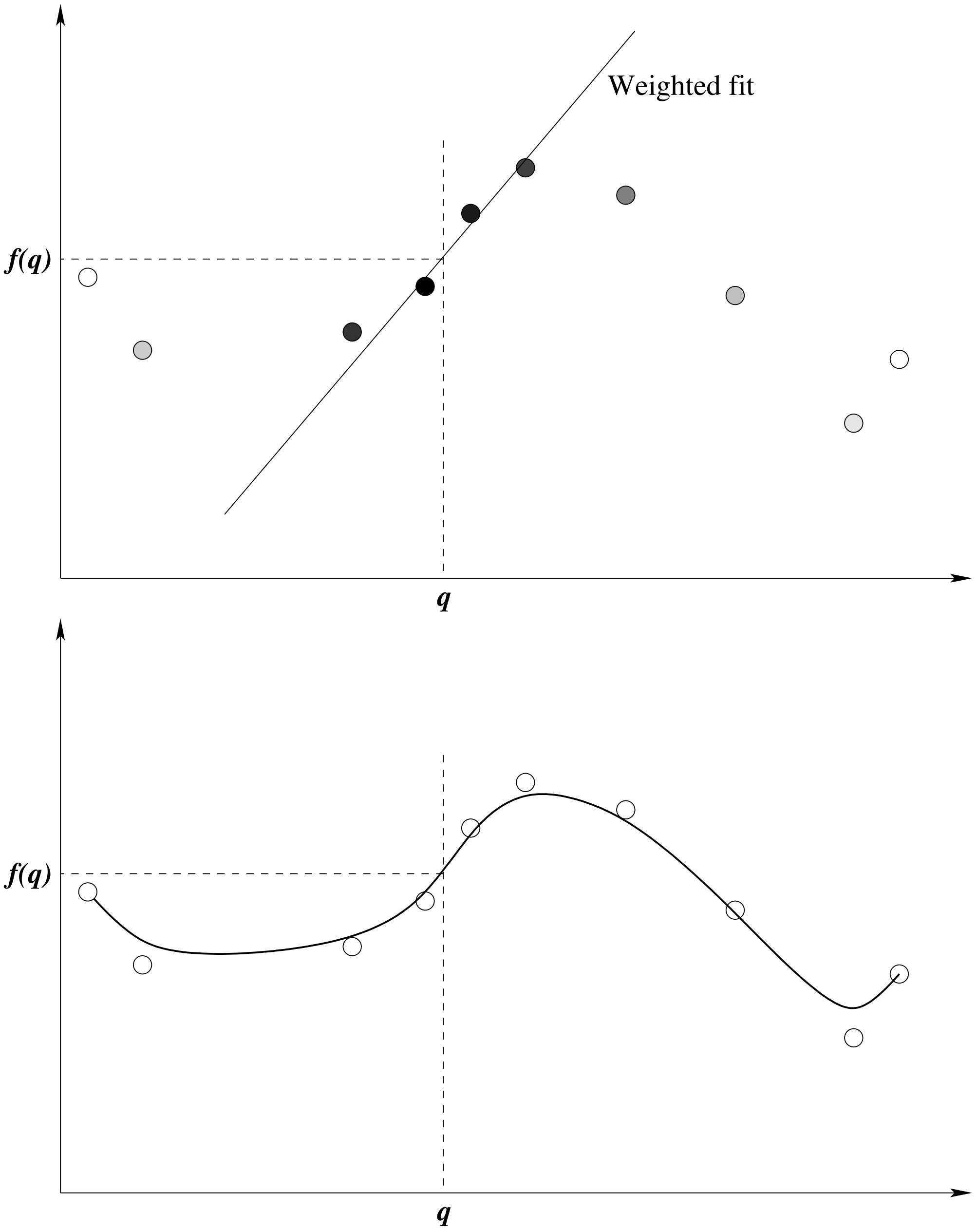


Figure 9.3: Top: evaluation of LWR model at query point $\boldsymbol{q}$, sample point significance is represented by the interior shade. Bottom: Evaluation over all points, each point requires a different linear fit.

9.2.1 Bayesian LWR

Up to this point, no assumption has been made on the *prior* probability distribution of coefficients to be determined. In some cases some more information is available about the task which can conveniently be added through a prior distribution.

In **Bayesian Locally Weighted Regression**, denoted as B-LWR, one specifies *prior information* about what values the coefficients should have. The usual power of Bayesian techniques derives from the *explicit* specification of the modeling assumptions and parameters (for example, a **prior distribution** can model our initial knowledge about the function) and the possibility to model not only the expected values but entire probability distributions. For example **confidence intervals** can be derived to quantify the uncertainty in the expected values.

The prior assumption on the distribution of coefficients w, leading to Bayesian LWR, is that it is distributed according to a multivariate Gaussian with zero mean and covariance matrix Σ, and the prior assumption on σ is that $1/\sigma^2$ has a Gamma distribution with k and θ as the shape and scale parameters. Since one uses a weighted regression, each data point and the output response are weighted using a Gaussian weighing function. In matrix form, the weights for the data points are described in $\ell \times \ell$ diagonal matrix $S = \text{diag}(s_1, \dots, s_\ell)$, while $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_\ell)$ contains the prior variance for the $\boldsymbol{w}$ distribution.

The local model for the query point $\boldsymbol{q}$ is predicted by using the marginal posterior distribution of $\boldsymbol{w}$ whose mean is estimated as

$$\bar{\boldsymbol{w}} = (\Sigma^{-1} + X^T S^2 X)^{-1} (X^T S^2 \boldsymbol{y}). \tag{9.3}$$

Note that the removal of prior knowledge corresponds to having infinite variance on the prior assumptions, therefore Σ^{-1} becomes null and equation (9.3) reduces to equation (9.2). The matrix $\Sigma^{-1} + X^T S^2 X$ is the weighted covariance matrix, supplemented by the effect of the $\boldsymbol{w}$ priors. Let's denote its inverse by $V_{\boldsymbol{w}}$. The variance of the Gaussian noise based on ℓ data points is estimated as

$$\sigma^2 = \frac{2\theta + (\boldsymbol{y}^T - \boldsymbol{w}^T X^T) S^2 \boldsymbol{y}}{2k + \sum_{i=1}^{\ell} s_i^2}.$$

The estimated covariance matrix of the $\boldsymbol{w}$ distribution is then calculated as

$$\sigma^2 V_{\boldsymbol{w}} = \frac{(2\theta + (\boldsymbol{y}^T - \boldsymbol{w}^T X^T) S^2 \boldsymbol{y})(\Sigma^{-1} + X^T S^2 X)}{2k + \sum_{i=1}^{\ell} s_i^2}.$$

The degrees of freedom are given by $k + \sum_{i=1}^{\ell} s_i^2$. Thus the predicted output response for the query point $\boldsymbol{q}$ is

$$\hat{y}(\boldsymbol{q}) = \boldsymbol{q}^T \bar{\boldsymbol{w}},$$

while the variance of the mean predicted output is calculated as:

$$Var(\hat{y}(\boldsymbol{q})) = \boldsymbol{q}^T V_{\boldsymbol{w}} \boldsymbol{q} \sigma^2. \tag{9.4}$$

9.3 LASSO to shrink and select inputs

When considering linear models, *ridge regression* was mentioned as a way to make the model more stable by penalizing large coefficients in a quadratic manner, as in equation (4.7).

Ordinary least squares estimates often have low bias but large variance; prediction accuracy can sometimes be improved by shrinking or setting to 0 some coefficients. By doing so we sacrifice a little bias to reduce the variance of the predicted values and hence may improve the overall prediction accuracy. The second reason is **interpretation**. With a large number of predictors (input variables), we often would like to determine a smaller subset that exhibits the strongest effects. The two standard techniques for improving the estimates, feature subset selection and ridge regression, have some drawbacks. Subset selection provides interpretable models but can be extremely variable because it is a discrete process - input variables (a.k.a. regressors) are either retained or dropped from the model. Small changes in the data can result in very different models being selected and this can reduce prediction accuracy. Ridge regression is a continuous process that shrinks coefficients and hence is more stable: however, it does not set any coefficients to 0 and hence does not give an easily interpretable model. The work in [358] proposes a new technique, called the **LASSO**, "least absolute shrinkage and selection operator." It shrinks some coefficients and sets others to 0, and hence tries to retain the good features of both subset selection and ridge regression.

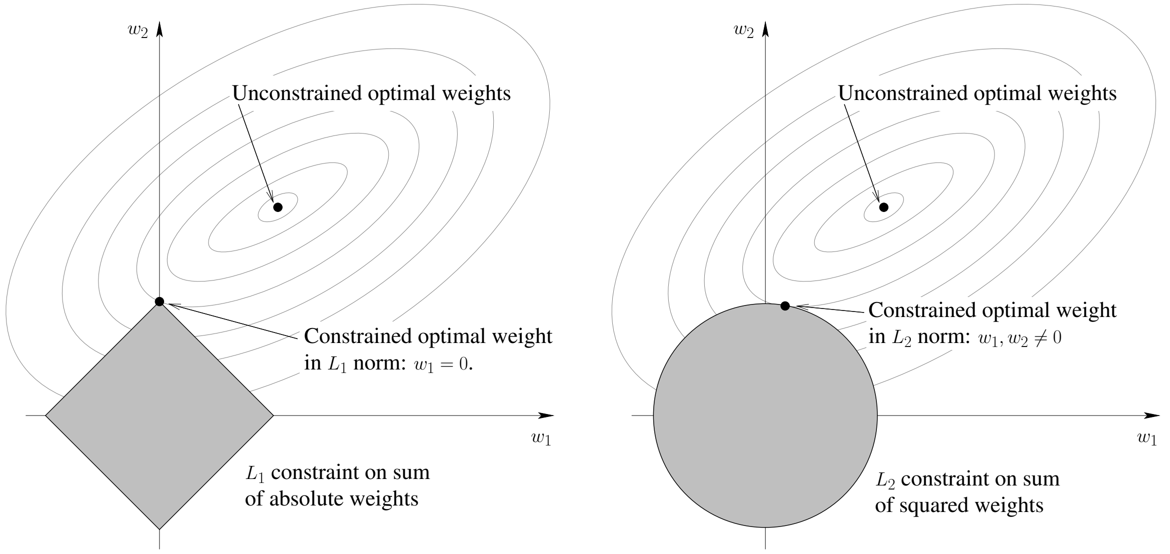

w_2
Unconstrained optimal weights
Constrained optimal weight
in L_1 norm: $w_1 = 0$.
w_1
L_1 constraint on sum
of absolute weights
w_2
Unconstrained optimal weights
Constrained optimal weight
in L_2 norm: $w_1, w_2 \neq 0$
w_1
L_2 constraint on sum
of squared weights

Figure 9.4: In LASSO, the best solution is where the contours of the quadratic error function touch the square, and this will sometimes occur at a corner, corresponding to some zero coefficients. On the contrary the quadratic constraint of ridge regression does not have corners for the contours to hit and hence zero values for the weights will rarely result.

LASSO uses the constraint that $\|\boldsymbol{w}\|_1$, the sum of the **absolute values of the weights** (the L_1 norm of the parameter vector), is no greater than a given value. LASSO minimizes the residual sum of squares subject to the sum of the absolute value of the coefficients being less than a constant. By a standard trick to transform a constrained optimization problem into an unconstrained one through Lagrange multipliers, explained in Section 26.5, this is equivalent to an unconstrained minimization of the *least squares* penalty with $\lambda\|\boldsymbol{w}\|_1$ added:

$$\text{LASSOerror}(\boldsymbol{w}; \lambda) = \sum_{i=1}^{\ell} (\boldsymbol{w}^T \cdot \boldsymbol{x}_i - y_i)^2 + \lambda \sum_{j=0}^{d} |w_j|. \tag{9.5}$$

One of the prime differences between LASSO and ridge regression is that in ridge regression, as the penalty is increased, all parameters are reduced while still remaining *non-zero*, while in LASSO, increasing the penalty will cause more and more of the parameters to be driven to *zero*. The inputs corresponding to weights equal to zero can be eliminated, leading to models with fewer inputs (**sparsification** of inputs) and therefore more interpretable. Fewer nonzero parameter values effectively reduce the number of variables upon which the given solution is dependent. In other words, LASSO is an embedded method to perform **feature selection as part of the model construction process**.

Let's note that the term that penalizes large weights in equation (9.5) does not have a derivative when a weight is equal to zero (the partial derivative jumps from minus one for negative values to plus one for positive values). The "trick" of obtaining a linear system by calculating a derivative and setting it to zero cannot be used. The LASSO optimization problem may be solved by using **quadratic programming** with linear inequality constraints or more general convex optimization methods. The best value for the LASSO parameter λ can be estimated via cross-validation.

Gist

Linear models are widely used but insufficient in many cases. Three examples of specific modifications have been considered in this chapter.

First, there can be reasons why the output needs to have a limited range of possible values. For example, if one needs to predict a probability, the output can range only between zero and one. Passing a linear combination of inputs through a “squashing” logistic function is a possibility. When the log-likelihood of the training events is maximized, one obtains the widely-used **logistic regression**.

Second, there can be cases when a linear model needs to be *localized*, by giving more significance to input points which are closer to a given input sample to be predicted. This is the case of **locally-weighted regression**.

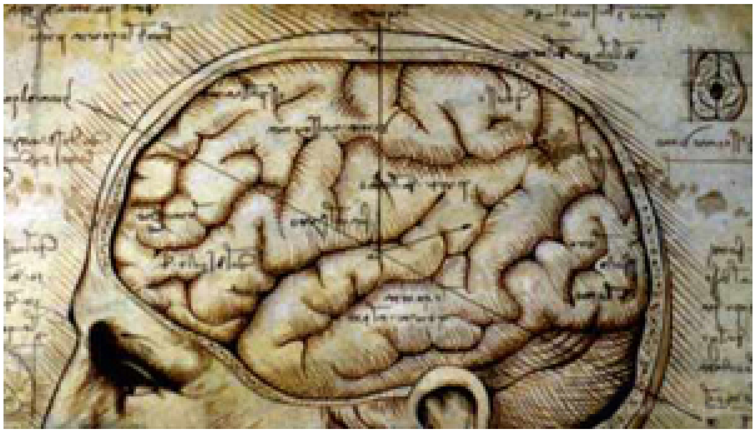
Last, the penalties for large weights added to the function to be optimized can be different from the sum of squared weights (the only case in which a linear equation is obtained after calculating derivatives). As an example, penalties given by a sum of absolute values can be useful to both reduce weight magnitude and *sparsify* the inputs. This is the case of the **LASSO** technique to shrink and select inputs. LASSO reduces the number of weights different from zero, and therefore the number of inputs which influence the output.

Before reading this chapter, to you a lasso was a long rope with a running noose at one end especially used to catch horses and cattle. Now you can catch more meaningful models too.

Chapter 10

Neural networks: multi-layer perceptrons

Quegli che pigliavano per altore altro che la natura, maestra de' maestri, s'affaticavano invano.
Those who took other inspiration than from nature, master of masters,
were laboring in vain.
(Leonardo Da Vinci)



Our **wet neural system**, composed of about 100 billion (100,000,000,000) computing units and about 10^{15} (1,000,000,000,000,000) connections is capable of surprisingly intelligent behaviors. Actually, the capabilities of our brain *define* intelligence. The computing units are specialized cells called **neurons**, the connections are called **synapses**, and computation occurs at each neuron by currents generated by electrical signals at the synapses, integrated in the central part of the neuron, and leading to electrical spikes propagated to other neurons when a threshold of excitation is surpassed. Neurons and synapses have been presented in Chapter 4 (Fig. 4.3). A way to model a neuron is through a linear discrimination by a weighted sum of the inputs passed through a "squashing" function (Fig. 4.4). The output level of the squashing function is intended to represent the spiking frequency of a neuron, from zero up to a maximum frequency.

A single neuron is therefore **a simple computing unit**, a scalar product followed by a sigmoidal function. By the way, the computation is rather noisy and irregular, being based on electrical signals influenced by chemistry, temperature, blood supply, sugar levels, etc. The intelligence of the system is coded in the interconnection strengths, and **learning occurs by modifying connections**. The paradigm is very different from that of "standard" sequential computers, which operate in cycles, fetching items from memory, applying mathematical operations and writing results back to memory. Neural networks do not separate memory and processing but operate via the flow of signals through the network connections.

The main mystery to be solved is how a system composed of many simple interconnected units can give rise to such incredible activities as recognizing objects, speaking and understanding, drinking a cup of coffee, fighting for your career. **Emergence** is the way in which **complex systems arise out of a multiplicity of relatively simple interactions**. Similar emergent properties are observed in nature, think about snowflakes forming complex symmetrical patterns starting from simple water molecules.

The real brain is therefore an incredible source of inspiration for researchers, and **a proof that intelligent systems can emerge from very simple interconnected computing units**. Ever since the early days of computers, the biological metaphor has been irresistible ("electronic brains"), but only as a simplifying analogy rather than a blueprint for building intelligent systems. As Frederick Jelinek put it, "**airplanes don't flap their wings**." Yet, starting from the sixties, and then again the late eighties, the principles of biological brains gained ground as a tool in computing. The shift in thinking resulted in a paradigm change, from artificial intelligence based on symbolic rules and reasoning, to artificial neural systems where knowledge is encoded in system parameters (like synaptic interconnection weights) and learning occurs by gradually modifying these parameters under the influence of external stimuli.

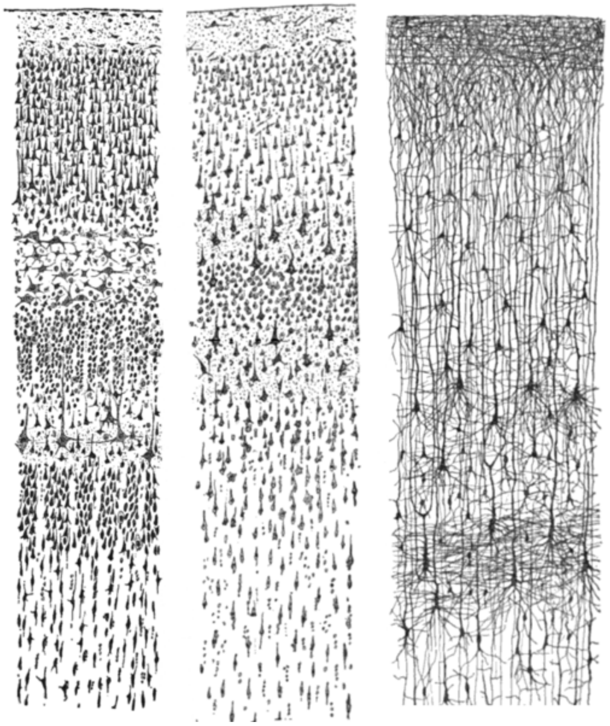


Figure 10.1: Three drawings of cortical lamination by Santiago Ramon y Cajal, each showing a vertical cross-section, with the surface of the cortex at the top. The different stains show the cell bodies of neurons and the dendrites and axons of a random subset of neurons.

Given that the function of a single neuron is rather simple, it subdivides the input space into two regions by a hyperplane, the complexity must come from having *more* layers of neurons involved in a complex action (like recognizing your grandmother in all possible situations). The "squashing" functions introduce critical nonlinearities in the system, without their presence multiple layers would still create linear functions (it is easy to check that the composition of linear functions remain linear). Organized layers are visible in the human cerebral cortex, the part of our brain which plays a key role in memory, attention, perceptual awareness, thought, language, and consciousness (Fig. 10.1).

For more complex "sequential" calculations like those involved in logical reasoning, feedback loops are essential but more difficult to simulate via artificial neural networks. As you can expect, the “high-level”, symbolic, and reasoning view of intelligence is complementary to the “low-level” sub-symbolic view of artificial neural networks. What is simple for a computer, like solving equations or reasoning, is difficult for our brain, what is simple for our brain, like recognizing our grandmother, is still difficult to simulate on a computer. The two styles of intelligent behavior are now widely recognized, leading also to popular books about “fast and slow thinking” [225].

In any case, “airplanes don’t flap their wings.” Even if real brains are a source of inspiration and a proof of feasibility, most artificial neural networks are actually run on standard computers, and the different areas of “neural networks”, “machine learning”, “artificial intelligence” are actually converging so that the different terms are now umbrellas that cover a continuum of techniques to address different and often complementary aspects of intelligent systems.

This chapter is focused on **feed-forward multilayer perceptron neural networks**, without feedback loops.

10.1 Multilayer Perceptrons (MLP)

The logistic regression model of Section 9.1 in Chapter 9 was a simple way to add the “minimal amount of non-linearity” to obtain an output which can be interpreted as a probability, by applying a sigmoidal transfer function to the unlimited output of a linear model. Imagine this as transforming a crisp plane separating the input space (output 0 on one side, output 1 on the other side, based on a linear calculation compared with a threshold) into a smooth and gray transition area, black when far from the plane in one direction, white when far from the plane in the other direction, gray in between[1] (Fig. 10.2).

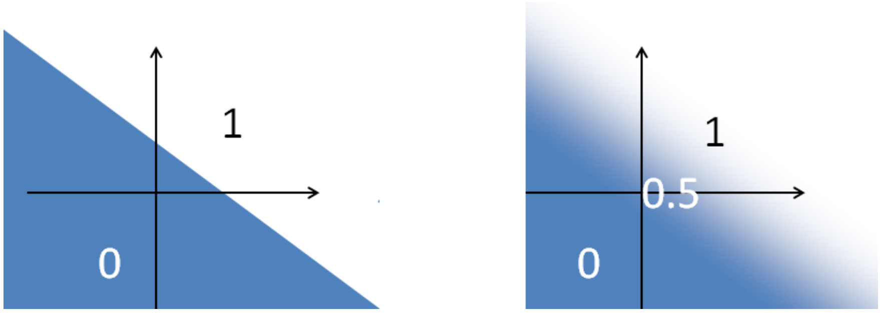


Figure 10.2: Effect of the logistic function. Linear model with threshold (left), smooth sigmoidal transition (right).

If one visualizes y as the elevation of a terrain, in many cases a mountain area presents too many hills, peaks and valleys to be modeled by a plane or maybe a single smooth transition region.

If linear transformations are composed, by applying one after another, the situation does not change: two linear transformation in a sequence still remain linear[2]. But if the output of the first linear transformation is transformed by a *nonlinear* sigmoid before applying the second linear transformation we get what we want: **flexible models capable of approximating all smooth functions**. The term **non-parametric models** is used to underline their flexibility and differentiate them from rigid models in which only the value of some parameters can be tuned to the data. An example of a parametric model is an oscillation $\sin(\omega x)$, in which the parameter ω has to be determined from the experimental data. The first linear transformation will provide a first “hidden layer” of outputs (hidden because internal and not directly visible as final outputs), additional transformations will produce the visible outputs from the hidden layers.

[1] As an observation, let’s note that logistic regression and an MLP network with no hidden layer and a single output value are indeed the same architecture, what changes is the function being optimized, the sum of squared errors for MLP, the $LogLikelihood$ for logistic regression.

[2] Let’s consider two linear transformations A and B. Applying B after A to get $B(A(\boldsymbol{x}))$ still maintains linearity. In fact, $B(A(a\boldsymbol{x} + b\boldsymbol{y})) = B(aA(\boldsymbol{x}) + bA(\boldsymbol{y})) = aB(A(\boldsymbol{x})) + bB(A(\boldsymbol{y}))$.

A multilayer perceptron neural network (MLP) is composed of a large number of highly interconnected units (*neurons*) working in parallel to solve a specific problem and organized in layers with a feed-forward information flow (no loops). The architecture is illustrated in Fig. 10.3.

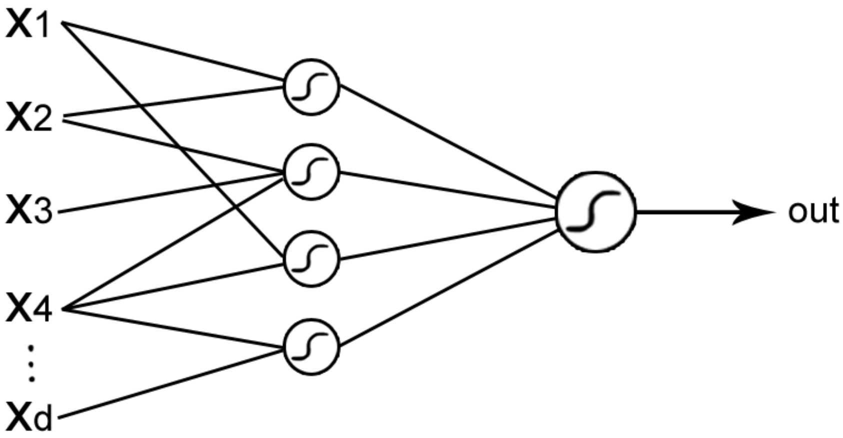


Figure 10.3: Multilayer perceptron: the nonlinearities introduced by the sigmoidal transfer functions at the intermediate (hidden) layers permit arbitrary continuous mappings to be created. A single hidden layer is present in this image.

The architecture of the multilayer perceptron is organized as follows: the signals flow sequentially through the different layers from the input to the output layer. The intermediate layers are called *hidden* layers because they are not visible at the input or at the output. For each layer, each unit first calculates a scalar product between a vector of weights and the vector given by the outputs of the previous layer. A *transfer function* is then applied to the result to produce the input for the next layer. A popular smooth and *saturating* transfer function (the output saturates to zero for large negative signals, to one for large positive signals) is the sigmoidal function, called sigmoidal because of the "S" shape of its plot. An example is the logistic transformation encountered before (Fig. 9.1):

$$f(x) = \frac{1}{1+e^{-x}}.$$

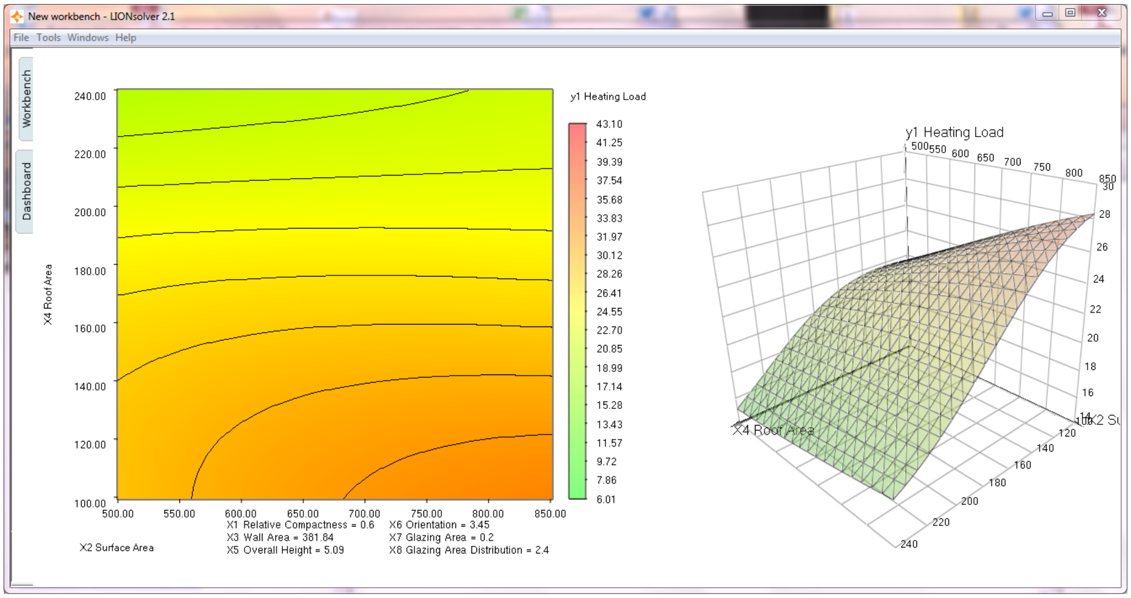
Other transfer functions can be used for the output layer; for example, the identity function can be used for unlimited output values, while a sigmoidal output function is more suitable for "yes/no" classification problems or to model probabilities.

A basic question about MLP is: **what is the flexibility of this architecture** to represent input-output mappings? In other words, given a function $f(\boldsymbol{x})$, is there a specific MLP network with specific values of the weights so that the MLP output closely approximates the function f? While perceptrons are limited in their modeling power to classification cases where the patterns (i.e., inputs) of the two different classes can be separated by a hyperplane in input space, MLPs are **universal approximators** [190]: an MLP with one hidden layer can approximate any smooth function to any desired accuracy, subject to a sufficient number of hidden nodes.

This is an interesting result: neural-like architectures composed of simple units (linear summation and squashing sigmoidal transfer functions), organized in layers with at least a hidden layer are what we need to model arbitrary smooth input-output transformations.

For colleagues in mathematics this is a brilliant "existence" results. For more practical colleagues the next question is: given the existence of an MLP approximator, how can one find it rapidly by starting from labeled examples?

After reading the previous chapter you should already know at least a possible training technique. Think about it and then proceed to the next section.



X1 Relative Compactness = 0.6
X3 Wall Area = 381.84
X5 Overall Height = 5.09
X6 Orientation = 3.45
X7 Glazing Area = 0.2
X8 Glazing Area Distribution = 2.4

Figure 10.4: Analyzing a neural network output with LIONsolver Sweeper. The output value, the energy consumed to heat a house in winter, is shown as a function of input parameters. Color coded output (left), surface plot (right). Nonlinearities are visible.

As an example of an MLP input-output transformation, Fig. 10.4 shows the smooth and nonlinear evolution of the output value as a function of varying input parameters. By using sliders one fixes a subset of the input values, and the output is color-coded for a range of values of two selected input parameters.

10.2 Learning via backpropagation

As usual, take a "guiding" function to be optimized, like the traditional sum-of-squared errors on the training examples, make sure it is smooth (differentiable), and use **gradient descent**. Iterate by calculating the gradient of the function with respect to the weights and by taking a small step in the direction of the negative gradient. If the gradient is different from zero, there is a sufficiently small step in the direction of the negative gradient which will decrease the function value.

The technical issue is now one of *calculating* partial derivatives by using the **chain rule** in calculus for computing the derivative of the composition of two or more functions. If f is a function and g is a function, then the chain rule expresses the derivative of the composite function $f \circ g$ in terms of the derivatives of f and g. For example, the chain rule for $(f \circ g)(x)$ is:

$$\frac{df}{dx} = \frac{df}{dg} \cdot \frac{dg}{dx}.$$

In MLP the basic functions are: scalar products, then sigmoidal functions, then scalar products, and so on until the output layer is reached and the error is computed. For MLP networks the gradient can be efficiently calculated, its calculation requires a number of operations proportional to the number of weights, and the actual calculation is done by simple formulas similar to the one used for the forward pass (from inputs to outputs) but now going in the contrary directions, from output errors backwards towards the inputs. The popular technique in neural networks known as **backpropagation** of the error consists precisely in the above exercise: gradient calculation and small step in the direction of the negative gradient [383, 384, 311].

It is amazing how a straightforward application of gradient descent took so many years to reach wide applicability in the late eighties, and brought so much fame to the researchers who made it popular. A possible excuse is that gradient descent is normally considered a "vanilla" technique capable of reaching only locally-optimal points (with zero gradient) without guarantees of global optimality. Experimentation on different problems, after initializing the networks with small and randomized weights, was therefore needed to show its practical applicability for training MLPs. In addition, let's remember that ML aims at *generalization*, and for this goal reaching global optima is not necessary. It may actually be counterproductive and lead to overtraining!

The use of gradual adaptations with simple and local mechanisms permits a close link with neuroscience, although the detailed realization of gradient descent algorithms with real neurons is still a research topic.

Let's note that, after the network is trained, calculating the output from the inputs requires a number of simple operations proportional to the number of weights, and therefore the operation can be extremely fast if the number of weights is limited.

Let us briefly define the notation. We consider the "standard" multilayer perceptron (MLP) architecture, with weights connecting only nearby layers and the sum-of-squared-differences *energy* function defined as:

$$E(w) \;=\; \frac{1}{2}\sum_{p=1}^{P} E_p \;=\; \frac{1}{2}\sum_{p=1}^{P}(t_p \;-\; o_p(w))^2, \tag{10.1}$$

where t_p and o_p are the target and the current output values for pattern p, respectively. The sigmoidal transfer function is $f(x) = 1/(1 + e^{-x})$.

The initialization can be done by having the initial weights randomly distributed in a range. Choosing an initial range, like $(-.5, .5)$ is not trivial, if the weights are too large, the scalar products will be in the saturated areas of the sigmoidal function, leading to gradients close to zero and numerical problems.

In the following sections we present two gradient-based techniques: standard *batch* backpropagation and a version with adaptive learning rate (*bold driver BP*, see [19]), and the on-line stochastic backpropagation of [311].

10.2.1 Batch and "Bold Driver" Backpropagation

The batch backpropagation update is a textbook form of gradient descent. After summing all derivatives related to each example and obtaining the gradient $g_k = \nabla E(w_k)$, the weights at the next iteration $k + 1$ are updated as follows:

$$w_{k+1} = w_k \;-\; \epsilon\; g_k. \tag{10.2}$$

The previous update, with a fixed *learning rate* ϵ, can be considered as a crude version of *steepest descent*, where the exact minimum along the gradient direction is searched at each iteration:

$$w_{k+1} = w_k - \epsilon_k g_k, \tag{10.3}$$

$$\text{where} \quad \epsilon_k \;\text{ minimizes }\; E(w_k - \epsilon g_k). \tag{10.4}$$

An application problem consists of picking a value of the learning rate which is appropriate for a specific learning task, not too small to avoid very long training times (caused by very small modifications of the weights at every iteration) and not too large to avoid oscillations leading to wild increases of the energy function (let's remember that a descent is *guaranteed* only if the step along the gradient tends to zero).

An heuristic proposal for avoiding the choice and for modifying the learning rate while the learning task runs is the **bold driver (BD)** method described in [19]. The learning rate increases exponentially if successive steps reduce the energy, and decreases rapidly if an "accident" is encountered (if E increases), until a suitable value is found. After starting with a small learning rate, its modifications are described by the following equation:

$$\epsilon(t) = \begin{cases} \rho\,\epsilon(t-1), & \text{if } E(w(t)) < E(w(t-1)); \\ \sigma^l\,\epsilon(t-1), & \text{if } E(w(t)) > E(w(t-1)) \text{ using } \epsilon(t-1), \end{cases} \tag{10.5}$$

where ρ is close to one ($\rho = 1.1$) in order to avoid frequent "accidents" because the energy computation is wasted in these cases, σ is chosen to provide a rapid reduction ($\sigma = 0.5$), and l is the minimum integer such that the reduced rate $\sigma^l \epsilon(t-1)$ succeeds in diminishing the energy.

The performance of this self-adaptive *bold driver* backprop is close and usually better than the one obtained by appropriately choosing a *fixed* learning rate. Nonetheless, being a simple form of *gradient descent*, the technique suffers from the common limitation of techniques that use the gradient as a search direction.

10.2.2 On-Line or stochastic backpropagation

Because the energy function E is a sum of many terms, one for each pattern, the gradient will be a sum of the corresponding partial gradients $\nabla E_p(w_k)$, the gradient of the error for the p-th pattern: $(t_p \; - \; o_p(w))^2$.

If one has one million training examples, first the contributions $\nabla E_p(w_k)$ are summed, and the small step is taken.

An immediate option comes to mind: how about taking a small step along a single negative $\nabla E_p(w_k)$ immediately after calculating it? If the steps are very small, the weights will differ by small amounts with respect to the initial ones, and the successive gradients $\nabla E_p(w_{k+j})$ will be very similar to the original ones $\nabla E_p(w_k)$.

If the patterns are taken in a random order, one obtains what is called **stochastic gradient descent**, a.k.a. **online backpropagation**.

By the way, because biological neurons are not very good at complex and long calculations, online backpropagation has a more biological flavor. For example, if a kid is learning to recognize digits and a mistake is done, the correction effort will tend to happen immediately after the recognized mistake, not after waiting to collect thousands of mistaken digits.

The stochastic on-line backpropagation update is given by:

$$w_{k+1} = w_k \; - \; \epsilon \, \nabla E_p(w_k), \tag{10.6}$$

where the pattern p is chosen randomly from the training set at each iteration and ϵ is the learning rate. This form of backpropagation has been used with success in many contexts, provided that an appropriate learning rate is selected by the user. The main difficulties of the method are that the iterative procedure is not guaranteed to converge and that the use of the gradient as a search direction is very inefficient for some problems[3]. The competitive advantage with respect to *batch* backpropagation, where the complete gradient of E is used as a search direction, is that the partial gradient $\nabla E_p(w_k)$ requires only a single forward and backward pass, so that the inaccuracies of the method can be compensated by the low computation required by a single iteration, especially if the training set is large and composed of redundant patterns. In these cases, if the learning rate is appropriate, the actual CPU time for convergence can be small.

Small batches BP is a third compromise option between the batch and online version. In this case, only a stochastic subset (a batch) of B patterns is run forward and back-propagated to accumulate the partial gradient. The weights are therefore modified every B forward passes. Of course, the extreme cases are online BP when B equals one, batch BP when B equals the total number of patterns.

The learning rate must be chosen with care: if ϵ is too small the training time increases without producing better generalization results, while if ϵ grows beyond a certain point the oscillations become gradually wilder, and the uncertainty in the generalization obtained increases.

10.2.3 Advanced optimization for MLP training

As soon as the importance of optimization for machine learning was recognized, researchers began to use techniques derived from the optimization literature that use **higher-order derivatives** information during the search, going *beyond gradient descent*. Examples are conjugate gradient and "secant" methods, i.e., methods that update an approximation of the second derivatives (of the Hessian) in an iterative way by using only gradient information. In fact, it is well

[3] The precise definition is that of *ill-conditioned* problems.

known that taking the gradient as the current search direction produces very slow convergence speed if the Hessian has a large *condition number*. In a pictorial way this corresponds to having "narrow valleys" in the search space leading to a zigzagging path, see Fig. 26.11. Techniques based on second order information are of widespread use in the neural net community, their utility being recognized in particular for problems with a limited number of weights ($<$ 100) and requiring high precision in the output values. A partial bibliography and a description of the relationships between different second-order techniques has been presented in [20]. Two techniques that use second-derivatives information (in an indirect and fast way): the conjugate gradient technique and the one-step-secant method with fast line searches (OSS), are described in [20], [19]. More details will be described in Chapter 26 dedicated to optimization of continuous functions.

Gist

Creating artificial intelligence based on the "real thing" is the topic of artificial neural networks research. **Multilayer perceptron neural networks** (MLPs) are a flexible (non-parametric) modeling architecture composed of layers of sigmoidal units interconnected in a feed-forward manner only between adjacent layers. A unit recognizing the probability of your grandmother appearing in an image can be built with our neural hardware (no surprise) modeled as an MLP network. Effective training from labeled examples can occur via variations of gradient descent, made popular with the term "error backpropagation." The weakness of gradient descent as optimization method does not prevent successful practical results.

There are indeed striking analogies between human and artificial learning schemes. In particular, increasing the effort during training pays dividends in terms of improved generalization. The effort with a serious and demanding teacher (diversifying test questions, writing on the blackboard, asking you to take notes instead of delivering pre-digested material) can be a pain in the neck during training but increases the power of your mind at later stages of your life. The German philosopher Hegel was using the term *Anstrengung des Begriffs* ("effort to define the concept") when defining the role of Philosophy.

Chapter 11

Deep and convolutional networks

As a single footstep will not make a path on the earth,
so a single thought will not make a pathway in the mind.
To make a deep physical path, we walk again and again.
To make a deep mental path, we must think over and over
the kind of thoughts we wish to dominate our lives.
(Henry David Thoreau)

In this period machine learning is experiencing a soft revolution, in which ideas born a long time ago enjoy a second youth. Deep learning and convolutional networks are a promising direction, but we consider also alternative and crucially different directions like reservoir and extreme computing in the next chapters.

An anecdote tells that a team of graduate students led by Professor Geoffrey E. Hinton decided to enter a contest at the last minute with a deep learning system developed with no specific domain knowledge and won the top prize in 2012. The system had to predict which molecule was most likely to be an effective medicine. Today many advanced applications of computer vision and speech recognition are based on deep networks.

This chapter presents **deep neural networks** and **convolutional networks**. The long-term dream of deep networks is that of developing intelligent systems in a completely automated manner directly from abundant data (both labeled and unlabeled), without human experts to extract useful features by hand before the system is trained. The plan is to have a hierarchy of levels in a feedforward network, self-organized so that the first layers extract basic building blocks (features) which are then combined to obtain more and more complex features in the subsequent layers (for example, features invariant under translation or rotation in image processing). **Convolutional networks** deal with **pre-wiring** an architecture which is appropriate for a domain (typically computer vision and speech processing), by inserting constraints, like locality of receptive fields, and by sharing weights. In our visual system and in image processing, basic local filtering operations like contrast enhancement or edge detection are applied over the entire image. It would be a waste of resources to ask ML to identify a different filter for every pixel and it would be masochistic to forget that the system is dealing with images, with a two-dimensional structure and local relationships.

11.1 Deep neural networks

There is abundant evidence from neurological studies that our brain develops higher-level concepts in stages, by first extracting **multiple layers of useful and gradually more complex representations**. In order to recognize your grandmother, first simple elements are detected in the visual cortex, like image edges (abrupt changes of intensity), then progressively higher-level concepts like eyes, mouth, and complex geometrical features, independently on the specific position in the image, illumination, colors, etc.

The fact that one hidden layer in MLPs is sufficient for the *existence* of a suitable approximation does not mean that *building* this approximation will be easy, requiring a small number of examples and a small amount of CPU time. In addition to neurological evidence in our brain, theoretical arguments demonstrate that some classes of input-output mappings are much easier to build when more hidden layers are considered [47].

The dream of ML research is to feed examples to an MLP with many hidden layers and have the MLP **automatically develop internal representations**, the activation patterns of the hidden-layer units. The training algorithm should determine the weights interconnecting the lower levels, closer to the sensory input, so that representations in the intermediate levels correspond to "concepts" which will be useful for the final complex classification task. Think about the first layers developing "nuggets" of useful regularities in the data.

This dream has some practical obstacles. When backpropagation is applied to an MLP network with many hidden layers, the partial derivatives associated to the weights of the first layers tend to be very small, and therefore subject to numerical estimation problems. This is easy to understand[1]: if one changes a weight in the first layers, the effect will be propagated upwards through many layers and it will tend to be confused among so many effects by hundreds of other units. Furthermore, saturated units (with output in the flat regions of the sigmoid) will squeeze the change so that the final effect on the output will be very small. In some cases internal representations in the first layers will not differ too much from what can be obtained by setting the corresponding weights randomly, and leaving only the topmost levels to do some "useful" work. From another point of view, when the number of parameters is very large with respect to the number of examples (and this is the case of deep neural networks) overtraining becomes more dangerous, it will be too easy for the network to accommodate the training examples without being forced to extract the relevant regularities, those essential for generalizing.

In the nineties, these difficulties shifted the attention of many users towards "simpler" models, based on linear systems with additional constraints, like the Support Vector Machines considered in Chapter 12.

More recently, a revival of **deep neural networks** (MLPs with many hidden layers) and more powerful training techniques brought deep learning to the front stage, leading to superior classification results in challenging areas like speech recognition, image processing, molecular activity for pharmaceutical applications. Deep learning **without any *ad hoc* feature engineering** (handcrafting of new features by using knowledge domain and preliminary experiments) lead to winning results and significant improvements over the state of the art [47].

The main scheme of the latest applications is as follows:

1. use unsupervised learning from many unlabeled examples to prepare the deep network in an initial state (**unsupervised pre-training**);

[1] If you are not familiar with partial derivatives, think about changing a weight by a small amount Δw and calculating how the output changes (Δf). A partial derivative is the limit of the ratio $\Delta f / \Delta w$ when the magnitude of the change Δw goes to zero.

2. use backpropagation only for the final tuning with the set of labeled examples, after starting from the initial network trained in an unsupervised manner.

The scheme is very powerful when the number of unlabeled (unclassified) examples is much larger than the number of labeled ones, and the classification process is costly. For examples, collecting huge numbers of unlabeled images by crawling the web is now very simple. Labeling them by humans to describe image content costs much more. The unsupervised system is in charge of extracting useful building blocks, like detectors for edges, for blobs, for textures of different kinds, in general, building blocks which appear in real images and not in random "broken TV screen" patterns.

11.1.1 Auto-encoders

An effective way to build internal representations in an unsupervised manner is through auto-encoders. One builds a network with a hidden layer and demands that the output simply reproduces the input. It sounds silly and trivial at first, but interesting work gets done when one squeezes the hidden layer, and therefore demands that the original information in the input is compressed into **an encoding $c(\boldsymbol{x})$ with less variables than the original ones** (Fig. 11.1). For sure, this compression will not permit a faithful reconstruction of *all* possible inputs. But this is positive for our goals: the internal representation $c(\boldsymbol{x})$ will be forced to discover regularities in the specific input patterns shown to the system, to extract useful and significant information from the original input.

For example, if images of faces are presented, some internal units will specialize to detect edges, other maybe will specialize to detect eyes, and so on.

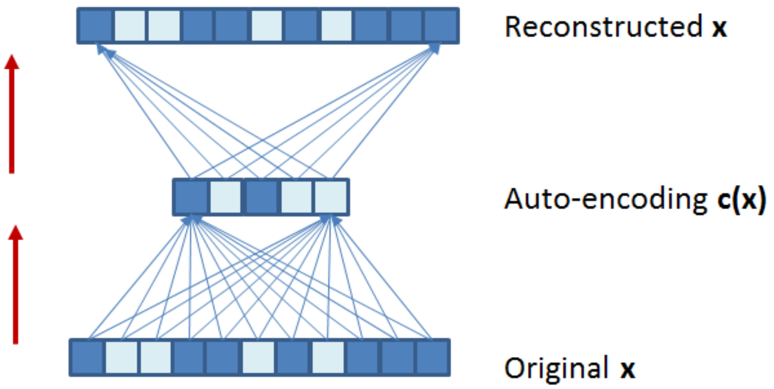


Figure 11.1: Auto-encoder.

The auto-encoder can be trained by backpropagation or variations thereof. Classification labels are not necessary. If the original inputs are labeled for classification, the labels are simply forgotten by the system in this phase. In addition, tons of unlabeled examples can be added for a more robust training (with better generalization) of the auto-encoder.

After the auto-encoder is built one can now transplant the hidden layer structure (weights and hidden units) to a second network intended for classification (Fig. 11.2), add an additional layer (initialized with small random weights),

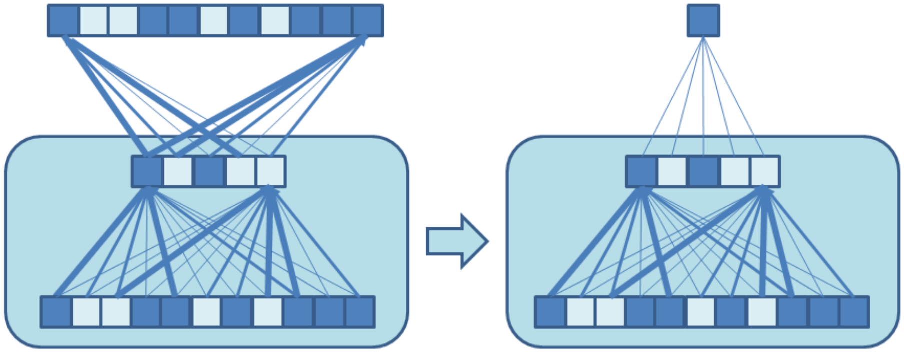


Figure 11.2: Using an auto-encoder trained from unlabeled data to initialize an MLP network.

and consider this “Frankenstein monster” network as the starting point for a final training phase intended to realize a classifier. In this final phase only a set of labeled pattern is used.

In many significant applications the final network has a better generalization performance than a network which could be obtained by initializing randomly all weights. Let’s note that the same properly-initialized network can be used for different but related supervised training tasks. The network is initialized in the same manner, but different labeled examples are used in the final tuning phase. **Transfer learning** is the term related to using knowledge gained while solving one problem and applying it to a different but related problem. For example, knowledge gained while learning to recognize people faces could apply when recognizing monkeys.

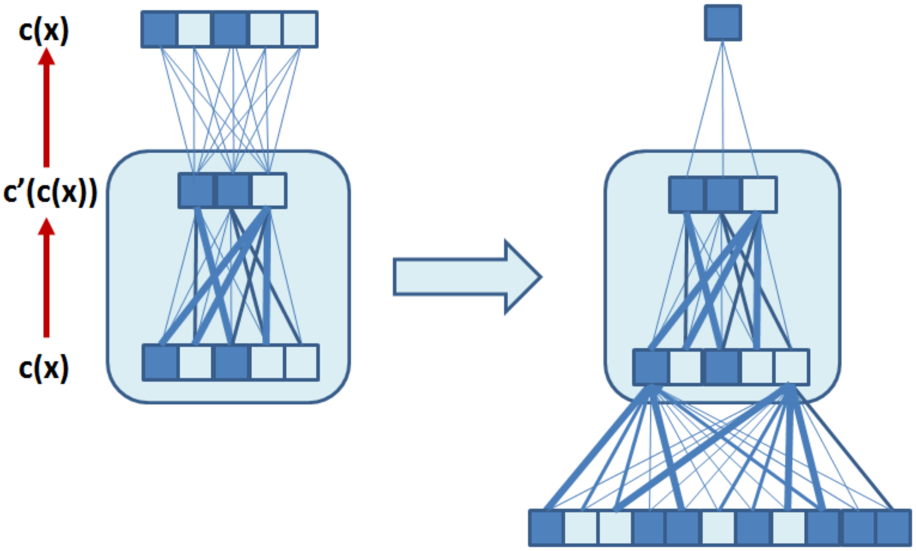


Figure 11.3: Recursive training of auto-encoders to build deeper networks.

The attentive reader may have noticed that up to now only one hidden layer has been created. But we can easily produce a chain of subsequent layers by iterating, compressing the first code $c(\boldsymbol{x})$, again by auto-encoding it, to develop a second more compressed code and internal representation $c'(c(\boldsymbol{x}))$. Again, the developed auto-encoding weights can be used to initialize the second layer of the network, and so on (Fig. 11.3).

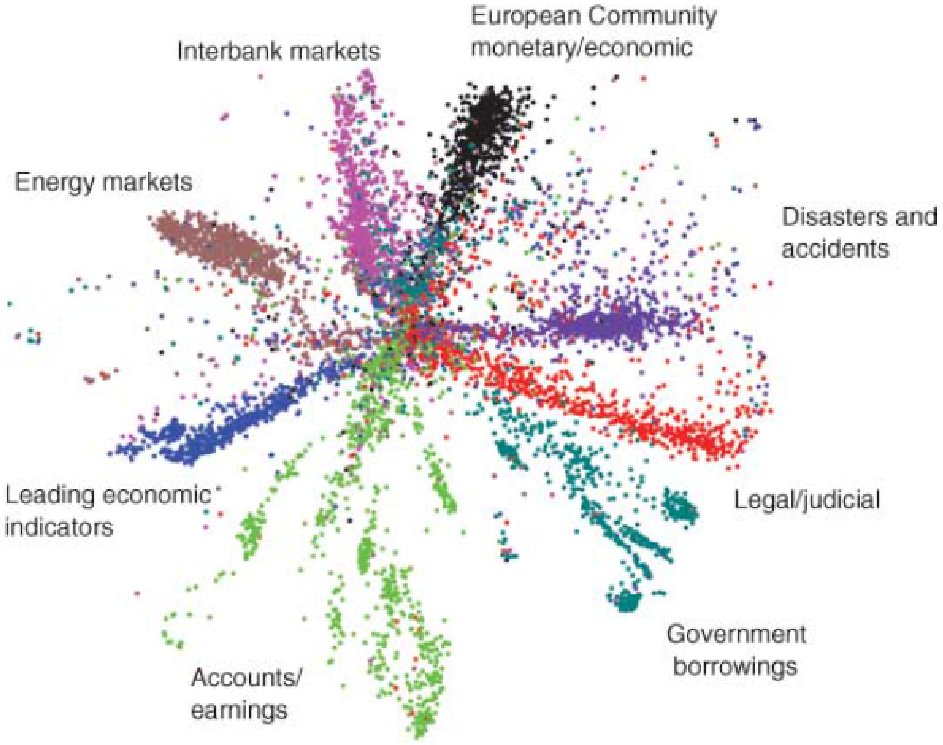


Figure 11.4: The codes produced by a 2000- 500-250-125-2 autoencoder on news stories by Reuters. Clusters corresponding to different topics, with different colors, are clearly visible (details in [181]).

In addition to being useful for pre-training neural networks, very **deep auto-encoders can be useful for visualization and clustering**. For example, news stories by Reuters[2] represented as a vector of document-specific probabilities of the 2000 commonest word stems, can be auto-encoded so that the bottleneck compressed layer contains only two units. The two-dimensional coordinates corresponding to story are visualized on a two-dimensional plane in Fig. 11.4. Different clusters approximately corresponding to the different topics are clearly visible in the two-dimensional space, the two (or more) coordinates in the bottleneck layer can therefore be used for clustering objects.

The optimal number of layers and the optimal number of units in the pyramidal structure is still a research topic, but appropriate numbers can be obtained pragmatically by using some form of cross-validation to select appropriate meta-parameters. More details in [47].

[2] The Reuter Corpus Volume 2 is available at http:// trec.nist.gov/data/reuters/reuters.html.

11.1.2 Random noise, dropout and curriculum

Now that you are getting excited about the idea of combining unsupervised pre-training with supervised final tuning to get deep and deeper network, so that less and less hand-made feature engineering will be required for state-of-the art performance, let's mention some more advanced possibilities which are now being transferred from pure research to the first real-world applications.

The first possibility has to do with injecting controlled amount of noise into the system [369] (**denoising auto-encoders**). The starting idea is very simple: corrupt each pattern $\boldsymbol{x}$ with random noisy (e.g., if the pattern is binary, flip the value of each bit with a given small probability) and ask the auto-encoding network to reconstruct the original noise-free pattern $\boldsymbol{x}$, to *denoise* the corrupted versions of its inputs. The task becomes more difficult, but asking the system to go the extra mile encourages it to extract even stronger and more significant regularities from the input patterns. This version bridges the performance gap with deep belief networks (DBN), another way to pre-train networks [180, 181], and in several cases surpasses it. Biologically, there is indeed *a lot* of noise in the wet brain matter. These results demonstrate that noise can in fact have a positive impact on learning!

Another way to make the learning problem harder but to increase generalization (by reducing overfitting) is through **random dropout** [182]: during stochastic backpropagation training, after presenting each training case, each hidden unit is randomly omitted from the network with probability 0.5. In this manner, complex co-adaptation on training data is avoided. Each unit cannot rely on other hidden units being present and is encouraged to become a detector identifying useful information, independently on what the other units are doing.

Interestingly, there is an intriguing similarity between dropout and the role of sex in evolution. One possible interpretation is that sex breaks up sets of co-adapted genes. Achieving a function by using a large set of co-adapted genes is not nearly as robust as achieving the same function, in multiple alternative ways, each of which only uses a small number of co-adapted genes. This allows evolution to avoid dead-ends in which improvements in fitness require coordinated changes to a large number of co-adapted genes. It also reduces the probability that small changes in the environment will cause large decreases in fitness a phenomenon similar to the "overfitting" in the field of ML [182].

In a way, randomly dropping some units is related to using different network architectures at different times during training, and then averaging their results during testing. Using ensembles of different networks is another way to reduce overtraining and increasing generalization, as it will be explained in future chapters. With random dropout the different networks are contained in the same complete MLP network (they are obtained by activating only selected parts of the complete network).

Another possibility to improve the final result when training MLP is through **curriculum learning** [48]. As in the human case, training examples are not presented to the network at the same time but in stages, by starting from the easiest cases first and then proceeding to the more complex ones. For example, when learning music, first the single notes are learned, then more complex symphonies. Pre-training by auto-encoding can be considered a preliminary form of curriculum learning. The analogy with the learning of languages is that first the learner is exposed to a mass of spoken material in a language (for example by placing him in front of a foreign TV channel). After training the ear to be tuned to characteristic utterances of the given spoken language, the more formal phase of training by translating phrases is initiated.

After all, magic systems for learning languages while you sleep and listen to recorded voices may not be a complete fraud :)

11.2 Local receptive fields and convolutional networks

Advanced animal brains are quick in learning how to process images and to recognize their content. An infant recognizes his mother already in the first days of life. This speed would be impossible without the help of a **pre-wired architecture** already available to process two-dimensional images. In particular, locality plays a big role: the first neurons which process nearby points in an image projected to the retina have local receptive fields and are mapped to nearby points in the visual cortex. Specialized low-level detectors like edge or movement detectors are available in biological brains.

Figure 11.5: *Bufo Bufo*, the common toad, was used in studies of toad form vision. Feature detectors in a frog retina are hard-wired and specialized to detect a fly at the distance that the frog could strike.

For example, when analyzing “on-off” ganglion cells in frogs – responding to both the transition from light to dark and from dark to light – with very restricted receptive fields (about the size of a fly at the distance that the frog could strike), it is difficult to avoid the conclusion that the ‘on-off’ units are matched to the stimulus and act as fly detectors [16] (Fig. 11.5).

When considering artificial neural networks, there is little doubt that recognizing images can be greatly simplified if some knowledge about image processing is pre-wired in the neural network. Only a masochist would forget the two-dimensional structure of the image and provide as input a one-dimensional array of pixel values at randomly scattered positions (if not convinced, apply a random permutation to the pixels of this page and try reading it).

In traditional models of pattern recognition, hand-designed features extract relevant information from the input and eliminates irrelevant variabilities. A trainable classifier like a MLP can then categorize the resulting feature vectors into classes. A potentially more interesting scheme is to eliminate the feature extractor, feeding the network with raw inputs, and to rely on back-propagation to turn the first few layers into an appropriate feature extractor. This brute-force approach faces difficulties related to the very large input dimension (causing many weights and possible over-training) and to the absence of any **built-in invariance** with respect to translations, rotations or local distortions of the inputs. For a frog, a fly remains a fly even if rotated and translated.

In principle, a sufficiently large fully-connected network could learn to produce outputs that are invariant with respect to such variations. However, learning such a task would probably result in multiple units with similar weight patterns positioned at various locations in the input. In **convolutional neural networks** (CNN) [249], some shift invariance is automatically obtained by forcing the replication of weight configurations across space. A kernel with local connectivity in the image plane is repeated at different positions in the image (the **weights are shared**). Local correlations are the reasons for the well-known advantages of extracting and combining local features before recognizing spatial or temporal objects. Convolutional networks force the extraction of local features by restricting the receptive fields of hidden units to be local.

The mathematical operation of applying the same local filter at different spatial positions is called **convolution**.

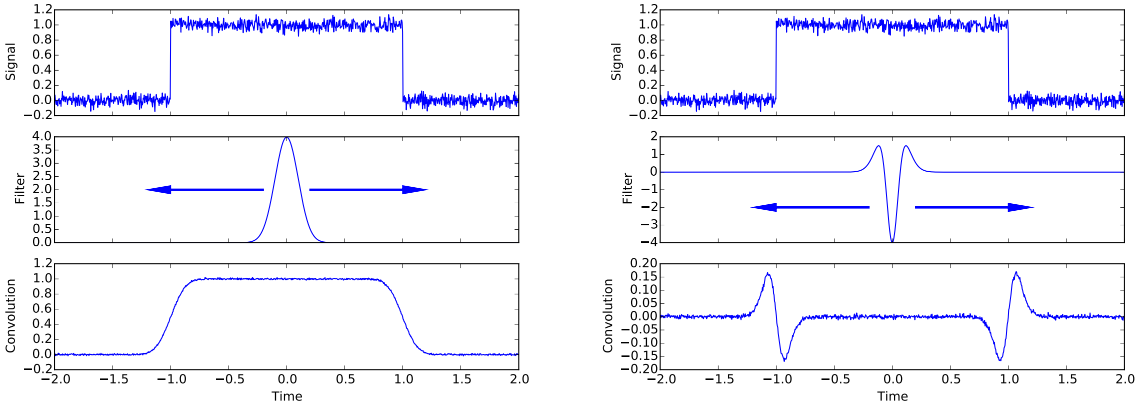


Figure 11.6: Two examples of convolution. Left: Gaussian smoothing; right: DoG border enhancement.

The use of localized kernels to extract local features is well exemplified by signal processing, where convolution is one of the most important mathematical tools. Fig. 11.6 shows two typical examples. On the left, a noisy signal is filtered by convolution with a Gaussian kernel; the outcome is a smoother version of the original signal. The procedure is called *blurring* (in computer vision), *low-pass filtering or de-noising* (signal processing), *smoothing out*. Mathematically, given a signal $s(t)$ and a filter $f(t)$, the convolution operation is given by

$$s * f(t) = \int_{-\infty}^{+\infty} s(x)f(t-x)\,\mathrm{d}x. \tag{11.1}$$

In other words, the filtering kernel f "sweeps" the signal by a weighted integral. If the Gaussian kernel has unit area, the result is a weighted average of the original signal. On the right of Fig. 11.6, a more interesting example uses the difference between two Gaussian kernels with different amplitudes. Two blurred versions of the signal with different smoothing windows are subtracted. The resulting kernel is called **Difference of Gaussians** (DoG), and its application highlights the points in which the signal has sudden, significant changes.

The convolution formula (11.1) can be easily extended in two dimensions and discretized for use in neural networks. To this aim, let x_{ij} be the pixels of an $m \times n$ image. The filtering kernel will be represented by an $(2r+1) \times (2r+1)$ matrix of weights w_{ij}, where the *radius* r is usually very small. Convolution produces a new $m \times n$ image whose pixels y_{ij} are

$$y_{ij} = \sum_{h=0}^{2r}\sum_{k=0}^{2r} w_{hk}x_{i+r+1-h,j+r+1-k}. \tag{11.2}$$

In the formula we assume that indices are zero-based. In order to obtain a resulting image of the same size as the original, we must also assume that the original image has an r-sized border in all directions; as an alternative, the resulting image will be smaller by r pixels in all directions.

Observe the "$t - x$" in equation (11.1): to retain many useful mathematical properties the convolution operator requires the two functions to be swept in opposite directions, as reproduced in (11.2). Most software packages can be configured to work either this way, or by having the kernel and the input swept in the same direction. In the latter case, the network is said to operate in *cross-correlation* mode, and the result is a proper inner product. The only actual difference between the two modes is the order in which the weights are stored, moving between the two representations only requires a 180° rotation of the kernels. In other terms, a convolution layer takes the inner product of the linear filter and the underlying receptive field.

Convolutional networks combine three ingredients to ensure some degree of shift and distortion invariance: **local receptive fields, shared weights** (or weight replication), and, sometimes, spatial or temporal subsampling (**pooling**).

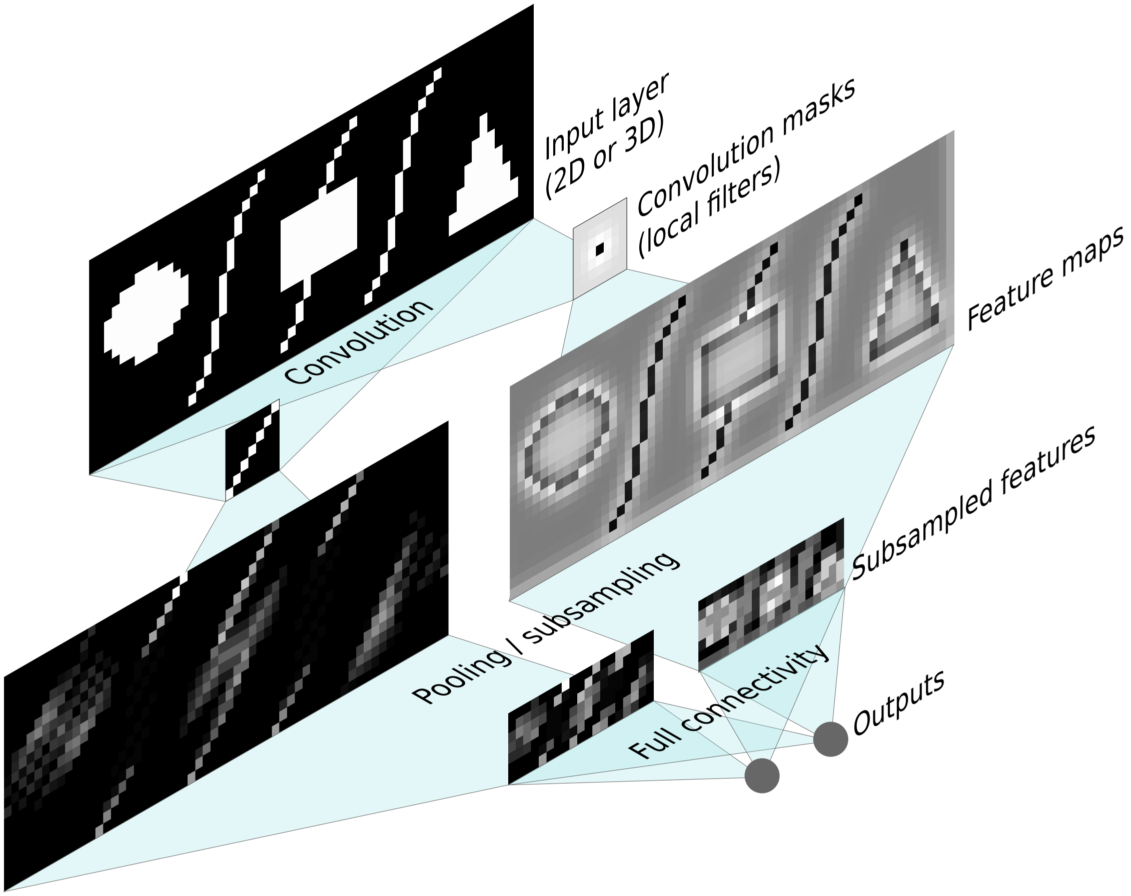


Figure 11.7: Basic convolutional network: the inputs (image pixels) are swept by a convolution operation against a small set of input weights acting as local feature extractors. The resulting feature maps are subsampled by a pooling operation, and the smaller set of neurons is passed through a traditional, completely connected output layer.

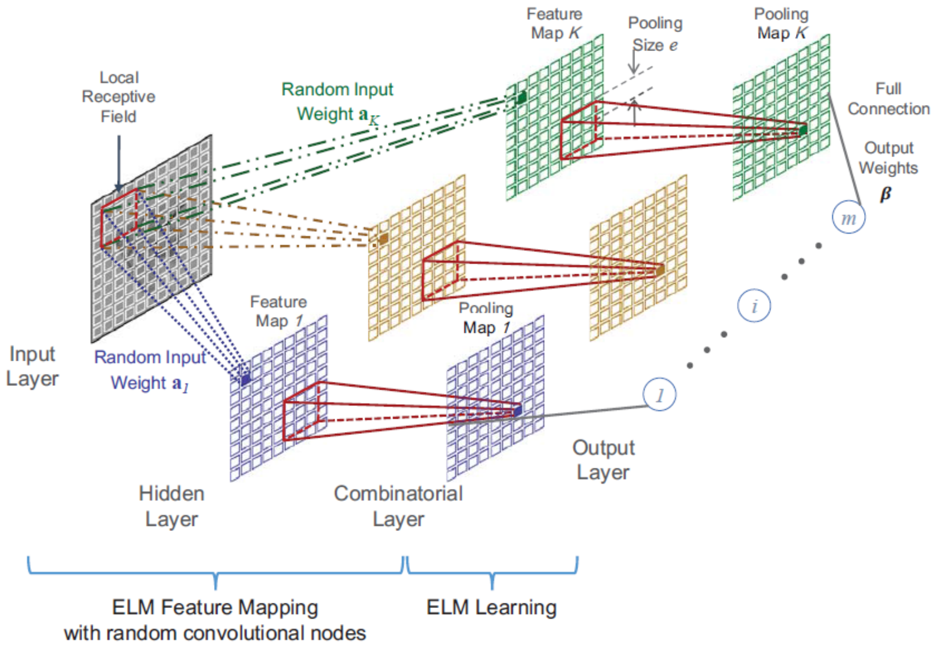


Figure 11.8: A structured architecture with local receptive fields (convolutional) and pooling layers (adapted from [165]).

As shown in Fig. 11.7, by applying the same local receptive fields throughout the image, neurons can extract elementary visual features such as oriented edges, end-points, corners, or similar patterns in speech spectrograms. These features are then combined by the higher layers.

The outputs of a set of neurons with shared weights, replicated at different points in the image, is called a **feature map**, obtained by convolution followed by a nonlinear activation function at every local portion of the input. In the upper portion of Fig. 11.7, an input image is "swept" by two filters, generating two feature maps whose neurons are more or less activated by the presence of the corresponding feature in the local receptive field. In the example, one filter has specialized to recognize slanted lines, the other has learned to enhance borders *à la* DoG.

Usually, each **convolutional layer** is followed by an additional **pooling layer** (see the bottom part of Fig. 11.7) which performs a local averaging and a sub-sampling, reducing the resolution of the feature map, and therefore reducing the sensitivity of the output to shifts and distortions. In its basic form, a pooling layer divides each feature layer into non-overlapping rectangles and applies a simple "summarizing" operation to each rectangle's pixels. Common operations are:

- the maximum value among all pixels in the rectangle (*max-pooling*);
- the average of pixel values in the rectangle (*average-pooling*);
- the square root of the sum of all squared pixel values (i.e., the *Frobenius norm* of the rectangle).

Deeper architectures can implement a cascade of convolutional and pooling layers, possibly enhancing the robustness of the output by means of other schemes such as the random dropout technique discussed in Section 11.1.2. Once the number of neurons is small enough, fully connected feed-forward layers complete the network.

Convolutional neural networks are still a hot research topic and a state-of-the-art tool for complex image and speech processing tasks, far too wide to be reviewed in this book. An example of the layered and structured architecture considered is shown in Fig. 11.8, for the recent proposal of randomly created weights for the units in the first layers [165]. The authors of [253] propose a kind of "fractal" network-in-network architecture, building micro neural networks with more complex structures to abstract the data within the receptive field (going beyond the linear scalar product between filter coefficients and image pixels in traditional CNN). The micro neural networks (MLPs) are then replicated over the image.

Gist

Deep neural networks composed of many layers are becoming effective (and superior to Support Vector Machines) through appropriate learning schemes, consisting of an unsupervised preparatory phase followed by a final tuning phase by using the scarce labeled examples.

Among the ways to improve generalization, the use of **controlled amounts of noise during training** is effective (noisy auto-encoders, random dropout). If you feel some noise and confusion in your brain, relax, it can be positive after all.

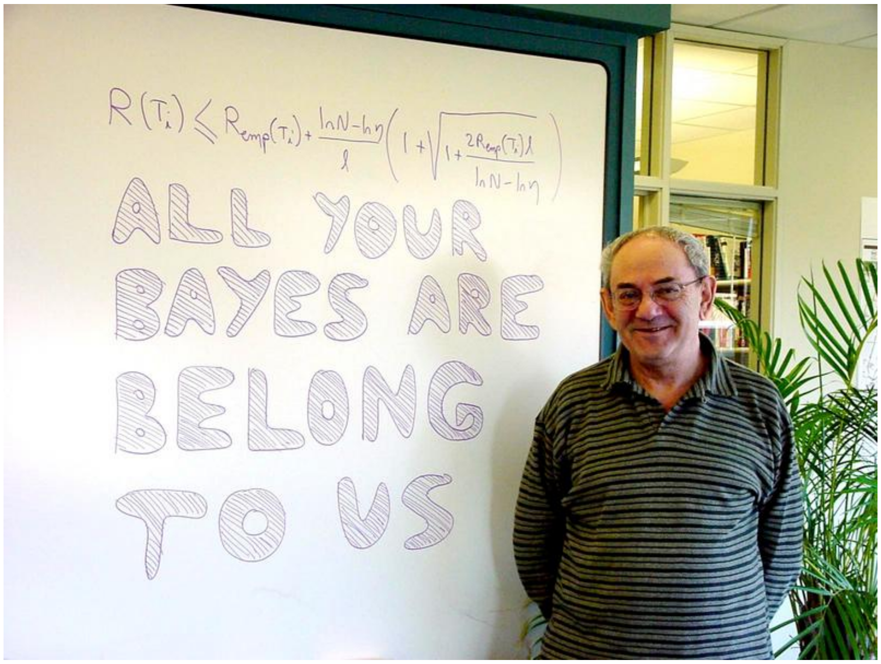
Convolutional neural networks are a good example of an idea inspired by biology that results in competitive engineering solutions and suggest **pre-wired architectures** with domain knowledge embedded in it.

Neural networks are like a glacial lake. You dive into the water, but you can't see how deep they are going to be.

Chapter 12

Statistical Learning Theory and Support Vector Machines (SVM)

Sembravano traversie ed eran in fatti opportunità.
They seemed hardships and were in fact opportunities.
(Giambattista Vico)


$R(T_i) \leqslant R_{emp}(T_i) + \frac{\ln N - \ln \eta}{l}\left(1 + \sqrt{1 + \frac{2R_{emp}(T_i)\,l}{\ln N - \ln \eta}}\right)$
ALL YOUR
BAYES ARE
BELONG
TO US

The order of chapters in this book has some connections with the history of machine learning[1]. Before 1980, most learning methods concentrated either on symbolic "rule-based" expert systems, or on simple sub-symbolic *linear discrimination* techniques, with clear theoretical properties. In the eighties, decision trees and neural networks paved the way to efficient learning of *nonlinear* models, but with little theoretical basis and naive optimization techniques based on gradient descent.

[1] The photo of prof. Vapnik is from Yann LeCun website *Vladimir Vapnik meets the video games sub-culture* at `http://yann.lecun.com/ex/fun/index.html#allyourbayes`

In the nineties, efficient learning algorithms for nonlinear functions based on statistical learning theory developed, mostly through the seminal work by Vapnik and Chervonenkis. **Statistical learning theory** (SLT) deals with fundamental questions about *learning from data*. Under which conditions can a model learn from examples? How can the measured performance on a set of examples lead to bounds on the generalization performance?

These theoretical results are everlasting, although the conditions for the theorems to be valid are almost impossible to check for most practical problems. In another direction, the same researchers proposed a resurrection of **linear separability** methods, with additional ingredients intended to improve generalization, with the name of **Support Vectors Machines (SVM)**.

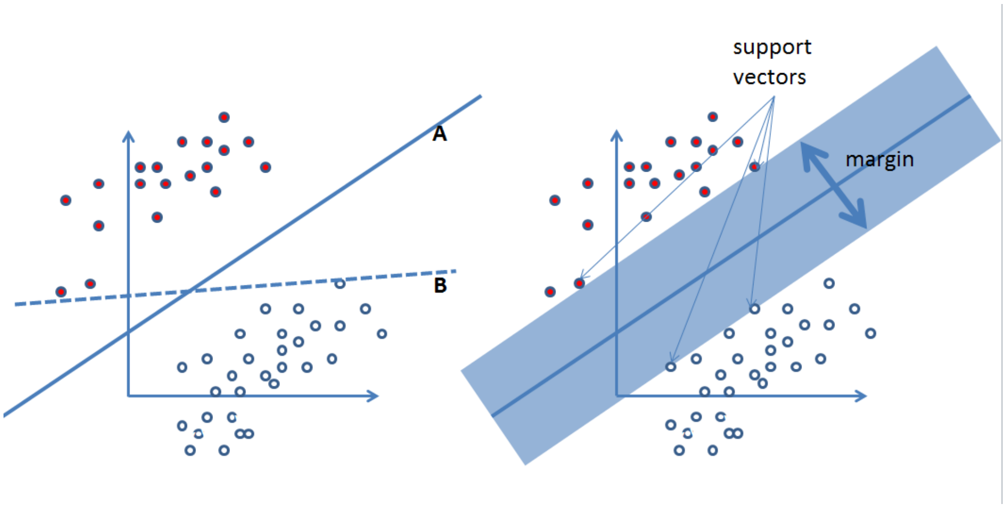


Figure 12.1: Explaining the basis of Support Vectors Machines. The *margin* of line A is larger than that of line B. A large margin increases the probability that new examples will fall in the right side of the separator line. *Support vectors* are the points touching the widest possible margin.

The term SVM sounds technical but the rationale is simple to grasp. Let's consider the two classes (dark and bright dots) in Fig. 12.1 (left) and the two possible lines A and B. They both linearly-separate the examples and can be two results of a generic ML scheme to separate the labeled training data. The difference between the two is clear when thinking about *generalization*. When the trained system will be used, new examples from the two classes will be generated with the same underlying probability distribution. Two clouds with a similar shape will be produced, but, for the case of line B, the probability that some of the new points will fall on the *wrong* side of the separator is bigger than for line A. Line B is passing very close to some training examples, it makes it just barely to separate them. Line A has the biggest possible distance from the examples of the two classes, it has the largest possible "safety area" around the boundary, a.k.a. *margin*. SVMs are **linear separators with the largest possible margin**, and the *support vectors* are the ones touching the safety *margin* region on both sides (Fig. 12.1, right). We encountered a similar issue with linear models for classification and least-squares (Section 4.3). Lest-squares minimizes the average squared error, SVMs minimize the maximum distance but the objective of a robust and safe boundary between classes is shared.

Asking for the maximum-margin linear separator leads to standard **Quadratic Programming (QP)** problems, which can be solved to optimality for problems of reasonable size. QP is the problem of optimizing a quadratic function of several variables subject to linear constraints on these variables. The issue with local minima potentially dangerous for MLP — Because local minima can be very far from global optima — disappears and this makes users feel relaxed. As you may expect, there's no rose without a thorn, and complications arise if the classes are *not* linearly separable. In this case one first applies **a nonlinear transformation** ϕ to the points so that they become (approximately) linearly separable. Think of ϕ as building appropriate features so that the transformed points $\phi(\boldsymbol{x})$ of the two classes *are* linearly separable. The nonlinear transformation has to be handcrafted for the specific problem, no general-purpose transformation is available.

To discover the proper ϕ, are we back to feature extraction and feature engineering? In a way yes, and after transforming inputs with ϕ, the **features in SVM are all similarities between an example to be recognized and the training examples**[2]. A critical step of SVM, which has to be executed by hand through some form of cross-validation, is to identify which similarity measures are best to learn and generalize, an issue related to selecting the so-called **kernel functions**.

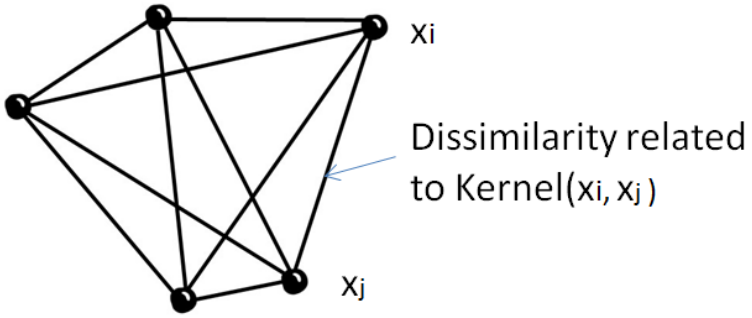


Figure 12.2: Initial information for SVM learning are similarity values between couples of input points $K(\boldsymbol{x}_i, \boldsymbol{x}_j)$, where K is known as *kernel function*. These values, under some conditions, can be interpreted as scalar products obtained after mapping the initial inputs by a nonlinear function $\phi(\boldsymbol{x})$, but the actual mapping does not need to be computed, only the kernel values are needed ("kernel trick").

SVMs can be seen as a way to **separate two concerns**: that of identifying a proper way of **measuring similarities** between input vectors, the *kernel functions* $K(\boldsymbol{x}, \boldsymbol{y})$, and that of **learning a linear architecture** to combine the outputs on the training examples, weighted by the measured similarities with the new input example. As expected, more similar input examples contribute more to the output, as in the more primitive nearest-neighbors classifiers encountered in Chapter 2. This is the way to grasp formulas like:

$$\sum_{i=1}^{\ell} y_i \lambda_i^* K(\boldsymbol{x}, \boldsymbol{x}_i),$$

(ℓ is the number of training examples, y_i is the output on training example $\boldsymbol{x}_i$, $\boldsymbol{x}$ is the new example to be classified) that we will encounter in the following theoretical description. Kernels calculate *dot products* (scalar products) of data points mapped by a function $\phi(\boldsymbol{x})$ without actually calculating the mapping, this is called the "**kernel trick**" (Fig. 12.2):

$$K(\boldsymbol{x}, \boldsymbol{x}_i) = \boldsymbol{\varphi}(\boldsymbol{x}) \cdot \boldsymbol{\varphi}(\boldsymbol{x}_i).$$

A symmetric and positive semi-definite *Gram Matrix* containing the kernel values for couples of points fuses information about data and kernel[3]. Estimating a proper *kernel matrix* from available data, one that will maximize generalization results, is an ongoing research topic.

Now that the overall landscape is clear, let's plunge into the mathematical details. Some of these details are quite complex and difficult to grasp. Luckily, you will not need to know the demonstration of the theorems to use SVMs, although a knowledge of the main math results will help in selecting meta-parameters, kernels, etc.

[2] Actually only *support vectors* will give a non-zero contribution.

[3] Every similarity matrix can be used as kernel, if it satisfies Mercer's theorem criteria.

12.1 Empirical risk minimization

We mentioned before that minimizing the error on a set of examples is not the only objective of a statistically sound learning algorithm, also the modeling architecture has to be considered. **Statistical Learning Theory** provides mathematical tools for *deriving unknown functional dependencies* on the basis of observations.

A **shift of paradigm** occurred in statistics starting from the sixties: previously, following Fisher's research in the 1920–30s, in order to derive a functional dependency from observations one had to know the detailed form of the desired dependency and to determine only the values of a finite number of *parameters* from the experimental data. The new paradigm does not require the detailed knowledge, and proves that some general properties of the set of functions to which the unknown dependency belongs are sufficient to estimate the dependency from the data. **Nonparametric techniques** is a term used for these flexible models, which can be used even if one does not know a detailed form of the input-output function. The MLP model described before is an example.

A brief summary of the main methodological points of Statistical Learning Theory is useful to motivate the use of Support Vector Machines (SVM) as a learning mechanism. Let $P(\boldsymbol{x}, y)$ be the unknown probability distribution from which the examples are drawn. The learning task is to learn the mapping $\boldsymbol{x}_i \to y_i$ by determining the values of the parameters of a function $f(\boldsymbol{x}, \boldsymbol{w})$. The function $f(\boldsymbol{x}, \boldsymbol{w})$ is called *hypothesis*, the set $\{f(\boldsymbol{x}, \boldsymbol{w}) : \boldsymbol{w} \in \mathcal{W}\}$ is called the *hypothesis space* and denoted by $\mathcal{H}$, and $\mathcal{W}$ is the set of abstract parameters. A choice of the parameter $\boldsymbol{w} \in \mathcal{W}$, based on the labeled examples, determines a "trained machine."

The *expected test error* or *expected risk* of a trained machine for the classification case is:

$$R(\boldsymbol{w}) = \int \|y - f(\boldsymbol{x}, \boldsymbol{w})\| \, \mathrm{d}P(\boldsymbol{x}, y), \tag{12.1}$$

while the *empirical risk* $R_{\text{emp}}(\boldsymbol{w})$ is the mean error rate measured on the training set:

$$R_{\text{emp}}(\boldsymbol{w}) = \frac{1}{\ell} \sum_{i=1}^{\ell} \|y_i - f(\boldsymbol{x}_i, \boldsymbol{w})\|. \tag{12.2}$$

The classical learning method is based on the **empirical risk minimization** (ERM) inductive principle: one approximates the function $f(\boldsymbol{x}, \boldsymbol{w}^*)$ which minimizes the risk in (12.1) with the function $f(\boldsymbol{x}, \hat{\boldsymbol{w}})$ which minimizes the empirical risk in (12.2).

The rationale for the ERM principle is that, if R_{emp} converges to R in probability (as guaranteed by the law of large numbers), the minimum of R_{emp} may converge to the minimum of R. If this does not hold, the ERM principle is said to be *not consistent*.

As shown by Vapnik and Chervonenkis, consistency holds if and only if convergence in probability of R_{emp} to R is *uniform*, meaning that as the training set increases the probability that $R_{\text{emp}}(\boldsymbol{w})$ approximates $R(\boldsymbol{w})$ uniformly tends to 1 on the whole $\mathcal{W}$. Necessary and sufficient conditions for the consistency of the ERM principle is the finiteness of the **Vapnik-Chervonenkis dimension (VC-dimension)** of the hypothesis space $\mathcal{H}$.

The VC-dimension of the hypothesis space $\mathcal{H}$ is, loosely speaking, the largest number of examples that can be separated into two classes in all possible ways by the set of functions $f(\boldsymbol{x}, \boldsymbol{w})$. The VC-dimension h measures the **complexity and descriptive power of the hypothesis space** and is often proportional to the number of free parameters of the model $f(\boldsymbol{x}, \boldsymbol{w})$.

Vapnik and Chervonenkis provide **bounds on the deviation of the empirical risk from the expected risk**. A bound that holds with probability $1 - p$ is the following:

$$R(\boldsymbol{w}) \leq R_{\text{emp}}(\boldsymbol{w}) + \sqrt{\frac{h\left(\ln \frac{2\ell}{h} + 1\right) - \ln \frac{p}{4}}{\ell}} \quad \forall \boldsymbol{w} \in \mathcal{W}.$$

By analyzing the bound, and neglecting logarithmic factors, in order to obtain a small expected risk, both the empirical risk *and* the ratio h/ℓ between the VC-dimension of the hypothesis space and the number of training examples have to be small. In other words, a valid generalization after training is obtained if the hypothesis space is sufficiently powerful to allow reaching a small empirical risk, i.e., to learn correctly the training examples, but not too powerful to simply memorize the training examples without extracting the structure of the problem. For a larger model flexibility, a larger number of examples is required to achieve a similar level of generalization.

The choice of an appropriate value of the VC-dimension h is crucial to get good generalization performance, especially when the number of data points is limited.

The method of **structural risk minimization** (SRM) has been proposed by Vapnik based on the above bound, as an attempt to overcome the problem of choosing an appropriate value of h. For the SRM principle one starts from a nested structure of hypothesis spaces

$$\mathcal{H}_1 \subset \mathcal{H}_2 \subset \cdots \subset \mathcal{H}_n \subset \cdots \tag{12.3}$$

with the property that the VC-dimension $h(n)$ of the set $\mathcal{H}_n$ is such that $h(n) \leq h(n+1)$. As the subset index n increases, the minima of the empirical risk decrease, but the term responsible for the confidence interval increases. The SRM principle chooses the subset $\mathcal{H}_n$ for which minimizing the empirical risk yields the best bound on the actual risk. Disregarding logarithmic factors, the following problem must be solved:

$$\min_{\mathcal{H}_n} \left(R_{\text{emp}}(\boldsymbol{w}) + \sqrt{\frac{h(n)}{\ell}} \right). \tag{12.4}$$

The SVM algorithm described in the following is based on the SRM principle, by minimizing a bound on the VC-dimension and the number of training errors at the same time.

The mathematical derivation of Support vector Machines is summarized first for the case of a linearly separable problem, also to build some intuition about the technique.

12.1.1 Linearly separable problems

Assume that the labeled examples are linearly separable, meaning that there exist a pair $(\boldsymbol{w}, b)$ such that:

$$\begin{aligned} \boldsymbol{w}\cdot\boldsymbol{x} + b &\geq 1 \quad \forall \boldsymbol{x} \in \text{Class}_1; \\ \boldsymbol{w}\cdot\boldsymbol{x} + b &\leq -1 \quad \forall \boldsymbol{x} \in \text{Class}_2. \end{aligned}$$

The hypothesis space contains the functions:

$$f_{\boldsymbol{w},b} = \text{sign}(\boldsymbol{w}\cdot\boldsymbol{x} + b).$$

Because scaling the parameters $(\boldsymbol{w}, b)$ by a constant value does not change the decision surface, the following constraint is used to identify a unique pair:

$$\min_{i=1,\ldots,\ell} |\boldsymbol{w}\cdot\boldsymbol{x}_i + b| = 1.$$

A structure on the hypothesis space can be introduced by limiting the norm of the vector $\boldsymbol{w}$. It has been demonstrated by Vapnik that if all examples lie in an n-dimensional sphere with radius R then the set of functions $f_{\boldsymbol{w},b} = \text{sign}(\boldsymbol{w}\cdot\boldsymbol{x} + b)$ with the bound $\|\boldsymbol{w}\| \leq A$ has a VC-dimension h that satisfies

$$h \leq \min\{\lceil R^2 A^2 \rceil, n\} + 1.$$

The geometrical explanation of why bounding the norm of $\boldsymbol{w}$ constrains the hypothesis space is as follows (see Fig. 12.3): if $\|\boldsymbol{w}\| \leq A$, then the distance from the hyperplane $(\boldsymbol{w}, b)$ to the closest data point has to be larger than $1/A$, because only the hyperplanes that do not intersect spheres of radius $1/A$ placed around each data point are considered. In the case of linear separability, minimizing $\|\boldsymbol{w}\|$ amounts to determining a separating hyperplane with the maximum *margin* (distance between the convex hulls of the two training classes measured along a line perpendicular to the hyperplane).

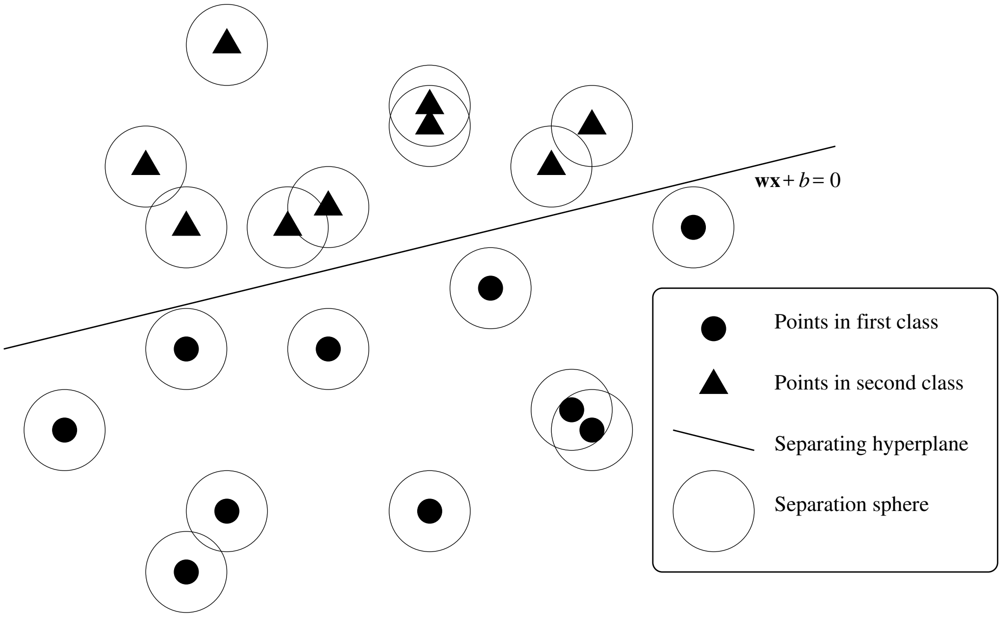


Figure 12.3: Hypothesis space constraint. The separating hyperplane must maximize the margin. Intuitively, no point has to be too close to the boundary so that some noise in the input data and future data generated by the same probability distribution will not ruin the classification.

The problem can be formulated as:

$$\begin{array}{ll} \text{Minimize}_{\boldsymbol{w},b} & \frac{1}{2}\|\boldsymbol{w}\|^2 \\ \text{subject to} & y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i+b)\geq 1 \quad i=1,\ldots,\ell. \end{array}$$

and solved by using standard **quadratic programming (QP)** optimization tools.

The dual quadratic program, after introducing a vector $\boldsymbol{\Lambda}=(\lambda_1,\ldots,\lambda_\ell)$ of non-negative Lagrange multipliers corresponding to the constraints, as explained in Section 26.5, is as follows:

$$\begin{array}{ll} \text{Maximize}_{\boldsymbol{\Lambda}} & \boldsymbol{\Lambda}\cdot\mathbf{1}-\frac{1}{2}\boldsymbol{\Lambda}\cdot D\cdot\boldsymbol{\Lambda} \\ \text{subject to} & \begin{cases}\boldsymbol{\Lambda}\cdot\boldsymbol{y}=0 \\ \boldsymbol{\Lambda}\geq 0\end{cases} ; \end{array} \tag{12.5}$$

where $\boldsymbol{y}$ is the vector containing the example classification, and D is a symmetric $\ell\times\ell$ matrix with elements $D_{ij}=y_iy_j\boldsymbol{x}_i\cdot\boldsymbol{x}_j$.

The vectors $\boldsymbol{x}_i$ for which $\lambda_i>0$ are called **support vectors**. In other words, support vectors are the ones for which the constraints in (12.5) are active. If $\boldsymbol{w}^*$ is the optimal value of $\boldsymbol{w}$, the value of b at the optimal solution can be computed as $b^*=y_i-\boldsymbol{w}^*\cdot\boldsymbol{x}_i$ for any support vector $\boldsymbol{x}_i$, and the classification function can be written as

$$f(\boldsymbol{x})=\text{sign}\left(\sum_{i=1}^{\ell}y_i\lambda_i^*\boldsymbol{x}\cdot\boldsymbol{x}_i+b^*\right).$$

Note that the summation index can as well be restricted to support vectors, because all other vectors have null λ_i^* coefficients. The classification is determined by a linear combination of the classifications obtained on the examples y_i weighted according to the scalar product between input pattern and example pattern (a measure of the “similarity” between the current pattern and example $\boldsymbol{x}_i$) and by parameter λ_i^*.

12.1.2 Non-separable problems

If the hypothesis set is unchanged but the examples are not linearly separable a penalty proportional to the constraint violation ξ_i (collected in vector Ξ) can be introduced, solving the following problem:

$$\begin{array}{ll} \text{Minimize}_{\boldsymbol{w},b,\Xi} & \frac{1}{2}\|\boldsymbol{w}\|^2 + C\left(\sum_{i=1}^{\ell}\xi_i\right)^k \\ \text{subject to} & \begin{cases} y_i(\boldsymbol{w}\cdot\boldsymbol{x}_i + b) \geq 1 - \xi_i & i = 1,\dots,\ell \\ \xi_i \geq 0 & i = 1,\dots,\ell \\ \|\boldsymbol{w}\|^2 \leq c_r; \end{cases} \end{array} \tag{12.6}$$

where the parameters C and k determine the cost caused by constraint violation, while c_r limits the norm of the coefficient vector. In fact, the first term to be minimized is related to the VC-dimension, while the second is related to the empirical risk. (See the above described SRM principle.) In our case, k is set to 1.

12.1.3 Nonlinear hypotheses

Extending the above techniques to nonlinear classifiers is based on mapping the input data $\boldsymbol{x}$ into a higher-dimensional vector of *features* $\boldsymbol{\varphi}(\boldsymbol{x})$ and using *linear* classification in the transformed space, called the *feature space*. The SVM classifier becomes:

$$f(\boldsymbol{x}) = \text{sign}\left(\sum_{i=1}^{\ell} y_i\lambda_i^*\boldsymbol{\varphi}(\boldsymbol{x})\cdot\boldsymbol{\varphi}(\boldsymbol{x}_i) + b^*\right).$$

After introducing the *kernel function* $K(\boldsymbol{x},\boldsymbol{y}) \equiv \boldsymbol{\varphi}(\boldsymbol{x})\cdot\boldsymbol{\varphi}(\boldsymbol{y})$, the SVM classifier becomes

$$f(\boldsymbol{x}) = \text{sign}\left(\sum_{i=1}^{\ell} y_i\lambda_i^* K(\boldsymbol{x},\boldsymbol{x}_i) + b^*\right),$$

and the quadratic optimization problem becomes:

$$\begin{array}{ll} \text{Maximize}_{\boldsymbol{\Lambda}} & \boldsymbol{\Lambda}\cdot\mathbf{1} - \frac{1}{2}\boldsymbol{\Lambda}\cdot D\cdot\boldsymbol{\Lambda} \\ \text{subject to} & \begin{cases} \boldsymbol{\Lambda}\cdot\boldsymbol{y} = 0 \\ 0 \leq \boldsymbol{\Lambda} \leq C\mathbf{1}, \end{cases} \end{array} \tag{12.7}$$

where D is a symmetric $\ell \times \ell$ matrix with elements $D_{ij} = y_i y_j K(\boldsymbol{x}_i,\boldsymbol{x}_j)$.

An extension of the SVM method is obtained by weighing in a different way the errors in one class with respect to the error in the other class, for example when the number of samples in the two classes is not equal, or when an error for a pattern of a class is more expensive than an error on the other class. This can be obtained by setting two different penalties for the two classes: C^+ and C^-. The function to minimize becomes:

$$\frac{1}{2}\|\boldsymbol{w}\|^2 + C^+(\sum_{i:y_i=+1}^{\ell}\xi_i)^k + C^-(\sum_{i:y_i=-1}^{\ell}\xi_i)^k.$$

If the feature functions $\boldsymbol{\varphi}(\boldsymbol{x})$ are chosen with care one can **calculate the scalar products without actually computing all features**, therefore greatly reducing the computational complexity.

The method used to avoid the explicit mapping is also called **kernel trick**. One uses learning algorithms that only require dot products between the vectors in the original input space, and chooses the mapping such that these high-dimensional dot products can be computed within the original space, by means of a **kernel function**.

For example, in a one-dimensional space a reasonable choice can be to consider monomials in the variable x multiplied by appropriate coefficients a_n:

$$\boldsymbol{\varphi}(x) = (a_0 1, a_1 x, a_2 x^2, \ldots, a_d x^d),$$

so that $\boldsymbol{\varphi}(x) \cdot \boldsymbol{\varphi}(y) = (1 + xy)^d$. In more dimensions, it can be shown that if the features are monomials of degree $\leq d$ then one can always determine coefficients a_n so that:

$$K(\boldsymbol{x}, \boldsymbol{y}) = (1 + \boldsymbol{x} \cdot \boldsymbol{y})^d.$$

The kernel function $K(\cdot, \cdot)$ is a convolution of the canonical inner product in the feature space. Common kernels for use in a SVM are the following.

1. Dot product: $K(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{x} \cdot \boldsymbol{y}$; in this case no mapping is performed, and only the optimal separating hyperplane is calculated.
2. Polynomial functions: $K(\boldsymbol{x}, \boldsymbol{y}) = (\boldsymbol{x} \cdot \boldsymbol{y} + 1)^d$, where the *degree* d is given.
3. Radial basis functions (RBF), like Gaussians: $K(\boldsymbol{x}, \boldsymbol{y}) = e^{-\gamma \|\boldsymbol{x} - \boldsymbol{y}\|^2}$ with parameter γ.
4. Sigmoid (or neural) kernel: $K(\boldsymbol{x}, \boldsymbol{y}) = \tanh(a\boldsymbol{x} \cdot \boldsymbol{y} + b)$ with parameters a and b.
5. ANOVA kernel: $K(\boldsymbol{x}, \boldsymbol{y}) = \left(\sum_{i=1}^{n} e^{-\gamma(x_i - y_i)}\right)^d$, with parameters γ and d.

When ℓ becomes large the quadratic optimization problem requires a $\ell \times \ell$ matrix for its formulation, so it rapidly becomes an unpractical approach as the training set size grows. A decomposition method where the optimization problem is split into an active and an inactive set is introduced in [284]. The work in [216] introduces efficient methods to select the working set and to reduce the problem by taking advantage of the small number of support vectors with respect to the total number of training points.

12.1.4 Support Vectors for regression

Support vector methods can be applied also for regression, i.e., to estimate a function $f(\boldsymbol{x})$ from a set of training data $\{(\boldsymbol{x}_i, y_i)\}$. As it was the case for classification, one starts from the case of linear functions and then preprocesses the input data $\boldsymbol{x}_i$ into an appropriate feature space to make the resulting model nonlinear.

In order to fix the terminology, the linear case for a function $f(\boldsymbol{x}) = \boldsymbol{w} \cdot \boldsymbol{x} + b$ can be summarized. The convex optimization problem to be solved becomes:

$$\begin{array}{ll} \text{Minimize}_{\boldsymbol{w}} & \frac{1}{2}\|\boldsymbol{w}\|^2 \\ \text{subject to} & \begin{cases} y_i - (\boldsymbol{w} \cdot \boldsymbol{x}_i + b) \leq \varepsilon \\ (\boldsymbol{w} \cdot \boldsymbol{x}_i + b) - y_i \leq \varepsilon, \end{cases} \end{array}$$

assuming the existence of a function that approximates all pairs with ε precision.

If the problem is not feasible, a *soft margin* loss function with slack variables ξ_i, ξ_i^*, collected in vector $\boldsymbol{\Xi}$, is introduced in order to cope with the infeasible constraints, obtaining the following formulation:

$$\begin{array}{ll} \text{Minimize}_{\boldsymbol{w}, b, \boldsymbol{\Xi}} & \dfrac{1}{2}\|\boldsymbol{w}\|^2 + C\left(\displaystyle\sum_{i=1}^{\ell} \xi_i^* + \sum_{i=1}^{\ell} \xi_i\right) \\ \text{subject to} & \begin{cases} y_i - \boldsymbol{w} \cdot \boldsymbol{x}_i - b \leq \varepsilon - \xi_i^* & i = 1, \ldots, \ell \\ \boldsymbol{w} \cdot \boldsymbol{x}_i + b - y_i \leq \varepsilon - \xi_i & i = 1, \ldots, \ell \\ \xi_i^* \geq 0 & i = 1, \ldots, \ell \\ \xi_i \geq 0 & i = 1, \ldots, \ell \\ \|\boldsymbol{w}\|^2 \leq c_r. \end{cases} \end{array} \tag{12.8}$$

As in the classification case, C determines the tradeoff between the flatness of the function and the tolerance for deviations larger than ε. Detailed information about support vector regression can be found also in [339].

Gist

Statistical Learning Theory (SLT) states the conditions so that learning from examples is successful, i.e., such that positive results on training data translate into effective generalization on new examples produced by the same underlying probability distribution. The **constancy of the distribution** is critical: a good human teacher will never train students on some examples just to give completely different examples in the tests. In other words, the examples have to be representative of the problem. The conditions for learnability mean that the hypothesis space (the "flexible machine with tunable parameters" used for learning) must be sufficiently powerful to allow reaching a good performance on the training examples (a small *empirical risk*), but not too powerful to simply memorize the examples without extracting the deep structure of the problem. The flexibility is quantified by the VC-dimension.

SLT demonstrates the existence of the Paradise of Learning from Data but, for most practical problems, it does not show the practical steps to enter it, and appropriate choices of kernel and parameters through intuition and cross-validation are critical to the success.

The latest results on deep learning and MLPs open new hopes that the "feature engineering" and kernel selection step can be fully automated. Research has not reached an end to the issue, there is still space for new disruptive techniques and for following the wild spirits of creativity more than the lazy spirits of hype and popular wisdom.

Chapter 13

Least-squares and robust kernel machines

Science may be described as the art of systematic over-simplification.
(Karl Popper)

The initial proposal of Support Vector Machines was based on the idea of mapping the data into a higher dimensional input space and of constructing an optimal separating hyperplane in this space, one maximizing the "safety" margin. As shown in Section 12.1.1, the requirement that points fall safely on the correct side of the separating hyperplane leads to **inequalities** like:

$$y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) \geq 1 \qquad i = 1, \ldots, \ell,$$

then corrected with the addition of a constraint violation ξ_i:

$$y_i(\boldsymbol{w} \cdot \boldsymbol{x}_i + b) \geq 1 - \xi_i \qquad i = 1, \ldots, \ell$$

The maximization of the margin leads to minimizing $\|\boldsymbol{w}\|$. The dual convex **quadratic program (QP)** obtained is solvable to optimality without the problem of local minima encountered in MLP and similar techniques.

Enthusiastic practitioners followed the SVM / convex QP wave, but two issues remained in the background. The first issue has to do with **identifying the proper kernel**: linear separability with good generalization requires a proper way of measuring similarities

$$K(\boldsymbol{x}, \boldsymbol{x}_i) = \boldsymbol{\varphi}(\boldsymbol{x}) \cdot \boldsymbol{\varphi}(\boldsymbol{x}_i)$$

between a point to be classified and the training examples. A crude analogy is that of a gentle teacher solving a big portion of the problem and leaving to the learner only a final and trivial part (QP optimization to identify the optimal hyperplane). Deep learning (Section 11.1) is a way of building intermediate features directly from the data in an automated manner.

A second issue has to do with computing times. QP is solvable, but CPU times increase very rapidly for nontrivial problems with many examples. QP is needed because of inequalities, so the temptation to abandon them in favor of simpler equalities is worth exploring. Encouraging equalities and penalizing mistakes in a quadratic manner leads to good old linear equations, faster to solve and easier to interpret. This chapter is dedicated to recent development in the area of **least-squares Support Vector Machines**. As we will see, quadratic penalties do not encourage **sparsity**, which can be recovered by other means. In addition, quadratic penalties can be fragile in the presence of **outliers** because big deviations are squared. Outliers can be caused by measurement errors, and one would like to avoid a few of them spoiling a modeling effort. A possible cure is by robust versions which limit the penalty for deviations which are suspiciously large.

The springs in the figure are related to the familiar physical interpretation of springs connecting data points and fitted models, with a quadratic potential energy.

13.1 Least-Squares Support Vector Machine Classifiers

After the support vector interpretation of ridge regression for function estimation in[313], kernel-based **Least-squares SVM classifiers** are proposed by Suykens and Vandewalle [355].

The least squares version of the SVM classifier is obtained by reformulating the minimization problem as:

$$\begin{array}{ll} \text{Minimize}_{\boldsymbol{w},b,e} & J_2(\boldsymbol{w}, e) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \frac{\gamma}{2}\sum_{i=1}^{\ell} e_{c,i}^2 \\ \text{subject to} & y_i\left[w^T\boldsymbol{\varphi}(\boldsymbol{x}_i) + b\right] = 1 - e_{c,i}, \quad i = 1, \ldots, \ell. \end{array}$$

The hyperparameter γ can be tuned to determine the appropriate amount of regularization versus the sum of squared errors.

The least squares SVM (LS-SVM) classifier formulation above implicitly corresponds to a regression interpretation with binary targets $y_i = \pm 1$.

Using $y_i^2 = 1$, we have

$$\sum_{i=1}^{\ell} e_{c,i}^2 = \sum_{i=1}^{\ell} (y_i e_{c,i})^2 = \sum_{i=1}^{\ell} \left[y_i - (\boldsymbol{w}^T\boldsymbol{\varphi}(\boldsymbol{x}_i) + b)\right]^2 = \sum_{i=1}^{\ell} e_i^2,$$

with $e_i = y_i - (\boldsymbol{w}^T\boldsymbol{\varphi}(\boldsymbol{x}_i) + b)$. This error also makes sense for least squares data fitting, so that the same end results holds for the regression case. Note that the cost function J_2 consists of a sum-squared-errors (SSE) fitting error and a regularization term penalizing large weights, which is also a standard procedure for training MLPs and is related to ridge regression, encountered in Section 4.7.

The solution of the LS-SVM regressor will be obtained by constructing the Lagrangian function:

$$\begin{aligned} L_2(\boldsymbol{w}, b, e, \boldsymbol{\alpha}) &= J_2(\boldsymbol{w}, e) - \sum_{i=1}^{\ell} \alpha_i \Big\{ \left[\boldsymbol{w}^T\boldsymbol{\varphi}(\boldsymbol{x}_i) + b\right] + e_i - y_i \Big\} \\ &= \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} + \frac{\gamma}{2}\sum_{i=1}^{\ell} e_i^2 - \sum_{i=1}^{\ell} \alpha_i \Big\{ \left[\boldsymbol{w}^T\boldsymbol{\varphi}(\boldsymbol{x}_i) + b\right] + e_i - y_i \Big\}, \end{aligned}$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_\ell)^T \in \mathbb{R}^\ell$ are the Lagrange multipliers, also called support values.

As usual, the requirement that the gradient is zero at the minimum leads to a linear system of equations instead of a quadratic programming problem (the derivatives of a quadratic form lead to a linear expression):

$$\begin{pmatrix} 0 & \mathbf{1}_\ell^T \\ \mathbf{1}_\ell & \Omega + \gamma^{-1} I_\ell \end{pmatrix} \begin{pmatrix} b \\ \boldsymbol{\alpha} \end{pmatrix} = \begin{pmatrix} 0 \\ \boldsymbol{y} \end{pmatrix}, \tag{13.1}$$

in which $\boldsymbol{y} = (y_1, \ldots, y_\ell)^T$, $\mathbf{1}_\ell = (1, \ldots, 1)^T$, I_ℓ is the $\ell \times \ell$ identity matrix, and $\Omega \in \mathbb{R}^{\ell \times \ell}$ is the kernel matrix defined by $\Omega_{ij} = \boldsymbol{\varphi}(\boldsymbol{x}_i)^T \boldsymbol{\varphi}(\boldsymbol{x}_j) = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$.

The "kernel trick" applies, one does not need to explicitly calculate the map $\boldsymbol{\varphi}$, only scalar products are needed. This trick is useful because the weight vector $\boldsymbol{w}$ can be infinite dimensional, and impossible to calculate in certain cases.

The classifier is found by solving the linear set of equations (13.1) instead of quadratic programming, and the resulting LS-SVM model for function estimation becomes

$$y(\boldsymbol{x}) = \sum_{k=1}^{\ell} \alpha_k K(\boldsymbol{x}, \boldsymbol{x}_k) + b.$$

A possibility is an RBF kernel characterized by the width parameter σ:

$$K(\boldsymbol{x}_1, \boldsymbol{x}_2) = e^{-\dfrac{\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|^2}{\sigma^2}}.$$

In this case, the support values $\alpha_k = \gamma e_k$ are proportional to the errors at the data points, while in the case of standard SVM most values are equal to zero.

An example of SVM in action to learn the two-spiral benchmark problem is shown in Fig.13.1.

13.2 Robust weighted least square SVM

The issues of robustness and sparse approximation for LS-SVM are studied in [354]. The linear system (13.1) can be efficiently solved either directly or by iterative methods such as conjugate gradient (Section 26.3.2). However, LS-SVM solutions have some potential drawbacks. The first drawback is that **sparseness is lost**. Every data point is contributing to the model and the relative importance of a data point is given by its support value. The second well-known drawback is that the use of a SSE cost function without regularization can lead to estimates which are **less robust with respect to outliers** in the data or when the assumption of a Gaussian distribution for the error variables is not correct.

The problem with outliers is that big errors become huge after squaring them. The cure is to discount very large errors (maybe caused by mistakes or very rare events) through **weighted least square** to produce a more robust estimate.

This is done by first applying an unweighted LS-SVM and then associating weights to the error variables based upon the resulting error variables from the first stage. One ends up solving a sequence of weighted LS-SVMs starting from the unweighted version. The motivation is to **adapt the underlying cost function to the training data**, instead of imposing the cost function beforehand (in a way, this is a form of meta-learning).

In order to obtain a robust estimate based upon the previous LS-SVM solution, in a subsequent step, one can weight the error variables $e_k = \alpha_k / \gamma$ by weighting factors v_k This leads to the optimization problem:

$$\min_{\boldsymbol{w}^*, b^*, e^*} \frac{1}{2} \boldsymbol{w}^{*T} \boldsymbol{w}^* + \frac{1}{2} \gamma \sum_{k=1}^{\ell} v_k e_k^{*2}.$$

The unknown variables for this weighted LS-SVM problem are denoted by the "$*$" symbol.

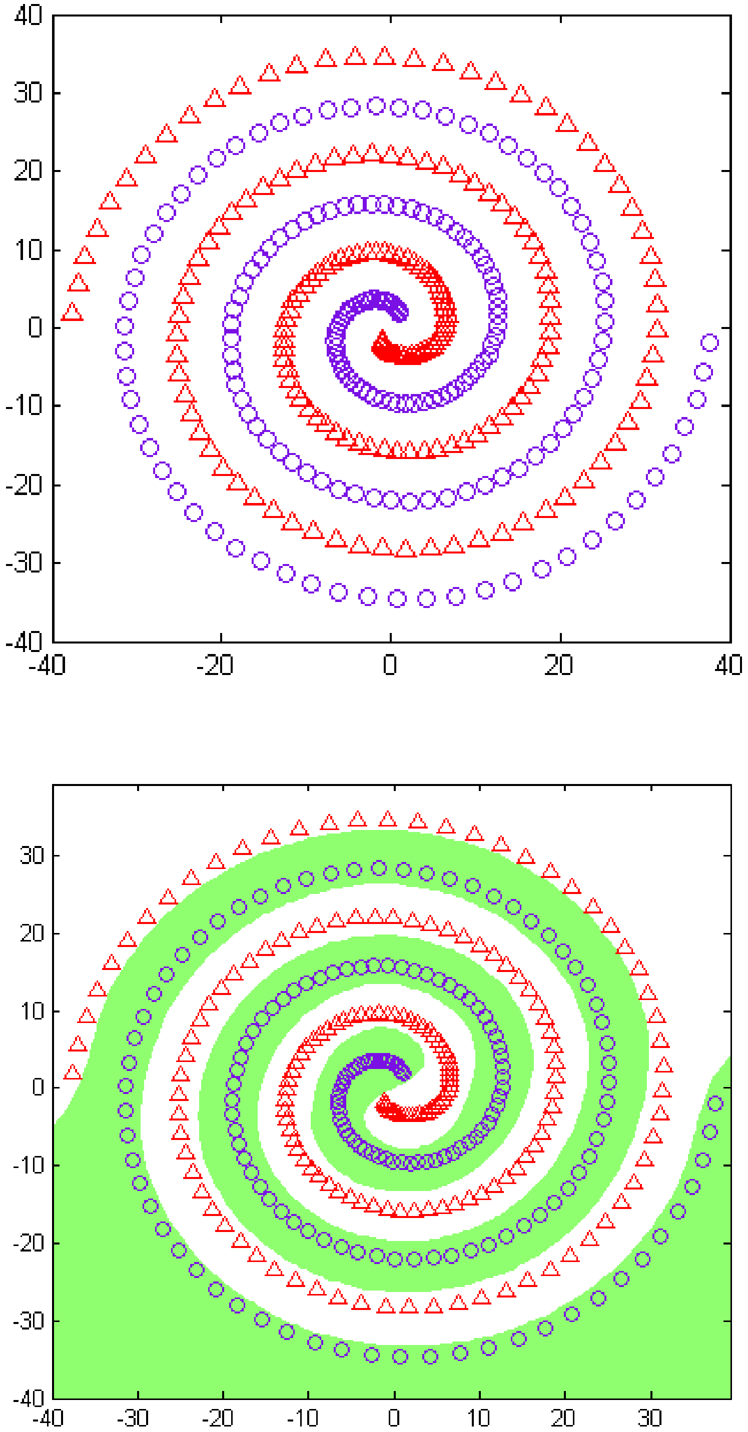


Figure 13.1: SVM tests on a two-spiral classification problem with the two classes indicated by circles and triangles. The figure shows the excellent generalization performance for an SVM.

```
Algorithm LS_SVM ( $\ell$ training data items)
    Find optimal $(\gamma, \sigma)$ by $k$-fold cross-validation with linear system (13.1).
    $e_k \leftarrow \alpha_k / \gamma$
    Compute $\hat{s}$ from the $e_k$ distribution using (13.2).
    Determine the weights $v_k$ based upon $e_k$, $\hat{s}$, as in (13.3).
    Solve (13.1) for $\boldsymbol{\alpha}^*$ and $b^*$, giving the model
        $y(\boldsymbol{x}) = \sum_{k=1}^{\ell} \alpha_k^* K(\boldsymbol{x}, \boldsymbol{x}_k) + b^*.$
```

Figure 13.2: The weighted LS-SVM algorithm

The choice of the weights v_k is based upon the error variables $e_k = \alpha_k/\gamma$ from the (unweighted) LS-SVM case. First one obtains $\hat{s}$, a robust estimate of the standard deviation of the LS-SVM error variables e_k:

$$\hat{s} = \frac{\text{IQR}}{2 \cdot 0.6745} \tag{13.2}$$

The interquartile range IQR is the difference between the 75th percentile and the 25th percentile. Of course, extreme cases like outliers do not count in this estimate, and this is why it is robust. In detail, robust estimates [309] can be obtained by taking:

$$v_k = \begin{cases} 1 & \text{if } |e_k/\hat{s}| < c_1 \\ \dfrac{c_2 - |e_k/\hat{s}|}{c_2 - c_1} & \text{if } c_1 \leq |e_k/\hat{s}| \leq c_2 \\ 10^{-4} & \text{otherwise.} \end{cases} \tag{13.3}$$

The constants c_1 and c_2 are typically chosen as $c_1 = 2.5$ and $c_2 = 3$. This is a reasonable choice taking into account the fact that, for a Gaussian distribution, very few residuals will be larger than $2.5\hat{s}$. Then errors which are suspiciously high with respect to a Gaussian distribution are discounted by giving them smaller and smaller weights.

If needed, the above procedure can be repeated iteratively, but in practice one single additional weighted LS-SVM step will often be sufficient. The final algorithm is shown in Fig. 13.2.

An important notion in robust estimation is the **breakdown point of an estimator**. It is the smallest fraction of contamination (with outliers) of a given data set that can cause an estimate which is arbitrarily far away from the estimated parameters obtained with the uncontaminated data set. Standard least-squares estimate in linear regression without regularization has a low breakdown point. Weighted LS-SVM greatly improves the breakdown point.

13.3 Recovering sparsity by pruning

While standard SVMs possess a sparseness property in the sense that many α_k values are equal to zero, this is not the case for LS-SVM's due to the fact that $\alpha_k = \gamma e_k$ from the conditions for optimality. Support values reveal the relative importance of the data points for contributing to the model.

While pruning methods for MLPs (such as *optimal brain damage* [250] and *optimal brain surgeon* [174]) involve Hessian matrices, the pruning in LS-SVMs proposed in [354] can be done based upon the solution vector itself. Sparseness can be imposed to the weighted LS-SVM solution by gradually pruning the sorted support value spectrum, i.e., by zeroing out the smaller α_i's: this way, less meaningful data points (as indicated by their support values) are removed and the LS-SVM is re-computed on the basis of the remaining points, while validating on the complete training data set.

By omitting a relative and small amount of the least meaningful data points (with α_k set to zero) and by re-estimating the LS-SVM, one obtains a sparse approximation. In order to guarantee a good generalization performance,

```
Algorithm LS_SVM_pruning ( $\ell$ training data items)
    $\ell' \leftarrow \ell$
    repeat until performance degrades
        Apply LS_SVM to the $\ell'$ training data
        Sort training data according to decreasing magnitudes $|\alpha_k^*|$
        Remove the last $M$ data items in the sorted $|\alpha_k^*|$ spectrum
        $\ell' \leftarrow \ell' - M$
```

Figure 13.3: The weighted LS-SVM pruning algorithm

in each of these pruning steps one can optimize (γ, σ), e.g., by defining an independent validation set, or 10-fold cross-validation. Figure 13.3 outlines the resulting algorithm.

Typically, doing a number of pruning steps without modification of (γ, σ) will be possible. When the generalization performance starts degrading (checked e.g. on a validation set or by means of cross-validation [365]) an update of (γ, σ) will be needed. The fact that (γ, σ) determination can be kept *localized* is a possible advantage of this method in comparison with other approaches which need to solve a QP problem for the several possible choices of the hyperparameters.

13.4 Algorithmic improvements: tuned QP, primal versions, no offset

Improvements to SVM are related both to detailed implementations of Quadratic Programming adapted to this scenario and to slight modifications of the problem definition, but with potentially big effects on CPU times and final performance [217].

The quadratic form in (12.7) involves a matrix that has a number of elements equal to the square of the number of training examples (matrix elements containing all possible kernel "similarities" between couples of examples). The first approach to splitting large SVM learning problems into a series of smaller optimization tasks is proposed in [62] as the "**chunking**" algorithm. It starts with a random subset of the data, solves this problem, and iteratively adds examples which violate the optimality conditions.

The work in [299] shows how much can be gained by passing from off-the-shelf QP software to a special-purpose implementation (and, incidentally, how much can be gained by studying the mathematical details of a problem). **Sequential Minimal Optimization** (SMO) proposes to break the large QP problem derived for SVM into a series of smallest possible QP problems. These small QP problems are solved analytically, avoiding a time-consuming numerical QP optimization as an inner loop. The amount of memory required for SMO is linear in the training set size, therefore SMO can handle very large training sets. Because large matrix computation is avoided, SMO scales somewhere between linear and quadratic in the training set size for various test problems, while a standard projected conjugate gradient (PCG) chunking algorithm scales somewhere between linear and cubic in the training set size. SMO's computation time is dominated by SVM evaluation, hence it is fastest for linear SVMs and sparse data sets.

An improved algorithm for training SVMs on large-scale problems (**SVMlight**) is proposed in [217]. The algorithm is based on a decomposition strategy and addresses the problem of selecting the variables for the working set in an effective and efficient way. Furthermore, a technique for "shrinking" the problem during the optimization process is introduced: during the optimization process it often becomes clear fairly early that certain examples are unlikely to end up as support vectors (SV), and by eliminating them the problem gets smaller. This is found particularly effective for large learning tasks where the fraction of SVs is small compared to the sample size. SVMlight's memory requirement is linear in the number of training examples and in the number of SVs.

Solving SVM in the primal space is proposed in [80]. Most literature on SVMs concentrates on the dual optimization problem. The authors of [80] argue that the primal problem can also be solved efficiently and that there is no reason for ignoring this possibility. On the contrary, from the primal point of view new families of algorithms for large scale SVM training can be investigated. The usual main reasons mentioned for solving this problem in the dual are:

1. The duality theory provides a convenient way to deal with the constraints.
2. The dual optimization problem can be written in terms of dot products, thereby making it possible to use kernel functions.

Newton optimization in the primal yields exactly the same computational complexity as optimizing the dual. When it comes to approximate solution, primal optimization can be superior because it is more focused on minimizing what we are interested in: the primal objective function. Primal optimization might have advantages for large scale optimization. Indeed, when the number of training points is large, the number of support vectors is also typically large and it becomes intractable to compute the exact solution. One has to resort to approximations, but introducing approximations in the dual may not be wise. There is indeed **no guarantee that an approximate dual solution yields a good approximate primal solution**.

In a different direction, [345] develops and analyzes a training algorithm for **support vector machine classifiers without offset**. Historically, SVMs were motivated by a geometrical illustration of their linear decision surface in the feature space, like in Fig. 12.3. This illustration justified the use of an offset b that moves the decision surface from the origin. However, this geometrical interpretation has serious flaws. Even if visualizations can be powerful, one should **never base algorithmic choices on simple illustrations in low-dimensional spaces**.

It turns our that SVM optimization with offset imposes more restrictions on solvers than the optimization problem without offset does. The offset leads to an additional equality constraint in the dual optimization problem, which in turn makes it necessary to update at least two dual variables at each iteration of commonly used solvers such as sequential minimal optimization (SMO) [299].

The authors of [345] develop algorithms for SVMs without offset. These algorithms not only achieve a classification accuracy that is comparable to the one for SVMs with offset, but also run significantly faster.

Gist

Least-squares Support Vector Machines require equalities instead of inequalities for classifying patterns (like the usual trick of mapping positive cases to $+1$, negative cases to -1). In this manner the quadratic penalty on the errors leads to **linear equations** after taking partial derivatives and demanding a zero gradient.

Quadratic penalties increase big deviations so that a few **outliers** can distort the model. **Robust statistics** produces methods that are not unduly affected by outliers, by limiting their effect on the goodness function to be minimized. Suspiciously large errors are discounted by giving them small weights and obtaining **robust weighted least square SVM**.

The sparseness which is lost in the quadratic formulation can be recovered through **pruning** techniques, so that less meaningful data points are removed and the LS-SVM is re-computed on the basis of the remaining points.

The antediluvian least-squares method minimizing the sum of squared residuals remains an effective pillar to support also recent methods like SVM. Never underestimate good old techniques and linear algebra when comparing with the latest proposals.

Chapter 14

Structured Machine Learning, Text and Web Mining

Wholly new forms of encyclopedias will appear, ready made with a mesh of associative trails running through them, ready to be dropped into the memex and there amplified.
(Vannevar Bush, 1945)

Up to now we have considered data with a flat structure, numbers conveniently collected in vectors. But there are interesting situations in which data (observations) come with a very structured form, imagine the graph of a **network** describing relationships between people or between genes (genetic regulatory networks), a causal network linking a hidden syndrome to symptoms, or imagine analyzing text or understanding language.

Structured machine learning refers to learning structured hypotheses from data with rich internal structure usually in the form of one or more relations[118]. The data might include structured inputs as well as outputs, parts of

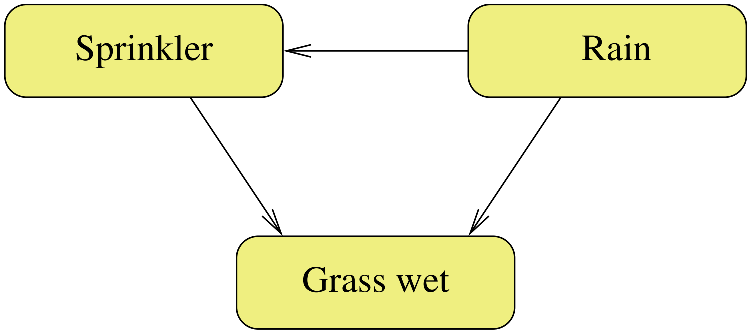


Figure 14.1: A simple Bayesian network: nodes and relationships.

which may be noisy, or missing. **Probabilistic graphical models** is an umbrella term to cover Bayesian networks, Markov networks and variations thereof.

Applications include a variety of tasks such as learning to parse and translate sentences, studying social networks, predicting the pharmacological properties of molecules, and interpreting visual scenes. Predictions can be about node properties (e.g., "Is a user in a social network going to vote democrat or republican?"), about link properties or link existence ("Will customer A buy product B?", "Are two proteins interacting?"), or about entire networks ("Is this a network of terrorists?"). An empirical fact which can be used for collective classifications is **homophily** (i.e., "love of the same"), the tendency of individuals to associate and bond with similar others. Linked entities are likely to share attribute values ("If A is a subscriber of a cellular company and B is connected to A, B is more likely to be a subscriber of the same company"), and entities sharing common neighbors are more likely to be linked ("friend of friends are friends").

The topic is rapidly getting very technical and we are forced to mention only some relevant models. In this introductory chapter we consider briefly Bayesian belief networks (Sec. 14.1), Markov networks (Sec. 14.2) and inductive logic programming (Sec. 14.3), and dedicate more space to text and web mining (from Sec. 14.4), also because of its relevance and concrete aspect which facilitates understanding.

14.1 Bayesian networks

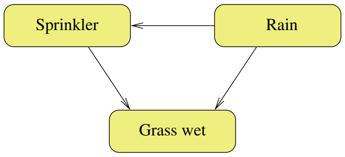
A **Bayesian network, or belief network** is a **graphical representation of uncertain knowledge**, easy to build and to interpret, yet with a formal probabilistic semantics making it suitable for statistical interpretation [176, 211].

Up to now, the objective has been that of maximizing some performance index (correct recognition, squared error, etc.). But there is another positive objective for intelligent systems, one that becomes a necessity for certain applications: **human understanding and high-level explanation**. In healthcare, purely automated systems identifying a diagnosis from symptoms and exams are not yet acceptable. A physician has to check and understand (and be responsible in case of lawsuits). An example of systems based on rules are decision trees (Chapter 6), but their structure based on deterministic hierarchical chain of "if ... then" rules limit their applicability. A long time ago, "**expert systems**" with high-level (symbolic) rules defined solely by experts were popular but soon encountered problems related to fragility, difficulty in maintenance for dynamic systems, exploding times for running the inference engine.

A Bayesian network is a useful compromise: **domain experts can define an initial network structure**, but it is amenable to refinement through **learning, by fine-tuning probabilities** or modifying some parts of the network structure.

In details, a Bayesian network is a probabilistic graphical model that represents a set of random variables and their conditional dependencies via **a directed acyclic graph (DAG)**. For example, it could represent the probabilistic relationships between diseases and symptoms. Given symptoms, the network can be used to compute the probabilities

Rain	Sprinkler F	Sprinkler T
F	0.6	0.4
T	0.99	0.01



Rain F	Rain T
0.8	0.2

Sprinkler	Rain	Sprinkler F	Sprinkler T
F	F	1.0	0.0
F	T	0.2	0.8
T	F	0.1	0.9
T	F	0.01	0.99

Figure 14.2: A simple Bayesian network: nodes and probability tables.

of various diseases. Nodes represent random variables: they can be observable quantities, latent variables, unknown parameters or hypotheses. Edges represent **conditional dependencies**. Each node is associated with a probability function that takes, as input, a particular set of values for the node's parent variables, and gives (as output) the probability of the variable represented by the node.

A toy example is in Fig. 14.1 Two events can cause grass to be wet: either the sprinkler is on or it's raining. Also, the rain has a direct effect on the use of the sprinkler (when it rains, the sprinkler is usually not turned on). All three variables have two possible values, T (for true) and F (for false). Possible probability tables for this examples are in Fig. 14.2.

The joint probability function is:

$$\Pr(G, S, R) = \Pr(G|S, R)\Pr(S|R)\Pr(R)$$

where the names of the variables have been abbreviated to G = "Grass wet" (yes/no), S = "Sprinkler turned on" (yes/no), and R = "Raining" (yes/no). The model can answer questions like "What is the probability that it is raining, given the grass is wet?"

Not surprisingly, Bayesian networks are related to the **Bayesian philosophy**. The probability of an event represents the **degree of belief** that the event will occur in an experiment. This is also called the subjective interpretation, different from the *frequentist* interpretation of probability (frequency in a series of repeated experiments). According to Bayes, the probability of event e depends on the state of knowledge ξ of the person providing the probability $p(e|\xi)$. One of the main motors for probabilistic reasoning is **Bayes' theorem**:

$$\Pr(X|Y, \xi) = \frac{\Pr(Y|X, \xi)}{\Pr(Y|\xi)}\Pr(X|\xi), \text{ for } \Pr(Y|\xi) > 0$$

The standard names for the probability of X before we know Y ($P(X|\xi)$) is the *prior*, the probability $P(X|Y, \xi)$ after we know Y is called the *posterior*. Because probabilities sum up to one, one can forget about the denominator and just remember:

$$P(X|Y, \xi) \propto P(Y|X, \xi)P(X|\xi)$$

To remember: "Posterior equals prior times likelihood". Important ingredients in the machinery of Bayes networks are the *chain rule*:

$$p(x_1, \dots, x_n|\xi) = \prod_{i=1}^{n} p(x_i|x_1, \dots, x_{i-1}, \xi) \tag{14.1}$$

the *generalized sum rule* (variable Y is *marginalized out*) :

$$\sum_{Y} P(X, Y|\xi) = P(X|\xi) \tag{14.2}$$

and the *expansion rule*:

$$P(X|\xi) = \sum_{Y} P(X|Y, \xi)P(Y|\xi) \tag{14.3}$$

Given a set of events $x_1, \dots, x_n$, the joint probability distribution function $p(x_1, \dots, x_n)$ contains the entire probabilistic knowledge. Unfortunately, dealing directly with a generic p.d.f. is out of question for computational reasons (the number of values to store is at least 2^n, in the lucky case of events with just two possibilities) and for understanding (we are very bad at reasoning with very large-dimensional tables).

Luckily, useful real-world Bayesian networks have a **very sparse structure**: the relevant tables are low-dimensional and the relationships are only among a limited set of nodes. In detail, in the factors of the chain rule of equation (14.1), for every x_i there will be a limited subset Π_i such that x_i and $\{x_1, \dots, x_n\}$ are conditionally independent given Π_i, i.e.,

$$p(x_i|x_1, \dots, x_{i-1}, \xi) = p(x_i|\Pi_i, \xi)$$

In the graph representing the Bayesian network, the parents of node x_i correspond to the set Π_i. In addition to the connectivity structure defining the parent - child relationship, the tables $p(x_i|\Pi_i, \xi)$ contain the relevant probability distributions.

Let's note that Bayesian networks are not uniquely defined: the **structure depends on variable order**, and a careless ordering may fail to reveal many conditional dependencies.

On the other hand, with a carefully selected ordering (guided by the knowledge and intuition of the domain expert), the joint probability distribution can be decomposed into manageable pieces. In this manner **probabilistic inference**, i.e., computing probabilities of interest from a joint probability distribution, becomes doable in acceptable times (no sums over 2^n or more possibilities!). In spite of the "*divide et impera*" approach, efficient probabilistic inference is not trivial and different algorithms have been proposed [176]. Exact inference in arbitrary Bayesian networks, and even approximate inference is NP-hard [106], but these negative results should not discourage, there is help for reasonably small networks, particular topologies, particular queries.

Unfortunately, rarely is the domain so clear and the probabilistic knowledge so refined to design a fully functional Bayesian network from scratch. In other words, this is another area in which huge **opportunities for learning from data** exist. In particular, one can **learn probabilities**. One can start with a prior distribution depending on available knowledge ξ and update probabilities with Bayes rule to obtain posterior distributions after running experiments. In other cases, the **structure of the network** is also uncertain and one may want to refine the structure when more and more data becomes available. Prior probabilities can be defined over network structures, then posterior probability distributions over structures can be derived.

Unfortunately, the number of possible structures to sum over explodes when the network is more than a small toy problem and radical approximations are needed. Luckily, even crude approximations that consider only **a single "good" network structure** can be sufficient. Identifying a good network compatible with the measured data can be done through **local search (LS)** mechanisms (LS is explained in Chapter 24). LS can be particularly effective when the score can be *updated* rapidly for small changes, like the addition or deletion of an edge, and not recomputed from scratch. In LS one needs heuristic scoring metrics to measure the "goodness of fit" of a particular network to prior knowledge and data. One can search for the network structure with the highest posterior probability (**maximum a posteriori – MAP – structure**). As it was the case for neural networks, overly-complex networks may easily lead to very large posterior probability and should be discouraged, for example through Akaike information criterion [7]. More sophisticated local search mechanism going beyond local optimality can be employed (Chapter 27).

As you imagine, the topic is rapidly getting very technical and we have to stop. But continue your exploration in case you encounter applications characterized by a rich structure of relationships (in some cases relationships of cause and effects), not excessively large, with abundance of existing domain knowledge and requiring high-level explanation. Notable cases are medical diagnosis, computational biology and bioinformatics (e.g., gene regulatory networks), semantic search, image processing, law, decision support systems, financial informatics (risk analysis). Generalizations of Bayesian networks that can represent and solve decision problems under uncertainty are called **influence diagrams**.

14.2 Markov networks

Markov random fields (or **Markov networks**) are based on *undirected* graphical models, possibly with cyclic dependencies. Different Markov properties can be assumed, like the fact that the variable associated to a node is *conditionally independent* of all other variables *given its neighbors*. For a concrete image, imagine particles moving among nodes (so that the probability of a node is related to the fraction of particles sitting in that specific node) and imagine that you sit at one node. The stochastic arrival or departure of particles depend only on the local situation and not on the distant nodes (and each particle forgets about the previous part of its trajectory). Markov random fields are studied in Statistical Physics to explain "spin glasses", and enjoy a large popularity in computer vision. A rich theory is available. To rapidly hint at some results, in a commonly used class of Markov random fields the joint probability density can be *factorized* according to the cliques of the graph (cliques are subset of nodes which are completely connected).

$$P(X=x)=\prod_{C\in \mathrm{cl}(G)} \phi_C(x_C) \tag{14.4}$$

This is a huge simplification if cliques are small (in a typical computer vision applications cliques can be associated to neighboring pixels in an image).

Consider a field where values at the nodes can be among a finite set. Any Markov random field (with a strictly positive density) can be written as log-linear model with feature functions f_k such that the full-joint distribution can be written as

$$P(X=x)=\frac{1}{Z}\exp\left(\sum_k w_k^\top f_k(x_{\{k\}})\right)$$

where the notation $w_k^\top f_k(x_{\{k\}})=\sum_{i=1}^{N_k} w_{k,i}\cdot f_{k,i}(x_{\{k\}})$ is simply a dot product over field configurations, and Z is the partition function (needed so that probabilities sum up to one):

$$Z=\sum_{x\in\mathcal{X}}\exp\left(\sum_k w_k^\top f_k(x_{\{k\}})\right).$$

Here, $\mathcal{X}$ denotes the set of all possible assignments of values to all the network's random variables. Usually, the feature functions $f_{k,i}$ are defined such that they are indicators of the clique's configuration, i.e. $f_{k,i}(x_{\{k\}})=1$ if $x_{\{k\}}$ corresponds to the $i-th$ possible configuration of the $k-th$ clique and 0 otherwise.

Gibbs sampling can be used in Markov networks to sample from the joint probability distribution. The intuition behind Gibbs sampling is to start from a configuration of $\mathbf{x}$ (a vector of random variables), then consider randomly one variable x_j at a time and update the current value with one derived from the conditional distribution specified by $p(x_j|x_1,\ldots,x_{j-1},x_{j+1},\ldots,x_n)$. The method is therefore very fast if conditional probabilities are a function of a small subset of local variables. Gibbs sampling is a **Markov chain Monte Carlo (MCMC)**algorithm for obtaining a sequence of observations which are approximated from a specified multivariate probability distribution. The samples in the generated **Markov chain** approximate the joint distribution of all variables, the expected value of any variable can be approximated by **averaging over all the samples**. But let's note: samples are not independent: subsequent samples are in fact highly correlated. It is common to ignore some number of samples at the beginning (the so-called *burn-in* period), and then consider only every n-th sample when averaging values to compute an expectation. Some additional black magic is involved in many applications in statistical inference. In machine learning, missing values for some input variables can be handled by simply fixing the values of all variables whose values are known, and sampling from the remainder.

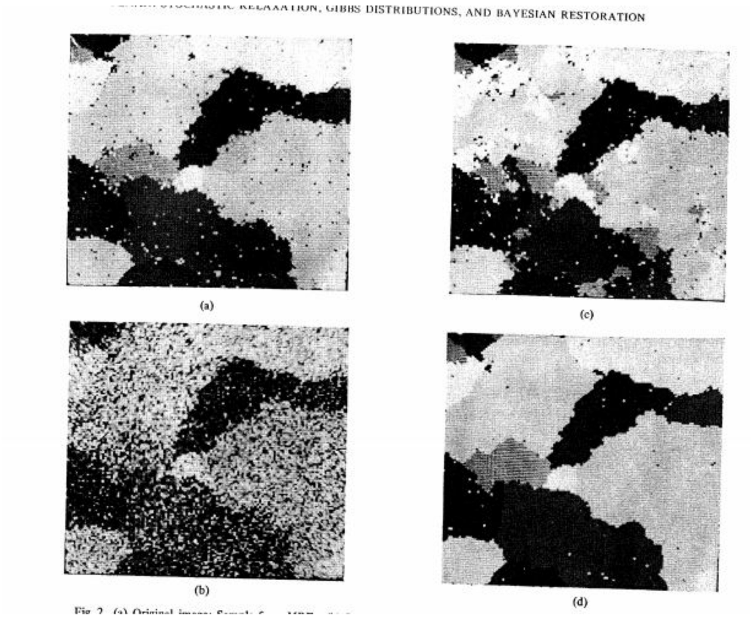

STOCHASTIC RELAXATION, GIBBS DISTRIBUTIONS, AND BAYESIAN RESTORATION
(a)
(c)
(b)
(d)
Fig. 2. (a) Original image

Figure 14.3: Gibbs sampling in computer vision (image restoration) from [143].

A very influential paper with applications in computer vision is [143]. The authors propose an analogy between images and statistical mechanics. Pixel gray levels and presence and orientation of edges are viewed as state of atoms in a lattice-like system (a Markov random field). The probability of a pixel value depends (mostly) on the probability of a set of neighboring pixels, which means that the probability density functions factorize as a product of "local" terms, easy and fast to calculate, see equation (14.4).

Maximum *a posteriori* (MAP) estimates of images given a degraded observation (with some noise at pixel levels, like in old-style television without robust error-correcting coding), are derived by Gibbs sampling and Simulated Annealing versions. A mental image is that the initial image is modified at randomized pixel locations, and flickers more at the beginning, less when an approximation of a stationary state maximizing the probability is reached. In spite of the enormous influence and number of theoretical studies originating from Statistics and Physics, like all MCMC methods, Gibbs sampling tends to be extremely slow for all apart simple and small-scale applications, and therefore should not generate excessive expectations.

14.3 Inductive logic programming (ILP)

The early phase of Artificial Intelligence concentrated on **symbolic approaches based on if-then rules (knowledge base)** and **inference engines**. Formal logic, knowledge representation and automated reasoning were under the spotlight.

The dream was to separate **knowledge acquisition**, in which a domain expert would make the critical information required for the system to work *explicit*, from **automated reasoning**. By removing the need to write conventional code, and therefore removing the need for trained programmers, experts could develop systems themselves trough **expert systems**. The use of rules to explicitly represent knowledge also enabled **explanation capabilities**, even in English (human) language.

In expert systems an inference engine is being driven by the antecedent (left hand side) or the consequent (right hand side) of the rule. In forward chaining an antecedent *fires* and asserts the consequent. For example, consider the following toy example with the rule:

$$R1 : Man(x) => Mortal(x)$$

A simple example of forward chaining would be to assert $Man(Socrates)$ to the system and then trigger the inference engine. It would match $R1$ and assert $Mortal(Socrates)$ into the knowledge base. Backward chaining is less straightforward: the system looks at possible conclusions and works backward to see if they might be true.

Logic programming is a programming paradigm based on formal logic at the base of this high-level approach to developing intelligent systems. A program written in a logic programming language is a set of sentences in logical form, expressing facts and rules about some problem domain. Prolog is a notable programming language in this area. In all of these languages, rules are written in the form of clauses:

$$H \quad :- \ B_1, \ldots, B_n.$$

and are read declaratively as logical implications:

$$H \text{ if } B_1 \text{ and } \ldots \text{ and } B_n.$$

H is called the head of the rule and $B_1, \ldots, B_n$ is called the body. Let's note that the "$: -$" symbol is used to fake a left arrow by standard keyboard symbols (keyboard design was for secretaries not for programmers!).

The knowledge-base and inference-engine dream generated hype and then following disillusion, when it turned out that passing from rapid prototypes to real-world systems in many cases created an explosion of CPU times for reasoning, difficulty in maintaining systems, **fragility** when application was at the boundary of the domain. While the rules for an expert system were more comprehensible than typical computer code they still had a formal syntax where a misplaced comma or other character could cause havoc as with any other computer language.

Nonetheless, research is still in specific areas like natural language processing (language parsing), bio-informatics, hardware-software verification. The new developments are mentioned in this book for completeness but also because ILP is deeply involved with **learning and optimization**, to simplify system developments, take account of examples in addition to rules, make the systems more robust and dynamic.

In particular, **Inductive logic programming (ILP)**[277] is a subfield of machine learning which uses logic programming as a uniform representation for *examples*, background knowledge and hypotheses. Given an encoding of the known background knowledge and a set of **examples** represented as a logical database of facts, an ILP system will **derive a hypothesised logic program** which entails all the positive and none of the negative examples. The term "inductive" here refers to a philosophical induction process of suggesting a theory to explain observed *facts*. Current research[118] deals with *reasoning about the identity* of objects (like recognizing that vehicles found in different images represent the same physical object), *inventing new objects* to achieve compact hypotheses which explain empirical observations (like inventing an unknown enzyme to explain effects in a metabolic network), *incremental theory revision* (background knowledge can be incomplete and incorrect, it can be revised when abundant experimental data are present), *logical experimental design* (optimal design of experiments to test hypothesis in laboratory settings).

Structured machine learning[118] is an umbrella term for ML techniques that involve predicting structured objects, like a parse tree (part-of-speech tagging natural language) or a symbolic interpretation of a visual scene, rather than scalar discrete or real values. Structured ML includes learning logical representations, like in ILP or Bayesian networks. The current research deals with handling uncertainty in a principled manner by incorporating probabilities into logical and relational representations. The long-term goal is to deal with the dynamic nature of systems, to deal with *shifting sands* of non-stationary distribution in order to achieve graceful degradation. From the computational point of view while searching for the best structure, dynamic programming (Viterbi and variations), local search, greedy search and **beam search** (which extends a greedy approach by considering a certain number B of interesting candidates to modify instead of a single one), are in the bag of tools to achieve acceptable CPU times to deal with real-world systems.

```
<html>
 <head>
  <title>Learning and Intelligent Optimization</title>
  <meta name="author" content="Roberto Battiti">
  <meta name="keywords" content="LION, ML, optimization, big data">
 </head>
 <body>
  <h1>The LION way is the future</h1>
  The reasons are explained in the
  <a href="intelligent-optimization.org"> LIONlab homepage </a>.
 </body>
</html>
```

Figure 14.4: An example of a web page written in HTML, the Hypertext Markup Language which is standard to describe the overall page structure.

Combining logical and statistical approaches is far from trivial but can produce advantages related to speed of development and human explanation in areas for which logical rules are present (e.g, natural language, robotics, vision). As an example, automated car driving requires both following many symbolic rules (including speed limits, road signs, safety requirements, etc.) and reacting very rapidly to unusual driving conditions or adapting the driving style in order to reduce fuel consumption, in some cases in sub-symbolic manners through learning-by-example.

14.4 Text and web mining: the context

When the data consist of a collection of documents, we can still use many of the techniques used to analyze numerical data but we need to adapt them, by suitably **preprocessing the documents and fine-tuning the ML methods**. Preprocessing transforms texts into vectors containing numeric values. Fine-tuning the ML methods has to deal with the fact that these vectors may possess a huge number of coordinates, that words have synonyms, that texts have a structure going beyond a bag of words, facts which require specific ad hoc metrics, feature selection and extraction.

Information retrieval deals mostly with searching for documents and for information within documents, and **web mining** is related to adapting methods to the context of the world wide web. The Web is an *unstructured* (or, at most, *semi-structured*) collection of data mostly in form of human-readable texts and images, connected by hyper-links. The Web is not a database: a complete description of data items structure (a *schema*) is missing, it is just a messy collection of human-readable data and human-exploitable hyper-links. There are efforts to help machines (computers) to automatically extract meaning from web pages through semantic support, but the task is daunting given the anarchic and continuously evolving structure of the web. “Semantic” means related to the “meaning” of the data items, and the so-called semantic web is an effort to add meta-data —data about the meaning of data— to enable automated agents and other software to access the Web more intelligently, for example understanding that a field is the name of a person, another field the age, another one the address, etc.

“**Big data**” is a popular marketing term for a collection of data sets so large, complex and unstructured that it becomes difficult to handle by using traditional data processing applications.

In addition to text, it is important to remember that web pages contain tags that modify the *appearance* and the *meaning* of the text, they contain links to other documents (**hyper-links**) and, in some cases, **meta-data** describing the meaning of the different parts. A short example of a page written in HTML is shown in Fig. 14.4. *No web page is an island entire of itself*: in fact hyperlinks help in searching for, ranking, and classifying pages in the web. Of course, similar linked structures are present in other areas, like social networks, bibliographic references in research papers, etc.

14.5 Retrieving and organizing information from the web

Before taking the plunge into the more interesting web mining tasks like ranking, clustering and classification, let's start with a short introduction about how to collect the raw content of the web pages (**crawling**), and structure it so that it is ready for further analysis (**indexing**). If you do not care about how the raw data is obtained and you are just interested in a high-level view, you may skip these sections and jump to Section 14.6.

The collected documents are processed into an **index** suitable for answering queries and retrieving information. Unlike the context of RDBMS (relational databases), *the order of answers is fundamental*: the user wants to see relevant data first. In other words: one aims at maximizing the probability that the first few answers will satisfy the user's needs. The union of a web crawler and a web index is a **search engine**.

In some cases **topic directories** are built to simplify searching. They are treelike structures (taxonomies), initially designed by hand. The process of organizing the documents can be automated by **clustering and unsupervised learning** methods. The purpose is the automated discovery of groups in the set of documents so that documents *inside* the same group are *more similar* than documents in different groups. As one may expect, similarity measures are a crucial issue when designing automated document clustering techniques.

14.5.1 Crawling

The processing of the web information starts with **crawling**, systematic methods to visit web pages and harvest the information contained therein. The basic crawling principle consists of visiting the web graph by starting from a given set of URLs, fetching and collecting the corresponding pages, scanning collected pages for hyperlinks to pages that have not been collected yet.

If you are familiar with *graphs*, nodes represent web pages, edges represent links and the task is to *visit the graph*, i.e., visit all nodes in a systematic manner while avoiding duplicate visits. While a basic crawler implementing a visit of the web graph can be put together with a little knowledge of the underlying communication protocol (HTTP), avoiding the many pitfalls requires careful design considerations:

- many web servers assume that a human mind is driving the web requests, therefore they assume that any attempt at fetching many pages per second is an attack, and respond by denying access;

- more and more pages on the Internet are dynamic in many subtle ways: their content depends on data previously input by the user, by pre-existing client cookies, even by the position the request is being originated from; therefore, any attempt to automatically collect all available information fails, and some user intelligence must be put into the system;

- resolving host names might take longer than fetching the data itself; in general, identifying the real bottleneck is not an easy task;

- the web is now dominated by virtual servers with their many-to-many relationships (Domain names to IP addresses, URLs to pages, not to mention mirrored or plagiarized info), so that identifying what has already been visited is becoming more and more difficult.

A minimal crawler architecture is shown in Fig. 14.5: a queue of still unvisited URLs is maintained; every time a page is fetched, it is scanned for new URLs. In order to overcome the aforementioned DNS bottleneck, a preliminary DNS request can be issued long before the URL is finally requested. Avoiding page and URL duplicates is also important, so various "is it new?" checkpoints can be placed throughout the workflow.

14.5.2 Indexing

Indexing is a required **preprocessing so that queries can be answered rapidly**. The simplest kind of queries, and by far the most used, involves one or more terms, in some cases combined by Boolean operators. For example one may

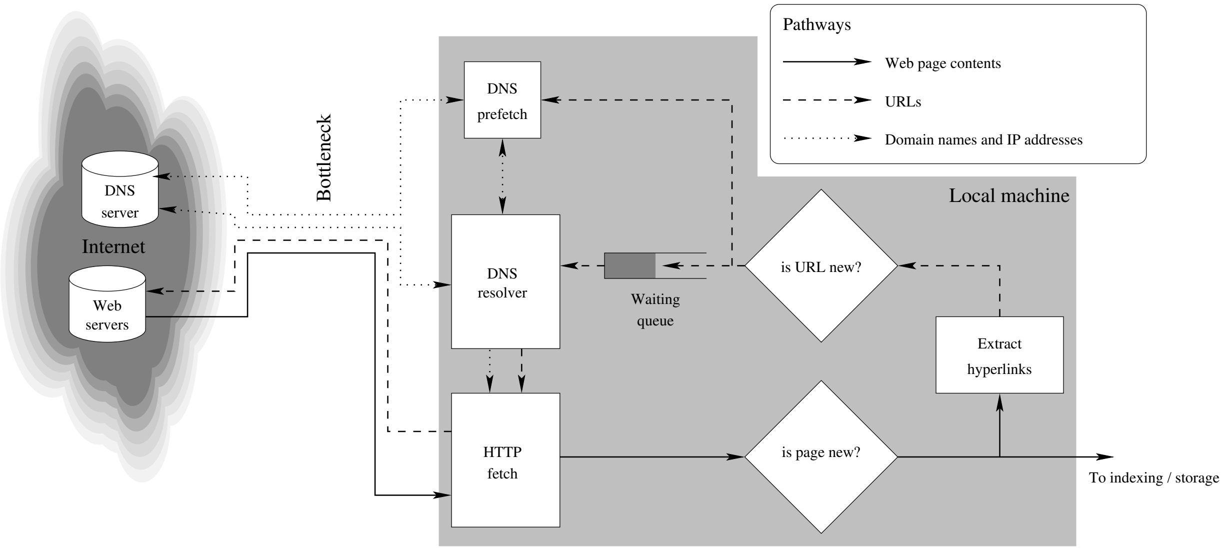


Figure 14.5: A basic crawler architecture: URLs are extracted from fetched pages and enqueued; domain names are pre-fetched to overcome the potential bottleneck.

search for: documents containing the word “Reactive” but not the word “Search”; documents containing the phrase “Reactive Search Optimization”; documents where “Reactive” and “Search” occur in the same sentence, etc.

Before building indices, documents undergo a sequence of cleaning steps, often including the following: HTML tags and other non-relevant markup items are filtered out (there are some exceptions: some meta-information should be retained, heading tags might provide information about the relevance and visibility of words); punctuation can be removed and replaced, if needed, by end-of-sentence markers; character casing is made uniform (e.g., all lowercase); the remaining text is *tokenized*, i.e., divided into words; very common words (“and”, “I”, “the”…), also known as *stopwords*, are removed; variant forms of the same word are collapsed to their *stem* (so that “play”, “playing” and “played” all correspond to the same token).

While not all of the original information is preserved in the process, from the information retrieval point of view, the lost part is mainly noise, and a user who sends the query “Shakespeare play” to a search engine will expect results containing the words “Shakespeare plays” too, with proper casing and plural forms.

Fig. 14.6 shows two sample documents[1], d_1 and d_2, where the subscript denotes the position of the token in the document:

A direct index is a table mapping term ID `tid` to document’s ID and position (`did`,`pos`). Such table, shown in the left-hand side of Fig. 14.6, makes searching for all documents containing a token very inefficient (one has to scan the entire table). An inverted index is a table obtained by “transposing” the previous one (right-hand side of Fig. 14.6), and giving for each token the list of documents that contain it.

14.6 Information retrieval and ranking

After the raw content of the web is properly saved and preprocessed (indexed), let’s now consider the more interesting task of searching for documents, and searching for information within documents, also called Information retrieval (IR). In general, one wants to retrieve documents which are *relevant* to a query and which are of *good quality*. If one

[1] WILLIAM SHAKESPEARE — *The Life and Death of Richard the Second*, Act IV, Scene 1.

d_1 = My$_1$ care$_2$ is$_3$ loss$_4$ of$_5$ care$_6$, by$_7$ old$_8$ care$_9$ done$_{10}$.

d_2 = Your$_1$ care$_2$ is$_3$ gain$_4$ of$_5$ care$_6$, by$_7$ new$_8$ care$_9$ won$_{10}$.

tid	did	pos
my	1	1
care	1	2
is	1	3
⋮	⋮	⋮
new	2	8
care	2	9
won	2	10

tid	pos list
my	d_1/1
care	d_1/2,6,9 // d_2/2,6,9
is	d_1/3 // d_2/3
loss	d_1/4
of	d_1/5 // d_2/5
by	d_1/7 // d_2/7
old	d_1/8
done	d_1/10
your	d_2/1
gain	d_2/4
new	d_2/8
won	d_2/10

Figure 14.6: Two documents (top) and their direct (left) and inverted (right) index, from [75].

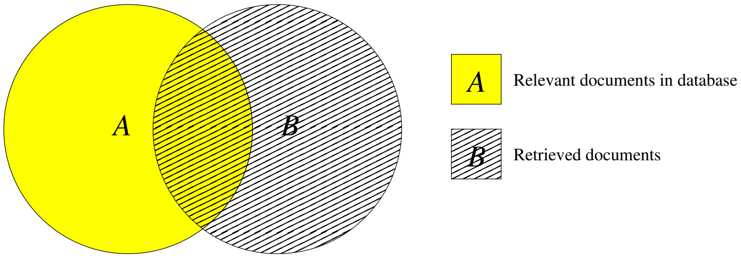


Figure 14.7: Information retrieval: relevant and retrieved documents.

searches for "loss" and "care" one may retrieve a piece by Shakespeare, as well as documents about, let's say, "hair loss care," which are probably of inferior quality, if you are interested in literature and not in hair loss.

Standard definitions of performance measures when retrieving documents are as follows. If A is the set of relevant documents, and B the set of retrieved documents, see also Fig. 14.7 and Fig. 3.5 in Section 4.3, one identifies:

- retrieved relevant items (true positives): $A \cap B$;
- retrieved irrelevant items (false positives): $B \setminus A$;
- unretrieved relevant items (false negatives): $A \setminus B$.

The **precision** of a retrieval system is defined as the fraction of retrieved documents that is relevant:

$$\text{precision} = \frac{|A \cap B|}{|B|}.$$

The **recall** of the system is defined as the fraction of relevant documents that is retrieved:

$$\text{recall} = \frac{|A \cap B|}{|A|}.$$

The recall measure usually is not so relevant for web searches, where the number of relevant documents typically is too large for a human to examine. For search engines, the order in which results are presented to the user is fundamental. In general, such order implies *ranking* the documents, so an adequate performance measure should favor those methods that place relevant documents in the highest ranks, and show them first in the user browser as response to a search.

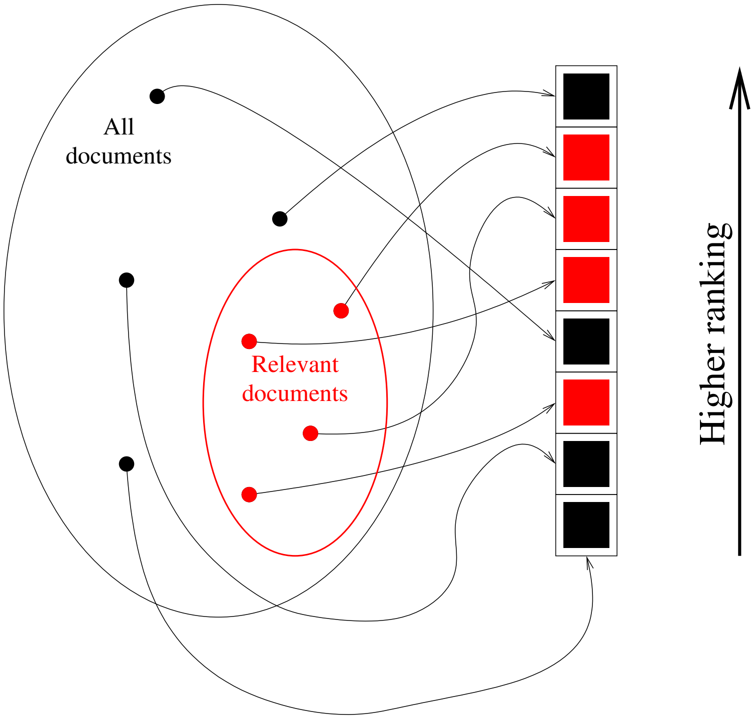


Figure 14.8: A ranking example.

Consider Fig. 14.8, where the darker dots represent relevant documents, while the ranking order is provided on the right. It is clear that the best ranking procedure should place the bright (red) elements in the top positions. Let's introduce more specialized definition of performance to take this into account.

Let D be a corpus of $n = |D|$ documents, and let q be a query. Define $D_q \subset D$ as the set of all relevant documents for query q. We assume that D_q represents the "desired" answer of the system. Let $(d_1^q, d_2^q, \ldots, d_n^q)$ be an ordering ("ranking") of D returned by the system in response to query q. Let $(r_1^q, r_2^q, \ldots, r_n^q)$ be defined as

$$r_i^q = \begin{cases} 1 & \text{if } d_i^q \in D_q \\ 0 & \text{otherwise.} \end{cases}$$

We can now define rank-dependent versions of the recall and precision figures, which will help us answer the question "how would we rate the performance of our system if we only took the top-k ranked answers?"

The recall at rank k is defined as the fraction of relevant documents found in the top k positions:

$$\text{recall}_q(k) = \frac{1}{|D_q|} \sum_{i=1}^{k} r_i^q,$$

and similarly for the precision:

$$\text{precision}_q(k) = \frac{1}{k}\sum_{i=1}^{k} r_i^q.$$

As usual, there are no free meals: when analyzing the ranked list, the recall can be increased by increasing k; but then, more and more irrelevant documents occur, driving down the precision (**precision-recall tradeoff**).

14.6.1 From Documents to Vectors: the Vector-Space Model

To use standard techniques designed for vector spaces to search, cluster, and classify documents, we first need to map each document to a vector (the **vector-space model**).

After preprocessing, our document is now a *bag of words*, actually a bag of tokens, and the most straightforward way to obtain a vector is to: i) fix a set of terms (tokens), ii) have a separate axis to represents each term (token), iii) set the value of the vector along the axis t to zero if the document does not contain the token t, to a number greater than zero if the document contains the token one or more times.

If $n(d,t)$ is the number of times that document d contains the term t, the **term frequency** TF(d,t) of term t in document d is defined as a figure that increases monotonically with the relative frequency of t in d. Some possible definitions are the following:

$$\begin{aligned}
\text{TF}(d,t) &= \frac{n(d,t)}{\sum_\tau n(d,\tau)} \\
\text{TF}_{\text{SMART}}(d,t) &= \begin{cases} 0 & \text{if } n(d,t)=0 \\ 1+\log\bigl(1+\log n(d,t)\bigr) & \text{otherwise.} \end{cases}
\end{aligned}$$

The TF$_{\text{SMART}}$ formula is meant to avoid an exaggerated value along a dimension if a term is present too many times. This was a frequent case in the initial years of the web, when simple search engines were just counting term occurrences. It used to be that many pages contained for example the term “sex” repeated hundreds of times, aiming at reaching a high rank for many users searches. Actually, the more recent search engines combat this kind of spamming by using the hyperlink information, as we will see later.

Actually, often the most interesting terms are the ones which do not appear in many documents (**rare terms** like “C++”, “Reactive Search Optimization”, “stochastic” are probably more informative than “is”, “nice”, “free”, “excellent”), and an **inverse document frequency** can be defined as a figure that monotonically *decreases* as the overall frequency of a term in the whole document corpus increases:

$$\text{IDF}(t) = \log\frac{1+|D|}{|D_t|},$$

where D_t is the set of documents containing term t, and the logarithm is used to avoid an exaggerated multiplier for very rare terms. Let’s note that the above methods to derive vectors are heuristic and not based on fundamental principles like information theory. If you think that the logarithm is not appropriate, feel free to experiment with other functions. After discounting the importance of weak terms appearing in too many documents, a specific document d in TF-IDF space (term-frequency inverse-document-frequency) is represented by vector

$$\boldsymbol{d} = (d_t)_{t\in\text{terms}} \in \mathbb{R}^{\text{terms}},$$

where component d_t is

$$d_t = \text{TF}(d,t)\,\text{IDF}(t).$$

A query q is a sequence of terms, therefore it admits a representation $\boldsymbol{q} = (q_t)$ in the same space as documents. Given the query $\boldsymbol{q}$ and the document $\boldsymbol{d}$, one can now measure their proximity, by considering vector-space similarity measures, as shown in Fig. 14.9. Two frequently used proximity measures in TF-IDF space are listed below.

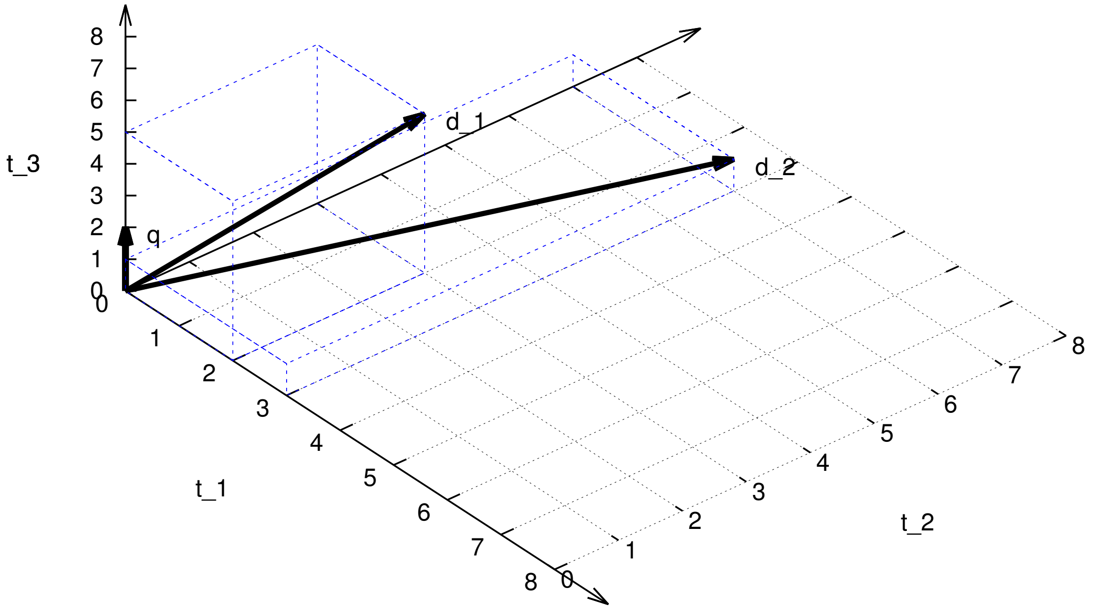


Figure 14.9: Geometric Interpretation.

- Euclidean distance $\|\boldsymbol{d}-\boldsymbol{q}\|$. To avoid artifacts, vectors should be normalized,i.e., an n-fold replica of document $\boldsymbol{d}$ should have the same similarity to $\boldsymbol{q}$ as $\boldsymbol{d}$ itself:

$$\left\| \frac{\boldsymbol{d}}{\|\boldsymbol{d}\|} - \frac{\boldsymbol{q}}{\|\boldsymbol{q}\|} \right\|.$$

- Cosine similarity, i.e., the cosine of the angle between vectors $\boldsymbol{d}$ and $\boldsymbol{q}$:

$$\frac{\boldsymbol{d}\cdot\boldsymbol{q}}{\|\boldsymbol{d}\|\;\|\boldsymbol{q}\|},$$

  see also equation (17.3).

An Information Retrieval system based on TF-IDF coordinates therefore works as follows. First build an inverse index with TF(t,d) and IDF(t) information. When given a query, map it onto TF-IDF space, sort documents according to the similarity metric, return the most similar documents. Searching methods can be extended in different ways, for example to search for phrases. The book [75] presents more details on the topic which cannot be presented in this short introductory chapter.

Please note that there is nothing magic in the traditional TF-IDF representation: it is just a heuristic recipe to give more weight to more informative words, so that the standard metrics given above can produce reasonable results. More sophisticated metric-learning or feature-selection methods based on information content (like mutual information) can lead to superior results but require a deeper knowledge.

14.6.2 Relevance feedback

As mentioned above, after transforming the query into a vector, a vector-similarity measure can be used to identify a set of most similar documents to return to the user.

Unfortunately, the average web query is as few as one or two terms long, and it is not surprising that a lot of irrelevant documents can be retrieved. This is why either a serious measure to rank qualitatively superior documents is needed (like PageRank in Section 14.7) or at least a way to rapidly get **feedback from the user** and use it to form a better query.

Rocchio's Method is based on updating the vector used for the first query to make it more similar to vectors describing documents that the user identifies as relevant (likes), and less similar to the ones classified as irrelevant (dislikes), as illustrated in Fig. 14.10. For a mental image, think about documents that the user liked *attracting* the query vector, and documents that he disliked *repelling it*. In details, the query vector is updated as:

$$\boldsymbol{q}' = \alpha \boldsymbol{q} + \beta \sum_{\boldsymbol{d}\in D_+} \boldsymbol{d} - \gamma \sum_{\boldsymbol{d}\in D_-} \boldsymbol{d},$$

where D_+ is a set of retrieved documents liked by the user, and D_- is a set of retrieved documents that the user dislikes. Parameters α, β and γ control the amount of modification. The careful reader may notice a resemblance with the way in which prototype vectors are updated in the self-organizing maps in Chapter 19.

14.6.3 More complex similarity measures

In a TF-IDF vector space, we can define the "similarity" between two items as a decreasing function of distance — its inverse, for example, although it goes to infinity when comparing an object to itself, requiring some correction. If the elements admit a set representation, another similarity criterion is available, the *Jaccard coefficient*. Let A and B be two (finite) sets, the Jaccard coefficient of A and B is defined as

$$r'(A,B) = \frac{A \cap B}{A \cup B}.$$

Its aim should be clear: compare what is common to the two sets (their intersection) to their total size. It varies between 0 and 1, where $r'(A,B) = 0$ implies that the two sets have no common element and $r'(A,B) = 1$ means that A and B are equal. An additional important property is that $1 - r'(A,B)$ is a *distance*, it obeys all the properties of a metric.

Let us adopt a more document-centric definition. If d is a document, let's define $T(d)$ as the set of tokens (terms) it contains. Note that, as always when referring to sets, elements have no multiplicity and we are just interested in a binary model where a term either occurs or does not. Then, the *Jaccard coefficient* of the two documents is

$$r'(d_1,d_2) = \frac{|T(d_1) \cap T(d_2)|}{|T(d_1) \cup T(d_2)|}.$$

The use of the Jaccard coefficient in search can be motivated as follows: a query is usually seen by the user as a set of terms without repetitions, and no user would ever write a query such as "reactive reactive search" into Google expecting it to return documents containing the word "reactive" twice as frequently as the word "search".

The skeleton of an algorithm for computing the *Jaccard coefficient* $r'(\cdot,\cdot)$ is the following one.

- For each $d \in D$:
  - for each term $t \in T(d)$: put record (t,d) on file f_1.

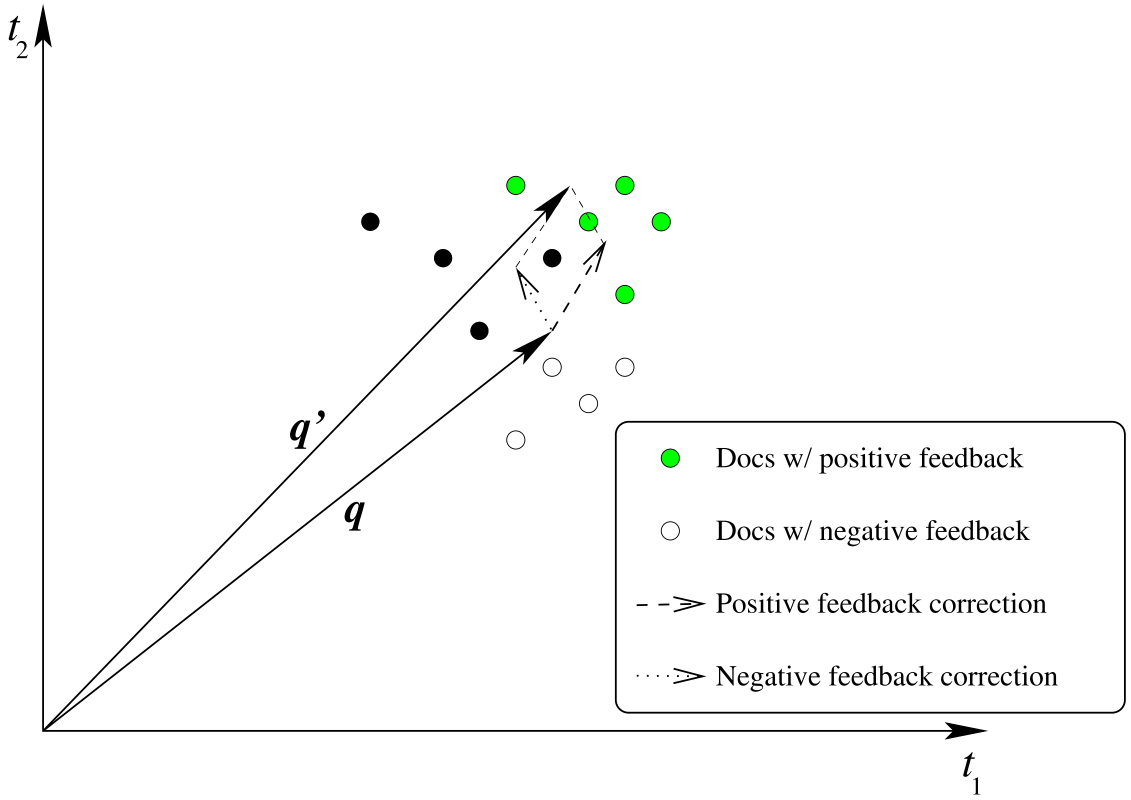

t_2
t_1
q'
q
Docs w/ positive feedback
Docs w/ negative feedback
Positive feedback correction
Negative feedback correction

Figure 14.10: Rocchio's method.

- Sort f_1 in (t, d) order and aggregate into form (t, D_t).
- For each term t scanned from f_1:
  - for each pair $d_1, d_2 \in D_t$: put record (d_1, d_2, t) on file f_2.
- Sort f_2 on (d_1, d_2) and aggregate by adding on the third field.

Some possible tricks to reduce the search cost are related to pre-computing the Jaccard coefficient for all pairs of documents and queries, which can require huge amounts of storage and CPU time, or reducing the set of pairs, by pre-associating every document or query to a list of a small and fixed number of the most similar documents. In addition, very frequent terms (having low IDF) can be omitted entirely from consideration.

In practice, in many cases one is interested in *approximating* the coefficient. An interesting randomized algorithm using random permutations is available.

If one uses probabilities, given sets A and B, one starts from this interesting equality:

$$\frac{|A \cap B|}{|A \cup B|} = \Pr(x \in A \cap B | x \in A \cup B).$$

If we can estimate the above probability, we can estimate the Jaccard coefficient. What we can do is to generate random elements in the set $S \subset \{1, \ldots, n\}$ and to estimate the probability by the ratio of events.

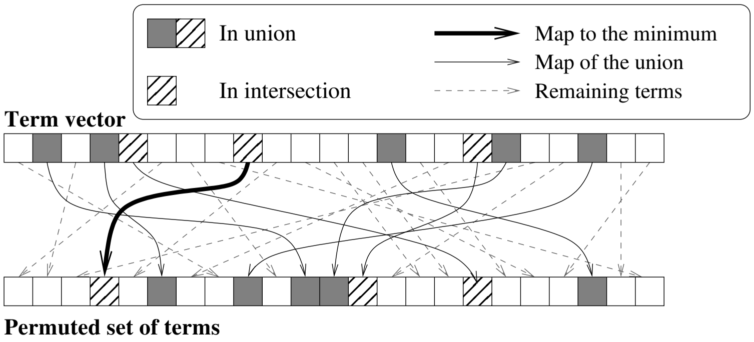


Figure 14.11: Building a permutation.

To select a random element from a set $S \subset \{1, \dots, n\}$ one can select a random permutation π on n elements and pick the element in S such that its image in π is minimum:

$$x = \arg\min_{x \in S} \pi(x) = \arg\min \pi(S)$$

When applied to $A \cup B$, this method locates an element in the intersection if and only if

$$\min \pi(A) = \min \pi(B).$$

We can therefore estimate the above ratio by applying random permutations and checking if the two minima are coincident.

Let's demonstrate why permutations work. Given sets $A, B \subset \{1, \dots, n\}$, to derive the probability that the two minima are coincident, let us count how many permutations $\pi : \{1, \dots, n\} \to \{1, \dots, n\}$ (of the $n!$ possible) have the property

$$\min \pi(A) = \min \pi(B)$$

by building one such permutation. From Fig. 14.11 it should be clear that:

- The image of $A \cup B$ (lighter and darker squares) can be chosen in $\binom{n}{|A \cup B|}$ different ways.
- Within such image, the minimum element can be chosen within the $|A \cap B|$ elements that form the intersection (thick arrow).
- The remaining elements in the image of $A \cup B$ can be permuted in $(|A \cup B| - 1)!$ ways (thin arrow).
- The elements not in $A \cup B$ can be permuted in any of $(n - |A \cup B|)!$ ways (light arrows).

After multiplying all these, one obtains:

$$\binom{n}{|A \cup B|} \cdot |A \cap B| \cdot (|A \cup B| - 1)! \cdot (n - |A \cup B|)! = n! \frac{|A \cap B|}{|A \cup B|},$$

and after dividing by the total number of permutations one derives the desired equality.

A randomized but inefficient algorithm is as follows:

- generate a set Π of m permutations on the set of terms;
- $k \leftarrow 0$

- for each $\pi \in \Pi$:
    - if $\min \pi(T(d_1)) = \min \pi(T(d_2))$ then $k \leftarrow k + 1$;
- estimate $r'(d_1, d_2) \approx \dfrac{k}{m}$.

By combining a randomized algorithm with suitable data structures working on external storage and simultaneous computation of the coefficients for many documents, one manages to deal with the enormous amount of documents contained in the world wide web!

14.7 Using the hyperlinks to rank web pages

There are so many web pages that the issue is not only that of retrieving a few set of pages relevant to the query, but that of retrieving a set of *high quality* and relevant pages. The issue predates the web and is encountered also when reading books, or papers. One would like to concentrate on good quality papers written on a subject, without wasting time on poor quality ones. In scientific communities, a paper is considered of good quality if it is *cited* by other good quality papers, meaning that some colleagues found the paper useful and acknowledged it by putting it the list of citations. For a more mundane analogy, a candidate for employment is valued if many other valued people recommend him. In general, see also Fig. 14.12, in a social network of relationships between people, a high reputation is obtained by having other highly-reputed people recommending you. It is not sufficient to convince many low-rank individuals to support you, there are no shortcuts!

After a seminal paper by Marchiori [260] highlighting the importance of *hyper-information* (information in the hyperlinks), Larry Page and Sergey Brin developed the PageRank algorithm, which follows the same basic social networks principles, by substituting “recommendations” and “citations” with hyperlinks [286] (the authors then became Google founders). They define a “measure of prestige” such that the prestige of a page is related to how many pages of prestige link to it. Let’s note that this is a *recursive definition*. To measure the prestige of a page one needs to have the prestige of pages pointing to it, and so on. In short, their solution is: start with an initial distribution of prestige values, iterate the prestige calculation for the different nodes, and stop when the values do not change too much after recalculation, as simple as that! At first reading, this process seems prone to pitfalls. What guarantee do we have that the process converges, hopefully to the same limiting distribution, not depending on the initial distribution of values?

Now: it is fascinating how the solution to this problem is related to basic linear algebra concepts of **eigenvalues and eigenvectors**, as well as concepts related to **Markov chains**. Let’s summarize the main relationships.

First, let’s see how iterating the prestige calculation after starting from an initial distribution is related to the classic **power iteration method for finding the dominant eigenvector** of a matrix. We proceed very rapidly, skipping mathematical details, only to give the flavor of the method.

The rank of a page is calculated by examining the incoming links (the hyper-links of other pages pointing to the given page). Each incoming link from page i contributes a partial rank equal to the rank of i divided by the number of i’s outgoing links, as shown in Fig. 14.13. The human motivation for the division is clear: a page of high rank but pointing to a very large number of pages is like a person of good quality but recommending a too large number of people. Without the division, the owner of a top-ranked page could influence all pages in the world just by putting an enormous number of outgoing links.

Given the above recalculation rule, once the network of hyper-links is given, the computation of new rank values $\mathbf{p}^k$ at iteration k is obtained by a *linear* transformation of the previous values through a matrix, which we denote as M, as follows:

$$\mathbf{p}^k = M\mathbf{p}^{k-1}.$$

The matrix M will depend only on the connectivity structure, on the links between pages. Now, after starting from the initial rank distribution $\mathbf{p}^0$ and executing k recalculations:

$$\mathbf{p}^k = M^k\mathbf{p}^0.$$

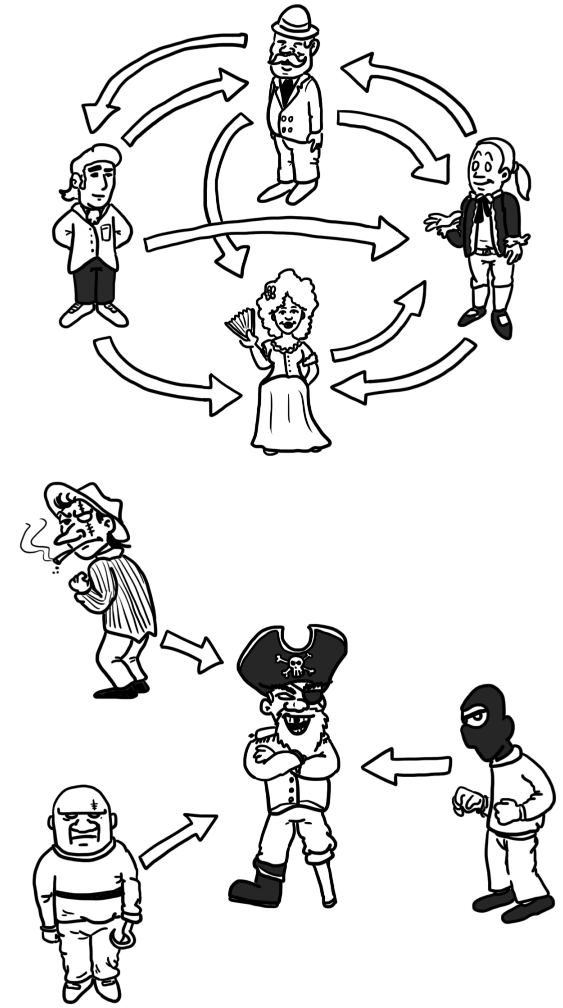


Figure 14.12: Prestige in social networks: recommendations from (or relationship with) high-rank individuals (above) are more effective to reach a high rank than recommendations by low-rank ones (below).

Assume that a basis of eigenvectors of M is available, let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the n eigenvalues, and let $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ be the corresponding eigenvectors. Suppose that λ_1 is the dominant eigenvalue, so that $|\lambda_1| > |\lambda_j|$ for $j > 1$.

The initial vector $\mathbf{p}^0$ can be written as a linear combination of the basis vectors:

$$\mathbf{p}^0 = c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \cdots + c_n\mathbf{v}_n.$$

If $\mathbf{p}^0$ is chosen randomly (with uniform probability), then $c_1 \neq 0$ with probability 1. Now, using linearity and the defining property of eigenvectors, one immediately obtains:

$$\begin{aligned} M^k\mathbf{p}^0 &= c_1 M^k\mathbf{v}_1 + c_2 M^k\mathbf{v}_2 + \cdots + c_n M^k\mathbf{v}_n \\ &= c_1\lambda_1^k\mathbf{v}_1 + c_2\lambda_2^k\mathbf{v}_2 + \cdots + c_n\lambda_n^k\mathbf{v}_n \\ &= c_1\lambda_1^k\left(\mathbf{v}_1 + \frac{c_2}{c_1}\left(\frac{\lambda_2}{\lambda_1}\right)^k\mathbf{v}_2 + \cdots + \frac{c_n}{c_1}\left(\frac{\lambda_n}{\lambda_1}\right)^k\mathbf{v}_n\right). \end{aligned}$$

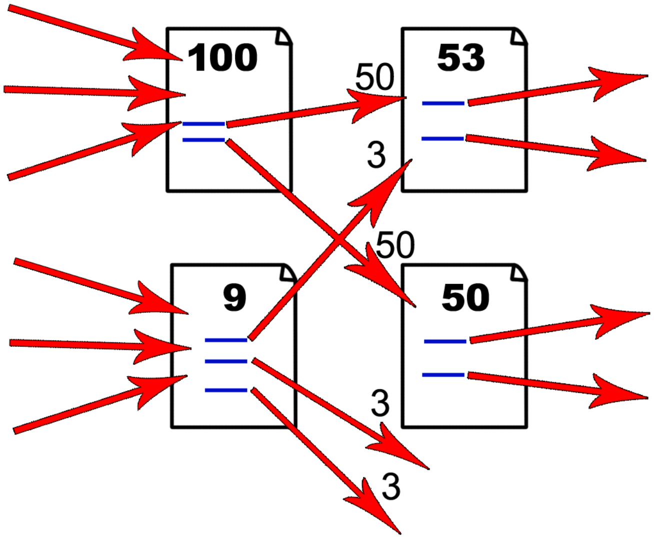


Figure 14.13: Recalculating the rank of a page in PageRank. The initial rank is distributed along the outgoing links (adapted from the original paper).

When the number of recalculations k, equal to the power of the matrix M^k, goes to infinity, all terms tend to zero apart from the one proportional to the dominant eigenvector. A simple iteration of matrix multiplication after starting from almost arbitrary initial conditions is indeed sufficient to extract the dominant eigenvector!

Let's now consider a different interpretation related to Markov chains, and imagine that you want to analyze a system representing the **movement of a web surfer** on the various web pages. Assume that a surfer is navigating through outgoing links forever, picking them uniformly at random. Let the starting page u be taken with probability p_u^0. Let E be the adjacency matrix of the web: $(u, v) \in E$ (or $E_{uv} = 1$) if and only if there is a link from page u to page v. What is the probability p_v^i of the surfer being at page v after i clicks?

Let's start with a single step. What is the probability p_v^1 that surfer is at page v after one step? Let

$$N_u = \sum_v E_{uv}$$

be the *out-degree* of page u (sum of u-th row of E). Suppose no parallel edges exist,

$$p_v^1 = \sum_{(u,v)\in E} \frac{p_u^0}{N_u}.$$

By normalizing E to have row sums equal to 1

$$L_{uv} = \frac{E_{uv}}{N_u},$$

we get

$$p_v^1 = \sum_u L_{uv} p_u^0 \qquad \text{or} \qquad \mathbf{p}^1 = L^T \mathbf{p}^0.$$

Let's now consider the situation after i steps:

$$\mathbf{p}^i = L^T \mathbf{p}^{i-1}.$$

If E is *irreducible* and *aperiodic* (none is actually true but the problem can be cured), then

$$\lim_{i\to\infty} \mathbf{p}^i = \mathbf{p},$$

where $\mathbf{p}$ is the principal eigenvector of L^T, a.k.a. its *stationary distribution*:

$$\mathbf{p} = L^T \mathbf{p} \qquad \text{(eigenvalue is 1).}$$

But p_u it the *prestige* of page u determined also by the previous interpretation. It is now clear how the prestige can be interpreted also as probability that a random surfer following links will be found at a given page.

Let's now deal with bad properties of real-world transition matrices. Surveys show that the Web is not strongly connected, and that random walks can be trapped into cycles. A possible fix is to introduce a "damping factor" corresponding to a user that occasionally stops following links: with an arbitrary probability d of going to a random page (even unconnected) at every step. The transition becomes:

$$\mathbf{p}^i = \left((1-d)L^T + \frac{d}{N}\mathbf{1}_N\right)\mathbf{p}^{i-1}.$$

The eigenvector of the matrix corresponding to the largest eigenvalue can be obtained as follows.

- Start with random vector $\mathbf{p} \leftarrow \mathbf{p}^0$;
- repeat:
  - update vector:
  $$\mathbf{p} \leftarrow \left((1-d)L^T + \frac{d}{N}\mathbf{1}_N\right)\mathbf{p};$$
  - from time to time, normalize it:
  $$\mathbf{p} \leftarrow \frac{\mathbf{p}}{\|\mathbf{p}\|_1}.$$

Normalization avoids very large components and therefore numerical problems with finite-precision computation. Of course, for the application we are not interested in *absolute* prestige values but in *relative* ones. The absolute values depend on the chosen range (one may measure prestige on a range from 0 to 10, or on a range from 0 to 100, etc.) but what is relevant is that a page is, say, three times more prestigious than another one. Normalization is a simple way to discount multiples of the given normalized eigenvector.

In practical applications, the notion of prestige is so fuzzy that nobody will ever care about obtaining the actual eigenvector with high precision! To have a flavor of how long is required for convergence, in his original paper Page says that 52 iterations are enough for about 3×10^8 pages, quite an exciting result paving the way to significant business applications.

14.8 Identifying hubs and authorities: HITS

Let's now consider a different analysis of the web. In a scientific community all good articles are either seminal (i.e., many others reference to them) or surveys (i.e., they reference to many others). In the web, pages may be *authorities* or *hubs* [146]. For example portals are very good hubs, even if they do not contain significant information, and they are used only as starting points to reach good quality pages.

To reflect this distinction, let's introduce *two* score measures, called **hubness** and **authority**:

$$\boldsymbol{h} = (h_u), \qquad \boldsymbol{a} = (a_u).$$

Let's now summarize the HITS algorithm (Hyperlink-Induced Topic Search). In the HITS algorithm, the first step is to retrieve the set of results to the search query. Given query q, let R_q be the *root set* returned by an IR system. The computation is performed only on this result set, not across all Web pages. Authority and hub values are defined in terms of one another in a mutual recursion.

The *expanded set* is formed by adding all nodes linked to the root set:

$$V_q = R_q \cup \{u : ((u \to v) \vee (v \to u)) \wedge v \in R_q\}.$$

Let E_q be the induced link subset, $G_q = (V_q, E_q)$. The recurrent relationship is defined as follows. Let the hub score h_u be proportional to sum of referred authorities, let the authority score a_u be proportional to the sum of referring hubs.

$$\begin{aligned} \boldsymbol{a} &= E^T \boldsymbol{h} \\ \boldsymbol{h} &= E \boldsymbol{a}. \end{aligned}$$

The iterated method is therefore given by:

- initialize $\boldsymbol{a}$ and $\boldsymbol{h}$ (e.g., uniformly) ;
- repeat:
  - $\boldsymbol{h} \leftarrow E\boldsymbol{a}$;
  - $\boldsymbol{a} \leftarrow E^T\boldsymbol{h}$;
  - normalize $\boldsymbol{h}$ and $\boldsymbol{a}$.

The top-ranking authorities and hubs are reported to the user.

The principal eigenvector identifies the largest dense bipartite subgraph. To find smaller sets, the other eigenvectors must be explored. There are iterative methods that remove known eigenvectors from a system: they reduce the search subspace once an eigenvector is identified.

Although of theoretical interest, HITS is not commonly used by search engines, also because pre-computing hubness and authority values for different queries is not doable in practice, the algorithm has to run after the query is executed and this makes the algorithm very heavy for general-purpose usage. Coming back to the PageRank algorithms, let's note that it is independent of page content and therefore a suitable combination with the content, depending on the query, must be executed. Google's way of combining query and ranking is unknown. Probably, empirical parameters and manual inspection are necessary.

14.9 Clustering

The motivations for clustering are related to the huge number of documents retrieved by web searches. To avoid overloading the user, identifying groups of closely related documents is useful, for example to show only a small number of representative prototypes.

Automatically identified clusters can also be a help for later manual classification à la Yahoo. In addition, if a user is interested in document d, he is likely to be interested in documents in the same cluster and therefore pre-computed clusters permit to obtain more documents similar to the one under examination on demand.

Let's note that queries can be ambiguous, especially *web* queries. For example, if one searches for `star`, one may look for movie stars, or for celestial objects, clearly two very different topics.

Mutual similarities in term vector space can help grouping similar documents together, i.e., to find “clusters” of documents. Let D be the corpus of documents (or other entities) to be grouped together by similarity. Items $d \in D$ are characterized either *internally* by some intrinsic property (e.g., terms contained, coordinates in TF-IDF space) or *externally* by a measure of distance $\delta(d_1, d_2)$ or similarity $\rho(d_1, d_2)$ between pairs. Examples are: Euclidean distance, dot product, Jaccard coefficient. After defining the metric, the usual bottom-up or top-down clustering techniques can be used. The methods are explained in Chapter 17 and 18.

Gist

Some interesting applications involve more **structure** than simple “flat” vectors of measures, for example **relationships between entities modeled by graphs and networks**. In this case **probabilistic graphical models** like Bayesian networks or Markov networks and Inductive Logic Programming can be used to describe the initial knowledge, refine it based on examples, build symbolic (human) explanations usable for debugging the knowledge and for explaining how a certain conclusion has been reached.

Web and text-mining are highly-relevant application areas with a vast expanse of data, some of it structured, some partially structured or not at all. **Crawling and indexing** are systematic methods to visit web pages, harvest the information contained therein and prepare data structures for searching, information retrieval and ranking.

By transforming text into vectors of data (e.g., frequencies of selected words as in the **vector-space model**) some traditional ML techniques can be reused, but the richer amount of structure in web documents permits a more focused analysis.

Web-mining schemes find explicit relationships between documents (web links), infer implicit ones (by clustering), rank the most relevant pages in a network of connected sites or identify the most relevant and well-connected person in a network of people. Abstraction helps to use similar tools for networks of pages and networks of people. As a notable example, the use of hyperlinks and linear algebra tools (eigenvectors and eigenvalues), previously used to rank researchers in bibliometrics, leads to a very powerful technique to **rank web pages**, now at the basis of Google search-engine technology.

From now on, you will look at your hyperlinks, Facebook “Likes” and Twitter “Followers” (or at the social network software which will be the most popular when you read this book) with new analytic and aware eyes.

Chapter 15

Democracy in machine learning

While in every republic there are two conflicting factions, that of the people and that of the nobles, it is in this conflict that all laws favorable to freedom have their origin.
(Machiavelli)

This is the final chapter in the supervised learning part. As you discovered, there are *many* competing techniques for solving the problem, and each technique is characterized by choices and meta-parameters: when this flexibility is taken into account, one easily ends up with **a very large number of possible models for a given task**.

When confronted with this abundance one may just select the best model (and best meta-parameters) and throw away everything else, or recognize that there's never too much of a good thing and try to use all of them, or at least the best ones. One already spends effort and CPU time to select the best model and meta-parameters, producing many models as a byproduct. Are there sensible ways to recycle them so that the effort is not wasted? Relax, this chapter does not introduce radically new models but deals with **using many different models in flexible, creative and effective ways**. The advantage is in some cases so clear that using many models will make a difference between winning and losing a competition in ML.

The *leitmotif* of this book is that many ML principles resemble some form of human learning. Asking a **committee of experts** is a human way to make important decisions, and committees work well if the participants have different competencies and comparable levels of professionalism. Diversity of background, culture, sex is assumed to be a critical component in successful innovative businesses. Democracy itself can be considered as a pragmatic way to pool knowledge from citizens in order to reach workable decisions (well, maybe not always optimal but for sure better than decisions by a single dictator).

We already encountered a creative usage of many classification trees as **classification forests** in Chapter 6 (Sec. 6.2). In this chapter we review the main techniques to make effective use of more and different ML models with a focus on the architectural principles and a hint at the underlying math.

15.1 Stacking and blending

If you are participating in a ML competition (or if you want to win a contract or a solution to a critical need in a business), chances are you will experiment with different methods and come up with a large set of models. Like for good coffee, blending them can bring higher quality.

The two straightforward ways to combine the outputs of the various models are by **voting** and by **averaging**. Imagine that the task is to classify patterns into two classes. In voting, each trained model votes for a class, votes are collected and the final output class is the one getting more votes, exactly as in a basic democratic process based on **majority**. If each model has a probability of correct classification greater than $1/2$, **and if the errors of the different models are uncorrelated, then the probability that the majority of M models will be wrong goes to zero** as the number of models grows. The demonstration is simple by measuring the area under the binomial distribution where more than $M/2$ models are wrong. Unfortunately errors tend to be *correlated* in practical cases. If a pattern is difficult to recognize, it will be difficult for *many* models, and the probability that many of them will be wrong will be higher than the product of individual mistake probabilities so that the advantage will be less dramatic. Think about stained digits in a zip code on a letter: the stain will create hard difficulties to *many* models and therefore correlate their mistakes.

If the task is to predict a probability (a posterior probability for a class given the input pattern), averaging individual probabilities is another option. By the way, averaging the results of experimental measures is the standard way to **reduce variance**. The "law of large numbers" in statistics explains why, under certain conditions, the average of the results obtained from a large number of trials tends to be close to the expected value, and why it tends to become closer as more trials are performed.

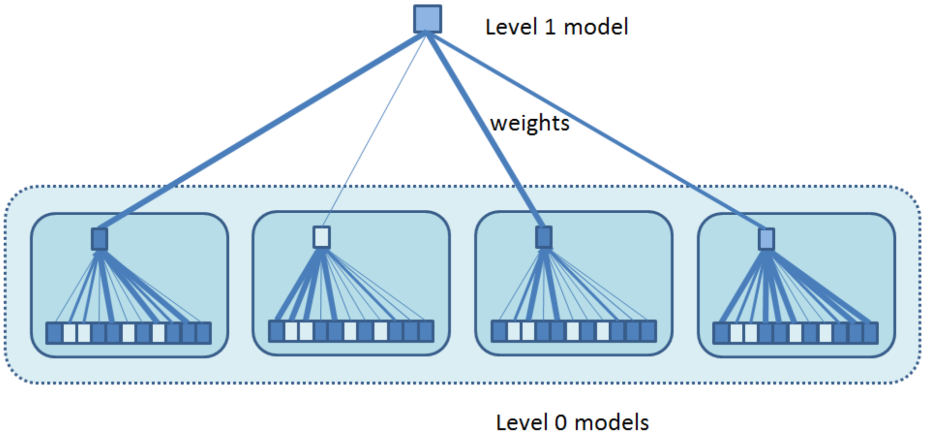


Figure 15.1: Blending different models by adding an additional model on top of them (stacking).

Although straightforward, averaging and voting share a weakness: they treat all models equally and the performance of the very best models can vanish amidst a mass of mediocre models. The more complex a decision, the more the different **experts have to be weighted, and often weighted in a manner which depends on the specific input**.

You already have a hammer for nailing also this issue of weighting experts: machine learning itself! Just add another linear model on top, connect the different outputs by the level-0 models (the experts) and let ML identify the optimal weights (Fig. 15.1). This is the basic idea of **stacked generalization** [385]. To avoid overtraining one must take care that the training examples used for training the stacked model (for determining the weights of the additional layer on top) were *never* used before for training the individual models. Training examples are like fish: they stink if you use them for too long!

Results in stacked generalization are as follows [359]:

- When you can, **use class probabilities** as outputs of the original level-0 models (instead of class predictions). Estimates of probabilities tell something about the *confidence*, and not just the prediction. Keeping them will give more information to the higher level.

- Ensure **non-negative weights** for the combination by adding constraints in the optimization task. They are necessary for stacked regression to improve accuracy. They are not necessary for classification task, but in both cases they increase the **interpretability** of the level-1 model (a zero weight means that the corresponding 0-level model is not used, the higher the weight, the more important the model).

If your appetite is not satisfied, you can experiment with more than one level, or with more structured combination. For example you can stack a level on top of MLPs and decision forests, or combine a stacked model already done by a group with your model by adding yet another level (Fig. 15.2). The more models you manage, the more careful you have to be with the "stinking example" rule above. The higher-level models do not need to be linear: some interpretability will be lost, but the final results can be better with nonlinear combining models.

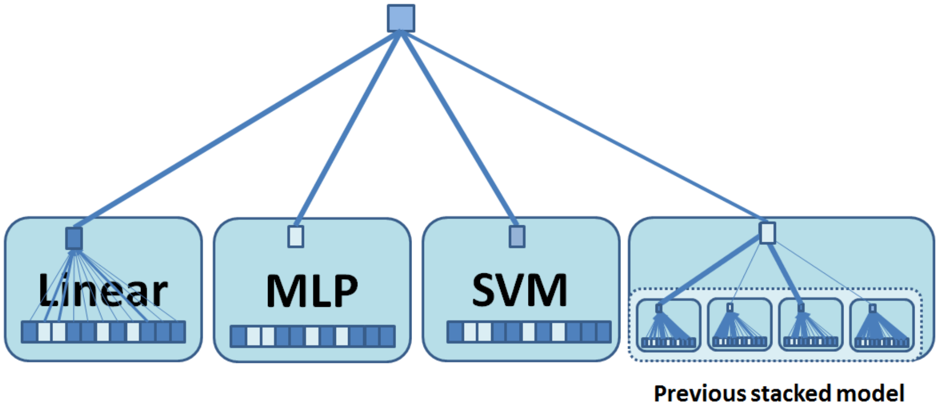


Figure 15.2: Stacking can be applied to different models, including previously stacked ones.

An interesting option is the **feature-weighted linear stacking** [332]. We mention it as an example of how a specific real-world application can lead to an elegant solution. In some cases, one has some additional information, called "**meta-features**" in addition to the raw input features. For example, if the application is to predict preferences for customers for various products (in a *collaborative filtering and recommendation* context), the reliability of a model can vary depending on the additional information. For example, a model *A* may be more reliable for users who rated many products (in this case, the number of products rated by the user is the "meta-feature"). To maintain linear regression while allowing for weights to *depend* on meta-features (so that model *A* can have a larger weight when used for a customer who rated more products), one can ask for weights to be *linear in the meta-features*. If $g_i(\boldsymbol{x})$ is the output for level-0 model i and $f_j(\boldsymbol{x})$ is the j-th meta-feature, weights will be

$$w_i(\boldsymbol{x}) = \sum_j v_{ij} f_j(\boldsymbol{x}),$$

where v_{ij} are the parameters to be learned by the stacked model. The level-1 output will be

$$b(\boldsymbol{x}) = \sum_{i,j} v_{ij} f_j(\boldsymbol{x}) g_i(\boldsymbol{x}),$$

leading to the following **feature-weighted linear stacking** problem:

$$\min_{(v_{ij})} \sum_{\boldsymbol{x}} \sum_{i,j} \big(v_{ij} f_j(\boldsymbol{x}) g_i(\boldsymbol{x}) - y(\boldsymbol{x})\big)^2.$$

Because the model is still linear in v, we can use standard linear regression to identify the optimal v. As usual, never underestimate the power of linear regression if used in proper creative ways.

15.2 Diversity by manipulating examples: bagging and boosting

For successful democratic systems in ML one needs **a set of accurate and diverse classifiers**, or regressors, also called **ensemble**, like a group of musicians who perform together. **Ensemble methods** is the traditional term for these techniques in the literature, **multiple-classifiers systems** is a synonym.

Different techniques can be organized according to the main way in which they create diversity [116].

Training models on **different subsets of training examples** is a possibility. In **bagging** ("bootstrap aggregation"), different subsets are created by random sampling *with replacement* (the same example can be extracted more than once). Each bootstrap replica contains about two thirds (actually $\approx 63.2\%$) of the original examples. The results of the different models are then aggregated, by averaging, or by majority rules. Bagging works well to improve *unstable* learning algorithms, whose results undergo major changes in response to small changes in the learning data. As described in Chapter 6 (Section 6.2), bagging is used to produce **classification forests** from a set of classification trees.

Cross-validated committees prepare different training sets by leaving out disjoint subsets of training data. In this case the various models are the side-effect of using cross-validation as ingredient in estimating a model performance (and no additional CPU is required).

A more dynamic way of manipulating the training set is via **boosting**. The term has to do with the fact that weak classifiers (although with a performance which must be slightly better than random) can be "boosted" to obtain an accurate committee [132]. Like bagging, boosting creates multiple models, but the model generated at each iteration is built in an **adaptive** manner, to directly improve the combination of previously created models. The algorithm `AdaBoost` maintains a set of weights over the training examples. After each iteration, weights are updated so that **more weight is given to the examples which are misclassified** by the current model (Fig. 15.3). Think about a professional teacher, who is organizing the future lessons to insist more on the cases which were not already understood by the students.

The final classifier $h_f(\boldsymbol{x})$ is given by a weighted vote of the individual classifiers, and the weight of each classifier reflects its accuracy on the weighted training set it was trained on:

$$h_f(\boldsymbol{x}) = \sum_l w_l h_l(\boldsymbol{x}).$$

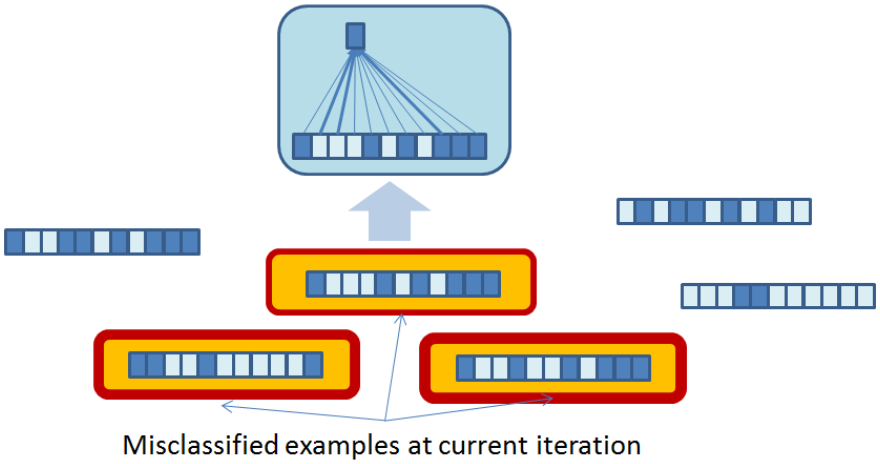


Figure 15.3: In boosting, misclassified examples at the current iteration are given more weight when training an additional model to be added to the committee.

Because we are true believers in the power of optimization, the best way to understand boosting is by the function it optimizes. Different variations can then be obtained (and understood) by changing the function to be optimized or by changing the detailed optimization scheme. To define the error function, let's assume that the outputs y_i of each training example are $+1$ or -1. The quantity $m_i = y_i h(\boldsymbol{x}_i)$, called the *margin* of classifier h on the training data, is positive if the classification is correct, negative otherwise. As explained later in Section 15.6, `AdaBoost` can be viewed as a **stage-wise algorithm** for minimizing the following error function:

$$\sum_i \exp\left(-y_i \sum_l w_l h_l(\boldsymbol{x}_i)\right), \tag{15.1}$$

the negative exponential of the margin of the weighted voted classifier. This is equivalent to **maximizing the margin on the training data**.

15.3 Diversity by manipulating features

Different **subsets of features** can be used to train different models (Fig. 15.4). In some cases, it can be useful to group features according to different characteristics. In [86] this method was used to identify volcanoes on Venus with human expert-level performance. Because the different models need to be accurate, using subsets of features works only when input features are highly redundant.

15.4 Diversity by manipulating outputs: error-correcting codes

Error-correcting codes (ECC) are designed so that they are robust with respect to a certain number of mistakes during transmission by noisy lines (Fig. 15.5). For example, if the codeword for "one" is "`111`" and that for "zero"

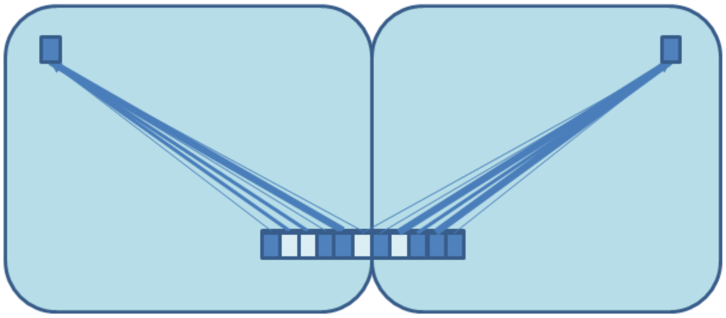


Figure 15.4: Using different subsets of features to create different models. The method is not limited to linear models.

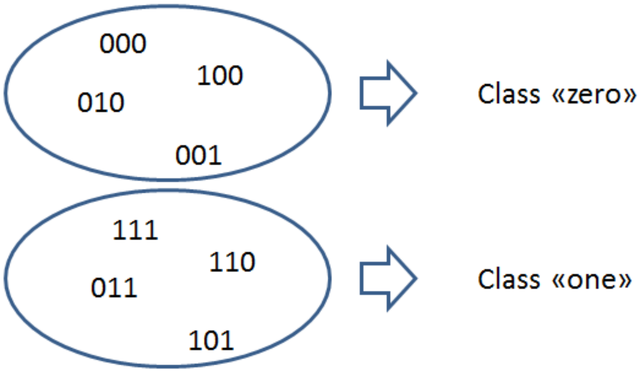


Figure 15.5: In error-correcting codes a redundant encoding is designed to resist a certain number of mistaken bits.

is “000”, a mistake in a bit like in “101” can be accepted (the codeword will still be mapped to the correct “111”). **Error-correcting output coding** is proposed in [117] for designing committees of classifiers.

The idea of applying ECC to design committees is that each output class j is encoded as an L-bit codeword C_j. The l-th trained classifier in the committee has the task to predict the l-th bit of the codeword. After generating all bits by the L classifiers in the committee, the output class is the one with the closest codeword (in Hamming distance, i.e., measuring the number of different bits). Because codewords are redundant, a certain number of mistakes made by some individual classifiers can be corrected by the committee.

As you can expect, the different ensemble methods can be combined. For example, error-correcting output coding can be combined with boosting, or with feature selection, in some cases with superior results.

15.5 Diversity by injecting randomness during training

Many training techniques have randomized steps in their bellies. This randomness is a very natural way to obtain diverse models (by changing the seed of the random number generator). For example, MLP starts from randomized initial weights. Tree algorithms can decide in a randomized manner the next feature to test in an internal node, as it was already described for obtaining decision forests.

Last but not least, most optimization methods used for training have space for randomized ingredients. For example, stochastic gradient descent presents patterns in a randomized order.

15.6 Additive logistic regression

We just encountered boosting as a way of sequentially applying a classification algorithm to re-weighted versions of the training examples and then taking a weighted majority vote of the sequence of models thus produced.

As an example of the power of optimization, boosting can be interpreted as a way to apply **additive logistic regression, a method for fitting an additive model $\sum_m h_m(\boldsymbol{x})$ in a forward stage-wise manner** [133].

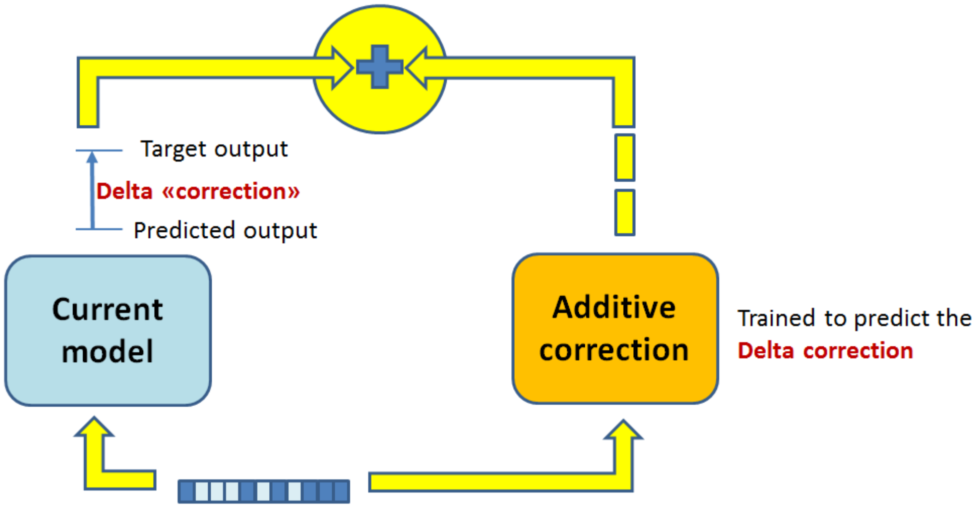


Figure 15.6: Additive model step: the error of the current model on the training examples is measured. A second model is added aiming at canceling the error.

Let's start from simple functions

$$h_m(\boldsymbol{x}) = \beta_m b(\boldsymbol{x}; \boldsymbol{\gamma}_m),$$

each characterized by a set of parameters $\boldsymbol{\gamma}_m$ and a multiplier β_m acting as a weight. One can build an additive model composed of M such functions as:

$$H_M(\boldsymbol{x}) = \sum_{m=1}^{M} h_m(\boldsymbol{x}) = \sum_{m=1}^{M} \beta_m b(\boldsymbol{x}; \boldsymbol{\gamma}_m).$$

With a **greedy forward stepwise approach** one can identify at each iteration the best parameters $(\beta_m, \boldsymbol{\gamma}_m)$ so that **the newly added simple function tends to correct the error of the previous model** $F_{m-1}(\boldsymbol{x})$ (Fig. 15.6). If least-squares is used as a fitting criterion:

$$(\beta_m, \gamma_m) = \arg\min_{(\beta,\gamma)} E\left[\left(y - F_{m-1}(\boldsymbol{x}) - \beta b(\boldsymbol{x};\gamma)\right)^2\right], \tag{15.2}$$

where $E[\cdot]$ is the expected value, estimated by summing over the examples. This greedy procedure can be generalized as **backfitting**, where one iterates by fitting one of the parameters couple (β_m, γ_m) at each step, not necessarily the last couple. Let's note that this method only requires an algorithm for fitting a *single* weak learner $\beta b(\boldsymbol{x};\gamma)$ to data, which is applied repeatedly to modified versions of the original data (Fig. 15.7):

$$y_m \leftarrow y - \sum_{k \neq m} h_k(\boldsymbol{x}).$$

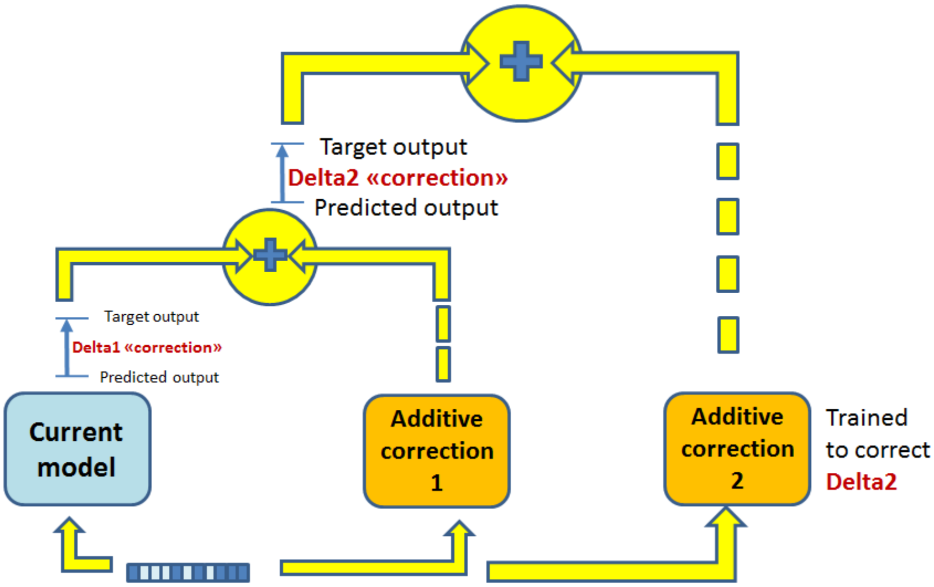


Figure 15.7: The greedy forward step-wise approach in additive models, one iterates by adding new components to cancel the remaining error.

For classification problems, using the squared-error loss (with respect to ideal 0 or 1 output values) leads to trouble. If one would like to estimate the posterior probability $\Pr(y = j|\boldsymbol{x})$, there is no guarantee that the output will be limited in the $[0, 1]$ range. Furthermore, the squared error penalizes not only real errors (like predicting 0 when 1 is requested), but also it **penalizes classifications which are "too correct"** (like predicting 2 when 1 is required).

Logistic regression comes to the rescue (Section 9.1): one uses the additive model $H(\boldsymbol{x})$ for predicting an "intermediate" value, which is then *squashed* onto the correct $[0, 1]$ range by the logistic function to obtain the final output in form of a probability.

An additive logistic model has the form

$$\ln \frac{\Pr(y = 1|\boldsymbol{x})}{\Pr(y = -1|\boldsymbol{x})} = H(\boldsymbol{x}),$$

where the *logit* transformation on the left monotonically maps probability $\Pr(y = 1|\boldsymbol{x}) \in [0, 1]$ onto the whole real axis. Therefore, the logit transform, together with its inverse

$$\Pr(y = 1|\boldsymbol{x}) = \frac{e^{H(\boldsymbol{x})}}{1 + e^{H(\boldsymbol{x})}}, \tag{15.3}$$

guarantees probability estimates in the correct $[0, 1]$ range. In fact, $H(\boldsymbol{x})$ is modeling the *input* of the logistic function in equation (15.3).

Now, if one considers the expected value $E\big[e^{-yH(\boldsymbol{x})}\big]$, one can demonstrate that this quantity is minimized when

$$H(x) = \frac{1}{2} \ln \frac{\Pr(y = 1|\boldsymbol{x})}{\Pr(y = -1|\boldsymbol{x})},$$

i.e., the symmetric logistic transform of $\Pr(y = 1|\boldsymbol{x})$ (note the factor $1/2$ in front). The interesting result is that `AdaBoost` builds an additive logistic regression model via Newton-like updates[1] for minimizing $E\big[e^{-yH(\boldsymbol{x})}\big]$. The technical details and additional explorations are in the original paper [133].

15.7 Gradient boosting machines

Boosting is a very active research area, with a lot of flexibility, speed of realization and successful applications. [135] develops a **general gradient-descent boosting paradigm for additive expansion based on any fitting criterion**. Special enhancements are derived in particular for the case in which additive components are regression trees.

While we refer to the original publication for all theoretical details, we follow the explanation of [84] for the case of convex and differentiable loss functions. The objective is to obtain an **ensemble of k trees**, such that the predicted output $\hat{y}_i$ is given by the sum of the individual trees:

$$\hat{y}_i \;=\; \sum_{k=1}^{K} f_k(\mathbf{x}_i), \quad f_k \in \mathcal{F} \tag{15.4}$$

where $\mathcal{F}$ is the space of regression trees. Each tree partitions the input space into T zones ("leaves"), each zone is associated with a constant output value w, the function $q(\mathbf{x})$ maps an input values to a specific leaf.

$$\mathcal{F} = \{f(\mathbf{x}) = w_{q(\mathbf{x})}\}, \;\; q : R^m \to T, \;\; \mathbf{w} \in R^T$$

To learn the model one minimizes a regularized objective function:

$$\mathcal{L} = \sum_i l(y_i, \hat{y}_i) + \sum_k \Omega(f_k) \tag{15.5}$$

where:

$$\Omega(f) = \gamma T + \frac{1}{2}\lambda \|\mathbf{w}\|^2 \tag{15.6}$$

The loss function l measures the difference between the predicted $\hat{y}_i$ and teh target y_i, **differentiable and convex**. The term Ω penalizes overly-complex models, with too many leaves or very large weights, aiming at a better generalization.

Let's now consider how the addition of a tree can reduce the regularized objective. The **greedy** aspect corresponds to adding at iteration t the tree which brings the largest possible reduction, by minimizing:

$$\mathcal{L}^{(t)} = \sum_i \Big[l(y_i, \hat{y}_i)^{(t-1)} + f_t(\mathbf{x}_i) \Big] + \Omega(f_t) \tag{15.7}$$

The previous trees are left untouched. Instead of minimizing $\mathcal{L}^{(t)}$ one minimizes its second-order Taylor expansion, remembering that the delta in its input parameter is in this case the additional contribution $f_t(\mathbf{x}_i)$.

$$\mathcal{L}^{(t)} \approx \sum_i \left[l(y_i, \hat{y}_i)^{(t-1)} + g_i f_t(\mathbf{x}_i) + \frac{1}{2} h_i f_t(\mathbf{x}_i)^2 \right] + \Omega(f_t) \tag{15.8}$$

[1] Optimization with Newton-like steps, as it will become clear in the future chapters, means that a quadratic approximation in the parameters is derived, and the best parameters are obtained as the minimum of the quadratic model.

where g_i and h_i are the first and second derivative of the loss function with respect to the predicted output: $g_i = \frac{\partial l(y_i, \hat{y}_i^{(t-1)})}{\partial \hat{y}_i^{(t-1)}}$, $h_i = \frac{\partial^2 l(y_i, \hat{y}_i^{(t-1)})}{\partial \hat{y}_i^{(t-1)2}}$. The derivatives have to be calculated at the current output value $\hat{y}_i^{(t-1)}$. Because we are minimizing, we can remove the constant term and we are left with:

$$\mathcal{L}^{(t)} = \sum_i \left[g_i f_t(\mathbf{x}_i) + \frac{1}{2} h_i f_t(\mathbf{x}_i)^2 \right] + \gamma T + \frac{1}{2}\lambda \sum_{j=1}^{T} {w_j}^2 \tag{15.9}$$

The tree model is simple, just *constant* values over separate regions. It makes sense to sum separately over the examples belonging to the different leaves (regions). Let's define $I_j = \{i | q(\mathbf{x}_i) = j\}$ as the set of examples with input values in leaf j. We can rewrite equation (15.9) as follows:

$$\mathcal{L}^{(t)} = \sum_{j=1}^{T} \left[(\sum_{i \in I_j} g_i) w_j + \frac{1}{2} (\sum_{i \in I_j} h_i + \lambda) {w_j}^2 \right] + \gamma T \tag{15.10}$$

If the tree structure $q(\mathbf{x})$ is fixed, the optimal weight ${w_j}^*$ is the one minimizing the parabola (let's remember that h_i are positive by assumption):

$${w_j}^* = \frac{\sum_{i \in I_j} g_i}{\sum_{i \in I_j} h_i + \lambda} \tag{15.11}$$

and the objective function value decreases by:

$$\Delta\mathcal{L}^{(t)}(q) = -\frac{1}{2} \sum_{j=1}^{T} \frac{(\sum_{i \in I_j} g_i)^2}{\sum_{i \in I_j} h_i + \lambda} + \gamma T \tag{15.12}$$

Conclusion: for a fixed tree, with simple and fast algebra, we can calculate the optimal values for the weight in the leaves (in the Taylor approximation), and the corresponding decrease in the objective function $\Delta\mathcal{L}$. if the tree is not fixed, we can now see if a local modification leads to a better $\Delta\mathcal{L}$ value! A simple local modification the addition of an additional split, leading to an additional leaf. The best possible split can be chosen greedily as the one leading to the best possible $\Delta\mathcal{L}$ in equation (15.11).

A greedy algorithm starts from a single leaf and iteratively adds branches to the tree. Assume that I_L and I_R are the sets of examples ending up in the left and right nodes after the split. Letting $I = I_L \cup I_R$, the loss reduction after the split is given by the difference of the above reductions in $\mathcal{L}$

$$\mathcal{L}_{split} = \frac{1}{2} \left[\sum_{j=1}^{T} \frac{(\sum_{i \in I_L} g_i)^2}{\sum_{i \in I_L} h_i + \lambda} + \frac{(\sum_{i \in I_R} g_i)^2}{\sum_{i \in I_R} h_i + \lambda} - \frac{(\sum_{i \in I} g_i)^2}{\sum_{i \in I} h_i + \lambda} \right] - \gamma T \tag{15.13}$$

The meaning of γ is evident. The split must lead to a reduction in $\mathcal{L}$ larger than γ to be accepted. If γ gets larger, more and more "insignificant" splits are avoided.

The basic algorithm for constructing the tree is evident. Start from an initial root (all examples in the same leaf), evaluate a set of candidate splits (each split is defined by a variable and a threshold) with the "loss reduction" formula (15.12), pick the best split. Repeat the entire process for all leaves and possible splits until no reduction is possible.

Additional flexibility can be obtained by: (i) adding a shrinkage parameter [136]. Shrinkage scales the newly added weights by a factor η after each step of tree boosting, reduces the influence of each individual tree and leaves space for future trees to improve the model, (ii) using sub-sampling (of features and of examples) to increase the diversity of the individual trees, going in the direction of random forests (see Chapter 6.2), (iii) using heuristics to consider only a subset of all possible splits (to reduce CPU time) (iv) dealing in an expicit manner with sparsity and missing values [84]. The increase in the number of parameters and possible choices demands more automated ways for choosing the meta-parameters appropriate for a specific task, for example by cross-validation, a hot area for future research.

15.8 Democracy for better accuracy-rejection compromises

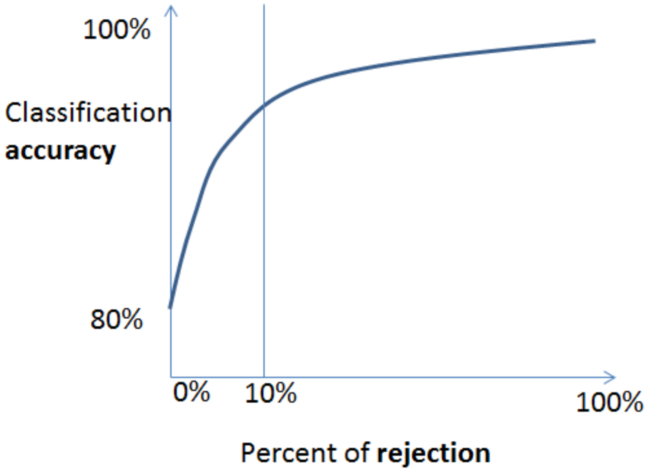


Figure 15.8: The accuracy-rejection compromise curve. Better accuracy can be obtained by rejecting some difficult cases.

In many practical applications of pattern recognition systems there is another "knob" to be turned: the fraction of cases to be rejected. **Rejecting some difficult cases and having a human person dealing with them** (or a more complex and costly second-level system) can be better than accepting and classifying everything. As an example, in optical character recognition (e.g., zip code recognition), difficult cases can arise because of bad writing or because of segmentation and preprocessing mistakes. In these cases, a human expert may come up with a better classification, or may want to look at the original postcard in the case of a preprocessing mistake. Let's assume that the ML system has this additional knob to be turned and some cases *can* be rejected. One comes up with an **accuracy-rejection curve** like the one in Fig. 15.8, describing the attainable accuracy performance as a function of the rejection rate.

For historical reasons, a used term is **receiver operating characteristic (ROC)**. A **ROC curve** is a graphical plot that illustrates the performance of a binary classifier system as its discrimination threshold is varied. The curve is created by plotting the true positive rate (TPR) against the false positive rate (FPR) at various threshold settings. The **area under the curve (AUC) or AUROC** criterion can be used to evaluate different classifiers.

$$AUC = \int_{\infty}^{-\infty} \text{TPR}(T)\text{FPR}'(T)\, dT \tag{15.14}$$

where T is the varying threshold parameter. AUC is equal to the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one.

If the system is working in an intelligent manner, **the most difficult and undecided cases will be rejected first**, so that the accuracy will rapidly increase even for modest rejection rates. A related "tradeoff" curve in signal detection is the *receiver operating characteristic (ROC)*, a graphical plot which illustrates the performance of a binary classifier system as its discrimination threshold is varied. It is created by plotting the fraction of true positives out of the total actual positives (TPR = true positive rate) vs. the fraction of false positives out of the total actual negatives (FPR = false positive rate), at various threshold settings.

For simplicity, let's consider a two-class problem, and a trained model with an output approximating the **posterior probability** for class 1. If the output is close to one, the decision is clear-cut, and the correct class is 1 with high probability. A problem arises if the output is close to 0.5. In this case the system is "undecided". If the estimated probability is close to 0.5, the two classes have a similar probability and mistakes will be frequent (if probabilities are correct, the probability of mistake is equal to 0.5 in this case). If the correct probabilities are known, the theoretically best **Bayesian classifier** decides for class 1 if $P(class = 1|x)$ is greater than $1/2$, for class 0 otherwise. The mistakes will be equal to the remaining probability. For example, if $P(class = 1|x)$ is 0.8, mistakes will be done with probability 0.2 (the probability that cases of class two having a certain x value are classified as class 1).

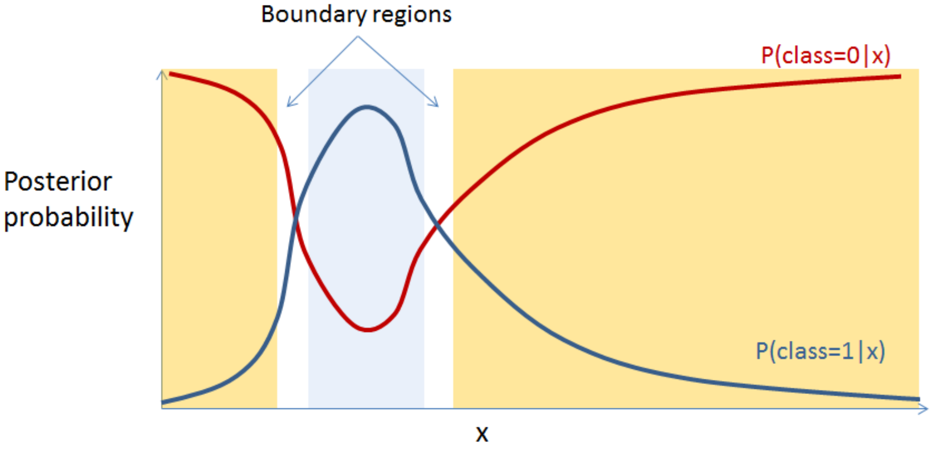


Figure 15.9: Transition regions in a Bayesian classifier. If the input patterns falling in the transition areas close to the boundaries are rejected, the average accuracy for the accepted cases increases.

Setting a positive threshold T on the posterior probability, demanding it to be greater than $(1/2 + T)$ is the best possible "knob" to increase the accuracy by rejecting the cases which do not satisfy this criterion. One is rejecting the patterns which are close to the boundary between the two classes, where cases of both classes are mixed with probability close to $1/2$ (Fig. 15.9).

Now, if probabilities are not known but are *estimated* through machine learning, having a committee of classifiers gives many opportunities to obtain more flexibility and realize superior accuracy-rejection curves [43]. For example, one can get **probabilistic combinations of teams**, or portfolios with more classifiers, by activating each classifier with a different probability. One can consider the agreement between all of them, or a **qualified majority**, as a signal of cases which can be assigned with high confidence, and therefore to be accepted by the system. Finally, even more flexibility can be obtained by considering the output probabilities (not only the classifications), averaging and thresholding. If there are more than two classes, one can require that the average probability is above a first threshold, while the distance with the second best class is above a second threshold.

Experiments show that superior results and higher levels of flexibility in the accuracy-rejection compromise can be easily obtained, by reusing in an intelligent manner the many classifiers which are produced in any case while solving a task.

Gist

Having a number of **different** but similarly **accurate** machine learning models allows for many ways of increasing performance beyond that of the individual systems (**ensemble methods, committees, democracy in ML**).

In **stacking or blending** the systems are combined by adding another layer working on top of the outputs of the individual models.

Different ways are available to create diversity in a strategic manner. In **bagging (bootstrap aggregation)**, the same set of examples is sampled with replacement. In **boosting**, related to additive models, a series of models is trained so that the most difficult examples for the current system get a **larger weight** for the latest added component. Using different subsets of features or different random number generators in randomized schemes are additional possibilities to create diversity. **Error-correcting output codes** use a redundant set of models coding for the various output bits to increase robustness with respect to individual mistakes.

Additive logistic regression is an elegant way to explain boosting via additive models and Newton-like optimization schemes. Optimization is boosting our knowledge of boosting.

Ensemble methods in machine learning resemble jazz music: the whole is greater than the sum of its parts. Musicians and models working together, feeding off one another, create more than they would by themselves.

Chapter 16

Recurrent networks and reservoir computing

Music is a reservoir... of sounds.
(Dexter Gordon)

A "pet hypothesis" which dominated neural networks and machine learning research for a long period is the idea that humans or computers spend huge efforts to extract building blocks (features) of growing complexity in order to solve complex tasks. Deep learning, supervised pre-training, stage-wise feature extraction are examples.

By negating the above hypothesis one obtains **reservoir learning**. The idea is to prepare a huge **reservoir of random features**, which are then tapped to build the final system, usually by a simple least-squares fit between the hidden outputs of the reservoir and the problem outputs. This sounds too quick and dirty to produce useful systems, but a growing amount of evidence shows that reservoir techniques are incredibly effective in many contexts. In some cases, they produce competitive results, or at least quick initial results which can be rapidly improved by an additional tuning phase.

The **biological plausibility** of these techniques is probably higher than that of complex training mechanisms if one thinks about the rapidity of learning to ride a bicycle, to sing a song, to pronounce a new word. The fact that a handful of examples is sufficient to learn can be explained by the availability of **"random" building blocks**, with a proper architecture, ready to be tapped and rapidly fine-tuned.

16.1 Recurrent neural networks

Up to now we considered machine learning systems without a notion of time, history and memory. Better said, time and iterations played a role only *during* training, but not when the system is operational. During operation, the outputs depends only on the inputs, in a "feed-forward" one-shot manner, no cycle involved. Biological systems do not always work in this simple way. On the contrary, when singing a song, the output depends not only on the current input but also on the previous inputs, on the previous history. The same is true for playing music, speaking, heart beating, breathing, walking, etc. which involve cycles, oscillations and a rich dynamical behavior going beyond single-step input-output machines (which realize mathematical *functions*).

Artificial **recurrent neural networks** (**RNNs**) are distinguished from the more widely used feed-forward neural networks because of cycles in their connection topology. Some outputs are fed back to some nodes of the network, so that they influence also future outputs, providing the network with some *memory* of the past. Depending on the model, the computation can proceed via synchronized steps (think about a global clock ticking to make each unit collect and process the current inputs to produce a new output), or in asynchronous mode (each unit wakes up at random times and updates its output), or via continuous dynamics regulated mathematically by differential equations. Figure 16.1 shows the basic structure of a recurrent network: hidden unit outputs can be fed back as inputs; outputs are fed back to hidden units and to output units. This latter requirement is important if subsequent outputs are strongly correlated and the network can better operate incrementally; depending on the case, some of these feedback channels may not be implemented.

Let's present a concrete example to develop some intuition. A recurrent network with no inputs, four hidden sigmoid units and two linear output units was trained to follow a circle (centered on the origin, radius 1, three turns of 16 steps each, initial transient of 4 steps). After a short training phase, the system follows an approximated circular trajectory shown in Fig. 16.2 The corresponding values for the four hidden units are shown in Fig. 16.3.

The existence of cycles has a profound impact (a recent review is [256]):

- A RNN can develop a self-sustained temporal activation dynamics along its recurrent connection pathways, even in the absence of input. A RNN is a **dynamical system**, while feedforward networks are functions.

- If driven by an input signal, a RNN preserves in its internal state a nonlinear transformation of the input history. It has a dynamical memory, and is able to process temporal context information.

From a dynamical systems perspective, there are two main classes of RNNs. The first class is characterized by an energy-minimizing stochastic dynamics and **symmetric connections** (the trajectory of the network outputs finds local minima of a suitable "energy" function, think about a kind of modified gradient descent). Known example are **Hopfield networks** derived from statistical physics [189], Boltzmann machines [6], and Deep Belief Networks [181]. These systems are mostly trained with **unsupervised learning**. Typical targeted functionalities in this field are *associative memories* (the retrieved memory correspond to local minima of the energy function), data compression, the unsupervised modeling of data distributions, and static pattern classification. The model is run for multiple time steps per single input instance to reach some type of convergence or equilibrium.

The second big class of RNN models typically features a deterministic update dynamics and **directed connections**. Systems from this class implement nonlinear filters, which transform an input time series into an output time series. The mathematical background consists of nonlinear dynamical systems. The standard training mode is **supervised**.

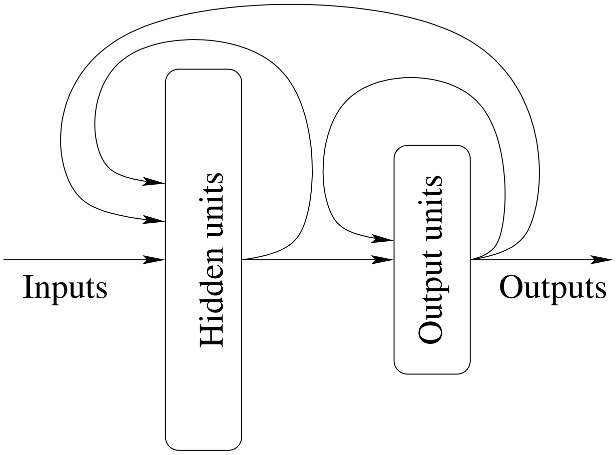


Figure 16.1: The basic scheme of a recurrent network.

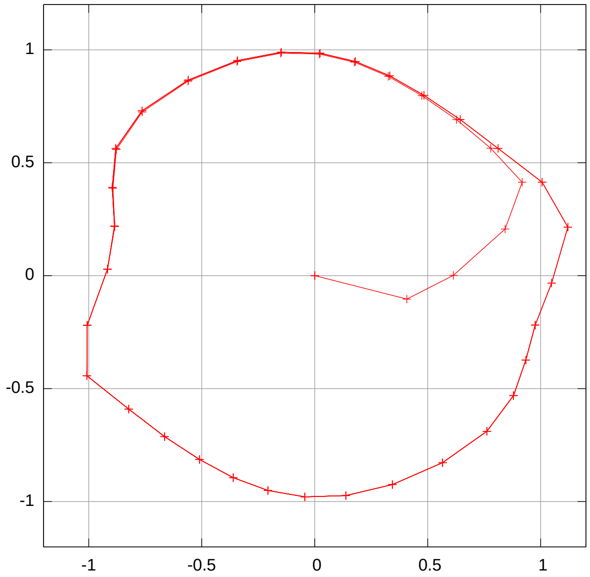


Figure 16.2: Recurrent network trained on a circular trajectory: output sequence starting from null inputs.

16.2 Energy-minimizing Hopfield networks

A **Hopfield network** (Fig.16.4), defined in [189], consists of binary threshold units, i.e., they only take on two different output values (normally 1 or -1), depending on whether the input exceeds a threshold or not. Symmetric weights w_{ij} connect pairs of units (with no self-connection: $w_{ii} = 0$). A unit is updated as follows:

$$s_i \leftarrow \begin{cases} +1 & \text{if } \sum_j w_{ij} s_j \geq \theta_i \\ -1 & \text{otherwise,} \end{cases} \tag{16.1}$$

where s_i is the output state of unit i and θ_i is the threshold. Updates can be performed **asynchronously** (a unit is picked at random and updated) or **synchronously** (all units are updated at the same time at the tick of a central clock). Asynchronous updates have a more biological or physical flavor (*spin glasses* are a related model in physics). The initial output values are progressively changed by the update rule so that the state depends on the initial condition but also on the sequence of updates. If an output is signalled by a flashing (+1) or inactive (-1) LED —actually this was a homework hardware realization by one of the authors— one observes a flickering pattern in time. The main question is: what is the possible *meaning* of this flickering pattern, which kind of computation can be executed? The answer by Hopfield is related to **optimizing a suitable energy function** (in math and physics called a *Lyapunov function*) :

$$E = -\frac{1}{2}\sum_{i,j} w_{ij} s_i s_j + \sum_i \theta_i s_i$$

One can easily demonstrate that, when units are chosen to be updated, with symmetric connections, the **energy E will either decrease or remain equal**. Under repeated updating the network will eventually converge to a state which is a local minimum in the energy function. Local minima in the energy function are **stable states** for the network. The flickering pattern will stabilize and show a stable pattern of light. The "meaning" of Hopfield networks is explained by a dynamical system which, when started from an initial input, **seeks out local minima in the attraction basin of the initial point**, like a drop of water flowing to a lake in a drainage basin. The facts that outputs are constrained in a box is crucial. If not, one is minimizing a quadratic form which could be unlimited (going to minus infinity).

Programming a Hopfield net amounts to **carving out appropriate local minima in the energy landscape**. The Hebbian learning rule for modifying weights during training was introduced by Donald Hebb in 1949 to explain "associative learning." The simultaneous activation of neuron cells leads to pronounced increases in synaptic strength between those cells: "Neurons that fire together, wire together. Neurons that fire out of sync, fail to link." The Hebbian rule is local and incremental. For the Hopfield Networks, it is implemented in the following manner, when learning N binary patterns:

$$w_{ij} = \frac{1}{N}\sum_{\mu=1}^{N} x_i^\mu x_j^\mu, \qquad i, j = 1, \ldots, n$$

where each pattern $\boldsymbol{x}^\mu = (x_1^\mu, \ldots, x_n^\mu)$ is an n-bit sequence, and n is also the number of neurons in the network. If the bits corresponding to neurons i and j are equal in pattern $\boldsymbol{x}^\mu$, then the product $x_i^\mu x_j^\mu$ will have a positive effect on the weight w_{ij} and the values of neurons i and j will tend to become equal. The opposite happens if the bits corresponding to neurons i and j are different.

Depending on the number of nodes in the network, the Hebbian rule will be able to "carve" in the energy landscape a set of local minima that are close to the N patterns used to train it, provided that N is not too large (a rule of thumb is that the number N of patterns should not exceed about 13.8% of the number n of neurons [177]). When the update rule (16.1) is repeatedly applied by first assigning a specific pattern $\boldsymbol{x}^\nu$ to the neurons, the network will settle to a local minimum, thereby retrieving the stored pattern that is closest to $\boldsymbol{x}^\nu$, as shown in Fig. 16.5.

With Hopfield nets one can build **content-addressable memory** systems: the network will converge to a "remembered" state if it is given only part of the content (with other bits set randomly). The net can be used to recover from a distorted input the trained state that is most similar to that input. This is called **associative memory**, related to

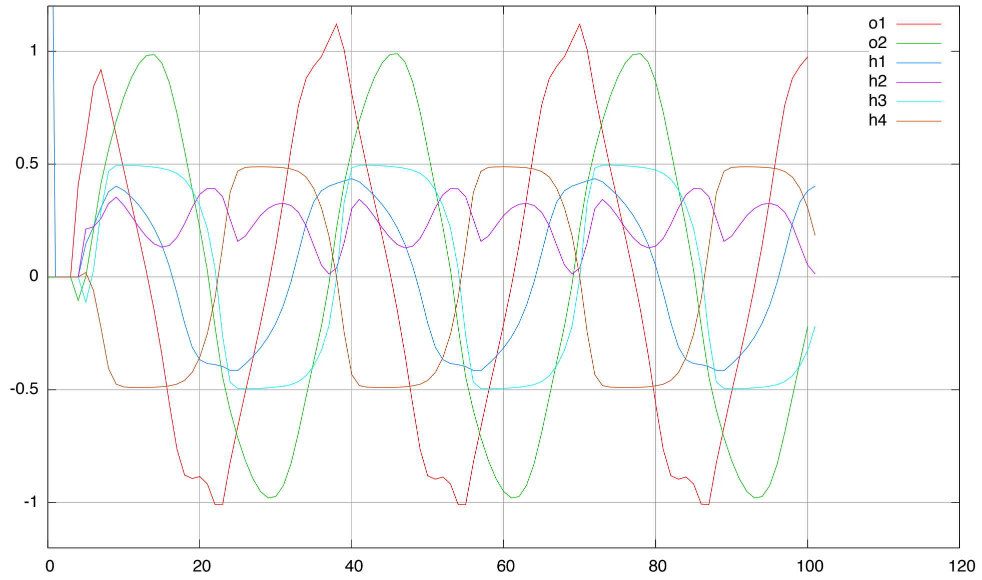


Figure 16.3: Recurrent network trained on a circular trajectory: outputs and hidden units.

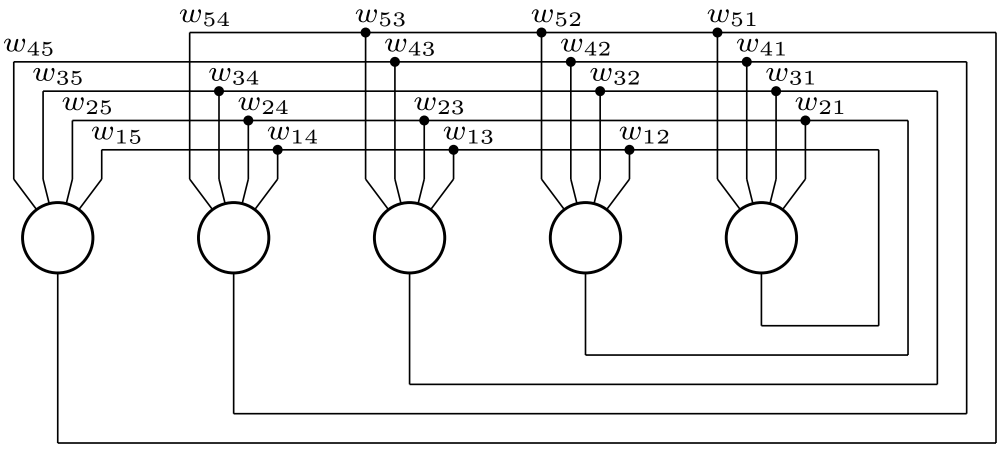


Figure 16.4: A Hopfield network with 5 neurons and feedback loops.

error-correcting codes. Generalizations with continuous weights have dynamics similar to gradient descent, with the descent direction modified with respect to the gradient (but still descending).

Although of formidable theoretical and scientific interest, real-world applications of Hopfield networks face some difficulties related to *spurious patterns*, i.e., local minima that do not correspond to programmed memories, and to *capacity limits*. When too many patterns are stored, one stored item can be confused with another upon retrieval. Note that human memory has similar characteristics, and semantically related items tend to confuse the individual and lead to the recollection of wrong patterns.

16.3 RNN and backpropagation through time

Let's now consider more general RNNs, without the requirement of symmetric weights and binary outputs (Fig. 16.1).

This kind of network can be simulated with a feed-forward network by **unrolling** it as shown in Fig. 16.6. The only change needed to a standard feed-forward MLP is to allow some of the inputs to be fed directly to the output neurons, in addition to the hidden layer(s). The standard training method is called "**backpropagation through time**" or BPTT, in which standard back-propagation for feed-forward networks is applied to the above unrolled model [379]. Recurrent neural networks, with output of some units fed back to other units, are difficult to train with derivative-based techniques because of the **vanishing and exploding gradient problems** [49]. Exploding gradients refers to the large increase in the norm of the gradient during training, caused by the explosion of the long-term components, which can grow exponentially more than short-term ones. The vanishing gradients problem refers to the opposite behavior, when long-term components go exponentially fast to norm 0, making it impossible for the model to learn correlation between temporally distant events. The problems are caused by the large number of iterations which can be present in RNN, which cause a small weight change to be exponentially increased or decreased. Modifications to cure the above problems (gradient norm clipping to deal with exploding gradients and soft constraints for the vanishing gradients problem) are presented in [293].

In a way, RNNs stress the limits of derivative-based techniques for optimization and motivate the adoption of derivative-free techniques or of radical changes in the training architecture like reservoir learning and extreme learning machines considered in the following sections.

16.4 Reservoir learning for recurrent neural networks

RNNs (of the second type that we introduced, i.e., without symmetry constraints) are highly promising tools for non-linear time series applications [256]. They are biologically plausible (recurrent connection pathways are present in brains) universal approximators of dynamical systems, under fairly mild and general assumptions.

A number of training algorithms proposed in the past suffer from the following shortcomings:

- The gradual change of network parameters during learning drives the network dynamics through **bifurcations**: the gradient information degenerates and may become ill-defined. Therefore, convergence cannot be guaranteed.
- Many costly update cycles may be necessary, resulting in excessive training times for large networks (with more than tens of units).
- Dependencies requiring long-range memory are hard to learn, because the necessary gradient information exponentially dissolves over time.
- Advanced training algorithms are complex with many global control parameters. They need skill and experience to be used.

In the current century a radically new approach is being proposed independently under the name of *Liquid State Machines* [258] and *Echo State Networks* [210], here collectively referred to as **Reservoir Computing** (RC). RC avoids the shortcomings of gradient-descent RNN by the following prescription (Fig.16.7):

- A recurrent network is **randomly created** and remains unchanged during training. This RNN is called the **reservoir**. It is passively excited by the input signal and maintains in its state a nonlinear transformation of the input history.
- The desired output signal is generated as a **linear function** of the neuron's signals from the input- excited reservoir. This linear combination is obtained by linear regression, for example by using least-squares.

Reservoir Computing is rapidly becoming one of the basic tools for RNN modeling, showing better modeling accuracy, universal modeling capacity for continuous-time, continuous-value real-time systems. RC can explains why biological brains can carry out accurate computations in spite of noisy physical components. Last but not least, models can be extended by adding more output units to the same reservoir, without interfering with the previous functionality.

In some cases, a completely random reservoir is not sufficient and the current research deals with developing suitable reservoir design and adaptation methods. RC is departing from a brute-force random approach and becoming a paradigm for using different methods for (i) producing/adapting the reservoir, and (ii) training different types of readouts. An updated review is presented in [256].

16.5 Extreme learning machines

A separate but related stream of research considers feed-forward systems, like multi-layer perceptrons, in which the initial layers are created randomly and only the final layer is trained by linear regression. **Extreme Learning Machines** are proposed in [194] by adopting the standard pseudo-inverse technique for least-squares fitting described in Section 4.1. Both ELM and RC overcome the problems associated with traditional neural network training algorithms, such as local minima and vanishing or exploding gradients, by **modifying only the output weights** using a simple and efficient linear regression algorithm. The main difference between the two approaches is that the reservoir of RC architectures contains recurrent connections, giving it a short-term memory, whereas ELMs are a pure feedforward architecture without short-term memory.

The "surprising" fact that useful learning occurs in MLP even if the initial layers are random has been observed starting from the initial developments in neural networks. For example, Rosenblatt [308] and other early investigators favored randomly chosen input feature detectors. E. Baum [44] claims that in some simulations one may fix the weights of the connections on one level and simply adjust the connections on the other level, with no significant gain by adjusting the weights on both levels simultaneously. More recently, an extensive theoretical and practical investigation is presented in [195], which coined the term "**Extreme Learning Machine**."

It is well known from linear algebra that, through matrix inversion, single-layer feed-forward networks (SLFNs) with N hidden nodes and randomly chosen input weights and hidden layer biases can exactly learn N distinct observations, under conditions of full matrix rank (linear independence). Of course, generalization is not guaranteed, but learning becomes a trivial one-shot operation by matrix inversion.

The work in [195] rigorously proves that the input weights and hidden layer biases of SLFNs can be randomly assigned if the activation functions in the hidden layer are infinitely differentiable. After they are chosen randomly, SLFNs can be considered as a linear system and the output weights can be analytically determined through simple generalized inverse (pseudo-inverse) operation of the hidden layer output matrices. Various generalizations considering different kinds of hidden nodes and architectures have been proposed (Fig. 16.8). In some cases, ELMs can learn much faster than traditional algorithms like back-propagation (BP), while obtaining better generalization performance, in particular if the norm of weights is controlled through the usual quadratic penalty. The number of hidden neurons leading to optimal performance can be much bigger that that for backpropagation learning, an indication that a large pool of random units needs to be created to tap a sufficient number of useful units to determine the outputs. A recent review is [193].

Related investigations are [214], which evaluates multi-stage architectures for object recognition and considers also random filters, and [382], which proposes the *no-prop* method (same as ELM, but with iterative least-squares techniques). Architecture with random weights are studied in [314]. They show that certain convolutional pooling architectures (sharing connection weights at different spatial positions in image processing) can be inherently frequency selective and translation invariant, even with random weights. Based on this they propose **using random weights to evaluate candidate architectures**, thereby sidestepping the time-consuming learning process. A surprising fraction of the performance of certain state-of-the-art methods can be attributed to the architecture alone, although subsequent fine-tuning usually does improve the final performance.

It is clear that Reservoir Computing and ELM follow similar research directions, although originally RC concentrated mostly on RNN, ELM on feed-forward systems. Reservoir computing and extreme learning are considered jointly in [73].

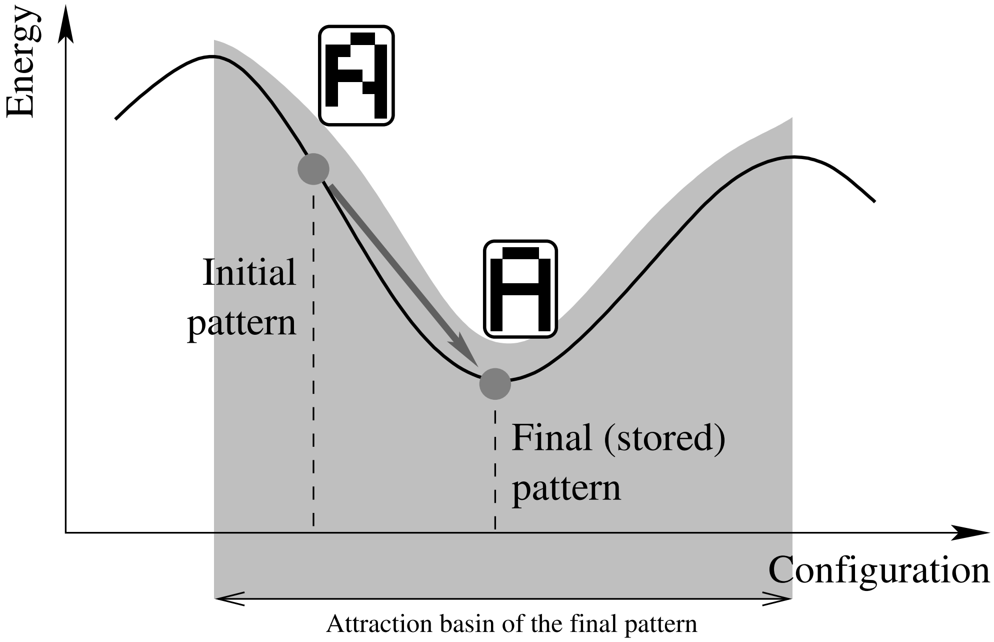


Figure 16.5: Energy Landscape of a Hopfield Network, highlighting the initial state of the network (up the hill), an attractor state to which it will eventually converge, and a basin of attraction (shaded).

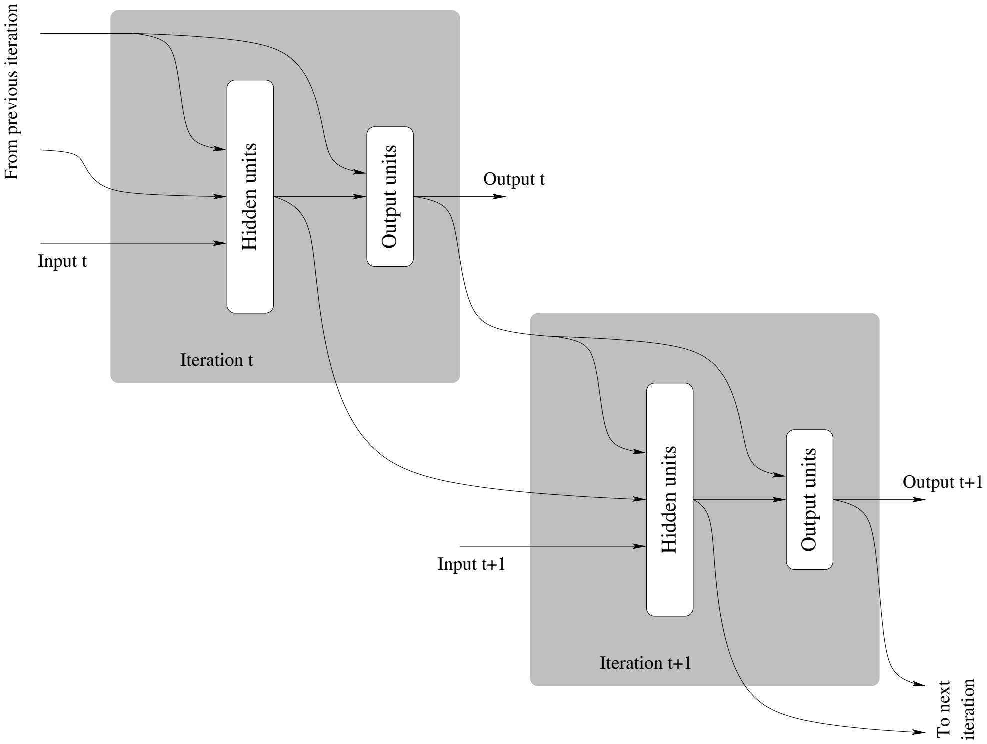


Figure 16.6: The basic recurrent network of Fig. 16.1 can be unrolled as a cascade of feed-forward networks, each fed by an iteration's inputs and by the previous iteration's hidden and output values.

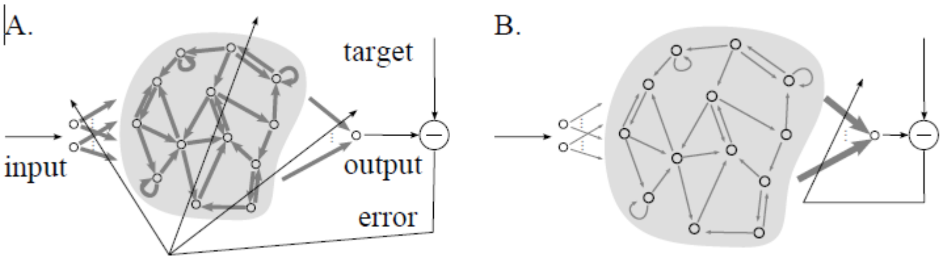


Figure 16.7: (Left) Traditional gradient-descent-based RNN training methods adapt all connection weights (bold arrows), (Right) In Reservoir Computing, only the RNN-to-output weights are modified (adapted from [256]) .

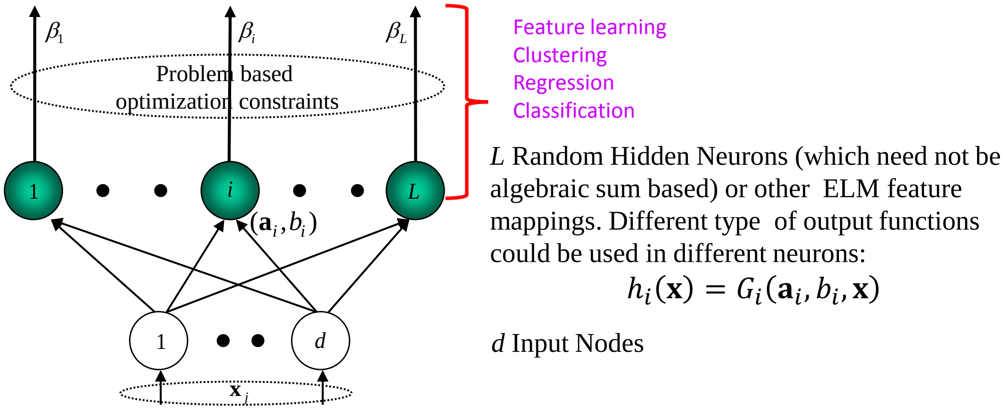

β_1
β_i
β_L
Problem based optimization constraints
Feature learning
Clustering
Regression
Classification
1
i
L
$(\mathbf{a}_i, b_i)$
L Random Hidden Neurons (which need not be algebraic sum based) or other ELM feature mappings. Different type of output functions could be used in different neurons:
$h_i(\mathbf{x}) = G_i(\mathbf{a}_i, b_i, \mathbf{x})$
1
d
d Input Nodes
$\mathbf{x}_j$

Figure 16.8: The hidden nodes in ELM can consist of different type of computational nodes (adapted from [193]).

Gist

Recurrent neural networks with feedback loops allow the transition from "mathematical functions" (feedforward networks) to full-fledged **dynamical systems** with evolution in time and internal memory.

Machine learning for recurrent neural networks is very hard, in particular for derivative-based methods. The many cycles involved can cause derivatives to explode or to vanish.

The recently proposed **reservoir computing** (RC) and **extreme learning machines** (ELM) methods take a radical approach, in a way contrary to that of deep learning, by creating vast amounts of **random building blocks** (random features), and limiting learning to a final linear combination layer. A specific problem "taps" the useful building blocks in the reservoir and weighs them appropriately to get the final solution.

Given the difficulties of realizing deep derivative-based techniques with noisy biological neural hardware, the success of this brute-force "randomized construction plus final tuning" approach gives new hope to explain parts of our brain and to engineer fast and flexible learning machines.

We are happy to live in a sparkling research period, when crazy and wildly different ideas advance the frontier of ML and neural networks through spectacular plot twists and paradigm changes.

Part II

Unsupervised learning and clustering

Chapter 17

Top-down clustering: K-means

First God made heaven and earth. The earth was without form and void, and darkness was upon the face of the deep; and the Spirit of God was moving over the face of the waters. And God said, "Let there be light"; and there was light. And God saw that the light was good; and God ***separated the light from the darkness. God called the light Day, and the darkness he called Night****. [...]*
So out of the ground the Lord God formed every beast of the field and every bird of the air, and brought them to the man to see what he would call them; and whatever the man called every living creature, that was its name. ***The man gave names*** *to all cattle, and to the birds of the air, and to every beast of the field.*
(Book of Genesis)

This chapter starts a new part of the book and enters a new territory. Up to now we considered *supervised* learning methods, while the issue of this part is: **What can be learned without teachers and labels**?

Like the energy emanating in the above painting by Michelangelo suggests, we are entering a more creative region, which contains concepts related to exploration, discovery, different and unexpected outcomes. The task is not to slavishly follow a teacher but to gain freedom in generating models. In most cases the freedom is not desired but it is the only way to proceed.

Let's imagine you place a child in front of a television screen. Even without a teacher he will immediately differentiate between a broken screen, showing a "snowy" random noise pattern, and different television programs like cartoons and world news. Most probably, he will show more excitement for cartoons than for world news and for random noise. The appearance of a working TV screen (and the appearance of the world) is not random, but highly structured, arranged according to explicit or implicit plans. For another example of unsupervised learning, let's assume that entities represent speakers of different languages, and coordinates are related to audio measurements of their spoken language (such as frequencies, amplitudes, etc.). While walking in an international airport, most people can readily identify clusters of different language speakers based on the audible characteristics of the language. We may for example easily distinguish English speakers from Italian speakers, even if we cannot name the language being spoken.

Modeling and understanding structure (forms, patterns, clumps of interesting events) is at the basis of our cognitive abilities. The use of *names* and language is deeply rooted in the organizing capabilities of our brain. In essence, a name is a way to group different experiences so that we can start speaking and reasoning. Socrates is a *man*, all men are *mortal*, therefore Socrates is mortal[1].

For example, animal species (and the corresponding names) are introduced to reason about **common characteristics** instead of individual ones ("The man gave names to all cattle"). In geography, continents, countries, regions, cities, neighborhoods represent clusters of geographical entities at different scales. Clustering is related to the very human activity of **grouping similar things together, abstracting** them and giving names to the classes of objects (Fig. 17.1). Think about categorizing men and women, a task we perform with a high degree of confidence in spite of significant individual variation.

Clustering has to do with **compression of information**. When the amount of data is too much for a human to digest, **cognitive overload** results and the finite amount of "working memory" in our brain cannot handle the task. Actually, the number of data points chosen for analysis can be reduced by using filters to restrict the range of data values. But this is not always the best choice, as in this case we are filtering data based on individual coordinates, while **a more global picture** may be preferable.

Clustering methods work by collecting similar points together in an intelligent and data-driven manner, so that attention can be concentrated on a small but relevant set of **prototypes**. The prototype summarizes the information contained in the subset of cases which it represents. When similar cases are grouped together, one can reason about groups instead of individual entities, therefore reducing the number of different possibilities.

As you imagine, the practical applications of clustering are endless. To mention some examples, in **market segmentation** one divides a broad marketplace into parts, or segments, and then implements strategies to target the common needs and desires of the segmented customers. In **finance**, clustering groups stocks with a similar behavior, for diversifying the portfolio and reducing risk. In **health care**, diseases are clusters of abnormal conditions that affect our body. In **text mining**, different words are grouped together based on the structure and meaning of the analyzed texts. A **semantic network** represents relations between concepts. It is a directed or undirected graph consisting of vertices, which represent concepts, and labeled edges, which represent relations. The different relations (e.g., "is an", "has", "lives in", ...) underline that there is no single way to group entities.

[1] To be honest, the radical simplification implied by giving names takes mysticism away from the world, a price to pay for conquering it with our technical means. Rainer Maria Rilke expresses this concept in his "In Celebration of Me" (1909):

> I am so afraid of people's words.
> They describe so distinctly everything:
> And this they call dog and that they call house,
> here the start and there the end.
> ...
> I want to warn and object: Let the things be!
> I enjoy listening to the sound they are making.
> But you always touch: and they hush and stand still.
> That's how you kill.

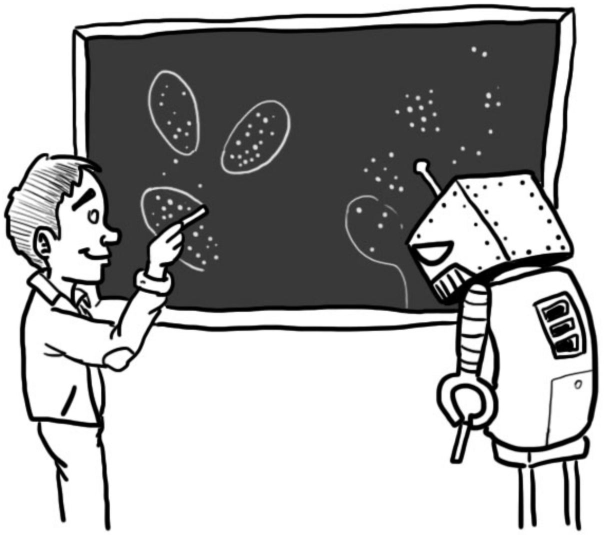


Figure 17.1: Clustering is deeply rooted into the human activity of grouping and naming entities.

17.1 Approaches for unsupervised learning

Given the creativity and different objectives of clustering, there are wildly different ways to proceed. It is traditional to subdivide methods into top-down and bottom-up techniques.

In **top-down or divisive clustering** one decides about a number of classes and then proceeds to separate the different cases into the classes, aiming at putting similar cases together. Let's note that classes do not have labels, only the subdivision matters. Think about organizing your laundry in a cabinet with a fixed number of drawers. If you are an adult person (if you are a happy teenager, please ask your mother or father) you will probably end up putting socks with similar socks, shirts with shirts, etc.

In **bottom-up or agglomerative clustering** one leaves the data speak for themselves and starts by merging (associating) the most similar items. As soon as larger groupings of items are created, one proceeds by merging the most similar groups, and so on. The process is stopped when the grouping makes sense, which of course depends on the specific metric, application area and user judgment. The final result will be a hierarchical organization of larger and larger sets (known as *dendrogram*), reflecting the progressively larger mergers. Dendrograms are familiar from natural sciences, think about the organization of zoological or botanical species.

More advanced and flexible unsupervised strategies are known under the umbrella term of **dimensionality reduction**: in order to reduce the number of coordinates to describe a set of experimental data one needs to understand the structure and the "directions of variation" of the different cases. If one is clustering people faces, the directions of variation can be related to eyes color, distance between nose and mouth, distance between nose and eyes, etc. All faces can be obtained by changing some tens of parameters, for sure much less than the total number of pixels in an image.

Another way to model a set of cases is to assume that they are produced by an underlying **probabilistic process**. By modeling it one understands the structure and the different clusters. **Generative models** aim at identifying and modeling the probability distributions of the process producing the observed examples. Think about grouping books by deriving a model for the topics and words used by different authors, without knowing the author names beforehand. An author will pick topics with a certain probability. After the topic is fixed, words related to the topic will be generated

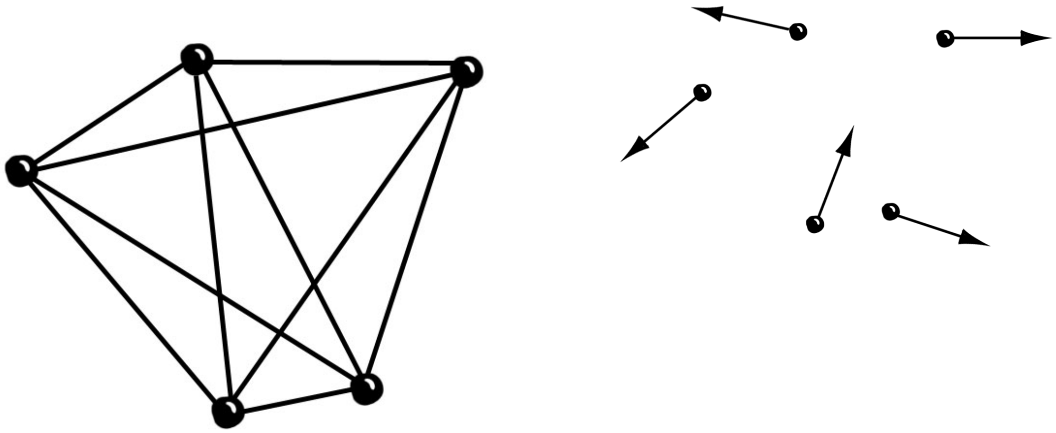


Figure 17.2: External representation by relationships (left) and internal representation with coordinates (right). In the first case mutual similarities between pairs are given, in the second case individual vectors.

with specific probabilities. For sure, the process will not generate masterpieces but similar final word probabilities, in many cases sufficient to recognize an unknown author.

Our visual system is extremely powerful at clustering salient parts of an image and **visualizations** like linear or nonlinear **projections** onto low-dimensional spaces (usually with two dimensions) can be very effective to identify structure and clusters "by hand" — well, actually "by eyes."

Last but not least, very interesting and challenging applications require a mixture of supervised and unsupervised strategies (**semi-supervised learning**). Think about "big data" applications related to clustering zillions of web pages. Labels can be very costly — because they can require a human person to classify the page — and therefore rare. By adding a potentially huge set of unlabeled pages to the scarce labeled set one can greatly improve the final result.

After clarifying the overall landscape, this chapter will focus on the popular and effective top-down technique known as **k-means clustering**.

17.2 Clustering: Representation and metric

There are two different contexts in clustering, depending on how the entities to be clustered are organized (Fig. 17.2). In some cases one starts from an **internal representation** of each entity (typically an M-dimensional vector $\mathbf{x}_d$ assigned to entity d) and derives mutual dissimilarities or mutual similarities from the internal representation. In this case one can derive **prototypes (or centroids)** for each cluster, for example by averaging the characteristics of the contained entities (the vectors). In other cases only an **external representation** of dissimilarities is available and the resulting model is an undirected and weighted graph of entities connected by edges.

For example, imagine that market research for a supermarket indicates that stocking similar foods on nearby shelves results in more revenue. An internal representation of a specific food can be a vector of numbers describing: type of food (1=meat, 2=fish...), caloric content, color, box dimension, suggested age of consumption, etc. Similarities can then be derived by comparing the vectors, by Euclidean metric or scalar products.

An external representation can instead be formed by polling the customers, asking them to rate the similarity of pairs of product X and Y (on a fixed scale, for example from 0 to 10), and then deriving external similarities by averaging the customer votes.

The effectiveness of a clustering method depends on the **similarity metric** (how to measure similarities) which needs to be strongly problem-dependent. The traditional Euclidean metric is in some cases appropriate when the different coordinates have a similar range and a comparable level of significance, it is not if different units of measure are used. For example, if a policeman compares faces by measuring eyes distance in millimeters and mouth-nose distance in kilometers, he will make the Euclidean metric almost meaningless. Similarly, if some data in the housing market represent the house color, it will not be significant when clustering houses for business purposes. Instead, the color can be extremely significant when clustering paintings of houses by different artists. The metric is indeed problem-specific, and this is why we denote the dissimilarity between entities $\mathbf{x}$ and $\mathbf{y}$ by $\delta(\mathbf{x},\mathbf{y})$, leaving to the implementation to specify how it is calculated.

If an internal representation is present, a metric can be derived by the usual **Euclidean distance**:

$$\delta_E(\mathbf{x},\mathbf{y}) = \|\mathbf{x}-\mathbf{y}\| = \sqrt{\sum_{i=1}^{M}(x_i-y_i)^2}. \tag{17.1}$$

In three dimensions this is the traditional distance, measured by squaring the edges and taking the square root. The notation $\|\mathbf{x}\|_2$ for a vector $\mathbf{x}$ means the Euclidean norm, and the subscript 2 is usually omitted.

Another notable norm is the Manhattan or taxicab norm, so called because it measures the distance a taxi has to drive in a rectangular street grid to get from the origin to the point x:

$$\delta_{\text{Manhattan}}(\mathbf{x},\mathbf{y}) = \|\boldsymbol{x}-\boldsymbol{y}\|_1 = \sum_{i=1}^{M}|x_i-y_i|. \tag{17.2}$$

As usual, there is no absolutely right or wrong norm. Taxicabs in New York prefer the Manhattan norm, while airplane pilots prefer the Euclidean norm (at least for short distances, then the curvature of earth requires still different distance measures based on geodetics). In some cases, the appropriate way to measure distances is recognized only *after* judging the clustering results, which makes the effort creative and open-ended.

Another possibility is that of starting from similarities given by scalar products of the two normalized vectors and then taking the inverse to obtain a dissimilarity. In detail, the normalized scalar product between vectors $\mathbf{x}$ and $\mathbf{y}$, by analogy with geometry in two and three dimensions, can be interpreted as the *cosine* of the angle between them, and is therefore known as **cosine similarity**:

$$\text{cosine-similarity}(\mathbf{x},\mathbf{y}) = \cos(\theta) = \frac{\mathbf{x}\cdot\mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|} = \frac{\sum_{i=1}^{M} x_i\, y_i}{\sqrt{\sum_{i=1}^{M}(x_i)^2}\,\sqrt{\sum_{i=1}^{M}(y_i)^2}}, \tag{17.3}$$

and after taking the inverse one obtains the dissimilarity:

$$\delta(\mathbf{x},\mathbf{y}) = \|\mathbf{x}\|\|\mathbf{y}\|/(\epsilon+\mathbf{x}\cdot\mathbf{y}),$$

ϵ being a small quantity to avoid dividing by zero.

Let's note that the cosine similarity depends only on the *direction* of the two vectors, and it does not change if components are multiplied by a fixed number, while the Euclidean distance changes if one vector is multiplied by a scalar value. A weakness of the standard Euclidean distance is that values for different coordinates can have very different ranges, so that the distance may be dominated by a subset of coordinates. This can happen if units of measures are picked in different ways, for example if some coordinates are measured in millimeters, other in kilograms, other in kilometers: it is always very unpleasant if the analysis crucially depends on picking a suitable set of physical units. To avoid this trouble we need to make values *dimensionless*, without physical units. Furthermore we may as well normalize them so that all values range between zero and one before measuring distances.

The above can be accomplished by defining:

$$\delta_{norm}(\mathbf{x},\mathbf{y}) = \sqrt{\sum_{i=1}^{M}\left(\frac{x_i-y_i}{\text{maxval}_i-\text{minval}_i}\right)^2}, \tag{17.4}$$

where M is the number of coordinates, minval_i and maxval_i are the minimum and maximum values achieved by coordinate i for all entities.

In the general case, a positive-definite matrix $\mathbf{M}$ can be determined to transform the original metric:

$$d_{ij} = \sqrt{(\boldsymbol{x}_i - \boldsymbol{x}_j)^T \mathbf{M} (\boldsymbol{x}_i - \boldsymbol{x}_j)}.$$

An example is the Mahalanobis distance which takes into account the correlations of the data set and is scale-invariant (it does not change if we measure quantities with different units, like millimeters or kilometers). More details about the Mahalanobis distance will be discussed in future chapters.

17.3 K-means for hard and soft clustering

Hard clustering partitions the entities D into k disjoint subsets $C = \{C_1, \ldots, C_k\}$ to reach the following objectives.

- Minimization of the average intra-cluster dissimilarities:

$$\min \sum_{d_1, d_2 \in C_i} \delta(\mathbf{x}_{d_1}, \mathbf{x}_{d_2}). \tag{17.5}$$

  If an internal representation is available, the cluster centroids $\mathbf{p}_i$ can be derived as the average of the internal representation vectors over the members of the i-th cluster $\mathbf{p}_i = (1/|C_i|) \sum_{d \in C_i} \mathbf{x}_d$.

  In these cases the intra-cluster distances can be measured with respect to the cluster centroid $\mathbf{p}_i$, obtaining the related but different minimization problems:

$$\min \sum_{d \in C_i} \delta(\mathbf{x}_d, \mathbf{p}_i). \tag{17.6}$$

- Maximization of inter-cluster distance. One wants the different clusters to be clearly separated.

As anticipated, the two objectives are not always compatible, clustering is indeed a **multi-objective optimization** task. It is left to the final user to weigh the importance of achieving clusters of very similar entities *versus* achieving clusters which are well separated, also depending on the chosen number of clusters.

Divisive algorithms are among the simplest clustering algorithms. They begin with the whole set and proceed to divide it into successively smaller clusters. One simple method is to decide the number of clusters k at the start and subdivide the data set into *k subsets*. If the results are not satisfactory, the algorithm can be reapplied using a different k value.

If one wants to represent groups of entities by a single vector, one can select the prototypes which minimize the average **quantization error**, the error incurred when the entities are substituted with their prototypes:

$$\text{Quantization Error} = \sum_d \|\mathbf{x}_d - \mathbf{p}_{c(d)}\|^2, \tag{17.7}$$

where $c(d)$ is the cluster associated with data d.

In statistics and machine learning, **k-means clustering** partitions the observations into k clusters represented by **centroids** (prototypes for cluster c, denoted as $\mathbf{p}_c$), so that each observation belongs to the cluster with the *nearest* centroid. The iterative method to determine the prototypes in k-means, illustrated in Fig. 17.3, consists of the following steps.

1. Choose the number of clusters k.

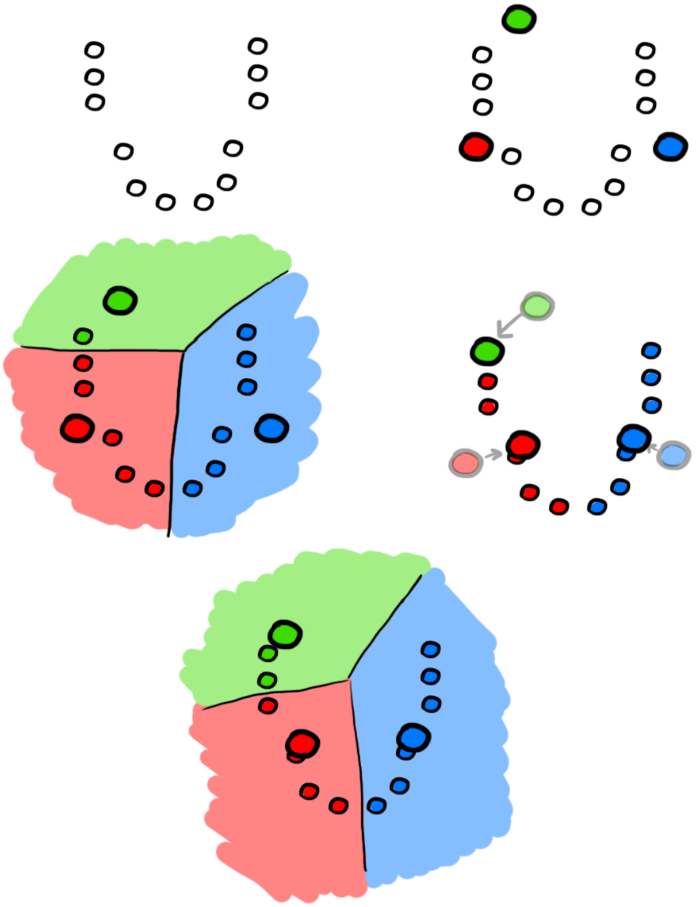


Figure 17.3: K-means algorithm in action (from top to bottom, left to right). Initial centroids are placed. Space is subdivided into portions close to the centroids (Voronoi diagram: each portion contains the points which have the given centroid as closest prototype). New centroids are calculated. A new space subdivision is obtained.

2. Randomly generate k clusters and determine the cluster centroids $\mathbf{p}_c$, or pick k randomly chosen training examples as cluster centroids. In other words, the initial centroid positions can be chosen randomly among the original data points.

3. Repeat the following steps until some convergence criterion is met, usually when the last assignment hasn't changed, or a maximum number of iterations has been executed.

   (a) Assign each point $\mathbf{x}$ to the nearest cluster centroid, the one minimizing $\delta(\mathbf{x}, \mathbf{p}_c)$.

   (b) Recompute the new cluster centroid by averaging the points assigned in the previous step:

$$\mathbf{p}_c \leftarrow \frac{\sum_{\text{entities in cluster } c} \mathbf{x}}{\text{number of entities in cluster } c}.$$

The main advantages of this algorithm are simplicity and speed, it can be used also on large datasets. **K-means clustering** can be seen as a skeletal version of the **Expectation-Maximization** algorithm[2]: if the assignment of the

[2] In statistics, an expectation-maximization (EM) algorithm is a method for finding maximum likelihood or maximum a posteriori (MAP)

examples to the cluster is known, then it is possible to compute the centroids and, on the other hand, once the centroids are known it is easy to calculate the cluster assignments. Because at the beginning both the cluster centroids (the parameters of the various clusters) and the memberships are unknown, one cycles through steps of assignment and recalculation of the centroid parameters, aiming at a consistent situation.

Given a set of prototypes, an interesting concept is the **Voronoi diagram**. Each prototype $\mathbf{p}_c$ is assigned to a Voronoi cell, consisting of all points closer to $\mathbf{p}_c$ than to any other prototype. The segments of the Voronoi diagram are all the points in the space that are equidistant to the two nearest sites. The Voronoi nodes are the points equidistant to three (or more) sites. An example is shown in Fig. 17.3.

Up to now we considered hard clustering, where the assignment of entities to clusters is crisp. In some cases a softer approach is more appropriate, in which **assignments are not crisp, but probabilistic or fuzzy**. The assignment of each entity is defined in terms of a probability (or fuzzy value) associated with its membership in different clusters, so that values sum up to one. Consider for example a clustering of bald versus non-bald people. A middle-aged man with some hair left on his head may feel he is mistreated if associated with the cluster of bald people. By the way, in this case it is also inappropriate to talk about a probability of being bald, and a fuzzy membership is more suitable: one may decide that the person belongs to the cluster of bald people with a fuzzy value of 0.4 and to the cluster of hairy people with a fuzzy value of 0.6.

In **soft-clustering**, the cluster membership can be defined as a decreasing function of the dissimilarities, for example as:

$$\text{membership}(\mathbf{x}, c) = \frac{e^{-\delta(\mathbf{x},\mathbf{p}_c)}}{\sum_c e^{-\delta(\mathbf{x},\mathbf{p}_c)}}. \tag{17.8}$$

For updating the cluster centroids one can proceed either with a **batch** or with an **online update**. In the online update one repeatedly considers an entity $\mathbf{x}$, for example by randomly extracting it from the entire set, derives its current fuzzy cluster memberships and updates all prototypes so that the closer prototypes tend to become even closer to the given entity $\mathbf{x}$:

$$\begin{aligned} \Delta\mathbf{p}_c &= \eta \cdot \text{membership}(\mathbf{x}, c) \cdot (\mathbf{x} - \mathbf{p}_c); && (17.9) \\ \mathbf{p}_c &\leftarrow \mathbf{p}_c + \Delta\mathbf{p}_c. && (17.10) \end{aligned}$$

With a physical analogy, in the above equations the prototype is pulled by each entity to move along the vector $(\mathbf{x} - \mathbf{p}_c)$, and therefore to become closer to $\mathbf{x}$, with a force proportional to the membership.

In the batch update, one first sums update contributions over all entities to obtain $\Delta_{total}\mathbf{p}_c$, and then proceed to update, as follows:

$$\mathbf{p}_c \leftarrow \mathbf{p}_c + \Delta_{total}\mathbf{p}_c. \tag{17.11}$$

When the parameter η is small, the two updates tend to produce very similar results, when η grows different results can be obtained. The online update avoids summing all contributions before moving the prototype, and it is therefore suggested when the number of data items becomes very large.

The k-means results can be visualized by a scatterplot display, as in Fig. 17.4. The k cluster prototypes are marked with large gray circles. The data points associated with a cluster are those for which the given prototype is the closest one among the k prototypes.

estimates of parameters in statistical models, where the model depends on unobserved latent variables. EM is an iterative method which alternates between performing an expectation (E) step, which computes the expectation of the log-likelihood evaluated using the current estimate for the latent variables, and a maximization (M) step, which computes parameters maximizing the expected log-likelihood found on the E step.

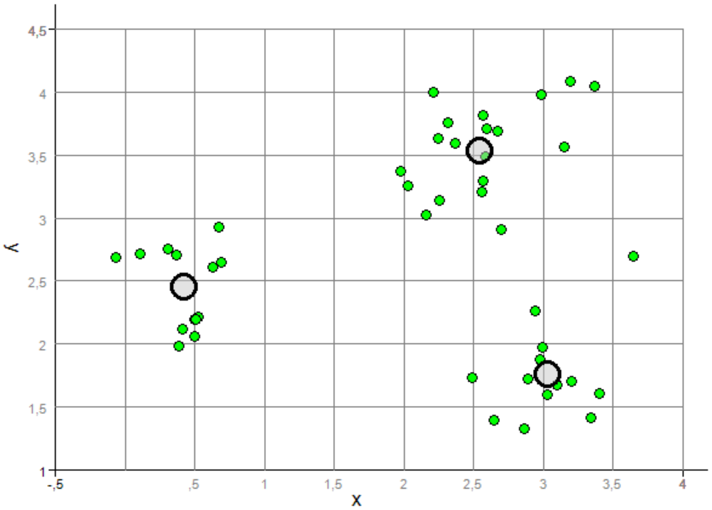


Figure 17.4: K-means clustering. Individual points and cluster prototypes are shown.

Gist

Unsupervised learning deals with building models using only input data, without resorting to classification labels. In particular, clustering aims at grouping similar cases together, dissimilar cases in different groups. The information to start the clustering process can be given as relationships between couples of points (**external representation**) or as vectors describing individual points (**internal representation**). In the second case, an average vector can be taken as a **prototype** for the members of a cluster.

The objectives of clustering are: compressing the information by abstraction (considering the groups instead of the individual members), identifying the global structure of the experimental points (which are typically not distributed randomly in the input space but “clustered” in selected regions), reducing the cognitive overload by using prototypes.

There is not a single “best” clustering criterion. Interesting results depend on the way to measure **similarities** and on the relevance of the grouping for the subsequent steps. In particular, one trades off two objectives: a high similarity among members of the same cluster and a high dissimilarity among members of different clusters.

In **top-down clustering** one proceeds by selecting the desired number of classes and subdividing the cases. K-means starts by positioning K prototypes, assigning cases to their closets prototypes, recomputing the prototypes as averages of the cases assigned to them, ...

Clustering gives you a new perspective to look at your *dog Toby*. *Dog* is a cluster of living organisms with four paws, barking and wagging their tails when happy, *Toby* is a cluster of all experiences and emotions related to your favorite little pet.

Chapter 18

Bottom-up (agglomerative) clustering

Birds of a feather flock together.
(Proverb: Those of similar taste congregate in groups)

Clustering methods require setting many parameters, such as the appropriate number of clusters in K-means, as explained in Chapter 17. A way to avoid choosing the number of clusters at the beginning consists of building progressively larger clusters, in a hierarchical manner, and leaving the choice of the most appropriate number and size of clusters to a subsequent analysis. This is called **bottom-up, agglomerative clustering**. Hierarchical algorithms find successive clusters by using previously established clusters, beginning with each element as a separate cluster and merging them into successively larger clusters. At each step the most similar groups are merged.

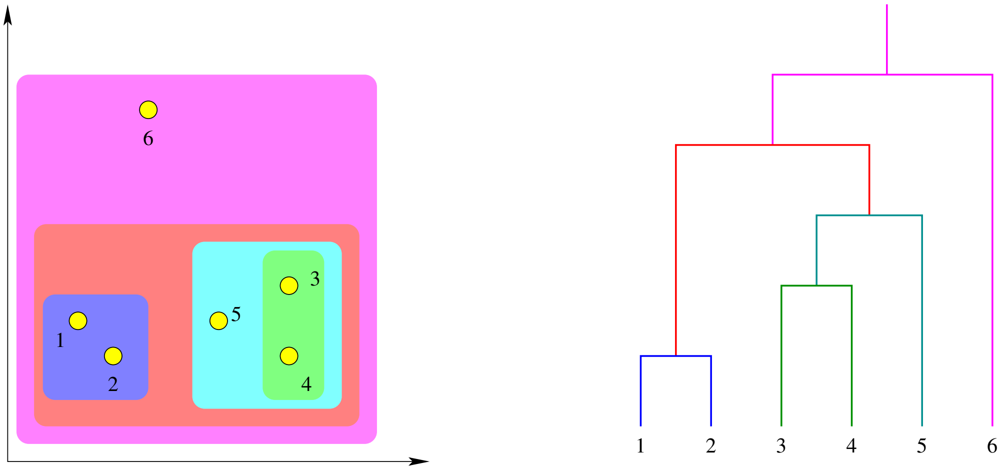


Figure 18.1: A dendrogram obtained by bottom-up clustering of points in two dimensions (with the standard Euclidean distance). Each point is an entity described by two numeric values.

18.1 Merging criteria and dendrograms

Let $\mathcal{C}$ represent the current clustering as a collection of subsets of entities, the individual clusters C. Thus $\mathcal{C}$ defines a partition: each entity belongs to one and only one cluster. Initially $\mathcal{C}$ consists of singleton groups, each with one entity.

As in top-down clustering, bottom-up merging also needs a measure of distance to guide the process. In this case, the relevant measure is the distance between two clusters $C, D \in \mathcal{C}$, let's call it $\overline{\delta}(C, D)$, which is derived from the original distance between entities $\delta(x, y)$. There are at least three different ways to define it, leading to very different results. In fact, it is possible to consider the average distance between pairs, the maximum, or the minimum distance, as follows:

$$\begin{aligned}
\overline{\delta}_{ave}(C, D) &= \frac{\sum_{x \in C,\, y \in D} \delta(x, y)}{|C| \cdot |D|}; \\
\overline{\delta}_{min}(C, D) &= \min_{x \in C,\, y \in D} \delta(x, y); \\
\overline{\delta}_{max}(C, D) &= \max_{x \in C,\, y \in D} \delta(x, y).
\end{aligned}$$

The algorithm now proceeds with the following steps:

1. find C and D in the current $\mathcal{C}$ with minimum distance $\overline{\delta}^* = \min_{C \neq D} \overline{\delta}(C, D)$;

2. substitute C and D with their union $C \cup D$, and register $\overline{\delta}^*$ as the distance for which the specific merging occurred;

until a single cluster containing all entities is obtained.

The history of the hierarchical merging process and the distance values at which the various merging operations occurred can be used to plot a **dendrogram** (from Greek *dendron* "tree", *-gramma* "drawing") illustrating the process in a visual manner, as shown in Fig. 18.1-18.2.

The dendrogram is a tree where the original entities are at the bottom and each merging is represented with a horizontal line connecting the two fused clusters. The position of the horizontal line on the Y axis shows the value of the distance $\overline{\delta}^*$ at which the fusion occurred. To reconstruct the clustering process, imagine that you move a horizontal

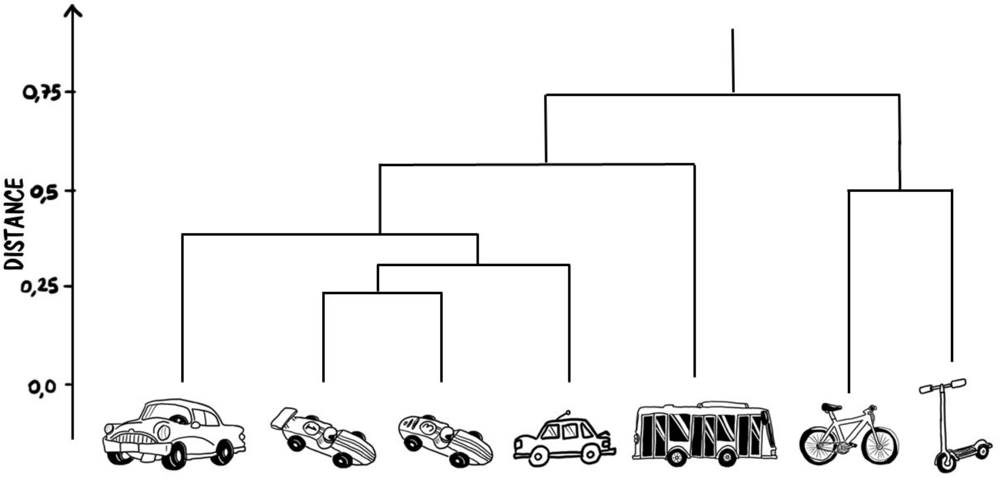


Figure 18.2: A dendrogram obtained by bottom-up clustering of vehicles.

ruler over the dendrogram, from the bottom to the top of the plot. Dendrograms are close cousins of the trees used in the natural sciences to visually represent related species, in which the root represents the oldest common ancestor species, and the branches indicate successively more recent divisions leading to different species.

By selecting a value of the desired distance level and cutting horizontally across the dendrogram, the number of clusters at that level and their members are immediately obtained, by following the subtrees down to the leaves. This provides a simple visual mechanism for analyzing the hierarchical structure and determining the appropriate number of clusters, depending on the application and also on the detailed dendrogram structure. For example, if a large gap in distance levels is present along the Y axis of the dendrogram, that can be a possible candidate level to cut horizontally and identify “natural” clusters.

18.2 A distance adapted to the distribution of points: Mahalanobis

The **Mahalanobis distance** was prompted by the problem of identifying the similarities of human skulls based on measurements (in 1927) and is now widely used to **take the data distribution into account when measuring dissimilarities**. The data distribution is summarized by the correlation matrix.

After a set of points are grouped together in a cluster one would like to describe the whole cluster in quantitative (*holistic*) terms, instead of considering just the cloud of points grouped together. In the following we assume that the clouds of points forming the clusters have simple ball-shaped or “elliptic” forms, excluding for the moment more complex arrangements like for example spirals, zigzagging or similar convoluted forms.

In addition, given a new test point in N-dimensional Euclidean space, one would like to estimate the probability that the new point belongs to the cluster. A first step can be to find the average or center of mass of the sample points. Intuitively, the closer the point in question is to this center of mass, the more likely it is to belong to the set.

However, we also need to know if the set is spread out over a large range or a small range, so that we can decide whether a given distance from the center can be considered large or not. The simplistic approach is to estimate the standard deviation σ of the distances of the sample points from the center of mass. If the distance between the test point and the center of mass is less than one standard deviation, then we might conclude that the new test point belongs to the set with a high probability. This intuitive approach can be made quantitative by defining the **normalized distance** between the test point and the set to be $(x - \mu)/\sigma$. By plugging this into the normal distribution we can derive the probability of the test point belonging to the set.

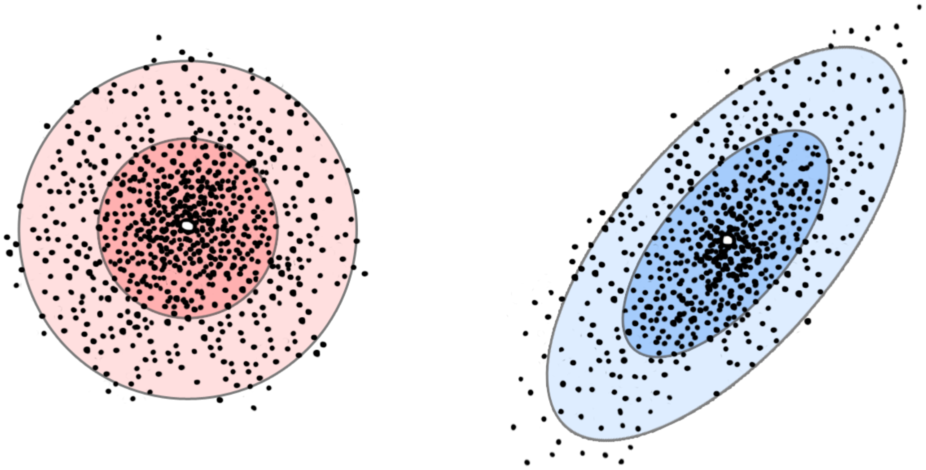


Figure 18.3: In the case on the left we can use the Euclidean distance as a dissimilarity measure, while in the other case we need to refer to the Mahalanobis distance, because the data are distributed in an ellipsoidal shape.

The drawback of the above approach is that it assumes that the sample points are distributed in a spherical manner. If the distribution is highly non-spherical, for instance ellipsoidal, then one would expect the probability of the test point belonging to the set to depend not only on the distance from the center of mass, but also on the direction. In those directions where the ellipsoid has a short axis the test point must be closer, while in those where the axis is long the test point can be further away from the center.

The ellipsoid that best represents the set's probability distribution can be estimated by building the **covariance matrix** of the samples.

Let $C = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_n\}$ be a cluster in D dimensions. The center $\bar{\boldsymbol{p}}$ of the cluster is the mean value:

$$\bar{\boldsymbol{p}} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{x}_i. \tag{18.1}$$

Let the covariance matrix components are defined as:

$$S_{ij} = \frac{1}{n}\sum_{k=1}^{n}(p_{ki} - \bar{p}_i)(p_{kj} - \bar{p}_j), \qquad i, j = 1, .., D. \tag{18.2}$$

The Mahalanobis distance is simply the distance of the test point from the center of mass divided by the width of the ellipsoid in the direction of the test point. Fig. 18.3 illustrates the concept. In detail, the **Mahalanobis distance** of a vector $\boldsymbol{x}$ from a set of values with mean $\boldsymbol{\mu}$ and covariance matrix $\mathbf{S}$ is defined as:

$$D_M(\boldsymbol{x}) = \sqrt{(\boldsymbol{x} - \boldsymbol{\mu})^T \mathbf{S}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})}. \tag{18.3}$$

The Mahalanobis distance can also be defined as a dissimilarity measure between two random vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ of the same distribution with the covariance matrix $\mathbf{S}$:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{(\boldsymbol{x} - \boldsymbol{y})^T \mathbf{S}^{-1} (\boldsymbol{x} - \boldsymbol{y})}. \tag{18.4}$$

If the covariance matrix is the identity matrix, the Mahalanobis distance reduces to the Euclidean distance. If the covariance matrix is diagonal, then the resulting distance measure is called the **normalized Euclidean distance**:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\sum_{i=1}^{D} \frac{(x_i - y_i)^2}{\sigma_i^2}}, \tag{18.5}$$

where σ_i is the standard deviation of the x_i over the sample set.

After clarifying the concepts of Mahalanobis distance and of the possible description of a cloud of points in a cluster through ellipsoids characterized by a fixed Mahalanobis distance from the barycenter, we are ready to understand the way in which clusters can be visualized.

18.3 Visualization of clustering and parallel coordinates

This section explains how clusters can be visualized in 3D (feel free to skip it without any effect on understanding the subsequent chapters). In order to graphically represent a cluster, one can visualize its **inertial ellipsoid**, whose surface is the locus of points having unit distance from the cluster's average position according to the Mahalanobis metric given by the cluster's dispersion. One starts by projecting the data points to three dimensions and calculating the corresponding 3x3 covariance matrix.

In graphical packages for three-dimensional rendering, points can be represented as row vectors of homogeneous coordinates in $\mathbb{R}^4$ with the infinite plane represented as $(x, y, z, 0)$, the projective coordinate transformation, mapping the unit sphere into the desired ellipsoid, is represented by the following matrix:

$$T_C = \begin{pmatrix} S_{11} & S_{12} & S_{13} & 0 \\ S_{21} & S_{22} & S_{23} & 0 \\ S_{31} & S_{32} & S_{33} & 0 \\ \bar{p}_1 & \bar{p}_2 & \bar{p}_3 & 1 \end{pmatrix}. \tag{18.6}$$

When moving between hierarchical clustering levels, cluster C will split into several clusters $C_1, \ldots, C_l$. To preserve the proper mental image, a parametric transition from ellipsoid T_C to its l offspring $T_{C_1}, \ldots, T_{C_l}$ will be animated and the ellipsoids

$$T_{C_i}^{\lambda} = (1 - \lambda)T_C + \lambda T_{C_i}, \qquad i = 1, \ldots, l$$

will be drawn with parameter λ uniformly varying from 0 to 1 in a given time interval (currently 1 second). This will effectively show the original ellipsoid *morphing* into its offspring.

Fig. 18.4 shows some clusters resulting from the analysis of a set of cars, characterized by a vector containing mechanical characteristics and price. The edge intensity is related to the object distances: the closer the objects the darker the color.

One can navigate up and down the clustering hierarchy until identifying a suitable number of clusters for conducting the analysis. Then prototypes can be examined to provide a summarized version of the data.

A particularly useful and direct tool to use for visualizing clusters of large-dimensional data is the **parallel coordinates** display. An example for the three clusters of the original Fisher Iris data is shown in Fig. 18.5. In a parallel coordinates plot, each vertical axe corresponds to a coordinate. A point in n-dimensional space is represented as a *polyline* (a line composed of attached segments) with vertices on the parallel axes. The position of the vertex on the i-th axis corresponds to the i-th coordinate of the point. By acting on filters, the number of points displayed can be reduced to concentrate on the most interesting ones. Furthermore, different ordering of the axes, colored lines, highlighting, background colors, etc. can add useful information to the plot. At a glance, both the individual items and the overall structure of clusters (or subset of items) is visible.

The parallel coordinates plot is probably the least known but simplest and most effective way to visualize n-dimensional points, as soon as n is larger than the two or three dimensions we can observe directly with our eyes. You do not need to be an engineer (the enlightened caste which is already using them) to use parallel coordinates plots.

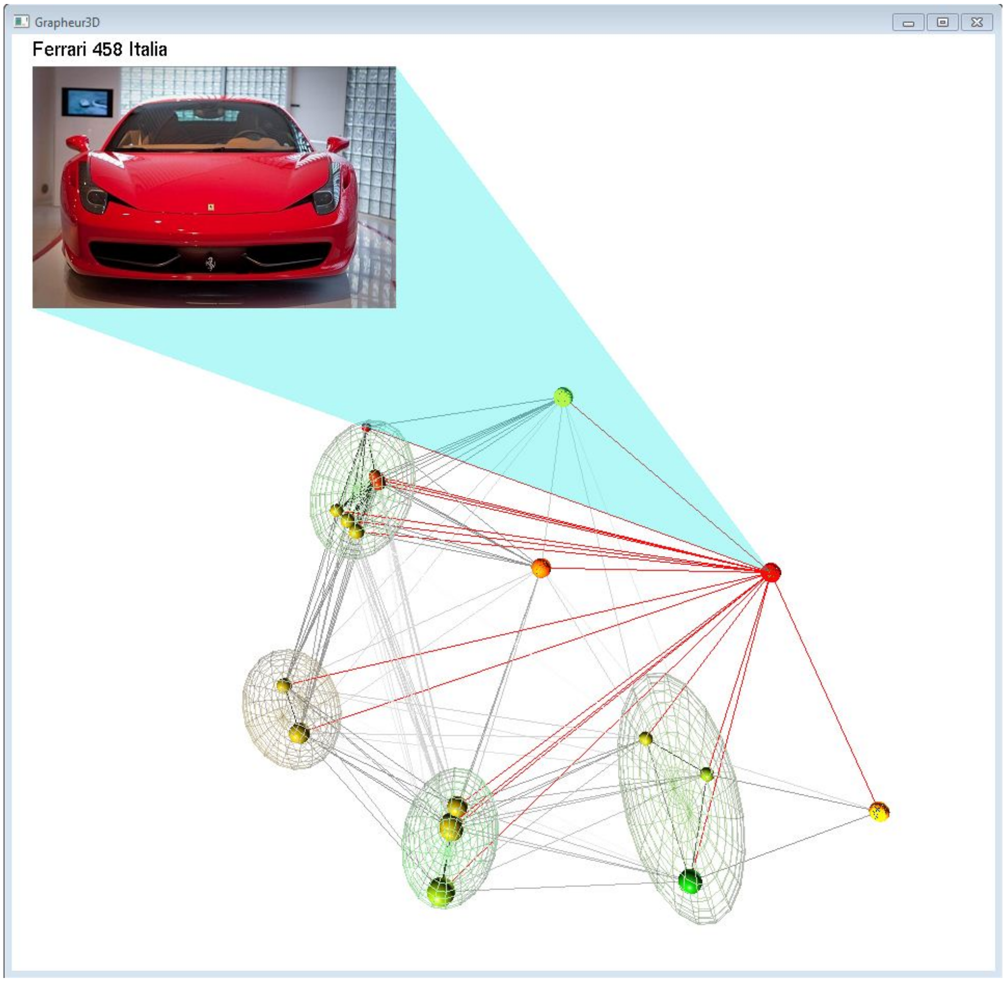


Figure 18.4: Clustering cars from mechanical characteristics.

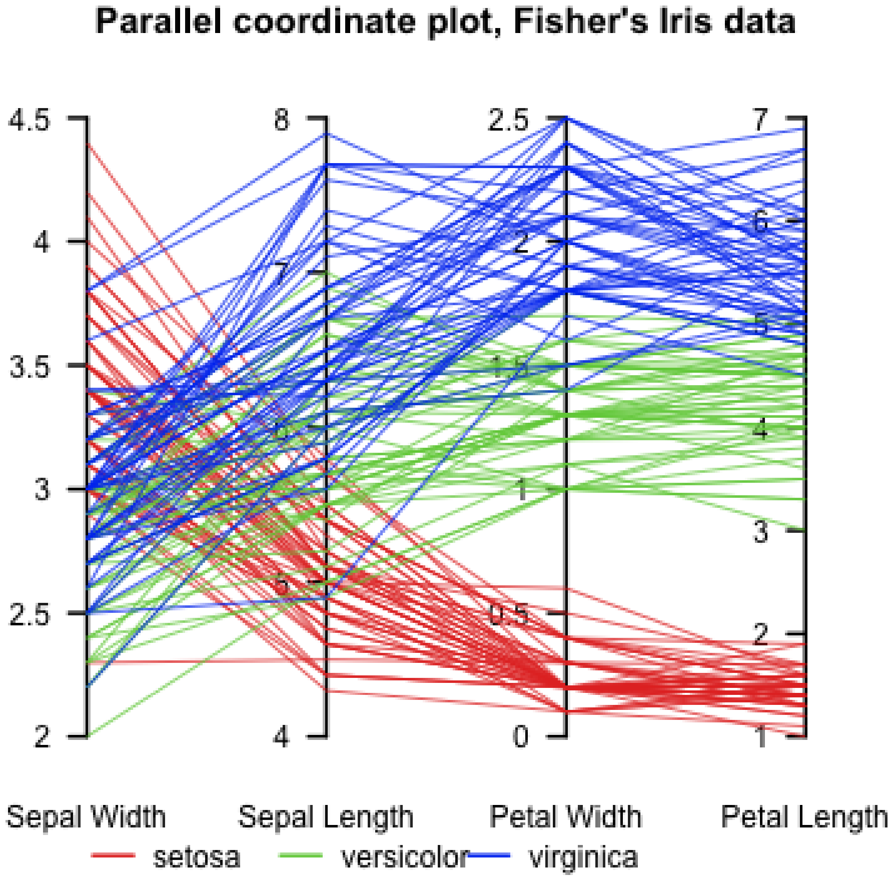


Figure 18.5: Parallel coordinates plot for Fisher Iris data (each flower is characterized by four geometrical measures). A vertical axe for each dimension. Each item is represented by a polyline cutting the i-th axe at the item's value of the i-th coordinate.

Gist

Agglomerative clustering builds **a tree (a hierarchical organization)** containing data points. If trees are unfamiliar to you, think about the folders that you may use to organize your documents, either physically or in a computer (docs related to a project together, then folders related to the different projects merged into a "work in progress" folder, etc.).

Imagine that you have no secretary and no time to do it by hand: a bottom-up clustering method can do the work for you, provided that you set up an appropriate way to measure similarities between individual data points and between sets of already merged points.

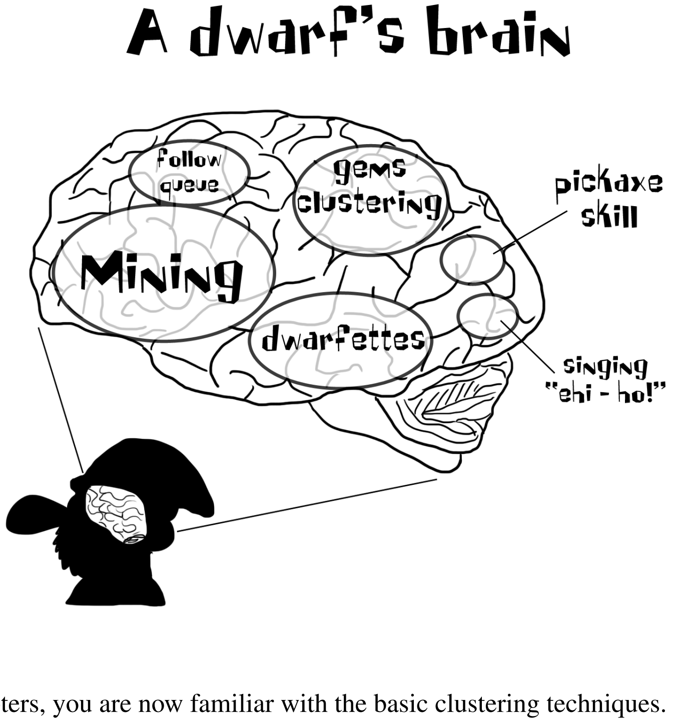
This method is called "**bottom-up**" because it starts from individual data points, merges the most similar ones and then proceeds by merging the most similar sets, until a single set is obtained. The number of clusters is not specified at the beginning: a proper number can be obtained by cutting the tree (a.k.a. **dendrogram**) at an appropriate level of similarity, after experimenting with different cuts.

Through agglomerative clustering, Santa can now organize all Christmas presents as a single huge red box. After one opens it one finds a set of boxes, after opening them, still other boxes, until the "leaf" boxes contain the actual presents.

Chapter 19

Self-organizing maps

The grandmother cell *is a hypothetical neuron*
that represents any complex and specific concept or object.
It activates when a person's brain "sees, hears, or otherwise sensibly discriminates"
such a specific entity as his or her grandmother.
(Jerry Lettvin, 1969)



From the previous chapters, you are now familiar with the basic clustering techniques. Clustering identifies group of similar data, in some cases with a hierarchical structure (groups, then groups containing groups, ...). If an internal representation is available, a group can be represented with a prototype. This chapter deals with **prototypes arranged according to a regular grid-like structure and influencing each other if they are neighbors in this grid**.

The idea is to **cluster data (entities) while at the same time visualizing this clustered structure on a two-dimensional map**. One wants a visualization that is at least approximately coherent with the clustering — this should be puzzling enough to continue reading.

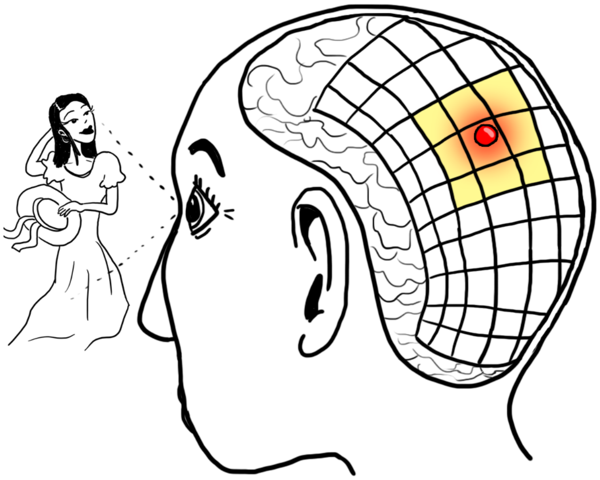


Figure 19.1: The presence of certain external stimuli activates a region in the brain ("*grandmother cell*"). In some areas, neurons are approximately organized according to a two-dimensional structure, like in the cortex, the surface layer of the brain where most high-level functionalities are located.

Let each cluster i be associated with a representative vector, a prototype $\mathbf{p}_i$. In the field of marketing, it is usual to identify different customer types, and describe them through prototypes (wealthy single individual, middle-class worker with family, etc.). A prototype will have the same number of coordinates as our entities and each component of the vector will describe a representative value for the given cluster, for example the average value of the entities contained in the cluster.

A coherent visualization demands that similar prototypes are placed in nearby positions in the 2D visualization space. Of course, for high-dimensional problems (problems with more than two coordinates), no exact solution is available and one aims at approximations which are sufficient for us to reason about the data. A **self-organizing map (SOM)** is a type of artificial neural network that is trained by using unsupervised learning to produce a two-dimensional representation of the training samples, called a map. This model was introduced as an artificial neural network by Teuvo Kohonen, and is also called a **Kohonen map**.

19.1 An artificial cortex to map entities to prototypes

A self-organizing map consists of component nodes or neurons. The arrangement of nodes is a regular placement in a two-dimensional grid. In some cases the grid is hexagonal, so that each node has six closest neighbors instead of four neighbors like in a traditional squared grid (Fig. 19.3). Associated with each node i is a prototype vector $\mathbf{p}_i$ of the same dimension as the input data vectors, *and* a position in the map space.

The analogy is again with our neural system: the **neurons are organized according to a physical network of connections in the brain, in practice two or three-dimensional**. Some neurons are tuned by evolution and training to fire electrical signals for particular events, as shown in Fig. 19.1. For example, a neuron may fire when your mother enters your visual field. The prototype is in this case given by visual features corresponding to your mother, the position is the physical position of the neuron in the brain.

Another principle of our neural systems is that, in many cases, **neurons that are neighbors tend to fire for similar input data** (a neighbor of the neuron firing for your mother presence may be close to one firing for an old photo of your mother). After training, the self-organizing map describes a mapping from a higher-dimensional input space to

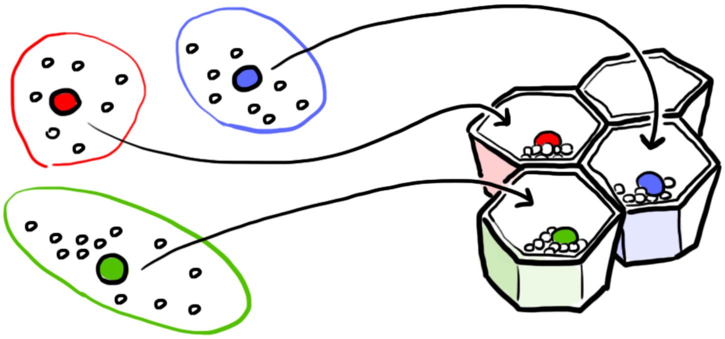


Figure 19.2: A SOM maps entities in a multi-dimensional space into cells in two-dimensional space. Each cell contains a prototype and the entities for which the prototypes is the most similar one.

a two-dimensional map space. Each cell in two dimensions corresponds to a neuron and contains a prototype vector. A generic entity is then mapped (or assigned) to the neuron with the prototype vector which is *nearest* to the vector describing the entity, as shown in Fig. 19.2. The training can start from a random initial configuration of the prototype vectors (for example picked to be equal to a random subset of entities) and then iterate by presenting and mapping randomly selected cases. The winning neuron $c(\mathbf{x})$, or c for brevity, is identified as the one with the prototype closest to the vector describing the current case $\mathbf{x}$:

$$c(\mathbf{x}) = \arg\min_i \|\mathbf{x} - \mathbf{p}_i\|. \tag{19.1}$$

Then the winning prototype $\mathbf{p}_{c(\mathbf{x})}$ is changed to make it more similar to the one of the current case presented to the network. In addition, the prototypes of *nearby* vectors are also changed in a similar manner, although by smaller and smaller amounts as the distance in the grid increases.

Think about a democratic system in which voters (entities) are asked to educate a set of regularly-arranged representatives (like in a chamber of the parliament) so that at least one of them represents a cluster of related ideas, and in which representatives sitting in nearby positions influence each other, and tend to become similar. Two "force fields" are active, attractive forces between entities and prototypes, and attractive forces between neighboring prototypes on the grid. Entities (voters) compete for prototypes: each entity is pulling its *winning* prototype and, to a less extent, the neighbors of the winning prototype, to move a bit towards itself, to make it progressively more similar. Of course, different entities are pulling in different directions and the resulting dynamical system is very complex.

After explaining the basic mechanism and motivations, let's now fix the details. In an online learning scheme, at each iteration t a random entity $\mathbf{x}$ is extracted, its winning neuron c is determined, and all prototype vectors $\mathbf{p}_i(t)$ at iteration (time) t are then modified as follows:

$$\mathbf{p}_i(t+1) \leftarrow \mathbf{p}_i(t) \;+\; \eta(t)\cdot \text{Act}\big(c(\mathbf{x}), i, \sigma(t)\big)\cdot(\mathbf{x} - \mathbf{p}_i(t)), \tag{19.2}$$

where $\eta(t)$ is a time-dependent small learning rate, $\text{Act}\big(c, i, \sigma(t)\big)$ is an **activation function** which depends on the distance between the two neurons in the 2D grid, and on a time-dependent radius $\sigma(t)$. The two neurons involved in the formula are: the winning neuron c for pattern $\mathbf{x}$, and the neuron i whose pattern $\mathbf{p}_i(t)$ is being updated. The modification mechanism resembles the update described in equation (17.9) for soft clustering in k-means, but with the important difference given by the regular two-dimensional organization of the neurons, which now determines the activation level.

To help convergence, usually the learning rate decreases in time, and the same happens for the radius parameter. The idea is that at the beginning the neuron prototypes are moving faster (*neural plasticity* is higher for young children!), and they tend to activate a larger set of neighbors, while movements are smaller and limited to a smaller set of neighbors in the last phase, when hopefully the arrangement already identified the main characteristics of the data distribution and only a fine-tuning is needed. The learning rate in some cases decreases like $\eta(t) = A/(B+t)$. A reasonable default can be $\eta(t) = 1/(20+t)$.

In batch training, all N entities $\mathbf{x}_j$ are presented to the SOM and their winning neurons $c(\mathbf{x}_j)$ are identified before proceeding to an update as follows:

$$\mathbf{p}_i(t+1) \leftarrow \frac{\sum_{j=1}^{N} \text{Act}\big(c(\mathbf{x}_j), i, \sigma(t)\big) \cdot \mathbf{x}_j}{\sum_{j=1}^{N} \text{Act}\big(c(\mathbf{x}_j), i, \sigma(t)\big)}. \tag{19.3}$$

Each prototype is updated with a weighted average over all entities, the weight being proportional to the vicinity in neuron grid space (usually two-dimensional) between the winning neuron prototype and the current prototype.

Because of the system complexity, one is encouraged to try different parameters and different time schedules until acceptable results are obtained. For example, a suitable neighborhood activation function can be:

$$\text{Act}\big(c, i, \sigma(t)\big) = \exp\left(-\frac{{d_{ci}}^2}{2\,\sigma^2(t)}\right), \tag{19.4}$$

where d_{ci} is the distance between the two neurons in the two-dimensional grid, and $\sigma(t)$ is a neighborhood radius, at the beginning including more neighbors than the closest ones, at the end including only a set of close neighbors. Be careful not to confuse the distance between neurons in the grid, as shown in Fig. 19.3, with the distance between prototype vectors in the original multi-dimensional space of the data!

Let TOT_{SOM} be the total number of SOM neurons, and TOT_{iter} the number of iterations executed. The default value starts from $\sqrt{\text{TOT}_{\text{SOM}}}$, a value close to the radius of the grid if the grid is a square one, and ends with the value 2, as follows:

$$\sigma(t) = \frac{(\text{TOT}_{\text{iter}} - t)\sqrt{\text{TOT}_{\text{SOM}}} + 2t}{\text{TOT}_{\text{iter}}}. \tag{19.5}$$

One should not be discouraged by the complexity intrinsic in this and in similar mapping tasks: in many cases acceptable results are obtained by considering simple default values for the basic parameters. On the other hand, it is not surprising that a basic mapping mechanism of our brain is indeed characterized by a high complexity level, we are intelligent and in part unpredictable human beings, aren't we?

19.2 Using an adult SOM for classification

Even if you do not want to indulge in the *debauchery of indices* of the above mathematical details, you can still use SOM effectively as a guide in reasoning about your problem. After training, the SOM can be used to classify new objects by finding the closest (winning) prototype and assigning the new object to the corresponding cell, as illustrated in Fig. 19.4. In many cases, after looking at the prototypes, it will be easy to give *names* to the different cells, to help reasoning and remembering. But let's note that cells may discover *unusual* combinations, leading to interesting insight and *detection of novel groups*, and not only to re-discovering trivial classifications.

Let's imagine that you trained your SOM on marketing data: each cell may represent a characteristic group of customers. Possible names could be: "wealthy-single-individual," "poor-family-with-kids," "senior-retired-person," "spoiled-adolescent," etc. When a new customer arrives, you may easily identify the appropriate prototype, for example to pick the best strategy to sell him your products. If you are a movie fan, and you train your SOM to classify different kinds of movies, you may use a SOM to classify a new movie, for example to predict if you will like it or not (with a high probability).

In a SOM, the quality of training can be measured by the **quantization error** (the average error incurred by substituting an entity $\mathbf{x}$ with its winning prototype vector $\mathbf{p}_{c(\mathbf{x})}$, i.e., the average distance from each data vector to its nearest prototype) or by the **topological error**, which is related to the failure to assign close vectors in the original high-dimensional space to close neurons in neuron-grid space (usually two-dimensional). The topological error can

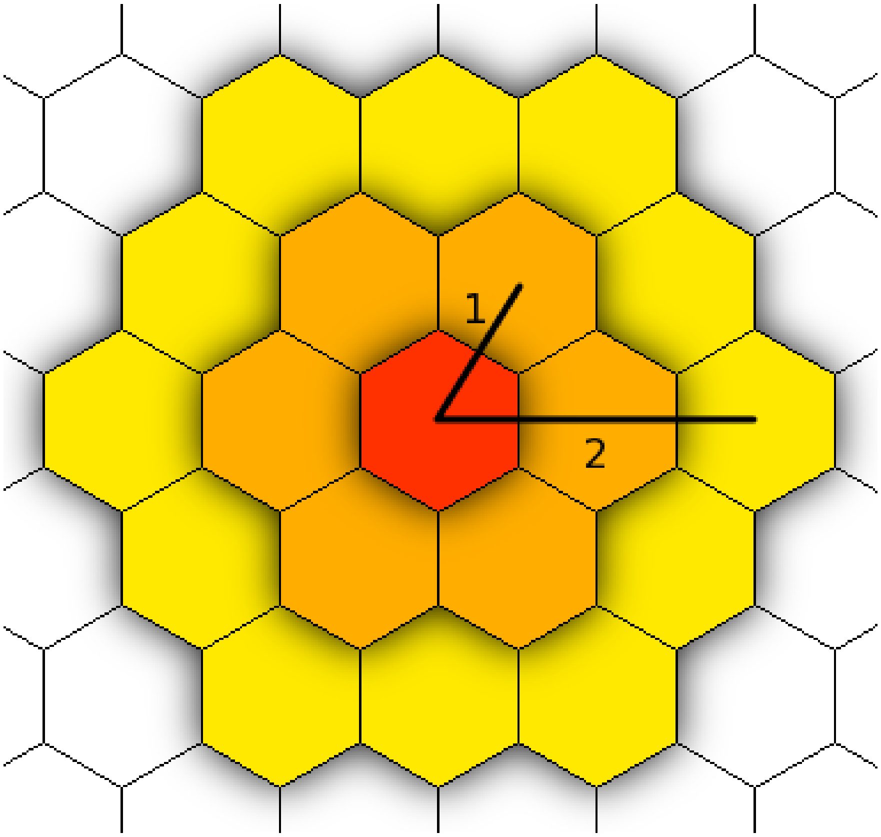


Figure 19.3: An example of neighborhood in a self organizing map: neighboring cell at distance 1 and 2 from the central are shown.

be evaluated as the fraction of all data vectors for which the first and the second nearest prototypes (in the original multi-dimensional space) are not represented by adjacent neurons in the grid mapping.

Color coding can be used to represent the value of the data point along a dimension, while the size of each hexagon can represent the value along another dimension (Fig. 19.5). The colored maps are called components or **component planes** and can be compared to identify local relationships. One can devise interesting new analysis techniques by combining the SOM map with a scatterplot display, or with a parallel coordinates plot (Fig. 18.5). For example, when the mouse pointer is moved over the SOM cells, the position of the prototype vector associated with each cell can be shown in a scatterplot or in a parallel coordinates plot. In this manner, details of relevant entities can be further analyzed.

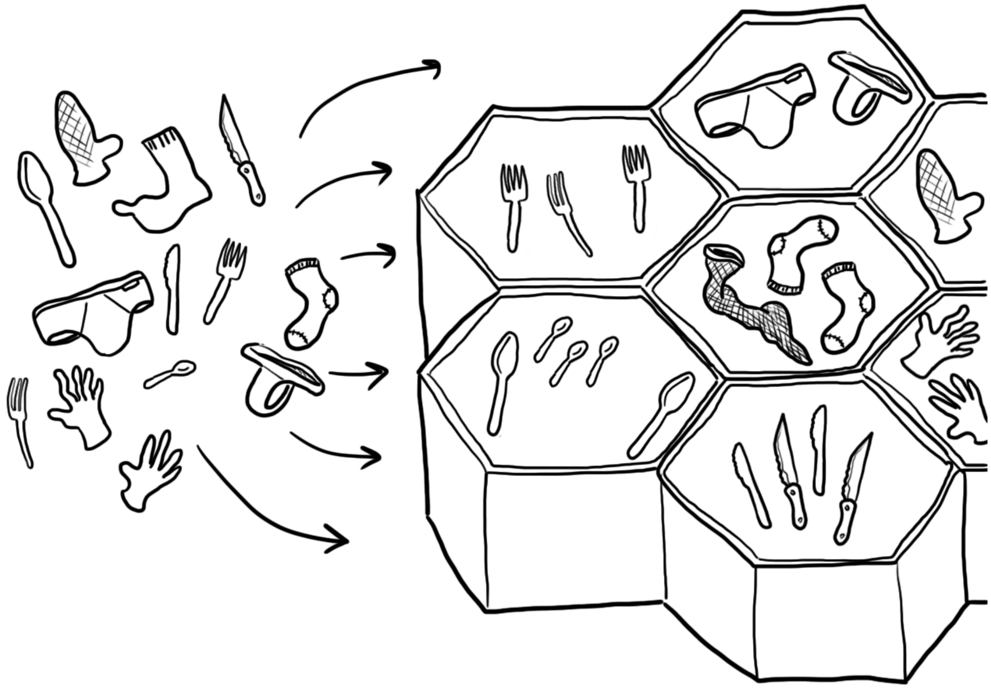
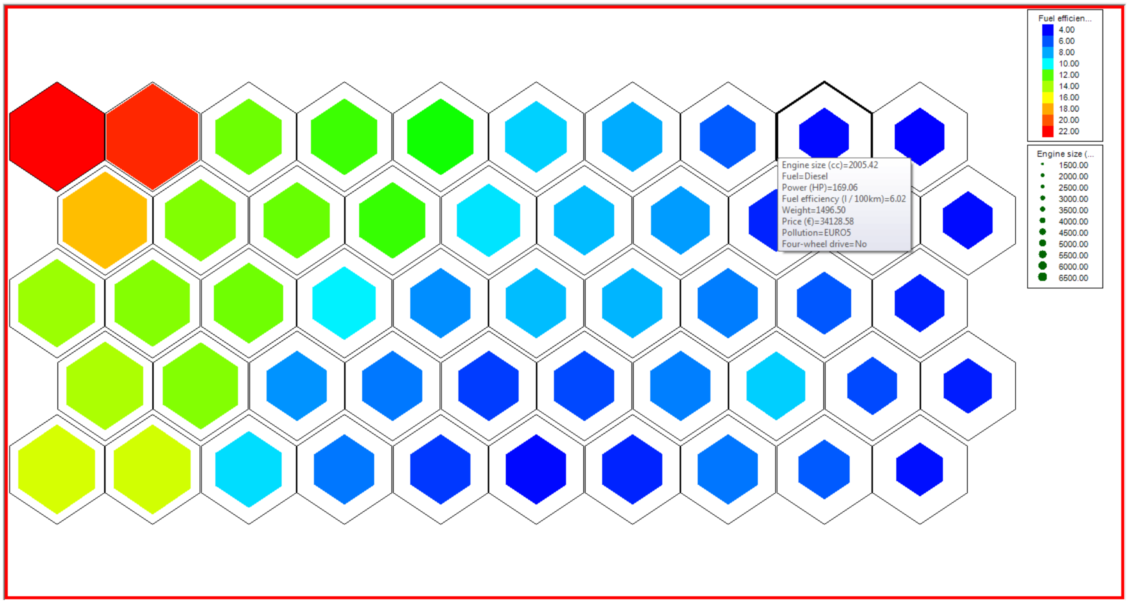


Figure 19.4: An analogy for the SOM: each cell is like a drawer in a well-organized piece of furniture. Neighboring drawers are used to contain similar objects.



Engine size (cc)=2005.42
Fuel=Diesel
Power (HP)=169.06
Fuel efficiency (l / 100km)=6.02
Weight=1496.50
Price (€)=34128.58
Pollution=EURO5
Four-wheel drive=No

Figure 19.5: A SOM, color and size depends on two coordinates of the prototype vectors. Prototypes can be examined by passing with the mouse over the cell (LIONoso.org software).

Gist

Self-organizing maps reach two objectives: placing a set of prototypes close to clusters of data points, and having the prototypes organized in a two-dimensional grid so that neighboring prototypes in the grid tend to be mapped to similar data points.

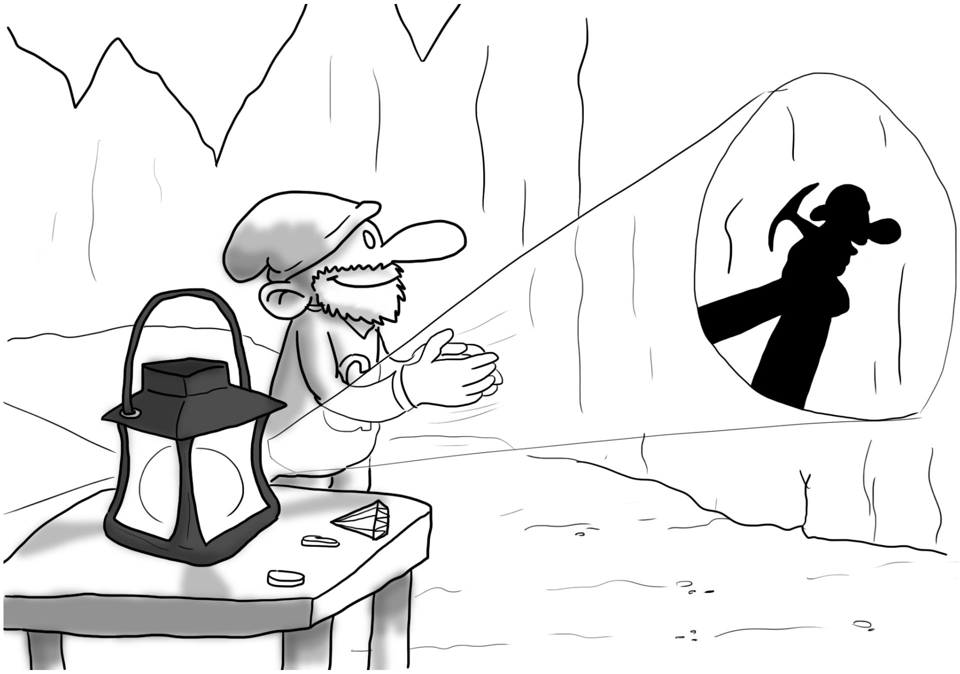
The motivations are in part biological (our neural cortex is approximately organized according to two- and three-dimensional arrangement of neurons) and in part related to visualization. A two-dimensional grid can be visualized on the screen, and the characteristics of the prototypes are not randomly scattered but slowly varying, because of the neighboring relationships, leading to more intelligible visualizations.

If data points are imagined as schooling fishes in the sea, a SOM is an elastic fisherman's network aiming at capturing the largest number of them without breaking up.

Chapter 20

Dimensionality reduction by projection

You, who are blessed with shade as well as light, you, who are gifted with two eyes, endowed with a knowledge of perspective, and charmed with the enjoyment of various colors, you, who can actually see an angle, and contemplate the complete circumference of a Circle in the happy region of the Three Dimensions – how shall I make it clear to you the extreme difficulty which we in Flatland experience in recognizing one another's configuration?
(Flatland - 1884 -Edwin Abbott Abbott)



In **exploratory data analysis** one is actually using the **unsupervised learning capabilities of our brain** to identify interesting patterns and relationships in the data. It is often useful to map entities to two dimensions, so that they can be analyzed by our eyes. The mapping has to preserve as much as possible the relevant information present in the original data, describing **similarities and diversities** between entities. For example, think about a marketing manager analyzing similarities and differences between customers, so that different campaigns can be tuned to the different groups, or think about the head of a human resources department who aims at classifying the competencies possessed by different employees. We would like to organize entities in two dimensions so that **similar objects are near each other and dissimilar objects are far from each other**. Let's note that there is a clear difference between this and SOM maps. In SOM, prototype vectors associated with a two-dimensional grid are moved (their coordinates are changed) to cover the original data space, whereas here the original points are mapped in different ways onto a two-dimensional surface.

Following the discussion in Chapter 17 (see Fig. 17.2), it's useful to recall the two ways in which initial information can be given to the system. A first possibility is that entities are characterized by an **internal structure (a vector of coordinates)**. In this case the raw coordinates can be used to *derive* a similarity measure, as by considering the Euclidean distance between the two corresponding vectors. A second possibility is that entities are endowed with an **external structure of pairwise relationships**, expressed by similarities or dissimilarities. We deal only with dissimilarities to avoid confusion and we leave to the reader the simple exercise of transforming the formulas to handle the other case. To establish a suitable notation, let the n entities be characterized by some mutual dissimilarities δ_{ij}. Some dissimilarities may be unknown.

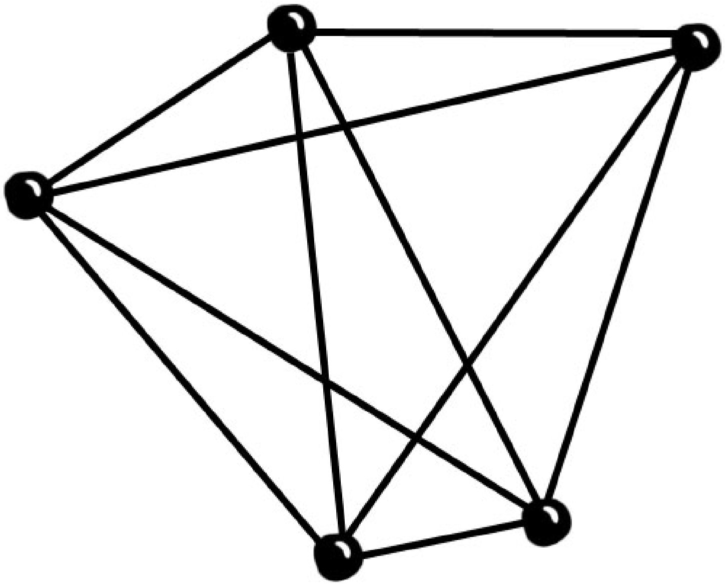


Figure 20.1: A graph with external dissimilarities (edges) between entities (nodes).

An appropriate model is an undirected graph, like the one illustrated in Fig. 20.1, in which each entity is represented by a node, and a connection with weight δ_{ij} is present between two nodes, if and only if a distance δ_{ij} is defined for the corresponding entities. The set of edges in the graph is denoted by E.

The two situations (coordinates or relationships) can be combined. In some cases the information given to the system consists of **both coordinates and relationships**. As a very concrete example, imagine that some automated clustering method has been applied to the data vectors. We can then declare two entities to be dissimilar ($\delta_{ij} = 1$) if and only if they do not belong to the same cluster. This additional information can be used to encourage a visualization where items coming *from the same cluster* tend to be close in the two-dimensional space. In other cases, indications about dissimilarities among items given by people can help for tuning the visualization and adapting it to the user's wishes.

A way to distinguish the different contexts has to do with the *level of supervision* in the visualization, i.e., the type of hints given to the process. The type of supervision ranges from a purely **unsupervised** approach (only coordinates are given) to a **supervised** approach (relationships or dissimilarities are fully specified), to mixed approaches combining unsupervised exploration in the vector space of coordinated and labeling methods.

After clarifying the context, depending on the available data, it is time to consider ways to use the data to produce useful visualizations. Methods derived from linear algebra are described in the following sections, while more general

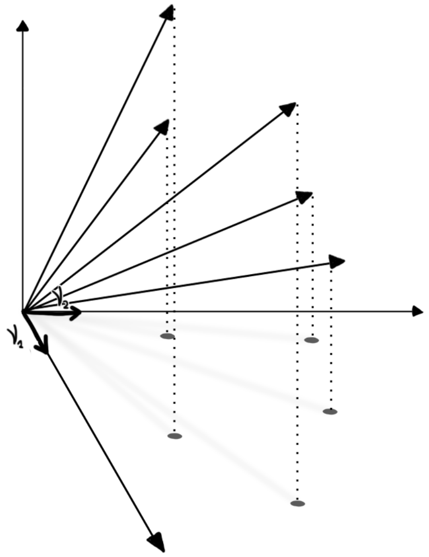


Figure 20.2: A projection: each dotted line connecting a vector to its projection is perpendicular to the plane defined by ν^1 and ν^2 (in this case the direction vectors are the X and Y axes, in general a projection can be on any plane identified by two linearly independent vectors).

nonlinear methods are described in future chapters. As usual, linear methods are simpler to understand, while nonlinear methods are in principle more powerful, although more complex.

20.1 Linear projections

This chapter starts from linear algebra, Let n be the number of vectors (entities), and let m be the dimension of each vector (the number of coordinates). For convenience, the n vectors can be stored as rows of an $n \times m$ matrix X. To help the reader, Latin indices i, j ranges over the data items, while Greek indices α, β range over the coordinates. Thus $X_{i\alpha}$ is the α-th coordinates of item i. For the rest of this chapter we assume that the **data is centered**, i.e., that the mean of each coordinate over the entire dataset is zero: $\sum_{i=1}^{n} X_{i\alpha} = 0$. If the original data are not centered, they can be preprocessed by a trivial translation. In other words, we are not interested in the absolute positions of the data points, but in their relative positions with respect to the other data. We denote by S the $m \times m$ biased **covariance matrix**: $S = \frac{1}{n} X^T X$, with the components: $S_{\alpha,\beta} = \frac{1}{n} \sum_{i=1}^{n} X_{i\alpha} X_{i\beta}$.

It is called covariance because each term measures how two coordinates tend to *vary together* for the different data points. The sum in the covariance will have a large positive value if positive values of the first coordinate tend to be accompanied by positive values of the second coordinate, and the same tends to be true for negative values. Actually, the covariance is changed if the values of a coordinate are multiplied by a constant (this happens every time one changes physical units, for example from millimeters to kilometers). A measure which does not depend on changes of physical units is the *correlation coefficient*, derived by dividing the covariance by the product of the standard deviations of the involved coordinates. (See Section 7.2.)

We consider a linear transformation L of the items to a space of dimension p, the usual value for p is two, but we keep this presentation more general. L is represented by a $p \times m$ matrix, acting on vector x by the usual matrix multiplication $y = Lx$. Each coordinate α of y is obtained by a scalar product of a row ν^α of L and the original coordinate vector x. The p rows $\nu^1, \ldots, \nu^p \in \mathbb{R}^m$ of L are called **direction vectors** and in the following we assume that they have unit norm $\|\nu^\alpha\| = 1$. Therefore each coordinate α in the transformed p-dimensional space is obtained by **projecting** the original vector x onto ν^α. If we project all items and we repeat for all coordinates we obtain the **coordinate vectors** $x^1 = X\nu^1, \ldots, x^p = X\nu^p$.

Among the possible linear transformations, interesting visualizations are obtained by **orthogonal projections**: the direction vectors $\nu^1, \ldots, \nu^p$ are mutually orthogonal and with unit norm: $\nu^\alpha \cdot \nu^\beta = \delta_{\alpha,\beta}, \alpha, \beta = 1, \ldots, p$, as illustrated in Fig. 20.2. Please note that here $\delta_{\alpha,\beta}$ is the usual Kronecker delta, equal to 1 if and only if the two indices are equal, not to be confused with dissimilarities! An example of orthogonal projection is a selection of a subset of the original coordinates (in this case $\nu^\alpha = (0, 0, \ldots, 1, \ldots, 0, 0)$, a vector with 1 for the selected coordinate and 0 in all other places). Other examples are obtained by first rotating the original vectors and then selecting a subset of coordinates.

The visualization is simple because it shows **genuine properties** of the data, corresponding to the intuitive notion of navigating in the original space, far from the data points, and looking at the data from different points of view[1]. Think about placing a two-dimensional screen at an arbitrary orientation, switching a lamp on (very far from the data), and observing the projected shadows. On the contrary, nonlinear transformations may deform the original data distribution in arbitrary and potentially very complex and counter-intuitive ways, as by viewing the world through a deforming lens.

As an additional feature of linear projections, it is easy to explain the p-dimensional coordinates because each one is a linear combination of the original coordinates (for example, the magnitude of the combination coefficients "explains" a lot about the relevance of the initial coordinates in the projection).

Last but not least, the storage requirements are limited to storing the direction vectors, and the computational complexity for projecting each point is the usual one for matrix-vector multiplication.

Now that the motivation is present, let's consider some of the most successful linear visualization methods.

20.2 Principal Components Analysis (PCA)

To *understand* the meaning of this historic transformation (PCA was invented in 1901 by Karl Pearson) it is useful to concentrate on what PCA is trying to accomplish. As usual, *optimization is the source of power* and helps us to understand the deep meaning of operations. Now, PCA finds the orthogonal projection that **maximizes the sum of all squared pairwise distances** between the projected data elements.

If dist^p_{ij} is the distance between the projections of two data points i and j:

$$\text{dist}^p_{ij} = \sqrt{\sum_{\alpha=1}^{p} ((X\nu^\alpha)_i - (X\nu^\alpha)_j)^2},$$

PCA maximizes:

$$\sum_{i<j} (\text{dist}^p_{ij})^2. \tag{20.1}$$

The objective is to spread the points as much as possible, but the fact of considering only projections implies that the mutual distances cannot increase beyond the original ones: $\text{dist}^p_{ij} \leq \text{dist}_{ij}$ (just consider Pythagoras theorem applied to the triangle defined by the original vector, the projection and the vector connecting the projection to the original vector). The best that we can obtain is to approximate as much as possible the original sum of squared distances:

$$\max_{\nu^1,\ldots,\nu^p} \sum_{i<j} (\text{dist}^p_{ij})^2 \leq \sum_{i<j} (\text{dist}_{ij})^2. \tag{20.2}$$

[1] Actually the mapping executed by our eye or by cameras is a perspective viewing projection so that the analogy is not to be taken literally.

After introducing the $n \times n$ *unit Laplacian* matrix L^u, as $L^u_{ij} = (n \cdot \delta_{ij} - 1)$, the optimization problem can be posed as the solution of:

$$\begin{aligned} \max_{\nu^1,\dots,\nu^p} \quad & \sum_{\alpha=1}^{p} (\nu^\alpha)^T X^T L^u X \nu^\alpha \\ \text{subject to} \quad & \nu^\alpha \cdot \nu^\beta = \delta_{\alpha,\beta}, \qquad \alpha, \beta = 1, \dots, p. \end{aligned} \tag{20.3}$$

The **Laplacian matrix** is in general a key tool for describing **pairwise relationships** between entities. In fact, it is used a lot in the study of graphs, where the pairwise relationship is given by weighted edges connecting two nodes. In general, it is an $n \times n$ symmetric positive semidefinite matrix, with zero row and column sums. Its usefulness is related to the possibility to express in a compact manner the **weighted sum of all pairwise squared distances**:

$$x^T L x = \sum_{i<j} -L_{ij}(x_i - x_j)^2. \tag{20.4}$$

Considering the p coordinate vectors introduced above, it is easy to check that:

$$\sum_{\alpha=1}^{p} (x^\alpha)^T L x^\alpha = \sum_{i<j} -L_{ij}\ (\text{dist}^p_{ij})^2. \tag{20.5}$$

The optimal solution of equation (20.3) is given by the p **eigenvectors with largest eigenvalues** of the $m \times m$ matrix $X^T L^u X$. For centered coordinates, this matrix is identical to the covariance matrix apart from a multiplicative factor (which does not influence the eigenvectors) $X^T L^u X = n^2 S$. The solutions for PCA is obtained by finding the **eigenvectors of the covariance matrix**. We prefer the above form with the Laplacian matrix which can be easily generalized to cases where we have additional information about relationships between data points. (See Section 20.3.) While we are not giving the details in this section, the fact that solutions are eigenvectors is again related to formulating the problem as a maximization task: the original quantity to be minimized is quadratic, and requiring zero gradient and satisfaction of constraints leads to linear (eigenvalue) equations.

As a side-effect of the above solution, PCA transforms a number of possibly correlated variables into a smaller number of uncorrelated variables called principal components. The first principal component accounts for as much of the variability in the data as possible, and each succeeding component accounts for as much of the remaining variability as possible. Another interesting explanations of PCA is that it minimizes the mean squared error incurred when approximating the data with their projection.

A geometric interpretation in three dimensions is shown in Fig. 20.3. If the data points form an m-dimensional ellipsoidal cloud, the eigenvectors of the covariance matrix are the principal axes of the ellipsoid. Principal component analysis reduces the dimensionality by restricting attention to the directions along which the scatter of the cloud is the greatest.

PCA is a simple and very popular transformation but with obvious limits (maybe too popular?). It simply performs a coordinate rotation that aligns the transformed axes with the directions of maximum variance. Having a larger variance is not always related to having a larger *information content*, for example it can be related to having a larger measurement noise. In addition, the variance along a coordinate can be easily enlarged by multiplying the coordinate by a constant, but the information content of course does not change. In other words, the PCA results depend on choosing appropriate physical units, a spherical cloud of points can become elongated for the superficial reason that millimeters instead of meters are used to measure a physical distance. Furthermore, because a sum of squared distances is involved in the optimization of equation (20.1), PCA is **sensitive to outliers**. Points which are very far from most of the other points contribute with large (squared) distances and encourage a choice of direction vectors which may be very different from those chosen if the outliers are eliminated. When PCA is used to identify promising features for classification in supervised learning, its main limitation is that it makes no use of the class label of the feature vector.

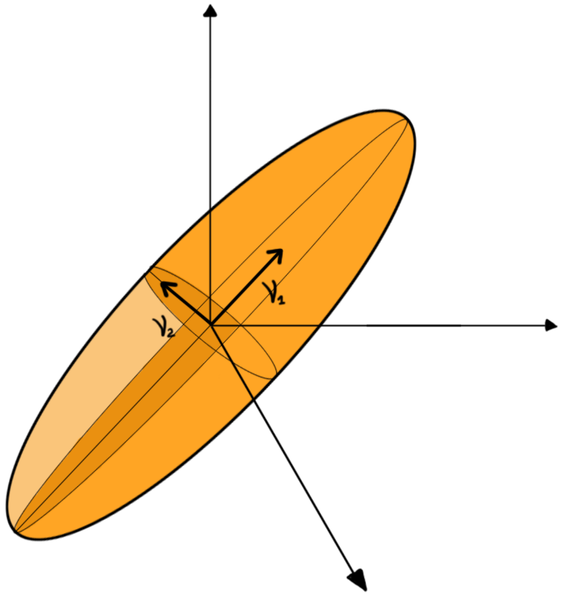


Figure 20.3: Principal component analysis, data are described by an ellipsoid. The first eigenvector is in the direction of the longest principal axis, the second eigenvector lies in a plane perpendicular to the first one, along the longest axis of the two-dimensional ellipse.

There is no guarantee that the directions of maximum variance will contain good features for discrimination, see also Chapter 7 about selecting and ranking features.

The computational cost is related to solving the eigenvalues-eigenvectors problem for a matrix of dimension $m \times m$. Let's note that the number of points n is not relevant, therefore the method is particularly fast when the number of initial coordinates is limited, even if the number of data points is very large. More details about PCA can be found in [238].

20.3 Weighted PCA: combining coordinates and relationships

As we mentioned before, in some cases additional information is available about the data in the form of *relationships* between (some) entities. For example, we may have a *class label*, so that some pairs are in the same class and we would like them to be close in the projected distance. Or we may have additional information about dissimilarities beyond what is obtained from the raw data coordinates.

Fortunately, we can extend PCA to incorporate additional information. For example, we can minimize a **weighted** sum of the squared projected distances:

$$\sum_{i<j} d_{ij} \cdot (\mathrm{dist}^p_{ij})^2. \tag{20.6}$$

If a weight d_{ij} is large, a large contribution to the function to be maximized is obtained if the corresponding dist^p_{ij} is also large. We can then interpret d_{ij} as weights measuring the importance that points i and j are placed far apart in the low dimensional projection space, let's call them dissimilarities. As in the unweighted case, we can now assign to the problem an $n \times n$ Laplacian matrix L^d:

$$L^d_{ij} = \begin{cases} \sum_{j=1}^{n} d_{ij} & \text{if } i = j \\ -d_{ij} & \text{otherwise} \end{cases}, \tag{20.7}$$

and obtain the optimal projection with the direction vectors given by the p highest eigenvectors of the matrix $X^T L^d X$.

We can now use the dissimilarity values to create different variations of PCA. In normalized PCA $d_{ij} = 1/\text{dist}_{i,j}$ to discount large original distances in the optimization. This can be useful to increase the original PCA robustness with respect to outliers.

In supervised PCA, with data labeled as belonging to different classes, we can set the dissimilarities d_{ij} to a small value ϵ if i and j belong to the same class, to a value 1 if they belong to different classes. This weighing instructs the projection that it is more important to put at large distances points of different clusters. If ϵ is zero, the internal structure of each cluster is set only indirectly according to the inter-cluster relationships of its members.

20.4 Linear discrimination by ratio optimization

Other possibilities to project points while considering also class labels arise by optimizing **ratios of quantities**. Obviously, maximizing a ratio reflects a **compromise** between maximizing the numerator and minimizing the denominator.

Let's consider a c-way classification problem, the standard case being with two output classes. Fisher analysis deals with finding a vector ν_F such that, when the original vectors are projected onto it, values of the different classes are separated in the best possible way.

A nice separation is obtained when the sample *means* of the projected points are as different as possible, when normalized with respect to the average *scatter* of the projected points. The division by the scatter corresponds to the intuition that what matters is not the separation of means *per se*, but the fact that values are sufficiently clustered around their means so that the classes can be clearly *separated*. This is not possible if they are scattered so that most values are mixed in the same area, even if the means are separated.

Let n_i be the number of points in the i-th cluster, let μ_i and S_i be the mean vector and the biased covariance matrix for the i-th cluster. The matrix $S_{\text{within}} = \frac{1}{n}\sum_{i=1}^{c} n_i S_i$ is the **average within-cluster covariance matrix** and $S_{\text{between}} = \frac{1}{n}\sum_{i=1}^{c} n_i \mu_i \mu_i^T$ the **average between cluster covariance matrix**.

In detail, the Fisher linear discriminant is defined as the linear function $y = \nu^T \mathbf{x}$ for which the following ratio is maximized:

$$\frac{\nu^T S_{\text{between}}\, \nu}{\nu^T S_{\text{within}}\, \nu}. \tag{20.8}$$

Think about **maximizing the ratio of between-class to within-class scatter**: we want to maximally separate the clusters (the role of the numerator where the projections of the means count) and keep the clusters as compact as possible (the role of the denominator).

It can be proved that the maximizer of Fisher's criterion is the same as the maximizer of:

$$\frac{\nu^T S_{\text{between}}\, \nu}{\nu^T\; S\; \nu}. \tag{20.9}$$

For the special but interesting case of two classes, see also Fig. 20.4, after specializing the above equations, the Fisher linear discriminant is defined as the linear function $y = \mathbf{w}^T \mathbf{x}$ for which the following criterion function is maximized:

$$\text{Separation}(\mathbf{w}) = \frac{\|\widetilde{m}_1 - \widetilde{m}_2\|^2}{\widetilde{s}_1^2 + \widetilde{s}_2^2}, \tag{20.10}$$

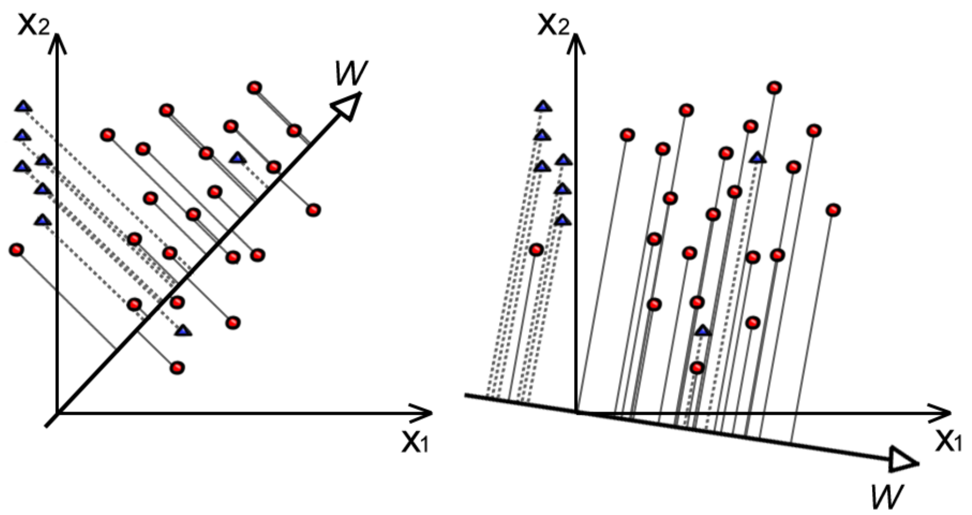


Figure 20.4: Fisher linear discrimination (triangles belong to one class, circles to another one): the one-dimensional projection on the left mixes projected points from the two classes, while the projection on the right best separates the projected sample means with respect to the projected scatter.

where $\widetilde{m}_i$ is the sample mean for the projected points $\widetilde{m}_i = (1/n_i)\sum_{y \in Class_i} y$, and $\widetilde{s}_i^2$ is the *scatter* of the projected samples of each class: $\widetilde{s}_i^2 = \sum_{y \in Class_i}(y - \widetilde{m}_i)^2$. Think about maximizing the ratio of between-class to total within-class scatter. The solution is:

$$\mathbf{w}_F = (S_w)^{-1}(\mathbf{m}_1 - \mathbf{m}_2), \tag{20.11}$$

where $\mathbf{m}_i$ is the d-dimensional sample mean for class i and S_w is the sum of the two scatter matrices S_i defined as follows:

$$S_i = \sum_{\mathbf{x} \in Class_i} (\mathbf{x}_i - \mathbf{m}_i)(\mathbf{x}_i - \mathbf{m}_i)^T. \tag{20.12}$$

An interesting application of Fisher linear projection is for selecting features in neural networks and general model-building techniques based on supervised learning. (See Section 20.4.1.)

20.4.1 Fisher discrimination index for selecting features

Let's consider a two-way classification problem (with two output classes) with input vectors of d dimensions. Fisher analysis deals with finding the vector $\mathbf{w}_F$ so that, when the original vectors are projected onto it, values of two classes are separated in the best possible way. The method has already been encountered in Section 20.4.

Let's remind that a nice separation of the projected points is obtained when the sample *means* of the projected points are as different as possible, when normalized with respect to the average *scatter* of the projected points. The division by the scatter corresponds to the intuition that what matters is not the separation of means *per se*, but the fact that values are sufficiently clustered around their means so that the two classes can be clearly separated. This is not possible if they are scattered so that most values are mixed in the same area, even if the means are separated.

We can now rate the importance of feature i according to the magnitude of the i-th component of the Fisher vector $\mathbf{w}_F$ defined in equations (20.11)–(20.12). Identifying the largest components in Fisher vector will heuristically identify the most relevant directions (coordinates) for separating the classes. In other words, if the direction of a coordinate vector is similar to the direction of the Fisher vector, projecting onto the given coordinate axis can be approximately used to separate the two classes, instead of projecting onto the original Fisher vector. Let's note that the criterion is empirical because it is based on *linear* projections: in some cases a *nonlinear* combination of features which rank poorly by the above Fisher criterion may do an excellent job in separating classes.

If the number of dimension d is very large, inverting the S_w matrix in equation (20.11) can be numerically difficult, and this first measure can be insufficient to correctly order many features.

A simpler and possibly more effective criterion to rank feature k, called **Fisher's discrimination index**, is to measure the Separation$(\mathbf{w})$ value defined in equation (20.10) when considering a vector $\mathbf{e}_k$ along the specific direction k (zero everywhere, 1 only in the k-th coordinate). In other words, we want to measure the discrimination which can be achieved if only the k-th coordinate of the points is considered.

20.5 Fisher's linear discriminant analysis (LDA)

The original Fisher method described above aims at finding a single direction vector (a single projection). For finding p direction vectors, the idea can be generalized to the popular technique known as Fisher's **linear discriminant analysis (LDA)**, which is based on maximizing the following ratio:

$$\begin{aligned} \max_{\nu^1,\ldots,\nu^p} \quad & \frac{\sum_{\alpha=1}^{p} (\nu^\alpha)^T \, S_{\text{between}} \, \nu^\alpha}{\sum_{\alpha=1}^{p} (\nu^\alpha)^T \, S \, \nu^\alpha} \\ \text{subject to} \quad & (\nu^\alpha)^T S \nu^\beta = \delta_{\alpha\beta}, \qquad \alpha, \beta = 1, \ldots, p. \end{aligned} \tag{20.13}$$

Although widely used, LDA, like the basic PCA, is sensitive to outliers and it does not take the shape and size of clusters into consideration. A more flexible generalization is based on maximizing a ratio of the following form:

$$\begin{aligned} \max_{\nu^1,\ldots,\nu^p} \quad & \frac{\sum_{i<j} d_{ij} (\text{dist}_{ij}^p)^2}{\sum_{i<j} \text{sim}_{ij} (\text{dist}_{ij}^p)^2} \\ \text{subject to} \quad & (\nu^\alpha)^T X^t L^s X \nu^\beta = \delta_{\alpha\beta}, \qquad \alpha, \beta = 1, \ldots, p, \end{aligned}$$

where d_{ij} are dissimilarity weights, sim_{ij} are similarity weights (they express the preference for placing two entities together in the projection), and L^s is the Laplacian matrix corresponding to the similarities

$$L_{ij}^s = \begin{cases} \sum_{j=1}^{n} \text{sim}_{ij} & \text{if } i = j \\ -\text{sim}_{ij} & \text{if } i \neq j \end{cases}. \tag{20.14}$$

After defining a generalized eigenvector problem of (A, B) as the solution of $Ax = \lambda Bx$, the optimal solution of equation (20.13) is given by the p highest generalized eigenvectors of $(X^T L^d X, X^T L^s X)$.

Apart from the mathematical details, remember that finding an optimal projection requires defining in measurable ways what is meant by optimality. Above we have seen ways of **combining unsupervised (based only on coordinates) and supervised information (based on relationships)**, and ways of giving different weights to different preferences for placing items distant or close.

After the user intelligence is spent on defining the optimization problem, what is left is to derive $m \times m$ matrices by the appropriate multiplications and to solve an $m \times m$ generalized eigenvector problem in an efficient and numerically stable way. Of course, the technique is very fast when the number of original coordinates m is limited, even if the number of points to project is very large.

Interestingly enough, eigenvectors will be encountered again in chapter 14 about web mining, for ranking web pages.

20.6 Projection Pursuit: searching for interesting structure guided by an explicit index

Projection pursuit (PP) is a catchy name proposed in [138] and based on [243] for exploratory data analysis based on the explicit definition of an objective function (called *projection index*). "Pursuit" refers to the systematic use of optimization techniques to identify the best projection, or at least a locally-optimal one, according to the index. Let's stress that structure can be obscured by projections but never enhanced (projection is a shadow of an actual structure in many dimensions) and therefore linear projections are always solid low-danger techniques.

Many of the methods of classical multivariate analysis (like PCA in Sec. 20.2 or LDA in Sec. 20.5) are special cases of PP, but this dedicated section underlines some interesting observations of the most advanced PP methods, following [134] and [197].

The purpose of *exploratory* projection pursuit is to discover non-obvious (non-linear) effects in the data by low-dimensional projections. The human gift for pattern recognition works best by observing data projected in two or three dimensions. Linear effects are "obvious" because they can be easily identified by PCA, i.e., by deriving and using the covariance structure of variable pairs.

20.6.1 Normal Gaussian distributions are non-interesting: sphering or whitening

If the cloud of data points follows with high fidelity an elliptically symmetric distribution like that of Fig. 20.6, the covariance matrix tells the whole story. A normal distribution (following a multi-dimensional Gaussian probability density function) is a paradigm of a non-interesting structure. If we project a normal distribution, we obtain another normal distribution, usually quite boring. Let's consider that a normal distribution can be the real-world equivalent of a constant value (if we measure the height of a person with more digits than required by our instrument's precision, we get an approximately normal distribution of values).

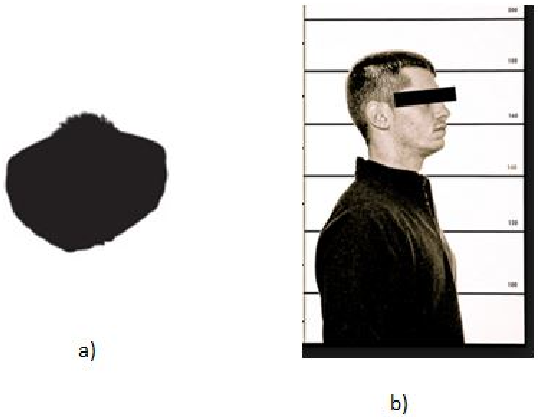


Figure 20.5: Projection Pursuit: if we project a human body, the interest of a projection is related to the amount of nonlinearity. A projection from above leads to a quasi-normal distribution (a), a lateral projection is of bigger use to identify people (b).

If the task confirms that normal distributions are of no interest, a "first aid" treatment of the data consists of **sphering** or **whitening**. *Sphering* means squeeze, stretch and rotate data until the ellipsoid describing the covariance structure (Fig. 20.6) becomes a sphere. The alternative term of "whitening" originates from signal processing and reminds that the input vector is transformed into a *white noise* vector, a signal whose samples are regarded as a sequence of serially uncorrelated random variables with zero mean and finite variance.

In detail, a **whitening transformation** is a decorrelation transformation that transforms an arbitrary set of variables having a known covariance matrix M into a set of new variables whose covariance is the identity matrix (meaning that they are uncorrelated and all have variance 1).

A first step consists of **centering** the data, by subtracting the average vector. Then the correlation matrix M is derived as the expected value of the outer product of X with itself, namely:

$$M = \mathrm{E}[XX^T]$$

When M is symmetric and positive definite (and therefore not singular), it has a positive definite symmetric square root $M^{1/2}$, such that $M^{1/2}M^{1/2} = M$. Since M is positive definite, $M^{1/2}$ is invertible, and the vector $Y = M^{-1/2}X$ has covariance matrix:

$$\mathrm{Cov}(Y) = \mathrm{E}[YY^T] = M^{-1/2}\,\mathrm{E}[XX^T](M^{-1/2})^T = M^{-1/2}MM^{-1/2} = I$$

and is therefore a white random vector.

If M is singular (and hence not positive definite), the vector X can still be mapped to a smaller white vector Y with m elements, where m is the number of non-zero eigenvalues of M.

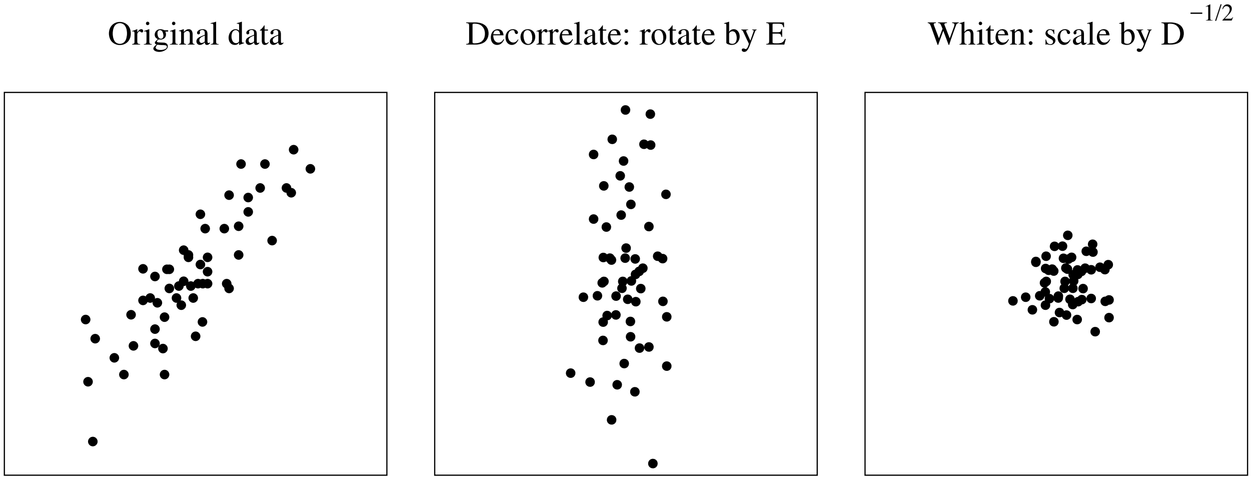


Figure 20.6: Sphering a data distribution.

A first underlying principle of PP is: the level of interest is proportional to the degree of nonlinear structure in the projection. **Normal distributions have no interest** and can be discounted by **whitening** or **sphering** the data points before proceeding with PP.

In many cases, one demands that PP results are invariant with respect to affine transformations of the data. In the real-world, an affine transformation can be related to changing offset and scale of measurement units (like in a Celsius to Fahrenheit conversion of temperatures) and it would be unpleasant if such a trivial change could create or destroy interesting structure (but remember that PCA results are going to be changed by an affine transformation: therefore PCA has to be used with great care and a high level of danger).

20.6.2 Index to measure non-normality

If it is confirmed that normal distributions and not of interest, one must pay attention to the fact that *most* projections have a natural tendency to obtain normal distributions.

This natural tendency is caused by the **central limit theorem (CLT)**[289]: given certain conditions, the arithmetic mean of a sufficiently large number of iterates of independent random variables will be *approximately normally distributed*, regardless of the underlying distribution.

The fact that most projections (arithmetic means of scaled single variables) tend to produce normal distribution, and therefore identifying one by manual search is close to impossible for high-dimensional data, is a strong motivation in favor of a systematic search of interesting ones by PP. One is searching for needles (non-normal projections) is a haystack of approximately normal ones.

Most PP applications seek distribution that exhibit clustering or other kinds of nonlinear structures in the main body of the distribution, and not so much in the tails. The most computationally attractive indices of non-normality are based on polynomial moments.

The procedure to obtain this measure of non-normality can be as follows. One seeks a linear combination:

$$X = \alpha^T Z$$

so that the projected probability density $p_\alpha(X)$ is different from a Gaussian (normal) distribution in its main body. After using the normal cumulative distribution function (cdf):

$$\Phi(X) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{X} \exp(-t^2/2) dt$$

and introducing the variable R

$$R = 2\Phi(X) - 1$$

R will be uniformly distributed in the interval $-1 \leq R \leq 1$ if X is normally distributed. In general, the density for the new variable R can be obtained as:

$$p_R(R) = \frac{1}{2} p_\alpha \left(\Phi^{-1} \left(\frac{R+1}{2} \right) \right) \Big/ g \left(\Phi^{-1} \left(\frac{R+1}{2} \right) \right)$$

where $g(X)$ is the standard normal density.

One can then measure the non-uniformity of R as the integral of the squared distance between the real probability density in the new variable R and the uniform probability density equal to $1/2$ over the entire interval.

$$\int_{-1}^{1} \left(p_R(R) - \frac{1}{2} \right)^2 dR.$$

The projection index to be maximized can be taken as a suitable approximation of the above integral. Traditionally, an expansion in terms of Legendre polynomials can be used [134]. It is of comfort that the final results of PP tend to be quite robust with respect to the details of the approximation as well as estimation of densities from data points.

Indices with derivatives which can be computed analytically can be used as ingredient in **gradient ascent** techniques to find local maxima of the index, but global derivative-free optimization schemes can be adopted if derivatives are not present (see Chapters 26 and 25).

The above derivation can be generalized for projections into more than one dimension. As a sub-optimal alternative, the different vector for the multi-dimensional projection can be determined in successive steps, with *greedy* versions of PP. The general idea is to identify a first projection and then to *remove the structure that makes the specific direction interesting*, otherwise one would re-discover the same direction again. The structure can be removed by applying a transformation that renders the projected density a normal distribution in the projected subspace [134], therefore lowering the local optimum responsible for identifying the first direction (see also Chapter 31 for ways of modifying the objective function to escape from previously fund local optima).

If one considers optimization, one has to be careful that a multiplicity of suboptimal local optima can be created by sampling fluctuations (high frequency ripples are superimposed on the main structure of the objective function). Optimization methods combining global search schemes with local convergence are recommended (Chapter 26).

Being an explanatory method, traditional PP can often discover strong nonlinear effects which cause the researcher to look harder at the data aiming at insight and understanding.

In a way, PP is valid when PCA does not offer any significant insight. PCA is very sensitive to the definition of units of measures and is easily misled by the overall distribution of data.

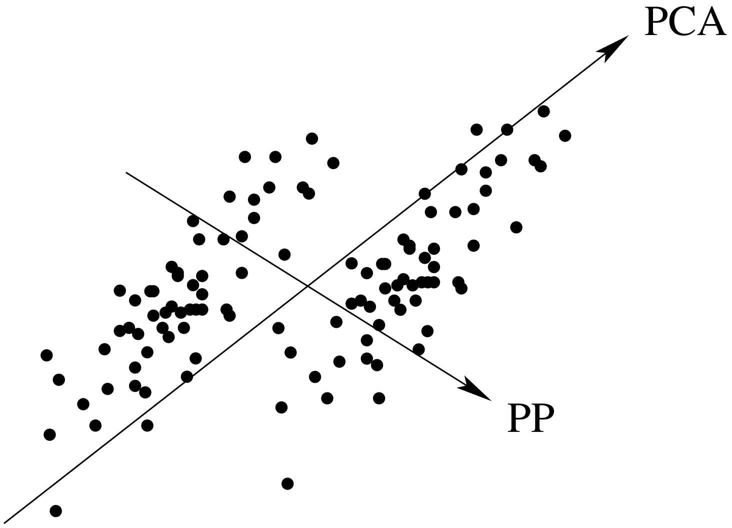


Figure 20.7: PCA and PP can identify very different directions for projecting data. In this case PCA identifies the overall direction of distribution but completely misses the clustering structure of the two clouds of points.

The usefulness of PP in finding projections can be seen in Fig. 20.7. The projection on the projection pursuit direction, which is horizontal, clearly shows the clustered structure of the data. The projection on the first principal component (vertical), on the other hand, fails to show this structure.

Gist

Visualizations (visual representations of abstract data) help the human unsupervised learning capabilities to extract knowledge from the data. Because visualizations are for our visual system, they are limited to the two dimensions of our retina (three in case of stereo vision).

A simple way to transform data into two-dimensional views is through projections (actually, projections can be to more than two or three dimensions if a computer is using the projected points). **Orthogonal projections** can be intuitively explained as looking at the data from different and distant points of view.

Because there are infinite ways to project data, the power of optimization comes to the rescue to select some of them through clear objectives. In particular, **Principal Component Analysis (PCA)** identifies the orthogonal projection that spreads the points as much as possible in the projection plane. In spite of its popularity, PCA can fail to produce relevant insight: having a larger variance is not always related to having the largest information content, or the best possible discrimination.

If **relationships** are available in addition to the raw coordinates (e.g., knowledge that some points are in the same or in different class), they can be used to modify PCA and obtain more meaningful projections.

When class labels are present, **Fisher discrimination** projects data so that the *ratio* of difference in the projected means of points belonging to different classes *divided* by the intra-class scatter is maximized.

Projection pursuit (PP) can be used for exploring data in order to find a few (typically one-two) directions so that the projection identifies interesting nonlinear effects in an automated fashion, guided by an objective function which measures deviations from Gaussian distributions.

If linear relationships identified by the covariance matrix are not considered of interest, a **whitening or sphering** transformation can render the data uncorrelated and with unit variance. What are left are the *nonlinear* effects.

Alchemists used projection to mix powdered philosopher's stone with molten base metals in order to transmute them into gold. You can use it for a more successful enterprise, to transform raw data points into precious and robust insight.

Chapter 21

Feature extraction and Independent Component Analysis

Like other parties of the kind, it was first silent, then talky, then argumentative, then disputatious,
then unintelligible, then altogether, then inarticulate, and then drunk.
George Gordon, Lord Byron

The previous chapter considered feature selection: the identification of a subset of informative attributes as a preprocessing phase before building ML models.

Now, in many real-world situations, the relevant measurements do not correspond to individual signals but to *combinations* of them. Human expertise can be complemented by automatic **feature construction** techniques. In some methods, feature construction is embedded in the machine learning process. For examples the "hidden units" of artificial neural networks in MLPs (Sec. 10.1) can be considered as automatically extracted attributes, internal representations of higher complexity and nonlinearity when one passes from the first to higher hidden layers. Deep learning (Sec. 11.1) aims at building features of progressively higher complexity in an automated fashion. But in this chapter we focus mostly on **explicit preprocessing efforts to construct features** guided by principles and dedicated objective functions to be optimized, often in an unsupervised manner.

For a concrete situation, imagine **two people talking at a cocktail party**, the signal recorded from a microphone will be a mixture of two voice signals, approximately a linear combination with coefficients related to the distance of the speakers. If one could extract from the raw measurements the individual voices, it is clear that subsequent intelligent processing (like natural language comprehension) will be greatly facilitated. Listening to an unborn baby's heartbeat is not direct. An ECG generates a pattern based on electrical activity of the heart, which closely follows heart function, but two signals originating from the mother's and the baby's heartbeats will be superimposed and need to be separated. In a similar way, many physical phenomena are characterized by a superposition of signals, an electroencephalogram (EEG) measurement by electrode on the human scalp contains contributions from many different brain regions, the height of a person is influenced by many causes (nutrition, genetics, work, age, etc.), the cash flow of a business depends on a variety of factors, in an image the intestity values are caused by the combinations of different objects and illumitation sources, in biology a gene expression level may be considered the sum of many different biological processes. In many application areas the **measurements provided by a device contain interesting phenomena mixed up, often in an approximately linear manner** [348, 202].

Identification of the basic factors (latent variables) controlling the output variability has value both for the subsequent intelligent analysis and for understanding more about the basic causes of a phenomenon.

One is left with the following challenge: can one identify a certain number of basic factors from a number of measurements in which the various factors are (often linearly) confused? Can one separate the source signals without a precise knowledge of the different signals (without requiring supervised learning) but only with generic high-level assumptions? **Blind Source Separation (BSS)** is a term used in signal processing to estimate individual source components from their mixtures at multiple sensors. It is called *blind* because it does not require any other information besides the mixtures (and some high-level structural assumptions).

In the language of Machine Learning, one is dealing with a special kind of **feature extraction**, in which the extraction is some combination of the basic raw figures, for example a suitable linear combination. This is different from feature selection in which no combination of different features is considered.

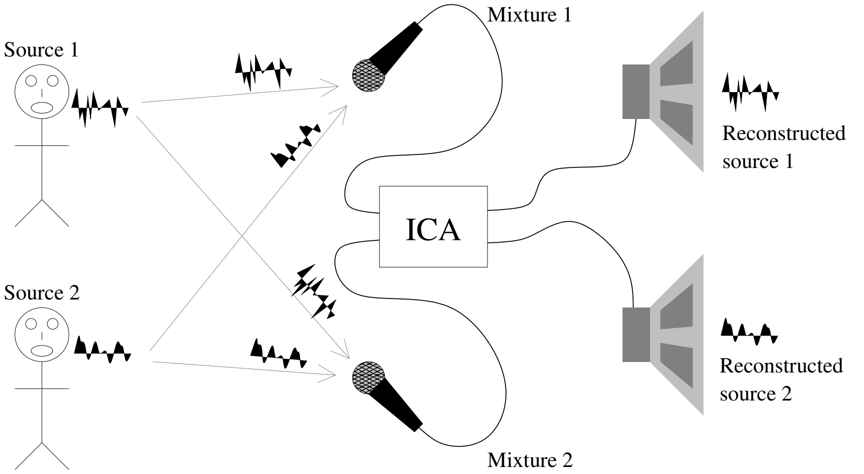


Figure 21.1: A practical context related to Independent Component Analysis. Two people are talking at a cocktail party.

In the following sections, first a review of simple "first-aid" feature transformation is given (Sec. 21.1). Then Independent Component Analysis (ICA) is presented as a way to identify basic hidden variables (sources) producing measured signals, in the assupmtion of independence and non-Gaussianity (Sec. 21.2). ICA searches for a linear transformation. More complex, possibly non-linear, transforms of raw features are considered when one aims at maximizing the Mutual Information between constructed features and output (Sec. 21.3). The transform is parametric, and the best parameter values can be identified by optimization.

This crucial feature-construction step can be the initial phase of a more complex process. After an initial set of features are constructed, they can be validated and selected with the feature selection techniques already explained in Chapter 7.

21.1 Simple preprocessing for feature extraction

In some cases, raw features make the machine learning problem difficult in a masochistic way. For example, a bad choice for the units of measurements (millimeters, kilometers, light-years) can cause large numerical errors in many algorithms (like gradient descent) or render some inputs negligible even if they contain precious information. Simple preprocessing methods should always be applied before considering more advanced feature extraction techniques. A list derived from [167] is the following one.

Standardization Consider inputs with widely different ranges, for example one measuring distances in meters, one measuring in light-years, or with a different offset like Celsius and Fahrenheit measurements of temperature. A classical centering and scaling of the data is often used:

$$x_i \leftarrow (x_i - \mu_i)/\sigma_i,$$

where μ_i and σ_i are the mean and the standard deviation of feature x_i over training examples. Of course, the same transformation will then be applied to new cases in generalization (with means and standard deviations measured on the *training* set).

Normalization If $\mathbf{x}$ is the vector of inputs and one thinks that the *direction* of the vector is more meaningful than its *magnitude* for subsequent processing, the vector should be divided by its norm:

$$\mathbf{x} \leftarrow \mathbf{x}/\|\mathbf{x}\|$$

where a suitable norm is considered. An example is the case where $\mathbf{x}$ describes a histogram of colors contained in an image (x_i is number of pixels with color i). It makes sense to normalize $\mathbf{x}$ by dividing it by the total number of counts in order to remove the dependence on the size of the image.

Whitening If one suspects that linear relationships are not significant a whitening or sphering transformation can be applied (Sec. 20.6.1). As in all cases, care must be used: in many cases linear relationships tell most of the story!

Signal enhancement by application-specific transforms or local filters The signal-to-noise ratio may be improved by applying signal or image-processing filters like background removal, de-noising, smoothing, or sharpening. A simple example of local filters are edge detection or edge enhancement, e.g., by convolutional methods using hand-crafted kernels. More complex but widely used global transformations techniques are Fourier transform and wavelet transforms.

Monomials with raw features If one suspects nonlinear dependencies, one can try to *increase* the dimensionality of the data by adding products of the original features $x_{k1}x_{k2}, ..., x_{kM}$, in the hope that a simpler model will be sufficient after this step (for example traditional least-squares or SVM).

Quantization of values In some cases, passing from a real value to a small set of integers can reduce noise and simplify processing (for example, to measure Mutual Information, as described in Sec. 7.6).

Transformation of variable type In some cases, categorical data should be transformed into numerical data. For example, if the age of a person is initially described with keywords ("child", "adolescent", "adult", "senior"), assigning numbers (1,2,3,4) will allow for using metric comparisons. In other cases, the contrary makes sense, if the initial numerical data is not related to metric comparisons but is to be intended as an ID for different categories, like people used to do in the old days, when memory was costly and using ID instead of keywords lead to some economy.

Other ways to construct features are described in different chapters, for example Principal Component Analysis (Sec. 20.2), Projection Pursuit (Sec. 20.6), Deep Learning (Chapter 11).

21.2 Independent Component Analysis (ICA)

The success of Independent Component Analysis (ICA) depends on a plausible assumption regarding the nature of the physical world: **the basic variables or signals are independent and non-Gaussian (non-normal)**. Independence means that the value of one signal cannot be used to predict anything about the other signals. Linear combinations of Gaussian variables are also Gaussian, this is why non-Gaussianity is important to identiify particular (optimal) linear transforms.

At a party, one assumes that the value of a voice signal from a speaker cannot be used to predict the voice signal of a second speaker. Like all approximations, this is not completely true, a speaker may start talking only when a second speaker is silent, but ICA methods tend to be quite robust. In practice, most measured signals are derived from many independent physical processes, and are therefore mixtures of independent signals. The emphasis on identifying structured (non-Guassian) distributions is shared with the Projection Pursuit method (Sec. 20.6). This is also what distinguishes ICA from Principal Component Analysis (PCA) described in Sec. 20.2 .

ICA is an unsupervised, **exploratory, or data-driven method**: one can simply measure a phenomenon without specific detailed knowledge, investigate the structure of the data when suitable hypotheses are not yet available.

Following [202], let the observed variables be $x_i(t), i = 1, ..., n, t = 1, ..., T$. Index t can be interpreted as time, or index of different observations.

One assumes that the observed variables can be modelled as linear combinations of hidden (latent) variables $s_j(t), j = 1, ..., m$, with some unknown coefficients a_{ij},

$$x_i(t) = \sum_{j=1}^{m} a_{ij} s_j(t), \mathrm{for all} i = 1, ..., n.$$

At a first look, the puzzling fact is that we observe only the variables $x_i(t)$, whereas both the mixing coefficients a_{ij} and the independent components $s_i(t)$ are to be estimated (no supervised knowledge of $s_i(t)$ is available). For sure, one can hope to estimate each component only up to a multiplying scalar factor: the same results is obtained by multiplying sources by α and dividing mixing coefficients by the same value (in measurements, this corresponds to using different fundamental units of length, mass, time, etc. - trivial changes indeed). In addition, the result is the same by permuting components and rows of the mixing matrix, one cannot expect a standard ordering of the components.

Let's forget about time and consider the x_i and the s_i as realizations of random variables. The different n measures x_i and s_i can be collected in vectors $\mathbf{x}$ and $\mathbf{s}$ so that the model becomes:

$$\mathbf{x} = \mathbf{A}\mathbf{s}$$

The main breakthrough in the theory of ICA was the realization that the puzzle can be solved by making **the unconventional assumption that the independent components are not Gaussian**, in addition to the assumtion that the components s_i are statistically independent (i.e., the joint probability density $p(s_1, ..., s_m)$ is the product of the marginal densities $\prod_j p_j(s_j)$). The second assuption appears also in standard Factor Analysis (a statistical method like PCA used to describe variability among observed, correlated variables in terms of a potentially lower number

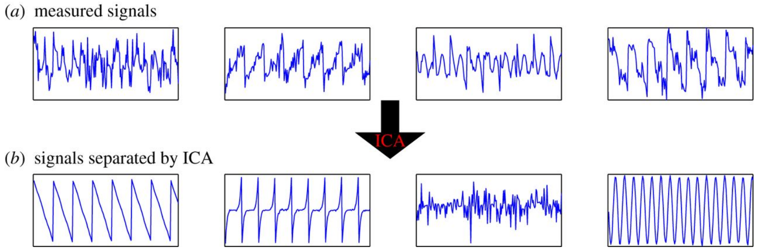


Figure 21.2: ICA objective is to recover from the different measurements in (a), the original source signals that were mixed together, as shown in (b). Source: [202].

of unobserved variables called factors) in which the factors are assumed uncorrelated and Gaussian, which implies statistical independence. Only in the non-Gaussian case independence means more than uncorrelatedness (lack of linear correlation).

As in the discussion about Mutual Information (Sec. 7.6), one can have variables with no linear correlation but high mutual dependency. As an example, consider a distribution which places equal probability to four points located in a cross-like manner in two dimensions: $(-1,0),(1,0),(0,-1),(0,1)$, the correlation is zero but knowledge of one variable (e.g., of x_1) helps when predicting the second one (e.g., $x_1 = -1$ implies $x_2 = 0$), a situation of positive mutual information.

The steps in ICA are the following ones. First, a **whitening** transformation (Sec. 20.6.1) discounts the "trivial" linear relationships to create white variables with zero correlation and unit variance.

The whitening matrix $\mathbf{V}$ can be easily found by PCA, the transformed matrix $\tilde{\mathbf{A}} = \mathbf{V}\mathbf{A}$ is now orthogonal, and the transformed variables are obtained as: $\mathbf{z} = \tilde{\mathbf{A}}\mathbf{x}$

After whitening, one can constrain the estimation of the mixing matrix to the space of orthogonal matrices, which reduces the number of free parameters and makes numerical optimization faster and more stable.

Let's note that whitening is not uniquely defined. If $\mathbf{z}$ is white, then any orthogonal transform $\mathbf{Uz}$, with $\mathbf{U}$ being an orthogonal matrix, is white as well. Mere information of uncorrelatedness does not lead to a unique decomposition and the assumpton of non-Gaussianity is crucial. For Gaussian variables, uncorrelatedness implies independence, whitening exhausts all the dependence information in the data, and we can estimate the mixing matrix only up to an arbitrary orthogonal matrix. For non-Gaussian variables, on the other hand, whitening does not at all imply independence, and there is much more nonlinear information in the data than what is used in whitening.

In fact, one can estimate $\tilde{\mathbf{A}}$ by maximizing some objective function that is related to a measure of non-Gaussianity of the components. As usual, a clear definition of the objectives is sufficient to tap the power of optimization. The main approaches to define an objective function for ICA are maximum-likelihood estimation [296], and minimization of the mutual information between estimated component signals [96], leading to similar objective functions.

The derivation based on the Mutual Information is as follows. After remembering equation (7.12) about the role of the Jacobian determinant in changing entropy after a transformation (because probability densities are transformed by volume changes), and the fact that the ICA transformation is linear (and therefore the Jacobian does not depending on $\mathbf{z}$), one gets ($\mathbf{s} = \tilde{\mathbf{A}}\mathbf{z}$) :

$$I(s_1, ..., s_m) = \sum_j H(s_j) - H(\mathbf{s}) = \sum_j H(s_j) - H(\mathbf{z}) - \log|\det \tilde{\mathbf{A}}|. \tag{21.1}$$

If one constrains the s_i to be uncorrelated and of unit variance then $\det \tilde{\mathbf{A}}$ has to be constant (volumes cannot change if the whitening-sphering transformation has to be preserved). But $H(\mathbf{z})$ is also constant w.r.t. the transformation weights and therefore one is left with a sum of entropies of the transformed variables (the hidden sources to be determined) [203].

If one remembers the definition of entropy as minus the average of the *logarithm* of probabilities (Sec. 7.6), assumes that probability is distributed equally on the measurements and neglects multiplicative constants, the objective function is usually formulated in terms of the inverse of the orthogonal matrix $\tilde{\mathbf{A}}$ (if a matrix is orthogonal its transpose is equal to its inverse), whose rows are denoted by $\mathbf{w}_i^T$, as:

$$\text{ICAobjective}(\mathbf{w}_i) = \sum_{i=1}^{n} \sum_{t=1}^{T} \log \text{pdf}_i(\mathbf{w}_i^T \mathbf{z}(t)),$$

where pdf_i is the probability density function of s_i, s_i being estimated by $\mathbf{w}_i^T \mathbf{z}(t)$.

This objective function depends only on the marginal densities of the estimated independent components $\mathbf{w}_i^T \mathbf{z}(t)$. Each term $\sum_{t=1}^{T} \log \text{pdf}_i(\mathbf{w}_i^T \mathbf{z}(t))$ can be interpreted as a measure of non-Gaussianity (entropy) of the estimated component. It is an estimate of the negative differential entropy of the components, which is *maximized* for a Gaussian variable (for fixed variance). Here one is going in the contrary direction, therefore away from Gaussianity!

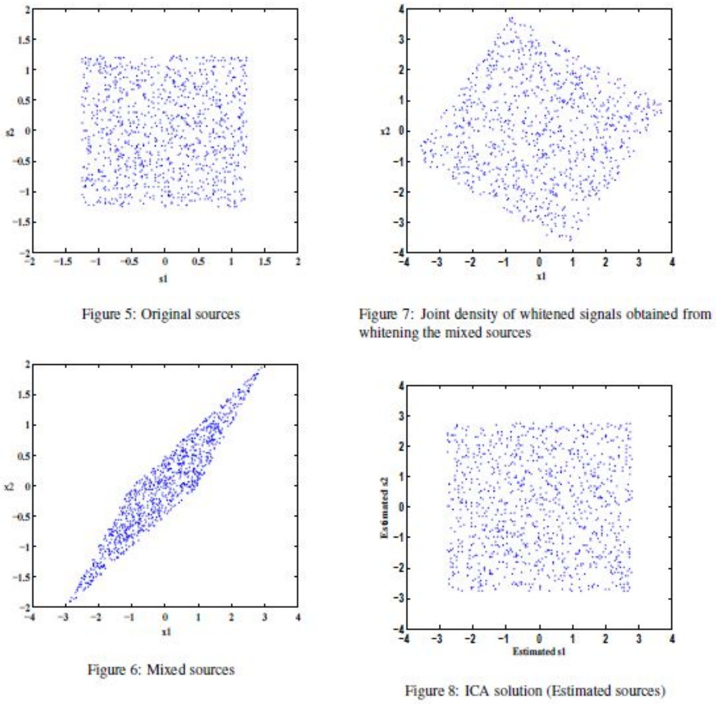


Figure 5: Original sources

Figure 7: Joint density of whitened signals obtained from whitening the mixed sources

Figure 6: Mixed sources

Figure 8: ICA solution (Estimated sources)

Figure 21.3: ICA at work. Original sources (a), measurements (b), whitened measurements (c), rotation to identify sources (c). For Gaussian signals, whitening would produce a sphere, no way to identify an optimal rotation leading to non-Gaussian signals!

Maximizing the nongaussianity of $\mathbf{w}_i^T \mathbf{z}(t)$ thus gives us one of the independent components. In fact, the optimization landscape in the m-dimensional space of vector **w** has $2m$ local maxima, two for each independent component, corresponding to s_i and $-s_i$ (recall that the independent components can be estimated only up to a multiplicative sign). To find several independent components, one needs to find all local maxima. Because the different independent components are uncorrelated, one can always constrain the search to the space that gives estimates uncorrelated (orthogonal) with the previous ones.

Rough approximations of the *log-pdf* are used in practice for computational reasons, and robust and fast optimization schemes are proposed for example in [201] (FastICA).

Fortunately for ICA, non-Gaussianity is quite widespread in many applications dealing with physical measurements, and therefore ICA has become a standard tool in machine learning and signal processing in the last decade. Some recent developments in ICA are: analysis of causal relations (structural equation modelling and identification of Bayesian networks), testing independent components (robustness of identification w.r.t. chance), analysing multiple datasets (like EEG signals related to different patients), modelling dependencies between the components (generalizing beyond the independence assumption), special versions for non-negative variables, time-varying signals, etc. [202].

Precise estimators of mutual information (MI) to find the least dependent components in a linearly mixed signal is considered in [347], using a recently proposed k-nearest-neighbor-based algorithm for the MI estimator. The obtained MILCA method (mutual-information-based **least dependent component** analysis) relaxes the assumption of strict independence, henceforth the name “least dependent”. After preprocessing the data (by centering, whitening, etc.), the “grouping property” of MI:

$$I(X,Y,Z) = I((X,Y),Z) + I(X,Y).$$

together with invariance under homeomorphisms of a single variable are used to obtain an incremental rule:

$$I(X',Y',Z,...) = I(X,Y,Z,...) + [I(X',Y') - I(X,Y)].$$

Since any such transformation in m dimensions can be factorized into pairwise transformations, this means that one only has to compute pairwise MIs for the minimization. Thus one needs to compute the full high-dimensional MI only once. In particular, any rotation can be represented as a product of rotations which act only in some 2x2 subspace. MILCA works with actual dependencies between reconstructed sources (as measured by mutual information). The estimated dependencies can be used to cluster sources, gaining additional insight. It is applied in the cited paper to a fetal ECG recording from the abdomen of a pregnant woman to extract a clean fetal ECG. Clustering identifies the two groups of mother- and child-related sources.

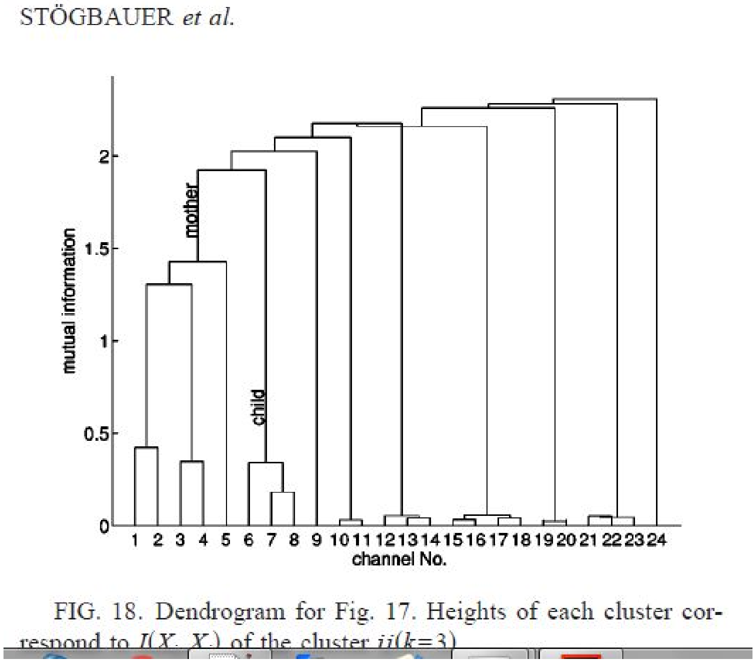


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FIG. 18. Dendrogram for Fig. 17. Heights of each cluster correspond to $I(X, X)$ of the cluster $ij(k=3)$

Figure 21.4: MILCA: Dendrogram built from the Mutual Information between sources. Heights of each cluster correspond to $I(X_i, X_j)$.

21.2.1 ICA and Projection Pursuit

As the careful reader probably noticed, ICA is deeply related to Projection Persuit (Sec. 20.6) Projection pursuit aims at finding "interesting" projections of multidimensional data for optimal visualization, density estimation and regression. In one-dimensional projection pursuit, one searches for directions such that the projections of the data have interesting distributions with non-trivial structure. In many cases the Gaussian distribution (in some cases corresponding to a constant factor modified by ramdom errors in the measurement apparatus) is the least interesting one, and the most interesting directions are those that show the **least Gaussian distribution**. This objective is shared by the ICA model.

As a difference to be noted, no data model or assumption about independent components is made in standard projection pursuit. If the ICA model holds, optimizing the ICA non-Gaussianity measures produces independent components; if the model does not hold, then what one gets are the projection pursuit directions.

21.3 Feature Extraction by Mutual Information Maximization

As mentioned in Sec. 7.6, the Mutual Information measure can be used to select features, in a manner which is independent of the particular ML model [21]. In the same way, the Mutual Information can be used to construct informative and non-redundant features. In supervised classification or regression, one can design parametric functions of the basic features. **Optimization of the Mutual Information between the constructed parametric features and the output** can be used to determine an optimal configuration of the parameters.

Estimating MI from a finite set of examples is computationally demanding. Therefore suitable approximations are usually derived to obtain affordable and effective algorithms. For example, a quadratic divergence measure, which does not require prior assumptions about class densities is considered in [362].

Finding a transform to lower dimensions might be easier than selecting features, which is by definition a discrete process, given an appropriate criterion that measures the joint "importance" of a set of features. If the criterion is differentiable with respect to the parameters of the transform, and if the transform is smooth, then one can learn the transform by some form of gradient-descent-optimization of the criterion. ICA (Sec. 21.2) can be used as a tool to find "interesting" projections of the data by finding linear projections that looks rich of clusters and non-Gaussian structure, but it is completely unsupervised with regard to the class labels, and may not be optimal to enhance class separability.

If $\mathbf{y}_i = g(\mathbf{w}, \mathbf{x}_i)$ is a feature transform parametrized by $\mathbf{w}$, the goal is now to find a differentiable estimate of the Mutual information from the examples so that gradient descent can produce better and better values of $\mathbf{w}$, as in Fig 21.5.

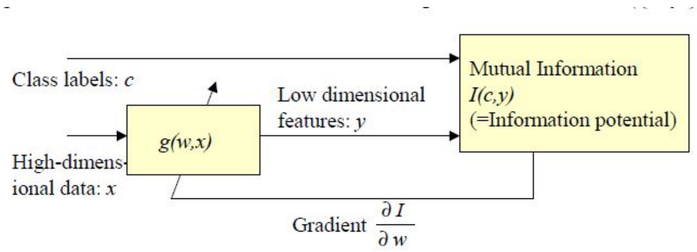

Class labels: c
High-dimens-ional data: x
$g(w,x)$
Low dimensional features: y
Mutual Information
$I(c,y)$
(=Information potential)
Gradient $\frac{\partial I}{\partial w}$

Figure 21.5: Learning feature transforms by maximizing the mutual information between class labels and transformed features (from [362]).

If the aim is not to compute an accurate value of the entropy of a particular distribution, but rather to find a distribution that maximizes or minimizes the entropy given some constraints, then a large number of entropy measures alternative to the original Shannon's definition can be used, producing the same distribution as the result of optimization [229]. In particular, **Renyi entropy** of order α is defined as:

$$H_{R_\alpha(X)} = \frac{1}{1-\alpha} \log \left(\sum_{i=1}^{n} p_i^\alpha \right)$$

where $\alpha \geq 0$ and $\alpha \neq 1$. As α approaches zero, the Renyi entropy increasingly weighs all possible events equally, regardless of their probabilities. The limit for $\alpha \to 1$ is the Shannon entropy.

It turns out that Renyi's quadratic measure (a function of the square of the density function), when combined with Parzen density estimation method using Gaussian kernels, provides significant computational savings: it can be estimated as a sum of local interactions, as defined by the kernel, over all pairs of samples. After completing the exercise to calculate derivatives in the given scheme [362] (Parzen windows and Renyi entropy), the method can be applied both to linear and non-linear tranforms.

The two main advantages of the method are that: i) it provides a non-parametric estimate of the mutual information without simplifying assumptions, like Gaussianity about the class densities, ii) it is usable with training datasets of the order of tens of thousands of samples. In static pattern recognition tasks, such feature transforms can extract more discriminatory information from the source features than alternative techniques like Fisher linear discriminant analysis (LDA) (Sec 20.5). Judging from the experiments, the method works extremely well only in transforms to low dimensions, approximately less than 10, probably because of limits in the the Parzen density estimation.

Gist

Feature extraction (or construction) goes beyond feature selection, aiming at **building more interesting features** from the raw data, in order to facilitate further processing and, hopefully, gain more insight about the modeled process.

Some **"first-aid" techniques** like normalization, quantization, application of application-dependent local or global filters should not be neglected, otherwise one risks masochism.

Raw measurements are often a combination (approximately linear) of basic signals or **hidden variables**. Identifying these factors of variations which explain the measurements variability, is invaluable. In the assumption of statistically independent signals and non-Gaussian (structured, high-entropy) probability distributions, the signals causing the phenomenon can be identified even before supervision is applied (**Independent Component Analysis**). Mixtures of source signals are almost always Gaussian (central limit theorem), and it is fairly safe to assume that non-Gaussian signals must, therefore, be source signals. Gaussian variables are forbidden for ICA!

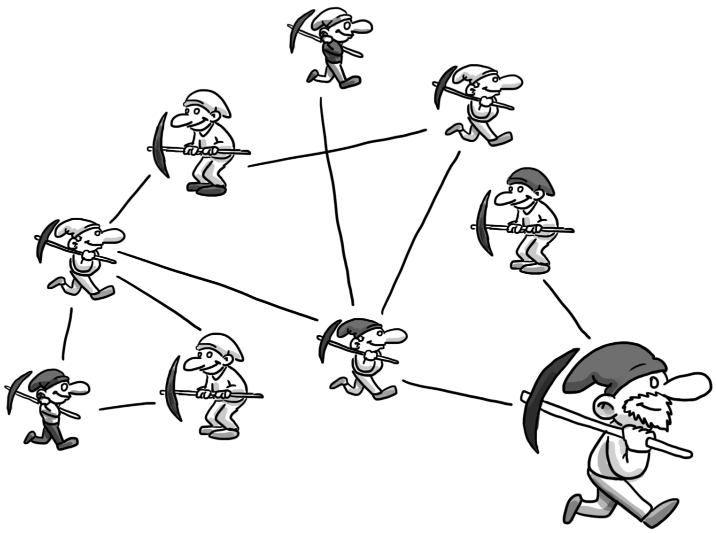
More complex, also non-linear, features can be constructed by considering parametric feature extractors, and by determining suitable parameters via **maximization of the Mutual Information between extracted features and output**. This is more easily said than done as Mutual Information is not easy to estimate, suitable approximations are often considered in practice.

If you listened to your unborn baby's heartbeat, now you know which methods you have to thank.

Chapter 22

Visualizing graphs and networks by nonlinear maps

No man is an Iland, intire of it selfe; [. . .]
any mans death diminishes me, because I am involved in Mankinde;
And therefore never send to know for whom the bell tolls;
It tolls for thee.
(John Donne, 1623)



After considering visualizations based on linear projections in Chapter 20, let's now consider more general ways to feed the human unsupervised learning capabilities and derive *insight* from data. We assume that the n entities to be displayed are not necessarily characterized by internal coordinates, but only by item-to-item (i.e., *external*) **relationships** such as dissimilarities between two items i and j denoted by d_{ij}. If items do have coordinates, such external relationships can be obtained by simple ways, as explained in Sec. 17.2.

In the general case, however, the external dissimilarity measure is not computed as a distance, and may not be available for every pair of items. An appropriate model for this situation is an **undirected weighted graph** $G(V, E)$, given by a set of vertices (or nodes) V, and edges $E \subset V \times V$. Each entity is represented by a node, and a connection (i, j) labeled d_{ij} is present between two nodes if and only if a dissimilarity is defined for the corresponding entities, as shown in Fig. 20.1. We assume that similarities are positive but we do not consider any other assumption (like the validity of triangular inequalities). For example, in marketing the similarity between two products could be derived by sampling customers and asking them to evaluate the product similarity along a given scale.

22.1 Multidimensional Scaling (MDS) Visualization by stress minimization

Given our eyes, visualization is only in two or three dimensions. The aim is therefore to place items on the 2D plane (or in 3D space) so that their **mutual distances are as close as possible to their dissimilarities**. In general, a perfect placement obeying all dissimilarities is impossible; therefore, a precise criterion is needed in order to define what placements can be considered as acceptable.

The problem is the following: given a set of items with (positive) dissimilarities d_{ij}, find the two-dimensional or three-dimensional coordinates $\boldsymbol{p}_i$ for all items that provide a convenient placement, one preserving the original dissimilarities as much as possible. The simplest objective is **stress minimization**, stress being the amount by which a *visualized* dissimilarity is compressed or expanded with respect to the original dissimilarity. It is intuitive, physical, and useful also as a starting point to understand more complex approaches.

A straightforward error measure quantifies by how much the distances in the plane are different with respect to the original dissimilarities. For simplicity we consider a two-dimensional visualization.

Let $\delta_{ij} = \sqrt{(\boldsymbol{p}_i - \boldsymbol{p}_j)^T(\boldsymbol{p}_i - \boldsymbol{p}_j)}$ be the distance between the coordinates of items i and j on the plane. A natural *global mapping error* can be defined as the sum of the squared individual errors:

$$\sum_{(i,j)\in E} (d_{ij} - \delta_{ij})^2.$$

No contribution to the error is present for missing edges (for couples of points without dissimilarity values). Additional flexibility can be obtained by adding an arbitrary weight w_{ij} representing the impact that an individual error has on the overall stress:

$$\text{global mapping error} = \text{Stress} = \sum_{(i,j)\in E} w_{ij}(d_{ij} - \delta_{ij})^2. \tag{22.1}$$

For example, if $w_{ij} = 1/{d_{ij}}^2$, one considers the *relative* errors $(\delta_{ij} - d_{ij})/d_{ij}$ instead of the absolute errors. The value $w_{ij} = 1$ is the default.

An exact solution reproduces all original dissimilarities: $\delta_{ij} = d_{ij}$, with zero error. Low error means that many distances tend to be rather close to the original ones. The problem is now to *minimize* the *global mapping error* by changing the point positions $\boldsymbol{p}_i$. The freedom in placing point in two dimensions is complete, and therefore the optimization problem has a very large number of dimensions, equal to twice the number of entities. The situation is different in Chapter 20 with mappings executed by a linear projection.

There is a nice physical model related to minimizing the above *global mapping error*, explaining the term *Stress* to denote the function to be minimized. A spring is attached to each pair of points with a length at rest equal to d_{ij}, the desired distance, and with an elastic constant (resistance to deformation) equal to the weight w_{ij}. The term $w_{ij}(\delta_{ij} - d_{ij})^2$ can be considered as the potential energy of a spring which is elongated or compressed with respect to the rest length. The initial position of the points can be chosen randomly and the movement is constrained to two dimensions. The system will start oscillating and, provided that some friction is present, oscillations will gradually be damped, leading to a stable situation, a locally optimal configuration of the overall stress function.

The physical system can of course be simulated on a computer, leading to what is called the **force-directed approach for drawing graphs**. Methods based on this approach consist of two main components. The first is the

model that quantifies the quality of a drawing (or of the two-dimensional map if you prefer a more technical term). The second is an **optimization method** for computing a drawing that is locally optimal with respect to this model. The resulting final layout brings the system to equilibrium, so that the total force on each vertex is zero, or equivalently, the potential energy is locally minimal with respect to the vertex positions.

If you do not like Physics but prefer Math, you can forget about simulating physical details like friction and concentrate on minimizing the stress function through gradient descent: calculate partial derivatives and use an optimization method to reach a global optimum, again *optimization is the source of power*!

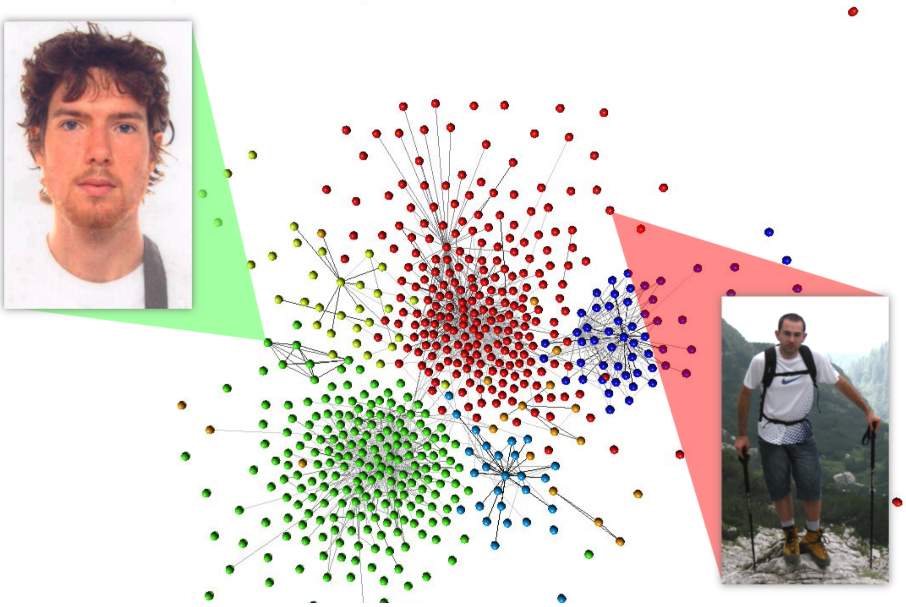


Figure 22.1: 2D Visualization by stress minimization.

Examples of visualizations are in Fig. 22.1, which shows a **social network** of friends interested in different mountaineering activities, and in Fig. 22.2, which shows a social network of politicians with similarities related to their activity in the parliament. Note how the main political groups are automatically *clustered* as an interesting side-effect of encouraging the placement of similar people in similar positions. Through a **focus and context visualization**, one can either concentrate on the local network of connections around a single politician (*focus*), or see also the *context* given by the complete set of connections (Fig. 22.3). It is therefore simple to navigate from an entity to a neighbor, to a neighbor of a neighbor, etc., to likewise track complex relationships in a fast and effective manner. Criminal investigations are another possible application of this method.

In addition to visualization, reducing data dimensionality by finding a mapping from the original space to one with a smaller number of dimensions (also called **Multidimensional Scaling (MDS)** [244] has value also to extract relevant features for subsequent processing by ML. In this case, the mapping is defined via parametric definitions so that is can be applied also to new points, when the ML system has is used for new points in generalization mode [61].

22.2 A one-dimensional case: spectral graph drawing

A paradigmatic case consists of mapping the set of n points to one dimension while keeping similar points as close as possible. As usual, one needs to define a quantity to minimize, related to the goodness of the one-dimensional drawing. Let x_i be the one-dimensional coordinate assigned to point i (and let $\boldsymbol{x}$ denote the vector of all such coordinates). A

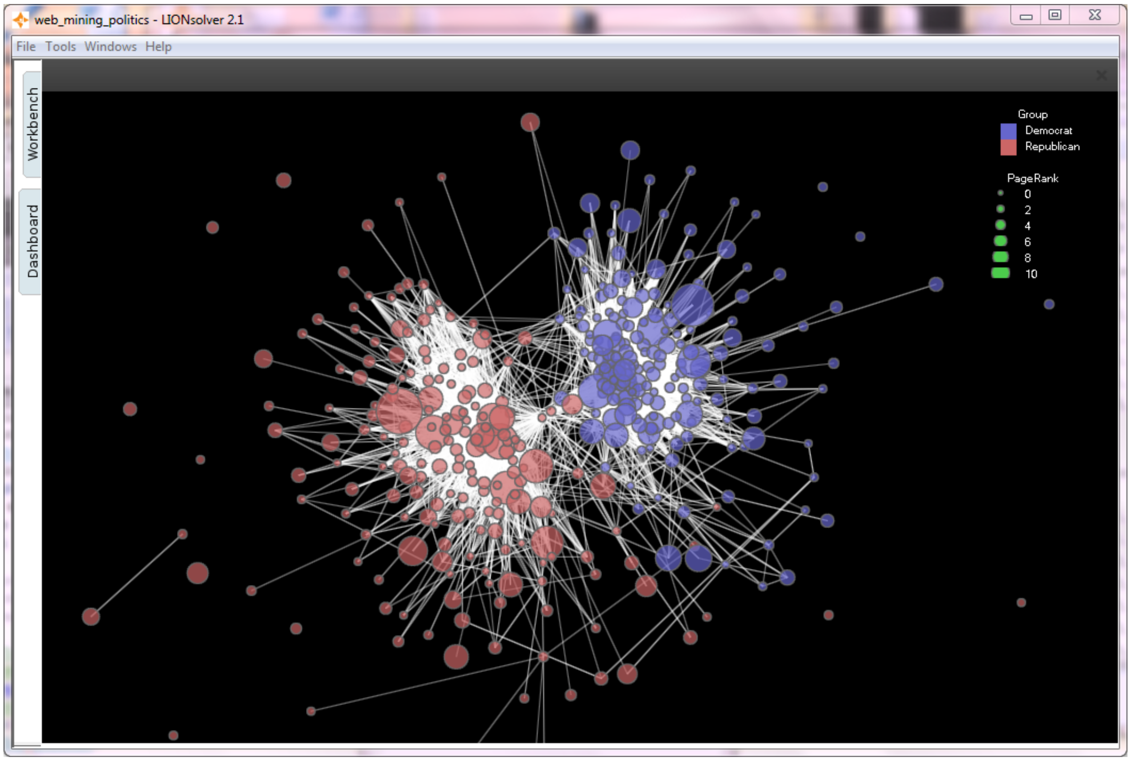


Figure 22.2: Social network analysis: visualizing the network of USA representatives. The two parties (which are not available to the clustering software) emerge as two very different clusters.

useful quantity is **Hall's energy**, first proposed in the 70's:

$$E_{\text{Hall}} = \frac{1}{2} \sum_{i,j=1}^{n} w_{ij}(x_i - x_j)^2. \tag{22.2}$$

The interpretation of this formula is to square the individual distances (so that the function will be differentiable and the differentiation will lead to linear equations) and sum them weighted by the similarities between pairs. When w_{ij} is large the function E_{Hall} gets a large contribution from the $(x_i - x_j)^2$ term and therefore this definition should encourage placing similar points at close positions, to avoid paying a large penalty and obtaining a large E_{Hall} value. Through Hall's energy, large similarities encourage close positions in the placement.

Stop for a minute to identify a serious weakness in the above definition and the proceed. Now one is completely free to pick a coordinate x_i for each point and by picking very small coordinates (or coordinates which are very similar) the energy goes to zero but we are left with a trivial solution: mapping all points to the same position. The definition can be repaired by considering that one is not interested in the *absolute* values of the coordinates but in their *relative* values. As usual, the optimized drawing should not depend on choosing meters or millimeters as units. One

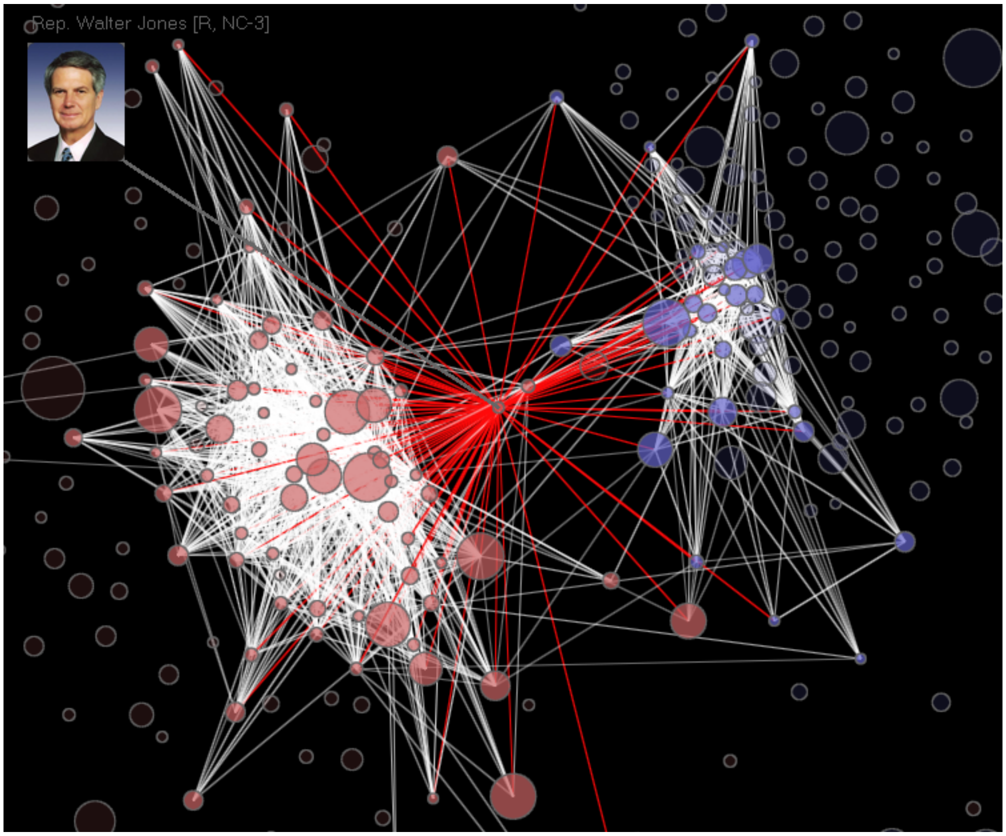


Figure 22.3: Navigating in a social network of politicians: the network of a single representative.

can therefore fix the length of the x vector to one and the problem becomes:

$$\text{minimize} \qquad \left(\sum_{(i,j)\in E} w_{ij}(x_i - x_j)^2 \right) \tag{22.3}$$

$$\text{subject to} \qquad \|\boldsymbol{x}\|^2 = \boldsymbol{x}^T\boldsymbol{x} = \sum_{i=1}^{n} x_i^2 = 1. \tag{22.4}$$

For convenience let $N(i) = \{j|(i,j) \in E\}$ be the neighborhood of node i and $\deg(i) = \sum_{j\in N(i)} w_{ij}$ its weighted degree. After defining the Laplacian matrix L^G associated with the graph:

$$L^G_{ij} = \begin{cases} \deg(i) & \text{if } i = j \\ -w_{ij} & \text{if } i \neq j \end{cases}, \tag{22.5}$$

one can obtain Hall's energy as $E_{\text{Hall}} = \boldsymbol{x}^T L^G \boldsymbol{x}$.

The energy and the constraint are invariant under translation. We can eliminate this degree of freedom by requiring that the mean of $\boldsymbol{x}$ be zero: $\sum_{i=1}^n x_i = \boldsymbol{x}^T\mathbf{1}_n = 0$ (where the vector $\mathbf{1}_n$ contains all 1's). Finally, the 1-dimensional optimal layout can be described as the solution of the following constrained minimization problem:

$$\begin{array}{ll} \text{minimize} & \boldsymbol{x}^T L^G \boldsymbol{x} \\ \text{subject to} & \begin{cases} \boldsymbol{x}^T \boldsymbol{x} = 1 \\ \boldsymbol{x}^T \mathbf{1}_n = 0 \end{cases} \end{array} .$$

By standard optimization and linear algebra results, provided that the graph is connected, the resulting minimum value of the energy is the so-called *algebraic connectivity* of the graph, i.e., the second smallest eigenvalue λ_1 of L^G (L^G is singular, therefore the smallest eigenvalue is $\lambda_0 = 0$), while the solution is the corresponding eigenvector $\boldsymbol{v}_1$, also known as the *Fiedler vector*. The result is elegant and it deserves an inspiring name: **spectral graph drawing**, or **spectral layout**. The term "spectral" has nothing to do with ghosts and scary movies but with the usage of eigenvectors and eigenvalues in Physics to study the distribution of energy emitted by a radiant source (spectrum), of vibration modes, etc.

Unfortunately elegance must be neglected when going to more than one dimension. Let's call the second dimension y. A trivial generalization will make the second vector coordinate $\boldsymbol{y}$ the same as $\boldsymbol{x}$, not a big gain: all points will be aligned on the diagonal line, not really a two-dimensional plot. To get something more usable we must force the solution value for the y coordinate to be different from the one for the x coordinate.

A reasonable requirement is to ask that the two coordinate vectors are not correlated ($\boldsymbol{y}^T \boldsymbol{x} = 0$), so that the additional dimension will give us some new information, "new" in the sense that it is not linearly related to the previous values, not in a deep information-theoretic meaning. The problem for $\boldsymbol{y}$ now becomes:

$$\begin{array}{ll} \text{minimize} & \boldsymbol{y}^T L^G \boldsymbol{y} \\ \text{subject to} & \begin{cases} \boldsymbol{y}^T \boldsymbol{y} = 1 \\ \boldsymbol{y}^T \mathbf{1}_n = 0 \\ \boldsymbol{y}^T \boldsymbol{x} = 0 \end{cases} \end{array} .$$

Potential difficulties are inherited from the difficulties in solving very large eigenvector problems. Multi-scale techniques and iterative techniques to calculate principal eigenvectors can help.

In spite of the elegance related to minimizing a simple function with a well known linear algebra result, there are no guarantees that the aesthetic properties of the layout correspond to the user preferences. In particular, there are no requirements forbidding the methods to place too many nodes too close together so that they become hardly visible. Furthermore, there is no guarantee that requiring an uncorrelated y coordinate corresponds to the best aesthetic results.

Real-world layouts typically require energies (functions to be minimized) designed in close agreement with the specific preferences. By defining a clear energy, one separates the concern about **the goal** (the desired layout characteristics) from the concern about **how the goal can be reached**, at least approximately, by optimization techniques.

22.3 Complex graph layout criteria

Let us consider the following simple graph connectivity matrix, where two nodes i and j are connected if and only if the matrix entry (i, j) is 1:

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

corresponding to a three-node graph whose only requirement is that node 2 has distance 1 from the other two nodes:

$$d_{12} = d_{23} = 1.$$

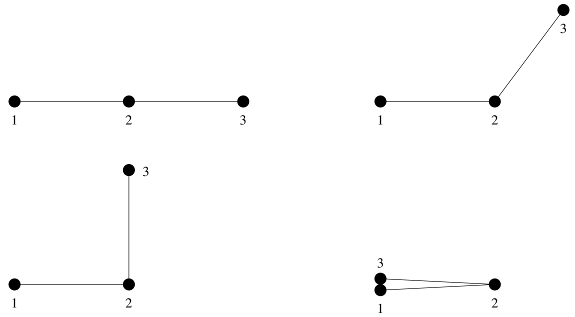


Figure 22.4: Equivalent stress-minimizing layouts when too few constraints are defined.

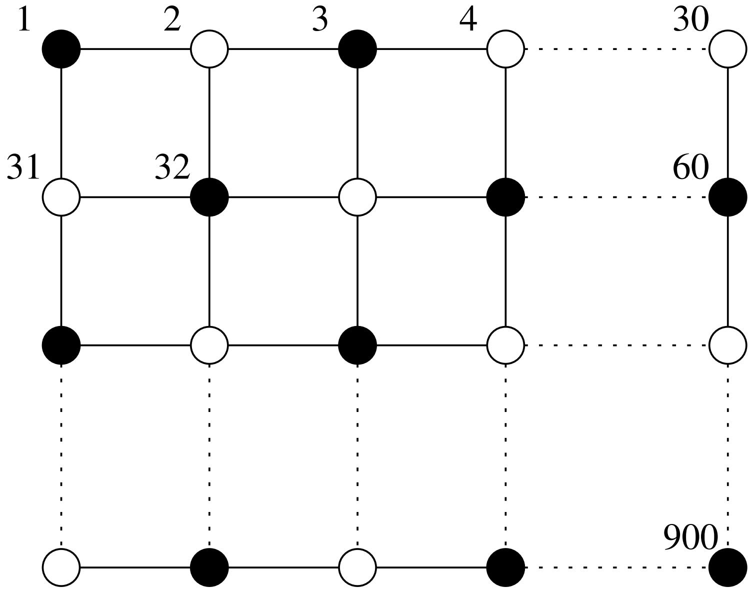


Figure 22.5: A 30 × 30 lattice with first-neighbor edges.

The layouts shown in Fig. 22.4 are perfectly equivalent from a stress-minimization approach: the absence of an edge (e.g., between nodes 1 and 3) implies that the mutual distance of the corresponding nodes is irrelevant if the energy function to be optimized contains only terms related to *connected* pairs.

The problem is even worse in large graphs where many indifferent pairs of nodes exist. Fig. 22.5 shows a 30 × 30 rectangular lattice where only first-neighborhood edges are defined (requiring unit distance between the endpoints). An "optimal" layout obtained by minimizing equation (22.1) is shown in Fig. 22.6. Many degenerate locally-optimal layouts exist. They can be obtained by alternately coloring nodes in black and white in a checkerboard fashion, so that black nodes are only connected to white ones and *vice versa*. A one-dimensional solution packing all black nodes at $x = 0$ and all white nodes at $x = 1$ trivially satisfies all distance constraints, so that the *global mapping error* defined in equation (22.1) is zero.

The introduction of a default large distance for unconnected nodes can easily solve the problem. Fig. 22.7 shows the optimal layout obtained by equation (22.1) on the same 30 × 30 lattice where disconnected nodes i and j have a large required distance $d_{ij} = 20$ with a very small weight $w_{ij} = 10^{-5}$. Observe that, the layout being unknown a priori, it is often difficult to define a convenient default distance. In the case of Fig. 22.7, for instance, the value of 20

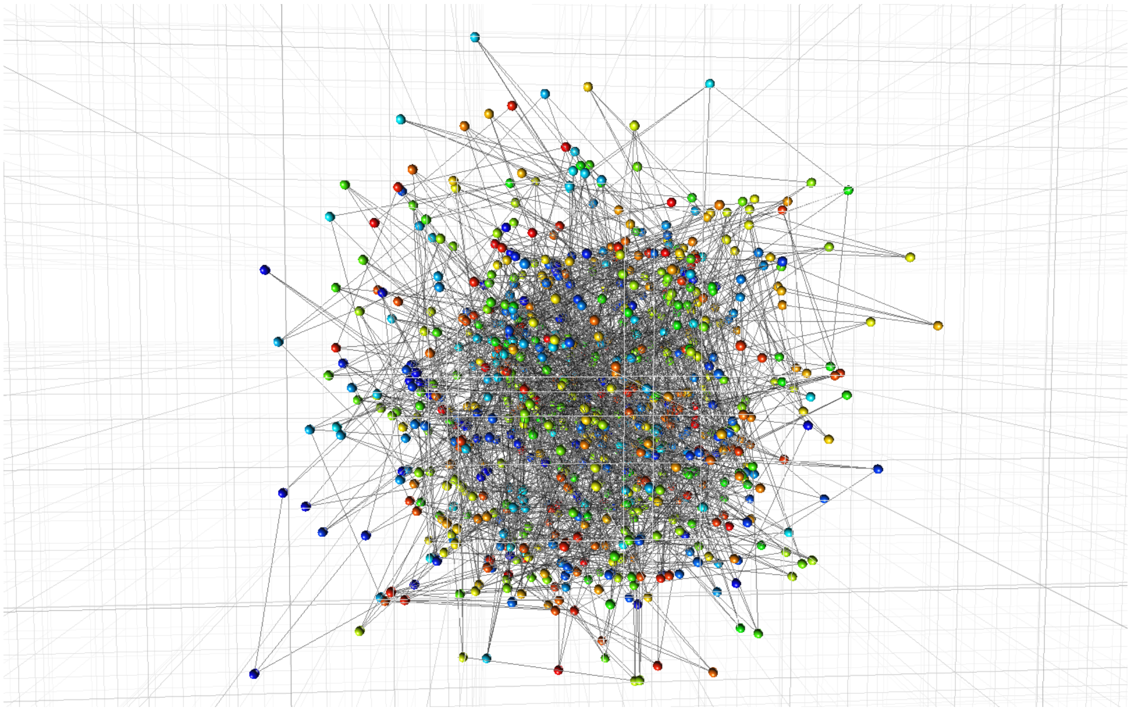


Figure 22.6: An "optimal" layout from the stress-minimization point of view, which is not optimal for understanding the network structure.

is too little to ensure a correct layout, and the overall graph bends into a spherical shape.

A second approach, shown in Fig. 22.8, is the completion of the distance matrix by the *shortest path* calculation. All distances between nodes which are not directly connected are set equal to the *shortest path* between such nodes. For instance, nodes 1 and 32 of the lattice shown in Fig. 22.5 have a shortest path length equal to 2 (one horizontal and one vertical edge). Without the requirement that shortest paths distances are reproduced, nothing prohibits nodes 1 and 32 to be placed at a very small distance in the visualization. As soon as the requirement is active, this bad behavior is discouraged by a large penalty and nodes tend to untangle, passing from configurations like that of Fig. 22.6 to configurations like that of Fig. 22.8.

Notice that the minimum path distance is always larger than the Euclidean distance in the grid layout. As an example, the shortest-path distance between the two diagonally extreme nodes 1 and 900 is $(30-1)\cdot 2 = 58$, while the expected Euclidean distance in the grid layout would be $(30-1)\cdot\sqrt{2} \approx 41.01$, hence the pillow-shaped layout of Fig. 22.8.

More complex functions to be minimized for graph layout consider **additional aesthetic criteria**, like minimizing the number of edge crossings, or guaranteeing a certain minimum angle between edges connected to a node (small angles make readability difficult), or allowing curved edges, etc. A complete enumeration is out of the scope of this introductory chapter. In all cases, after defining in quantitative terms a suitable compromise between the desirable aesthetic criteria, one has to search for an effective minimization algorithm (the source of power!), in most cases looking for an approximate but fast solution.

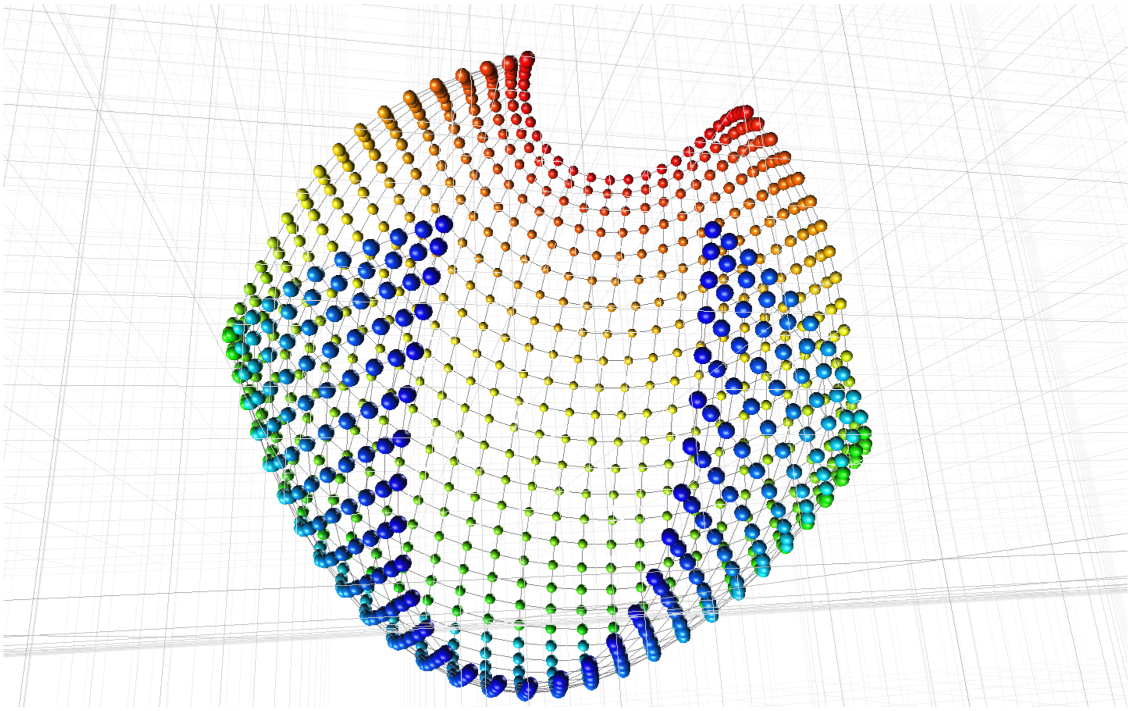


Figure 22.7: First solution to missing constraints: add a default repulsion.

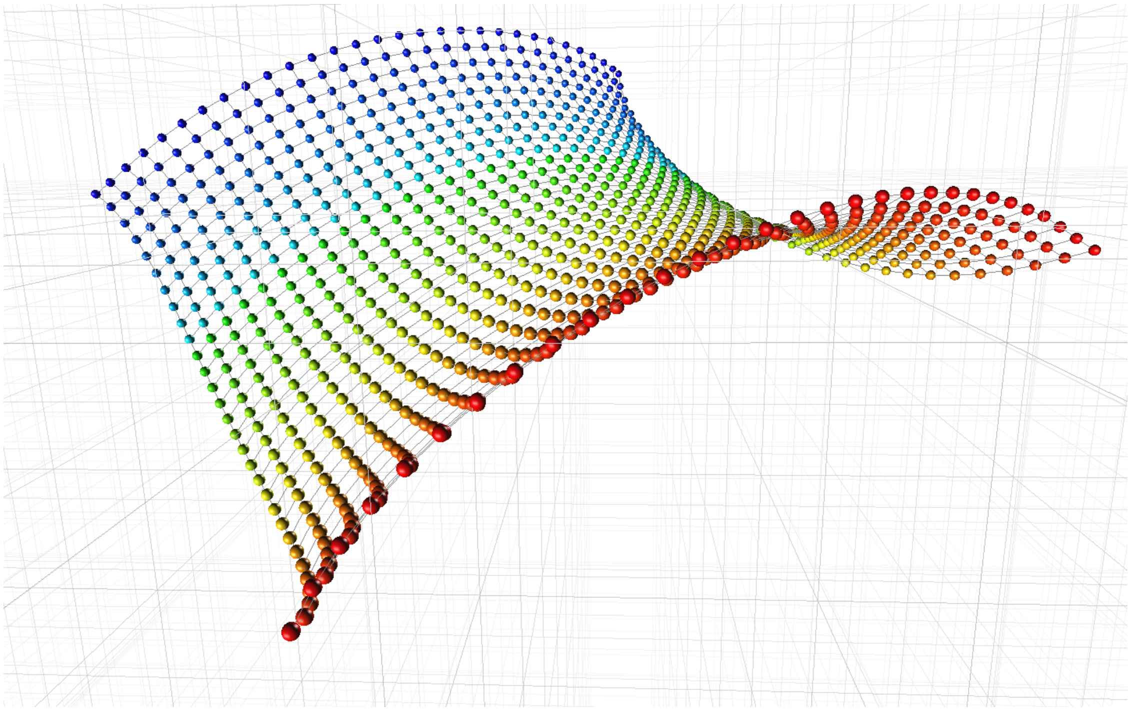


Figure 22.8: Second solution to missing constraints: complete distances by computing the minimum path between nodes.

Gist

Graph layout techniques can be used to visualize relationships between entities.

If some dissimilarities are available, drawing entities in two dimensions so that similar items are close to each other is precious to identify groups (clusters) and relationships between groups.

Stress minimization resorts to a physical model. Each dissimilarity value generates a spring between entities in n dimensions. The task is to "sandwich" the network by squeezing it to a plane, while minimizing the elongation or shortening of the various springs. By the way, if springs are substituted with rigid bars, squeezing becomes impossible: in general an exact solution to map points to a plane and maintain *all* dissimilarity values unchanged does not exist. If you imagine each point as a person at a party, everybody will move on the floor to be away from disagreeable people and close to likeable ones. The fact that everybody moves at the same time can make parties (and visualizations) very stressing (suboptimal).

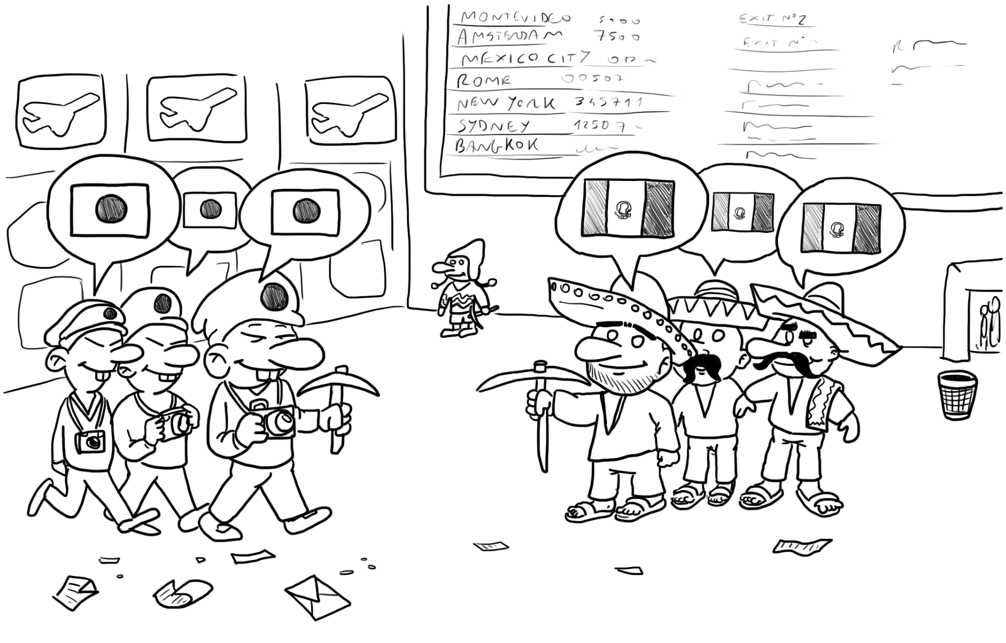
As for clustering, there is not an absolute best graph (or network) layout. Through optimization one defines the **objectives** (the quantitative meaning of "optimal layout") and then identifies the best possible mapping which maximizes them. Often one tries many possibilities before identifying a proper visualization.

Social network analysis is used to study networks of interacting persons. In business, a similarity between employees can be defined by the number of messages they exchange. If you design a layout of the network of employees with this metric you will easily identify clusters of colleagues working together, maybe loser connections between different groups, and maybe some isolated individuals who either concentrate a lot, or prefer the telephone, or ... are not too committed to the business.

Chapter 23

Semi-supervised learning

A mind is a fire to be kindled, not a vessel to be filled.
(Plutarch)



Let us consider the international airport example which motivated unsupervised learning methods in Chapter 19: you walk through a gate and clearly identify clusters of people speaking different languages, even if the language names are unknown. Now, if *some* people languages are identified, for example if some people are waving flags or wearing costumes of their countries, for sure one could select only the labeled speakers and run a supervised learning algorithm to map phonetic characteristics to languages.

The question now is: can one also use some information from the *unlabeled* people to improve language classification? Let us note that clusters of people usually speak the same language ("birds of a feather flock together") and we may be tempted to label some of the unknown speakers with the same language as the one spoken by at least one member of the same cluster. If the assumption is true, one greatly increases the number of examples and can improve the overall generalization capability of the trained classifier. For example, young children clustered with their older and identified parents can be added to the database so that even young people voices (usually with higher frequencies) can be correctly classified.

In a similar manner, one can use some supervised data to aid unsupervised learning and clustering. This is the underlying idea of semi-supervised learning: **use both the labeled examples and also (some) unlabeled ones to improve the overall classification accuracy**.

If the assumptions work, one gets a very valuable performance boost in all cases when **labeled examples are scarce and unlabeled ones abundant**. Think for example at web pages: human labeling is very costly and only a minuscule subset of web pages are labeled. By contrast, an enormous and growing number of unlabeled pages is present.

23.1 Learning with partially unsupervised data

Semi-supervised learning (SSL) uses both supervised and unsupervised data to improve performance. The standard form of supervision are **labels** associated with some examples. In this case the training set X is divided into a labeled portion $X_L = \{x_1, \dots, x_l\}$, for which labels $Y_L = \{y_1, \dots, y_l\}$ are given, and an unlabeled portion $X_U = \{x_{l+1}, \dots, x_{l+u}\}$.

Other forms of supervision can be related to constraints or **hints** given to the system [4]. For example, the hints can take the form “the output function must be growing as a function of one input coordinate,” while constraints can be formulated as “these two points must be in the same class” (**must-link**) or “these two points cannot be in the same class” (**cannot-link**).

A first idea, originated in the sixties [320] is the so-called self-learning or **self-labeling** method where a wrapper algorithm repeatedly uses a supervised learning method. Initially, learning is executed on the labeled examples. Then, some additional unlabeled examples are labeled by using the current trained system, and learning is repeated by adding the newly labeled examples. Heuristically, one could try adding labels to the examples which are labeled with the largest confidence. Although appealing, the effect of the wrapper depends on the supervised method enclosed and it is unclear when self-labeling is effective.

A context related to SSL was introduced by Vapnik as **transductive learning**. Inductive learning wants to derive a prediction function valid for arbitrary inputs, while transductive learning just aims at predicting only a fixed set of test points, by using all available information. Usually, transductive learning is based on a **labeled graph representation of the data**, labeled nodes are classified training examples, edges represent similarity/dissimilarity relationships or constraints. A combinatorial optimization on the labels to maximize an overall consistency measure is then performed.

In general, SSL looks promising if the unsupervised information about the density $p(x)$ is useful in deriving $p(y|x)$. By analogy with the supervised learning smoothness assumption, the **semi-supervised smoothness assumption** states that if two input points x_1 and x_2 *in a high-density region* are close, the corresponding outputs y_1 and y_2 should also be close. By transitivity, if two points are linked by a path in a high density region (they belong to the same cluster) their outputs should be close. If points are close but in a low-density area, the requirement that outputs are similar is less stringent.

If we equate unsupervised learning with clustering, the **cluster assumption** states that if two points are in the same cluster, they are likely to belong to the same class. In this case, the use of unlabeled points is useful to find boundaries between clusters with better accuracy, and then improve the overall classification by the above assumption.

An equivalent formulation is the **low-density separation assumption**: decision boundaries between different classes should lie in low-density regions, and should not split single clusters, as shown in Fig. 23.1.

The above assumptions correspond very closely to the international airport analogy: if one wants to separate different languages he had better not split clusters of people but draw boundaries in empty areas.

A different paradigm is the assumption that data lie approximately on a **low-dimensional manifold**, as shown in Fig. 23.2. A manifold is a mathematical space that on a small enough scale resembles Euclidean space of a specific dimension. For example, a line and a circle are one-dimensional manifolds, a plane and a sphere (the surface of a ball) are two-dimensional manifolds. More formally, every point of an n-dimensional manifold has a neighborhood homeomorphic to an open subset of the n-dimensional space R^n. The curse of dimensionality for input data of very

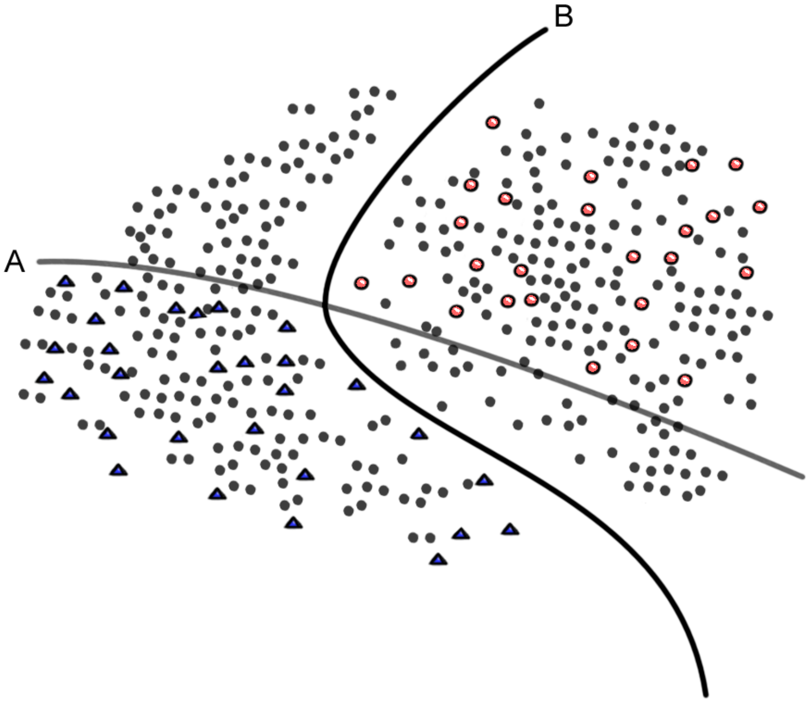


Figure 23.1: Low-density separation assumption. Even if boundary A correctly separates the labeled examples, boundary B is better because it crosses a low-density region. Information about unlabeled data produces a better classification.

large dimensions is avoided by first identifying a manifold where most data lie. Then an appropriate metric is given by **geodesic distances** on the manifold (the analogy is with distances covered by airplanes on the Earth surface), and the standard smoothness assumption is considered on the low-dimensional manifold. The more data is available, the better one identifies the relevant manifold and the corresponding metric to use in supervised learning (consider for example a nearest-neighbor classifier, where the vicinity is given by geodesic distances on the manifold).

23.1.1 Separation in low-density areas

Some SSL techniques are based on encouraging the separation between classes (the decision boundaries) to pass through low-density areas, away from most data examples.

An immediate algorithm is obtained by adopting a margin-maximization algorithm like SVM and maximizing the margin for both labeled and unlabeled examples, this is called **transductive SVM** (TSVM). To the function to be minimized one adds a term like:

$$\lambda_2 \sum_{unlabeled\ data\ i} (1 - |f(x_i)|), \tag{23.1}$$

$f(x_i)$ being the classification function which has to be greater than 1 for one class, less than -1 for the other class. The

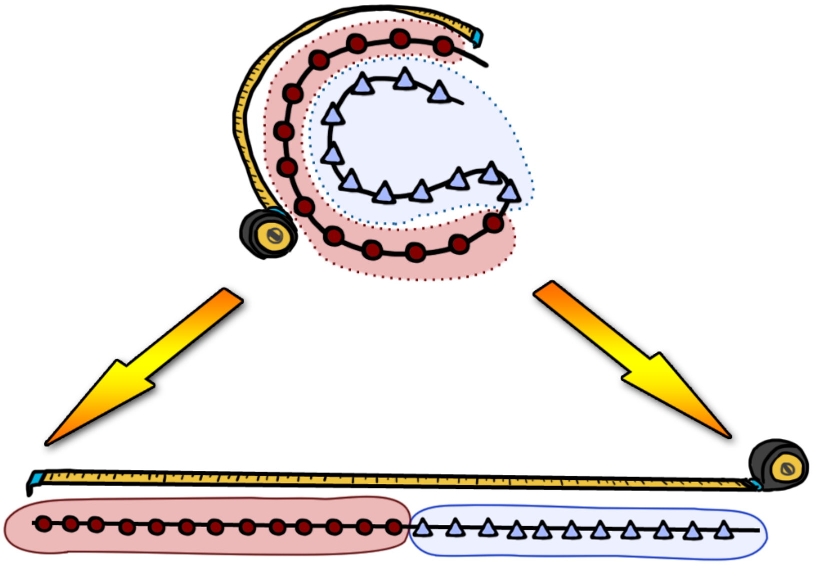


Figure 23.2: The geodesic distance can help to separate classes lying on a manifold.

penalty introduced in the function is of λ_2 when $f(x_i) = 0$, and it linearly becomes equal to zero when $f(x_i)$ becomes 1 or, in the other direction, when $f(x_i)$ becomes -1 (the penalty has a triangular form centered around zero). In other words, a penalty is incurred if an unlabeled data point falls in the "gray" boundary region where $|f(x_i)| \leq 1$: therefore unlabeled data tend to **guide the linear boundary away from the dense regions**. The corresponding problem is not convex and therefore robust heuristic optimization schemes have to be adopted, for example *deterministic annealing* strategies which start from an easy problem and gradually transform it into the TSVM optimization function [333]. The continuation approach of [78] follows a similar paradigm of first optimizing an "ironed" version of the function and then gradually introducing finer and finer details.

23.1.2 Graph-based algorithms

The graph-based methods are based on representing the problem as a graph, where nodes correspond to examples and edges are labeled with the pairwise similarity w_{ij} of two nodes i and j. As usual, one can think in terms of similarities, or in terms of dissimilarities/distances.

An approximation of the **geodesic distance of two points along the manifold** can be approximated by deriving the **minimum-path distances** between couples of points from the initial pairwise distances.

Let's introduce the matrix $\mathbf{W}$ to represent similarities $\mathbf{W}_{ij} = w_{ij}$ if the edge is present, zero otherwise, and the diagonal degree matrix $\mathbf{D}$, so that $\mathbf{D}_{ii} = \sum_j w_{ij}$.

The basic method to encourage **smoothness along light edges** (smoothness when connected nodes are similar) is related to defining and using the **graph Laplacian** operator. The normalized $\mathcal{L}$ and non-normalized combinatorial graph Laplacian operator $\mathbf{L}$ are defined as:

$$\mathcal{L} = \mathbf{I} - \mathbf{D}^{-1/2}\,\mathbf{W}\,\mathbf{D}^{-1/2}, \tag{23.2}$$

$$\mathbf{L} = \mathbf{D} - \mathbf{W}. \tag{23.3}$$

The graph Laplacian is related to the more traditional Laplace operator (denoted with ∇^2) used for continuous functions $f(x_1, \ldots, x_n)$:

$$\nabla^2 \phi = \sum_{i=1}^{n} \frac{\partial^2 f}{\partial {x_i}^2}. \tag{23.4}$$

In fact, the Laplacian matrix of a lattice, when applied to the values of f at the vertices, corresponds to the finite-differences approximation of the continuous operator on a regular grid of points. The Laplacian matrix of a graph can be seen as a generalization of the lattice definition.

The Laplacian $\nabla^2 f(\boldsymbol{x})$ of a function f at a point $\boldsymbol{x}$, up to a constant depending on the dimension, is the rate at which the average value of f over spheres centered at $\boldsymbol{x}$, deviates from $f(\boldsymbol{x})$ as the radius of the sphere grows. Zero means that the average value on a sphere is equal to the value at the center.

A motivation for the Laplacian appearing in physics is that solutions to $\nabla^2 f = 0$ in a region U are functions that make the Dirichlet energy functional stationary:

$$E(f) = \frac{1}{2} \int_U \|\nabla f\|^2 \, \mathrm{d}x. \tag{23.5}$$

The **smoothing action** is clear: one aims at identifying locally optimal configurations that minimize the average square of the gradient modulus. Once again, the optimization point of view clarifies the meaning.

Iterative ways to solve the above $\nabla f = 0$ equation on a grid involves repeatedly substituting the value at a grid point with a weighted average of the values on its neighbors.

A similar smoothing action is obtained on graphs, the goal is to obtain a distribution of values on the graph so that **the value at a node is equal to the weighted average of the neighboring values**.

A semi-supervised learning using Gaussian fields and harmonic function is proposed in [392]. Classification algorithms for Gaussian fields can be seen as a form of nearest-neighbor approach, where the nearest labeled examples are computed by a random walk on the graph. The method's equations are related to electrical networks and to spectral graph theory. The problem is represented as a graph, with some nodes labeled with $y \in 0, 1$ (for simplicity we consider a binary labeling). Weighted edges represent similarities: w_{ij} is large for similar cases. For example $w_{ij} = \exp\{-\|\mathbf{x}_i - \mathbf{x}_j\|^2_{\mathbf{A}}\}$ for a suitable metric. The strategy is to first compute a "smooth" real-valued function f for all nodes and then assign labels based on f. The "smoothness" desire of having similar values between similar points is expressed by formulating the problem as one of minimizing the quadratic energy function

$$E(f) = \frac{1}{2} \sum_{i,j} w_{ij} (f(i) - f(j))^2. \tag{23.6}$$

The minimum energy function is *harmonic*: it satisfies $Lf = 0$ on unlabeled points, and is equal to the label value on the labeled ones. L is the graph Laplacian defined above, and the harmonic property means that the value of f at an unlabeled point is equal to the weighted average of f at neighboring points:

$$f(j) = \frac{\sum_i w_{ij} f(i)}{\sum_i w_{ij}}. \tag{23.7}$$

In matrix notation: $f = \mathbf{P} f$, where $\mathbf{P} = \mathbf{D}^{-1}\ \mathbf{W}$. This is consistent with the intuitive notion of smoothness with respect to the similarity relationships. The graph-based smoothing operation is illustrated in Fig. 23.3.

A simple rule is to label a node i with 1 if $f(i) > 1/2$, 0 otherwise.

The connection with **random walk** is as follows: imagine a walker starting from an unlabeled node i and moving to a neighbor j with probability $\mathbf{P}_{ij}$. The walk stops when the first labeled node is encountered. Then $f(i)$ is the probability that the walker stops at a node labeled 1.

The **electrical network** interpretation is as follows: nodes labeled 1 are connected to a positive voltage source, nodes labeled 0 to ground. Edges are resistors with conductance w_{ij}. Then f is the resulting voltage on the unlabeled nodes, which minimizes the energy dissipation. Ways to incorporate class prior knowledge (desirable proportions of the two classes) by modifying the threshold to label the nodes, as well as possible ways to learn a weight matrix $\mathbf{W}$ from labeled and unlabeled data are described in [392].

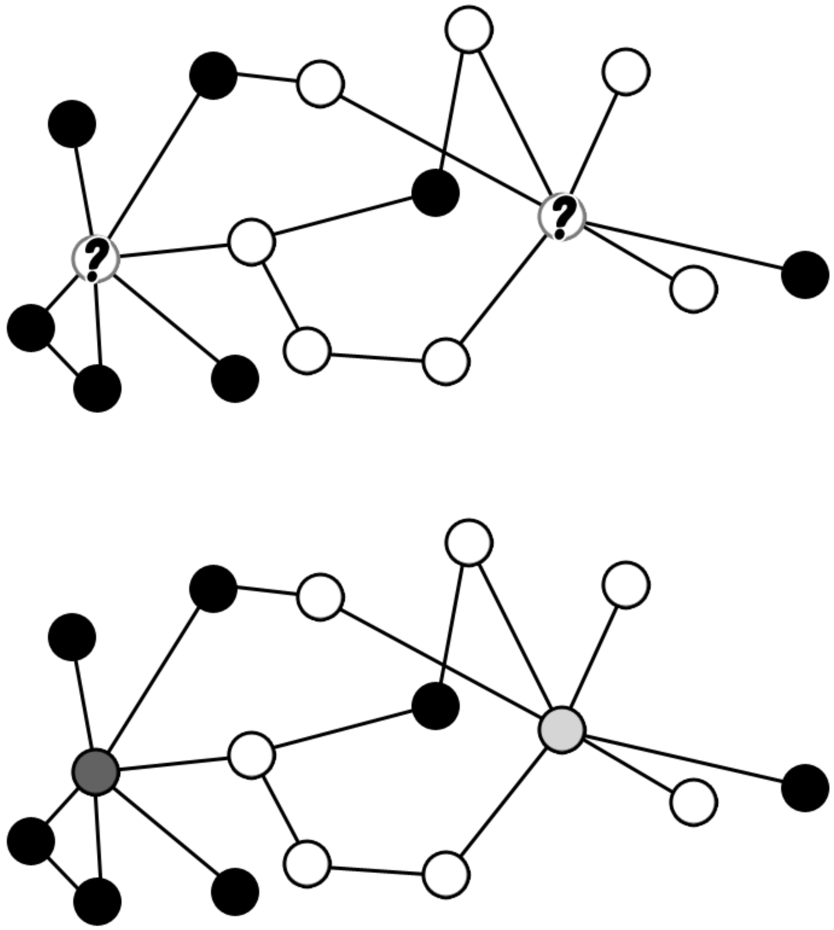


Figure 23.3: The values of the unknown nodes in the graph are computed as the average of the neighbors.

23.1.3 Learning the metric

Some semi-supervised algorithms proceed in two steps: first **a new metric or representation is identified** by performing an unsupervised step on all data (ignoring the existence of labels), then a pure supervised learning phase is executed by using the newly identified metric or representation.

The two steps are in fact implementing the semi-supervised smoothness assumption, by ensuring that the new metric or representation satisfies that distances are small in the high density regions.

Let's note that some graph-based methods are closely related to this way of proceeding: the construction of the graph from the data can be seen as an unsupervised change of representation.

23.1.4 Integrating constraints and metric learning

In many cases, when dealing with an optimization problem defined over more than one variable, a sequential method which first minimizes over the first variable, then over the second (leaving the first variable untouched) etc. gives in general a solution which can be improved if all variables are considered at the same time. This is clear because the freedom of movement in the input space is increased: in the first case one moves only along coordinate axes, in the second case one moves freely in input space looking for locally optimal points.

This holds also for SSL. For example the work in [53] shows how to combine constraints and metric learning into semi-supervised clustering.

Constraint-based clustering approaches start from pairwise *must-link* or *cannot-link* constraints (requests that two points do or do not belong to the same cluster) and insert into the objective function to be minimized a penalty for violating constraints. By the way, constraints can be derived from the labels but also from other sources of information. For example, the Euclidean K-means algorithm partitions the points into k sets so that the function:

$$\sum_i \|\mathbf{x}_i - \boldsymbol{\mu}_{l_i}\|^2$$

is locally minimized. In it, the vector $\boldsymbol{\mu}_{l_i}$ is the winning centroid associated with point $\mathbf{x}_i$, the one minimizing the distance.

If two sets of must-link pairs $\mathcal{M}$ and cannot-link pairs $\mathcal{C}$ are available, one can encourage a placement of the centroids in order to satisfy the constraints by adding a penalty w_{ij} for a single violation of a constraint in $\mathcal{M}$ and a penalty $\overline{w}_{ij}$ for a single violation of a constraint in $\mathcal{C}$, obtaining the following function to be minimized ("**pairwise constrained K-means**"):

$$E_{\text{pckmeans}} = \sum_i \|\mathbf{x}_i - \mu_{l_i}\|^2 + \sum_{(\mathbf{x}_i,\mathbf{x}_j)\in\mathcal{M} \text{ and } l_i \neq l_j} w_{ij} + \sum_{(\mathbf{x}_i,\mathbf{x}_j)\in\mathcal{C} \text{ and } l_i = l_j} \overline{w}_{ij}. \tag{23.8}$$

Pairwise constraints can also be used for **metric learning**. If the metric is parametrized with a symmetric positive-definite matrix $\mathbf{A}$ as follows,

$$\|\mathbf{x}_i - \mathbf{x}_j\|_{\mathbf{A}} = \sqrt{(\mathbf{x}_i - \mathbf{x}_j)^T \mathbf{A} (\mathbf{x}_i - \mathbf{x}_j)},$$

the problem amounts to determining appropriate values of the matrix coefficients. If the matrix is diagonal, the problem becomes that of *weighing* the different features.

The constraints represent the user's view of similarities: they can be used to change the metric to reflect this view, by minimizing the distance between must-link instances and at the same time maximizing the distance between cannot-link instances. After the metric is modified, one can use a traditional clustering algorithm like K-means.

Asking for a single metric for the entire space can be inappropriate and a different metric $\mathbf{A}_h$ can be used for each k-means cluster h. The MPCK-MEANS algorithm in [53] uses the method of Expectation-Maximization, see also Section 17.3, and alternates between cluster assignment in the E-step, and centroid estimation and metric learning in the M-step.

Constraints are used during cluster initialization and when assigning points to clusters. The distance metric is adapted by re-estimating $\mathbf{A}_h$ during each iteration based on the current cluster assignment and constraint violations. An interesting paper dealing with metric learning for text documents is [248]. More details about semi-supervised learning are present in [79] and [391].

Gist

In many cases labeled examples are scarce and costly to obtain, while tons of unlabeled cases are available, usually sleeping in business databases or in the web.

Semi-supervised learning schemes use *both* the available labeled examples *and* the unlabeled ones to improve the overall classification accuracy.

The distribution of all examples can be used to encourage ML classification schemes to create boundaries between classes passing through **low-density areas** (transductive SVM).

If the problem is modeled as a **graph** (entities and relationships labeled with distances) smoothing operations on graphs can be used to transfer the information of some labeled nodes to the neighboring nodes (graph Laplacian).

The distribution of examples can be used to **learn a metric**, a crucial component to proceed with supervised learning.

A space alien arriving on Earth could combine the zillions of information bits in web pages plus some labeled information obtained by a human pen pal (or by a Yahoo-like directory) for an intensive course to understand human civilization before conquering us. Terrestrial businesses use similar techniques to mine data and conquer more customers.

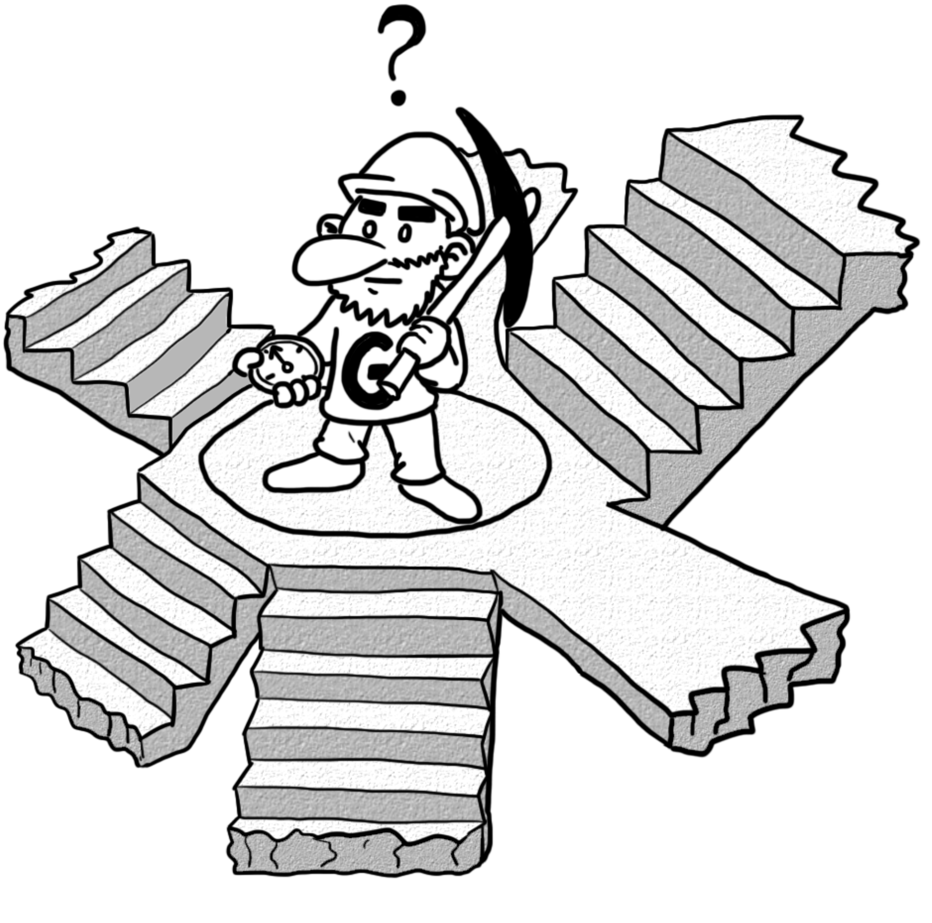
Part III

Optimization: basics

Chapter 24

Greedy and Local Search

Ognuno ha sulle proprie spalle la responsabilità delle proprie scelte. È un bel peso.
Everybody carries on his shoulders the responsibility of his choices. It is a heavy weight.
(Romano Battiti)



Many issues in everyday's life are related to solving optimization problems, to improve solutions, or to find solutions which are so good that no other solution is better (called "global optima").

For example, a salesman is given a list of cities and their mutual distances, and wants to find the *shortest possible tour* that visits each of them. This is called the **Traveling Salesman Problem** (TSP) and its relevance is obvious, to reduce travel costs and carbon dioxide emissions. TSP was first formulated in 1930 and it still is an extremely difficult problem, one of the most intensively studied in optimization. An **instance** of a problem is a specific case to be solved. In TSP a possible instance is to find a tour visiting Trento, Bologna, Napoli, Milano and Manarola. Even though finding optimal solutions for large TSP instances is computationally difficult, in most cases practically impossible, a large number of **heuristics** are known, so that even instances with tens of thousands of cities can be effectively solved in practice. Heuristics are algorithms without formal proof of convergence or guarantees of approximation but often effective in practice.

In abstract and general terms, in optimization one is given a function f defined on a set of possible input values $\mathcal{X}$. In TSP, f is the tour length, and $\mathcal{X}$ is the set of all possible tours visiting the cities, i.e., of their permutations. The function $f(\mathcal{X})$ to be optimized is called with more poetic names in some communities: *fitness* function, *goodness* function, *objective* function. If $\mathcal{X}$ is defined by a discrete set of possibilities (like binary values, permutations, integers) one speaks about **discrete optimization**. On the contrary, **continuous optimization** considers real-valued inputs.

One aims at finding the input configuration leading to the least possible value of the function f. Often a set of **constraints** on $\mathcal{X}$ have to be satisfied for a solution to be considered **admissible**. If one wants to pick quantities for possible foods in order to minimize the daily cost of a diet, useful constraints are to be placed on the minimum amount of calories and of vitamins. The solution corresponding to fasting costs zero but will lead to starvation, and is thefore not admissible.

This chapter presents the basic building blocks of **greedy and local search**, the more advanced Reactive Search Optimization (RSO) will be presented in Chapter 27. To avoid confusion, let's note that the term "local search" has nothing to do with the search for information or web pages, like in Google or similar services. To avoid confusions, remember to make it clear if you speak to normal people, who may think about local search of restaurants in the neighborhood of their current GPS position. In optimization one searches here for actions, decisions, effective innovations, aiming at improving solutions to problems, optimal solutions when possible, or at least approximations thereof.

Our optimization part starts with a chapter about greedy and local search for discrete optimization for many reasons. First, most real-world problems have to do with **choices among a discrete set of alternatives**. If one uses a computer even real numbers are actually approximated by a representation with a small number of bits. Understanding the main methods is much simpler with discrete local search than with methods based on real variables and derivatives.

Second, improving situations by a sequence of small greedy and local steps is deeply rooted in our human nature, as reflected in many quotes and proverbs across cultures: "little things make big things happen," "it does not matter how slowly you go so long as you do not stop" (Confucius), "the drop carves the stone" (Latin), "bean by bean the sack gets full" (Greek)... In passing, let's note that everybody's life can be seen as a running optimization algorithm: most of the changes are localized, dramatic changes do happen, but not so frequently. Imagine that you just found a partner, a possible companion for your life. Local changes are frequent in the initial part of a relationship. For example, you may convince your partner to dress in a better way, to avoid eating garlic, or to change opinions about various issues. You may have to stand worsening changes, like having your partner watching football games in the weekend, to eventually obtain improvements, in the form of a more relaxed partner. Or you may finally decide that small changes are not sufficient and that the way out is a drastic *diversification* or *restart* (finding a better partner).

Although the terminology can vary among different authors, there is a deep **connection between the greedy and local aspects**. In both cases the focus is limited to **profiting from a current tentative solution**, in a **short-sighted** manner.

In some cases one searches in the neighborhood of a complete admissible solution by small perturbations (a.k.a. **perturbative local search**), in other cases one gradually modifies and extends a partial solution (**constructive greedy search**).

The examples in this chapter are mostly for discrete optimization problems because of their simplicity, but we will encounter similar local search principles also for continuous optimization in Chapter 25.

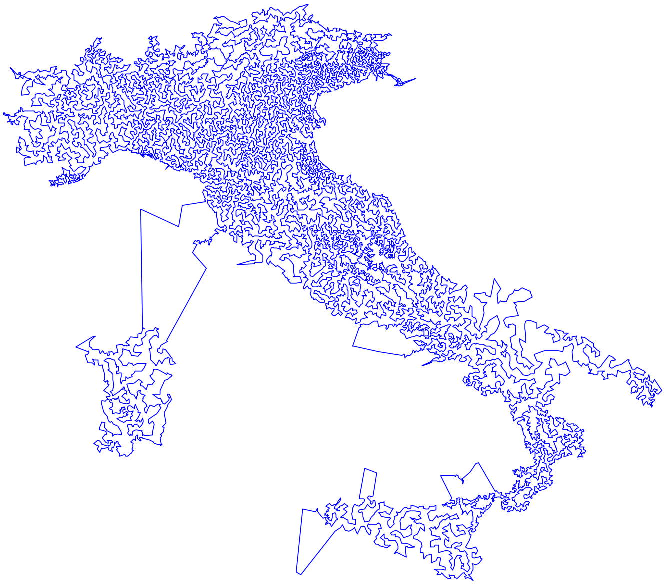


Figure 24.1: The Traveling Salesman Problem: the shortest tour of 16862 cities in Italy.

24.0.1 Case study: the Traveling Salesman Problem

The **Traveling Salesman Problem**, is paradigmatic and very relevant for both practical applications and theoretical reasons. The practical application can be read out from the name: imagine a salesman who has to visit a certain number of customers in different cities, and wants to minimize the fuel consumption, or the time dedicated to travel. Variations with more constraints and complexity consider multiple travelers, trucks with different capacities, time requirements for pickup and delivery of goods, etc. (vehicle routing, pickup and delivery with time windows [122]).

An illustration is in Fig. 24.1: a tourist wants to tour all Italian cities while minimizing time, or fuel consumption in case he travels with an SUV.

In an instance of TSP, one is given a set of n cities and the matrix of distances $d_{ij} > 0$ between couples of cities. A *tour* is a closed path visiting every city exactly once. The problem is to find a tour with minimum length. We can represent a tour with a cyclic permutation π of $\{1, ..., n\}$, where $\pi(i)$ is the city visited in the i-th place.

One can easily generalize the problem to any graph (V, E) not necessarily related to geography. The **decision version** (with "yes" or "no" answer) of the generalized TSP is: given a complete graph $(V, V \times V)$, a "cost" function $c : V \times V \to \mathbb{Z}$, and a maximum cost $k \in \mathbb{Z}$, is there a tour with total cost at most k? The requirement of complete connectivity means that an admissible tour can be found immediately, just generate a random permutation. If the graph is not complete, even determining if there is a tour, also called Hamiltonian path, is NP-complete (extremely unlikely to be solved in reasonable CPU times).

A fast algorithms for TSP is unlikely to exist, in fact TSP also belongs to the dreadful family of NP-complete problems. Of course, if one presents us with a solution we can easily check that the distance is k in polynomial time (actually this is the "meaning" of NP).

A brute-force **exhaustive search** algorithm is obvious: generate all possible tours and calculate the corresponding distances. Unfortunately, we need to examine $(n-1)! = (n-1) \times (n-2) \times (n-3) ... \times 1$ permutations (not $n!$

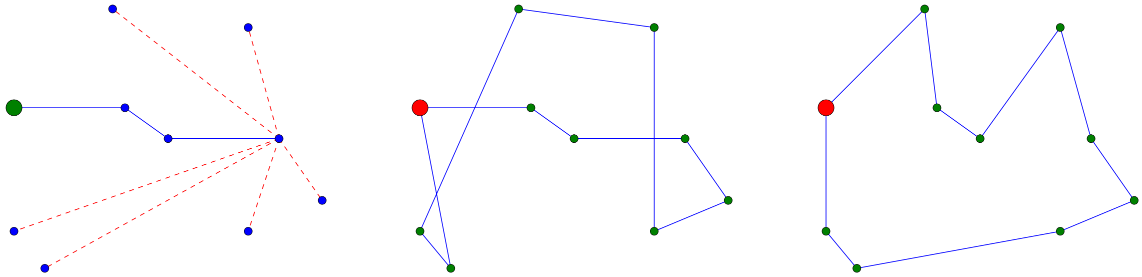


Figure 24.2: A 10 city TSP instance. Left: greedy construction after three steps from the initial city (larger dot); the algorithm will now choose the shortest among the dashed edges; center: the completed greedy solution; right: the optimal solution.

because we can change the starting point of the tour and still get the same tour). As you know, the factorial is growing *very* rapidly. If you do not know, calculate 3000! to get a couple of pages full of digits.

There is a lesson here: brute-force algorithms can solve small instances (10 cities are OK) and make a nice demo, but going to the real application will rapidly lead to unacceptable CPU times.

As a small digression, the TSP is an interesting problem for which **special versions** have pleasant properties. In particular, if the cost function satisfies the **triangle inequality** $c(u, v) \leq c(u, w) + c(w, v)$ (moving directly from u to v is always cheaper than passing through an intermediate point w), a **polynomial-time approximation algorithm** exists at less than twice the optimal cost. Without triangle inequality a ρ-approximated algorithm cannot be found unless $P = NP$. Real-world salesmen are lucky, because the Euclidean distance, as well as distances on the Earth surface, satisfies the triangle inequality. **Approximation algorithms with guaranteed approximation ratios** are a growing area of research.

24.1 Greedy constructions

In greedy algorithms "better an egg today than a hen tomorrow".

In some cases a solution can be built through a sequence of decisions, each step involving a small part of a solution. In the Traveling Salesman Problem a tour can be built by joining together partial tour segments. A **greedy algorithm** always makes the choice that looks best at the moment. For example, a greedy strategy for the TSP starts from a random initial city, and moves to the nearest city that hasn't been visited yet. This greedy choice is repeated until all cities have been visited (Fig. 24.2).

A greedy algorithm is therefore **shortsighted**: it can make commitments to certain choices too early, which prevent it from finding the best overall solution later. A choice cannot be undone during future steps. An example is shown in Fig. 24.2: ten cities are in such positions that a short-sighted salesman takes a much longer tour than the optimal one.

We will later explore other constructive strategies such as dynamic programming (see Sec. 34.2), where a solution is built by combining optimal solutions to subproblems. The simpler greedy algorithms, instead, skip the exhaustive examination of possibilities to select only the (locally) most appealing combination.

24.1.1 Greedy algorithms for minimum spanning trees

Greedy algorithms rarely find optimal solutions to problems, but there are happy exceptions.

A general way to prove the optimality of a greedy algorithm is as follows:

1. Formulate the problem in an *inductive* way: one makes a choice, and is left with a subproblem to solve.

2. Prove that there is always an optimal solution that *starts with the greedy choice*. In other words, prove that at least *a* globally optimal solution can be reached be completing the current partial solution given by greedy choice (at least one optimal solution is preserved).

3. Demonstrate that, after the greedy choice, one is left with a subproblem so that combining the optimal solution of the subproblem with the greedy choice, one arrives at an optimal solution of the original problem.

Examples of greedy algorithms are Kruskal's and Prim's algorithms for finding *minimum spanning trees* in graphs, and the algorithm for finding optimum Huffman trees for compressed codes. We also encountered greedy algorithms in this book when dealing with trees (Chapter 6).

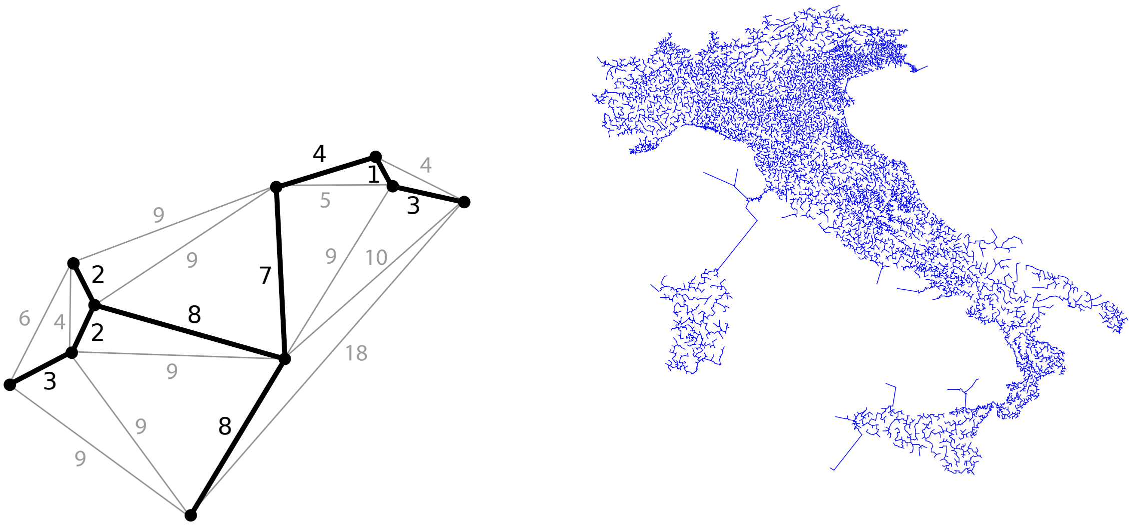


Figure 24.3: Minimum spanning trees. Left: a graph with varying edge costs; right: 16862 Italian cities.

Let's consider the **minimum spanning tree (MST) problem** [102]. The objective is to build a tree connecting all vertices of a connected, undirected graph, with the minimal total cost of the selected edges. Note that some edges can be missing, although there must be a way to pass from two arbitrary nodes by following selected edges (this is the meaning of connectedness).

For a concrete application, consider a company in telecommunications or electricity distribution in need to wire a new area. The company has to serve a number of existing or planned locations (houses, factories: the vertices of the graph) and to follow existing infrastructures (roads, tunnels, sewers: the edges of the graph), each associated to a different cost due to their length and to other features (need to open trenches in roads, put poles). Costs depend on many factors other than distance, so a direct connection between two nodes might be more expensive than a detour through multiple intermediate nodes, and the triangle inequality no longer applies. The minimum-cost connection of all nodes won't contain any cycles (otherwise we could spare one connection), therefore it is a tree. The practical "meaning" of a tree (useful to fix ideas and remember abstract concepts) is therefore: "connect all nodes without waste." Cycles are a waste of resources because they imply at least two ways to reach a node, going in the two directions of the cycle. Trees are born to be greedy.

The main difference between MST and TSP is precisely that one does not look for a tour, but for a tree. This "small" differences make MST a very friendly problem, which can be solved to optimality in polynomial CPU time.

For the abstract formulation of the **minimum spanning tree** problem, let $G = (V, E)$ be an undirected graph, V being the set of vertices, E the set of edges (connections between vertices). For each edge $(u, v) \in E$, the cost $c(u, v)$

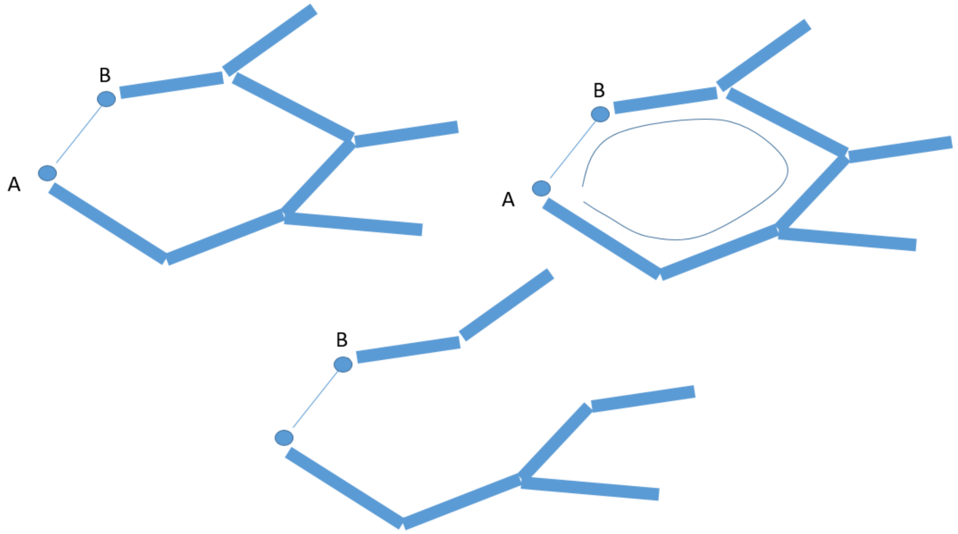


Figure 24.4: Adding the lightest edge is safe for MST. If an optimal solution does not contain it, we can do a substitution. Add the lightest edge to the optimal tree, and obtain a *cycle*, because A and B are already connected in an optimal tree. Then cut an edge of the cycle different from our lightest edge (with cost equal or larger!) and get a tree with the same or lower cost. Actually the cost cannot be lower because our tree was optimal but it can have the same cost (one can have more optimal solutions).

to connect u and v is given. One aims at finding a subset $T \subseteq E$ that connects all vertices without cycles and with the minimum possible total cost:

$$c(T) = \sum_{(u,v)\in T} c(u,v)$$

Let's concentrate on a core spanning-tree algorithm. The starting idea of the greedy construction is to grow the tree by adding one edge at a time to a set of edges A. Let's build some intuition. One is already thinking "greedily" and is therefore tempted to start from the least costly edge (the lightest edge). Is it safe to add it to the initial tree? Or can one miss an optimal solution? The fact that it is safe is demonstrated in Fig. 24.4 with the "substitution" argument.

In the analysis of algorithms one often considers **invariants** (logical assertions that are always true during the execution) and **progress properties** (changing in time).

A useful invariant here is:

Prior to each iteration, A is a subset of some minimum spanning tree.

If we manage to keep the invariant and increase the size of A (progress) we are done.

At a certain step, a **safe edge** for A is one which can be added to A while maintaining the invariant.

The generic algorithm is therefore as follows:

In the beginning, when A is the empty set, the invariant is true. We also demonstrated that the property holds if the first edge in A is one of the lightest edges. If the invariant holds at the beginning of a new iteration, and the tree is not complete, at least a safe edge must exist (picture in your mind the complete minimum spanning tree of which A is, by definition, a subset). Let's see how we can find it.

A **cut** $(S, V - S)$ of a graph is a partition of its vertices (imagine cutting some edges to separate two parts of the graph); an edge **crosses** a cut if its two endpoints belong to different partitions. A cut is said to respect an edge subset A if none of A's edges crosses it. An edge crossing the cut is **light** if its cost is minimum among all crossing edges.

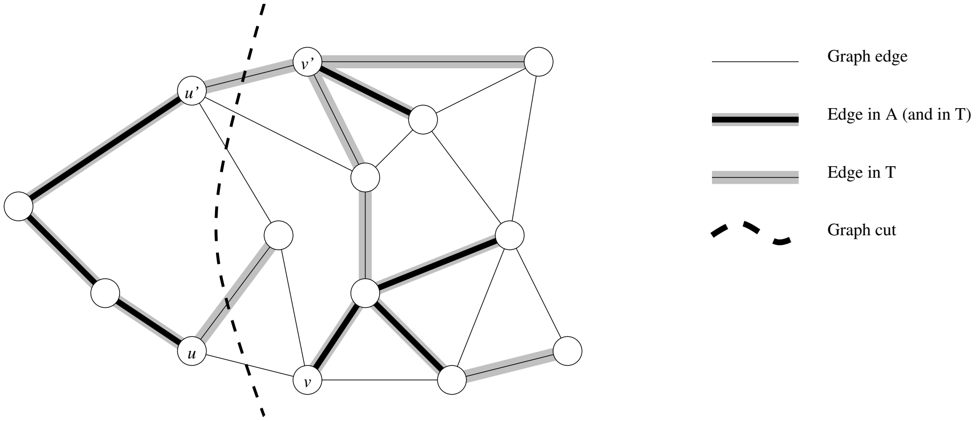


Figure 24.5: Minimum spanning tree construction. Dark thick edges are the partial MST A, gray edges are a complete MST T. The cut respects A. If (u, v) is light in the cut, then we can take any MST T and, if it doesn't contain (u, v), find an edge $(u', v') \in T$ with equal cost and replace it.

Now, let A be the current subset of E included in some minimum spanning tree, and let $(S, V - S)$ be any cut of G that respects A. A light edge (u, v) crossing the cut is safe for A. Suppose in fact that a minimum spanning tree T contains A, but not the light edge (u, v), as in Fig. 24.5. Then $T \cup \{(u, v)\}$ contains a cycle, and at least one other edge (u', v') in the cycle crosses the cut. Let $T' = T \cup \{(u, v)\} \setminus \{(u', v')\}$. Then T' is also a tree (we just cut the cycle in a different place), and since T is minimum and (u, v) is light, then (u', v') is light too (otherwise T' would have a total cost less than T). Therefore T' is a minimum spanning tree, A is a subset of T', and (u, v) is safe for A because it also belongs to T'.

This simple fact allows us to greedily find an edge to extend a partial MST to completion: just **cut the graph without crossing any edge of the current solution, and take one of the lowest-cost crossing edges**. The greedy property is apparent if you imagine that the algorithms has to pay money corresponding to the cost of the new edge to add at each iteration.

To summarize, we demonstrated that a greedy action maintains the invariant of producing a subset of an optimal spanning tree. Because the tree size is limited, the algorithm will converge producing an optimal solution.

Different MST greedy algorithms make different choices as to the cut to consider:

- Prim's algorithm maintains A as a connected tree whose vertices define the cut S. Every time, therefore, a least-cost edge is added going from the current tree to a new node, which will be added to the cut S for the next iteration.

- Kruskal's algorithm maintains A as a forest of partial trees (initially all disconnected nodes in V) and repeatedly adds a least-cost edge between two different trees.

Both algorithms can be made to run in $O(E \log V)$ time by using *binary heap* data structures [102]. With *Fibonacci heaps*, Prim's algorithms runs in time $O(E + V \log V)$ an improvement for dense graphs with $|E|$ much larger than $|V|$.

24.2 Local search based on perturbations

Aside from a small family of lucky problems, the greedy construction approach often leads to suboptimal solutions. Indeed, many problems have been shown to possess "pathological" instances for which a greedy algorithm produces a very bad solution, although in many cases better than a random solution.

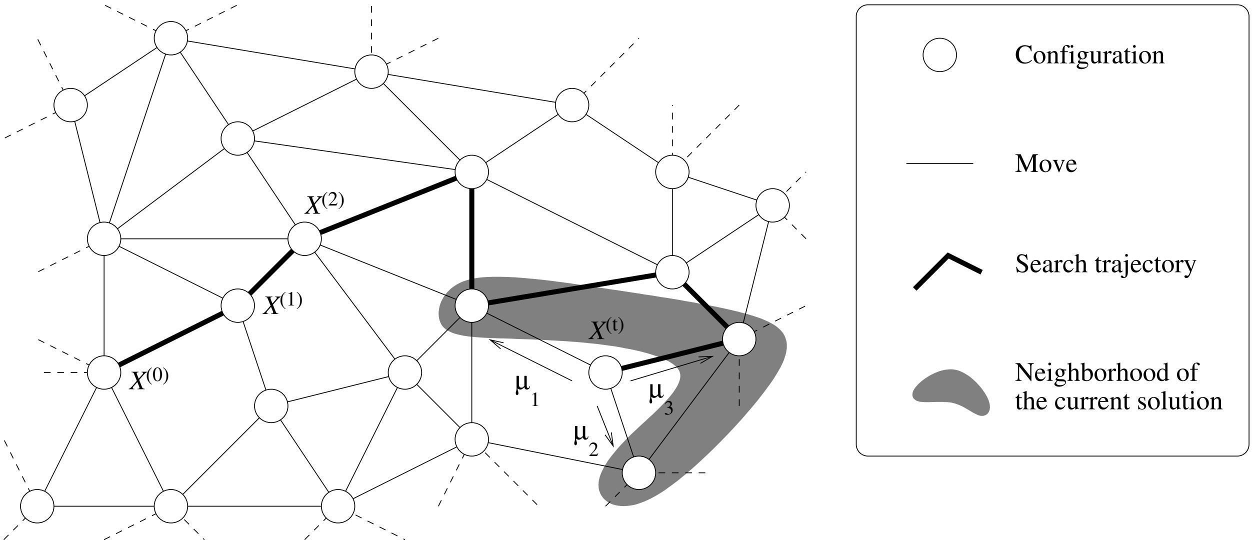


Figure 24.6: The local search heuristics in action.

This Section discusses what to do next. Suppose that you have an initial, suboptimal solution to a problem, be it obtained by a greedy algorithm or by any other means (e.g., randomly). A basic problem-solving strategy consists of starting from such initial tentative solution and trying to improve it through **repeated local (small) changes**. At each repetition, the current configuration is slightly modified (*perturbed*) and the function to be optimized is calculated. The change is kept if the new solution is better, otherwise another change is tried.

Let's define the notation. $\mathcal{X}$ is the search space, i.e., the set of all solutions, also known as "configurations," to a given problem instance; for example, in TSP $\mathcal{X}$ is the set of all possible city permutations. Given a configuration $X \in \mathcal{X}$, we can apply to it set of "perturbations" to transform it into other configurations; let us call such perturbations, or "moves", $\mu_0, \ldots, \mu_M$. Since we are considering an iterative process, let us call the initial configuration $X^{(0)}$, while the configuration at step ("time") t will be $X^{(t)}$. Every configuration after the first is generated by perturbing the previous one. The **neighborhood** $N(X^{(t)})$ of point $X^{(t)}$ is the set of configurations that can be obtained by perturbing the current one:

$$N(X^{(t)}) = \{\mu_i(X^{(t)}), i = 0, \ldots, M\}.$$

If the search space is given by binary strings with a given length L: $\mathcal{X} = \{0,1\}^L$, the moves can be those changing (or complementing or *flipping*) the individual bits, and therefore M is equal to the string length L.

We can abstractly represent the search space as a graph as in Fig. 24.6: configurations are nodes in the graph, while moves between configurations are represented by edges. The *search trajectory* $(X^{(0)}, X^{(1)}, X^{(2)}, \ldots, X^{(t)})$ is a path in this graph. The neighborhood $N(X^{(t)})$ is the set of first neighbors of $X^{(t)}$ within the graph. In the example, the current configuration can be perturbed in three different ways (μ_1, μ_2 and μ_3); two perturbations, μ_1 and μ_3, lead to previously visited configurations, while μ_3 generates a new one.

Local search starts from an admissible configuration $X^{(0)}$ and builds a **trajectory** $X^{(0)}, \ldots, X^{(t+1)}$. The successor of the current point is a point in the neighborhood with a lower value of the function f to be minimized:

$$Y \quad \leftarrow \quad \text{IMPROVING-NEIGHBOR}(\ N(X^{(t)})\ ) \tag{24.1}$$

$$X^{(t+1)} \quad = \quad \begin{cases} Y & \text{if } f(Y) < f(X^{(t)}) \\ X^{(t)} & \text{otherwise (search stops).} \end{cases} \tag{24.2}$$

IMPROVING-NEIGHBOR returns an improving element in the neighborhood. In a simple case this is the element with the lowest f value, but other possibilities exist, for example the *first improving* neighbor encountered.

If no neighbor has a better f value, i.e., if the configuration is a **local minimizer**, the search stops. Let's note that maximization of a function f is the same problem as minimization of $-f$. Like all symmetric situations, this fact can create some confusion of terminology. For example, *steepest descent* assumes a minimizing point of view, while *hill climbing* assumes the opposite point of view. In most of the book we will base the discussion on minimization, and *local minima* will be the points which cannot be improved by moving to one of their neighbors. Local optimum is a term which can be used both for maximization and minimization.

Local search is surprisingly effective because most combinatorial optimization problems have a very **rich internal structure** relating the configuration X and the f value. The analogy when the input domain is given by real numbers in $\mathbb{R}^n$ is that of a continuously differentiable function $f(x)$ optimized with gradient descent (a.k.a. steepest descent).

A **neighborhood** is suitable for local search if it reflects the problem structure. For example, if the solution is given by a permutation (in the Traveling Salesman Problem a permutation of the cities to be visited) an improper neighborhood choice would be to consider single-bit changes of a binary string describing the current solution, which would immediately cause *illegal configurations*, not corresponding to encodings of permutations. A better neighborhood can be given by all *transpositions* which exchange two elements and keep all others fixed. In general, a sanity check for a neighborhood controls if the f values in the neighborhood are correlated to the f value of the current point. If one starts at a good solution, solutions of similar quality can, on the average, be found more *in its neighborhood* than by sampling a completely unrelated random point. In addition, sampling a random point generally is much more expensive than sampling a neighbor, provided that the f value of the neighbors can be updated ("**incremental evaluation**") and it does not have to be recalculated from scratch, as we will see n the next Section.

24.3 Local search and big valleys

Local search stops at local minima but it can be the initial building block of more complex schemes, which will be presented in future chapters. For many optimization problems of interest, a closer approximation to the global optimum is required, and therefore more complex schemes are needed in order to continue the investigation into new parts of the search space, i.e., to *diversify* the search and encourage *exploration*. Here a second structural element comes to the rescue, related to the overall distribution of local minima and corresponding f values. In many relevant problems local minima tend to be *clustered*, furthermore good local minima tend to be closer to other good minima. **Promising local minima like to be in good company**. Let us define as **attraction basin** associated with a local optimum the set of points X which are mapped to the given local optimum by the local search trajectory. An hydraulic analogy, where the local search trajectory is now the trajectory of drops of water pulled by gravity, is that of *watersheds*, regions bounded peripherally by a divide and draining ultimately to a particular lake.

Now, if local search stops at a local minimum, **kicking** the system to a close attraction basin can be much more effective than restarting from a random configuration. If evaluations of f are incremental, completing a sequence of steps to move to a nearby basin can also be *much faster* than restarting with a complete evaluation followed by a possibly long trajectory descending to another local optimum.

This structural property is also called **Big Valley property** (Fig. 24.7). To help the intuition, one may think about a smooth f surface in a continuous environment, with basins of attraction which tend to have a nested, "fractal" structure. According to Mandelbrot, a fractal is generally "a rough or fragmented geometric shape that can be subdivided into parts, each of which is (at least approximately) a reduced-size copy of the whole," a property called self-similarity[1].

A second continuous analogy is that of a (periodic) function containing components at different wavelengths when analyzed with a Fourier transform. If you are not an expert in Fourier transforms, think about looking at a figure with defocusing lenses. At first the large scale details will be revealed, for example a figure of a distant person, then, by focusing, finer and finer details will be revealed: face arms and legs, then fingers, hair, etc. The same analogy holds for music diffused by loudspeakers of different quality, allowing higher and higher frequencies to be heard. At each scale the sound is not random noise and a pattern, a non-trivial structure is always present. This **multi-scale** structure, where smaller valleys are nested within larger ones, is the basic motivation for methods like Variable Neighborhood

[1] The term *fractal* derives from the Latin *fractus* meaning "broken" or "fractured."

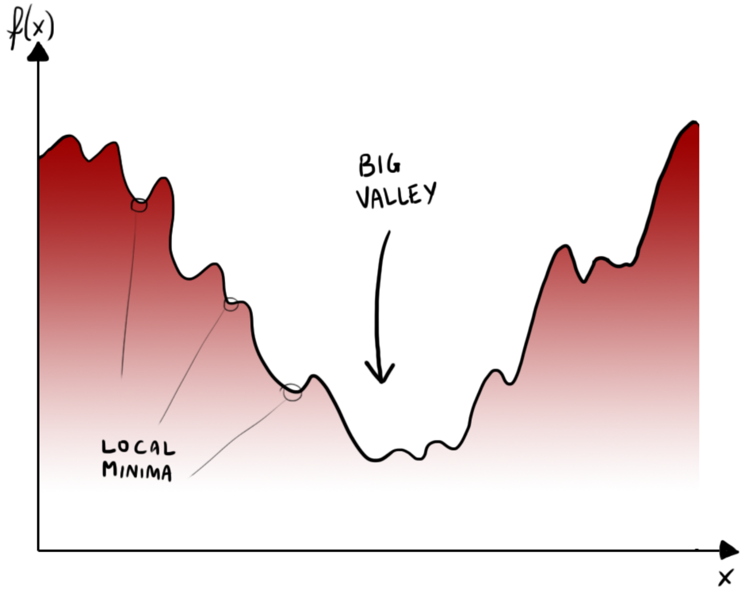


Figure 24.7: Structure in optimization problems: the “big valley” hypothesis.

Search (VNS) and Iterated Local Search (ILS), see for example [27] for a much more extended presentation and discussion of techniques, and [26] for a shorter presentation.

24.3.1 Local search and the TSP

Let’s see how Local search comes to the rescue to improve tours in TSP. A random permutation can give us a first tour, or a greedy algorithm can be used to identify a first one with more intelligence. Local modifications of the tour can be obtained by removing some edges of the tour and reconnecting in a different way to obtain a legal tour again. Fig. 24.8 shows a *2-change* local move: two different edges are eliminated and a different legal tour is obtained by reconnecting the nodes. The *2-change neighborhood* of a tour is given by all tours which can be obtained by applying all possible $2 - changes$.

The size of the neighborhood is polynomial, of order $O(n^2)$. In addition, **calculating the change in tour length** after a 2-change is very fast: subtract the cost of the two eliminated edges, add the cost of the two new edges (**incremental evaluation**). The advantage with respect to calculating a new path cost becomes enormous for a large number of cities (4 operations w.r.t. n operations). This means that local search can analyze in a given CPU time a number of possible configurations along a search trajectory which is much larger that the number of unrelated configurations which could be analyzed in the same time.

Of course, 2-changes can be easily generalized to k-changes (obtained by removing k different edges and reconnecting in a different manner). However, more complex neighborhoods imply larger numbers of neighbors to explore, and a tradeoff between improvement and step complexity must be sought, possibly by means of an adaptive technique such as Variable Neighborhood Search (VNS, see Sec. 28.1).

Note that the neighborhood choice does not only imply a slower or faster convergence towards a (local) optimum:

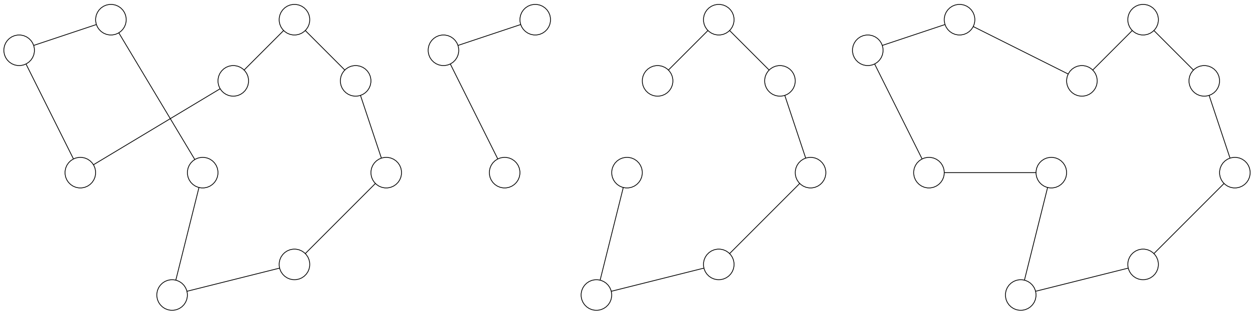


Figure 24.8: The Traveling Salesman Problem: a 2-change local move. Left to right: two edges are removed, leaving the tour partitioned, and the two segments are joined in the opposite way.

configurations that are locally optimal for a given neighborhood may be improved if more perturbations (e.g., a larger neighborhood) are allowed. Particularly bad choices of local moves mean that even simple instances of a problem can get stuck at an unsatisfactory local optimum, as shown in Fig. 24.9 where a TSP instance with 20 cities in a loop is initialized with a random configuration and solved by repeatedly selecting two cities and swapping them in the visiting order.

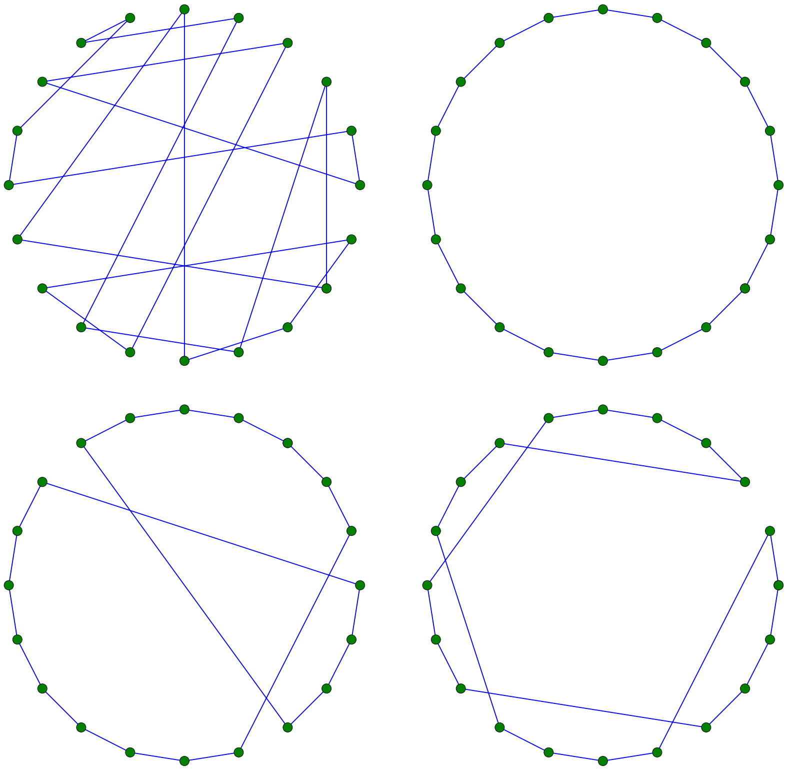


Figure 24.9: TSP configurations for a 20-city ring instance. Clockwise from top left: an initial random configuration, the optimal tour, two local minima. The local minima cannot be further improved by the chosen perturbation function, which consists in swapping the order of visit of two cities. A different local move (e.g., 2-swap) would improve the result.

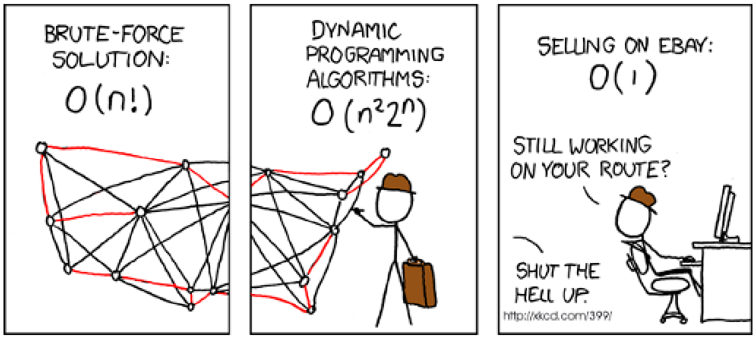


Figure 24.10: Do modern salesmen need TSP at all?

Gist

Greedy and local search are simple, human and effective ways to identify improving solutions for discrete optimization problems. They generate a sequence of changes, each change being *local*, i.e., affecting only a limited portion of the current solution. The **greedy principle** is related to short-sighted changes. The changes look appealing but maybe jeopardize reaching better solutions later on.

In a **greedy construction**, complete and admissible solutions are built is steps, by starting from incomplete ones and by fixing one element of the solution at a time. The single steps are not undone in the future steps.

In **perturbative local search**, one works with a complete solution and searches for a small (local) change leading to an improvement. The motivations for the relative success of local search is related to the rich structure of many problems a.k.a. **big valley** hypothesis. Local minima can often be reached by starting from nearby good tentative solutions. Local search tends to be fast because the **incremental evaluation** of neighbors of the current solution can be much faster that evaluating a new solution from scratch.

Greedy constructions and local search can be combined: one can build an initial complete solution with greedy construction and then improve it with local search.

Local search stops at **locally-optimal points**, when no improving neighbor exists. Additional **diversification** means are needed to escape from local attractors and avoid the search trajectory being *entrapped*, with little possibility of escaping from the attraction basin.

Local search is based on what is perhaps the oldest optimization method – trial and error. The idea is simple and natural and it is surprising to see how successful local search has been on a variety of difficult problems.

Chapter 25

Stochastic global optimization

While discrete variables have been considered in Chapter 24, in this chapter we search for **global optima of function of continuous (real) variables**. Having real variables means that "brute force" techniques like exhaustive enumeration of all possible solutions are impossible. In fact, the possible solutions are infinite! One may consider a range for each variable and *discretize* (for example $x \in [3, 22]$, with possible values $3.0, 3.1, 3.2, 3.3, ..., 21.9, 22.0$), but this dirty trick can lead to solutions of inferior quality. If the proper formulation is as a continuous problem, one should respect it. We will see in this Chapter that **throwing random points onto the input space** can be a robust brute-force method for the continuous optimization case.

Imagine to optimize (e.g., minimize) an objective function f through a so called **black-box interface**: the algorithm can query the value $f(\boldsymbol{x})$ for a sample point $\boldsymbol{x}$, but it cannot "look inside" f to see how it works: it cannot obtain gradient information, and it cannot make any assumptions on its analytic form (e.g., linear, quadratic, logarithmic, etc.). A black-box interface is optimal from the point of view of **separation of concerns**: to be as generally applicable as possible, optimization routines do not need to know anything about the application domain. With separation of concerns, an optimization expert can improve profits for a financial institution or improve survivability of patients cured for cancer without any knowledge of economics or medicine.

In these cases an optimization scheme has to make do with just function evaluations. Of course, it can still decide *where* to place sample points, and it can use the information obtained to build internal models of the function and tune its own meta-parameters. A large amount of *stochasticity* in the generation of sample points usually helps to improve robustness and avoid that some false initial assumptions lead the optimization to deliver low-quality local optima. *Simplicity and ease of implementation* of the schemes are valuable: in many cases sophisticated schemes improve performance on some specialized tasks but can produce inferior results on different problems.

The simplicity, separation of concerns and general-purpose character of **Stochastic Global Optimization (SGO)** leads to a rapidly growing number of applications in engineering, computational chemistry, finance and medicine. An up-to-date book presenting this topic is [390]: this chapter is a brief overview highlighting some important points and theoretical findings.

SGO is a suite of methods ranging from the simple *global random search* to methods based on *probabilistic assumptions* about the objective function. They are not a panacea and the "**curse of dimensionality**" is unavoidable when the number of variables increases, and it leads to an exponential increase in the computational complexity. This is caused by the fact that neighbours are becoming exponentially isolated from each other as the dimension increases (in a ball of radius r in a large-dimensional space, most points fall in a narrow crust near the surface of the ball).

Many algorithms have been proposed heuristically, in some cases based on sexy analogies with natural processes, like **evolutionary algorithms** and **simulated annealing**. Heuristic global optimization algorithms are very popular in applications, often without a sound theoretical basis. After some basic notions and definitions are given is Sec. 25.1, we start from Pure Random Search (PRS) in Sec. 25.3, develop our intuition with some statistics in Sec. 25.4, discuss probabilistic and statistical models in Secs. 25.5 and 25.6.

25.1 Stochastic Global Optimization Basics

Let $f(\boldsymbol{x})$ be the (real-valued) function to optimize on the feasible region A, usually some region of a multi-dimensional real space $A \subseteq \mathbb{R}^n$.

Global optimization problem:

$$\begin{array}{rl} \text{Given} & f : A \rightarrow \mathbb{R} \\ \text{find} & \boldsymbol{x}^* \in A \\ \text{such that} & f(\boldsymbol{x}^*) \leq f(\boldsymbol{x}) \text{ for every } \boldsymbol{x} \in A. \end{array}$$

A point $\boldsymbol{x}^*$ satisfying the above condition is called a **global optimum**, by definition it is the best possible solution to the problem.

Imagine that the optimization scheme generates a sequence of input values $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots$, let the **record value** (the best-so-far value) at iteration n be $\hat{y}_n = \min_{i=1,\ldots,n} f(\boldsymbol{x}_i)$, and let $\hat{\boldsymbol{x}}_n$ be the sequence of record points (inputs) corresponding to the record values. The sequence $\hat{y}_1, \hat{y}_2, \ldots$ never increases, and only decreases (i.e., improves) at iterations in which a new record value is found.

The objective of global optimization is to have the sequence of record points $\hat{\boldsymbol{x}}_n$ approach the minimum $\boldsymbol{x}^*$ as n increases.

As one can expect, the development of efficient global optimization methods is more difficult than that of the local optimization methods, the diversity of multi-modal functions is simply too large. Do not expect universal strategies for global optimization and be prepared to live with a wide variety of alternative approaches. In addition, be prepared to **combine robust global schemes with fast local search schemes**.

Multistart local search is one of these possibilities, consisting of firing more runs of local search starting from a set of interesting points. In particular,it can be worth making several iterations of a local descent immediately after obtaining a new record point. In addition, every global optimization procedure should finish with a local descent from one or several of the best points $\hat{\boldsymbol{x}}_i$.

The "global" schemes should narrow down the area of search for the minimizer $\boldsymbol{x}^*$ (hopefully the area should be in the **region of attraction** of $\boldsymbol{x}^*$), leaving the problem of finding the exact location of $\boldsymbol{x}^*$ to a local optimization technique.

As we have already seen in the local search scenario in Chapter. 24, the region of attraction can be different for different methods. In particular, some techniques are able to jump over high-frequency components of the objective function and to reach the global optimum even if started far, provided that the low-frequency structure gives consistent information about locating the minimum value.

This situation is illustrated in Fig. 25.1. The objective function (solid line) has a large number of local minima; however, a local search procedure might as well be oblivious to its roughness and, due to fairly large steps (the grey arrows), only be sensitive to the overall trend. In this case, the procedure correctly identifies the region in which the true global minimum lies (left-hand side of Fig. 25.1). The dashed line is a "model" of the function, built by considering the sample points, that captures its large-scale behavior without bothering about fine-grained details. On the other hand, as shown in the right-hand side, a particularly needle-like minimum might escape this procedure and lie outside the most promising region identified by the model.

Most if not all wide-purpose stochastic global optimization schemes are "once scorned, now respectable" heuristic methods [386] without formal proofs of efficiency. Most theoretical results are related only to asymptotic convergence. In the absence of strong assumptions about an optimization problem, the only converging algorithms are those generating **everywhere dense sequences of observation points**. If A is compact and f continuous in the neighborhood of a local minimizer, an algorithm converges ($y_{on} \to m$ as $n \to \infty$) if and only if the algorithm generates a sequence of points x_i which is everywhere dense in A. Much stronger assumptions like "limited variation" or Lipschitz continuity (see below) are needed to ensure convergence also for sparser sequences of sample points.

Randomness can appear in many ways in global optimization: because of random errors in the evaluation of f (a frequent case in the real world), because of the randomized generation of sample points, or because of probabilistic assumptions about the objective function. We do not insist on deterministic methods in this chapter, they are used rarely only with specific constraints on the function f, in particular limited-variability.

Deterministic global optimization schemes aim at reducing the **worst-case** difference w.r.t. the optimal value. Proofs are complex and conditions of validity very fragile. If optimization has to be repeated for many different functions with similar characteristics, one can take a more realistic direction by assuming **statistical models of the functions** to be optimized and aiming at some **average optimality** criteria (for example demanding that the *average* error converges rapidly to zero).

Global random search algorithms are very popular because they tend to be simple, insensitive to the structure of the objective function and of the feasibility region, easily modifiable to **guarantee theoretical convergence**. In spite of these positive facts, convergence if often more loved by theoreticians than by practitioners because it can be painfully slow, and practical efficiency can depend a lot on tuning algorithm parameters to the instances to be solved, so that automated self-tuning methods can be of value, as well as a sound **experimental approach** in the design and test of competitive algorithms.

25.2 A digression on Lipschitz continuity

Elegant deterministic global optimization schemes can be obtained with strong assumptions about the function to be optimized. One of the "natural" assumptions for many phenomena in the physical world is "**limited-variability**," a.k.a. **Lipschitz continuity**. A function is Lipschitz continuous if its change in value is bounded by the corresponding change in the evaluation point (multiplied by a constant factor); i.e., there is a constant $K \geq 0$ such that, for all $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ in the function's domain,

$$|f(\boldsymbol{x}_1) - f(\boldsymbol{x}_2)| \leq K\|\boldsymbol{x}_1 - \boldsymbol{x}_2\|.$$

For each point evaluated x, a **cone** $f(\boldsymbol{x}) - K\|\boldsymbol{x} - \boldsymbol{x}'\|$ defines an area on the plot in which the function cannot enter (because it cannot change too fast), and therefore an underestimate.

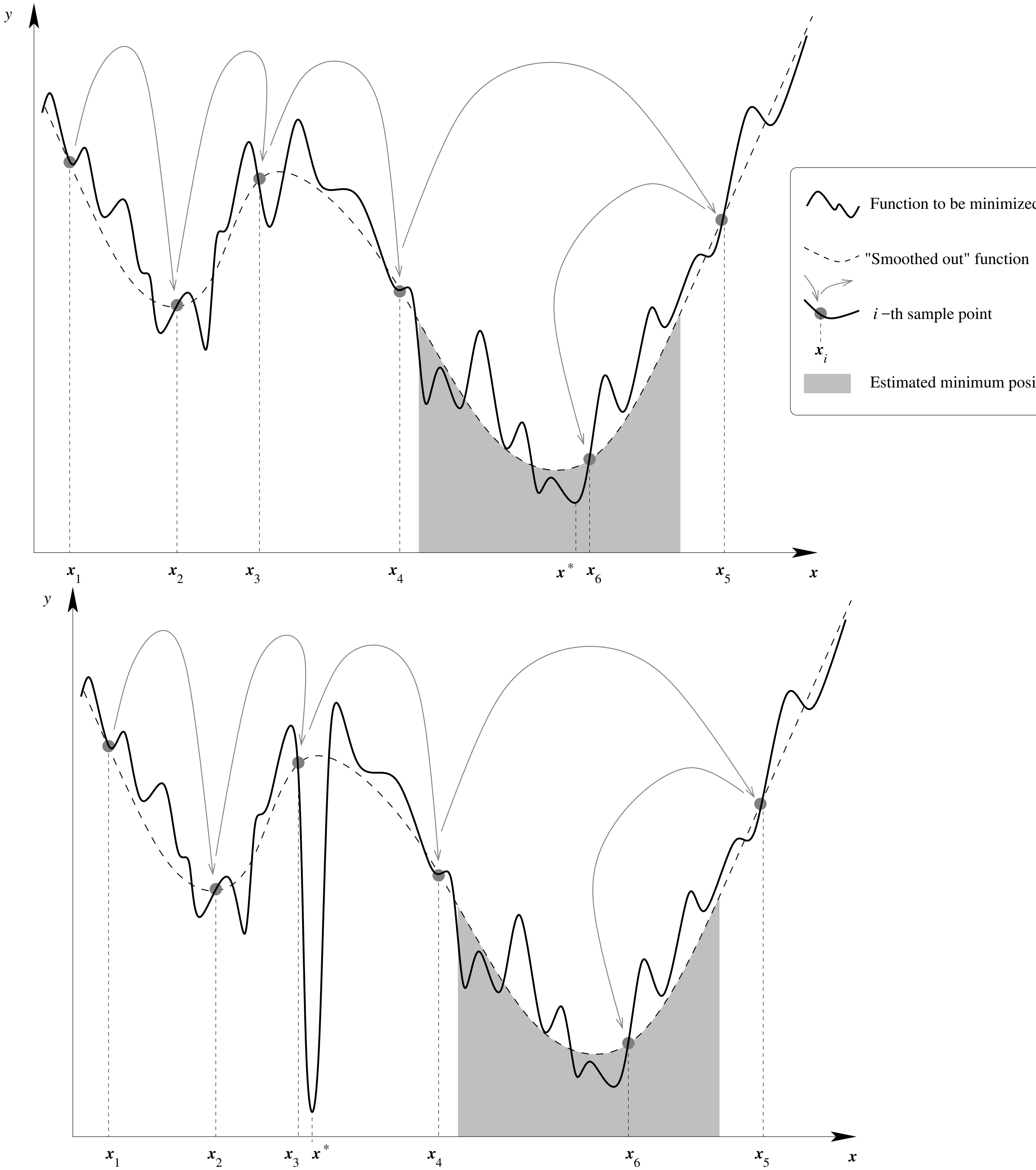


Figure 25.1: Top: function f (solid line) and a low-frequency, smoothed-out version (dashed line) leading to the region in which the global minimum lies. Bottom: a lesser well-behaved function where the global minimum lies at an unexpected position.

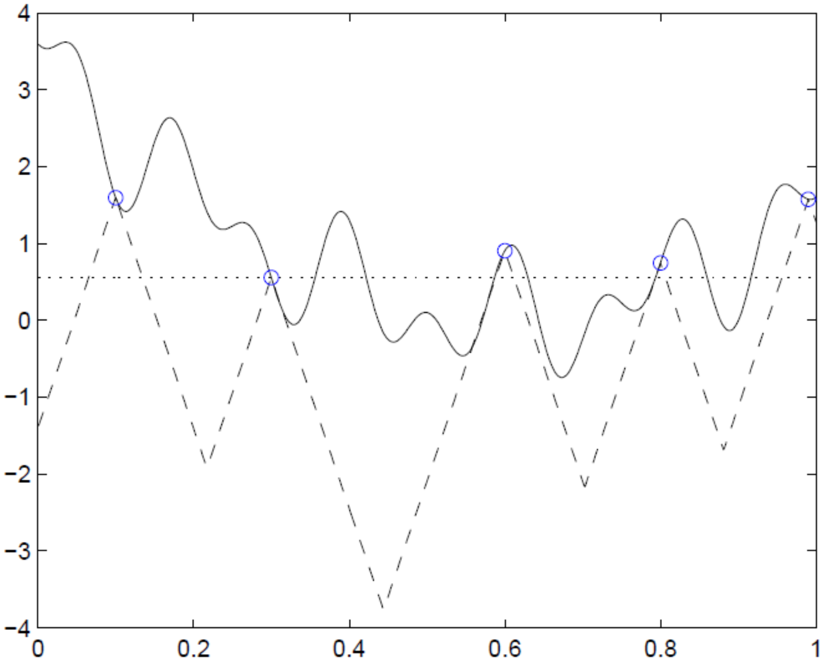


Figure 25.2: Pijavski-Shubert optimization scheme. The values of the objective function at t^k marked with dots determine the saw-tooth underestimate H^K (image derived from [390]).

Fig. 25.2 shows a function, same sampled points, and the current underestimate. It makes sense to place the next observation (sample) at the point of *minimum of the underestimate*, as in a well-known algorithm by Pijavski-Shubert.

Branch and Bound can be applied in a way similar to that for discrete problems: the admissible region A can be partitioned in subareas. If the underestimate over an area is too bad (so that the current record cannot be beaten), the area is cut and not considered for sampling. Advanced partitioning (and sampling) methods are presented in [327, 328]. As you can imagine, the situation for which a non-trivial Lipschitz constant K is known (and therefore underestimates are very tight) are very rare, but one can aim at estimating it in an online and local manner while the global optimization scheme is working [352], in a way similar to the RSO methods for discrete optimization considered in Chapter 27.

The idea of 'branching and bounding' can be extended to incorporate stochastic techniques. Branching of the feasible region A into a tree of subsets $A_i(i = 1, ..., l)$ is done in a similar manner. In global random search algorithms, the test points $x_j \in A_i$ are random; therefore, statistical methods can be used for estimating the attainable minimum on a specific region: $m_i = \inf_{x \in A_i} f(x)$ and for testing hypotheses about the values m_i, see Section 25.4.

25.3 Pure random search (PRS)

PRS is based on the **repeated generation of random points to be evaluated**, typically with the same probability distribution on the admissible region A, like a *uniform distribution*. It sounds too easy to work, but PRS is a solid building block not to be scorned, against which more sophisticated algorithms should be benchmarked. It is often found as a component of other more complex global optimization schemes, and its asymptotic properties, such as convergence rates, are easy to study.

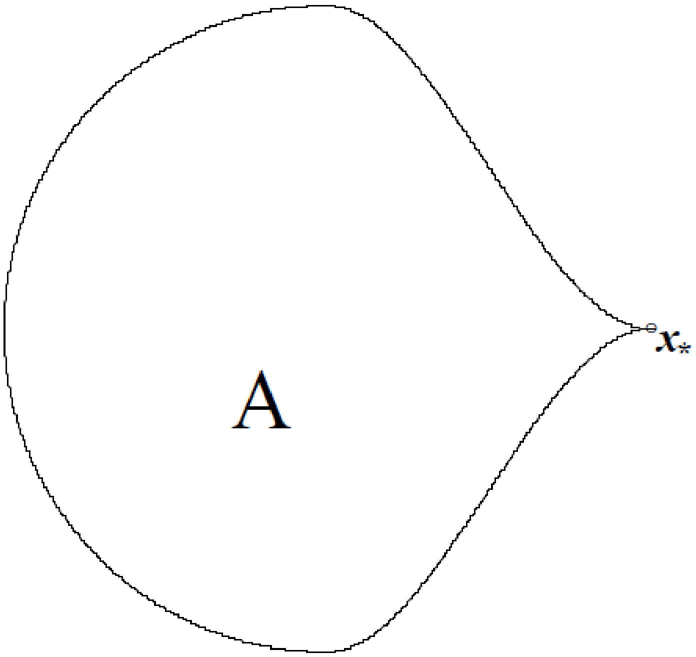


Figure 25.3: A pathological situation for PRS: the minimizer x^* is at a cusp of A so that the portion of a small ball centered around it which is feasible goes rapidly to zero.

In the following, we assume that the feasible region A and function f satisfy assumptions to avoid pathological cases, assumptions like smooth boundaries of A, small balls centered on minimizers having an approximately constant proportion of points in A, see Fig. 25.3 and [390] for the complete list.

Let's consider a general global random search in which point $\boldsymbol{x}_j$ in the sequence is generated from a probability distribution $P_j(\boldsymbol{x})$, which (for generality's sake) is allowed to be different at each iteration and to depend on the previous function evaluations. Because reaching the *exact* minimizer has probability zero (we are in a continuous setting), it is better to allow for some slack. Let's consider balls of a certain radius around points: $B(\boldsymbol{x}, \epsilon) = \{\boldsymbol{x}' \in A : \|\boldsymbol{x}' - \boldsymbol{x}\| \leq \epsilon\}$.

A classical form of the **convergence theorem** (derived from the "zero-one law" in classical probability theory, and rediscovered many times by different researchers) is the following one.

Let f have a finite number of minimizers, let $\boldsymbol{x}^*$ be such a minimizer, m be the minimum value, and f be continuous in the vicinity of $\boldsymbol{x}^*$. Also assume that

$$\sum_{j=1}^{\infty} \inf p_j\big(B(\boldsymbol{x}^*, \epsilon)\big) = \infty$$

for any $\epsilon > 0$, and the infimum is taken over all possible previous histories (sequence of evaluated points and function values). Then, for any $\delta > 0$ the sequence of points $\boldsymbol{x}_j$ with distribution P_j falls infinitely often into the set $W_\delta = \{\boldsymbol{x} \in A : f(\boldsymbol{x}) - m \leq \delta\}$, therefore δ-close to the optimal value.

Imagine placing arbitrarily small balls around each point (including the global optima). If, for all possible histories of stochastic sample generation, the probability distributions $p_j(\boldsymbol{x})$ guarantee that each ball is hit with probability which sum up to infinity, ***an arbitrary δ-close approximation of the optimum will be found infinitely often, with probability one***. In particular, a uniform probability distribution $P_j = P_{\text{uniform}}$ is an immediate way to satisfy the above requirements.

Before you jump on your chair to celebrate, let's remember that, more than this kind of convergence, you are probably more interested in the **rate of convergence**, i.e., in how many iterations you will have to wait in practice before arriving sufficiently close to the minimum, which is the topic of the following discussion.

Because a uniform probability distribution "does not learn" from the previous history of the search, to speedup the convergence in practice, a popular choice combines a "smart" probability density $Q_j(\boldsymbol{x})$, which takes into account what can be learnt from the previously evaluated points, plus a fraction of uniform probability density $P(\boldsymbol{x})$, as:

$$P_j(\boldsymbol{x}) = \alpha_j P(\boldsymbol{x}) + (1 - \alpha_j) Q_j(\boldsymbol{x})$$

so that the above convergence theorem still holds. In general, the distribution $Q_j(\boldsymbol{x})$ should egnerate more points in the most interesting areas. The different methods differe by the way in which they measure the interest level. For example, sampling from Q_j can consist of running a local search descent from the current record value, which is for sure an interesting point.

To take home: **convergence is not difficult to prove**, just mix some uniform probability with your favourite smart ("learning") sampling strategy. Note: this may satisfy your colleagues in maths, but not necessarily your colleagues in applied areas looking for *fast* optimization methods, producing high-quality solutions in a finite CPU time, not for infinite time!

25.3.1 Rate of Convergence of Pure Random Search

"Abandon all hope, you who enter here" was written at the entrance of Dante's Inferno.

In a similar manner, to start your global optimization effort without being fooled by marketing hype, a useful exercise is to derive the **rate of convergence** of PRS. It is a simple application of basic rules about deriving probabilities of repeated unlucky events.

Imagine that the different samples $\boldsymbol{x}_j$ are **independent and identically distributed (i.i.d)** with distribution $p(\boldsymbol{x})$, and let our objective be to hit the "target" set $B(\boldsymbol{x}^*, \epsilon) = \{\boldsymbol{x} \in A : \|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \epsilon\}$ with one or more of the points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$. A "success" event means that some $\boldsymbol{x}_j$ hits B, "failure" is the alternative event.

A single sampling event has success probability $p(B)$, which we assume to be strictly positive for all values of ϵ. It looks like throwing a dice with many faces, and calculating the probability that we get a particular face in a sequence of trials. PRS generates a sequence of **independent Bernoulli trials**. We fail in the sequence only if we fail in all trials.

In our case:

$$\Pr\{\boldsymbol{x}_j \notin B\} = 1 - p(B), \quad \text{for all } j.$$

Because of the independent generation of sample points, probabilities are multiplied:

$$\Pr\{\boldsymbol{x}_1 \notin B, \ldots, \boldsymbol{x}_n \notin B\} = \big(1 - p(B)\big)^n.$$

Because $p(B)$ is positive, this probability tends to zero when $n \to \infty$, and the probability that at least one $\boldsymbol{x}_j$ lies in B tends to one.

The average number of PRS iterations required for a first hit of our ball (and therefore solving the problem) is:

$$E(\text{first hitting time}) = \frac{1}{p(B)}.$$

If the distribution is uniform we can continue our exercise to reflect on concrete rates of convergence. In this case, for a d-dimensional problem:

$$p(B) = \frac{\text{vol}(B)}{\text{vol}(A)} = \frac{\pi^{d/2}\epsilon^d}{\Gamma(d/2+1)\text{vol}(A)}$$

in which $\Gamma(\cdot)$ is the Gamma function (an extension of the factorial function) and we used the formula for the volume of a d-dimensional Euclidean ball of radius ϵ.

In the interest of brevity one can consider approximations. If one wants to hit the ϵ-ball B with probability at least $1 - \gamma$, one needs to perform at least the following number of PRS iterations:

$$N^* \approx -\ln\gamma \cdot \frac{\Gamma(d/2+1)}{\pi^{d/2}\epsilon^d} \cdot \text{vol}(A).$$

The dependence on γ is not crucial: what is more alarming is the exponential increase w.r.t. the dimension d. This should not be a surprise. We are searching for a ball with radius equal to ϵ in a simple d-dimensional box of volume 1. If we shoot one random point we hit the target with probability proportional to ϵ in one dimension, ϵ^d in d dimensions, vanishing exponentially to zero when the dimension increases. Fig. 25.4 shows the simpler cases of $d = 1, 2, 3$ and a radius $\epsilon = 0.05$; them measure $p(B)$ goes from $2 \cdot 0.05 = 0.1$ in the 1-dimensional case to $4 \cdot \pi \cdot 0.05^3/3 \approx 0.0005$ in three dimensions.

If you are into combinatorics rather than geometry, you can also see the optimal point $\boldsymbol{x}^*$ as an array of d entries (its coordinates). For a randomly generated array $\boldsymbol{x}_j$ to be close to $\boldsymbol{x}^*$, each of its entries x_{jk} must be close to the corresponding entry x^*_k of the optimal point. Imagine how unlikely it is to generate $d = 100$ independent numbers, and finding that each of them is not farther than ϵ from a target value! Clearly, hitting an ϵ-ball is even harder than that; asymptotically, however, hitting a ball is not so different from hitting a cube: when d is fixed and $\epsilon \to 0$, the number of iterations for success increases approximately as:

$$N^* = O\left(\frac{1}{\epsilon^d}\right).$$

“Abandon all hope, you who enter here”. If the number of dimensions is large, there is no magic algorithm to rapidly approximate the global optimum for a generic function in less than exponential number of iterations. If there is hope, it is related to **functions with special forms, so that regularities can be learnt** from an initial sampling, albeit in approximated form, and used to identify shortcuts leading rapidly to close approximations of the optimal solution.

The question is: what is the chance that we will encounter this kind of highly-structured objective functions in real applications? Luckily for us, the chance is not negligible. Think about three-dimensional protein folding. Identifying

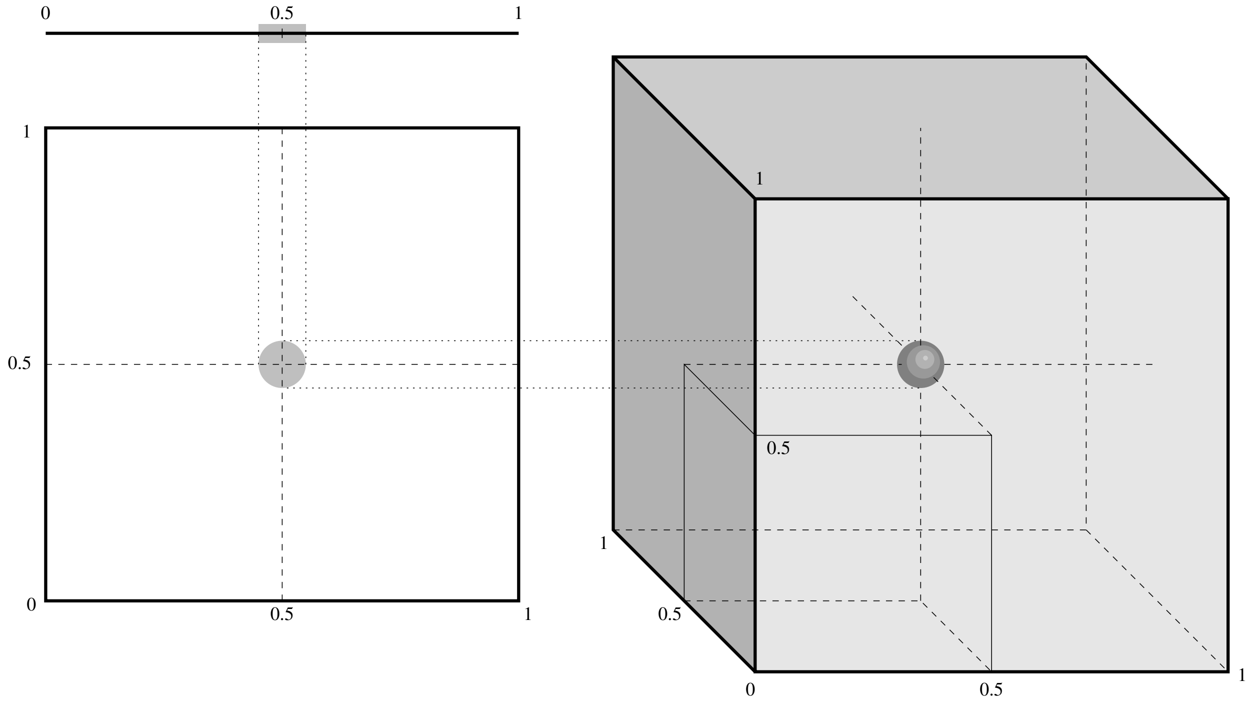


Figure 25.4: The curse of dimensionality: balls of the same radius in spaces of increasing dimensionality become harder and harder to hit due to their growingly negligible size w.r.t. the total volume.

the optimal structure (minimizing the potential energy) seems daunting but mother Nature does it rapidly with very noisy and humid hardware in our cells.

The bottom line is that convergence of some global optimization algorithms may please a theoretician but may not mean much in practice.

25.4 Statistical inference in global random search

If you are an expert in statistics, **order statistics** can be used to derive probabilities of extreme events of interest. In order statistics one starts from a probability distribution and derives distributions for the minimum (or maximum or k-th) **record value** in a sample of a certain size. In addition to optimization, results in this area, also under the name of **extreme value theory**, are applied to **estimating the risk of extreme, rare events**, like earthquakes, floods, beating records in athletic disciplines. We summarize some concepts pointing to useful references if you are interested in further investigations.

The objective is to answer questions of this kind: what is the probability to get a new record value in the next n iterations? What is the average waiting time? What is the probability that we already found a locally optimal point (or an approximation thereof)? Interesting asymptotic distributions arise when the number of iterations becomes very large. Some results are, at the beginning, counter-intuitive. For example, on average one has to make infinitely many iterations of PRS to get an improvement over the current best value. Of course, this result refers to an unbounded search domain and no prior knowledge about the function structure, so be patient! Some potentially useful results are related to statistical inference about the optimal value, which can be used for a statistically sound termination criterion. For example, **maximum likelihood estimations** of m can be derived, as well as **confidence intervals**. All techniques in statistics must be used with extreme competence and care. In certain cases one demands a large number of sample points in the vicinity of the global optimizer in order to derive estimates, bounds, etc. But reaching the region of attraction of the global minimizer can be extremely difficult so that statistical inference will be made about some other local minimum!

A couple of interesting applications of statistical inference in global optimization are **branch and probability bound** and **random multistart**.

Branch and probability bound generalizes branch and bound to continuous variables when no error-proof bound is available. It consists of several iterations with the following steps:

1. split (branch) the set of admissible values into subsets, obtaining a tree organization;
2. decide about the potential value of the individual subsets for further investigation;
3. select the most interesting subsets for additional splits.

Hyper-rectangles are a frequent and easy choice for subdividing the input space. Statistical techniques to judge about the potential value of a subset Z are based on the (statistical) rejection of the hypothesis that the global minimum m cannot be reached in Z. Statistics can be obtained by sampling Z, or by running short local search streams starting in Z. In practice, *branch and probability bound* methods can be used for low-dimensional problems (up to about 10 dimensions). For much larger dimensions, the number of tree nodes explodes and the efficiency of the statistical procedures degrades.

Random multistart is another simple method consisting of repeating local search from random initial points, and running each search until a local minimum is met, or a close approximation thereof. An interesting question to answer is: given that multistart already found a certain set of locally-optimal points, some of them multiple times, what is the probability that all local optima have been found (including therefore the global optimum)? Let our continuous function f have a finite but unknown number L of local optimizers $\boldsymbol{x}^{*(1)}, \ldots, \boldsymbol{x}^{*(L)}$, and let $\theta_i = p(A_i^*)$ be the probability of "hitting" the attraction basin A_i^* of the local minimizer $\boldsymbol{x}^{*(i)}$. The size and form of the attraction basins depends on the specific local search scheme (which may for example filter out very small sub-basins).

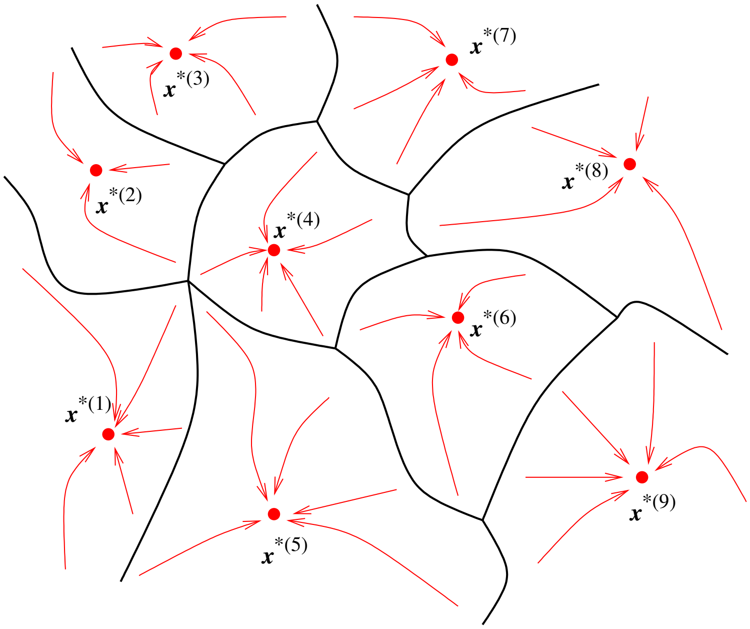


Figure 25.5: Attraction basins around locally optimal points.

By definition, $\theta_i > 0$ and $\sum_i \theta_i = 1$ (every local search will eventually end up on a local minimizer). Let n_i be the number of generated initial points belonging to the i-th basin, out of a sample of n points. The random vector $(n_1, \ldots, n_L)$ follows the **multinomial distribution**:

$$\text{Pr}(n_1, ..., n_L) = \frac{n!}{n_1!...n_L!}\theta_1^{n_1}...\theta_L^{n_L}.$$

Statistical inference can be used to estimate the number of trials n^* with a probabilistic guarantee that all local minimizers have been found.

If the number of local minimizers L is known, at least as an upper bound L, we can obtain the following approximation for the number of starts of local search which guarantee to find all local minima with probability at least γ:

$$n^* \approx L \ln L + L \ln(-\ln \gamma)$$

If the number of local minimizers is not known, a Bayesian approach with an *a priori* distribution for the number of local minima can be used (but the practical issue becomes that of identifying a proper *a priori* probability, a kind of magic art in the absence of information about the possible function to be minimized).

25.5 Markov processes and Simulated Annealing

This section presents ideas which can be seen as stochastic modifications of Local Search, and which apply for both continuous and discrete optimization problems.

Local search stops at a locally optimal point. Now, for problems with a rich internal structure encountered in many applications (remember the “big valley” hypothesis), *searching in the vicinity of good local minima* may lead to the discovery of even better solutions. In this section the neighborhood structure is *fixed*, but the move generation and acceptance are stochastic and one also permits a “controlled worsening” of solution values to escape from the local attractor.

Now, if one is sitting on a local minimum and extends local search by *accepting worsening moves* (moves leading to worse f values) the trajectory moves to a neighbor of a local minimum. But the danger is that, after raising the solution value at the new point, the local minimum will be chosen again at the next iteration, leading to an endless cycle of “trying to escape and falling back immediately to the starting point.” This situation surely happens in the deterministic case if the local minimum is *strict* (all neighbors have worse f values) and if more than one intermediate step is needed before points with f values better than that of the local minimum become accessible. Better points can become accessible when they can be reached from the current solution point by a local search trajectory. The situation becomes more chaotic in stochastic versions, but still one may be stuck jumping around in an attraction basin around a local optimizers for very long times.

The **Simulated Annealing (SA)** method has been investigated to avoid deterministic cycles and to allow for worsening moves, while still biasing the exploration so that low f values are visited more frequently than large values. The terms and the initial application comes from annealing in metallurgy, a process involving heating and controlled cooling of a metal to increase the size of its crystals and reduce their defects. The heat causes the atoms to be shaken from their initial positions, a local minimum of the internal energy, and wander randomly through states of higher energy; the slow cooling gives them more chances of finding states with lower internal energy than the initial one, corresponding to a stronger metal.

We summarize the technique and hint at mathematical results.

25.6 Simulated Annealing and Asymptotics

In the general model of Pure Random Search the probability distribution $p_j(\boldsymbol{x})$ for generating the j-th sample can depend on the previously extracted points (and on the corresponding objective function values). A radical simplification, but possible improvement w.r.t. using a uniform distribution P, is to have P_j just depend on the latest generated point and f value. The sequence of sample points becomes a **Markov chain**. Markov is synonymous with **memory-less**: the entire previous history of the search process (points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{j-2}$ and corresponding f values) is forgotten to keep only the latest point. As you can imagine, Markovian algorithms are often practically inefficient because of their poor use of information and learning-while-searching possibilities. Nonetheless, they have enjoyed a huge popularity, partly caused by intriguing analogies with physical processes, partly because many mathematicians could demonstrate asymptotic theorems, rather useless to get practical guidelines, but helpful to obtain an aura of respectability.

The Simulated Annealing method [234] is based on the theory of Markov processes. The trajectory is built in a randomized manner: the successor of the current point is chosen stochastically, with a probability that depends only on the current point and not on the previous history.

$$\begin{aligned}
\boldsymbol{x}' &\leftarrow \textsc{Neighbor}(\ N(\boldsymbol{x}_j)\ ) \\
\boldsymbol{x}_{j+1} &\leftarrow \begin{cases} \boldsymbol{x}' & \text{if } f(\boldsymbol{x}') \leq f(\boldsymbol{x}_j) \\ \boldsymbol{x}' & \text{if } f(\boldsymbol{x}') > f(\boldsymbol{x}_j) \text{, with probability } p = e^{-\frac{f(\boldsymbol{x})-f(\boldsymbol{x}_j)}{T}} \\ \boldsymbol{x}_j & \text{otherwise.} \end{cases}
\end{aligned} \tag{25.1}$$

The neighbor of the current point can be obtained in discrete problems by applying a limited set of local changes to the current solution. In continuous problem it can be obtained by sampling with a probability distribution centered on the current point, e.g., with a Gaussian distribution.

SA introduces a *temperature* parameter T which determines the probability that worsening moves are accepted: a larger T implies that more worsening moves tend to be accepted, and therefore a larger diversification occurs. The rule in equation (25.1) is called *exponential acceptance rule*. If T goes to infinity, then the probability that a move is accepted becomes 1, whether it improves the result or not, and one obtains a **random walk**. *Vice versa*, if T goes to zero, only improving moves are accepted as in the standard local search. Being a Markov process, SA is characterized by a memory-less property: if one starts the process and waits long enough, the memory about the initial configuration is lost, the probability of finding a given configuration at a given state will be stationary and only dependent on the value of f. If T goes to zero **the probability will peak only at the globally optimal configurations**. This basic result raised high hopes of solving optimization problems through a simple and general-purpose method, starting from seminal work in physics [268] and in optimization [298, 87, 234, 2].

Unfortunately, after some decades it became clear that SA is not a *panacea*. Furthermore, most mathematical results about **asymptotic convergence** (converge of the method when the number of iterations goes to infinity) are quite **irrelevant for optimization**. First, one does not care whether the *final* configuration at convergence is optimal or not, but that an optimal solution (or a good approximation thereof) is encountered —and memorized— during the search. Second, asymptotic convergence usually requires a patience which is excessive considering the limited length of our lives. Actually, repeated local search [126], and even pure random search [88] have better asymptotic results for some problems.

A practitioner has to place asymptotic results in the background and develop heuristics where high importance is attributed to **learning from a task in an online manner during the search**. In the following we briefly consider some asymptotic convergence results of SA.

25.6.1 Asymptotic convergence results

Let $(\mathcal{X}, f)$ be an instance of a combinatorial optimization problem, $\mathcal{X}$ being the search space and f being the objective function. Let $\mathcal{X}^*$ be the set of optimal solutions. One starts from an initial configuration $X^{(0)}$ and repeatedly applies equation (25.1) to generate a trajectory $X^{(t)}$. Under appropriate conditions, the probability of finding one of the optimal solutions tends to one when the number of iterations goes to infinity:

$$\lim_{k\to\infty} \Pr(X^{(k)} \in \mathcal{X}^*) = 1. \tag{25.2}$$

Let $\mathcal{O}$ denote the set of possible outcomes (states) of a sampling process, let $X^{(k)}$ be the stochastic variable denoting the outcome of the k-th trial, then the elements of the *transition probability matrix* P, given the probability that the configuration is at a specific state j given that it was at state i before the last step, are defined as:

$$p_{ij}(k) = \Pr(X^{(k)} = j | X^{(k-1)} = i). \tag{25.3}$$

A *stationary distribution* of a finite time-*homogeneous* (meaning that transitions do not depend on time) Markov chain is defined as the stochastic vector $\boldsymbol{q}$ whose components are given by

$$q_i = \lim_{k\to\infty} \Pr(X^{(k)} = i | X^{(0)} = j), \text{ for all } j \in \mathcal{O} \tag{25.4}$$

If a stationary distribution exists, one has $\lim_{k\to\infty} \Pr(X^{(k)} = i) = q_i$. Furthermore $\boldsymbol{q}^T = \boldsymbol{q}^T P$, the distribution is not modified by a single Markov step.

If a finite Markov chain is homogeneous, *irreducible* (for every i, j, there is a positive probability of reaching i from j in a finite number of steps) and *aperiodic* (the greatest common divisor $\gcd(\mathcal{D}_i) = 1$, where $\mathcal{D}_i$ is the set of all integers $n > 0$ with $(P^n)_{ii} > 0$), there exist a unique stationary distribution, determined by the equation:

$$\sum_{j\in\mathcal{O}} q_j p_{ji} = q_i \tag{25.5}$$

Unfortunately the rate of convergence of SA is very slow, being based similar arguments as for the convergence of pure random search.

Homogeneous model

In the homogeneous model one considers a sequence of infinitely long homogeneous Markov chains, where each chain is for a fixed value of the temperature T.

Under appropriate conditions [1] (the generation probability must ensure that one can move from an arbitrary initial solution to a second arbitrary solution in a finite number of steps) the Markov chain associated to SA has a stationary distribution $q(T)$ whose components are given by:

$$q_i(T) = \frac{e^{-f(i)/T}}{\sum_{j\in\mathcal{X}} e^{-f(j)/T}} \tag{25.6}$$

and

$$\lim_{T\to 0} q_i(T) = q_i^* = \frac{1}{|\mathcal{X}^*|} I_{\mathcal{X}^*}(i) \tag{25.7}$$

where $I_{\mathcal{X}^*}$ is the characteristic function of the set $\mathcal{X}^*$, equal to one if the argument belongs to the set, zero otherwise.

It follows that:

$$\lim_{T\to 0} \lim_{k\to\infty} \Pr_T(X^{(k)} \in \mathcal{X}^*) = 1 \tag{25.8}$$

The algorithm asymptotically finds an optimal solution with probability one, “converges with probability one.”

Inhomogeneous model

In practice one cannot wait for a stationary distribution to be reached. The temperature must be lowered before converging. At each iteration k one has therefore a different temperature T_k, obtaining a non-increasing sequence of values T_k such that $\lim_{k\to\infty} T_k = 0$.

If the temperature decreases in a sufficiently slow way:

$$T_k \geq \frac{A}{\log(k + k_0)} \tag{25.9}$$

for $A > 0$ and $k_0 > 2$, then the Markov chain converges in distribution to q^* or, in other words

$$\lim_{k \to \infty} \Pr(X^{(k)} \in \mathcal{X}^*) = 1 \tag{25.10}$$

The theoretical value of A depends on the depth of the deepest local, non-global optimum, a value which is not easy to calculate for a generic instance.

The above cited asymptotic convergence results of SA in both the homogeneous and inhomogeneous model are unfortunately *irrelevant for the application of SA to optimization*. In any finite-time approximation one must resort to approximations of the asymptotic convergence. The "speed of convergence" to the stationary distribution is determined by the second largest eigenvalue of the transition probability matrix $P(T)$ (not easy to calculate!). The number of transitions is at least *quadratic* in the total number of possible configurations in the search space [1]. For the inhomogeneous case, it can happen (e.g., Traveling Salesman Problem) that the *complete enumeration of all solutions* would take less time than approximating an optimal solution arbitrarily closely by SA [1].

In addition, repeated local search [126], and even random search [88] has better asymptotic results. According to [1] "approximating the asymptotic behavior of SA arbitrarily closely requires a number of transitions that for most problems is typically larger than the size of the solution space. Thus, the SA algorithm is clearly unsuited for solving combinatorial optimization problems to optimality." Of course, SA can be used in practice with fast *cooling schedules*, i.e., ways to progressively reduce the temperature during the search, but then the asymptotic results are not directly applicable. The optimal finite-length annealing schedules obtained on specific simple problems do not always correspond to those expected from the limiting theorems [351].

More details about cooling schedules can be found in [273, 196, 169]. Extensive experimental results of SA for graph partitioning, coloring and number partitioning are presented in [219, 220]. A comparison of SA and Reactive Search Optimizaiton (RSO) is presented in [38, 39].

The authors share with [390] an overall skepticism about using **Markov Chain Montecarlo** (MCMC) methods for efficiently optimizing functions, even in small dimensions.

25.7 The Inertial Shaker algorithm

A suggestion derived from our experience with optimization is: **Be lazy! Always try simple methods first, add complication only if motivated by a measurable improvement.**

The simpler **Inertial Shaker (IS)** technique, outlined in Fig. 25.6 can be a practical choice to go beyond Pure Random Search, while allowing on-the-job learning to rapidly adapt the probability of generating the next sample.

In IS the generation probability is uniform over a **search box** identified by vectors parallel to the coordinate axes (therefore the search box is defined by a single vector $\boldsymbol{b}$. In addition, a *trend direction* is identified by averaging a number of previous displacements [36]: the *find_trend* function used at line 7 simply returns a weighted average of the m_{disp} previous displacements:

$$\boldsymbol{\delta}_t = \mathit{amplification} \cdot \frac{\displaystyle\sum_{u=1}^{T} \boldsymbol{\delta}_{t-u} e^{-\frac{u}{(\mathit{history\_depth})^2}}}{\displaystyle\sum_{u=1}^{T} e^{-\frac{u}{(\mathit{history\_depth})^2}}},$$

where *amplification* and *history_depth* are defined in the algorithm, while m_{disp} is chosen in order to cut off negligible exponential weights and to keep the past history reasonably small.

f	(input)	Function to minimize
$\boldsymbol{x}$	(input)	Initial and current point
$\boldsymbol{b}$	(input)	Box defining search region $\mathcal{R}$ around $\boldsymbol{x}$
$\boldsymbol{\delta}$	(parameter)	Current displacement
amplification	(parameter)	Amplification factor for future displacements
history_depth	(parameter)	Weight decay factor for past displacement average

```
function InertialShaker (f, $\boldsymbol{x}$, $\boldsymbol{b}$)
    $t \leftarrow 0$
    repeat
        $success \leftarrow$ double_shot_on_all_components ( $\boldsymbol{\delta}$)
        if $success$ = true
            $\boldsymbol{x} \leftarrow \boldsymbol{x} + \boldsymbol{\delta}$
            find_trend ( $\boldsymbol{\delta}$)
            if f( $\boldsymbol{x} + \boldsymbol{\delta}$) < f( $\boldsymbol{x}$)
                $\boldsymbol{x} \leftarrow \boldsymbol{x} + \boldsymbol{\delta}$;
                increase amplification and history_depth
            else
                decrease amplification and history_depth
    until convergence criterion is satisfied
    return $\boldsymbol{x}$;
```

Figure 25.6: The Inertial Shaker algorithm, from [36].

Fig. 25.9 shows how the double-shot strategy is applied to all components of the search position $\boldsymbol{x}$. A displacement is applied at every component as long as it improves the result. If no improvement is possible, then the function returns `false`, and the search box is accordingly shrunk.

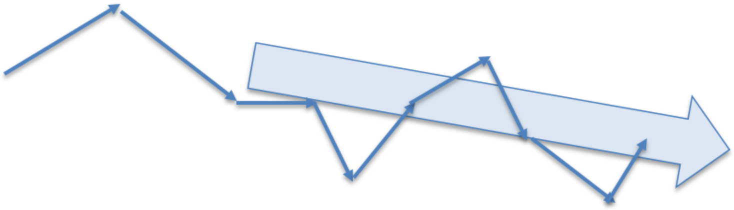


Figure 25.7: An illustration of the trend direction in the Inertial Shaker.

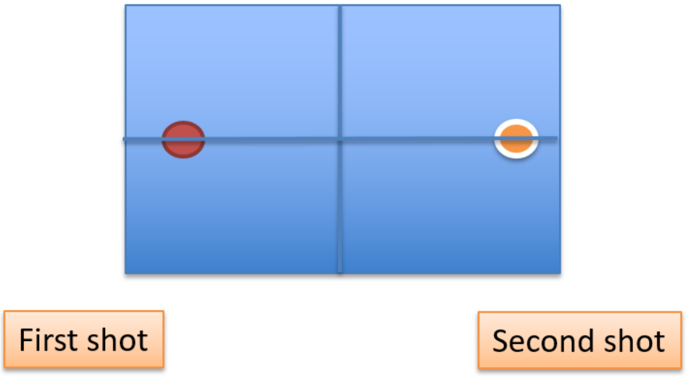


Figure 25.8: An illustration of the “double shot” in the Inertial Shaker.

f	Function to minimize
$\boldsymbol{x}$	Current position
$\boldsymbol{b}$	Vector defining current search box
$\boldsymbol{\delta}$	Displacement

```
function double_shot_on_all_components (f, $\boldsymbol{x}$, $\boldsymbol{b}$, $\boldsymbol{\delta}$)
    success ← false
    $\hat{\boldsymbol{x}} \leftarrow \boldsymbol{x}$
    for $i \in \{1, \ldots, n\}$
        $E \leftarrow$ f( $\hat{\boldsymbol{x}}$)
        r ← random in $[-b_i, b_i]$
        $\hat{x}_i \leftarrow \hat{x}_i + r$
        if $f(\hat{\boldsymbol{x}}) > E$
            $\hat{x}_i \leftarrow \hat{x}_i - 2r$
            if $f(\hat{\boldsymbol{x}}) > E$
                $b_i \leftarrow \rho_{\text{comp}} b_i$
                $\hat{x}_i \leftarrow \hat{x}_i + r$
            else
                $b_i \leftarrow \rho_{\text{exp}} b_i$
                success ← true
        else
            $b_i \leftarrow \rho_{\text{exp}} b_i$
            success ← true
    if success = true
        $\boldsymbol{\delta} \leftarrow \hat{\boldsymbol{x}}$ - $\boldsymbol{x}$
    return success
```

Figure 25.9: The double-shot strategy from [36]: apply a random displacement within the search box to all coordinates, keep the improving steps; return `false` if no improvement is found.

Gist

Stochastic Global Optimization is simple and robust technique relying on the **random generation of sample points** in the search space. It is a bit like in the piñata or *pentolaccia* game in which a blindfolded kid tries to break a container filled with treats. If one is patient, sooner or later a random point will fall in the vicinity of a global optimum. **Asymptotic convergence** can be demonstrated but it is irrelevant in practice

The **curse of dimensionality** is unavoidable: when the dimension is large there are just too many places to hide the global optimum and the number of sample grows exponentially. But there is still hope if the objective function has a very rich structure with regularities (e.g., a "big valley" structure), a frequent case in practical applications

Simulated Annealing goes beyond local optima by allowing for controlled worsening of the current solutions, and it generates Markov chains (memory-less).

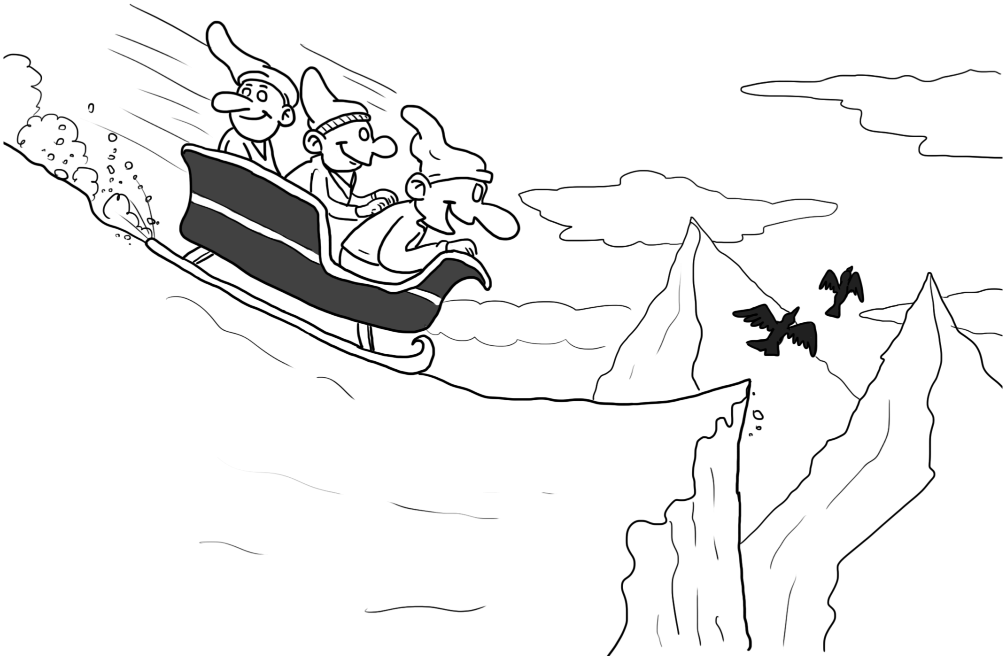
The more effective methods in SGO use some form of learning from the past generated samples along the search directory. **Statistical inference and "learning" techniques** can be used to modify probabilities of generating new samples, so that they are more concentrated on interesting regions.

The **Inertial Shaker** is a pragmatic example: samples are generated from a search box. Both the search box and a the trend direction are adapted (learnt) during the run.

Chapter 26

Derivative-Based Optimization

In this world - I am gonna walk
Until my feet - refuse to take me any longer
Yes I' m gonna walk - and walk some more.
(Macy Gray and Zucchero Fornaciari)



Most if not all problems can be cast as finding the optimal value for a suitable *objective function*, subject to constraints. If you are buying a house, you will have a bounded budget and objectives like number of rooms, neighborhood, view, vicinity to workplace, schools, etc. If you are searching for a partner you will have objectives like intelligence, beauty, companionship, etc. If you are running a company you will aim at maximizing profit, given constraints regarding your resources of people and equipment… You may notice that defining the proper function to be optimized is not trivial (think about the preference function for your preferred partner) but, once this crucial preliminary work is finished, one is left with the problem of **minimizing or maximizing a function which maps independent variables to an output value**. Maximizing means identifying the input values causing the maximum output value. If constraints are given, the input needs to be **feasible**, i.e., it needs to satisfy all constraints.

Methods to optimize functions are **the source of power** for most problem-solving and decision making activities, either explicitly or implicitly, a sound motivation for understanding the basic ideas and tools. While one does not need to know the underlying math before using the technology, mastering the basis facilitates faster and more effective choices. We consider the following related problems.

- **Nonlinear equations**, i.e. solving a set of nonlinear equations (individual functions f_i are collected in vector F):

  $$\begin{aligned}&\text{Given } F : \mathbb{R}^n \longrightarrow \mathbb{R}^n\\ &\text{find } x^* \in \mathbb{R}^n \ \text{ such that } F(x^*) = 0 \in \mathbb{R}^n.\end{aligned}$$

  The solution x^*, if it exists, minimizes $\sum_{i=1}^{n}(f_i(x))^2$. This is obvious because the sum of squares is not negative, and equal to zero if and only if all individual functions evaluate to zero.

- **Unconstrained minimization**:

  $$\begin{aligned}&\text{Given } f : \mathbb{R}^n \longrightarrow \mathbb{R}\\ &\text{find } x^* \in \mathbb{R}^n \ \text{ such that } f(x^*) \leq f(x) \ \text{ for every } x \in \mathbb{R}^n.\end{aligned}$$

  A point x^* satisfying the above condition is called a *global optimum*, by definition it is the best possible solution to the problem: no other solution is better.

In this chapter we collect some basic and traditional methods to optimize **smooth functions of continuous variables** (of real numbers), with some demonstrations about their convergence properties.

In mathematics, a function is smooth if a **derivative** exists. You may recollect the mathematical definition of derivative $f'(a)$ of function f at point a, as the limit for a step h going to zero of the difference in function value divided by the step:

$$f'(a) \;=\; \lim_{h\to 0}\frac{f(a+h)-f(a)}{h}. \tag{26.1}$$

What does this abstract definition have in common with learning, making approximated models, optimizing? A lot.

The practical “meaning” of the derivative is that, if x values are very close to a starting point of interest a (so that the displacement $h = x - a$ is small) one can use it to obtain a good **local approximation** as:

$$f(a+h) \;\approx\; f(a) + f'(a)\; h \tag{26.2}$$

The approximation is linear in the displacement h and it gets better and better when h becomes very small. The original functions can be approximated, in a local area, with its **tangent line**, which is linear and therefore easier to handle (with linear algebra!).

Counter-examples where derivatives do not exist are discontinuous functions (with sudden jumps) which cannot be approximated with a straight line at the jump position, or functions with sharp corners, which again do not have a single well-defined tangent line. A ski on a gentle slope is a nice image for a derivative of a smooth function. Skiing works because tangent lines are a good approximation to the slope. A ski on a spiky rock gets broken because there is no local smooth distribution of forces along a tangent line.

Like skis are tools for descending slopes, first and second derivatives are **useful tools to build local models** to improve a tentative configuration x. The improvements are typically obtained in an iterative manner, from an initial point x_1, to an improving point x_2 (with a different local model), to an improving x_3 (with a different local model)...

If the model is linear, one gets only indications about possible descent directions. In one dimension, after knowing the derivative at point x_1, one knows whether to do a small step to the right or to the left, depending on the slope. For sure, the step has to be *sufficiently small*. If the derivative is not zero, the model given by the tangent line does not lead to a well-defined minimization problem, the y value is unbounded and goes to minus infinity. A *quadratic* model using also the second derivatives can lead to a well-defined minimization problem if the parabola is U-shaped (opening to the top). In this case, one can to define the next point x_2 as the minimum of the parabolic model. A quadratic model built by using the fist and second derivatives of the function in Fig. 26.3 is shown in Fig. 26.2.

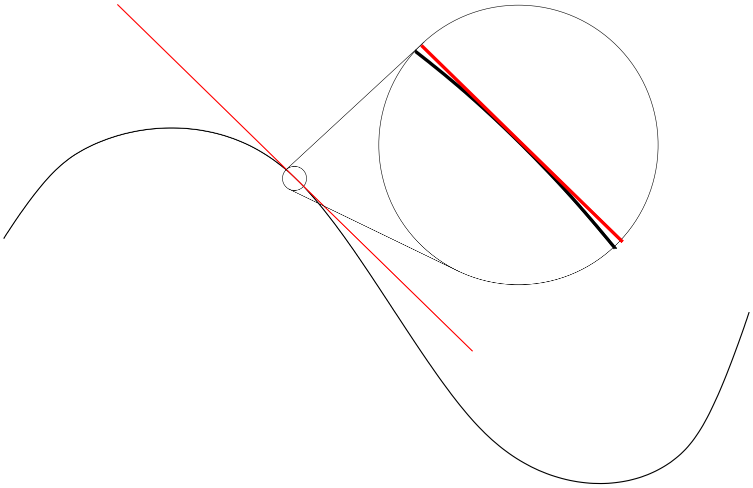


Figure 26.1: The graph of a function, drawn in black, and a tangent line to that function, drawn in red. The circular inset shows that the tangent line is a good local model of the function when one stays close to the point of interest.

26.1 Optimization and machine learning

To increase our motivation before jumping into the more terse mathematical results, let's note that there is a strong connection between machine learning and optimization.

When going in the direction of using **optimization for learning**, for sure *optimization* has to be used to select, among a class of models, one that is most consistent with the data provided for learning, one that better explains the observed data. An example is the usual "sum of squared differences" used in fitting curves and in supervised learning. Of course, the final scope of learning is *generalization*, but this only means that the function to be minimized will contain more pieces, to take the *model complexity* into account, so that simpler models will be favored over more complex ones.

When going in the contrary direction of using **learning for optimization**, some forms of *learning* are also used in efficient optimization algorithms. Preliminary examples of "learning" methods, although the inventors did not use that term, can be found in standard techniques for continuous optimization, where local models (obtained by using local information about function and derivatives) are constructed, whose validity can be limited to regions around the current point (*model-trust-regions* methods). Both the models and the *trust-regions* are typically adapted during a sequence of steps homing at a local minimizer.

While these techniques are traditionally associated with continuous optimization, the same principle of having a **local model learned during optimization** (or parameters tuned to the instance and local properties) can be useful in the different context of discrete (combinatorial) optimization, see for example the local search (Chapter 24) and Reactive Search Optimization (RSO) techniques [26] (Chapter 27).

A *leitmotiv* of many methods is to build the final solution by **a sequence of steps which modify a tentative solution**. At each step a **local model of the function** being optimized is built and used for a local move, modifying the tentative solution by small changes. The methods are therefore *short-sighted* and there is no guarantee of convergence to the global optimum. Nonetheless, in practice the presence of local minima (where local searchers will be stuck) did not prevent gradient-descent, local search and related techniques from becoming probably the simplest and most successful problem-solving machines.

Let us now see how the principle of having a *flexible local model (with parameters) learned during optimization of a given instance* acts in the case of continuous functions. The purpose of the following sections is to taste some of the most basic and successful paradigms of continuous optimization, with emphasis on intuition more than on mathematical details, that can be found in [115].

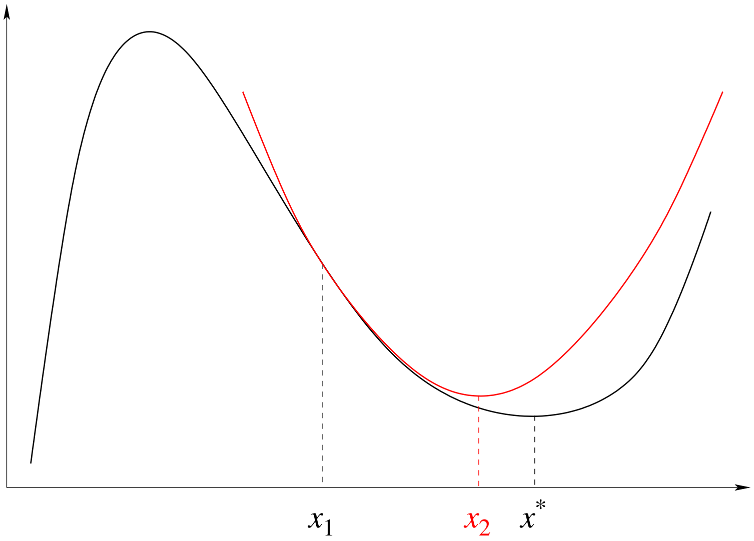


Figure 26.2: The graph of a function, drawn in black, and a local quadratic model at point x_1. The minimizer of the parabola x_2 is close to the (local) minimizer x^* of the function.

A discrimination has to do with the **availability of derivatives** of the function to be minimized. In most real-world cases derivatives are not available, actually in many cases the relationship between inputs and outputs can be *discontinuous*, or some inputs can be *discrete* (for example integer values). Try asking a businessman for the derivative of profit as a function of significant business choices, we doubt that you will get an answer!

If you are lucky and you are dealing with a function $f(x)$ of real numbers, which is continuous and differentiable, standard methods can be used. In particular, we summarize methods for one-dimensional optimization (Section 26.2), then review techniques for solving models (quadratic positive definite forms) in more dimensions (Section 26.3) and methods that use the model-solving techniques for the optimization of nonlinear functions of many variables (Section 26.4).

If your function does not have derivatives, you may consider the methods based on function evaluations only, like those described in Chapter 25.

26.2 Derivative-based techniques in one dimension

Intuition is easier in one dimension and let's therefore start with some classical results for functions of one variable. The historic, and still fundamental way to find a point where a differentiable function $f(x)$ is equal to zero, a.k.a. a **root**, is to start with a point *sufficiently close* to the target and iterate the two following steps:

1. find a **local solvable model**,
2. solve the local model.

The local model around the current point x_c can be derived from **Taylor series approximation** by stopping at the quadratic term:

$$f(x) = f(x_c) + f'(x_c)(x - x_c) + \frac{f''(x_c)(x - x_c)^2}{2!} + \dots,$$

or from Newton's theorem:

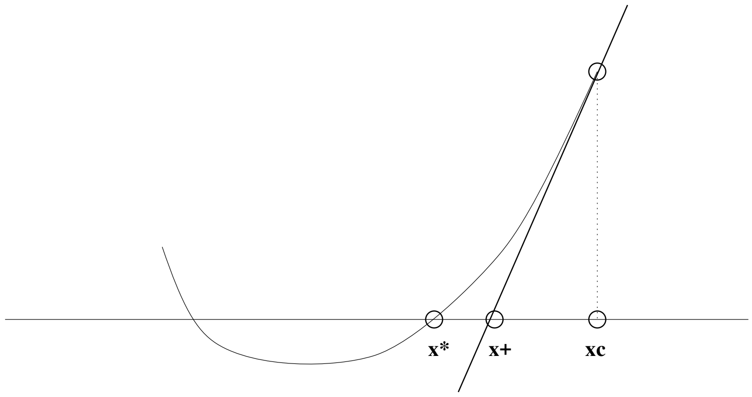


Figure 26.3: Local model for Newton's method.

$$f(x) = f(x_c) + \int_{x_c}^{x} f'(z)\ \mathrm{d}z \approx f(x_c) + f'(x_c)(x - x_c).$$

A **local model** (actually an **affine model**) around the current estimate x_c is therefore

$$M_c(x) = f(x_c) + f'(x_c)(x - x_c),$$

and by finding the root of the model one gets a prescription for the next value x_+ of the current estimate (the local step is from x_c to x_+), as illustrated in Fig. 26.3:

$$x_+ = x_c - \frac{f(x_c)}{f'(x_c)}.$$

If the function is linear, convergence occurs in one step. If the function is nonlinear, let us study the *local convergence* properties of Newton's method: we demonstrate that, if one starts with a point x_c sufficiently close to the root, one will eventually converge to it. The proof proceeds by *bounding the lack of linearity* of the model, and by demonstrating that the **distance to the target root is contracted at every step**.

The lack of linearity, or the error by using the model is:

$$f(x) - M_c(x) = \int_{x_c}^{x} [f'(z) - f'(x_c)]\ \mathrm{d}z.$$

We need now to bound the variation of a function proportionally to the difference in its inputs.

Definition 1 (Lipschitz continuity) *A function g is Lipschitz continuous with constant γ in a set X ($g \in Lip_\gamma(X)$) if for every $x, y \in X$:*

$$|g(x) - g(y)| \leq \gamma |x - y|.$$

Lemma 1 *Let $f' \in Lip_\gamma(D)$ for an open interval D. Then for any $x, y \in X$:*

$$|f(y) - f(x) - f'(x)(y - x)| \leq \gamma \frac{(x - y)^2}{2}.$$

Proof.

$$|f(y) - f(x) - f'(x)(y - x)| = \int_0^1 [f'(x + t(y - x)) - f'(x)](y - x)\ \mathrm{d}t,$$

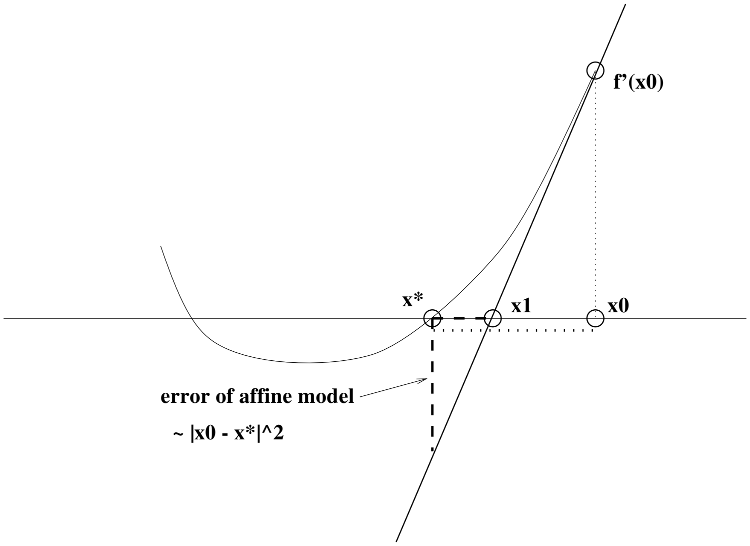


Figure 26.4: Convergence is guaranteed if the starting point x_0 is close to x^*.

and by using the triangle inequality and Lipschitz continuity:

$$\leq |y-x| \int_0^1 \gamma |t(y-x)| \, \mathrm{d}t = \gamma |y-x|^2/2.$$

We are now ready to demonstrate the **convergence theorem of Newton's method in one dimension**. Fig. 26.4 can help to follow the demonstration.

Theorem 1 *Let $f : D \longrightarrow \mathbb{R}$ for open interval D, $f' \in Lip_\gamma(D)$ (Lipschitz), $|f'(x)| \geq \rho$ (derivative bounded away from zero) in D.*

If $f(x) = 0$ has a solution $x^* \in D$, then the solution can be found by Newton method if the starting point x_0 is sufficiently close:
there is $\eta > 0$ such that if $|x_0 - x^*| < \eta$, the sequence:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

exists and converges to x^*. In addition:

$$|x_{k+1} - x^*| \leq \frac{\gamma}{2\rho} |x_k - x^*|^2.$$

Proof. Find a starting *ball* such that:

$$|x_{k+1} - x^*| \leq \tau |x_k - x^*| \text{ for a } \tau \in (0,1),$$

this would also imply that the point *remains* in the ball. Let's see.

$$x_1 - x^* = x_0 - x^* - \frac{f(x_0)}{f'(x_0)} = x_0 - x^* - \frac{f(x_0) - f(x^*)}{f'(x_0)},$$

$$= \frac{1}{f'(x_0)}[f(x^*) - f(x_0) - f'(x_0)(x^* - x_0)] = \frac{1}{f'(x_0)}[f(x^*) - M_0(x^*)],$$

where we identify the *error of the affine model* based on x_0 at x^*, bounded by $\frac{\gamma}{2}|x_0 - x^*|^2$. Therefore

$$|x_1 - x^*| \leq \frac{\gamma}{2|f'(x_0)|}|x_0 - x^*|^2 \leq \frac{\gamma}{2\rho}|x_0 - x^*|^2.$$

The distance is contracted if $\frac{\gamma}{2\rho}|x_0 - x^*| < 1$, or

$$|x_0 - x^*| \leq \frac{2\rho}{\gamma}\tau,$$

and contraction is obtained if one starts from the ball of radius:

$$\eta = \tau\frac{2\rho}{\gamma} \text{ (possibly reduced to fit the interval } D).$$

The above theorems guarantee **convergence in a fast (quadratic) manner, provided that one starts already sufficiently close to the target root**. This can be the case if a good approximation of the solution is already obtained, but, in general, one starts far away and does not have any guarantee that the starting point will be such that the steps will eventually lead to the solution.

The issue is **global convergence**. In practice, in the absence of strong guarantees, many techniques are **hybrid**, using Newton method when it works, otherwise falling back to a slower but safe global method, like the **bisection** method, as illustrated in Fig. 26.5.

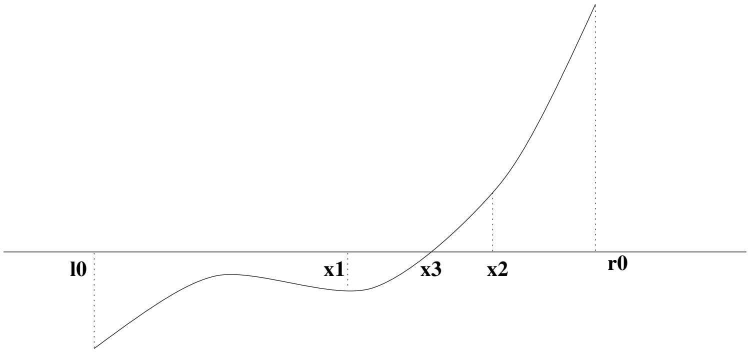


Figure 26.5: The bisection method. The initial interval is divided into two equal parts. One of the two sub-intervals is chosen depending on a test at the middle point. The subdivision is repeated for the chosen interval...

In the **bisection method for root finding**, one looks for a root of a continuous function by subdividing an initial interval (from l_0 to r_0) into two equal parts, observing the f value at the middle point x_1 and then continuing the search by considering only the left or the right sub-interval (while of course maintaining the invariant that the picked sub-interval contains the root). The function is continuous (smoothness implies continuity) and therefore it cannot have abrupt jumps. If the value is negative at l_0 and positive at r_0, there must be an internal point with value zero. If the value at x_1 is negative, at least one root must be in the right sub-interval. If the value at x_1 is positive, at least one root must be in the left sub-interval. One picks the appropriate sub-interval and iterates.

The bisection method is simple and effective, and it converges in a logarithmic number of steps. In fact, each step divides the interval into two equal parts, so that the length of the interval is divided by 2^s after s steps. It is unfortunate that this simple method is not easily extended to more than one dimension.

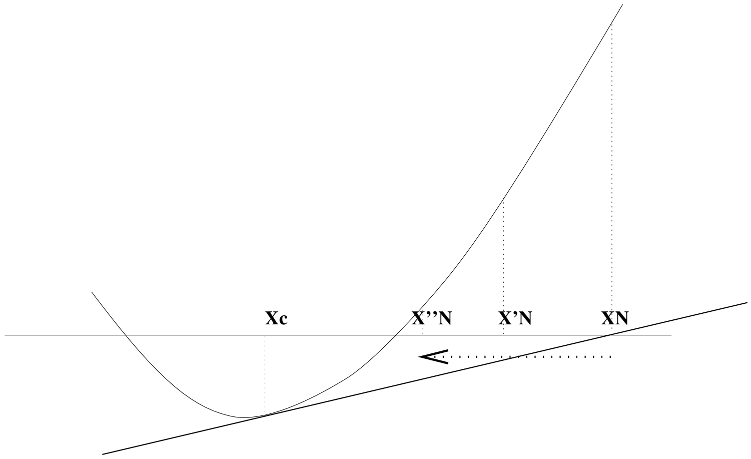


Figure 26.6: Backtracking: Newton step gives the direction.

```
function hybrid_quasi_newton ($f : \mathbb{R} \to \mathbb{R}$, $x_0$)
    while not finished
        Make local model of $f$ around $x_k$, find $x_N$ that solves the model;
        if $x_{k+1}$ is acceptable then move
        else pick $x_{k+1}$ by using a safe global strategy.
```

Figure 26.7: The hybrid quasi-Newton algorithm.

Fig. 26.6 illustrates the idea of **backtracking**: if Newton's step leads too far, beyond the position of the root, one reverts the direction coming back closer to the root position. One moves from Newton point x_N towards the starting point x_c until one finds x_+ with $|f(x_+)| < |f(x_c)|$.

A generic scheme for **hybrid methods** is to combine global convergence and fast local convergence, as illustrated in Fig. 26.7. One should try Newton step first but always insisting that the iteration decreases some measure of the closeness to a solution.

26.2.1 Derivatives can be approximated by the secant

If derivatives are not available or they are too costly to calculate, one can approximate them with the *secant* passing through two points (with a finite-difference approximation). The **secant method** consists of using the previous iterate x_- as follows:

$$a_c = \frac{f(x_c) - f(x_-)}{x_c - x_-}.$$

A convergence theorem is valid although the convergence rate is now slower (linear).

Theorem 2 *Let $f : D \longrightarrow \mathbb{R}$ for open interval D, $f' \in Lip_\gamma(D)$ (Lipschitz), $|f'(x)| \geq \rho$ (derivative bounded away from zero) in D.*

If $f(x) = 0$ has a solution $x^* \in D$, then there exist positive constants η, η' such that if $0 < |h_k| \leq \eta'$ and if $|x_0 - x^*| < \eta$, then the sequence

$$x_{k+1} = x_k - \frac{f(x_k)}{a_k}\ ,\ a_k = \frac{f(x_k + h_k) - f(x_k)}{h_k}$$

converges $q - linearly$ *to* x^*.

The lesson is that methods based on derivatives can often be used as starting points to develop methods without derivatives. The approximations will sacrifice some efficiency but convergence can still be obtained.

26.2.2 One-dimensional minimization

Up to now we discussed finding a root, a point where the value of f is equal to zero. To minimize a differentiable function one starts from this necessary condition [1]: the minimum must be at a point with $f'(x^*) = 0$. It all amounts to finding a *root* of the derivative function and we now know how to solve it! We can use the Hybrid Newton's method, plus the requirement that $f(x_k)$ decreases. After substituting the original function f with the first derivative f' one obtains

$$x_+ = x_c - \frac{f'(x_c)}{f''(x_c)}.$$

Note that the affine model of f' implies a **quadratic model** of f around x_c:

$$m_c(x) = f(x_c) + f'(x_c)(x - x_c) + \frac{1}{2} f''(x_c)(x - x_c)^2.$$

The iteration will converge locally and Q-quadratically to x^* of $f(x)$ if $f''(x^*) \neq 0$ and f'' satisfies the Lipschitz condition near x^*. If it is necessary, one backtracks until $f(x_+) < f(x_c)$.

26.3 Solving models in more dimensions (positive definite quadratic forms)

Before using local quadratic models for optimization, let's increase our motivation by confirming that these local models can actually be *solved*. Let's now consider more than one variable. Solving the local quadratic model amounts to solving a quadratic form. An plot of a quadratic positive-definite form is shown in Fig. 26.8.

Newton's method now requires that the **gradient** of the model be equal to zero. Given a step s the quadratic model is

$$Q(s) = \sum_{i=1}^{n} g_i s_i + \sum_{i=1}^{n} \sum_{j=1}^{n} H_{ij} s_i s_j \equiv g^T s + \frac{1}{2} s^T H s.$$

After deriving the gradient, one demands

$$\begin{aligned} \nabla Q(s) &= 0 = g + Hs; && (26.3) \\ Hs^N &= -g \ \ \text{(Newton equation)}\,. && (26.4) \end{aligned}$$

The solution of the linear system can be found in one step of cost $O(n^3)$ for the matrix inversion [2].

Because of the finite-precision computation carried out by computers one has to deal with issues of **numerical stability**: with some techniques the errors accumulate in a dangerous way, and one may end up with a numerical solution which is wildly different from the exact mathematical solution (reachable only if real numbers could be represented with infinite precision in computers).

Ill-conditioning is a term used to measure how the solution is sensitive to changes in the data (because of finite precision computation). Fig. 26.9 shows an example in two dimensions (two similar equations corresponding to almost parallel lines in the plane).

[1] Sufficient additional condition is $f''(x^*) > 0$, e.g., use Taylor series with remainder:

$$f(x) - f(x^*) = f'(x^*)(x - x^*) + \frac{1}{2} f''(\bar{x})(x - x^*)^2.$$

[2] Actually matrix inversion can be done with $O(n^{\log_2 7})$ or even better asymptotic requirements with more refined techniques, which are nonetheless not often used in practice because of complexity and numerical computing issues.

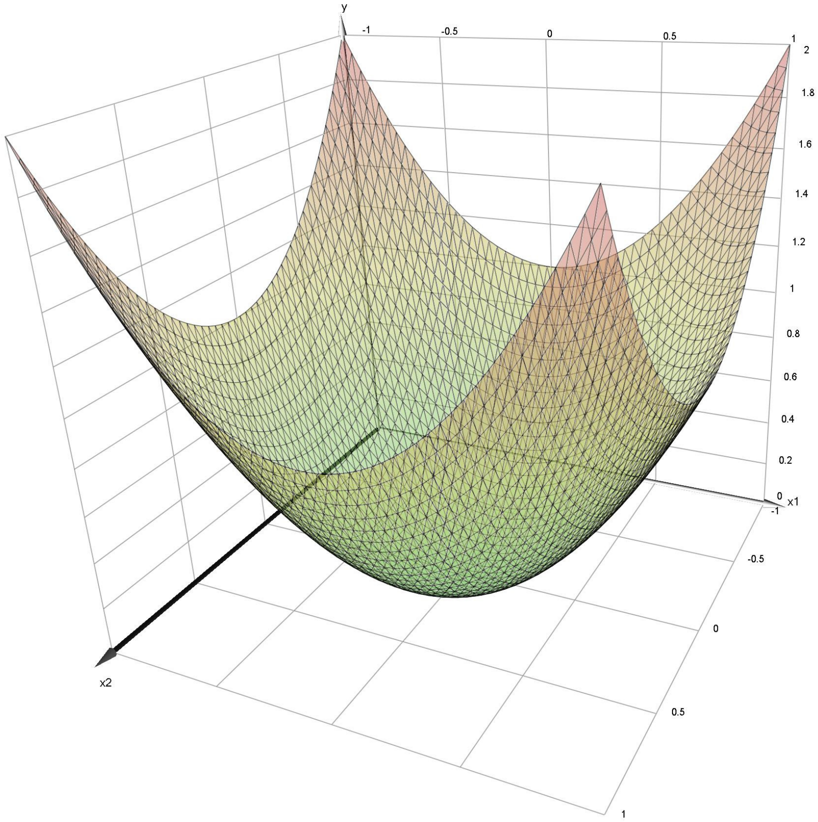


Figure 26.8: Quadratic positive definite f of two variables.

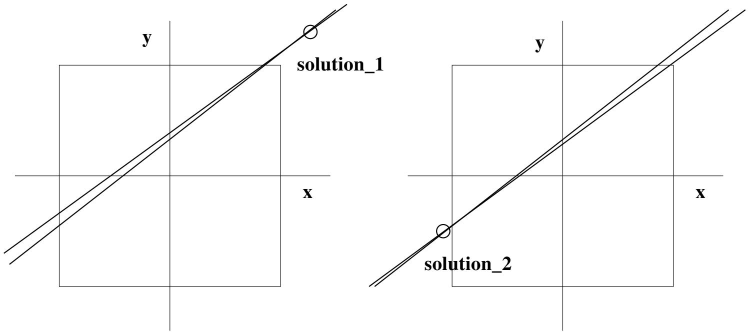


Figure 26.9: Ill-conditioning: solution is very sensitive to changes in the data. In this case two linear equations are very similar and a small change in the line direction is sufficient to shift the solution by a large amount.

In detail, one introduces the **condition number** $\kappa(H)$ of a matrix H defined as $\|H\|\,\|H^{-1}\|$, where $\|*\|$ is the matrix operator norm induced by the vector norm: $\|H\| = \max_x(\|Hx\|/\|x\|)$. The conditioning number is the ratio of the maximum to the minimum stretch induced by H and measures the **sensitivity of the solution of a linear system to finite-precision arithmetic**. If a linear system $Hx = b$ is perturbed in the following way with an error proportional to ϵ:

$$(H + \epsilon F)s(\epsilon) = g + \epsilon f, \tag{26.5}$$

the relative error in the solution can be bounded as:

$$\frac{\|s(\epsilon) - s\|}{\|s\|} \leq \kappa(H)\;(\frac{\|\epsilon F\|}{\|H\|} + \frac{\|\epsilon f\|}{\|g\|}) + O(\epsilon^2).$$

For the case of symmetric and positive definite matrices, an extremely stable triangular decomposition can be found with **Cholesky factorization**. Writing H (symmetric positive definite) as

$$H = LDL^T,$$

with L unit lower-triangular, D diagonal with strictly positive elements (LDL^T factorization).

Because the diagonal is strictly positive:

$$H = LD^{1/2}D^{1/2}L^T = \bar{L}\bar{L}^T = R^TR,$$

where R is a general upper triangular, the Cholesky factor can be considered the **"square root" of the matrix** H, a generalization of the usual square root for the case of matrices.

R can be computed directly from the element-by-element equality:

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix} = \begin{pmatrix} r_{11} & & & \\ r_{21} & r_{22} & & \\ \vdots & \vdots & \ddots & \\ r_{n1} & r_{n2} & \dots & r_{nn} \end{pmatrix} \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1n} \\ & r_{22} & \dots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{pmatrix}.$$

Let's equate element (1,1):

$$a_{11} = r_{11}^2, \;\; r_{11} = \sqrt{a_{11}},$$

continue with first row:

$$a_{12} = r_{11}r_{12}, \;\; a_{13} = r_{11}r_{13}, \dots.$$

After the entire first row is known, start with second row, element:

$$a_{22} = r_{12}^2 + r_{22}^2.$$

The above process needs about $\frac{1}{6}n^3$ multiplications and additions and n square roots (which are avoided if LDL^T is used). No dramatic growth in the elements of R occurs because the following holds:

$$a_{kk} = r_{1k}^2 + r_{2k}^2 + \dots + r_{kk}^2.$$

Now the original equation becomes

$$R^TRs = g, \tag{26.6}$$

and it can be solved by back-substitution (repeatedly solving for one variable and substituting into the remaining equations). Peel off factors in this way:

$$R^Ts_1 \;=\; -g \;\; \text{use forward substitution;} \tag{26.7}$$

$$Rs \;=\; s_1 \;\; \text{use backward substitution.} \tag{26.8}$$

The cost for solving the equation is $O(n^2)$ and therefore the dominant cost is in the factorization.

Figure 26.10: Two gradient-descent experts on the mountains surrounding Trento, Italy.

26.3.1 Gradient or steepest descent

In many cases, finding the minimum of the quadratic model by matrix inversion is not the most efficient and robust manner if the linear system becomes very large, a frequent case in machine learning. Furthermore, in many cases the H matrix of second partial derivatives is not available or it is too costly to calculate.

In all these cases **gradient descent** is a possible simple strategy to gradually improve a starting solution aiming at a locally optimal configuration.

If the gradient is different from zero, and one moves along the negative gradient:

$$x_+ = x_c - \epsilon \nabla f,$$

considering the Taylor expansion of equation 4.4, there is a sufficiently small ϵ so that the function decreases $f(x_+) < f(x_c)$. Although naive and requiring some care to choose a small ϵ value, the above technique is used in many different applications (see for example the popular error back-propagation method for training neural networks in Chapter 10).

Steepest descent has very natural and intuitive interpretations. A drop of water on a surface moves according to the local gradient scouting for local minima, at least approximately. Skiers, like those in Fig. 26.10, know very well the meaning of steepest descent, and the fact that skis must be positioned perpendicularly to the gradient to stop. Discrete analogies of steepest descent have been encountered in Chapter 24 in the form of *local search*. The idea is that a search process decides about a local step by sampling the function values at neighboring configurations and then deciding. **No form of global vision is available to guide the search, only local information**.

In addition to being a descent direction, it is well known that the negative gradient $-g$ is the direction of *fastest* descent. A method which looks promising is to execute a one-dimensional minimization while moving along the gradient direction:

$$\min_t Q(x_c - gt).$$

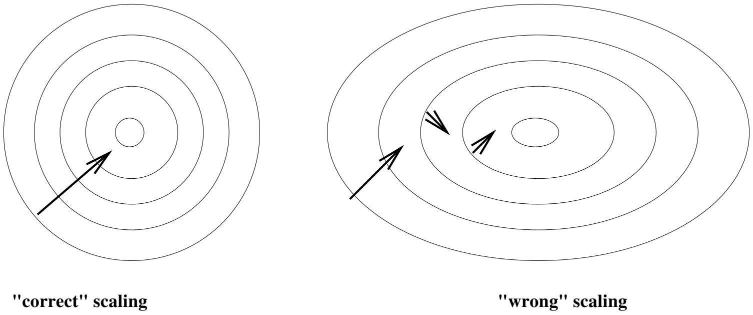


Figure 26.11: The gradient is not always an appropriate direction when searching for a minimizer.

Unfortunately, the intuition is wrong: in many cases spending a lot of effort in minimizing along the gradient direction is not the best way to solve a minimization problem.

The problem is caused by the fact that, when the matrix is *ill-conditioned*, the gradient direction does not point towards the optimal value but tends more and more to point in a perpendicular direction! Ill-conditioning in two dimensions can be visualized by thinking about contour lines becoming more and more *stretched* along a specific direction, see Fig. 26.11. When one follows the gradient, the resulting trajectory *zigzags* and the time to reach the minimum increases.

It can be shown that, when steepest descent is used to minimize a quadratic function $Q(s) = g^T s + \frac{1}{2} s^T H s$ (H symmetric and positive definite) the convergence can become very slow. In detail, by using the condition number κ, when κ increases, the difference between the current value and the best value is multiplied at each iteration by a number which tends to 1:

$$\begin{aligned} |Q(s_{k+1}) - Q(s_*)| &\approx \left(\frac{\eta_{max} - \eta_{min}}{\eta_{max} + \eta_{min}}\right)^2 |Q(s_k) - Q(s_*)| \\ &\approx \left(\frac{\kappa - 1}{\kappa + 1}\right)^2 |Q(s_k) - Q(s_*)|. \end{aligned}$$

If you permit us a far-fetched analogy, the above case may have some implication for life: being greedy and aiming at minimizing as much as possible along an appealing local direction can make one miss more “global” opportunities.

26.3.2 Conjugate gradient

The concept of **non-interfering directions** motivates the conjugate gradient method (CG) for minimization. Two directions are *mutually conjugate* with respect to the matrix H if

$$p_i^T H p_j = 0 \quad \text{when} \quad i \neq j. \tag{26.9}$$

After minimizing in direction p_i, the gradient at the minimizer will be perpendicular to p_i. If a second minimization is in direction p_{i+1}, the change of the gradient along this direction is $g_{i+1} - g_i = \alpha H p_{i+1}$ (for some constant α). The matrix H is indeed the Hessian, the matrix containing the second derivatives, and in the quadratic case the model coincides with the original function. Now, if equation (26.9) is valid, this change is *perpendicular* to the previous direction ($p_i^T(g_{i+1} - g_i) = 0$), therefore the *gradient at the new point remains perpendicular* to p_i and the previous minimization is not spoiled. For a quadratic function the conjugate gradient method is guaranteed to converge to the minimizer in at most $(n + 1)$ function and gradient evaluations (at least for infinite-precision calculations). For a general function the steps must be iterated until a suitable approximation to the minimizer is obtained.

Let us introduce the vector $y_k = g_{k+1} - g_k$. The first search direction p_1 is given by the negative gradient $-g_1$. Then the sequence x_k of approximations to the minimizer is defined by:

$$\begin{aligned} x_{k+1} &= x_k + \alpha_k p_k, && (26.10)\\ p_{k+1} &= -g_{k+1} + \beta_k p_k, && (26.11) \end{aligned}$$

where g_k is the gradient, α_k is chosen to minimize E along the search direction p_k and β_k is given by:

$$\beta_k = \frac{y_k^T g_{k+1}}{g_k^T g_k} \qquad \text{(Polak-Ribiere choice)}, \tag{26.12}$$

or by:

$$\beta_k = \frac{g_{k+1}^T g_{k+1}}{g_k^T g_k} \qquad \text{(Fletcher-Reeves choice)}. \tag{26.13}$$

The different choices coincide for a quadratic function [331]. A major difficulty with the above forms is that, for a general function, the obtained directions are *not* necessarily descent directions and numerical instability can result.

The use of a *momentum* term to avoid oscillations in *back-propagation* [311] can be considered as an approximated form of conjugate-gradient.

26.4 Nonlinear optimization in more dimensions

Let's now consider the convergence properties of Newton's method in more dimensions. The method consists of solving the quadratic model:

$$m_c(x_c + p) = f(x_c) + \nabla f(x_c)^T p + \frac{1}{2} p^T \nabla^2 f(x_c) p,$$

and iterating, as shown in Fig. 26.12.

If the initial point is *close* to the minimizer x^* and $\nabla^2 f(x^*)$ is positive definite, the method converges Q-quadratically to x^*.

The possible problems arise if:

- the Hessian is not positive definite: there are directions of negative curvature $p^T H p < 0$, which means that the quadratic local model can assume arbitrarily large negative values when the step length along p increases to infinity;
- the Hessian is singular or ill-conditioned, leading to the impossibility or numerical difficulty of inverting the matrix.

The above problems lead to what are called **Modified Newton's methods**, which change the local model to obtain a sufficiently positive-definite and non-singular matrix. Furthermore they deal with global convergence, indefinite H, and iterative approximations to H. The method is to **combine a fast tactical local method with a robust strategic method** to assure global convergence.

26.4.1 Global convergence through line searches

Global convergence is obtained by adopting line searches along the identified direction: one tries Newton's method *first* and then possibly *backtracks*. Of course one needs to ensure that the direction is indeed a *descent direction*! Fortunately, if H (that is symmetric) is positive definite, Newton's direction *is* a descent direction:

$$\frac{df}{d\lambda}(x_c + \lambda s^N) = \nabla f(x_c)^T s^T = -\nabla f(x_c)^T H_c^{-1} \nabla f(x_c) < 0.$$

```
function multi_dimensional_newton ($f : \mathbb{R}^n \to \mathbb{R}$, $\boldsymbol{x}_0 \in \mathbb{R}^n$)
                                                  f is twice continuously differentiable
    while not finished
        solve $\nabla^2 f(\boldsymbol{x}_c) s^N = -\nabla f(\boldsymbol{x}_c)$;
        $\boldsymbol{x}_{k+1} \leftarrow \boldsymbol{x}_k + s^N$.
```

Figure 26.12: Newton method in more dimensions.

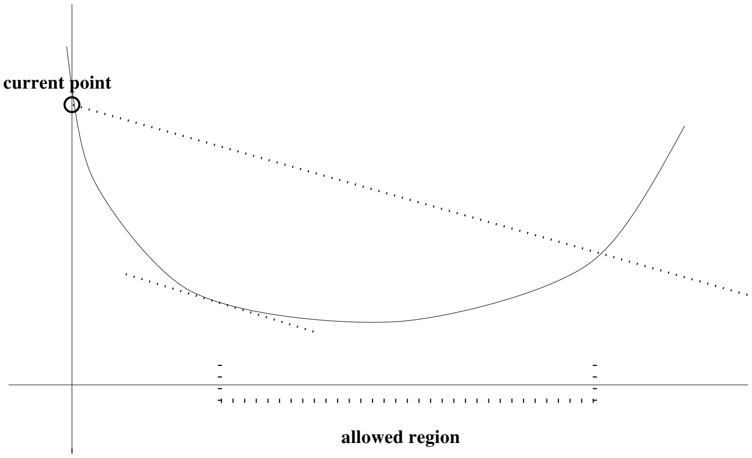


Figure 26.13: Armijo - Goldstein conditions.

If the Hessian has to be approximated, for sure one wants to maintain the *symmetry* and *positive definiteness*, so that the descent direction is guaranteed.

A way to ensure global convergence is to demand that the f value decreases by a sufficient amount with respect to the step length, that the step is long enough and that the search direction is kept away from being orthogonal to the gradient. A popular way to guarantee the above points is by Armijo and Goldstein conditions [157], also illustrated in Fig. 26.13:

1.
$$f(x_c + \lambda_c p) \leq f(x_c) + \alpha \lambda_c \nabla f(x_c)^T p,$$
where $\alpha \in (0, 1)$ and $\lambda_c > 0$;

2.
$$\nabla f(x_c + \lambda_c p)^T p \geq \beta \nabla f(x_c)^T p,$$
where $\beta \in (\alpha, 1)$.

If the Armijo-Goldstein conditions are satisfied at each iteration and if the error is bounded below, one has the following **global convergence** property:
$$\lim_{k \to \infty} \nabla f(x_c) = 0,$$
provided that each step is away from orthogonality to the gradient:
$$\lim_{k \to \infty} \nabla f(x_c) s_k / \|s_k\| \neq 0.$$

If the Armijo-Goldstein conditions are maintained, one can use **fast approximated one-dimensional searches** without losing global convergence [115].

26.4.2 Cure for indefinite Hessians

If the Hessian is indefinite one can use the **modified Cholesky** method. Let's consider the spectral decomposition:

$$H = U\Lambda U^T = \sum_{i=1}^{n} \eta_i u_i u_i^T,$$

where Λ is diagonal and Λ_{ii} is the eigenvalue η_i.

It is easy to see what will happen if η_i are negative (no minimum exists: values can grow to minus infinity) or close to zero (the inverse will have eigenvalues close to infinity).

If H is not positive definite or it is ill-conditioned one remedies in a very direct way by adding a simple diagonal matrix:

$$H' = \nabla f(x_c) + \mu_c I, \;\; \mu_c > 0$$

to correct the Hessian so that $\nabla^2 f(x_c) + \mu_c I$ is positive definite and well conditioned.

This leads to the **modified Cholesky factorization**: one finds the Cholesky factors of a different matrix $\bar{H}_c$, differing only by a diagonal matrix K with non-negative elements:

$$\bar{H}_c = LDL^T = H_c + K,$$

where all elements in D are positive and all elements of L are uniformly bounded

$$d_k > \delta, \;\; |l_{ij}|\sqrt{d_k} \leq \beta,$$

see [147] for an appropriate choice of β. The modified Cholesky factorization is used to correct Hessian [115, 20] so that $\nabla^2 f(x_c) + \mu_c I$ is positive definite and well conditioned.

This amounts to adding a positive definite quadratic form to our original model. The effect is that large steps tend to be penalized.

26.4.3 Relations with model-trust region methods

The previous techniques were based on finding a *search direction* and moving by an acceptable amount in that direction ("step-length-based methods").

Because the last modification consisted of adding to the local model a quadratic term:

$$m_{modified}(x_c + s) = m_c(x_c + s) + \mu_c s^T s,$$

one may suspect that minimizing the new model is equivalent to minimizing the original one with the constraint that the step s not be too large.

This can be executed by choosing first the maximum step length and then using the full (and not one-dimensional) quadratic model to determine the appropriate direction. In **model-trust region methods** the model is trusted only within a region, that is updated by using the experience accumulated during the search process.

Theorem 3 *Suppose that we are looking for the step s_c that solves:*

$$\begin{aligned} \min m_c(x_c + s) &= f(x_c) + \nabla f(x_c)^T s + \frac{1}{2} s^T H_c s & (26.14)\\ \textit{subject to } \|s\| \leq \delta_c. && (26.15) \end{aligned}$$

The above problem is solved by:

$$s(\mu) = -(H_c + \mu I)^{-1} \nabla f(x_c), \tag{26.16}$$

for the unique $\mu \geq 0$ such that the step has the maximum allowed length ($\|s(\mu)\| = \delta_c$), unless the step with $\mu = 0$ is inside the trusted region ($\|s(0)\| \leq \delta_c$), in which case $s(0)$, the Newton step, is the solution.

The diagonal modification of the Hessian is a **compromise between gradient descent and Newton's method**: when μ tends to zero the original Hessian is (almost) positive definite and the step tends to coincide with Newton's step; when μ has to be large the diagonal addition μI tends to dominate and the step tends to one proportional to the negative gradient:

$$s(\mu) = -(H_c + \mu I)^{-1} \nabla f(x_c) \approx -\frac{1}{\mu} \nabla f(x_c).$$

There is no need to decide from the beginning, the algorithm selects in an adaptive manner the move that is appropriate to the local configuration of the error surface.

26.4.4 Secant methods

Secant techniques are useful if the Hessian is not available or costly to calculate.

In one dimension the second derivative can be approximated with the slope of the secant through the values of the first derivatives at two near points:

$$\frac{d^2 f(x)}{dx^2}(x_2 - x_1) \approx \left(\frac{df(x_2)}{dx} - \frac{df(x_1)}{dx} \right). \tag{26.17}$$

In more dimensions one equation is not sufficient. Let the current and next point be x_c and x_+, respectively, and let's define $s_c = x_+ - x_c$ and $y_c = \nabla f(x_+) - \nabla f(x_c)$ (difference of gradients). The analogous "secant equation" is

$$H_+ s_c = y_c. \tag{26.18}$$

The above equation does not determine a unique H_+ but leaves the freedom to choose from a $(n^2 - n)$ dimensional affine subspace $Q(s_c, y_c)$ of matrices obeying equation (26.18).

A possibility to cure this issue is to use the previous "history." In other words, equation (26.18) will not be used to *determine* but to *update* a previously available approximation.

In particular (Broyden method), one can use a *least change* principle, finding the matrix in $Q(s_c, y_c)$ ("quotient") that is closest to the previously available matrix. This is obtained by *projecting* the matrix onto $Q(s_c, y_c)$, in the Frobenius norm (matrix as a long vector).

The resulting Broyden's update is

$$(H_+)_1 = H_c + \frac{(y_c - H_c s_c) s_c^T}{s_c^T s_c}. \tag{26.19}$$

Unfortunately, Broyden's update does not guarantee a *symmetric* matrix (remember that we want *descent* directions).

Projecting Broyden's matrix onto the subspace of *symmetric* matrices is not enough: the obtained matrix may be out of $Q(s_c, y_c)$.

Fortunately, if the two above projections are repeated, the obtained sequence $(H_+)_t$ converges to a matrix that is both symmetric and in $Q(s_c, y_c)$. This is the *symmetric* secant update of Powell:

$$H_+ = H_c + \frac{(y_c - H_c s_c) s_c^T + s_c (y_c - H_c s_c)^T}{s_c^T s_c} - \frac{< y_c - H_c s_c, s_c > s_c s_c^T}{(s_c^T s_c)^2}. \tag{26.20}$$

We are closer to a satisfactory update, but we insist on a *positive definite* approximation of the Hessian. The matrix H_+ is symmetric and positive definite if and only if $H_+ = J_+ J_+^T$, for some non-singular J_+. A proper update can be obtained by using Broyden's method to derive a suitable J_+.

The resulting update is historically known as the Broyden, Fletcher, Goldfarb, and Shanno (BFGS) update [68] and is given by:

$$H_+ = H_c + \frac{y_c y_c^T}{y_c^T s_c} - \frac{H_c s_c s_c^T H_c}{s_c^T H_c S_c}. \tag{26.21}$$

The positive-definite secant update converges $q - superlinearly$ [68].

It is possible to take the initial matrix H_0 as the identity matrix, so that the first step is along the negative gradient.

ϵ	Learning rate
$\bar{\epsilon}$	Average learning rate
$\boldsymbol{w}_{\text{curr}}$	Weights
$\boldsymbol{d}$	Search direction

```
procedure oss_minimize
    begin_or_restart
    $\epsilon \leftarrow 10^{-5}$
    $\bar{\epsilon} \leftarrow 10^{-5}$
    $\boldsymbol{w}_{\text{curr}} \leftarrow$ random initial weights
    iterations ← 1
    while convergence criterion is not satisfied
        if iterations is multiple of $N$
            begin_or_restart
        iterations ← iterations + 1
        $\boldsymbol{d} \leftarrow$ find_search_direction                See Eq. (26.22)
        if fast_line_search( $\boldsymbol{d}$) = false
            begin_or_restart
procedure begin_or_restart
    find the current energy value
    $\epsilon \leftarrow \bar{\epsilon}$
    $\boldsymbol{d} \leftarrow -g$
    fast_line_search( $\boldsymbol{d}$)
```

Figure 26.14: The one-step secant algorithm (Part I), from [19].

26.4.5 Closing the gap: second-order methods with linear complexity

Computing the exact Hessian requires order $O(n^2)$ operations and order $O(n^2)$ memory to store the Hessian components, in addition the solution of the equation to find the step (or search direction) in Newton's method (see Fig. 26.12) requires $O(n^3)$ operations, at least when using traditional linear algebra routines. Fortunately, some second-order information can be calculated by starting from the last gradients, and therefore reducing the computation and memory requirements to find the search direction to $O(n)$. The term "secant methods" used in [115] is reminiscent of the fact that derivatives are approximated by the secant through two function values.

Historically the one-step-secant method *OSS* is a variation of what is called *one-step (memory-less) Broyden-Fletcher-Goldfarb-Shanno* method, see [331]. The **OSS method** has been used for multilayer perceptrons in [19] and [31]. The main procedures are illustrated in Fig. 26.14–26.15.

Note that BFGS (see [376]) stores the whole approximated Hessian, while the *one-step* method requires **only vectors** computed from gradients. In fact, the new search direction p_+ is obtained as:

$$p_+ = -g_c + A_c s_c + B_c y_c, \tag{26.22}$$

where the two scalars A_c and B_c are the following combination of scalar products of the previously defined vectors s_c, g_c and y_c (last step, gradient and difference of gradients):

$$A_c = -\left(1 + \frac{y_c^T y_c}{s_c^T y_c}\right)\frac{s_c^T g_c}{s_c^T y_c} + \frac{y_c^T g_c}{s_c^T y_c} \;\; ; \;\; B_c = \frac{s_c^T g_c}{s_c^T y_c}.$$

The search direction is the negative gradient at the beginning of learning and it is restarted to $-g_c$ every N steps (N being the number of weights in the network).

The fast one-dimensional minimization along the direction p_c is crucial to obtain an efficient algorithm. This part of the algorithm (derived from [115]) is described in Fig. 26.15. The one-dimensional search is based on the backtracking strategy. The last successful learning rate λ is increased ($\lambda \leftarrow \lambda \times 1.1$) and the first tentative step is executed. To use the same notation as that of Fig. 26.14–26.15 let us denote with E ("energy") the function to be optimized. If the new value E is not below the "upper-limiting" curve, then a new tentative step is tried by using successive quadratic interpolations until the requirement is met. Note that the learning rate is decreased by L_{decr} after each unsuccessful trial. Quadratic interpolation is not wasting computation. In fact, after the first trial one has exactly the information that is needed to fit a parabola: the value of E_0 and E_0' at the initial point and the value of E_λ at the trial point. The parabola $P(x)$ is

$$P(x) = E_0 + E_0' x + \left[\frac{E_\lambda - E_0 - \lambda E_0'}{\lambda^2} \right] x^2, \tag{26.23}$$

and the minimizer λ_{min} is

$$\lambda_{min} = \frac{-E_0'}{2\left[\frac{E_\lambda - E_0 - \lambda E_0'}{\lambda^2}\right]} \leq \frac{1}{2(1 - G_{\text{decr}})} \lambda. \tag{26.24}$$

If the "gradient-multiplier" G_{decr} in Fig. 26.14 is 0.5, the λ_{min} that minimizes the parabola is less than λ.

26.5 Constrained optimization: penalties and Lagrange multipliers

Imagine that you are the owner of a factory and you want to maximize production. With unconstrained optimization your workers may complain if asked to work day and night without pauses, lunches and vacation. A reasonable constraint can be that each worker has to work for exactly 48 hours per week. Truck drivers have safety requirements on the number of continuous driving hours before a break is required, otherwise they risk falling asleep while driving (e.g., drive for no more that 6 hours).

A general **constrained minimization problem** is:

$$\begin{array}{rlll} \min & f(\mathbf{x}) & & \\ \text{subject to} & g_i(\mathbf{x}) = c_i & \text{for } i = 1, \ldots, n & \text{Equality constraints} \\ & h_j(\mathbf{x}) \geqq d_j & \text{for } j = 1, \ldots, m & \text{Inequality constraints} \end{array} \tag{26.25}$$

where $g_i(\mathbf{x}) = c_i$ for $i = 1, \ldots, n$ and $h_j(\mathbf{x}) \geq d_j$ for $j = 1, \ldots, m$ are constraints that are required to be satisfied. **Hard constraints** need to be satisfied for a solution to be feasible. Even for smooth objective functions, hard constraints complicate matters by introducing unsurmountable walls in the input parameter space.

Some ways to take care of constraints are problem-specific, e.g. they are easily handled in Linear and Quadratic Programming tasks (Chapter 33). But there are two simple general-purpose ways to address constraints. Both ways **transform an optimization problem with constraints into an unconstrained one** and are widely used.

The first method considers that **hard constraints are very rare in practice**. 48 working hours can be surpassed in some cases provided that overtime is paid more than the standard rate. In engineering, all physical measures are in any case subject to stochastic errors. If a truck on a freeway cannot weigh more than 10 tons, a policeman will hopefully not confiscate it if the maximum weight is surpasses by one gram. **Soft constraints** can be violated but there is a **penalty** to be paid, henceforth the name of **penalty method**. The harder the constraint, the higher the penalty.

For each equality constraint a quadratic penalty can be added for violation, leading to a **penalized objective function**:

$$\min f(\mathbf{x}) + \sum_i \gamma_i (g_i(\mathbf{x}) - c_i)^2 \tag{26.26}$$

If the constraint is not satisfied, a penalty proportional to γ_i times the (quadratic) violation is paid. Of course, different penalties are possible, e.g., absolute values, logarithmic, or different formulas for inequality constraints.

One may be tempted to set γ_i to a huge positive value to bring the constraint very close to perfect satisfaction. In fact, even a small violation of the constraint will cause an explosion of the penalty in the objective function. Unfortunately, very large constraints imply that very steep walls (although not perpendicular) will be created in the penalized objective, creating numerical problems and difficulties in the practical minimization. In practice, the proper γ_i values are a result of a tradeoff between minimizing f and accepting some violation. One can start with tentative values, see the results, discuss acceptability of constraint violation, repeat with different γ_i values until satisfied. Multiple-objective optimization (Chapter 40) gives equal standing to the initial objective and to the constraint violations, leading to a more systematic management of the solution.

If the function is smooth and has partial derivatives, a second possibility in mathematical optimization is the method of **Lagrange multipliers**. The problem is transformed into an unconstrained one by adding each constraint multiplied by a parameter λ_i (a Lagrange multiplier).

$$\min f(\mathbf{x}) + \sum_i \lambda_i g_i(\mathbf{x}) \tag{26.27}$$

Minimizing the transformed function yields a *necessary* condition for optimality. Additional checks are therefore necessary (for example, the identified point can be a saddle point and not a global minimum), but in many cases, in the presence of a single global optimum, the method of **Lagrange multipliers** will deliver the correct solution.

Let's develop some intuition with a graphical analysis.

Consider a two-dimensional problem:

$$\begin{array}{ll} \text{maximize} & f(x,y) \\ \text{subject to} & g(x,y) = c. \end{array}$$

We can visualize contours of f given by

$$f(x,y) = d$$

for various values of d and the contour of g given by $g(x,y) = c$, as shown in Fig. 26.17.

Suppose we walk along the contour line with $g = c$. In general the contour lines of f and g may be distinct, so the contour line for $g = c$ will intersect with or cross the contour lines of f. This is equivalent to saying that while moving along the contour line for $g = c$ the value of f can vary. Only when the contour line for $g = c$ meets contour lines of f tangentially, do we neither increase nor decrease the value of f — that is, when the contour lines touch but do not cross.

The contour lines of f and g touch when the **tangent vectors of the contour lines are parallel**. Since the gradient of a function is perpendicular to the contour lines, this is the same as saying that the gradients of f and g are parallel. Thus we want points (x,y) where $g(x,y) = c$ and

$$\nabla f(x,y) = \lambda \nabla g(x,y).$$

The above analysis is valid for more than two input dimensions. If the two gradients are *not* parallel at the minimizer, a local direction $\Delta\mathbf{x}$ can be found which is perpendicular to the constraint gradient, and therefore keeps the constraint satisfied in the linear approximation of Taylor series, but not perpendicular to the gradient of the original objective function. A small step along $\Delta\mathbf{x}$ (or minus $\Delta\mathbf{x}$) will therefore lead to smaller f values, contradicting the assumption of minimality.

The Lagrange multiplier λ specifies how one gradient needs to be multiplied to obtain the other one!

Because of linearity of the gradient, requiring $\nabla f(x,y) - \lambda \nabla g(x,y) = 0$ is the same as requiring $\nabla \left[f(x,y) - \lambda g(x,y) \right] = 0$. But this is the necessary condition for a stationary point of function:

$$f(x,y) - \lambda g(x,y)$$

the original function minus the constraint multiplied by the Lagrange multiplier.

The above can be generalized for more constraints and for inequality constraints.

A practical application of Lagrange multipliers is in economics. Let's remember that the gradient is used to find a first-order difference when $\mathbf{x}$ is changed, and that the two gradients are parallel and related by the λ^* multiplier. A Lagrange multiplier can be interpreted as the "marginal" change in the optimal value of the objective function (profit) due to **a change (relaxation) of a given constraint**. In such a context λ^* is the marginal cost of the constraint, and is referred to as the **shadow price**.

The shadow price can provide decision-makers with insights. For instance if a constraint limits the amount of labor available to 40 hours per week, the shadow price tells how much you should be willing to pay for an additional hour of labor. If pay more than the shadow price, the increase in in the total production value (the objective function) will be less that your labor cost.

Applications of Lagrange multipliers in ML are for example in the LASSO technique in Section 9.3, of in SVM in Section 12.1.1.

$\boldsymbol{d}$	Search direction
$\boldsymbol{g}$	Function gradient
$\boldsymbol{w}$	Weights
d_{l}	Projection of $\boldsymbol{d}$ along the gradient
E	Current energy
E_{saved}	Best energy
ok	Improving step found
trials	Number of iterations
MAXTRIALS	Maximum allowed number of iterations
L_{decr}	Step decrease at each iteration

```
procedure fast_line_search ( $\boldsymbol{d}$)
    $d_{\text{l}} \leftarrow \boldsymbol{g} \cdot \boldsymbol{d}$
    if $d_{\text{l}} > 0$
        $\boldsymbol{d} \leftarrow -\boldsymbol{g}$; $d_{\text{l}} \leftarrow \boldsymbol{g} \cdot \boldsymbol{d}$
    $E_{\text{saved}} \leftarrow E$
    $\epsilon \leftarrow L_{\text{incr}}\, \epsilon$; ok ← false; trials = 0
    repeat
        trials ← trials + 1
        $\boldsymbol{w} \leftarrow \boldsymbol{w}_{\text{curr}} + \epsilon\, \boldsymbol{d}$
        $E \leftarrow E(\boldsymbol{w})$
        if $E < E_{\text{saved}} + G_{\text{decr}} d_{\text{l}} \epsilon$
            ok ← true
        else
            $\epsilon_{\text{quad}} \leftarrow$ parabola_minimizer($E_{\text{saved}}$, $d_{\text{l}}$,f)        See Eq. (26.24)
            $\boldsymbol{w} \leftarrow \boldsymbol{w}_{\text{curr}} + \epsilon_{\text{quad}}\, \boldsymbol{d}$
            $E \leftarrow E(\boldsymbol{w})$
            if $E < E_{\text{saved}} + G_{\text{decr}} d_{\text{l}} \epsilon_{\text{quad}}$
                ok ← true; $\epsilon \leftarrow \epsilon_{\text{quad}}$
            else
                $\epsilon \leftarrow L_{\text{decr}}\, \epsilon$
    until ok = true or trials > MAXTRIALS
    if ok = true
        $\boldsymbol{p} \leftarrow \epsilon\, \boldsymbol{d}$
        $\boldsymbol{w}_{\text{curr}} \leftarrow \boldsymbol{w}$
        g ← $\nabla_{\boldsymbol{w}} E(\boldsymbol{w})$
        $\bar{\epsilon} \leftarrow 0.9\, \bar{\epsilon} + 0.1\, \epsilon$
    return ok
```

Figure 26.15: The one-step secant algorithm (Part II), from [19]: fast one-dimensional search along the chosen direction $\boldsymbol{d}$.

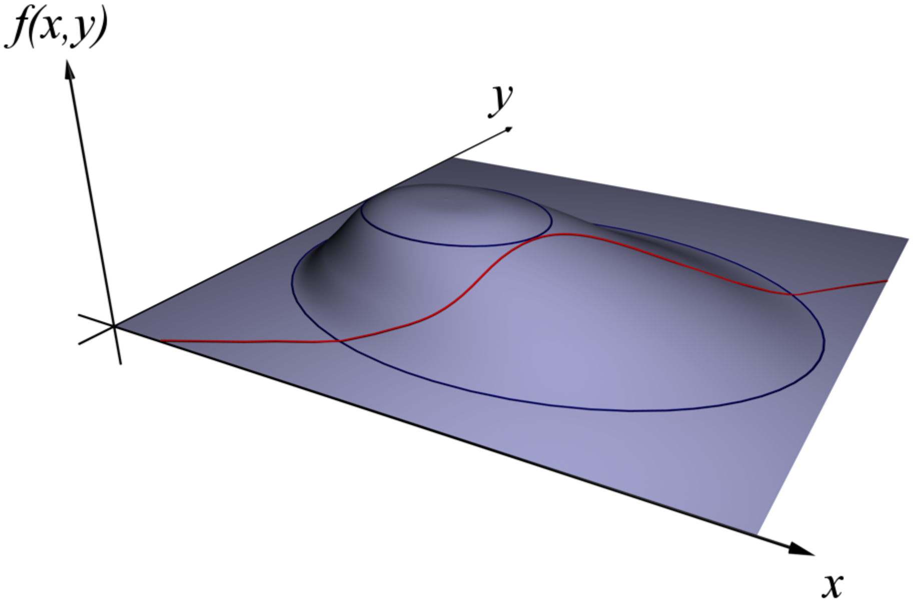


Figure 26.16: Find x and y to maximize $f(x, y)$ subject to a constraint (shown in red) $g(x, y) = c$.

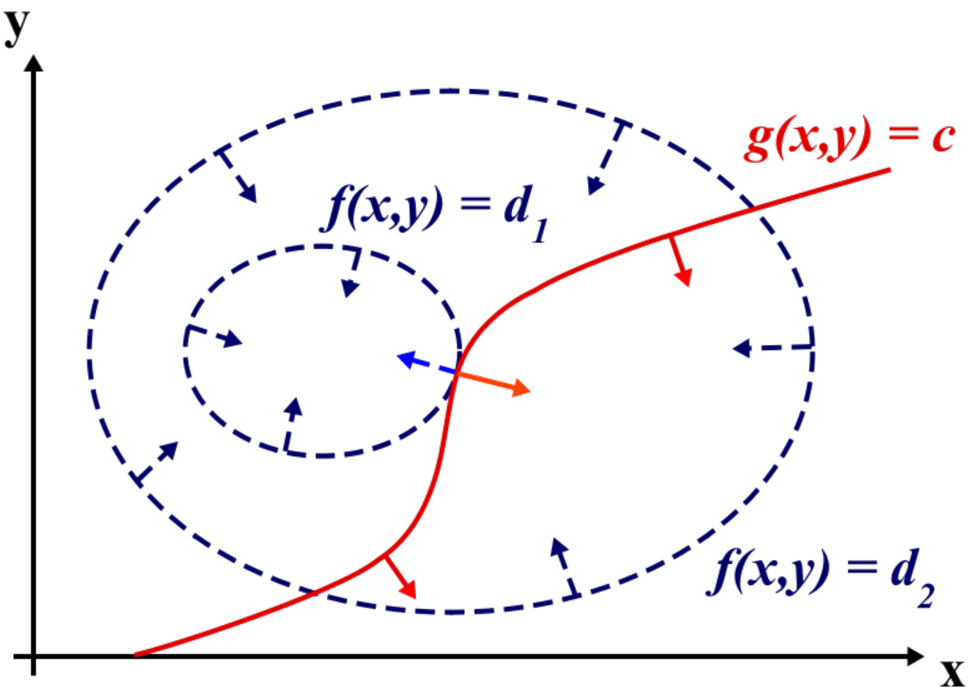


Figure 26.17: Lagrange multipliers.

Gist

Optimization of functions (models) with real numbers as input parameters is an old area, starting approximately during the second world war, and now reaching high levels of sophistication. The purpose is to design **automated techniques to identify inputs leading to maximum (or minimum) output values**.

In spite of the mathematical sophistication, the basis of most optimization techniques is very understandable, even if you do not remember anything from your courses in calculus (the mathematical study of change). A **drop of water** fallen from the sky reaches the sea without any conscious mathematical finesse.

The basic steps are as follows. Start from an initial value for the input parameters. Apply small local changes to the various inputs and test their effects (are they leading to higher or smaller output values?). Based on the test results decide whether to accept the local change or not. Repeat until there is progress, leading to better and better output values.

If one can calculate *derivatives*, one has a simple way to predict the effect of small local changes. In fact, you can consider the **derivative as a local predictor of change**. If the step is sufficiently small, the approximation "*change equals derivative times step*" tends to be very good. If derivatives are not available, one can test small changes directly (like in RAS) and keep **locally adapted models** to reduce wasted function evaluations. Local adaptation occurs by **learning from the previous steps of the search**.

Understanding the principles, even without math theorems, is sufficient to use optimization software with competence, and to avoid most pitfalls. After all, you do not need calculus and mathematical analysis to ski without falling down and with a reasonable guarantee to reach your gondola ski lift.

Part IV

Learning for intelligent optimization

Chapter 27

Reactive Search Optimization (RSO): Online Learning Methods

This then is the first duty of an educator:
to stir up life but leave it free to develop
(Maria Montessori)

After considering basic Local Search and memory-less (Markovian) search, this chapter presents the more advanced schemes for using machine learning to improve optimization,

In many cases a single relevant instance has to be solved, so that online learning schemes for optimization (**Reactive Search Optimization, RSO**) are of particular interest.

Even if the initial optimization problem is black-box, the more points are generated in input space and evaluated, the more knowledge is accumulated, in implicit form. Data about the past history of the search can be exploited to generate internal explicit models and improve the efficiency and effectiveness of the future optimization effort. In a way, RSO tends towards **truly intelligent problem-solving machines, which learn and self-improve the more they work**, in a way similar to humans, or similar to reactive biological systems. Think about the lifelong learning of a violinist, from the first mechanical and "symbolic" rule-based movements, to the real mastery of a Paganini.

The above figure shows an example in the history of bicycle design. Do not expect historical fidelity here, this book is about the LION way and not about bike technology. The first model is a starting solution with a single wheel, it works but it is not optimal yet. The second model is a randomized attempt to add some pieces to the original design, the situation is worse. One could revert back to the initial model and start other changes. But let's note that, if one *insists* and proceeds with a second addition, one may end up with the third model, clearly superior from a usability and safety point of view. This story has a lesson: **local search by small perturbations is a tasty ingredient but additional spices are in certain cases needed** to obtain superior results.

Reactive Search Optimization (RSO) advocates the integration of online machine learning techniques into optimization heuristics. The word *reactive* hints at a ready response to events during the search through an internal feedback loop for **online self-tuning and dynamic adaptation**. In RSO the past history of the search and the knowledge accumulated while moving in the configuration space is used for self-adaptation in an automated manner: the algorithm maintains the internal flexibility needed to address different situations during the search, but the adaptation is automated, and executed *while* the algorithm runs on a single instance and reflects on its past experience. Machine learning is therefore an essential ingredient in the RSO soup, as illustrated in Fig. 27.1.

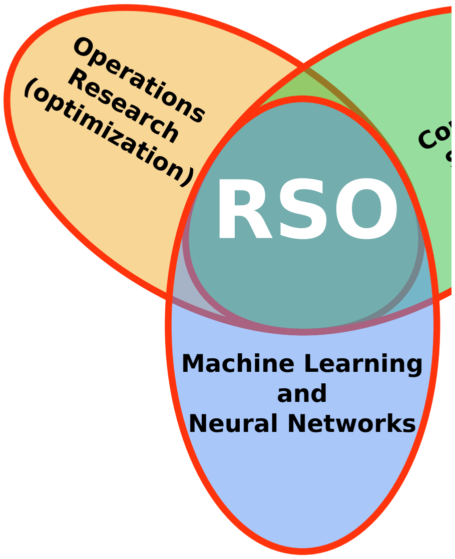


Figure 27.1: RSO is at the intersection of optimization, computer science (algorithms and data structures) and machine learning.

Reactive Search Optimization adopts ideas and methods from machine learning and statistics, in particular reinforcement learning, active or query learning, and neural networks. Let's note that the effort towards adaptive and self-tuning optimization schemes is deeply rooted also in the generation of adaptive probability density functions in stochastic global optimization (Chapter 25) or in the use of derivative-based local models in continuous optimization (Chapter 26). RSO deals with the systematic application of ML into optimization, also for solving a single instance!

The following sections are mostly dedicated to discrete optimization, but with some examples also for functions of real variables. After an introduction (Sec. 27.1), we present some notable ways of reacting from the search history to affect different parameters or critical choices of the search mechanism, in particular reacting on temporary prohibition periods (Sec. 27.2), adapting the neighborhood in variable-neighborhood search (Chapter 28), iterating local search to escape from an attractor (Chapter 29), self-tuning the temperature in Simulated Annealing (Chapter 30), dynamically adapting fitness surfaces or the amount of stochasticity (Chapter 31).

27.1 RSO: Learning while searching

Let's cite the main motivations for passing from simple local search to Reactive Search Optimization, by summarizing the more extended presentations of the subject [25, 27, 26].

Many problem-solving methods are characterized by a certain number of **choices and free parameters**, whose appropriate setting and tuning is complex. In some cases the parameters are tuned through a feedback loop that includes **the user as a crucial learning component**: different options are developed and tested until acceptable results are obtained. The quality of results is not automatically transferred to different instances and the feedback loop can require a slow "trial and error" process when the algorithm has to be tuned for a specific application. In Machine Learning a rich variety of "design principles" is available that can be used in the area of parameter tuning and optimal choice for heuristics. The lack of human intervention does not imply higher unemployment rates for researchers. On the contrary, one is now loaded with a heavier task: **the algorithm developer must transfer his intelligent expertise into the algorithm** itself, a task that requires the exhaustive description of the tuning phase in the algorithm. The algorithm complexity will increase, but the price is worth paying if the two following objectives are reached.

- **Reproducibility of results** through complete and unambiguous documentation. The algorithm becomes self-contained and its quality can be judged independently from the designer or specific user. This requirement is particularly important for science, in which objective evaluations are crucial. The widespread usage of software archives further simplifies the test and simple re-use of heuristic algorithms.

- **Automation**. The time-consuming handmade tuning phase is now substituted by an automated process, as illustrated in Fig. 27.2. Let us note that only the final user will typically benefit from an automated tuning process. On the contrary, the algorithm designer faces a longer and harder development phase. There are no free meals: complexity does not disappear, it is only shifted from the decision maker to the method (and software) designer.

The metaphors for Reactive Search Optimization derive mostly from the individual human experience. Its motto is "**learning on the job**." As already mentioned, real-world problems have a rich structure. While many alternative solutions are tested in the exploration of a search space, patterns and regularities appear. The human brain quickly learns and drives future decisions based on previous observations. This is the main inspiration source for inserting online machine learning techniques into the optimization engine of RSO. Memetic algorithms share a similar focus on learning, although their concentration is on cultural evolution, describing how societies develop over time, more than on the capabilities of a single individual.

Nature and biology-inspired metaphors for optimization abound today. It is to some degree surprising that most of them derive from genetics and evolution, or from the emergence of collective behaviors from the interaction of simple living organisms which are mostly hard-wired with little or no learning capabilities. One almost wonders whether this is related to ideological prejudices in the spirit of Jean-Jacques Rousseau, who believed that man was good when in the state of nature but is corrupted by society, or in the spirit of the "evil man against nature" principle of commercial Hollywood B-movies. Metaphors can lead us astray from our main path: we are strong supporters of a pragmatic approach, **an algorithm is effective if it solves a problem in a competitive manner without requiring an expensive tailoring**, not because it corresponds to one's favorite elaborate, fanciful or sexy analogies. Furthermore, at least for a researcher, in most cases an algorithm is of scientific interest if there are ways to analyze its behavior and explain *why and when* it is effective. Seminal papers related to using memory in a strategic manner to guide heuristics to continue exploration beyond local minima are the ones by Fred Glover about tabu search, scatter search and path relinking, and related metaheuristics, see for example [150], [153] and the amusing [152]. Other inspiring papers that

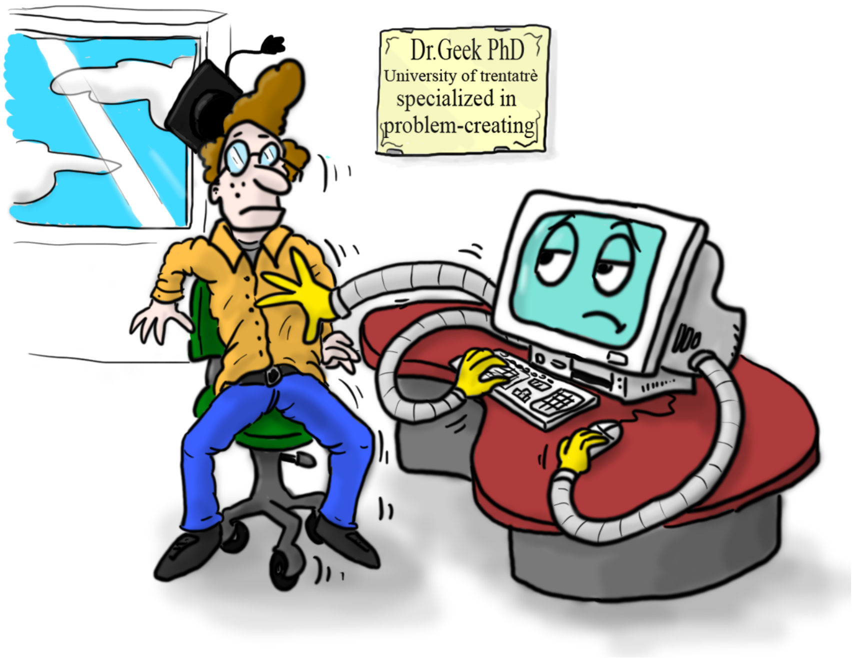


Figure 27.2: Algorithms with self-tuning capabilities like RSO make life simpler for the final user. Complex problem solving does not require technical expertise but is available to a much wider community of final users (adapted from [27]).

you may want to read to get a taste of related topics are [275] about memetic algorithms, [388] about evolving neural networks, [56] about meta-heuristics, and [200] about performance prediction and automated tuning.

27.2 RSO based on prohibitions

The idea of using **prohibitions to encourage creativity and diversification**, i.e., to encourage a decision maker, an engineer, or a designer, to consider radically new alternatives, is deeply rooted in the practice of research. Quoting from Konrad Lorenz, the Austrian Nobel-prize winner and creator of modern ethology, "*it is a good morning exercise for a research scientist to discard a pet hypothesis every day before breakfast. It keeps him young*." What a brilliant illustration of the fact that you want to *prohibit* the consideration of old solutions in order to be truly creative.

In the initial figure, one has to prohibit the consideration of monocycles and insist with local changes to eventually invent bicycles, although the process may include some intermediate inferior designs. Success is fueled by persistence and acceptance of repeated failure.

As mentioned above, local search generates a *trajectory* $X^{(t)}$ of points in the admissible search space. The successor of a point X is selected from a *neighborhood* $N(X)$ that associates to the current point X a subset of $\mathcal{X}$. A point X is *locally optimal with respect to* N, or a *local minimum* if: $f(X) \leq f(Y)$ for all $Y \in N(X)$. For the following discussion we consider the case in which $\mathcal{X}$ consists of binary strings with a finite length L: $\mathcal{X} = \{0,1\}^L$ and the neighborhood is obtained by applying the *elementary moves* $\mu_i (i = 1, ..., L)$ that change the i-th bit of the string $X = [x_1, ..., x_i, ..., x_L]$:

$$\mu_i([x_1, ..., x_i, ..., x_L]) = [x_1, ..., \bar{x}_i, ..., x_L]; \tag{27.1}$$

where $\bar{x}_i$ is the negation of the i-th bit: $\bar{x}_i \equiv (1 - x_i)$.

To avoid entrapment in local attraction basins, one can bias the search toward points with low f values but incorporate **reactive prohibition strategies** to discourage the repetitions of already-visited configurations. Local moves are executed even if f increases with respect to the value at the current point, to exit from local minima of f. But soon as a move is applied, **the inverse move is temporarily prohibited** (the name "tabu search" derives from this prohibition).

In detail, at a given iteration t, the set of moves $\mathcal{M}$ is partitioned into the set $\mathcal{T}^{(t)}$ of the *tabu* moves, and the set $\mathcal{A}^{(t)}$ of the admissible moves. Superscripts with parenthesis are used for quantities that depend on the iteration. At the beginning, the search starts from an initial configuration $X^{(0)}$, that is generated randomly, and all moves are admissible: $\mathcal{A}^{(0)} = \mathcal{M}$, $\mathcal{T}^{(0)} = \emptyset$. The search trajectory $X^{(t)}$ is then generated, by applying the best admissible move $\mu^{(t)}$ from the set $\mathcal{A}^{(t)}$:

$$X^{(t+1)} = \mu^{(t)}(X^{(t)}) \quad \text{where} \quad \mu^{(t)} = \arg \min_{\nu \in \mathcal{A}^{(t)}} f(\nu(X^{(t)})).$$

In isolation, the "modified greedy search" principle *can* generate cycles. For example, if the current point $X^{(t)}$ is a strict local minimum, the cost function at the next point must increase: $f(X^{(t+1)}) = f(\mu^{(t)}(X^{(t)})) > f(X^{(t)})$, and there is the possibility that the move at the next step will be its *inverse* ($\mu^{(t+1)} = {\mu^{(t)}}^{-1}$) so that the state after two steps will come back to the starting configuration

$$X^{(t+2)} = \mu^{(t+1)}(X^{(t+1)}) = {\mu^{(t)}}^{-1} \circ \mu^{(t)}(X^{(t)}) = X^{(t)}.$$

At this point, if the set of admissible moves is the same, the system will be trapped forever in a cycle of length 2. In this example, the cycle is avoided if the inverse move ${\mu^{(t)}}^{-1}$ is prohibited at time $t+1$. In general, the inverses of the **moves executed in the most recent part of the search are prohibited for a period** T. For binary strings a move coincides with its inverse: a move is prohibited if and only if its most recent use has been at time $\tau \geq (t - T^{(t)})$. The period is finite because the prohibited moves can be necessary to reach the optimum in a later phase of the search. In prohibition-based-RSO (tabu-RSO for short) the prohibition period $T^{(t)}$ is time-dependent.

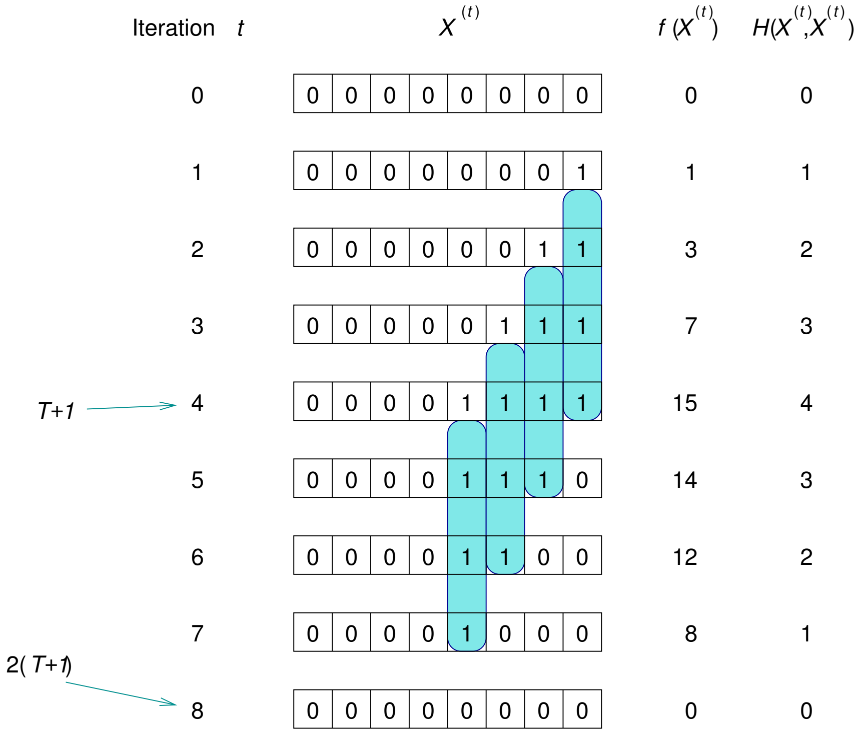
The diversification effect of prohibiting moves on the search trajectory has been clarified by the **fundamental relationships between prohibition and diversification** demonstrated by Battiti in [42]. Let $H(X,Y)$ be the Hamming distance between two strings X and Y, defined as the number of corresponding bits that are different in the two strings. Now, if only allowed moves are executed, and T satisfies $T \leq (n-2)$, which guarantees that at least two moves are allowed at each iteration, one obtains the following.

- The Hamming distance H between a starting point and successive points along the trajectory is strictly increasing for $T+1$ steps:
$$H(X^{(t+\tau)}, X^{(t)}) = \tau \quad \text{for} \quad \tau \leq T+1.$$
- The minimum repetition interval R along the trajectory is $2(T+1)$:
$$X^{(t+R)} = X^{(t)} \;\Rightarrow\; R \geq 2(T+1).$$

The above relationships clearly show how **the prohibition is related to the amount of diversification**: the larger T, the larger is the distance H that the search trajectory must travel before it is allowed to come back to a previously visited point. But T cannot be too large, otherwise a shrinking number of moves will be allowed after an initial phase, leading to less freedom of movement.

The demonstration of the relationships is immediate as soon as one notices that, after a bit is changed, it is "frozen" for the next T iterations. To visualize this behavior, Fig. 27.3 shows the evolution of the configuration $X^{(t)}$, when the function to be optimized is given by $f(X) \equiv \ number(X)$, where $number(X)$ is obtained by considering X as the standard binary encoding of an integer number. The prohibition T is equal to three.

In a physical analogy, as soon as a bit is changed, an *ice cube* is placed on it so that it will not be changed during the future T iterations. When the period T elapses, the ice cube melts down and the bit can be changed again. The situation in which a bit is "frozen" and cannot be changed is shown with a shaded box in Fig. 27.3. In the example, the configuration starts with the all-zero string, a locally optimal point. At iteration 0, the best move changes the least



Iteration t	$X^{(t)}$								$f(X^{(t)})$	$H(X^{(t)},X^{(t)})$
0	0	0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	1	1	1
2	0	0	0	0	0	0	1	1	3	2
3	0	0	0	0	0	1	1	1	7	3
4	0	0	0	0	1	1	1	1	15	4
5	0	0	0	0	1	1	1	0	14	3
6	0	0	0	0	1	1	0	0	12	2
7	0	0	0	0	1	0	0	0	8	1
8	0	0	0	0	0	0	0	0	0	0

Figure 27.3: An example of the relationship between prohibition T, and diversification measured by the Hamming distance $H(X^{(t)}, X^{(0)})$. T = 3 in the example. Figure adapted from [42].

significant bit. At iteration 1 the least significant bit is frozen and the best *allowed* move changes the second bit. The maximum Hamming distance is reached at iteration $(T+1)$, then the distance decreases and the initial configuration is repeated at iteration $2(T+1)$. When a cycle like the one above is generated, the set of configurations visited during the initial part, up to $H = T+1$, is *different* from the set visited when H decreases back toward zero. In other words, the trajectory looks like **a lasso around a local optimum**, and one does not waste CPU time to revisit previously visited configurations. In general, after visiting a locally optimal point, better values can be obtained by visiting other local optima. Of course, as soon as a local minimizer is found, all points in its *attraction basin* (i.e., all points that are mapped to the given minimizer by the local search dynamics) are not of interest. In fact, by definition, their f value is equal to or larger than the value at the local minimizer. The value of T should be chosen so that a new attraction basin leading to a new and possibly better local minimizer can be reached after reaching Hamming distance $T+1$.

Because the minimal Hamming distance required (a sort of *attraction radius* for the given attraction basin) is not known, one should **determine T in a reactive way**, by learning the proper value *while* the search executes. The basic prohibition mechanism cannot guarantee the absence of cycles [37, 40]. In addition, the choice of a fixed T without *a priori* knowledge about the possible search trajectories that can be generated in a given $(\mathcal{X}, f)$ problem is difficult. If the search space is inhomogeneous, a size T that is appropriate in a region of $\mathcal{X}$ may be inappropriate in other regions. For example, T can be too small and insufficient to avoid cycles, or too large, so that only a small fraction of the movements are admissible and the search is inefficient.

Tabu-RSO uses a simple mechanism to change T during the search so that the value $T^{(t)}$ is appropriate to the local structure of the problem (therefore the term “reactive”). The underlying design principle is that of determining, for a given local configuration, **the minimal prohibition value which is sufficient to escape** from an attraction basin around a minimizer, as illustrated in Fig. 27.4. The basic principle is that T is equal to one at the beginning (only immediately returning to a just left configuration is prohibited), T increases if the trajectory is *trapped* in an attraction basin around a local optimum (repetitions of previously visited configuration can signal this situation), and T decreases if unexplored search regions are visited, leading to different local optima. If the problem is so simple that a single local optimum is present, and therefore it coincides with the global optimum, the power of tabu-RSO is not needed, although not dangerous. Tabu-RSO will simply discover the optimal solution, save it, and then search for an (impossible) improvement. It has to be noted that most real-world problems are infested with many locally optimal points, so that tabu-RSO is crucial to transform a local search building block into an effective and efficient solver.

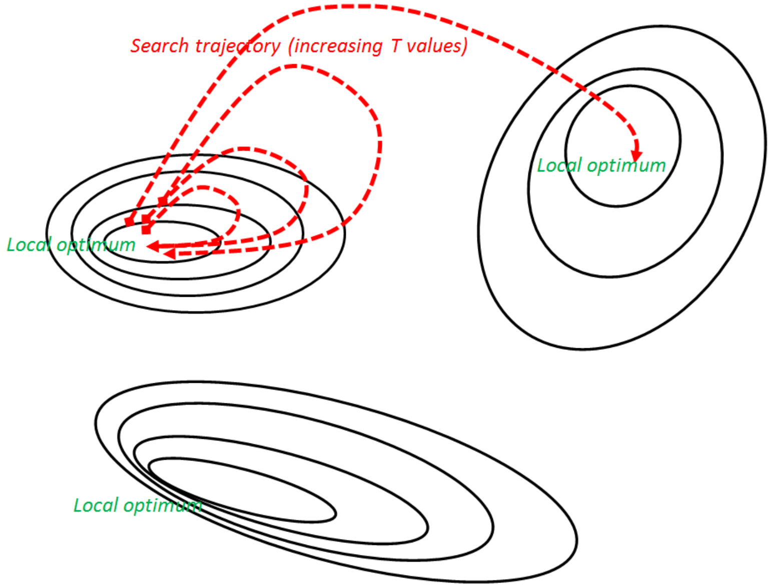


Figure 27.4: RSO with prohibitions in action. Three locally optimal points are shown together with contour lines of the function to be optimized. When starting from a locally optimal point, RSO executes loops which reach bigger and bigger distances from the attractor, until another attraction basin is encountered (if present).

The overhead (additional CPU time and memory) introduced by the reactive mechanisms is of small number of CPU cycles and bytes, approximately constant for each step in the search process. By using *hashing* functions[1] to store and retrieve the relevant data, the additional memory required can be reduced to some bytes per iteration, while the time is reduced to that needed to calculate a memory address from the current configuration and to execute a small number of comparisons and updates of variables [37]. RSO with prohibitions has been used for problems ranging from combinatorial optimization to the minimization of continuous functions and to sub-symbolic machine learning tasks, a partial list is contained in [26].

[1] Hashing is a nice trick — although maybe not well known outside of the computer science community — to create *dictionaries* (associations of data with keywords), so that retrieval is fast and approximately constant-time, on average. A *hash function* is a deterministic procedure that takes an arbitrary block of data (in our case the keyword) and returns a limited-size integer, the hash value, such that a change to the data will typically change the hash value. The obtained integer can be used as a memory *address* to store the block of data, so that lookup is immediate: get the hash value and go the memory address to read the data. Technical details related to having different keywords sharing by chance the same address can be resolved by *chaining*, i.e., associating a linked list of data items with the memory address.

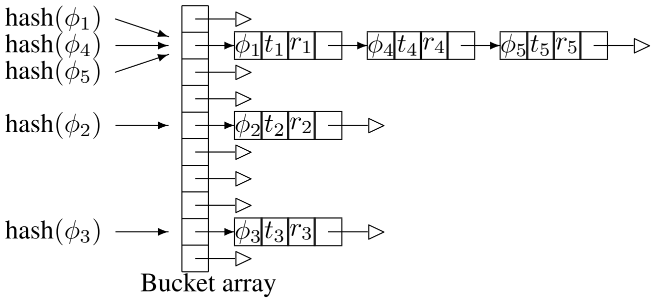


Figure 27.5: Open hashing scheme: items (configuration, or compressed hashed value, etc.) are stored in "buckets." The index of the bucket array is calculated from the configuration.

27.3 Fast data structures for using the search history

The storage and access of the past events is executed through the well-known *hashing* or radix-tree techniques in a CPU time that is approximately constant with respect to the number of iterations. Therefore the overhead caused by the use of the history is negligible for tasks requiring a non-trivial number of operations to evaluate the cost function in the neighborhood.

An example of a memory configuration for the hashing scheme is shown in Fig. 27.5. From the current configuration phi one obtains an index into a "bucket array." The items (configuration or hashed value or derived quantity, last time of visit, total number of repetitions) are then stored in linked lists starting from the indexed array entry. Both storage and retrieval require an approximately constant amount of time if: i) the number of stored items is not much larger than the size of the bucket array, and ii) the hashing function scatters the items with a uniform probability over the different array indices. More precisely, given a hash table with m slots that stores n elements, a load factor $\alpha = n/m$ is defined. If collisions are resolved by chaining, searches take $O(1 + \alpha)$ time, on average.

27.3.1 Persistent dynamic sets

Persistent dynamic sets are proposed to support memory–usage operations in history-sensitive heuristics in [24, 22].

Ordinary data structures are *ephemeral* [119], meaning that when a change is executed the previous version is destroyed. Now, in many contexts like computational geometry, editing, implementation of very high level programming languages, and, last but not least, the context of history-based heuristics, multiple versions of a data structure must be maintained and accessed. In particular, in heuristics one is interested in *partially persistent* structures, where all versions can be accessed but only the newest version (the *live* nodes) can be modified. A review of *ad hoc* techniques for obtaining persistent data structures is given in [119] that is dedicated to a systematic study of persistence, continuing the previous work of [285].

Hashing combined with persistent red-black trees

The basic observation is that, because Tabu Search is based on local search, configuration $X^{(t+1)}$ differs from configuration $X^{(t)}$ only because of the addition or subtraction of a single index (a single bit is changed in the string). It is therefore reasonable to expect that more efficient techniques can be devised for storing *a trajectory of chained configurations* than for storing arbitrary states. The expectation is indeed true, although the techniques are not for beginners. You are warned, proceed only if not scared by advanced data structures.

Let us define the operations INSERT(i) and DELETE(i) for inserting and deleting a given index i from the set. As cited above, configuration X can be considered as a set of indices in $[1, L]$ with a possible realization as a balanced red-black tree, see [46, 166] for two seminal papers about red-black trees. The binary string can be immediately obtained from the tree by visiting it in symmetric order, in time $O(L)$. INSERT(i) and DELETE(i) require $O(\log L)$ time, while at most a single node of the tree is allocated or deallocated at each iteration. Re-balancing the tree after insertion or deletion can be done in $O(1)$ rotations and $O(\log L)$ color changes [357]. In addition, the amortized number of color changes per update is $O(1)$, see for example [259].

Now, the REM method [148, 149] is closely reminiscent of a method studied in [285] to obtain partial persistence, in which the entire update sequence is stored and the desired version is rebuilt from scratch each time an access is performed, while a systematic study of techniques with better space-time complexities is present in [312, 119]. Let us now summarize from [312] how a partially persistent red-black tree can be realized. An example of the realizations that we consider is presented in Fig. 27.6.

The trivial way is that of keeping in memory all copies of the ephemeral tree (see the top part of Fig. 27.6), each copy requiring $O(L)$ space. A smarter realization is based on *path copying*, independently proposed by many researchers, see [312] for references. Only the path from the root to the nodes where changes are made is copied: a set of search trees is created, one per update, having different roots but sharing common subtrees. The time and space complexities for INSERT(i) and DELETE(i) are now of $O(\log L)$.

The method that we will use is a space-efficient scheme requiring only linear space proposed in [312]. The approach avoids copying the entire access path each time an update occurs. To this end, each node contains an additional "extra" pointer (beyond the usual left and right ones) with a time stamp. When attempting to add a pointer to a node, if the extra pointer is available, it is used and the time of the usage is registered. If the extra pointer is already used, the node is copied, setting the initial left and right pointers of the copy to their latest values. In addition, a pointer to the copy is stored in the last parent of the copied node. If the parent has already used the extra pointer, the parent, too, is copied. Thus copying proliferates through successive ancestors until the root is copied or a node with a free extra pointer is encountered. Searching the data structure at a given time t in the past is easy: after starting from the appropriate root, if the extra pointer is used the pointer to follow from a node is determined by examining the time stamp of the extra pointer and following it if and only if the time stamp is not larger than t. Otherwise, if the extra pointer is not used, the normal left-right pointers are considered. Note that the pointer direction (left or right) does not have to be stored: given the search tree property it can be derived by comparing the indices of the children with that of the node. In addition, colors are needed only for the most recent (live) version of the tree. In Fig. 27.6 NULL pointers are not shown, colors are correct only for the live tree (the nodes reachable from the rightmost root), extra pointers are dashed and time-stamped.

The worst-case time complexity of INSERT(i) and DELETE(i) remains $O(\log L)$, but the important result derived in [312] is that the amortized space cost per update operation is $O(1)$. Let us recall that the total amortized space cost of a sequence of updates is an upper bound on the actual number of nodes created.

Let us now consider the context of history-based heuristics. Contrary to the popular usage of persistent dynamic sets to search past versions at a specified time t, one is interested in checking whether a configuration has already been encountered in the previous history of the search, at *any* iteration.

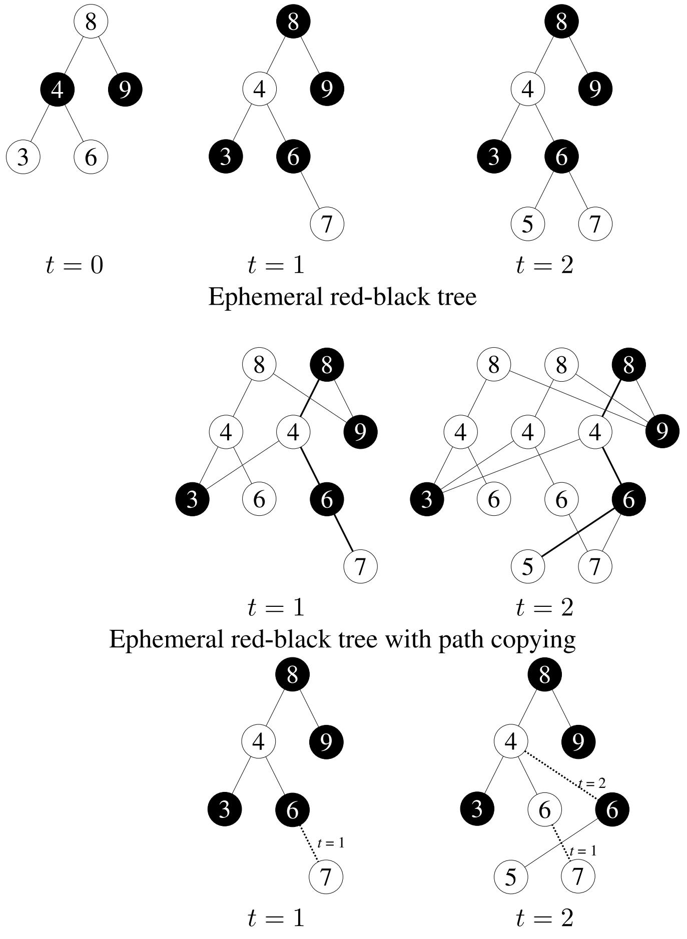
A convenient way of realizing a data structure supporting X-SEARCH(X) is to combine *hashing* and *partially persistent dynamic sets*, see Fig. 27.7. From a given configuration X an index into a "bucket array" is obtained through a hashing function, with a possible incremental evaluation in time $O(1)$. Collisions are resolved through chaining: starting from each bucket header there is a linked list containing a pointer to the appropriate root of the persistent red-black tree and satellite data needed by the search (time of configuration, number of repetitions).

As soon as configuration $X^{(t)}$ is generated by the search dynamics, the corresponding persistent red-black tree is updated through INSERT(i) or DELETE(i). Let us now describe X-SEARCH$(X^{(t)})$: the hashing value is computed from $X^{(t)}$ and the appropriate bucket searched. For each item in the linked list the pointer to the root of the past version of the tree is followed and the old set is compared with $X^{(t)}$. If the sets are equal, a pointer to the item on the linked list is returned. Otherwise, after the entire list has been scanned with no success, a NULL pointer is returned.

In the last case a new item is linked in the appropriate bucket with a pointer to the root of the live version of the tree (X-INSERT(X, t)). Otherwise, the last visit time t is updated and the repetition counter is incremented.

After collecting the above cited complexity results, and assuming that the bucket array size is equal to the maximum number of iterations executed in the entire search, it is straightforward to conclude that each iteration of *reactive-TS* requires $O(L)$ average-case time and $O(1)$ amortized space for storing and retrieving the past configurations and for establishing prohibitions.

In fact, both the hash table and the persistent red-black tree require $O(1)$ space (amortized for the tree). The worst-case time complexity per iteration required to update the current $X^{(t)}$ is $O(\log L)$, the average-case time for searching and updating the hashing table is $O(1)$ (in detail, searches take time $O(1 + \alpha)$, α being the load factor, in our case upper bounded by 1). The time is therefore dominated by that required to compare the configuration $X^{(t)}$ with that obtained through X-SEARCH$(X^{(t)})$, i.e., $O(L)$ in the worst case. Because $\Omega(L)$ time is needed during the neighborhood evaluation to compute the f values, the above complexity is optimal for the considered application to history-based heuristics.



Ephemeral red-black tree

Ephemeral red-black tree with path copying

Ephemeral red-black tree with limited node copying

Figure 27.6: How to obtain a partially persistent red-black tree from an ephemeral one (top), containing indices 3,4,6,8,9 at t=0, with subsequent insertion of 7 and 5. Path copying (middle), with thick lines marking the copied part. Limited node copying (bottom) with dashed lines denoting the “extra” pointers with time stamp.

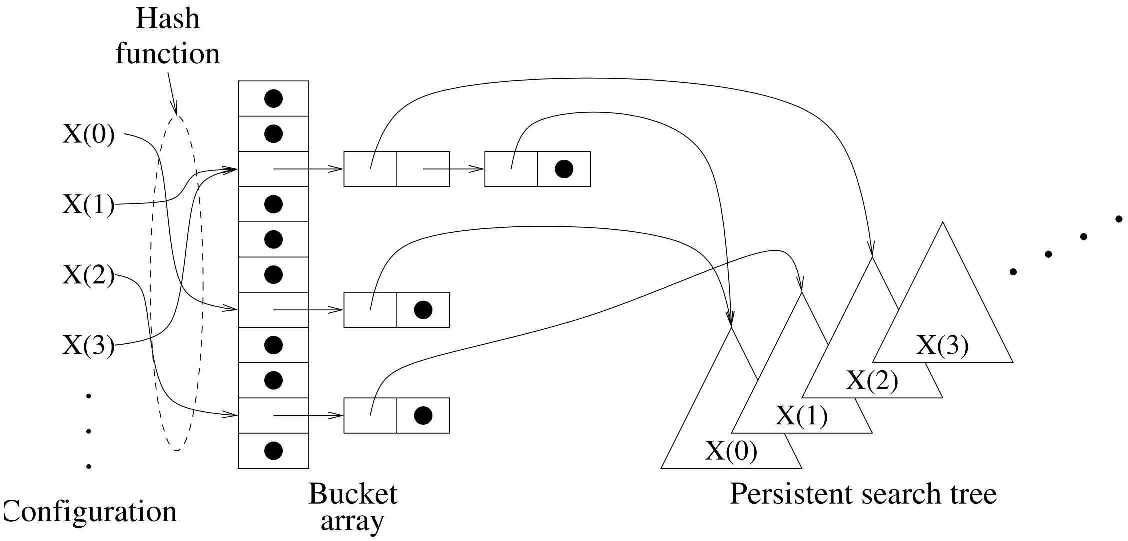


Figure 27.7: Open hashing scheme with persistent sets: a pointer to the appropriate root for configuration $X^{(t)}$ in the persistent search tree is stored in a linked list at a "bucket." Items on the list contain satellite data. The index of the bucket array is calculated from the configuration through a hashing function.

Gist

Reactive Search Optimization (RSO) uses learning and adaptation during the optimization process, so that the search technique can be fine-tuned to the instance being solved and to the local characteristics around the current tentative solution. RSO deals with designing **an intelligent module overseeing the basic local search process**, balancing diversification and intensification, optimizing components of the optimization process itself (meta-optimization or meta-heuristics).

Reactive Search Optimization **adapts in an online manner meta-parameters of heuristics**. In particular prohibition mechanisms ("stay away from this area") can be used to encourage diversification and discovery of improving solutions. It is well known that real creativity and innovation requires staying away from current solutions ("lateral thinking", "out-of-the-box thinking" are popular terms in the management literature). In a similar manner, prohibition mechanisms added to simple local-search schemes can be a very direct manner to continue the search beyond local optimality.

Reactive Search Optimization schemes require **saving and retrieving past configurations**, operations which can be very fast with appropriate data structures.

Let's note that the term reactive as "**readily responsive to a stimulus**" used in our context is not in contrast with proactive as "acting in anticipation of future problems, needs, or changes." In fact, in order to obtain a reactive algorithm, the designer needs to be proactive by appropriately planning modules into the algorithm, to endow it with the capability of autonomous response. In other words, **Reactive Search Optimization algorithms need proactive algorithm designers**.

Chapter 28

Adapting neighborhoods and selection

Speak through me, O Muse,
of that man of many devices
who wandered much
once he'd sacked the sacred citadel of Troy.
(Odyssey by Homer, as translated by Stein,
Charles)

It looks like there is little online learning to be considered for a simple technique like local search. Nonetheless, we already encountered a first possibility, that of prohibiting some local moves in Chapter 27. This chapter considers a more structured organization of the possible local moves. Various possible moves are collected into a set of different neighborhoods, which are chosen in a strategic manner depending on the current state of the search.

As a mythological analogy consider how Odysseus (or Ulysses in Roman myths) escaped from the Sirens, beautiful yet dangerous creatures, who lured nearby sailors with their enchanting music and voices to shipwreck on the rocky coast of their island. He had all of his sailors plug their ears with beeswax and tie him to the mast. He ordered his men to leave him tied tightly to the mast, no matter how much he would beg. What a nice analogy of the effort and different set of moves required to escape from the attraction of a local minimum.

Let's recollect the building block of local search considered in Section 24.2 In the function IMPROVING-NEIGHBOR one has to decide about a *neighborhood* (a set of local moves to be applied) and about a *way to pick one of the neighbors* to be the next point along the search trajectory. Selecting a **neighborhood structure appropriate to a given problem** is the most critical issue in LS. Let's concentrate on *online* learning strategies which can be applied *while* local search runs on a specific instance. They can be applied in two contexts: selection of the neighbor or selection of the neighborhood.

Let's start from the first context where a neighborhood is chosen before the run is started, and only the selection of an improving neighbor is dynamic. The average progress in the optimization per unit of computational effort (the average "speed of descent" Δf_{best} per second) will depend on two factors: the average *improvement per move* and the average *CPU time per move*. There is a trade-off: the longer to evaluate the neighborhood, the better the chance of identifying a move with a large improvement, but the shorter the total number of moves which one can execute in the CPU time allotted. The optimal setting depends on the problem, the specific instance, and the local configuration of the f landscape.

The immediate brute-force approach consists of considering **all neighbors**, by applying all possible basic moves, evaluating the corresponding f values and moving to the neighbor with the best value, breaking ties randomly if they occur. The best possible neighbor is chosen at each step. To underline this fact, the term "**best-improvement** local search" is used.

A second possibility consists of evaluating **a sample of the possible moves**, a subset of neighbors. In this cases IMPROVING-NEIGHBOR can return the first candidate with a better f value. This option is called **first-move**. If no such candidate exists the trajectory is at a local optimum. A randomized examination order can be used to avoid spurious effects. FIRSTMOVE is clearly adaptive: the exact number of neighbors evaluated before deciding the next move depends not only on the instance but on the particular local properties in the configuration space around the current point. One expects to evaluate a small number of candidates the early phase of the search, whereas identifying an improving move will become more and more difficult during the later phases, close to local optimality. The analogy is that of learning a new language: the progress is fast at the beginning but it gets slower and slower after reaching an advanced level. To summarize, FIRSTMOVE works according to "keep evaluating until either an improving neighbor is found or all neighbors have been examined".

28.1 Variable Neighborhood Search: Learning the neighborhood

There are cases when the definition of a *fixed* neighborhood for a problem is not an optimal choice because **adapting the neighborhood to the local configuration** around the current point is beneficial.

A possible way of tuning the neighborhood considers **a set of neighborhoods**, defined *a priori* at the beginning of the search, and then aims at using the most appropriate one during the search, as illustrated in Fig. 28.1. This is the seminal idea of the Variable Neighborhood Search (VNS) technique, see [171].

Let the set of neighborhoods be $\{N_1, N_2, ..., N_{kmax}\}$. A proper VNS strategy has to deal with the following issues:

1. Which neighborhoods to use and how many of them. Larger neighborhoods may include smaller ones or be disjoint.

2. How to schedule the different neighborhoods during the search (order of consideration, transitions between different neighborhoods)

3. Which neighborhood evaluation strategy to use (first move, best move, sampling, etc.)

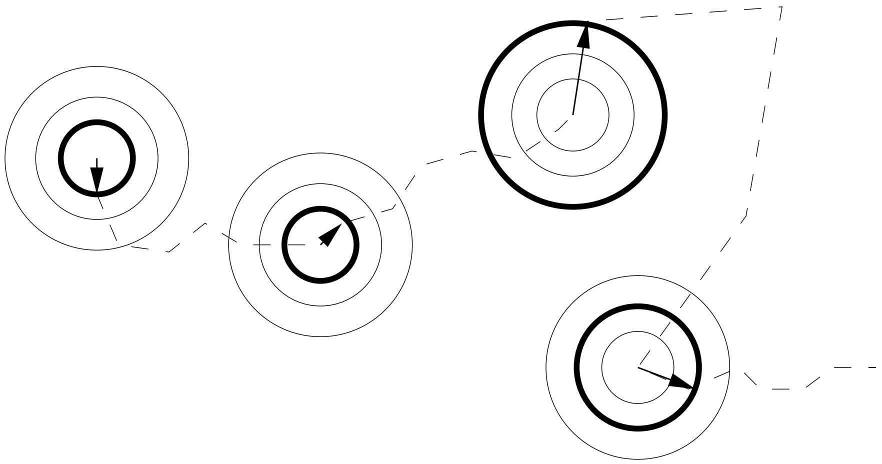


Figure 28.1: Variable neighborhood search: the used neighborhood ("circle" around the current configuration) varies along the search trajectory.

The first issue can be decided based on detailed problem knowledge, preliminary experimentation, or simply availability of off-the-shelf software routines for the efficient evaluation of a set of neighborhoods.

The second issue leads to a range of possible techniques. A simple implementation can just **cycle randomly among the different neighborhoods** during subsequent iterations: no online learning is present but possibly more robustness for solving instances with very different characteristics or for solving an instance where different portions of the search space have widely different characteristics.

Let's note that **local optimality depends on the neighborhood**: as soon as a local minimum is reached for a specific N_k, improving moves can in principle be found in other neighborhoods N_j with $j \neq k$. A possibility to use online learning is based on the principle "**intensification first, minimal diversification only if needed**" which we often encounter in heuristics [37]. One orders the neighborhoods according to their *diameter*, or to the *strength* of the perturbation executed. For example, if the search space is given by binary strings, one may consider as N_1 all changes of a single bit, N_2 all changes of two bits, etc. If local search makes progress one sticks to the default neighborhood N_1. As soon as a local minimum with respect to N_1 is encountered one tries to go to greater Hamming distances from the current point aiming at discovering a nearby attraction basin, possibly leading to a better local optimum.

Fig. 28.2 illustrates the reactive strategy: point a corresponds to the local minimum, point b is the best point in neighborhood N_1, and point c the best point in N_2. The value of point c is still worse, but the point is in a different attraction basin so that a better point e could now be reached by the default local search. The best point d in N_3 is already improving on a.

From the example one already identifies two possible strategies. In both cases one uses N_1 until a local minimum of N_1 is encountered. When this happens one considers N_2, N_3, ... In the first strategy one stops when an improving neighbor is identified (point d in the figure). In the second strategy one stops when one encounters a neighbor in a different attraction basin with an improving local minimum (point c in the figure). How does one know that c is in a different basin? One can perform a local search run from it and of look at which point the local search converges.

For both strategies, one reverts back to the default neighborhood N_1 as soon as the *diversification* phase considering neighborhoods of increasing diameter is successful. Note a strong similarity with the design principle of Reactive Tabu Search, see Sec. 27.2, where diversification through prohibitions is activated when there is evidence of entrapment in an attraction basin and gradually reduced when there is evidence that a new basin has been discovered.

Many VNS schemes using the set of different neighborhoods in an organized way are possible [173]. Variable Neighborhood Descent (VND), see Fig. 28.3, uses the default neighborhood first, and the ones with a higher number

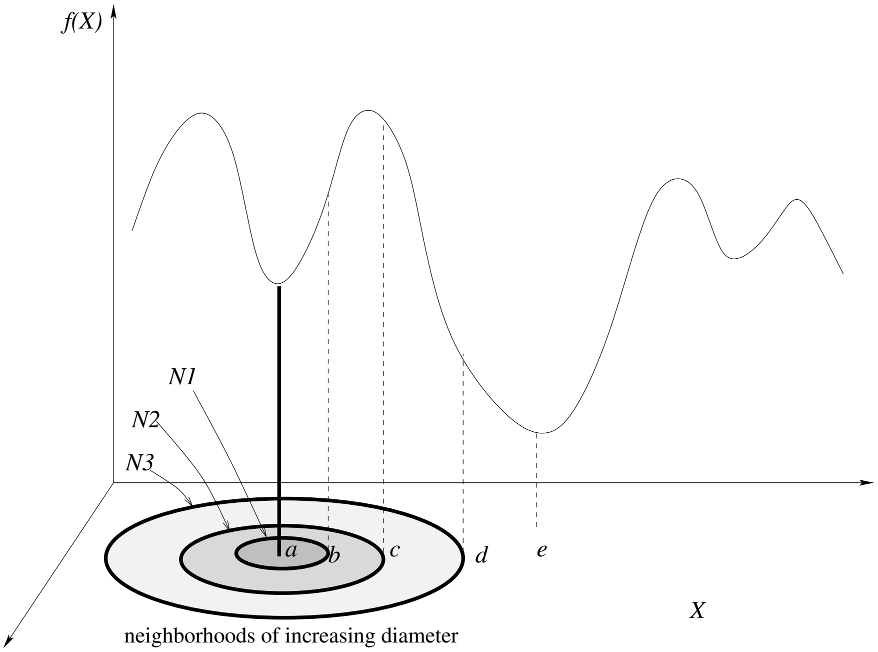


Figure 28.2: Variable neighborhoods of different diameters. Neighboring points are on the circumferences at different distances. The figure is intended to help the intuition: the actual neighbors considered in the text are discrete.

only if the default neighborhood fails (i.e., the current point is a local minimum for N_1), and only until an improving move is identified, after which it reverts back to N_1. When VND is coupled with an ordering of the neighborhoods according to the *strength* of the perturbation, one realizes the principle "**use the minimum strength perturbation leading to an improved solution**."

REDUCED-VNS is a stochastic version where only one random neighbor is generated before deciding about moving or not. Line 5 of Fig. 28.3 is substituted with:

$$X' \leftarrow \textsc{RandomExtract}(N_k(X))$$

SKEWED-VNS modifies the move acceptance criterion by **accepting also worsening moves if they lead the search trajectory sufficiently far** from the current point ("I am not improving but at least I keep moving without worsening too much during the diversification"), see Fig. 28.4. This version requires a suitable distance function $\rho(X, X')$ between two solutions to get controlled diversification (e.g., $\rho(X, X')$ can be the Hamming distance for binary strings), and it requires a *skewness* parameter α to regulate the trade-off between movement distance and willingness to accept worse values. By looking at Fig. 28.2, one is willing to accept the worse solution c because it is sufficiently far to possibly lead to a different attraction basin. Of course, determining an appropriate metric and skewness parameter is not a trivial task in general.

Other versions of VNS employ a stochastic move acceptance criterion, in the spirit of Simulated Annealing as implemented in the large-step Markov-chain version [264, 262], where "kicks" of appropriate strength are used to exit from local minima, see also Chapter 29 about Iterated Local Search.

An explicitly reactive-VNS is considered in [64] for the VRPTW problem (vehicle routing problem with time windows), where a construction heuristic is combined with VND using first-improvement local search. Furthermore, the objective function used by the local search operators is modified to consider the waiting time to escape from a local minimum. A preliminary investigation about a self-adaptive neighborhood ordering for VND is presented in [192].

```
function VariableNeighborhoodDescent ($N_1, \ldots, N_{k_{\max}}$)
    repeat until no improvement or max CPU time elapsed
        $k \leftarrow 1$                                  default neighborhood
        while $k \leq k_{\max}$:
            $X' \leftarrow$ BestNeighbor ($N_k(X)$)            neighborhood exploration
            if $f(X') < f(X)$
                $X \leftarrow X'$ ; $k \leftarrow 1$                   success: back to default neighborhood
            else
                $k \leftarrow k + 1$                         try with the following neighborhood
```

Figure 28.3: The VND routine. Neighborhoods with higher numbers are considered only if the default neighborhood fails and only until an improving move is identified. X is the current point.

```
function SkewedVariableNeighborhoodSearch ($N_1, \ldots, N_{k_{\max}}$)
    repeat until no improvement or max CPU time elapsed
        $k \leftarrow 1$                                  default neighborhood
        while $k \leq k_{\max}$
            $X' \leftarrow$ RandomExtract ($N_k(X)$)
            $X'' \leftarrow$ LocalSearch($X'$)                shake local search to reach local minimum
            if $f(X'') < f(X) + \alpha\rho(X, X'')$
                $X \leftarrow X''$ ; $k \leftarrow 1$                  success: back to default neighborhood
            else
                $k \leftarrow k + 1$                         try with the following neighborhood
```

Figure 28.4: The Skewed-VNS routine. Worsening moves are accepted provided that the change leads the trajectory sufficiently far from the starting point. X is the current point. $\rho(X, X'')$ measures the solution distance.

Ratings to the different neighborhoods are derived according to their observed benefits in the past and used periodically to order the various neighborhoods.

To conclude this section, let's note some similarities between VNS and the adaptation of the search region in stochastic search technique for continuous optimization. In both cases the neighborhood is adapted to the local position in the search space. In addition to many specific algorithmic differences, let's note that the set of neighborhoods is discrete in VNS while it consists of a portion of $\mathbb{R}^n$ for continuous optimization. Neighborhood adaptation in the continuous case, see for example the Reactive Affine Shaker algorithm [36] in Sec. 32.1, is considered to speed-up convergence to a local minimizer, not to jump to nearby valleys.

Gist

Local search heuristics build upon the definition of a suitable neighborhood (set of basic moves to apply to tentative solutions). Unfortunately, it is difficult to know *a priori* which neighborhood will produce the best results. In addition, configurations which are locally optimal for one neighborhood can be further improved by a different neighborhood.

Variable Neighborhood Search (VNS) organizes the neighborhoods as sets of different strengths (amount of perturbation), it uses the simplest neighborhood at the beginning, until a local minimum is reached. At this point, neighborhoods leading to bigger perturbations are tried. Like the flexible Ulysses, the man of many devices, rapidly adapts to new contexts to escape Polyphemus and the Sirens, **VNS adapts the neighborhood in a reactive fashion to the characteristics of a specific problem instance and to the local situation along the search trajectory** to escape locally optimal points.

VNS is a king of greedy strategy about the use of neighborhoods (therefore a kind of meta-greedy-strategy).

Chapter 29

Iterated local search

Our greatest weakness lies in giving up. The most certain way to succeed is always to try just one more time.
(Thomas A. Edison)

If a **local search "building block"** is available, for example as a concrete software toolkit, how can it be used by some upper layer coordination mechanism to get better results? An answer is given by *repeating* calls to the local search routine each time starting from a properly chosen configuration. If the starting configuration is random, one starts from scratch and discards knowledge about the previous searches. This trivial form actually is called simply **repeated local search**. It has no memory and just keeps trying, like the mythological Sisyphus, punished for his deceitfulness and forced to roll an immense boulder up a hill, only to watch it roll back down, repeating this action for eternity.

Learning implies that the previous history, for example the memory about the previously found local minima, is mined to produce better and better starting points. The implicit assumption is again that of a clustered distribution of local minima: determining good local minima is easier when starting from a local minimum with a low f value than when starting from a random point. It is also faster because trajectory lengths from a local minimum to a nearby

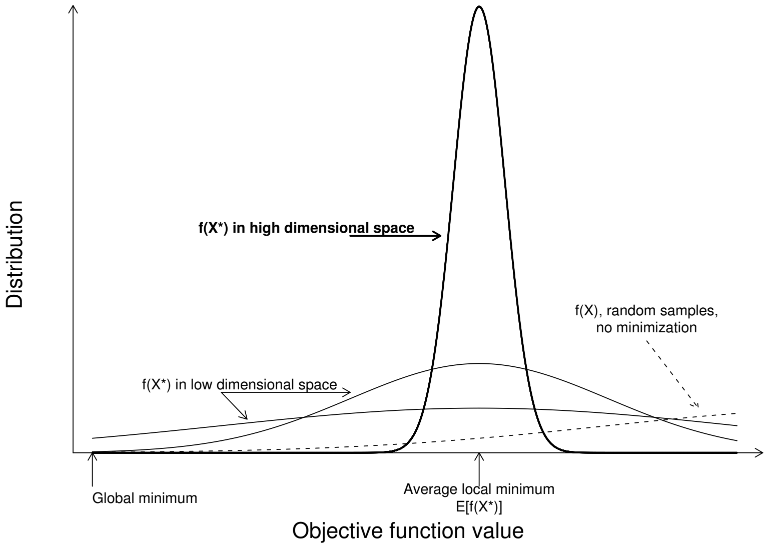


Figure 29.1: Probability of low f values is larger for local minima in $\mathcal{X}^*$ than for a point randomly extracted from $\mathcal{X}$. Large-dimensional problems tend to have a very spiky distribution for $\mathcal{X}^*$ values.

one tend to be shorter. Furthermore an incremental evaluation of f can often be used instead of re-computation from scratch if one starts from a new point. *Updating* f values after a move can be much faster than computing them from scratch. As usual, the only caveat is to avoid confinement in a given attraction basin, so that the "kick" to transform a local minimizer into the starting point for the next run has to be appropriately strong, but not too strong to avoid reverting to memory-less random restarts (if the kick is stochastic). **Iterated Local Search** is based on building a sequence of locally optimal solutions by: (i) perturbing the current local minimum; (ii) applying local search after starting from the modified solution.

As it happens with many simple — but sometimes very effective — ideas, the same principle has been rediscovered multiple times, for example in [45]. One may also argue that iterated local search shares many design principles with variable neighborhood search. A similar intuition is present in the iterated Lin-Kernighan algorithm of [221], where a local minimum is modified by a 4-change (a "big kick" eliminating four edges and reconnecting the path) and used as a starting solution for the next run of the Lin-Kernighan heuristic. In the stochastic local search literature based on Simulated Annealing, the work about large-step Markov chain of [264, 262, 263, 370] contains very interesting results coupled with a clear description of the principles.

Our description follows mainly [254]. LOCALSEARCH is seen by ILS as a black box. It takes as input an initial configuration X and ends up at a local minimum X^*. Globally, LOCALSEARCH maps from the search space $\mathcal{X}$ to the reduced set $\mathcal{X}^*$ of local minima. Obviously, the values of the objective function f at local minima are better than the values at the starting points, unless one is so lucky to start already at a local minimum. If one searches for low-cost solutions, sampling from $\mathcal{X}^*$ is therefore more effective than sampling from $\mathcal{X}$, this is in fact the basic feature of local search, see Fig. 29.1.

One may be tempted to sample in $\mathcal{X}^*$ by repeating runs of local search after starting from different random initial points. Unfortunately, general statistical arguments [316] related to the "law of large numbers" indicate that when the size of the instance increases, the *probability distribution of the cost values f tends to become extremely peaked about*

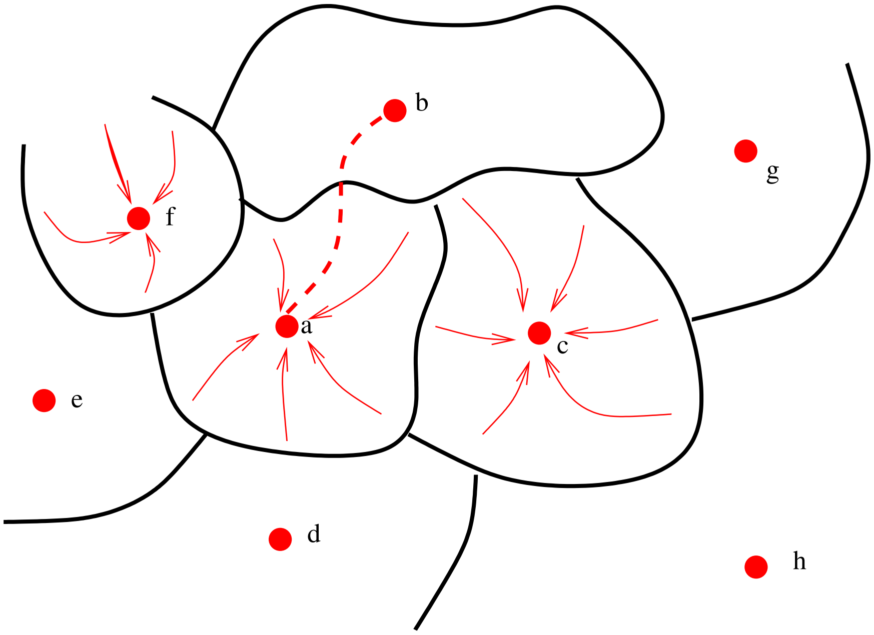


Figure 29.2: Neighborhood among attraction basins induced a neighborhood definition on local minima in $\mathcal{X}^*$.

the mean value $E[f(x^*)]$, mean value which can be offset from the best value f_{best} by a fixed percent excess. If we repeat a random extraction from $\mathcal{X}^*$ we are going to get very similar values with a large probability.

Relief comes from the rich structure of many optimization problem, which tends to cluster good local minima together. Instead of a random restart it is better to search in the neighborhood of a current good local optimum. What one needs is a **hierarchy of nested local searches**: starting from a proper neighborhood structure on $\mathcal{X}^*$ (proper as usual means that it makes the internal structure of the problem "visible" during a walk among neighbors). Hierarchy means that one uses local search to identify local minima, and then defines a local search *in the space of local minima*. One could continue, but in practice one limits the hierarchy to two levels. The sampling among $\mathcal{X}^*$ will therefore be *biased* and, if properly designed, can lead to the discovery of f values significantly lower than those expected by a random extraction in $\mathcal{X}^*$.

A neighborhood for the space of local minima $\mathcal{X}^*$, which is of theoretical interest, is obtained from the structure of the *attraction basins* around a local optimum. An attraction basin contains all points which are mapped to the given optimum by local search. The local optimum is an *attractor* of the dynamical system obtained by applying the local search moves. By definition, two local minima are neighbors if and only if their attraction basins are neighbors, i.e., they share part of the boundary. For example, in Fig. 29.2, local minima b, c, d, e, f are neighbors of local minimum a. Points g, h are not neighbors of a.

A weaker notion of closeness (neighborhood) which permits a fast stochastic search in $\mathcal{X}^*$ and which does not require an exhaustive determination of the attraction basins geography — a daunting task indeed — is based on creating a *randomized path* in $\mathcal{X}$ leading from a local optimum to one of the neighboring local optima, see the path from a to b in the figure.

A final design issue is how to build the path connecting two neighboring local minima. An heuristic solution is the following one, see Fig. 29.3 and Fig. 29.4: generate a sufficiently strong perturbation leading to a new point and then apply local search until convergence at a local minimum. The perturbation strength and the acceptance decision can change in a *reactive* manner, depending on the history of search. For example, the perturbation can become *stronger* if the recent history indicates that the search is trapped in the neighborhood of a local minimum, it can become *lighter* if

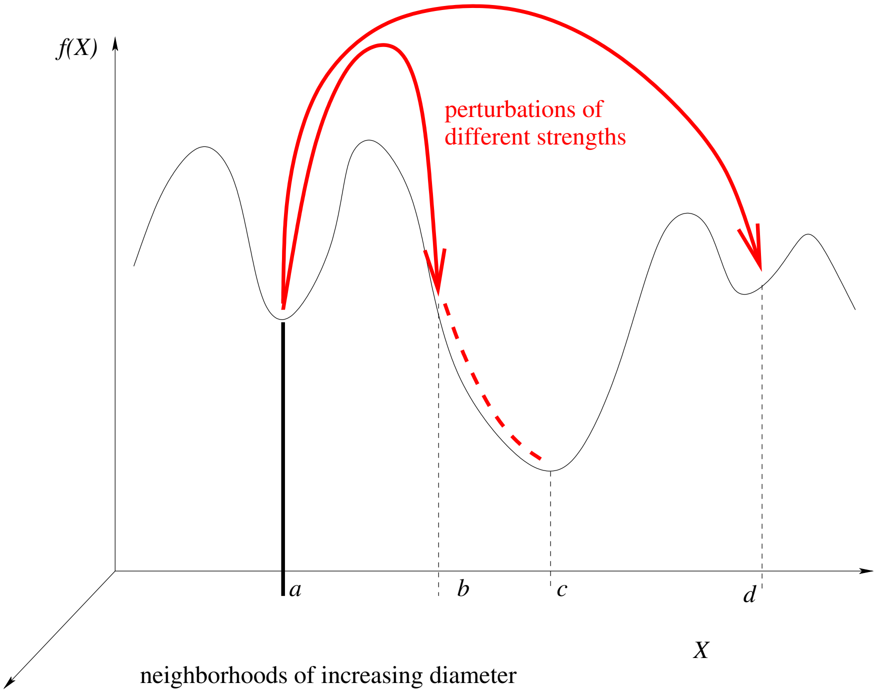


Figure 29.3: ILS: a perturbation leads from a to b, then local search to c. If perturbation is too strong one may end up at d therefore missing the closer local minima.

```
function IteratedLocalSearch ()
    $X^0 \leftarrow$ InitialSolution()
    $X^* \leftarrow$ LocalSearch ($X^0$)
    repeat
        $X' \leftarrow$ Perturb ($X^*$, history)
        $X^{*'} \leftarrow$ LocalSearch ($X'$)
        $X^* \leftarrow$ AcceptanceDecision ($X^*$, $X^{*'}$, history)
    until (no improvement or termination condition)
```

Figure 29.4: Iterated Local Search. The perturbation strength and the acceptance decision depend on the history of the search process.

new record values are generated after the most recent kicks (an evidence that new local optima are being visited after the kicks).

One has to adapt the appropriate *strength* of the perturbation to avoid cycling and keep exploring. If the perturbation is too small, one risks that the solution returns back to the starting local optimum. As a result, if the perturbation and local search are deterministic, an endless cycle would be produced.

Learning based on the previous search history is of paramount importance to avoid cycles and similar traps. The principle of "intensification first, minimal diversification only if needed" can be applied, together with stochastic elements to increase robustness and discourage cycling. As we have seen for VNS, minimal perturbations maintain the trajectory in the starting attraction basin, while excessive ones bring the method closer to a random sampling, therefore loosing the boost from the problem structure properties. A possible solution consists of perturbing by a short random walk of a length which is *adapted* by statistically monitoring the progress in the search.

It is already clear that the design principles underlying many superficially different techniques are in reality strongly related. We already mentioned the issue related to designing a proper perturbation, or "kick," or selecting the appropriate neighborhood, to lead a solution away from a local optimum, as well as the issue of using online reactive learning schemes to increase the adaptation and robustness.

Gist

Local search mechanisms are simple to build and run but stop at the first locally optimal point encountered along the search trajectory.

Repeated local search consists of repeating local search after starting from different (possibly randomized) initial solutions. The best solutions found in all repetitions in then returned. Repeated local search is oblivious (memory-less).

In most cases better results cab be obtained by the smarter **iterated local search**, which can be seen as **local search among locally optimal points**. Kicks (perturbations) are applied to push a local optimum sufficiently away that the trajectory will not fall back to the starting point, but not too far away to make it similar to random search (and therefore not exploiting the rich "Big-Valley" problem structure).

In a soccer analogy, a player kicks the ball and passes it to a different player to reach the goal, but if the kick is too strong the referee will signal with a flag that the ball wnet off the field of play, leaving to wasted time in the action.

Chapter 30

Online learning in Simulated Annealing

“The poets did well to conjoin music and medicine, in Apollo, because the office of medicine is but to tune the curious harp of man’s body and reduce it to harmony.”
(Francis Bacon, The Advancement Of Learning)

A notable feature of simulated annealing is its asymptotic convergence, a notable drawback is its *asymptotic* convergence. For a practical application of SA, if the local configuration is close to a local minimizer and the temperature is already very small in comparison to the upward jump which has to be executed to escape from the attractor, although the system will *eventually* escape, an enormous number of iterations can be spent around the attractor. Given a finite patience time, all future iterations can be spent while “circling like a fly around a light-bulb” (the light-bulb being a local minimum). Animals with superior cognitive abilities get burnt once, learn, and avoid doing it again!

The memoryless property (current move depending only on the current state, not on the previous history) makes SA look like a dumb animal indeed. It is intuitive that a better performance can be obtained by using memory, by self-analyzing the evolution of the search, and by activating more direct *escape* strategies. One needs a better time-management than the “let’s go to infinite time” principle. In the following sections we summarize the main memory-based approaches developed in the years to make SA a competitive strategy.

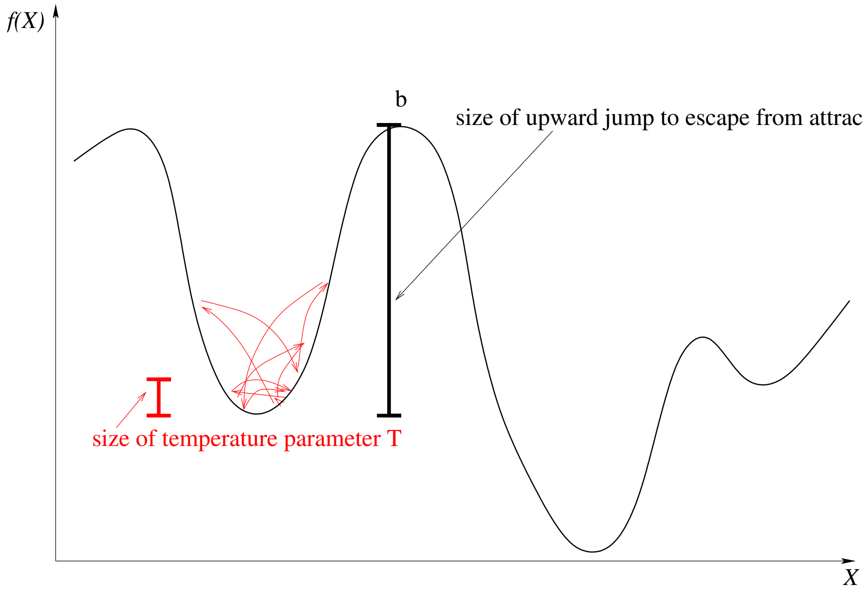

f(X)
b
size of upward jump to escape from attracto
size of temperature parameter T
X

Figure 30.1: Simulated Annealing: if the temperature is very low w.r.t. the jump size SA risks a practical entrapment close to a local minimizer.

30.1 Combinatorial optimization problems

Even if a vanilla version of a cooling schedule for SA is adopted (starting temperature T_{start}, geometric cooling schedule $T_{t+1} = \alpha \, T_t$, with $\alpha < 1$, final temperature T_{end}), a sensible choice has to be made for the three involved parameters T_{start}, α, and T_{end}. If the scale of the temperature is wrong, extremely poor results are to be expected. The work [380] suggests to estimate the distribution of f values, note that f is usually called "energy" when exploiting the physical analogies of SA. The standard deviation of the energy distribution defines the maximum-temperature scale, while the minimum change in energy defines the minimum-temperature scale. These temperature scales tell us where to begin and end an annealing schedule.

The analogy with physics is pursued in [247], where concepts related to *phase transitions* and *specific heat* are used. A **phase transition** is related to solving a sub-part of a problem. Before reaching the state after the transition, big reconfigurations take place and this is signaled by *wide variations* of the f values. In thermodynamics and statistical mechanics, the specific heat describes how the average function value (energy value) changes with temperature. A phase transition occurs when the specific heat is maximal, a quantity estimated by the ratio between the estimated variance of the objective function and the temperature: ${\sigma_f}^2/T$. After a phase transition corresponding to the big reconfiguration, finer details in the solution have to be fixed, and this requires a slower decrease of the temperature. It is a very bad idea to stop SA immediately after a phase transition, when new record values keep being generated. Concretely, one defines two temperature-reduction parameters α and β, monitors the evolution of f along the trajectory and, after the phase transition takes place at a given T_{msp}, one switches from a faster temperature decrease given by α to the slower one given by β. The value T_{msp} is the temperature corresponding to the maximum specific heat, when the scaled variance reaches its maximal value.

A monotonic decrease of the temperature has some weaknesses: for fixed values of T_{start} and α in the vanilla version one will reach an iteration so that the temperature will be so low that *practically* no tentative move will be accepted with a non-negligible probability (given the finite users' patience). The best value reached so far, f_{best}, will remain stuck in a helpless manner even if the search is continued for very long CPU times, see also Fig. 30.1. In other words, given a set of parameters T_{start} and α, the useful span of CPU time is practically limited. After the initial period the temperature will be so low that the system *freezes* and, with large probability, no tentative moves will be accepted anymore within the finite span of the run. In many cases one would like to obtain an **anytime algorithm**, so that longer allocated CPU times are related to possibly better and better values until the user decides to stop. Anytime algorithms — by definition — return the best answer possible even if they are not allowed to run to completion, and may improve on the answer if they are allowed to run longer.

Let's note that, in many cases, the stopping criterion should be decided *a posteriori*, for example after estimating that additional time has little probability to improve significantly on the result.

To avoid this problem is related to a monotonic temperature decrease, one considers **non-monotonic cooling schedules**, see [97, 283, 3]. A very simple proposal [97] suggests to reset the temperature once and for all at a constant temperature high enough to escape local minima but also low enough to visit them, for example, at the temperature T_{found} when the best heuristic solution is found in a preliminary SA simulation.

The basic design principle for a non-monotonic schedule is related to: i) exploiting an attraction basin rapidly by decreasing the temperature so that the system can settle down close to the local minimizer, ii) *increasing the temperature* to diversify the solution and visit other attraction basins, iii) decreasing again after reaching a different basin. As usual, the temperature increase in this kind of non-monotonic cooling schedule has to be rapid enough to avoid falling back to the current local minimizer, but not too rapid to avoid a random-walk situation (where all random moves are accepted) which would not capitalize on the local structure of the problem ("good local minima close to other good local minima"). The implementation details have to do with **determining an entrapment** situation, for example from the fact that no tentative move is accepted after a sequence t_{max} of tentative changes, and determining the detailed temperature decrease-increase evolution as a function of events occurring during the search. Possibilities to increase the temperature include resetting the temperature to $T_{\text{reset}} = T_{\text{found}}$, the temperature value when the current best solution was found [283]. If the reset is successful, one may progressively reduce the reset temperature: $T_{\text{reset}} \leftarrow T_{\text{reset}}/2$. Alternatively [3] geometric **re-heating** phases can be used, which multiply T by a heating factor γ larger than one at each iteration during reheat. Enhanced versions involve a learning process to choose a proper value of the heating factor depending on the system state. In particular, γ is close to one at the beginning, while it increases if, after a fixed number of escape trials, the system is still trapped in the local minimum. More details and additional bibliography can be found in the cited papers.

Let's note that similar "strategic oscillations" have been proposed in tabu search, in particular in the reactive tabu search [37] see Sec. 27.2, and in variable neighborhood search, see Sec. 28.1.

Experimental evidence shows that the *a priori* determination of SA parameters and acceptance function does not lead to efficient implementations [278]. Adaptations may be done "*by the algorithm itself using some learning mechanism* or by the user using his own learning mechanism." The authors appropriately note that the optimal choices of algorithm parameters depend not only on the problem but also on the particular instance and that a proof of convergence to a globally optimum is not a selling point for a specific heuristic: in fact a simple random sampling, or even exhaustive enumeration (if the set of configurations is finite) will eventually find the optimal solution, although they are not the best algorithms to suggest. A simple adaptive technique suggested in [278] is the SEQUENCEHEURISTIC: a perturbation leading to a worsening solution is accepted if and only if a fixed number of trials could not find an improving perturbation. This method can be seen as deriving evidence of "entrapment" in a local minimum and reactively activating an escape mechanism. In this way the temperature parameter is eliminated. The positive performance of the SEQUENCEHEURISTIC in the area of design automation suggests that the success of SA is "due largely to its acceptance of bad perturbations to escape from local minima rather than to some mystical connection between combinatorial problems and the annealing of metals" [278].

30.2 SA for global optimization of continuous functions

The application of SA to continuous optimization (optimization of functions defined on real variables in $\mathbb{R}$) is pioneered by [101]. The basic method is to generate a new point with a random step along a direction $\boldsymbol{e}_h$, to evaluate the function and to accept the move with the probability given in equation (25.1). One cycles over the different directions $\boldsymbol{e}_h$ during successive steps of the algorithm. A first critical choice has to do with the range of the random step along the chosen direction. A fixed choice obviously may be very inefficient: this opens a first possibility for *learning* from the local f surface. In particular a new trial point $\boldsymbol{x}'$ is obtained from the current point $\boldsymbol{x}$ as:

$$\boldsymbol{x}' = \boldsymbol{x} + \text{Rand}(-1,1) v_h \boldsymbol{e}_h$$

where $\text{Rand}(-1,1)$ returns a random number uniformly distributed between -1 and 1, $\boldsymbol{e}_h$ is the unit-length vector along direction h, and v_h is the step-range parameter, one for each dimension h, collected into the vector $\boldsymbol{v}$. The exponential acceptance rule is used to decide whether to update the current point with the new point $\boldsymbol{x}'$. The v_h value is adapted during the search with the aim of maintaining the number of *accepted* moves at about one-half of the total number of tried moves. Although the implementation is already reactive and based on memory, the authors encourage more work so that a "good monitoring of the minimization process" can deliver precious feedback about some crucial internal parameters of the algorithm.

In Adaptive Simulated Annealing (ASA), also known as very fast simulated re-annealing [205], the parameters that control the temperature cooling schedule and the random step selection are automatically adjusted according to algorithm progress. If the state is represented as a point in a box and the moves as an oval cloud around it, the temperature and the step size are adjusted so that all of the search space is sampled at a coarse resolution in the early stages, while the state is directed to promising areas in the later stages [205].

Gist

The use of Simulated Annealing for optimization has been motivated with **asymptotic convergence results**. When the number of iterations goes to infinity and the temperature is decreased slowly, the probability of observing a global optimum goes to one. Unfortunately, life is too short for asymptotic results, even the life of the universe is too short in some cases.

The problem is that the temperature parameter, when compared with the step in function value which must be executed to escape from a local attraction basin, can be so low that all future steps can be spent in the neighborhood of a single local optimum, in spite of the theoretical asymptotic convergence.

One has to **abandon vanilla "Markov-process" SA** in favor of more pragmatic versions which estimate progress, determine a possible entrapment, and activate direct ways of escaping, e.g., by raising the temperature (**re-heating**). The conditions for the validity of most math theorems are not valid anymore, theoretical analysis becomes very complex if not impossible, but better local optima can be determined in most practical cases.

Traditional SA can be compared to **a fly randomly circling around a light bulb**, getting burnt again and again, with no memory and no learning possibility. The light bulb is an analogy for a local optimum entrapping a search directory. When touching something hot, a kid will get burnt once, maybe twice, but then online learning takes place. Which process sounds more sensible?

Chapter 31

Dynamic landscapes and noise levels

'Morsel' is a perfect word. Forming those six letters on the lips and tongue prompts an instantaneous physiological reaction. The mouth waters. The lips purse.
(Shawn Amos)

This chapter considers reactive modification of the objective function in order to support appropriate diversification of the search process. Contrary to the prohibition-based techniques of Sec. 27.2 the focus is not that of pushing the search trajectory away from a local optimum though explicit and direct prohibitions but on **modifying the objective function so that previous promising areas in the solution space appear less favorable**, and the search trajectory will be gently pushed to visit new portions of the search space. To help the intuition, see also Fig. 31.1, one may think about pushing up the search landscape at a discovered local minimum, so that the search trajectory will flow into neighboring attraction basins. For a physical analogy, think about you sitting in a tent while it is raining outside. A

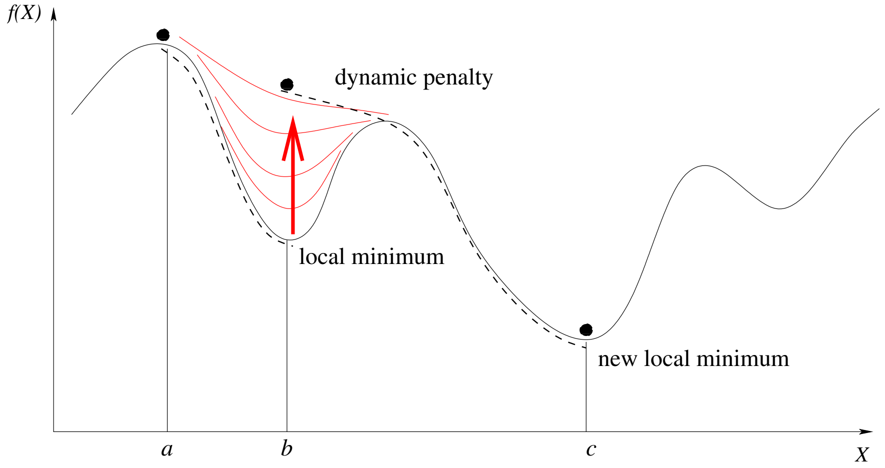


Figure 31.1: Transformation of the objective function to gently push the solution out of a given local minimum.

```
GSAT-WITH-WALK
for $i \leftarrow 1$ to MAX-TRIES
    $X \leftarrow$ random truth assignment
    for $j \leftarrow 1$ to MAX-FLIPS
        if Rand(0,1)< $p$ then
            $var \leftarrow$ any variable occurring in some unsatisfied clause
        else
            $var \leftarrow$ any variable with largest $\Delta f$
        FLIP($var$)
```

Figure 31.2: The "GSAT-with-walk" algorithm. Rand$(0,1)$ generates random numbers in the range $[0,1]$

way to eliminate dangerous pockets of water stuck on flat convex portions is to gently push the tent fabric from below until gravity will lead water down.

As with many algorithmic principles, it is difficult to pinpoint a seminal paper in this area. The literature about stochastic local search for the Satisfiability (SAT) problem is of particular interest. Different variations of local search with randomness techniques have been proposed for Satisfiability and Maximum Satisfiability (MAX-SAT) starting from the late eighties, for some examples see [164], [324], and the updated review of [208]. These techniques were in part motivated by previous applications of "min-conflicts" heuristics in the area of Artificial Intelligence, see for example [161] and [271].

Before arriving at the objective function modifications, let's summarize the influential algorithm GSAT [324]. It consists of multiple runs of LS$^+$ local search, each one consisting of a number of iterations that is typically proportional to the problem dimension n. Let f be the number of satisfied clauses. At each iteration of LS$^+$, a bit which maximizes Δf is chosen and flipped, even if Δf is negative, i.e., after flipping the bit the number of satisfied clauses decreases.

The algorithm is briefly summarized in Fig. 35.16. A certain number of tries (MAX-TRIES) is executed, where each try consists of a number of iterations (MAX-FLIPS). At each iteration a variable is chosen by two possible criteria and then flipped by the function FLIP, i.e., x_i becomes equal to $(1 - x_i)$. One criterion, active with *noise* probability p, selects a variable occurring in some unsatisfied clause with uniform probability over such variables, the other one is the standard method based on the function f given by the number of satisfied clauses. For a generic move μ applied at iteration t, the quantity $\Delta_\mu f$ (or Δf for short) is defined as $f(\mu\ X^{(t)}) - f(X^{(t)})$. The straightforward book-keeping part of the algorithm is not shown. In particular, the best assignment found during all trials is saved and reported at the end of the run. In addition, the run is terminated immediately if an assignment is found that satisfies all clauses. Different noise strategies to escape from attraction basins are added to GSAT in [322, 323]. In particular, the GSAT-with-walk algorithm.

The breakout method suggested in [274] for the constraint satisfaction problem measures the cost as the sum of the weights associated to the violated constraints (to the nogoods). Each weight is one at the beginning, at a local minimum the weight of each nogood is increased by one until one escapes from the given local minimum (a breakout occurs).

Clause–weighting has been proposed in [321] in order to increase the effectiveness of GSAT for problems characterized by strong asymmetries. A positive weight is associated to each clause to determine how often the clause should be counted when determining which variable to flip. The weights are dynamically modified and the qualitative effect is that of "filling in" local optima while the search proceeds. Clause–weighting and the breakout technique can be considered as "reactive" techniques where a repulsion from a given local optimum is generated in order to induce an escape from a given attraction basin. The local adaptation is clear: weights are increased until the original local minimum disappears, and therefore the current weights depend on the local characteristic of a specific local minimum point.

In detail, a weight w_i is associated to each clause, and the guiding evaluation function becomes not a simple count of the satisfied clauses but a sum of the corresponding weights. New parameters are introduced and therefore new possibilities for tuning the parameters based on feedback from preliminary search results. The algorithm in [325] suggests a different way to use weights to encourage more priority on satisfying the "most difficult" clauses. One aims at **learning how difficult a clause is to satisfy**. These hard clauses are identified as the ones which remain unsatisfied after a try of local search descent followed by plateau search. Their weight is increased so that future runs will give them more priority when picking a move. If weights are only increased, after some time their size becomes large and their relative magnitude will reflect the overall statistics of the SAT instance, more than the local characteristics of the portion of the search space where the current configuration lies. To combat this problem, two techniques are proposed in [130], either *reducing* the clause weight when a clause is satisfied, or by a weight decay scheme (each weight is reduced by a factor ϕ before updating it). Depending on the size of the increments and decrements, one achieves "continuously weakening incentives not to flip a variable" instead of the strict prohibitions of Tabu Search. The second scheme takes the *recency of moves* into account, the implementation is through a weight decay scheme updating so that each weight is reduced before a possible increment by δ if the clause is not satisfied:

$$w_i \leftarrow \ \phi \, w_i + \delta$$

where one introduces a decay rate ϕ and a "learning rate" δ. A faster decay (lower ϕ value) will limit the temporal extension of the context and imply a faster forgetting of old information. The effectiveness of the weight decay scheme is interpreted by the authors as "learning the best way to conduct local search by discovering the hardest clauses relative to recent assignments." Some collateral damage (*warping* effects) can be caused clause-weighting dynamic local search on the fitness surface [360]. The fitness surface is changed in a *global* way after encountering a local minimum. Points which are very far from the local minimum, but which share some of the unsatisfied clauses, will also see their values changed. This does not correspond to the naive "push-up" picture where only the area close to a specific local minimum is raised, and the effects on the overall search dynamics are far from simple to understand. Be aware of dangerous analogies!

A more recent proposal of a dynamic local search (DLS) for SAT is in [361]. The authors start from the Exponentiated Sub-Gradient (ESG) algorithm [317], which alternates search phases and weight updates, and develop a scheme with low time complexity of its search steps: Scaling and Probabilistic Smoothing (SAPS). Weights of satisfied clauses are multiplied by α_{sat}, while weights of unsatisfied clauses are multiplied by α_{unsat}, then all weights are smoothed towards their mean $\bar{w}$: $w \leftarrow w \, \rho + (1 - \rho) \, \bar{w}$. A *reactive version* of SAPS (RSAPS) is then introduced that adaptively tunes one of the algorithm's important parameters.

31.1 Guided local search

While we concentrated on the SAT problem above, a similar approach has been proposed with the term of Guided Local Search (GLS) [371, 373] for other applications. GLS aims at enabling intelligent search schemes that exploit problem- and search-related information to guide a local search algorithm in a search space. Penalties depending on solution features are introduced and dynamically manipulated to distribute the search effort over the regions of a search space.

Let us stop for a moment with an historical digression to show how many superficially distinct concepts are in fact deeply related. Inspiration for GLS comes from a previously proposed neural net algorithm (GENET) [375] and from tabu search [148], simulated annealing [234], and tunneling [252]. The use of "neural networks" for optimization consists of setting up *a dynamical system whose attractors correspond to good solutions of the optimization problem*. Once the dynamical system paradigm is in the front stage, it is natural to use it not only to search for but also to escape from local minima. According to the authors [372], GENET's mechanism for escaping resembles *reinforcement learning* [18]: patterns in a local minimum are stored in the constraint weights and are discouraged to appear thereafter. GENET's learning scheme can be viewed as a method to *transform the objective function so that a local minimum gains an artificially higher value*. Consequently, local search will be able to leave the local minimum state and search other parts of the space. In tunneling algorithms [252] the modified objective function is called the tunneling function. This function allows local search to explore states which have higher costs around or further away from the local minimum, while aiming at nearby states with lower costs. In the framework of continuous optimization similar ideas have been rediscovered multiple times. Rejection-based stochastic procedures are presented in [252, 15, 282]. Citing from a seminal paper [252], one combines "a minimization phase having the purpose of lowering the current function value until a local minimizer is found and a tunneling phase that has the purpose of finding a point ... such that when employed as starting point for the next minimization phase, the new stationary point will have a function value no greater than the previous minimum found." The "strict" prohibitions of tabu search become "softer" penalties in GLS, which are determined by *reaction to feedback from the local optimization heuristic under guidance* [373].

A complete GLS scheme [373] defines appropriate solution features f_i, for example the presence of an edge in a TSP path, and combines three ingredients:

feature penalties p_i to diversify the search away from already-visited local minima (the *reactive* part)

feature costs c_i to account for the *a priori* promise of solution features (for example the edge cost in TSP)

a neighborhood activation scheme depending on the current state.

The *augmented cost function* $h(X)$ is defined as:

$$h(X) = f(X) + \lambda \sum_i p_i \, I_i(X) \tag{31.1}$$

where $I_i(X)$ is an indicator function returning 1 if feature i is present in solution X, 0 otherwise. The augmented cost function is used by local search instead of the original function.

Penalties are zero at the beginning: there is no need to escape from local minima until they are encountered! Local minima are then the "learning opportunities" of GLS: when a local minimum of h is encountered the augmented cost function is modified by updating the penalties p_i. One considers all features f_i present in the local minimum solution X' and increments by one the penalties which maximize:

$$I_i(X') \, \frac{c_i}{1 + p_i} \tag{31.2}$$

The above mechanism kills more birds with one stone. First a higher cost c_i, and therefore an inferior *a priori* desirability for feature f_i in the solution, implies a higher tendency to be penalized. Second, the penalty p_i, which is also a counter of how many times a feature has been penalized, appears at the denominator, and therefore discourages penalizing features which have been penalized many times in the past. If costs are comparable, the net effect is that penalties tend to alternate between different features present in local minima.

GLS is usually combined with "fast local search" FLS. FLS includes implementation details which speedup each step but do not impact the dynamics and do not change the search trajectory, for example an incremental evaluation of the h function, but it also includes qualitative changes in the form of *sub-neighborhoods*. The entire neighborhood is broken down into a number of small sub-neighborhoods. Only active sub-neighborhoods are searched. Initially all of them are active, then, if no improving move is found in a sub-neighborhood, it becomes inactive. Depending on the move performed, a number of sub-neighborhoods are activated where one expects improving moves to occur as a result of the move just performed. For example, after a feature is penalized, the sub-neighborhood containing a move eliminating the feature from the solution is activated. The mechanism is equivalent to prohibiting examination of the inactive moves, in a tabu search spirit. As an example, in TSP one has a *sub-neighborhoods* per city, containing all moves exchanging edges where at least one of the edges terminates at the given city. After a move is performed, all *sub-neighborhoods* corresponding to cities at the ends of the edges involved in the move are activated, to favor a chain of moves involving more cities.

While the details of *sub-neighborhoods* definition and update are problem-dependent, the lesson learned is that much faster implementations can be obtained by avoiding a brute-force evaluation of the neighborhood, the motto is "evaluate only a subset of neighbors where you expect improving moves." In addition to a faster evaluation per search step one obtains a possible additional diversification effect related to the implicit prohibition mechanism. This technique to speedup the evaluation of the neighborhoods is similar to the "don't look bits" method in [50]. One flag bit is associated to every node, and if its value is 1 the node is not considered as a starting point to find an improving move. Initially all bits are zero, then if an improving move could not be found starting at node i the corresponding bit is set. The bit is cleared as soon as an improving move is found that inserts an edge incident to node i.

The parameter λ in equation (31.1) controls the importance of penalties w.r.t the original cost function: a large λ implies a large diversification away from previously visited local minima. A reactive determination of the parameter λ is suggested in [373].

While the motivations of GLS are clear, the interaction between the different ingredients causes a somewhat complicated dynamics. Let's note that different units of measure for the cost in equation (31.1) can impact the dynamics, something which is not particularly desirable: if the cost of edge in TSP is measured in kilometers the dynamics is not the same as if the cost is measured in millimeters. Furthermore, the definition of costs c_i for a general problem is not obvious and the consideration of the "costs" c_i in the penalties in a way duplicates the explicit consideration of the real problem costs in the original function f. In general, when penalties are added and modified, a desired effect (minimal required diversification) is obtained *indirectly* by modifying the objective function and therefore by possibly causing *unexpected effects*, like new spurious local minima, or shadowing of promising yet-unvisited solutions. For example, an unexplored local minimum of f may not remain a local minimum of h and therefore it may be skipped by modifying the trajectory.

A penalty formulation for TSP including memory-based trap-avoidance strategies is proposed in [374]. One of the strategies avoids visiting points that are close to points visited before, a generalization of the STRICT-TS strategy [23]. A recent algorithm with an *adaptive clause weight redistribution* is presented in [206], it adopts resolution-based preprocessing and reactive adaptation of the total amount of weight to the degree of stagnation of the search. Stagnation is identified after a long sequence of flips without improvement, long periods of stagnation will produce "oscillating phases of weight increase and reduction."

31.2 Adapting noise levels

Up to know we have seen how to modify the objective function or the LS rules in a dynamic manner depending on the search history and current state in order to deviate the search trajectory away from local optimizer. Another possibility to reach similar (stochastic) deviations of the trajectory is by adding a controlled amount of randomized movements. *Clinamen* is the name the philosopher Lucretius gave to the spontaneous microscopic swerving of atoms from a vertical path as they fall, considered in discussions of possible explanation for free will. A kind of algorithmic *clinamen* can be used to influence the diversification of an SLS technique. A related usage of “noise” is also considered in Sec 25.5 about Simulated Annealing, in which upward moves are accepted with a probability depending on a temperature parameter.

An opportunity for self-adaptation considering different amounts of randomness is given by **adaptive noise** mechanism for WalkSAT. In WalkSAT [322], one repeatedly flips a variable in an unsatisfied clause. If there is at least one variable which can be flipped without breaking already satisfied clauses, one of them is flipped. Otherwise, a noise parameter p determines if a random variable is flipped, or if a greedy step is executed, with probability $(1-p)$, favoring minimal damage to the already satisfied clauses.

In [265] it appears that appropriate noise settings achieve a good balance between the greedy “steepest descent” component and the exploration of other search areas away from already considered attractors. The work in [265] considers this generalized notion of a noise parameter and suggests tuning the proper noise value for a specific instance by testing different settings through a preliminary series of short runs. Furthermore, the suggested statistics to monitor, which is closely related to the algorithm performance, is the *ratio* between the average final values obtained at the end of the short runs and the variance of the f values over the runs. Quite consistently, the best noise setting corresponds to the one leading to the lowest empirical ratio increased by about 10%. faster tuning can be obtained if the examination of a predefined series of noise values is substituted with a faster adaptive search which considers a smaller number of possible values, see [294] which uses Brent’s method [67]. An adaptive noise scheme is also proposed in [188], where the noise setting p is dynamically adjusted based on search progress. Higher noise levels are determined in a reactive manner if and only if there is evidence of search stagnation. In detail, if too many steps elapse since the last improvement, the noise value is increased, while it is gradually decreased if evidence of stagnation disappears. A different approach based on optimizing the noise setting on a given instance prior to the actual search process (with a fixed noise setting) is considered in [294].

Gist

Imagine dynamic pricing for street parking: the higher the price, the more people will avoid parking at city centers. The “fitness landscape” for the appeal of parking spaces changes and drivers modify their trajectories to stay in the periphery.

In a similar manner, when local minima are discovered and saved in memory, and therefore they become uninteresting for additional explorations, **artificially raising the value of the objective function** can be a way to encourage the search process to stay away from the known local minima. Unfortunately, depending on how dynamic penalties are placed, some new promising solutions cab be hidden, so that the method has to be used with great care.

Adapting the level of randomness during the search is a second mechanism to tradeoff intensification and exploration. By turning the “noise knob” one transforms a greedy perturbative search more and more into a random walk. One aims at a compromise which is appropriate for the local characteristics along the optimization trajectory of a specific instance.

Chapter 32

Adaptive Random Search

Men nearly always follow the tracks made by others and proceed in their affairs by imitation, even though they cannot entirely keep to the tracks of others or emulate the prowess of their models. So a prudent man should always follow in the footsteps of great men and imitate those who have been outstanding. If his own prowess fails to compare with theirs, at least it has an air of greatness about it. He should behave like those archers who, if they are skilful, when the target seems too distant, know the capabilities of their bow and aim a good deal higher than their objective, not in order to shoot so high but so that ***by aiming high they can reach the target***.”
(Niccolo Machiavelli)

In many real-world situations partial derivatives cannot be used because the function is not differentiable or because computing derivatives is too expensive. This motivates the study of optimization techniques based only on the knowledge of function values, like variants of the **adaptive random search** algorithm based on the theoretical framework of [340].

The general scheme starts by choosing an initial point in the configuration space and an initial *search region* surrounding it and proceeds by iterating the following steps.

1. A new candidate point is generated by **sampling the search region** according to a given probability measure.
2. The **search region is adapted** according to the value of the function at the new point. It is compressed if the new function value is greater than the current one (unsuccessful sample) or expanded otherwise (successful sample).
3. If the sample is successful, the new point becomes the current point, and the **search region is moved** so that the current point is at its center for the next iteration.

For effective implementations, simple search regions around the current point suffice, for example regions defined by *boxes* (with edges given by a set of linearly independent vectors) with uniform probability distributions inside the box. In this case generating a random displacement is simple: the basis vectors are multiplied by random numbers in the real range (-1.0, 1.0) and added: $\boldsymbol{\delta} = \sum_j \text{Rand} \times \boldsymbol{b}_j$.

The requirement that the box edges are parallel to the coordinate axes can be relaxed so that the frames can be compressed or expanded along arbitrary directions by using affine transformations, as explained in the following section.

32.1 RAS: adaptation of the sampling region

A simple but surprisingly effective self-adaptive and derivative-free method is the **Reactive Affine Shaker (RAS)** algorithm [69], based on [36]. RAS adapts a search region by an affine transformation. An affine transformation (from the Latin, *affinis*, "connected with") between two vector spaces consists of a linear transformation followed by a translation:

$$x \mapsto Ax + b.$$

Geometrically, an affine transformation in Euclidean space preserves:

- (i) the collinearity relation between points; i.e., the points which lie on a line continue to be collinear after the transformation,
- (ii) ratios of distances along a line; i.e., for distinct collinear points $p_1$1,$p_2$2,$p_3$3, the ratio $|p_2 - p_1|/|p_3 - p_2|$ is preserved. In general, an affine transformation is composed of linear transformations (rotation, scaling or shear) and a translation (or "shift").

In RAS, the region is translated when a successful sample is found, elongated along arbitrary success directions, and compressed along the unsuccessful ones. The modification takes into account the *local knowledge* derived from trial points generated with a uniform probability in the search region. The aim is to scout for local minima in the attraction basin where the initial point falls, by adapting the step size and direction to maintain heuristically **the largest possible movement per function evaluation**. The design is complemented by the analysis of some strategic choices, like the double-shot strategy and the initialization [69]. Let's now comment on the name (Reactive Affine Shaker). The solver's movements try to minimize the number of jumps towards the minimum region, and this is achieved by constantly changing the movement direction and size. Search region and therefore step adjustments are implemented by a feedback loop guided by the evolution of the search itself, therefore implementing a "reactive" self-tuning mechanism. The generation of samples is *tuned to the local properties* of the f surface, in the spirit of the Reactive Search Optimization principles explained in Chapter 24. The constant change in step size and direction creates a "shaky" trajectory, with abrupt leaps and turns.

The pseudo-code of the RAS algorithm is shown in Fig. 32.1. At every iteration, a displacement $\boldsymbol{\Delta}$ is generated so that the point $\boldsymbol{x} + \Delta$ is uniformly distributed in the local search region $\mathcal{R}$ (line 4). To this end, the basis vectors are multiplied by different random numbers in the real range $[-1, 1]$ and added:

$$\boldsymbol{\Delta} = \sum_j \text{Rand}(-1, 1)\boldsymbol{b}_j.$$

f	(input)	Function to minimize
$\boldsymbol{x}$	(input)	Initial point
$\boldsymbol{b}_1, \ldots, \boldsymbol{b}_d$	(input)	Vectors defining search region $\mathcal{R}$ around $\boldsymbol{x}$
ρ	(input)	Box expansion factor
t	(internal)	Iteration counter
$\mathbf{P}$	(internal)	Transformation matrix
$\boldsymbol{x}$, $\boldsymbol{\Delta}$	(internal)	Current position, current displacement

```
function ReactiveAffineShaker ($f$, $\boldsymbol{x}$, ( $\boldsymbol{b}_j$), $\rho$)
    $t \leftarrow 0$;
    repeat
        $\boldsymbol{\Delta} \leftarrow \sum_j \text{Rand}(-1,1)\boldsymbol{b}_j$;
        if $f(\ \boldsymbol{x} + \boldsymbol{\Delta}) < f(\ \boldsymbol{x})$
            $\boldsymbol{x} \leftarrow \boldsymbol{x} + \boldsymbol{\Delta}$;
            $\mathbf{P} \leftarrow \mathbf{I} + (\rho - 1)\frac{\boldsymbol{\Delta}\boldsymbol{\Delta}^T}{\| \boldsymbol{\Delta} \|^2}$;
        else if $f(\ \boldsymbol{x} - \boldsymbol{\Delta}) < f(\ \boldsymbol{x})$
            $\boldsymbol{x} \leftarrow \boldsymbol{x} - \boldsymbol{\Delta}$;
            $\mathbf{P} \leftarrow \mathbf{I} + (\rho - 1)\frac{\boldsymbol{\Delta}\boldsymbol{\Delta}^T}{\| \boldsymbol{\Delta} \|^2}$;
        else
            $\mathbf{P} \leftarrow \mathbf{I} + (\rho^{-1} - 1)\frac{\boldsymbol{\Delta}\boldsymbol{\Delta}^T}{\| \boldsymbol{\Delta} \|^2}$;
        $\forall j\ \boldsymbol{b}_j \leftarrow \mathbf{P}\ \boldsymbol{b}_j$;
        $t \leftarrow t+1$
    until convergence criterion;
    return $\boldsymbol{x}$;
```

Figure 32.1: The Reactive Affine Shaker pseudo-code.

Rand$(-1, 1)$ represents a call of the random-number generator. If one of the two points $\boldsymbol{x} + \Delta$ or $\boldsymbol{x} - \Delta$ improves the function value, then it is chosen as the next point. Let us call $\boldsymbol{x}'$ the improving point. In order to enlarge the box along the promising direction, the box vectors $\boldsymbol{b}_i$ are modified as follows.
The direction of improvement is $\boldsymbol{\Delta}$. Let us call $\boldsymbol{\Delta}'$ the corresponding vector normalized to unit length:

$$\boldsymbol{\Delta}' = \frac{\boldsymbol{\Delta}}{\|\boldsymbol{\Delta}\|}.$$

Then the projection of vector $\boldsymbol{b}_i$ along the direction of $\boldsymbol{\Delta}$ is

$$\boldsymbol{b}_i|_{\boldsymbol{\Delta}} = \boldsymbol{\Delta}'(\boldsymbol{\Delta}' \cdot \boldsymbol{b}_i) = \boldsymbol{\Delta}'\boldsymbol{\Delta}'^T\boldsymbol{b}_i.$$

To obtain the desired effect, this component is enlarged by a coefficient $\rho > 1$, so the expression for the new vector $\boldsymbol{b}_i'$ is

$$\begin{aligned} \boldsymbol{b}_i' &= \boldsymbol{b}_i + (\rho - 1)\boldsymbol{b}_i|_{\boldsymbol{\Delta}} \qquad (32.1) \\ &= \boldsymbol{b}_i + (\rho - 1)\boldsymbol{\Delta}'\boldsymbol{\Delta}'^T\boldsymbol{b}_i \\ &= \boldsymbol{b}_i + (\rho - 1)\frac{\boldsymbol{\Delta}\boldsymbol{\Delta}^T}{\|\boldsymbol{\Delta}\|^2}\boldsymbol{b}_i \\ &= P\boldsymbol{b}_i, \end{aligned}$$

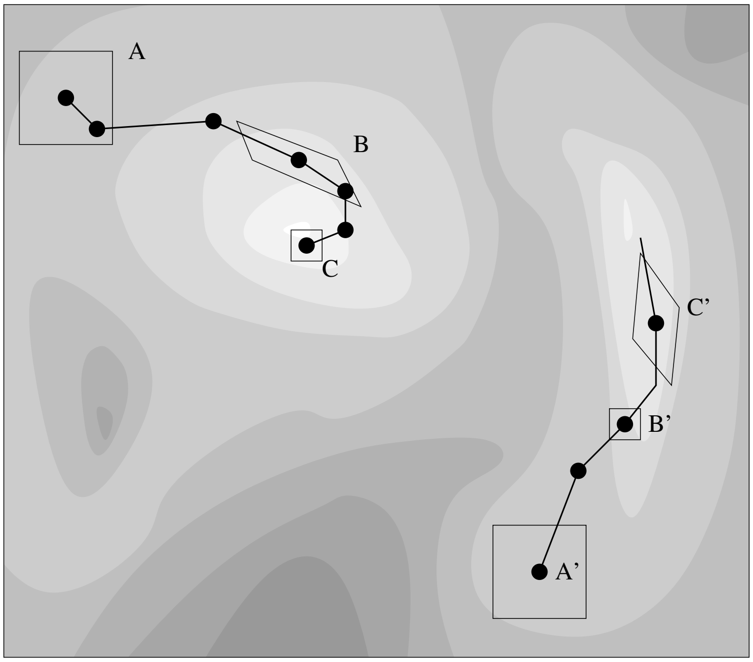


Figure 32.2: Reactive Affine Shaker geometry: two search trajectories leading to two different local minima, adapted from [69].

where

$$P = \mathbf{I} + (\rho - 1)\frac{\boldsymbol{\Delta}\boldsymbol{\Delta}^T}{\|\boldsymbol{\Delta}\|^2}. \tag{32.2}$$

The fact of testing the function improvement on both $\boldsymbol{x} + \boldsymbol{\Delta}$ and $\boldsymbol{x} - \boldsymbol{\Delta}$ is called *double-shot strategy*: if the first sample $\boldsymbol{x}+\boldsymbol{\Delta}$ is not successful, the specular point $\boldsymbol{x}-\boldsymbol{\Delta}$ is considered. This choice drastically reduces the probability of generating two consecutive unsuccessful samples. For a mental image, consider fitting a *plane* around the current point: if a step increases f, the opposite step decreases it. Going from mental images to math, if one considers differentiable functions and small displacements, the directional derivative along the displacement is proportional to the scalar product between displacement and gradient $\boldsymbol{\Delta} \cdot \nabla f$. If the first is positive, a change of sign will trivially cause a negative value, and therefore a decrease in f for a sufficiently small step size. The empirical validity for general functions, not necessarily differentiable, is caused by the correlations and structure contained in most of the functions corresponding to real-world problems.

If the double-shot strategy fails, then the affine transformation (32.1) is applied by replacing the expansion factor ρ with its inverse ρ^{-1} (line 12 of Fig. 32.1), causing a compression of the search area.

An illustration of the geometry of the Reactive Affine Shaker algorithm is shown in Fig. 32.2, where the function to be minimized is represented by a contour plot showing *isolines* at fixed values of f, and two trajectories (ABC and A'B'C') are plotted. The search regions are shown for some points along the search trajectory. The design criteria of RAS are given by an *aggressive search for local minima*: the search speed is increased when steps are successful (points A and A'), reduced only if no better point is found after the double shot. When a point is close to a local minimum, the repeated reduction of the search frame produces a very fast convergence of the search (point C). Note that another cause of reduction for the search region can be a narrow descent path (a "canyon", such as in point B'), where only a small subset of all possible directions improves the function value. However, once an improvement is found, the search region grows in the promising direction, causing a faster movement along that direction.

f	(input)	Function to minimize
ρ,	(input)	Box expansion factor
$L_1, \ldots, L_d, U_1, \ldots, U_d$	(input)	Search range
$L'_1, \ldots, L'_d, U'_1, \ldots, U'_d$	(input)	Initialization range
$\boldsymbol{b}_1, \ldots, \boldsymbol{b}_d$	(internal)	Vectors defining search region $\mathcal{R}$ around $\boldsymbol{x}$
$\boldsymbol{x}$, $\boldsymbol{x}'$	(internal)	Current position, final position of run

```
function RepeatedReaciveAffineShaker ($f$, $\rho$, $(L'_j)$, $(U'_j)$, $(L_j)$, $(U_j)$)
    $\forall j\ \boldsymbol{b}_j \leftarrow \frac{U_j - L_j}{4} \cdot \boldsymbol{e}_j$;
    pardo
        $\boldsymbol{x} \leftarrow$ random point $\in [L'_1, U'_1] \times \cdots \times [L'_d, U'_d]$;
        $\boldsymbol{x}$' $\leftarrow$ ReactiveAffineShaker($f$, $\boldsymbol{x}$, ( $\boldsymbol{b}_j$), $\rho$);
    return best position found;
```

Figure 32.3: The RAS algorithm, from [69].

32.2 Repetitions for robustness and diversification

In general, an effective estimation of the number of steps required for identifying a global minimum is clearly impossible. Even when a local minimum is found, it is generally impossible to determine whether it is global or not, in particular if the knowledge about the function derives only from evaluations of $f(x)$ at selected points, which is a frequent case in dealing with real-world applications.

Because RAS does not include mechanisms to escape from local minima, it should be stopped as soon as the trajectory is sufficiently close to a local minimizer. For instance, a single RAS run can be terminated if the search region becomes smaller than a threshold value. In fact, the box tends to reduce its volume in proximity of a local minimum because of repeated failures in improving the function value.

RAS searches for local minimizers and is stopped as soon as one is found. A simple way to continue the search is to **restart from a different initial random point**. This approach is equivalent to a "population" of RAS searchers, in which each member of the population is *independent*, completely unaware of what other members are doing (Fig. 32.3). More complex ways of coordinating a team of searchers are considered in the *C-LION* framework in Chapter 38.

Gist

Adaptive random search adapts a current **search region around the current tentative solutions**. New points are sampled from the search region. Depending on finding better or worse solutions, the search region is then adapted. In particular Reactive Affine Shaker (RAS) stretches or squeezes the search region along the direction of the latest successful or unsuccessful step, respectively.

This chapter concludes our presentation of RSO. To summarize, Reactive Search Optimization can **adapt in an online manner** at least the following choices or meta-parameters: prohibition periods ("stay away from this area"), neighborhood ("if no improving move, get another neighborhood"), iterations – not simply repetitions – of local search ("kick the system to a new attractor and call LS"), dynamic modifications of the objective function ("push up so that a local minimum disappears") amount of randomness in SA and other stochastic schemes ("noise level up to jump out of an attractor").

Part V

Special optimization problems and advanced topics

Chapter 33

Linear and Quadratic Programming

I think many people's deviant behavior starts with dreams because dreams are so non-linear... as if there's an assumption that everything has to be linear or has to be plotted.
(Robyn Hitchcock)

In the previous chapters we consider general-purpose methods for solving optimization problems, both discrete and continuous. But before considering the above techniques, it is worth checking if your problem belongs to **a few**

categories which can be solved exactly in acceptable (polynomial) time. These cases are not so frequent but some of them are incredibly useful for relevant applications.

Full-fledged real world applications with realistic constraints can *rarely* be solved to optimality (in the worst case) in acceptable CPU time. In theoretical computer science one abstracts from particular hardware and operating systems and studies how the worst-case CPU time grows when the input size grows. One does not care about constants but about rate-of-growth. A CPU time which increases as a polynomial in the input size n (e.g., like n^2 or n^5) is usually considered affordable. For sure, it is better than an exponential increase like 2^n which makes solving large-size problems impossible.

On the other hand, **a demonstration of global optimality is not required by most applications**, and it your problem cannot be solved in polynomial time in the worst case (for the worst possible input configuration) it does not mean that your problem cannot be addressed in practice. First, the input configurations causing very large CPU times can be very rare. Second, if a business obtains a 10% increase in profit by some optimization technique, the proof is in the pudding and it may be of academic interest to demonstrate that the optimal solution would have been an increase of 10.5%.

In any case, before starting your solution effort, you should always check that your problem is not in the list of those solvable in acceptable CPU time, with dedicated algorithms (updated lists of problems can be found in the web). Even if your case does not correspond exactly to one of these notable problems, in some cases you can consider radical simplifications leading to solvable cases, insight and deeper knowledge.

While we cannot cover many specialized cases in this introductory book, one interesting case is **Linear Programming (LP)**, the solution of problems with a **linear objective function and linear constraints**. By the way, "programming" has nothing to do with the modern meaning related to software, but with the organized solution with help of a tabular representation (a *tableau*). **Linear Optimization** can be a modern name, but less used. Let's consider the **diet problem**, originally motivated the 1930s by the Army's desire to minimize the cost of feeding GIs in the field while still providing a healthy diet. Its goal is to select a set of food quantities that will satisfy a set of daily nutritional requirement at minimum cost. The constraints regulate the minimum and maximum number of calories and the amount of vitamins, minerals, fats, sodium, etc. in the diet. LP is considered in Sec. 33.1.

Integer Linear Programming (ILP) has the same objective function and constraints, with the additional requirements that input values are integers, which makes the problem much more difficult to solve (Sec. 33.2). Imagine a diet problem in which foods are not "continuous-valued" like flour, but can be bought in boxes like canned soup in a supermarket.

Because the number of interesting problems is simply to large to consider in a single book, we concentrate on some relevant algorithm design principles, with at least a concrete example for each case: Linear and Quadratic Programming in this Chapter, Branch and bound (Sec. 34.1), Dynamic Programming (Sec. 34.2), Perturbative and Constructive Greedy in the introductory sections (Sec. 24.1).

33.1 Linear Programming (LP)

The diet problem can be easily stated as follows:

- Minimize the cost of food eaten during one day
- Subject to the requirements that the diet satisfy a person's nutritional requirements and that not too much of any one food be eaten.

The decision variables are the quantities for the different foods in an optimal diet. After knowing the relevant constants like the *cost per unit of weight* and the *content per unit of weight* of nutrients, vitamins etc., for the different foods, it is straightforward to demonstrate that both the objective function and the constraints are **linear functions of the decision variables**. In fact, the cost is a sum over all foods of "quantity times unitary cost", and the constraints will bound above or below sums over all foods of "quantity times unitary content". E.g., a sum will require calories to be in a certain range, another sum will require vitamin A to be in a second range, etc. In addition to the historic diet problem, the number of applications of LP is wide and growing, including scheduling flight crews, drilling for oil based on geological surveys, solving many graph-related and combinatorial problems[102].

Let's now develop some **geometrical intuition** about minimizing a linear function subject to linear constraints. We already encountered linear functions and constraints (of the form $\boldsymbol{w} \cdot \boldsymbol{x}$) in the Chapters 4 and 5 about linear models . If x is one-dimensional, a linear function is a straight line, constraints are inequalities like $a \leq x$ or $x \leq b$. If there are values of x satisfying the inequalities, and the slope of the line is different from zero, it should be evident that an optimal solution will be one of the boundary values (a or b). Proof by contradiction: if optimal value x is an interior point, we can move it right or left (depending on the slope) to get a lower f value, a contradiction. Be careful: constraints like $a < x$ are *not* acceptable (imagine $f(a)$ is the minimum value). In fact, given a point close to a we could always find a smaller x value with a smaller f value: one needs **compact sets**, closed —that is, containing all its limit points— and bounded.

In higher dimensions constraints become planes and then hyper-planes, linear functions become inclined planes and gently varying functions (boring, without any curvature, with straight and equally-separated contour lines). For a concrete image, imagine a two-dimensional example, an inclined billiard table with four different legs. Minimization means leaving a billiard ball to reach the lowest possible position. Guess what, the billiard ball will stop at a corner. If the two lowest legs are equal, the ball may stop at another position along the lowest edge, but we can easily move it to one corner without spending energy.

Let's us now move from intuition to math. Linear programming is a technique for the optimization of a linear objective function, subject to linear equality and linear inequality constraints. LP can be expressed in **canonical** form as

$$\begin{aligned} \text{maximize} \quad & \boldsymbol{c}^T \boldsymbol{x} \\ \text{subject to} \quad & A\boldsymbol{x} \leq \boldsymbol{b} \qquad (33.1) \\ \text{and} \quad & \boldsymbol{x} \geq 0 \\ & \qquad (33.2) \end{aligned}$$

where $\boldsymbol{x}$ represents the vector of n variables (to be determined), $\boldsymbol{c}$ and $\boldsymbol{b}$ are vectors of coefficients, A is an $m \times n$ matrix of coefficients, one row for each of the m constraints. If the form is not canonical, simple transformations can lead to it [102].

There are two standard ways to reason about LP: **the geometrical and the algebraic view**. Let's consider the geometric way first.

The inequalities $Ax \leq b$ and $x \geq 0$ are the constraints which specify a geometrical figure known as **convex polytope** over which the objective function is to be optimized.

Each constraint, the scalar product between a row of matrix and the vector of variables: $A_i \cdot \mathbf{x} \leq b_i$, defines a half-space of points satisfying it. Because *all* constraints have to be satisfied, the *intersection* of the half-spaces, when bounded and non-empty, defines the **convex polytope**. Interestingly, the geometrical features can be defined also as the convex hull of a set of vertices of the polytope.

Convexity plays a big role. A set is **convex** if, given any two points A, B in that set, the line AB joining them lies entirely within that set. The demonstration that the LP polytope is convex is simple: a half-space is convex, and the intersection of convex spaces is convex (the line AB belongs to all half-spaces and therefore to the intersection).

The polytope boundary consists of *facets* of dimension $d - 1$ (where one or more constraints are satisfied with equality), *vertices* (faces of dimension zero, i.e., points) and *edges*, faces of dimension one, i.e., line segments.

The LP polytope contains an **infinite** number of points. A brute-force algorithm of the kind "consider all feasible points and output one with maximum value of the objective function" is impossible.

Luckily, an optimal solution can always be found at a vertex. For a demonstration, convexity and linearity are the keys. First, because the feasible region is convex and the objective function is linear, **a local optimum is a global optimum**. The demonstration is easy, imagine the above does not hold, there will be a point $\mathbf{x}_{loc}$ which is locally optimal but with a global optimum point $\mathbf{x}_{opt} \neq \mathbf{x}_{loc}$ of higher objective value. If one considers the line segment *connecting* the two points, because of convexity belonging to the feasible region, the objective along this segment

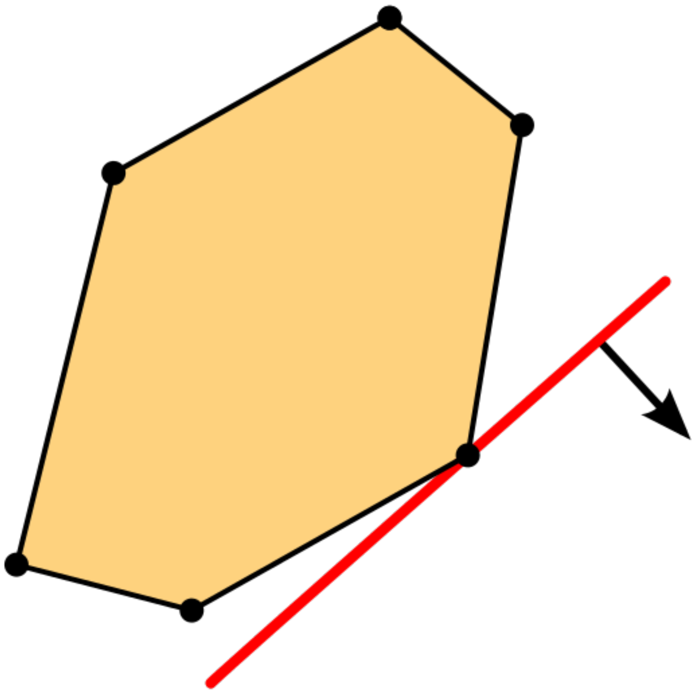


Figure 33.1: A a simple linear program with two variables and six inequalities. The set of feasible solutions is depicted in yellow and forms a polygon, a 2-dimensional polytope. The linear cost function is represented by the red line and the arrow: The red line is a level set of the cost function, and the arrow indicates the direction in which we are optimizing. Contour lines are also shown.

will increase. In particular, it will increase also for points along the segment in all local balls surrounding the local optimum, a contradiction with the fact that is is locally optimal.

In addition, a **global optimum can always be found among the vertices**. The proof is again by contradiction. Assume that a local optimum x_{opt} is in the interior of the LP polytope. If the gradient of the linear objective function is non-zero($\mathbf{c} \neq 0$), one can more away from the local optimum along the line $\mathbf{x}_{opt} + t\mathbf{c}$ $(t \geq 0)$ and obtain higher objective values, until a point on the boundary is met. If the point on the boundary is not a vertex, one considers the vectors spanning the facet or edge. Either the gradient is perpendicular (in which case moving along the faces will not change the objective), or its projection defines a direction to follow to get even higher objective values. In all cases one can safely move (getting higher or equal objective values) until a vertex is reached.

This is an important result: instead of considering an infinite number of points one can consider **only the vertices**. Actually, not all of them have to be checked. By the above conclusions that local optimality is sufficient one derives the **simplex algorithm** for LP, possibly among the ten most used algorithms in the world. The term simplex has to do with its operation on simplicial cones, the corners (i.e., the *neighborhoods of the vertices*) of the polytope.

The high-level description of the simplex algorithm is as follows.

- It starts at some vertex. If the problem is solvable (the feasible region is not empty), an initial vertex can be determined by applying the simplex algorithm to a modified and easily solvable version of the original program.
- A sequence of **local search** (LS) steps are executed, in which the possible neighbors (in local search terminology) of the current vertex are the vertices that can be reached by moving along an edge. LS always moves to an improving local vertex (one with higher objective value). Different versions have to do with rules for picking an

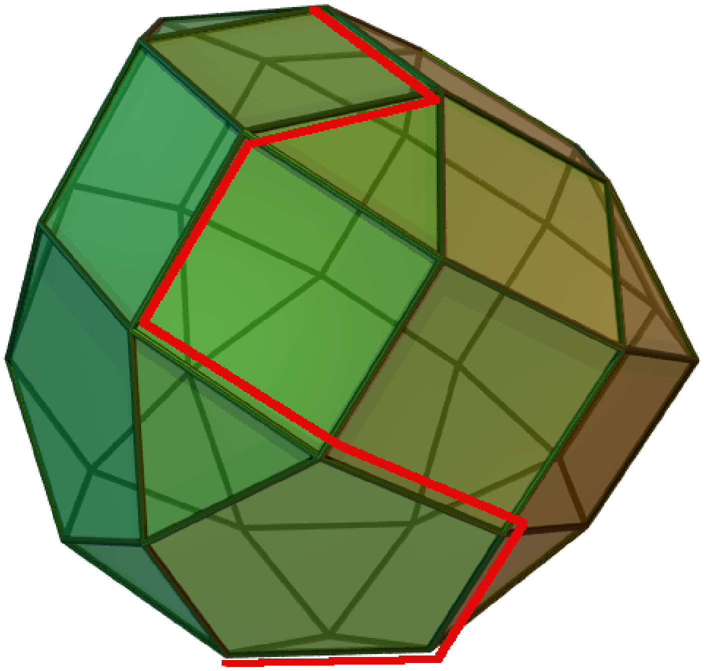


Figure 33.2: The simplex algorithm for solving LP problems.

improving vertex. In the LP terminology, a **pivot** is related to this passage to a neighboring vertex, and **pivoting rules** are LS rules for selecting an improving neighbor.

- Simplex terminates when it reaches a **local maximum**, a vertex from which all neighboring vertices have a smaller objective value. Because of convexity of feasible region and linearity of objective function, this is actually a global optimum.

The simplex algorithm works by constructing a feasible solution at a vertex of the polytope and then **walking along a path on the edges of the polytope** to vertices with non-decreasing values of the objective function until an optimum is reached.

A couple of questions are related to convergence (in a finite number of steps) and computational complexity (number of operations as a function of the dimension of the problem). For the first issue, the simple version above has to be cured o avoid possible cycles (endless repetitions of a sequence of vertices) in rare but possible situations. This "stalling" is possible only in the *degenerate* case of neighboring vertices with equal objective values. A randomized rule for picking a vertex in case of ties is a simple way to cure cycling. For the second issues, unfortunately he worst-case complexity of simplex method as formulated by Dantzig is exponential time. An exponential number of iterations is rarely encountered for many practical problems, but there is no guarantee.

The existence of solutions algorithms for LP with guaranteed polynomial complexity has been an open problem in computer science for many years. The LP problem was first shown to be solvable in polynomial time by Leonid Khachiyan in 1979, but a larger breakthrough in the field came in 1984 when Narendra Karmarkar introduced a new **interior-point method**. Nonetheless, the simplex algorithms with smart pivoting rules is still the *de facto* standard for most applications of LP.

33.1.1 An algebraic view of linear programming

Although the geometric view is intuitive, the algebraic view is useful to derive a workable algorithm. We refer to [287, 102] for detailed demonstrations and give only a short summary here. A first observation is that the boundaries of the polytope corresponds to some inequalities in the constraints becoming equality (the constraint is *tight* or *active*). If one sits at a vertex, a small change in some directions will make the point exit the feasibility region.

Now, dealing with equalities only is simpler than dealing with inequalities. Luckily, one can transform an LP problem into the **slack form**:

$$\begin{array}{cl} \text{maximize} & \mathbf{c}^{\mathrm{T}}\mathbf{x} \\ \text{subject to} & A\mathbf{x} = \mathbf{b} \\ \text{and} & \mathbf{x} \geq \mathbf{0} \end{array} \tag{33.3}$$

by a simple trick of adding additional **slack variables**. For each constraint:

$$\sum_{j=1}^{n} a_{ij} x_j \leq b_i \tag{33.4}$$

one introduces a new variable s and rewrites the above inequality as the two contraints:

$$\sum_{j=1}^{n} a_{ij} x_j + s = b_i \tag{33.5}$$

$$s \geq 0 \tag{33.6}$$

A constraint is satisfied if and only if there is a non-negative *slack* or difference between the left- and right-hand of equation (33.4).

If A is the $m \times n$ matrix, with $m < n$, the algebraic definition of a corner is obtained as follows. There are m linearly independent columns A_j of A, which make up a basis $\mathcal{B} = \{\mathcal{A}_{|\infty}, ..., \mathcal{A}_{|\Updownarrow}\}$ of the linear space spanned by all columns (A is of (full) rank, and "row rank equals column rank", therefore rank is the minimum of the two dimensions). We can collect the columns of the basis $\mathcal{B}$ as an $m \times m$ nonsingular (invertible) matrix $B = [A_{j_i}]$. Being a basis, all vectors in R^m can be derived by linear combination, in particular the vector $\mathbf{b}$, the other columns are not involved (their coefficient in the linear combination is zero).

A **basic solution** corresponding to the basis $\mathcal{B}$ is a vector $\mathbf{x} \in R^n$ with elements different from zero only for indices corresponding to the basis columns. In detail:

$$\begin{array}{ccll} x_j & = & 0 & \text{for} A_j \notin \mathcal{B} \\ x_{j_k} & = & \text{the } k\text{-th component of } B^{-1}\mathbf{b}, & k = 1, ..., m \end{array}$$

The connection between geometry and algebra is that **basic feasible solutions correspond to vertices** of the polytope.

When LP is formulated in the slack form, the simplex algorithm works with the system of equalities by rewriting it in an equivalent form. After a number of iterations, the system is rewritten so that the solution is immediate to obtain. In a way, **the simplex algorithm can be considered as a kind of "Gaussian elimination for inequalities"**.

At each step, the linear program is reformulated so that the current basic solution has a greater objective value. The action of moving along the edge of the polytope from a vertex to a neighboring one corresponds to changing the basis B. At each step one chooses a nonbasic variable (initially set to zero - not in the basis) which appears with a positive coefficient in the objective (if one increases the variable, the objective increases). The variable is raised away from zero until a constraint becomes tight (some basis variable becomes zero). At this point, one can rewrite the slack form, exchanging the roles of the basic and non-basic variables (a column exits the base B and a new column enters). After rewriting, if all multiplicative constants in the objective function are negative, we are done. By increasing non-basic variables we can only worsen the solution and therefore the vertex (basic feasible solution) is optimal. **Pivoting** corresponds of course to having a new non-basic variable enter the basis (entering variable) and a basic variable exit (leaving variable).

33.2 Integer Linear Programming

An Integer Linear Programming problem (ILP) is an LP problem with the additional constraints that the variables **x** must take on **integral values**. Imagine the diet problem, in which foods can only be bought in boxes of 1,2,3 ... kilograms.

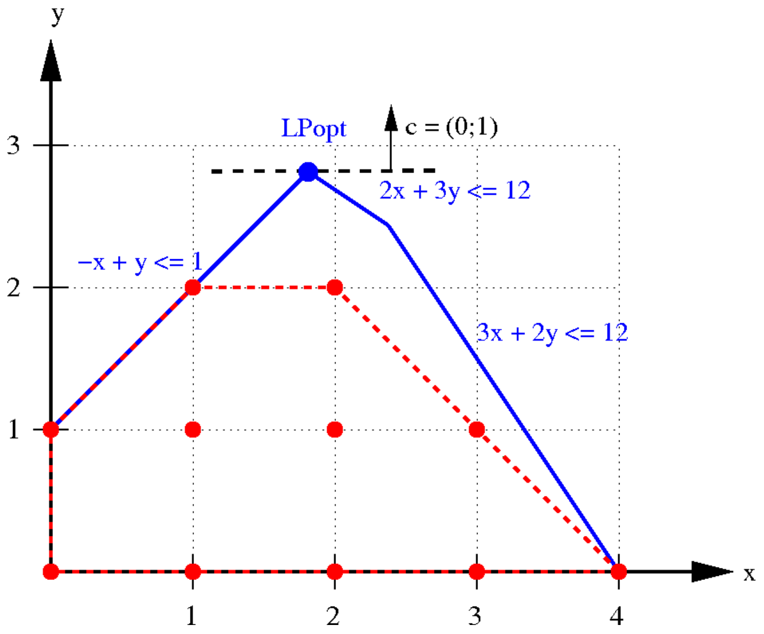


Figure 33.3: Integer Linear Program and relaxation.

Now, it can be demonstrated that ILP is NP-hard, therefore belonging to a hard class of problems for which there is unlikely to be a polynomial-time algorithm in the worst case. What looks like a "small" change in the definition (from real values to integers) completely changes the theoretical hardness of the problem. Actually, the problem is so hard that just determining whether an ILP problem has a feasible solution is NP-hard.

Intuitively, the feasible region is not a nice polytope anymore but a set of dots corresponding to integer (feasible) coordinates. No way to move continuously from vertex to vertex!

A heuristic way to proceed is to simply remove the constraint that **x** is integral, and solve the corresponding LP (called the **LP relaxation of the ILP**). The optimal LP value is for sure an *upper bound* (when one relaxes to real values, in particular one considers also integral values, and therefore has *more* possibilities to improve a solution). One can then round the entries of the solution to the LP relaxation to the nearest integers. Of course, a solution obtained by rounding may not be optimal, it may not even be feasible (it may violate some constraint). ILP problems can be solved with heuritic local search techniques (but of course abandoning hopes of guaranteed optimality in polynomial times).

33.3 Quadratic Programming (QP)

In addition to Linear Programming, a notable special case is that of **Quadratic Programming (QP)**, the problem of optimizing a *quadratic* function of several variables subject to linear constraints on these variables. An example has been encountered in dealing with Support Vector Machines (Chapter 12). Quadratic Programming is defined as:

$$\text{minimize}\tfrac{1}{2}\mathbf{x}^T Q\mathbf{x} + \mathbf{c}^T\mathbf{x} \quad \text{subject to} \quad A\mathbf{x} \leq \mathbf{b}.$$

For positive-definite Q, the ellipsoid method solves the problem in polynomial time. But if Q is indefinite, the problem becomes NP-hard. The mental image for positive-definite Q is that of Fig. 26.8. QP is considered to be solvable in practice for dimensions ranging up to thousands of variables (depending on the problem characteristics).

An excellent introduction of some classic algorithms for discrete (combinatorial) are [287] and [102], an updated "Bible of algorithms". More than on a list of special cases it is more interesting to concentrate on **high-level algorithm design principles** for optimization problems (with some concrete examples), in addition to the case of Local Search considered in Section 24.2.

Gist

Linear Programming, the solution of optimization problems with linear objective functions and linear constrains, creates mental images of gentle slopes and straight walls, and of balls ending up in low corners. LP is among the most widely used problems.

The analysis of LP and the development of the simplex algorithm is an elegant mixture of continuous (infinite) but convex feasible areas, and local search among the discrete set of vertices. The two different views (geometric and algebraic) are useful to develop insight about the problem structure and its solution.

LP can be solved in polynomial time, although the most used algorithm (the simplex) has no worst-case guarantee of always converging in a polynomial number of steps.

Remember that small changes in the definition can make huge changes in the difficulty of solving the problem: if input values are constrained to be integers the problem (ILP) becomes one of the hardest to be solved to optimality. But useful bounds and heuristic solutions can be obtained by relaxation: the problem is solved with continuous variables (LP) and the results is then rounded to the nearest integers.

Quadratic Programming can be used to solve efficiently problems with quadratic objective functions and linear constraints.

If you encounter an LP or QP in your business, enjoy, there is a wide variety of off-the-shelf software which can be immediately used for its solution.

Chapter 34

Branch and bound, dynamic programming

Big fish eats little fish.

The number of different optimization problems is so large that one can easily feel lost in a maze of details. Luckily, in many cases some **common underlying algorithm design principles** can be used for their solution. We therefore concentrate on the most relevant algorithmic patterns in addition to greedy and local search: Branch and Bound (Sec. 34.1) and Dynamic Programming (Sec. 34.2), with at least a concrete example for each algorithmic principle.

Branch and bound is a little smarter than the exhaustive enumeration of all possible solutions. When **branching** one considers all possible ways of fixing the value of a variable in the solution (leading to a subtree - a branch - in the visual representation of the process). In the construction of a complete solution from a partial one, a **bound** is associated to the current partial solution. One knows that, in whatever manner a solution is completed, one cannot obtain more than the value given by the bound. If this value is surpassed by the current "record" solution, the completion of the tentative solution is aborted and some iterations are spared.

Dynamic Programming is based on decomposing a problem, finding solutions to smaller instances, and re-using them to build solutions to larger and large instances, in a bottom-up manner. Because smaller instances are found many times, it makes sense to store their solutions in an organized memory structure. In an analogy, the big problem contains little problems in its bellies, which can be eaten to build the complete solutions.

34.1 Branch and bound

If one needs to find a best configuration out of a finite set, a brute-force algorithm is **exhaustive search**: generate all possible configuration and evaluate the corresponding objective-function values, deliver the best one.

If a configuration corresponds to picking specific values for a set of variables, the entire set of configurations can be organized as a **solution tree**: the root is the starting situation (no decision yet taken - no value given to the variables)), the first level corresponds to different (but finite) ways of assigning a value to the first variable, the second-level children correspond to the different values for the second variable, etc. **Complete solutions** correspond to the leaves of the tree, while internal nodes are **partial solutions**. Let's note that the tree is not unique, variables can be ordered in different ways and not necessarily balances (some variables can be assigned values conditionally on the values of other ones). Exhaustive search then is implemented by generating the entire tree and examining its leaves.

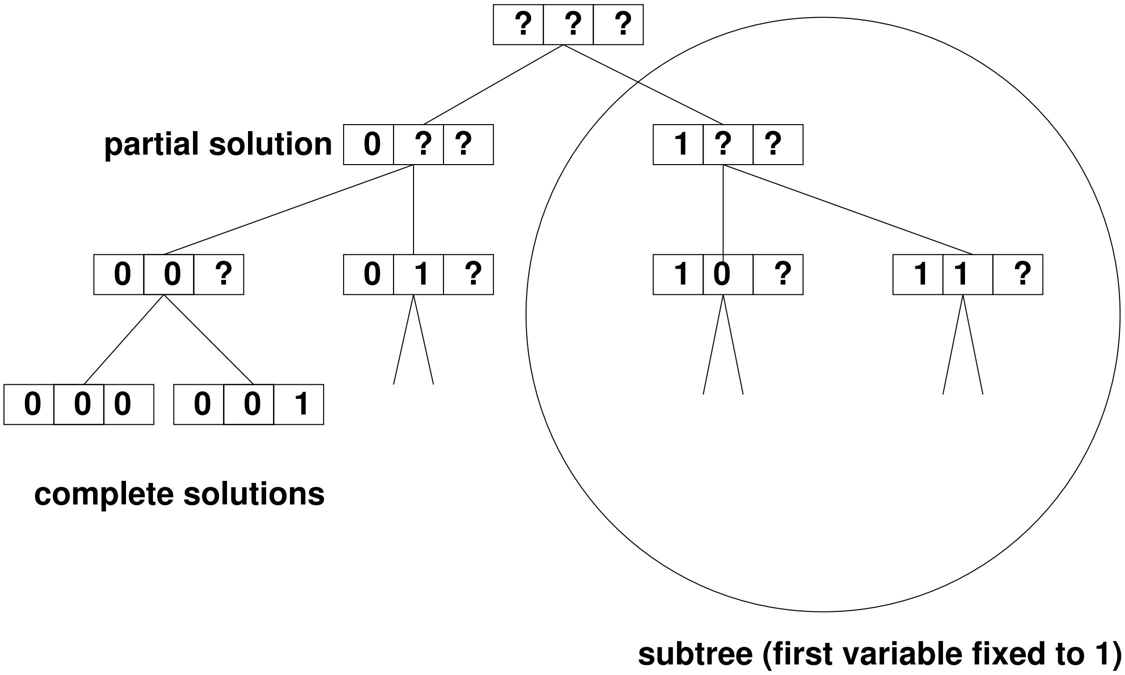


Figure 34.1: A solution tree for a binary sting with three variables.

As a concrete example, if the solution consists of a binary string, after a specific subset of bits is fixed (to 1 or 0) in a **partial solution**, one is left with the possibility to fix in all possible ways the remaining variables ("free variables"). When then the first free variable is fixed to zero one gets the left subtree, when it is fixed to one one gets the right subtree (Fig 34.1).

As you imagine, exhaustive search is too simple to be a practical solution for most cases: the difficulty lies in the enormous number of leaves, which can grow exponentially (e.g., if C values are possible for n variables, the total number of possibilities is C^n).

A trembling flame of hope in the tunnel of exhaustive search, which is some cases can lead to a notable saving of CPU time, is called **Branch and Bound (BB or B&B)**. The core idea is that some parts of the trees can be "**pruned**" (do not need to be generated) because one can demonstrate that **some partial solutions have no hope of becoming optimal** when completed. **B&B** was used al lot in the early stages of Artificial Intelligence. A generalization of branch and bound also subsumes the A*, B* and alpha-beta search algorithms from artificial intelligence [279]. In most cases, although a lot of CPU time can be spared, the total remains exponential and the size of instances which can be solved to optimality increases only by a small quantity. Nonetheless, B&B can be used also with early stopping and therefore becomes a useful heuristic when an optimal solution cannot be guaranteed in the allotted CPU time.

B&B is an algorithm design paradigm, mostly for discrete and combinatorial optimization problems. It consists of a systematic enumeration of candidate solutions by means of state space search. Before we considered nodes as decision points (fixing the value of a variable). An alternative and complementary view is to associates nodes with **sets of solutions**, the complete slutions which can be obtained by fixing the remaining free variables in all possible ways. The full set of candidate solutions is at the root. The algorithm explores branches of this tree, which represent subsets of the solution set (all leaves of the subtree originating at a node). **Branching** means assigning a value to a variable in a partial solution and finding, in a recursive manner, the best value in the corresponding subtree. Before enumerating the candidate solutions of a branch, the branch is checked against an **optimistic bound** on the optimal solution, and is discarded if it cannot produce a better solution than the current record value (the best value found so far by the algorithm). We talk about "optimistic" bound to avoid the usual confusion between upper or lower bound, depending on the max or min direction of optimization. The advantage w.r.t. exhaustive search depends on the existence, quality and speed of computation of the *optimistic bound* used for pruning. If the bound is tight, a big fraction of the search space can be cut.

To summarize (and after deciding for minimization), branch-and-bound aims at minimizing the value of a real-valued function $f(x)$, in which $x \in S$, the set of admissible, or candidate solutions, also called **search space**. A B&B algorithm operates according to two principles:

1. It recursively splits the search space into smaller spaces (**branching**), then minimizing $f(x)$ on these smaller spaces.

2. It keeps track of an **optimistic bound** on the minimum value which can be reached by completing a given partial solution in all possible ways. If the bound is larger than the current record value, the current subtree is pruned, and control is returned to the first encountered higher level in the tree which has alternative ways to fix variables not yet explored. This operation is called **backtracking**.

If one eliminates backtracking one obtains a single construction. The construction is greedy if the most promising choice is executed at each step. Greedy is myopic and cannot undo early choices. With backtracking, early choices will be undone in a systematic manner, until all possibilities are eventually tried. As one can imagine, programming languages with **recursive function calls** permit very elegant software implementations of branch-and-bound methods.

In visiting the solution tree starting from the root, like in all graph visits, one can proceed depth-first or breadth-first. The **depth-first** variant (going down the tree to produce an initial complete solution) quickly produces complete solutions, and therefore record values. Intelligent implementations aim at producing a first high-quality solution early in the search, so that its record value will help in pruning many future subtrees.

Fig. 34.3 shows a toy example related to maximizing the number of queens which can be placed on a chessboard so that no queen can attack another queen. For each positioned queen, no other queen can be placed in the same row, in the same column and in the two diagonals centered on the queen (Fig. 34.3). The first level of the tree is given by placing the first queen in all possible squares in the first row. The second level is obtained by placing the second queen in all possible *admissible* squares in the second row. The inadmissible squares do not lead to a subtree to explore, and are immediately dismissed. Each subtree is deepened until no additional queen can be placed. When this happens, the system backtracks to the first higher level in the tree with alternatives which have not been tried yet. A simple optimistic bound on the *new* queens that can be placed is given by the number of free squares remaining after eliminating all rows, columns and diagonals in which a queen is already placed.

Notice that Branch and Bound (much like Brute Force enumeration of all possible solutions) creates a search tree that explodes exponentially as the problem size increases. Therefore it will hit the same scalability wall, only a little bit later. In spite of its popularity in the initial study of Artificial Intelligence, Branch And Bound is unusable for most real-world problem due to its CPU time requirements. In any case, careful implementations are in some cases crucial to pass from solving problems with a few variables (say up to 5 or 10) to solving bigger problems, say with up to 20 or 30 variables. In some cases this permits to go from toy problems to cases which are closer to more complex real-world

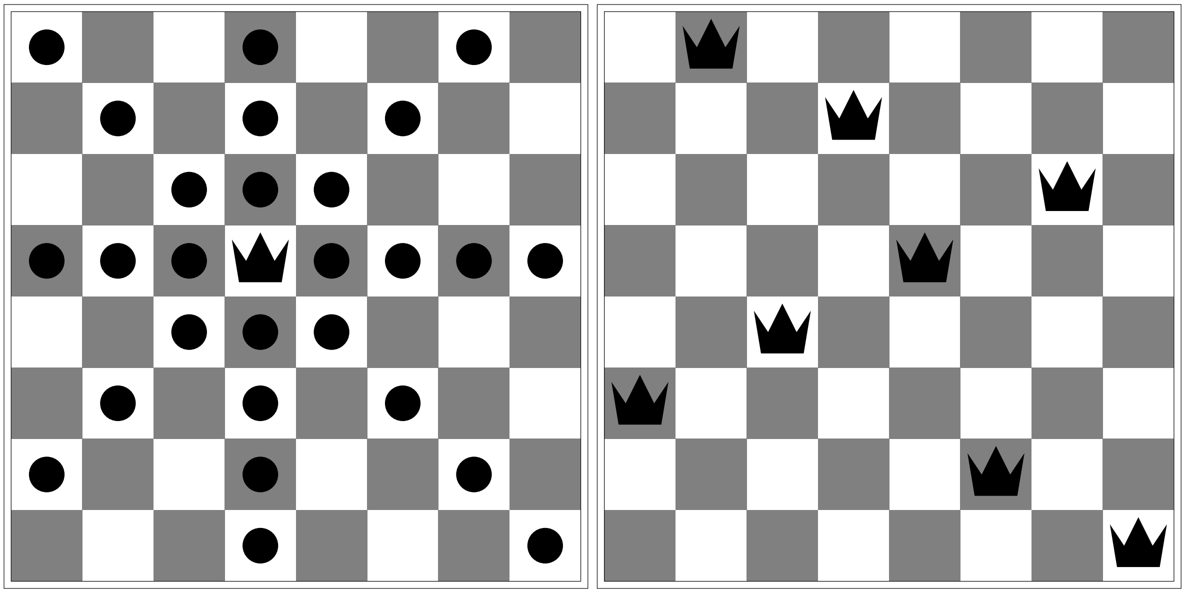


Figure 34.2: In chess, a queen is allowed to "take" any other queen on the board by moving along row, column or diagonals (left). Eight queens (right), is this a solution so that no queen can eat another one?

situations. On the other hand, when used as an heuristic (with early termination and no proof of optimality) B&B can be competitive if one employs smart bounds and rapid creation of good record values.

34.2 Dynamic programming

In some cases, the optimal solutions has a **structure with interesting nesting characteristics**, which can help in building it efficiently and in demonstrating its optimality. In Dynamic Programming, "*big fish eat little fish*", big problems have **shared optimal subproblems** in their bellies.

Dynamic programming (DP) shares with the general divide-and-conquer method the principle of solving problems by combining solutions to subproblems, with the specific flavor that the subproblems are not independent, i.e., **problems share subproblems**. DP solves each subproblem *only once* and then saves its result in a table, therefore avoiding useless re-computation. As it was the case for LP, "programming" has nothing to do with software but with the use of a tabular solution method.

DP algorithms, originally studied by R. Bellman in 1955, are developed according to four steps:

1. Study and characterize the structure of an optimal solution (how it *contains solutions to smaller instances*).

2. *Define the value* of an optimal solution *in a recursive manner* from the values of solutions of subproblems.

3. *Compute the value* of the optimal solution in a bottom-up manner (by starting from the smallest subproblems).

4. *Construct* an optimal solution from information computed while finding the value.

The above may sound abstract but dynamic programming is actually fundamental in making cellular phones work (Viterbi's algorithm), in bio-informatics (finding longest common subsequences in DNA), scheduling to maximize profit, in calculating shortest paths, and in hundreds of concrete applications including menial ones like pretty-printing and LaTEx formatting. Some for of DP has been used also for making this book look nice!

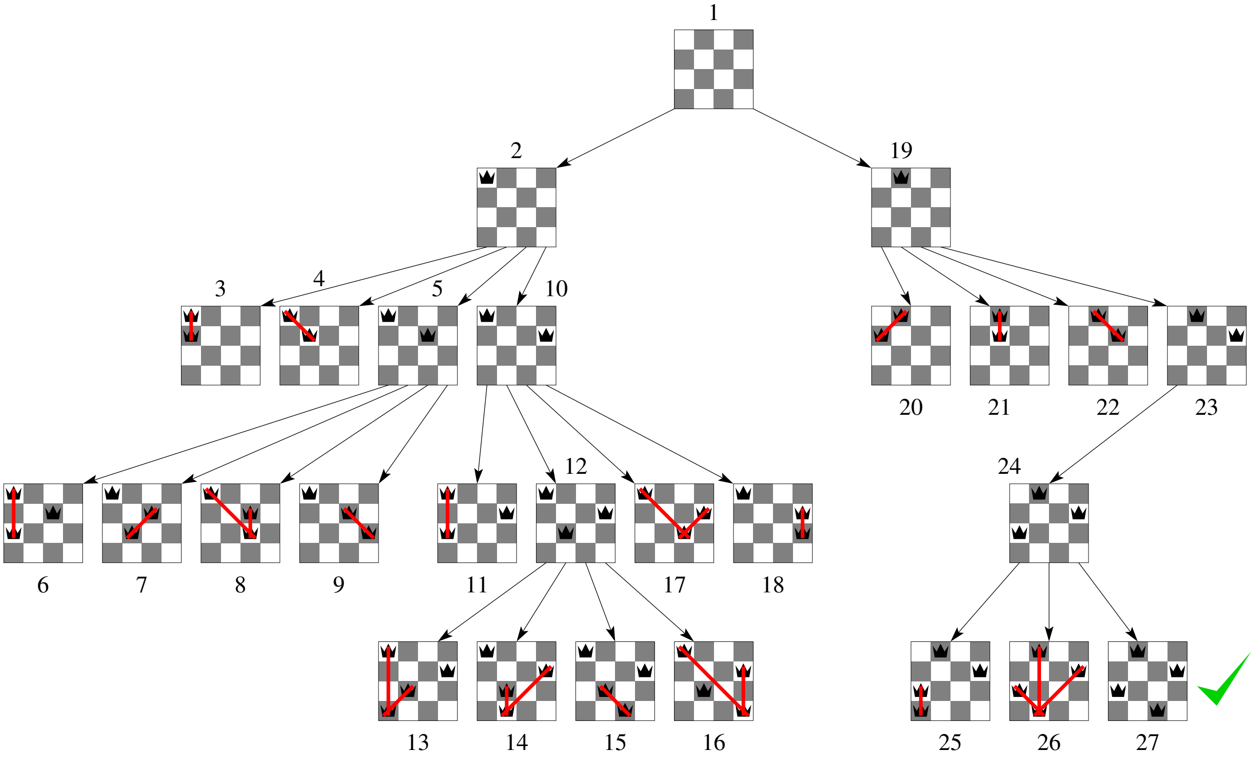


Figure 34.3: Branch and bound in action to maximize the number of queens placed on a 4×4 chessboard. Queens are positioned one row after another one. Positions are shown up to the first legal solution.

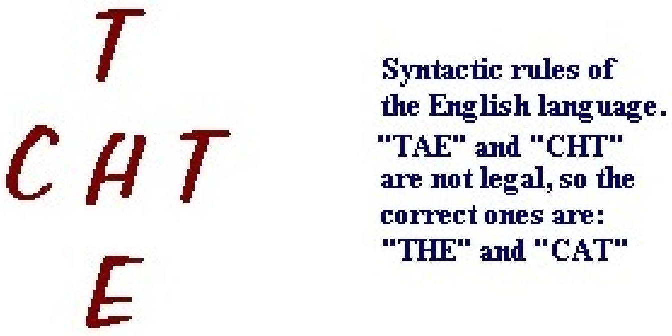


Figure 34.4: Viterbi's dynamic programming algorithm applied to text recognition.

We focus on **Viterbi's algorithm** here.

To help the intuition, let's consider a simplified problem of text recognition first (Fig. 34.4, 34.5). Recognition of characters from a text source can be done Optical Character Recognition (OCR) machines. The recognition of text can work by trying to recognize *individual* characters but the error rate can be large if the image is corrupted by noise or if the same letter can be written in many different ways. Imagine interpreting a hand-written prescription of medicines by doctors. Pharmacists can do it because they have a large amount of additional background information.

A model going beyond individual characters considers the fact that written text is a *sequence* generated from an underlying correct word or phrase. The probability of recognizing a character at a certain position depends on the underlying sequence, and therefore on the context given by additional nearby characters. In Fig. 34.4 ("THE-CAT" example) the recognition of the central ambiguous character as "H" or "A" is for sure influenced by the presence of a previous character "T" or "C". In the same manner, our brain recognizes spoken words and phrases even in very noisy and difficult situations, by considering its sequential nature and a lot of additional contextual knowledge.

Sequences abound in the real-world, as well as simple models to calculate overall probabilities of complete sequences. As noted before when discussing **maximum a posteriori (MAP) probability**, the principle of **searching for the most probable sequence given the observed signals and given a model of sequence generation** is a sound heuristic principle for identifying a "hidden" explanation of the observation. The "hidden" explanation of a recording is the correct phrase which originated the specific utterance.

Very useful and used models of sequences generated by an underlying hidden process are called **hidden Markov model (HMM)**. The intention is to model a system with a **hidden state** (not directly measurable) which produces one among a set of output signals (or symbols), with a probability for each symbol. In addition, the hidden state changes probabilistically in discrete time (1,2,3...), with a certain transition probability. One measures the output signals and aims at identifying **the most probable sequence of hidden states** producing the observed sequence of signals. Events are independent so that probabilities are multiplied. We can view the probability of a *path* (a specific sequence if hidden states in time) as the probability that a "random walk" beginning at time one with a given probability of being in the different initial states will follow the given path.

If you want, you can introduce a fictitious state 0 with a probability π_i of transiting to state i at time 1.

Mathematically the **hidden Markov model** is characterized by a state space S, initial probabilities π_i of being in state i, transition probabilities $a_{i,j}$ from state i to state j, and emission probabilities $b_{i,o}$ that state i emits a certain observation o.

Say we observe outputs $y_1, \dots, y_T$.

Let $V_{t,k}$ is the probability of the most probable state sequence ending at time t with k as its final (hidden) state. The best way to reason about the **shared optimal substructure** of the optimal solution is to consider its structure *in time*. Assume that $(s_1, ..., s_{t-1}, k)$ is the optimal sequence (the most probable one) ending at state k at iteration t, and consider the most probable sequences stopping one iteration before, at $t-1$. Let $V_{t-1,x}$ be the probability of the most probable path reaching configuration x at the previous time. Two other events must happen to reach k, a transition from x to k and the emission of the measured signal y_t. Because we are searching for the most probable sequence, we must maximize the probability over all possible previous points x.

Therefore, the most likely state sequence $x_1, \dots, x_T$ that produces the observations is given by the recurrence relations:

$$\begin{array}{rcl} V_{1,k} & = & \mathrm{P}\big(y_1 \mid k \big) \cdot \pi_k \\ V_{t,k} & = & \max_{x \in S} \big(\mathrm{P}\big(y_t \mid k \big) \cdot a_{x,k} \cdot V_{t-1,x} \big) \end{array}$$

After determining the optimal value, the Viterbi path can be retrieved by saving **back pointers** that remember which state x was the winning one in the second equation. Let $\mathrm{Ptr}(k,t)$ be the function that returns the value of x used to compute $V_{t,k}$ if $t > 1$, or k if $t = 1$. Then:

$$\begin{array}{rcl} x_T & = & \arg\max_{x \in S} (V_{T,x}) \\ x_{t-1} & = & \mathrm{Ptr}(x_t, t) \end{array}$$

The complexity of this algorithm is $O(T \times |S|^2)$ while a complexity of a brute-force scheme considering all possible paths is $O(|S|^T)$. The reduction in CPU time is enormous for long sequences.

To illustrate how the Viterbi algorithm works, consider the short example in Fig. 34.5. One assumes a 4-letter alphabet, $A = \{T, A, C, O\}$, and the observed string given by the OCR machine is $Z = -CAT-$, where "$-$" denotes blank or space. The features vectors $z1, z2$, and $z3$ are obtained when the feature extractor looks at C,A,T. The available and relevant information that Viterbi's algorithm traverses to make a decision on the word, is expressed in

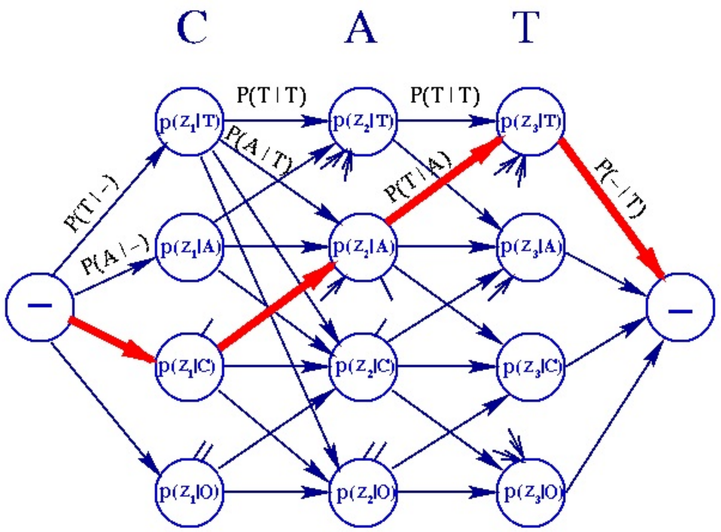


Figure 34.5: Viterbi's dynamic programming algorithm applied to text recognition.

terms of a directed graph or **trellis** as in Fig. 34.5. All nodes (except the blank nodes "-") and edges have probabilities associated with them. The edge probabilities (Markov transition probabilities between letters) remain fixed no matter what sequence of letters is presented to the machine. They represent *static information*. The node probabilities (likelihood of the feature vectors obtained from the characters), on the other hand, are a function on the actual characters presented to the machine. They represent *dynamic information*. We see from the figure that any path from the start node to the end node (the "–" nodes) represents a sequence of letters but not necessarily a valid word. Consider the bold path, which represent the letter sequence CAT. The aim is to find the letter sequence which maximizes the product of the probabilities of its corresponding path.

The pseudo-code of the algorithm is shown in Fig.34.6. Two support matrices are used to save values of the optimal subproblems (T_1) and to save the previous state in the temporal path, so that the optimal solution can be reconstructed at the end.

Andrew Viterbi proposed its algorithm in 1967 as a decoding algorithm for "convolutional codes" over noisy digital communication links. Being an application of dynamic programming, it has, however, a history of multiple invention.

A Dynamic Programming algorithm called the Bellman-Ford Algorithm is used to for the **single-source shortest path problem**, while the Floyd-Warshall algorithms can be used to find **shortest paths between all pairs** of vertices. The starting observation is that a shortest path between two vertices contains other shortest paths within it (otherwise one could substitute sub-paths obtaining shortest overall paths).

Similar algorithms, with generalizations, are now in wide use for maximization problems involving probabilities like statistical parsing, to find the most likely assignment of all or some subset of latent variables in some graphical models, e.g., Bayesian networks, Hidden Markov Models (HMM), and Markov random fields. The latent variables need in general to be connected in a way somewhat similar to an HMM, with a limited number of connections between variables and some type of linear structure among them.

O	Set of observations emitted by states
S	Set of states
$\boldsymbol{\pi}$	Initial probabilities for states
$\boldsymbol{y}$	Observed outputs
A	Matrix of transition probabilities between states
B	Matrix of emission probabilities

```
function Viterbi ($O$, $S$, $\boldsymbol{\pi}$, $\boldsymbol{y}$, $A$, $B$)
    for each state $s_i$
        $T_1[i,1] \leftarrow \pi_i \cdot B_{i,y_1}$
        $T_2[i,1] \leftarrow 0$
    for i $\leftarrow$ 2, 3, ..., $T$
        for each state $s_j$
            $T_1[j,i] \leftarrow \max_k(T_1[k,i-1] \cdot A_{kj} \cdot B_{j,y_i})$
            $T_2[j,i] \leftarrow \arg\max_k(T_1[k,i-1] \cdot A_{kj} \cdot B_{j,y_i})$
    $z_T \leftarrow \arg\max_k(T_1[k,T])$
    $x_T \leftarrow s_{z_T}$
    for i $\leftarrow$ $T$, $T$-1, ..., 2
        $z_{i-1} \leftarrow T_2[z_i, i]$
        $x_{i-1} \leftarrow s_{z_{i-1}}$
    return $\boldsymbol{x}$
```

Figure 34.6: Viterbi algorithm pseudo-code.

Gist

When solving problems with a set of discrete variables, **brute-force** exhaustive generation of all possible solutions has a clear scalability issue: the CPU time explodes in an exponential manner when the number of variables grows. One can imagine producing a tree, in which an additional variable is set to all possible values at a node, generating the corresponding sub-trees (**branching**). Branching alone amounts to brute-force enumeration of candidate solutions and testing them all. To improve the performance, Branch and Bound keeps track of an **optimistic bound** on the solution which can be obtained by completing a partial solution. This bound is compared with the current record value at each iteration to “prune” the search space, eliminating partial solutions that are doomed (one is sure that their completions will not contain any optimal solution). When a node in the tree is doomed, the search **backtracks** and continues from an upper-layer node which contains new subtrees to explore.

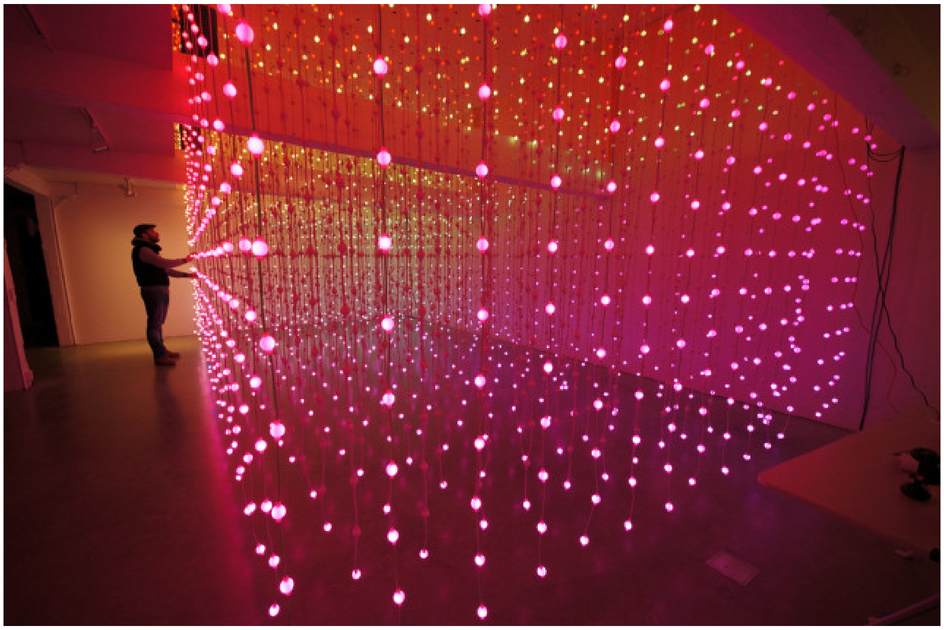
The popularity of B&B in the initial part of Artificial Intelligence is somewhat surprising: given only toy problems can be solved because of its exponential running times. For sure, the human species would not have survived in the forest with B&B when confronted by very fast predators.

The core idea of **dynamic programming** is to avoid repeated work by remembering partial results. It works when one can demonstrate that an **optimal solution contains optimal solutions to smaller subproblems**. The smaller subproblems can be solved once and saved in memory to build solutions to many larger and larger problems. In some happy cases this process leads to an enormous reduction of CPU times (and better scalability) w.r.t. the brute-force solution. Cellular phones would be impossible without Viterbi’s algorithm.

Chapter 35

Satisfiability

I can't get no satisfaction
'Cause I try and I try and I try and I try
(The Rolling Stones)



It is difficult to think about a problem which is more relevant for the applications and more interesting from an algorithmic point of view than **satisfiability of Boolean formulas**. It is the problem of determining if there exists an interpretation that satisfies a given Boolean formula. In other words, it asks whether the variables of a given Boolean formula can be consistently replaced by the values TRUE or FALSE so that the formula evaluates to TRUE.

Many instances of SAT that occur in practice, for example in **symbolic artificial intelligence, circuit design and automatic theorem proving**. While the roots of formalised logic go back to Aristotle, the dream of automating the derivation of all mathematical truth using axioms and inference rules of formal logic had a huge expansion in the twentieth century. Applications in integrated circuit design and verification are of particular commercial interest, given the huge losses caused by mistakes in the design of logic circuits. Solving *SAT* is a prototypical form of the more general **onstraint programming (CP)** method, searching for a state of the world in which a large number of constraints are satisfied at the same time. The constraints are expressed as Boolean formulas of binary variables (with two values usually called “true” and “false”).

In spite of their far-reaching mathematical interest, as an additional bonus, SAT and MAX-SAT are surprisingly easy to define and visualize, and therefore helpful to make abstract procedures very concrete in our minds. This chapter is somewhat more detailed than the other ones, and it requires therefore more effort and concentration, because most of the algorithmic building blocks for solving optimization problems can be encountered for *SAT* in a simple and terse version, with clear advantages for learning. In addition of the already presented topics, *SAT* gives the opportunity to discuss **approximation algorithms** (with guaranteed performance ratio) and **randomized algorithms** in which random numbers are used in the solution.

To start with a toy concrete example, let’s consider the organization of a meeting. Consider the following constraints: John can only meet either on Monday, Wednesday or Thursday, Catherine cannot meet on Wednesday, Anne cannot meet on Friday, Peter cannot meet neither on Tuesday nor on Thursday. Question: Is the meeting possible and when can it take place?

The constraints can be encoded into the following Boolean formula:

$$(Mon \bigvee Wed \bigvee Thu) \bigwedge (\neg Wed) \bigwedge (\neg Fri) \bigwedge (\neg Tue \bigwedge \neg Thu)$$

The formula can be satisfied by setting Monday to TRUE, and the other days to FALSE, and therefore the meeting can take place on Monday. Sure, this can also be easily solved by hand, but imagine defining meetings in a large university subject to many constraints regarding professors, classrooms, etc. Even approximated solutions become very hard!

In the following sections, by following mostly [35], we summarize the main methods, considering both exact (complete) and approximated approaches.

35.1 Satisfiability and maximum satisfiability: definitions

In the Maximum Satisfiability (*MAX–SAT*) problem one is given a Boolean formula in conjunctive normal form, i.e., as a conjunction of clauses, each clause being a disjunction. The task is to find an assignment of truth values to the variables that satisfies the maximum number of clauses.

SAT is the decision version of the problem, i.e., to assess if *all* clauses can be satisfied or not. A *MAX–SAT* solution solves *SAT* if the maximum number of clauses satisfied is equal to the total number of clauses.

In our work, n is the number of variables and m the number of clauses, so that a formula has the following form:

$$\bigwedge_{1\leq i\leq m} (\bigvee_{1\leq k\leq |C_i|} l_{ik})$$

where $|C_i|$ is the number of literals in clause C_i and l_{ik} is a literal, i.e., a propositional variable u_j or its negation $\overline{u_j}$, for $1 \leq j \leq n$. The set of clauses in the formula is denoted by **C**. If one associates a *weight* w_i to each clause C_i one obtains the weighted *MAX–SAT* problem, denoted as *MAX W–SAT*: one is to determine the assignment of truth values to the n variables that maximizes the sum of the weights of the satisfied clauses. Of course, *MAX–SAT* is contained in *MAX W–SAT* (all weights are equal to one). In the literature one often considers problems with different numbers k of literals per clause, defined as *MAX–k–SAT* , or *MAX W–k–SAT* in the weighted case. In some papers *MAX–k–SAT* instances contain *up to* k literals per clause, while in other papers they contain *exactly* k literals per clause. We consider the second option unless otherwise stated.

MAX–SAT is of considerable interest not only from the theoretical side but also from the practical one. On one hand, the decision version *SAT* was the first example of an $\mathcal{NP}$–complete problem [100], moreover *MAX–SAT* plays an important role in the characterization of different approximation classes [13]. On the other hand, many issues in mathematical logic and symbolic **artificial intelligence** can be expressed in the form of satisfiability or some of its variants, like **constraint satisfaction**. Some relevant applications are consistency in expert system knowledge bases [281], integrity constraints in databases [11, 142], approaches to inductive inference [187, 227], asynchronous circuit synthesis [209, 302].

We summarize the basic approaches for the exact or approximated solution of the *MAX W–SAT* and *MAX–SAT* problem, to give a panoramic view of the extreme diversity of methods.

The presentation of algorithms for the *SAT* is limited to a quick overview.

35.1.1 Notation and graphical representation

MAX–SAT is easy to define and excellent to visualize, and therefore to remember.

A clause will be represented either as $C = \overline{u} \vee v \vee z$ or as a set of literals, as in $C = \{\overline{u}vz\}$.

For the following discussion, it can be useful to help the intuition with a graphical representation of a formula in conjunctive normal form, as depicted in Fig. 35.1. In the figure, one has a case of *MAX 3–SAT* : all clauses have three literals and the formula is:

$$(u_1 \vee \overline{u_3} \vee u_5) \wedge (\overline{u_2} \vee \overline{u_4} \vee \overline{u_5}) \wedge (\overline{u_1} \vee u_3 \vee \overline{u_4})$$

Truth values to variables are assigned by placing a black triangle to the left if the variable is **true**, to the right if it is **false**. Each literal is depicted with a small circle, placed to the left if the corresponding variable is **true**, to the right in the other case. If a literal is *matched* by the current assignment (e.g., if the literal asks for a **true** value and the variable is set to **true**, or if is asks for **false** and the variable is **false**), it is shown with a gray shade. The *coverage* of a clause is the number of literals in the clause that are matched by the current assignment, and it is illustrated by placing a black square in the appropriate position of an array with indices ranging from 0 to the number of literals in each clause $|C|$.

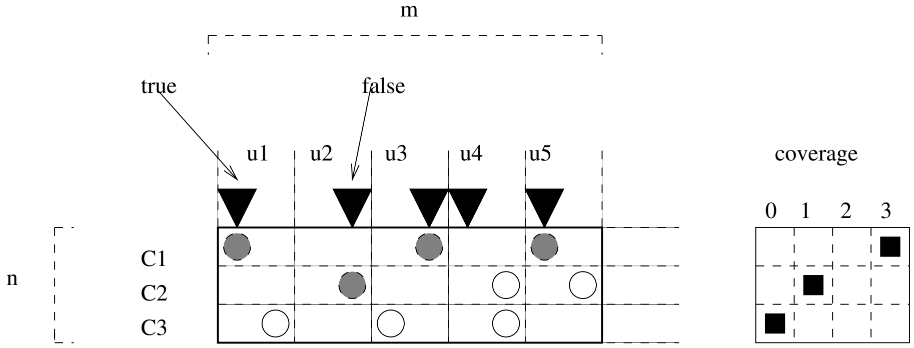


Figure 35.1: A formula in conjunctive normal form (CNF).

35.2 Resolution and Linear Programming

35.2.1 Resolution and backtracking for *SAT*

A simple approach to solve *SAT* consists of the smart generation and test of all possible truth assignment, adapting the Branch and Bound method described in Section 34.1 to the particular structure os *SAT* .

In the adaptation, a basic tool is that of **resolution**, given by the **recursive replacement of a formula by one or more formulae, the solution of which implies the solution of the original formula**.

In *resolution* a variable is selected and a new clause, called the *resolvent* is added to the original formula. The process is repeated to exhaustion or until an empty clause is generated. The original formula is not satisfiable if and only if an empty clause is generated [307].

One aims at demonstrating that the problem *cannot* be satisfied, if one fails, the problem is satisfiable.

Let us now consider some details: A clause R is the *resolvent* of clauses C_1 and C_2 iff there is a literal $l \in C_1$ with $\bar{l} \in C_2$ such that $R = (C_1 \setminus \{l\}) \cup (C_2 \setminus \{\bar{l}\})$ and $u(l)$, the variable associated to the literal, is the only variable appearing both positively and negatively.

For the two clauses $C_1 = (l \vee a_1 \vee ... \vee a_A)$ and $C_2 = (\bar{l} \vee b_1 \vee ... \vee b_B)$ the resolvent is therefore the clause $R = (a_1 \vee ... \vee a_A \vee b_1 \vee ... \vee b_B)$. The resolvent is a logical consequence of the logical *and* of the two clauses. Therefore, if the resolvent is added to the original set of clauses, the **set of solutions does not change**. It is immediate to check that, if both C_1 and C_2 are satisfied, i.e., have at least one matched literal, the resolvent must also be satisfied. In fact, if it is not, in the original clauses there are no matched literals apart from either $\bar{l}$ or l, but this implies that both clauses cannot be satisfied (see also Fig. 35.2 for a graphical illustration).

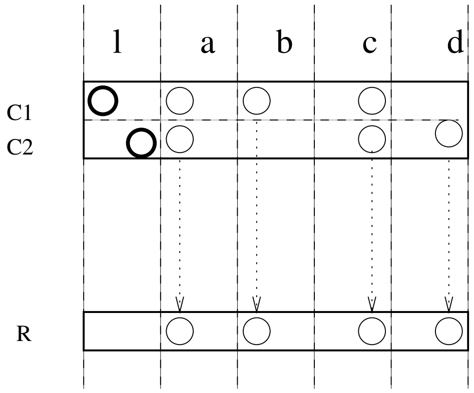


Figure 35.2: How to construct a resolvent, an example with variables l, a, b, c, d.

Davis and Putnam [111] started in 1960 the investigation of useful strategies for handling resolution. In addition to applying transformations that preserve the set of solutions they eliminate one variable at a time in a chosen order by using all possible resolvents on that variable. During resolution the lengths and the number of added clauses can easily increase and become extremely large.

```
DPLL( C : set of clauses )
Input: Boolean CNF formula C = $\{C_1, C_2, \ldots, C_m\}$
Output: Yes or No (decision about satisfiability)
    if C is empty  then return Yes
    if C  contains an empty clause  then return No
    if  there is a pure literal $l$ in C  then return DPLL(C($l$))
    if  there is a unit clause $\{l\} \in$ C then return DPLL(C($l$))
    Select a variable $u$ in C
    if DPLL(C($u$)) = Yes then return Yes
    else return DPLL(C($\overline{u}$))
```

Figure 35.3: The DPLL algorithm by Davis, Logemann and Loveland in recursive form. The recursive calls are executed on the problems derived after setting the truth value of the selected variable.

Davis, Logemann and Loveland [110] avoid the memory explosion of the original DP algorithm by replacing the resolution rule with the *splitting rule* (Davis, Putnam, Logemann and Loveland, or DPLL algorithm for short). In splitting, a variable u in a formula is selected. Now, if there exist a satisfying truth assignment for the original formula then either u is **true** or $\overline{u}$ is **true** in the assignment. In the first case the formula obtained by eliminating all clauses containing u and by deleting all occurrences of $\overline{u}$ must be satisfied, see Fig 35.4. This derived formula is called $\mathbf{C}(u)$ in Fig. 35.3. In the second case, the formula obtained by eliminating all clauses containing $\overline{u}$ and all occurrences of u must be satisfied. *Vice versa*, if both derived formulae cannot be satisfied, neither can the original problem.

A *tree* is therefore generated. At the root one has the original problem and no variables are assigned values. At each node of the tree one generates two children by *selecting* one of the yet unassigned variables in the problem

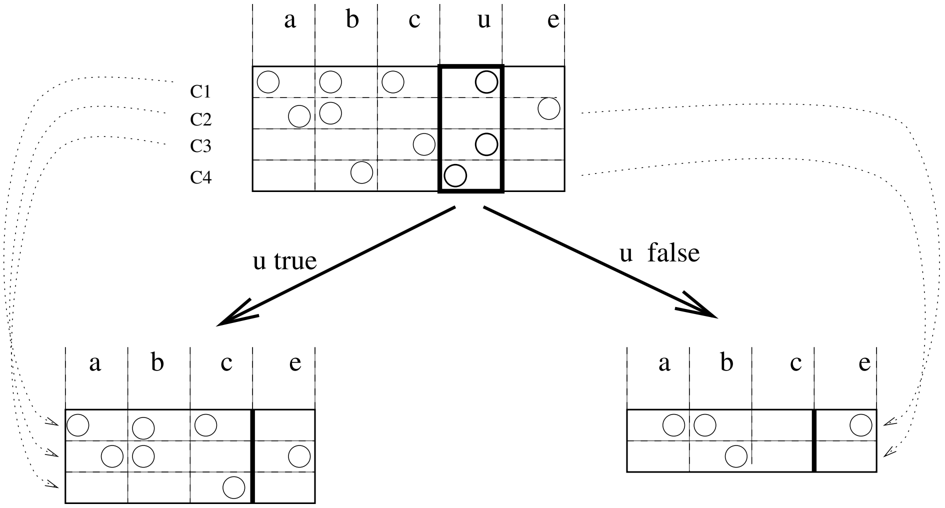


Figure 35.4: Example of splitting on a variable u.

corresponding to the node and by generating the two problems derived by setting the variable to **true** or **false**. A trivial upper bound on the number of nodes in the tree is proportional to the number of possible assignments, i.e., $O(2^n)$. In fact, sophisticated techniques are available to reduce the number of nodes, that nonetheless remains exponential in the worst case.

The techniques include:

- avoiding the examination of a subtree when the fate of the current problem is decided (problems with an empty clause have no solutions, problems with no clauses have a solution). If the current problem cannot be solved, or if it is solved but one wants all possible solutions, one *backtracks* to the first unexplored branch of the tree. Note that, when splitting is combined with a depth-first search of the tree (as in the DPLL algorithm) one avoids the memory explosion because only one subproblem is active at a given time.
- *selecting* the next variable for the splitting based on appropriate criteria. For example, one can prefer variables that appear in clauses of length one (*unit clause rule*), or select a *pure literal* (such that it occurs only positive, or only negative), or select a literal occurring in the *smallest clause*.

Interesting reviews are [163], and [246]. A parallel implementation in given in [57].

35.2.2 Integer programming approaches

The *MAX W–SAT* problem has a natural integer linear programming formulation (*ILP*), see Section 34.1. Let $y_j = 1$ if Boolean variable u_j is **true**, $y_j = 0$ if it is **false**, and let the Boolean variable $z_i = 1$ if clause C_i is satisfied, $z_i = 0$ otherwise. The integer linear program is:

$$\max \sum_{i=1}^{m} w_i \, z_i$$

subject to the following constraints:

$$\begin{aligned} \sum_{j \in U_i^+} y_j + \sum_{j \in U_i^-} (1 - y_j) \quad &\geq \quad z_i \ , \ i = 1, \cdots, m \\ &y_j \in \{0,1\} \ , \ j = 1, \cdots, n \\ &z_i \in \{0,1\} \ , \ i = 1, \cdots, m \end{aligned}$$

where U_i^+ and U_i^- denote the set of indices of variables that appear unnegated and negated in clause C_i, respectively.

Because the sum of the $z_i\ w_i$ is maximized and because each z_i appears as the right-hand side of one constraint only, z_i will be equal to one if and only if clause C_i is satisfied.

If one neglects the objective function and sets all z_i variables to 1, one obtains an integer programming feasibility problem associated to the *SAT* problem [55].

The integer linear programming formulation of *MAX–SAT* suggests that this problem could be solved by a standard **branch-and-bound** method. A tree is generated, see also the DPLL method, where the root corresponds to the initial instance and two children are obtained by *branching*, i.e., by selecting one free variable and setting it **true** (left child) and **false** (right child). An *upper bound* on the number of satisfied clauses can be obtained by using a **linear programming relaxation**: the constraints $y_j \in \{0,1\}$ and $z_i \in \{0,1\}$ are replaced by $y_j \in [0,1]$ and $z_i \in [0,1]$. One obtains a Linear Programming (*LP*) problem that can be solved in polynomial time and, because the set of admissible solutions is enlarged with respect to the original problem, one obtains an upper bound.

Unfortunately this is not likely to work well in practice [172] because the solution $y_j = 1/2, j = 1, \cdots, n$, $z_i = 1, i = 1, \cdots, m$ is feasible for the *LP* relaxation unless there exist some constraint containing only one variable. The bounds so obtained would be very poor.

Better bounds can be obtained by using Chvátal cuts. In [187] it is shown that the resolvents in the propositional calculus correspond to certain cutting planes in the integer programming model of inference problems.

A general cutting plane algorithm for *ILP* , see for example [287], works as follows. One solves the *LP relaxation* of the problem: if the solution is integer the algorithm terminates, otherwise one adds linear constraints to the *ILP* that do not exclude integer feasible points. The constraints are added one at a time, until the solution to the *LP* relaxation is integer.

LP relaxations of integer linear programming formulations of *MAX–SAT* have been used to obtained upper bounds in [170, 387, 155]. A linear programming and rounding approach for *MAX 2–SAT* is presented in [85].

35.3 Continuous approaches

The *ILP* feasibility problem obtained from *SAT* as described in the previous section is solved with an **interior point algorithm** in [227, 228], which applies a function minimization method based on *continuous* mathematics to the inherently discrete *SAT* problem.

In [228] the application is to a problem of **inductive inference**, in which one aims at identifying a hidden Boolean function using outputs obtained by applying a limited number of random inputs to the hidden function. The task is formulated as a *SAT* problem, which is in turn formulated as an integer linear program:

$$A^T y \leq c\ ,\ y \in \{-1,1\}^n \tag{35.1}$$

where A^T is an $m \times n$ real matrix and c a real m vector.

The interior point algorithm is based on finding a local minimum in the box $-1 \leq y_j \leq 1$ of the *potential function*:

$$\phi(y) = \log \left\{ \frac{n - y^T y}{\prod_{k=1}^{m} (c_k - {a_k}^T y)^{1/m}} \right\} \tag{35.2}$$

by an iterative method. The denominator of the argument of the log is the geometric mean of the *slacks* (a_k is the k-th column of matrix A). It is shown that, if the integer linear program has a solution, y^* is a global minimum of this potential function if and only if y^* solves the integer program. The next iterate y^{k+1} (interior point solution, i.e., such that $A^T y < c$) is obtained by moving in a descent direction Δy from the current iterate y^k such that $\phi(y^{k+1}) = \phi(y^k + \alpha \Delta y) < \phi(y^k)$. Each iteration in [228] is based on the *trust region approach* of continuous optimization where the Riemannian metric used for defining the search region is dynamically modified.

In some techniques the *MAX–SAT* (or *SAT*) problem is transformed into an **unconstrained optimization problem** on the real space R^n and solved by using existing global optimization techniques.

Some examples of this approach include the UniSAT models [207] and the *neural network* approaches [222, 76]. In general, these techniques do not have performance guarantees because they assure only the local convergence to a locally optimal point, not necessarily the global optimum. The local convergence properties of some optimization algorithms are considered in [162]. To obtain these results, one assumes that the initial solution is "sufficiently close" to the optimal solution.

35.4 Approximation algorithms

MAX–SAT is a playground for algorithms with **guaranteed quality of approximation**. The basic principle is to guarantee that the delivered result will be within a certain percentage of the optimal solution, which is of interest for many applications. Let's remember that the real world is complex and noisy so that small differences in the solutions can become irrelevant when compared with experimental noise and approximations related to defining the problem. For a detailed treatment of complexity classes we refer to [35], we focus here on some notable approximated algorithms.

The two first approximate algorithms for *MAX W–SAT*were proposed by Johnson [218] and use **greedy construction** strategies. The original paper [218] demonstrated for both of them a performance ratio $1/2$. Actually the second one reaches a performance ratio $2/3$ [83].

The first algorithm chooses, at each step, the literal that occurs in the maximum number of clauses. If the literal is positive, the corresponding variable is set to **true**; if the literal is negative, the corresponding variable is set to **false**. The clauses satisfied by the literal are deleted from the formula and the algorithm stops when the formula is satisfied or all variables have been assigned values. More formally, this procedure is developed in algorithm GreedyJohnson1 of Fig. 35.5.

```
GreedyJohnson1
Input: Boolean CNF formula $\mathbf{C} = \{C_1, C_2, \ldots, C_m\}$;
Output: Truth assignment $U$;
△ The satisfied clauses will be incrementally inserted in the set S;
△ $U$ is the truth assignment;
△ for every literal $l$, $u(l)$ is the corresponding variable;
    $\mathbf{S} \leftarrow \emptyset$; Left $\leftarrow \mathbf{C}$; $V \leftarrow \{u \mid u$ variable in $\mathbf{C}\}$;
    repeat
        Find $l$, with $u(l) \in V$, that is in max. no. of clauses in Left
        Solve ties arbitrarily
        Let $\{C_{l_1}, \ldots, C_{l_k}\}$ be the clauses in which $l$ occurs
        $\mathbf{S} \leftarrow \mathbf{S} \cup \{C_{l_1}, \ldots, C_{l_k}\}$
        Left $\leftarrow$ Left $\setminus \{C_{l_1}, \ldots, C_{l_k}\}$
        if $l$ is positive then $u(l) \leftarrow$ true else $u(l) \leftarrow$ false
        $V \leftarrow V \setminus \{u(l)\}$
    until no literal $l$ with $u(l) \in V$ is contained in any clause of Left
    if $V \neq \emptyset$ then forall $u \in V$ do $u \leftarrow$ true
    return $U$
```

Figure 35.5: The GreedyJohnson1 algorithm, a $k/(k+1)$-approximate algorithm.

Theorem 35.4.1 *Algorithm* GreedyJohnson1 *is a polynomial time 1/2-approximate algorithm for MAX–SAT .*

Proof. One can prove that, given a formula with m clauses, algorithm GreedyJohnson1 always satisfies at least $m/2$ clauses, by induction on the number of variables. Because no optimal solution can be larger than m, the theorem follows. The result is trivially true in the case of one variable. Let us assume that it is true in the case of $i-1$ variables $(i > 1)$ and let us consider the case in which one has i variables. Let u be the last variable to which a truth value has been assigned. We can suppose that u appears positive in k_1 clauses, negative in k_2 clauses and does not appear in $m - k_1 - k_2$ clauses. Without loss of generality suppose that $k_1 \geq k_2$. Then, by inductive hypothesis, algorithm GREEDYJOHNSON1 allows us to choose suitable values for the remaining $i-1$ variables in such a way to satisfy at least $(m - k_1 - k_2)/2$ clauses; if according to the algorithm we now choose u = **true** we satisfy

$$\frac{m - k_1 - k_2}{2} + k_1 \geq \frac{m}{2}$$

clauses.

□

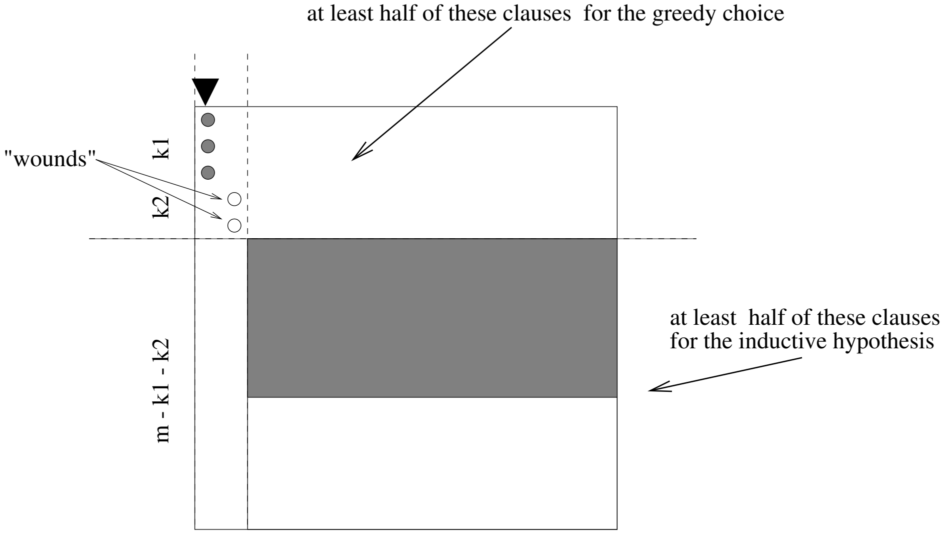

at least half of these clauses for the greedy choice
"wounds"
k1
k2
m - k1 - k2
at least half of these clauses
for the inductive hypothesis

Figure 35.6: Illustration of the GREEDYJOHNSON1 algorithm.

Let us note that one does not use the fact that the chosen literal occurs in the *maximum* number of clauses for the above proof. What is required is that, given an unset variable that appears in at least an unsatisfied clause, the variable is set to **true** or **false** in a way that maximizes the number of newly satisfied clauses.

This result can be made more specific by considering the number of variables in a clause.

Theorem 35.4.2 *Let k be the minimum number of variables occurring in any clause of the formula. For any integer $k \geq 1$, algorithm* GREEDYJOHNSON1 *achieves a feasible solution y of an instance x such that*

$$\frac{m(x,y)}{m^*(x)} \geq 1 - \frac{1}{k+1}.$$

Proof. Because of the greediness, when literal l is picked in line 3 of Fig. 35.5, the number of newly satisfied clauses is at least as large as the number of new *wounds*, defined as the number of occurrences of literal $\bar{l}$ in clauses of LEFT that will never be matched in the future steps, given the choice of l, see Fig. 35.6. When the algorithm halts, the only clauses remaining in LEFT are those that have a number of wounds equal to the number of their literals, and hence are *dead*. This means that, when the algorithm halts, there are at least $k|\text{LEFT}\ |$ wounds, and therefore $|S| \geq k|\text{LEFT}\ |$. Thus $m^* \leq m = |S| + |\text{LEFT}\ | \leq \frac{(k+1)}{k}|S|$. The bound follows.

□

Note that, according to the definition of performance ratio, algorithm GreedyJohnson1 is $\frac{k}{k+1}$–approximate. In particular, for $k = 1$, the performance ratio is $1/2$, for $k = 2$ the performance ratio is $2/3$, for $k = 3$ the performance ratio is $3/4$ and so on. This means that the goodness of the algorithm improves for larger values of k. Therefore the worst case is given by $k = 1$, that is, when one has unit clauses (clauses with just one literal).

Johnson introduced a second algorithm (GreedyJohnson2). This algorithm improves the performance ratio and obtains a bound $2/3$ [83]. Until very recently, only a performance ratio $1/2$ was demonstrated [218]. The original theorem in [218] is here presented, because of its simplicity and paradigmatic nature and because it gives a better performance as a function of k, the minimum number of literals in some clause. In the algorithm one associates a *mass* $w(C_i) = 2^{-|C_i|}$ to each clause. The term *mass* is used instead of the original term "weight" in order to avoid confusions with the clause *weight* in the *MAX W–SAT* problem. The mass will be proportional to the weight in the version of the algorithm for the *MAX W–SAT* problem ($w(C_i) = w_i\ 2^{-|C_i|}$). In [218] the analysis of the performance of algorithm GreedyJohnson2 leads to the following:

```
GreedyJohnson2
Input: Boolean CNF formula $\mathbf{C} = \{C_1, C_2, \ldots, C_m\}$;
Output: Truth assignment $U$;
△ The satisfied clauses will be incrementally inserted in the set S;
△ $U$ is the truth assignment;
△ for every literal $l$, let $u(l)$ be the corresponding variable;
1    $\mathbf{S} \leftarrow \emptyset$;  Left $\leftarrow \mathbf{C}$;  $V \leftarrow \{u \mid u$ variable in $\mathbf{C}\}$;
2    Assign to each clause $C_i$ a mass $w(C_i) = 2^{-|C_i|}$
3    repeat
4        Determine $u \in V$, appearing in at least a clause $\in$ Left
5        Let CT be the clauses $\in$ Left cont. $u$, CF those cont. $\overline{u}$
6        if $\sum_{C_i \in \mathbf{CT}} w(C_i) \geq \sum_{C_i \in \mathbf{CF}} w(C_i)$ then
7            $u(l) \leftarrow$ true
8            $\mathbf{S} \leftarrow \mathbf{S} \cup \mathbf{CT}$
9            Left $\leftarrow$ Left $\setminus$ CT
10           forall $C_i \in$ CF do $w(C_i) \leftarrow 2 \cdot w(C_i)$
11       else
12           $u(l) \leftarrow$ false
13           $\mathbf{S} \leftarrow \mathbf{S} \cup \mathbf{CF}$
14           Left $\leftarrow$ Left $\setminus$ CF
15           forall $C_i \in$ CT do $w(C_i) \leftarrow 2 \cdot w(C_i)$
16   until no literal $l$ in any clause of Left is such that $u(l)$ is in $V$
17   if $V \neq \emptyset$ then forall $u \in V$ do $u \leftarrow$ true
18   return $U$
```

Figure 35.7: The GreedyJohnson2 algorithm, a $(1 - 1/2^k)$-approximate algorithm.

Theorem 35.4.3 *Let k be the minimum number of clauses occurring in any clause of the formula. For any integer $k \geq 1$, algorithm* GreedyJohnson2 *achieves a feasible solution y of an instance x such that*

$$\frac{m(x,y)}{m^*(x)} \geq 1 - \frac{1}{2^k}.$$

Proof. Initially, because each clause has at least k literals, the total mass of all the clauses in Left cannot exceed $m/2^k$. During each iteration, the total mass of the clauses in Left cannot increase. In fact, the mass removed from Left is at least as large as the mass added to those remaining clauses which receive new *wounds*, see lines 6–15 of

Fig. 35.7. Therefore, when the algorithm halts, the total mass still cannot exceed $m/2^k$. But each of the *dead* clauses in LEFT when the algorithm halts must have been wounded as many times as it had literals, hence must have had its mass doubled that many times, and so must have final mass equal to one. Therefore $|\text{LEFT }| \leq m/2^k$, and so $|S| \geq m(1 - 1/2^k)$ and the bound follows.
□

Again, for larger values of k, algorithm GREEDYJOHNSON2 obtains better performance ratios and, generally speaking, because $1 - \frac{1}{2^k} > 1 - \frac{1}{k+1}$ for any integer $k \geq 2$, algorithm GREEDYJOHNSON2 has a better performance than that of algorithm GREEDYJOHNSON1.

The performance ratio $2/3$ has been proved in a paper by Chen, Friesen, and Zheng [83]. Because they consider the *MAX W–SAT* problem, line 2 in Fig. 35.7 must be modified to take the weights w_i into account: the *mass* becomes $w(C_i) = w_i \; 2^{-|C_i|}$. The preceding bound $1/2$ depends on the fact that the only upper bound used in the above proofs was given by the total weight of the clauses; of course this upper bound can be far from the optimal value. The novelty of the approach of [83] is that the performance ratio can be derived by using the correct value of the optimal solution. In order to prove that algorithm GREEDYJOHNSON2 has this better performance ratio let us introduce a generalization of the algorithm. It is important to stress that this generalization is introduced to perform a more accurate analysis of the performance ratio and it is used in the following as a theoretical tool.

The difference between GREEDYJOHNSON2 and its generalization is rather subtle. The generalized algorithm, that we denote as GENJOHNSON2, considers an arbitrary Boolean array $b[1..n]$ of size n as additional input, and examines b to decide what to do if an equality is present in line 6 of Fig. 35.7. Let us assume that the variable one is considering is u_j. In line 6 of GREEDYJOHNSON2 in Fig. 35.7, when $\sum_{C_i \in \mathbf{CT}} w(C_i) = \sum_{C_i \in \mathbf{CF}} w(C_i)$, the **if** condition is true and u_j is set to **true**. Now, instead, when one obtains an equality one considers two different cases: if the variable $b[j]$ is **true** u_j is set to **true**; if the variable $b[j]$ is **false** u_j is set to **false**.

This generalized algorithm is then used in the proof with this Boolean array equal to the optimal assignment. Of course the optimal assignment cannot be derived in polynomial time but here we are not interested in running an algorithm but in performing a theoretical analysis.

We will prove that GENJOHNSON2 has a performance ratio $2/3$ and this fact will imply that also GREEDYJOHNSON2 has performance ratio $2/3$.

Let us give some definitions needed in the proof.

Definition 2
- *A literal is positive if it is a Boolean variable u_i for some i.*
- *A literal is negative if it the negation $\bar{u}_i$ of a Boolean variable for some i.*

Definition 3 *Assume that algorithm* GENJOHNSON2 *is applied to a formula* **C** *and consider a fixed moment in the execution.*

- *A literal l is active if it has not been assigned a truth value yet.*
- *A clause C_j is killed if all literals in C_j are assigned value* **false**.
- *A clause C_j is negative if it is neither satisfied nor killed, and all active literals in C_j are negative literals.*

Definition 4 *Let $0 \leq t \leq n$. Assume that in* GENJOHNSON2 *the t–th iteration has been completed (a truth assignment has been given to t variables). Then $\mathbf{S}^t$ denotes the set of satisfied clauses, $\mathbf{K}^t$ denotes the set of killed clauses, $\mathbf{N}_i^t$ denotes the set of negative clauses with exactly i active liberals.*

Without less of generality, one assumes that each clause in the formula has at most r literals. The proof of the performance ratio $2/3$ depends on the following Lemma.

Given a set of clauses **C**, let us define as $w(\mathbf{C})$ the sum of the weights of all clauses of **C**.

Lemma 2 *For any formula* $\mathbf{C}$ *of MAX W–SAT and for any Boolean array* $b[1..n]$*, when the algorithm* GENJOHNSON2 *is applied on* $\mathbf{C}$ *the following inequality holds at all iterations* $0 \le t \le n$*:*

$$w(\mathbf{S}^t) \ge 2w(\mathbf{K}^t) + \sum_{i=1}^{r} \frac{1}{2^{i-1}} w(\mathbf{N}_i^t) - A_0 \tag{35.3}$$

where $A_0 = \sum_{i=1}^{r} \frac{1}{2^{i-1}} w(\mathbf{N}_i^0)$

The proof of the Lemma proceeds by induction on t and can be found in [83].

Theorem 35.4.4 *The performance ratio of algorithm* GREEDYJOHNSON2 *is* $2/3$*.*

Proof. Let $\mathbf{C}$ be an instance of *MAX W–SAT* and let U_0 an optimal truth assignment for $\mathbf{C}$. Now one considers another formula $\mathbf{C}'$ that is derived from $\mathbf{C}$ as follows. If $U_0(u_t) = \textbf{false}$ for a variable u_t then one negates u_t (u_t and $\bar{u}_t$ are interchanged) in $\mathbf{C}'$. No change on the weights is done. Therefore there exists a one–to–one correspondence between the set of clauses in $\mathbf{C}$ and the set of clauses in $\mathbf{C}'$; moreover the corresponding clauses have the same weight. In addition, the Boolean array $b[1..n]$ is constructed such that $b[j]$ = **false** if and only if $U_0(u_j) = \textbf{false}$.

It is easy to see (for the details, see again [83]) that

- the weight of an optimal assignment to $\mathbf{C}'$ is equal to the weight of an optimal assignment to $\mathbf{C}$.
- the truth assignment for $\mathbf{C}$ found by GREEDYJOHNSON2 and the truth assignment for $\mathbf{C}'$ found by GENJOHNSON2 have the same weight.

This means that, if we prove that GENJOHNSON2 has a performance ratio $2/3$ on the formula $\mathbf{C}'$, the theorem is shown.

Note that the truth assignment $U_0^{'}$ for $\mathbf{C}'$ that gives value **true** to all variables corresponds to the optimal truth assignment U_0 for $\mathbf{C}$. Therefore $U_0^{'}$ is optimal for $\mathbf{C}'$.

When GENJOHNSON2 stops, that is, for $t = n$, $\mathbf{S}^n$ is the set satisfied by the algorithm and $\mathbf{K}^n$ is the set of clauses not satisfied. $\mathbf{N}_i^n$ is the empty set for any i.

Applying the inequality 35.3 of Lemma 2 to this case, one obtains:

$$w(\mathbf{S}^n) \ge 2w(\mathbf{K}^n) - A_0. \tag{35.4}$$

On the other hand, A_0 can be upperbounded in the following way:

$$A_0 = \sum_{i=1}^{r} \frac{1}{2^{i-1}} w(\mathbf{N}_i^0) \le \sum_{i=1}^{r} w(\mathbf{N}_i^0) \le 2\sum_{i=1}^{r} w(\mathbf{N}_i^0). \tag{35.5}$$

From inequalities 35.4 and 35.5 one has:

$$\frac{3}{2} w(\mathbf{S}^n) \ge w(\mathbf{S}^n) + w(\mathbf{K}^n) - \sum_{i=1}^{r} w(\mathbf{N}_i^0) \tag{35.6}$$

Note that, on one hand, $w(\mathbf{S}^n)$ is the weight of the truth assignment found by GENJOHNSON2. On the other hand, $\mathbf{S}^n \cup \mathbf{K}^n$ is the whole set of clauses in $\mathbf{C}'$ and the optimal truth assignment $U_0^{'}$ for $\mathbf{C}'$ that gives value **true** to all variables satisfies all clauses in $\mathbf{C}'$ except those belonging to $\mathbf{N}_i^0$ for $i = 1, 2, \ldots, r$.

Therefore an optimal truth assignment for $\mathbf{C}'$ has weight exactly

$$w(\mathbf{S}^n) + w(\mathbf{K}^n) - \sum_{i=1}^{r} w(\mathbf{N}_i^0).$$

Then the inequality 35.6 says that the weight of the truth assignment found by GENJOHNSON2 is at least $2/3$ of the weight of an optimal assignment to $\mathbf{C}'$. In consequence, the weight of the assignment constructed by the original GREEDYJOHNSON2 algorithm for the instance $\mathbf{C}$ is at least $2/3$ of the weight of an optimal assignment to $\mathbf{C}$, thus proving the theorem.
□

35.4.1 Randomized algorithms for *MAX W–SAT*

A randomized $1/2$–approximate algorithm for *MAX W–SAT*

One of the most interesting approaches in the design of new algorithms is the use of *randomization*. During the computation, random bits are generated and used to influence the algorithm process.

In many cases randomization allows to obtain better (expected) performance or to to simplify the construction of the algorithm. Particularly in the field of approximation, randomized algorithms are widely used and, for many problems, the algorithm can be "derandomized" in polynomial time while preserving the approximation ratio. However, it is important to note that, often, the derandomization leads to algorithms which are very complicated in practice.

Let us now use this approach to present more efficient approximate algorithms for *MAX W–SAT*. More precisely, this section introduces two different randomized algorithms that achieve a performance ratio of $3/4$. Moreover, it is possible to derandomize these algorithms, that is, to obtain deterministic algorithms that preserve the same bound $3/4$ for every instance.

The derandomization is based on the *method of conditional probabilities* that has revealed its usefulness in numerous cases and is a general technique that often permits to obtain a deterministic algorithm from a randomized one while preserving the quality of approximation.

Let us first present the algorithm RANDOM, a simple randomized algorithm, that, while just achieving a performance ratio $1/2$, will be used in the following subsections as an ingredient to reach the performance ratio $3/4$.

```
RANDOM
Input: Set C of weighted clauses in conjunctive normal form
Output: Truth assignment $U$, $\mathbf{C}'$, $\sum_{C_j \in \mathbf{C}'} w_j$
    Independently set each variable $u_i$ to true with probability $1/2$
    Compute $\mathbf{C}' = \{C_j \in \mathbf{C} : C_j \text{ is satisfied } \}$
    Compute $\sum_{C_j \in \mathbf{C}'} w_j$
```

Figure 35.8: The RANDOM algorithm, a randomized $(1 - 1/2^k)$-approximate algorithm.

It is difficult to think about a simpler (randomized) algorithm! Because the algorithm is randomized, one is interested in the **expected performance** when the algorithm is run with different sequences of random bits (i.e., with different random assignments).

Lemma 3 *Given an instance of MAX W–SAT in which all clauses have at least k literals, the expected weight W of the solution found by algorithm* RANDOM *is such that*

$$W \geq (1 - \frac{1}{2^k}) \sum_{C_j \in \mathbf{C}} w_j.$$

Proof. The probability that any clause with k literals is not satisfied by the assignment found by the algorithm is 2^{-k} (all possible k matches must fail). Therefore the probability that a clause is satisfied is $1 - 2^{-k}$. Then

$$W = (1 - \frac{1}{2^k}) \sum_{C_j \in \mathbf{C}} w_j.$$

□

As an immediate consequence of Lemma 3, one obtains the following Corollary.

Corollary 1 *Algorithm* RANDOM *finds a solution for MAX W–SAT whose expected value is at least one half of the optimum value.*

The performance of algorithm RANDOM is the same, in a probabilistic setting, as that of algorithm GREEDYJOHNSON2.

Actually it is possible to show that, by applying the method of conditional probabilities to derandomize [35] algorithm RANDOM, one essentially obtains algorithm GREEDYJOHNSON2.

For $k = 1$, algorithm RANDOMachieves an expected performance ratio $1/2$. The performance of the algorithm improves if we increase the number of literals. In particular, for $k = 2$, that is for formulae which do not contain unit clauses, one obtains an expected value which is at least $3/4$ of the optimal value. Therefore if one could discard unit clauses, one would already have a $3/4$-approximate algorithm for *MAX W–SAT*, after applying the derandomization. This observation will reveal its usefulness in the following.

A randomized $3/4$-approximate algorithm for *MAX W–SAT*

This subsection presents an algorithm that considerably improves the performance of algorithm RANDOM, and obtains a performance ratio $3/4$.

First of all we consider a generalization of algorithm RANDOM. In the previous case the value of every variable was chosen randomly and uniformly, that is with probability $1/2$; now the value of variable u_i is chosen with probability p_i, obtaining algorithm GENRANDOM.

```
GENRANDOM
Input: Set C of weighted clauses in conjunctive normal form
Output: Truth assignment $U$, $\mathbf{C}'$, $\sum_{C_j \in \mathbf{C}'} w_j$
    Independently set each variable $u_i$ to true with probability $p_i$
    Compute $\mathbf{C}' = \{C_j \in \mathbf{C} : C_j$ is satisfied $\}$
    Compute $\sum_{C_j \in \mathbf{C}'} w_j$
```

Figure 35.9: The GENRANDOM algorithm.

The expected number of clauses satisfied by algorithm GENRANDOM can be immediately computed as a function of p_i.

Lemma 4 *The expected weight W of the set of clauses* **C** *is:*

$$W = \sum_{C_j \in C} w_j (1 - \prod_{i \in U_j^+} (1 - p_i) \prod_{i \in U_j^-} p_i)$$

where U_j^+ (U_j^-) denotes the set of indices of the variables appearing unnegated (negated) in the clause C_j.

Proof. It is an obvious generalization of the proof given in the particular case $p_i = 1/2$.

□

Now, if one manages to find suitable values p_i such that $W \geq 3/4\ m^*(\mathbf{C})$ for every formula **C**, one would obtain a $3/4$-approximate randomized algorithm.

To aim at this result, let us consider the representation of the instances of *MAX W–SAT* as instances of an integer linear programming problem (*ILP*) already presented in Section 2:

$$max \sum_{C_j \in \mathbf{C}} w_j z_j$$

subject to :

$$\sum_{i \in U_j^+} y_i + \sum_{i \in U_j^-} (1 - y_i) \geq z_j, \forall C_j \in \mathbf{C}$$

$$y_i \in \{0, 1\}, 1 \leq i \leq n$$

$$z_j \in \{0, 1\}, \forall C_j \in \mathbf{C}$$

Let $u_1, \ldots, u_n$ be the Boolean variables appearing in the formula. An instance of *MAX W–SAT* is equivalent to an instance of *ILP* if we choose the following conditions:

- $y_i = 1$ iff variable u_i is **true**;
- $y_i = 0$ iff variable u_i is **false**;
- $z_j = 1$ iff clause C_j is satisfied;
- $z_j = 0$ iff clause C_j is not satisfied.

The linear inequality states the fact that a clause can be satisfied ($z_j = 1$) only if at least one of its literals is matched.

One cannot compute the optimal value in polynomial time because *ILP* is $\mathcal{NP}$–complete. However let us consider the *LP* relaxation (by *relaxation* one means that the set of admissible solution increases with respect to that of the original problem) in which one relaxes the conditions $y_i, z_j \in \{0, 1\}$ with the new constraints $0 \leq y_i, z_j \leq 1$. It is known that *LP* can be solved in polynomial time finding a solution

$$(y^* = (y_1^*, \ldots, y_n^*), z^* = (z_1^*, \ldots, z_m^*))$$

with value $m^*_{LP}(x) \geq m^*_{ILP}(x)$, for every instance x, where $m^*_{LP}(x)$ and $m^*_{ILP}(x)$ denote the optimal value of the *LP* and *ILP* instances, respectively. The upper bound is obvious given that the set of admissible solutions is enlarged by the relaxation.

Let us consider algorithm GENAPPROX, see Fig. 35.10, that works as follows: first it solves the linear programming relaxation and so computes the optimal values (y^*, z^*); then, given a function g to be specified later, it computes, for each i, $i = 1, \ldots, n$, the probabilities $p_i = g({y^*}_i)$. By Lemma 4 we know that a solution of weight:

$$W = \sum_{C_j \in \mathbf{C}} w_j (1 - \prod_{i \in U_j^+} (1 - p_i) \prod_{i \in U_j^-} p_i)$$

must exist; by applying the method of conditional probabilities, such solution can be deterministically found.

If the function g can be computed in polynomial time then algorithm GENAPPROX runs in polynomial time. In fact the linear relaxation can be solved efficiently and the computation of the feasible solution can be computed in polynomial time with the method of conditional probabilities explained before.

The quality of approximation naturally depends on the choice of the function g. Let us suppose that this function finds suitable values such that:

$$(1 - \prod_{i \in U_j^+} (1 - p_i) \prod_{i \in U_j^-} p_i) \geq \frac{3}{4} z_j^*.$$

```
GENAPPROX
 Input: Set C of clauses in disjunctive normal form
 Output: Set $\mathbf{C}'$ of clauses, $W = \sum_{C_j \in \mathbf{C}'} w_j$
    Express the input C as an equivalent instance $x$ of ILP
    Find the optimum value $y^*, z^*$ of $x$ in the linear relaxation
    Choose $p_i \leftarrow g({y^*}_i)$, $i = 1, 2, \ldots, n$, for a suitable function $g$
    $W \leftarrow \sum_{C_j \in \mathbf{C}} w_j (1 - \prod_{i \in X_j^+} (1 - p_i) \prod_{i \in X_j^-} p_i)$
    Apply the method of conditional probabilities to find
     a feasible solution $\mathbf{C}' = \{C_j \in \mathbf{C} : C_j \text{ is satisfied}\}$ of value $W$
```

Figure 35.10: The GENAPPROX algorithm, deterministic version.

If this inequality is satisfied, then the algorithm is a $3/4$-approximate algorithm for *MAX W–SAT*. In fact one has :

$$\begin{aligned} W &= \sum_{C_j \in \mathbf{C}} w_j (1 - \prod_{i \in U_j^+} (1 - p_i) \prod_{i \in U_j^-} p_i) \geq \frac{3}{4} \sum_{C_j \in \mathbf{C}} w_j z_j^* = \\ &= \frac{3}{4} m^*_{\mathit{LP}}(x) \geq \frac{3}{4} m^*_{\mathit{ILP}}(x) \end{aligned}$$

More generally if one has :

$$(1 - \prod_{i \in U_j^+} (1 - p_i) \prod_{i \in U_j^-} p_i) \geq \alpha z_j^*$$

one obtains a α-approximate algorithm.

A first interesting way of choosing the function g consists of applying the following technique, called *Randomized Rounding*, to get an integral solution from a linear programming relaxation. In order to get integer values one rounds the fractional values, that is each variable y_i is independently set to 1 (corresponding to the Boolean variable u_i being set to **true**) with probability y_i^*, for each $i = 1, 2, \ldots, n$. Hence the use of the randomized rounding technique is equivalent to choosing $p_i = g(y_i^*) = y_i^*, i = 1, 2, \ldots, n$.

Lemma 5 *Given the optimal values (y^*, z^*) to LP and given any clause C_j with k literals, one has*

$$(1 - \prod_{i \in U_j^+} (1 - y_i^*) \prod_{i \in U_j^-} y_i^*) \geq \alpha_k z_j^*$$

where

$$\alpha_k = 1 - \left(1 - \frac{1}{k}\right)^k .$$

Proof. Let us consider a clause C_j and, for the sake of simplicity, let us assume that every variable is unnegated. If a variable u_i would appear negated in C_j, one could substitute u_i by its negation $\overline{u}_i$ in every clause and also replace y_i by $1 - y_i$. So we can assume $C_j = u_1 \vee \cdots \vee u_k$ with the associated condition $y_1^* + \cdots + y_k^* \geq z_j^*$. The Lemma is proved by showing that:

$$1 - \prod_{i=1}^{k} (1 - y_i^*) \geq \alpha_k z_j^* .$$

In the proof we exploit the geometric inequality based on the properties of the arithmetic mean: given a finite set of nonnegative numbers $\{a_1, \ldots, a_k\}$,

$$\frac{a_1 + \cdots + a_k}{k} \geq \sqrt[k]{a_1 a_2 \cdots a_k} .$$

Now we apply the geometric inequality to the set $\{1 - y_1^*, \ldots, 1 - y_k^*\}$. Because $\sum_{i=1}^{k} \frac{1-y_i^*}{k} = 1 - \frac{\sum_{i=1}^{k} y_i^*}{k}$, one has

$$1 - \prod_{i=1}^{k}(1 - y_i^*) \geq 1 - (1 - \frac{\sum_{i=1}^{k} y_i^*}{k})^k \geq 1 - (1 - \frac{z_j^*}{k})^k.$$

We note that the function $g(z_j^*) = 1 - (1 - \frac{z_j^*}{k})^k$ is concave in the interval $[0,1]$; hence it is sufficient to prove that $g(z_j^*) \geq \alpha_k z_j^*$ at the extremal points of the interval. Because one has

$$g(0) = 0 \text{ and } g(1) = \alpha_k$$

the Lemma is shown.

□

One can conclude that algorithm GENAPPROX with the choice $p_i = y_i^*$ reaches an approximation ratio equal to α_k. In particular for $k = 2$, the ratio is 3/4. Note that, because α_k is decreasing with k, algorithm GENAPPROX is an α_k–approximation algorithm for formulae with *at most* k literals per clause.

Moreover, it is well known that $\lim_{k\to\infty}(1 - \frac{1}{k})^k = \frac{1}{e}$; hence for arbitrary formulae one finds approximate solutions whose value is at least $1 - \frac{1}{e}$ times the optimal value. Because $1 - \frac{1}{e} = 0.632\ldots$, the randomized rounding obtains a better performance than RANDOM, but it looks as if one is far from achieving a $3/4$-approximation ratio.

Luckily, with a suitable merging of the above algorithm with RANDOM one obtains the desired performance ratio. Firstly let us recall that RANDOM is a $3/4$-approximation algorithm if all clauses have *at least* two literals. On the other hand, GENAPPROX is a $3/4$-approximation algorithm if we work with clauses with *at most* two literals. One algorithm is good for large clauses, the other for short ones. A simple combination consists of running both algorithm and choosing the best truth assignment obtained. Let us now consider the expected value obtained from the combination.

Theorem 35.4.5 *Let W_1 be the expected weight corresponding to $p_i = 1/2$ and let W_2 be the expected weight corresponding to $p_i = y_i^*$, $i = 1, 2, \ldots, n$. Then one has :*

$$\max(W_1, W_2) \geq \frac{3}{4} m^*_{LP}(x), \textit{ for any instance } x.$$

Proof. Because $\max(W_1, W_2) \geq \frac{W_1+W_2}{2}$, it is sufficient to show that $\frac{W_1+W_2}{2} \geq \frac{3}{4} m^*_{LP}(x)$ for any x. Let us denote by $\mathbf{C}^k$ the set of clauses with exactly k literals. By Lemma 3, because $0 \leq z_j^* \leq 1$ one has

$$W_1 = \sum_{k\geq 1} \sum_{C_j \in \mathbf{C}^k} \gamma_k w_j \geq \sum_{k\geq 1} \sum_{C_j \in \mathbf{C}^k} \gamma_k w_j z_j^* \tag{35.7}$$

where $\gamma_k = (1 - \frac{1}{2^k})$.

Moreover, by applying Lemma 5, one obtains:

$$W_2 \geq \sum_{k\geq 1} \sum_{C_j \in \mathbf{C}^k} \alpha_k w_j z_j^*. \tag{35.8}$$

Summing 35.7 and 35.8 one has :

$$\frac{W_1 + W_2}{2} \geq \sum_{k\geq 1} \sum_{C_j \in \mathbf{C}^k} \frac{\gamma_k + \alpha_k}{2} w_j z_j^*.$$

We note that $\gamma_1 + \alpha_1 = \gamma_2 + \alpha_2 = 3/2$ and for $k \geq 3$ one has that $\gamma_k + \alpha_k \geq 7/8 + 1 - \frac{1}{e} \geq 3/2$; Therefore:

$$\frac{W_1 + W_2}{2} \geq \sum_{k\geq 1} \sum_{C_j \in \mathbf{C}^k} \frac{3}{4} w_j z_j^* = \frac{3}{4} m^*_{LP}(x).$$

□

Note that it is not necessary to separately apply the two algorithms but it is sufficient to randomly choose one of the two algorithms with probability $1/2$, as it is done in algorithm 3/4–APPROXIMATE SAT.

```
3/4–APPROXIMATE SAT
Input: Set C of clauses in conjunctive normal form
Output: Set C′ of clauses, $W = \sum_{C_j \in \mathbf{C}'} w_j$
    Express the input C as an equivalent instance $x$ of ILP
    Find the optimum value $(y^*, z^*)$ of $x$ in the linear relaxation
    With probability $1/2$ choose $p_i = 1/2$ or $p_i = y_i^*, i = 1, 2, \ldots, n$
    $W \leftarrow \sum_{C_j \in \mathbf{C}} w_j (1 - \prod_{i \in U_j^+} (1 - p_i) \prod_{i \in U_j^-} p_i)$
    Apply the method of conditional probabilities to find a feasible
     solution $\mathbf{C}' = \{C_j \in \mathbf{C} : C_j \text{ is satisfied}\}$ of value $W$
```

Figure 35.11: The 3/4–APPROXIMATE SAT algorithm: deterministic with performance ratio 3/4.

Corollary 2 *Algorithm* 3/4–APPROXIMATE SAT *is a $3/4$-approximation algorithm for MAX W–SAT.*

Proof. The proof derives from the above theorem and from the use of the method of conditional probabilities.
□

35.5 Local search for *SAT*

MAX–SAT is among the problems for which perturbative local search, described in Section 24.2, has been very effective: different variations of local search with randomness techniques have been proposed for *SAT* and *MAX–SAT* starting from the late eighties, see for example [164, 324], motivated by previous applications of “min-conflicts” heuristics in the area of Artificial Intelligence [270].

The general scheme is based on generating a starting point in the set of admissible solution and trying to improve it through the application of simple *basic* moves. If a move (“trial”) is successful one accepts it, otherwise (“error”) one keeps the current point. Of course, the successfulness of a local search technique depends on the neighborhood chosen and there are often trade-offs between the size of the neighborhood (and the related computational requirements to calculate it) and the quality of the obtained local optima.

In addition, as it will be demonstrated in Sec. 35.5.2, the use of a guiding function different from the original one can in some cases guarantee local optima of better quality.

Because this presentation is dedicated to the *MAX–SAT* problem, the search space that we consider is given by all possible truth assignments. Of course, a truth assignment can be represented by a binary string. For this presentation, let us consider the elementary changes to the current assignment obtained by changing a single truth value. The definitions are as follows.

Let $\mathcal{U}$ be the discrete search space: $\mathcal{U} = \{0,1\}^n$, and let $f : \mathcal{U} \longrightarrow R$ (R are the real numbers) be the function to be maximized, i.e., in our case, the number of satisfied clauses. In addition, let $U^{(t)} \in \mathcal{U}$ be the current configuration along the *search trajectory* at iteration t, and $N(U^{(t)})$ the neighborhood of point $U^{(t)}$, obtained by applying a set of basic moves μ_i $(1 \leq i \leq n)$, where μ_i complements the i-th bit u_i of the string: μ_i $(u_1, u_2, ..., u_i, ..., u_n) = (u_1, u_2, ..., 1 - u_i, ..., u_n)$. Clearly, these moves are idempotent ($\mu_i^{-1} = \mu_i$).

$$N(U^{(t)}) = \{U \in \mathcal{U} \text{ such that } U = \mu_i \, U^{(t)}, i = 1, ..., n\}$$

The version of *local search* (LS) that we consider starts from a random initial configuration $U^{(0)} \in \mathcal{U}$ and generates a search trajectory as follows:

$$V = \textsc{Best-Neighbor}(\ N(U^{(t)})\ ) \tag{35.9}$$

$$U^{(t+1)} = \begin{cases} V & \textbf{if} \quad f(V) > f(U^{(t)}) \\ U^{(t)} & \textbf{if} \quad f(V) \leq f(U^{(t)}) \end{cases} \tag{35.10}$$

where $\textsc{Best-Neighbor}$ selects $V \in N(U^{(t)})$ with the best f value and ties are broken randomly. V in turn becomes the new current configuration if f improves. Other versions are satisfied with an improving (or non-worsening) neighbor, not necessarily the best one. Clearly, local search stops as soon as the first local optimum point is encountered, when no improving moves are available, see eqn. 35.10. Let us define as LS$^+$ a modification of LS where a specified number of iterations are executed and the candidate move obtained by $\textsc{Best-Neighbor}$ is *always* accepted even if the f value remains equal or worsens.

35.5.1 Quality of local optima

Let m^* be the optimum value and k the minimum number of literals contained in the problem clauses.

For the following discussion it is useful to consider the different degree of *coverage* of the various clause for a given assignment. Precisely, let us define as $\textsc{Cov}_s$ the subset of clauses that have exactly s literals matched by the current assignment, and by $\textsc{Cov}_s(l)$ the number of clauses in $\textsc{Cov}_s$ that contain literal l.

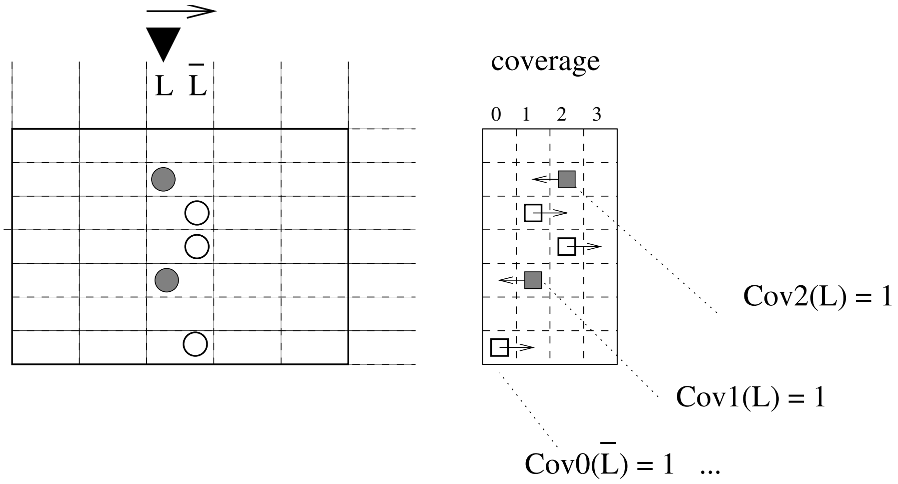


Figure 35.12: Literal L is changed from **true** to **false**.

One has the following theorem [172]:

Theorem 35.5.1 *Let m_{loc} be the number of satisfied clauses at a local optimum of any instance of MAX–SAT with at least k literals per clause. m_{loc} satisfies the following bound*

$$m_{loc} \geq \frac{k}{k+1} m$$

and the bound is sharp.

Proof. By definition, if the assignment U is a local optimum, one cannot flip the truth value of a variable (from **true** to **false** or *vice versa*) and obtain a net increase in the number of satisfied clauses f. Now, let $(\Delta f)_i$ by the increase in

f if variable u_i is flipped. By using the above introduced quantities one verifies that:

$$(\Delta f)_i = -\textsc{Cov}_1(u_i) + \textsc{Cov}_0(\overline{u_i}) \le 0 \tag{35.11}$$

In fact, when u_i is flipped one looses the clauses that contain u_i as the single matched literal, i.e., $\textsc{Cov}_1(u_i)$ and gains the clauses that have no matched literal and that contain $\overline{u_i}$, i.e., $\textsc{Cov}_0(\overline{u_i})$.

After summing over all variables:

$$\sum_{i=1}^{n} \textsc{Cov}_0(\overline{u_i}) \le \sum_{i=1}^{n} \textsc{Cov}_1(u_i) \tag{35.12}$$

$$k|\textsc{Cov}_0| \le |\textsc{Cov}_1| \le m_{loc} \tag{35.13}$$

where the equality $\sum_{i=1}^{n} \textsc{Cov}_0(\overline{u_i}) = k|\textsc{Cov}_0|$ and $\sum_{i=1}^{n} \textsc{Cov}_1(u_i) = |\textsc{Cov}_1|$ have been used. The equality are demonstrated by counting how many times a clause in $\textsc{Cov}_0$ (or $\textsc{Cov}_1$) is uncountered during the sum. For example, because all literals are unmatched for the clauses in $\textsc{Cov}_0$, each of them will be encountered k times during the sum.

The conclusion is immediate:

$$m = m_{loc} + |\textsc{Cov}_0| \le (1 + \frac{1}{k})m_{loc} = \frac{k+1}{k} m_{loc} \tag{35.14}$$

□

The intuitive explanation is as follows: if there are too many clauses in $\textsc{Cov}_0$, because each of them has k unmatched literals, there will be at least one variable whose flipping will satisfy so many of these clauses to lead to a net increase in the number of satisfied clauses.

There is therefore a very simple local search algorithm that reaches the same bound as the GREEDYJOHNSON1 algorithm. One starts from a truth assignments and keeps flipping variables that cause a net increase of satisfied clauses, until a local optimum is encountered. Of course, because one gains at least one clause at each step, there is an upper bound of m on the total number of steps executed before reaching the local optimum.

The following corollary is immediate:

Corollary 3 *If m_{loc} is the number of satisfied clauses at a local optimum, then:*

$$m_{loc} \ge \frac{k}{k+1} m^* \tag{35.15}$$

Besides *MAX–SAT* , many important optimization problems share the property that the ratio between the value of the local optimum and the optimal value is bounded by a constant. It is possible to define a class $\mathcal{GLO}$ composed of these problems. It is of interest to note that the closure of $\mathcal{GLO}$ coincides with $\mathcal{APX}$ [14].

35.5.2 Non-oblivious local optima

In the design of efficient approximation algorithms for *MAX–SAT* a recent approach of interest is based on the use of *non-oblivious functions* independently introduced in [8] and in [335].

Let us consider the classical local search algorithm LS for *MAX–SAT* , here redefined as *oblivious* local search (LS-OB). Clearly, the feasible solution found by LS-OB typically is only a *local* and not a *global* optimum.

Now, a different type of local search can be obtained by using a *different* objective function to direct the search, i.e., to select the best neighbor at each iteration. Local optima of the standard objective function f are not necessarily local optima of the different objective function. In this event, the second function causes an *escape* from a given local optimum. Interestingly enough, suitable *non-oblivious* functions f_{NOB} improve the performance of LS if one considers both the worst-case performance ratio and, as it has been shown in [34], the actual average results obtained on benchmark instances.

Let us mention a theoretical result for *MAX 2–SAT* . The d-neighborhood of a given truth assignment is defined as the set of all assignment where the values of at most d variables are changed. The theoretically-derived non–oblivious function for *MAX 2–SAT* is:

$$f_{NOB}(U) = \frac{3}{2}|\text{Cov}_1| + 2|\text{Cov}_2|$$

Theorems 7-8 of [335] state that:

Theorem 35.5.2 *The performance ratio for any oblivious local search algorithm with a d-neighborhood for MAX 2–SAT is* $2/3$ *for any* $d = o(n)$*. Non-oblivious local search with an 1-neighborhood achieves a performance ratio* $3/4$ *for MAX 2–SAT .*

Proof. While one is referred to the cited papers for the complete details, let us only demonstrate the second part of the theorem. The proof is a generalization of that for Theorem 35.5.1. Let the non-oblivious function be a weighted linear combination of the number of clauses with one and two matched literals:

$$f_{NOB} = a|\text{Cov}_1| + b|\text{Cov}_2|$$

Let $(\Delta f)_i$ by the increase in f if variable u_i is flipped. By using the definition of local optimum and the quantities introduced in Sec. 35.5.1 one has that $(\Delta f)_i \leq 0$ for each possible flip of a variable u_i. After expressing $(\Delta f)_i$ by using the above introduced quantities, one obtains:

$$-a|\text{Cov}_1(u_i)| - (b-a)|\text{Cov}_2(u_i)| + a|\text{Cov}_0(\overline{u_i})| + (b-a)|\text{Cov}_1(\overline{u_i})| \leq 0 \qquad (35.16)$$

In fact, when u_i is flipped, all clauses that contain it decrease their coverage by one, while the clauses that contain $\overline{u_i}$ increase it by one, see also Fig. 35.12. As usual, let us assume that no clause contains both a literal and its negation.

After summing over all variables and collecting the sizes of the sets Cov_i one obtains:

$$\sum_{i=1}^{n} (\Delta f)_i \leq 0 \qquad (35.17)$$

$$\frac{b-a}{a}|\text{Cov}_2| + \frac{2a-b}{2a}|\text{Cov}_1| \geq |\text{Cov}_0| \qquad (35.18)$$

Now one can fix the relative size of the values a and b in order to get the best possible bound. This occurs when the coefficients of the terms $|\text{Cov}_2|$ and $|\text{Cov}_1|$ in equation 35.18 are equal, that is, for $b = \frac{4}{3}a$.

For these values one obtains the following bound:

$$|\text{Cov}_2| + |\text{Cov}_1| \geq 3\ |\text{Cov}_0| \qquad (35.19)$$

The number of satisfied clauses must be larger than three times the number of unsatisfied ones, which implies that $|\text{Cov}_0| \leq \frac{1}{4}m$, or $m_{loc} \geq \frac{3}{4}m$.
□

Therefore LS-NOB, by using a function that weights in different ways the satisfied clauses according to the number of matched literals, improves considerably the performance ratio, even if the search is restricted to a much smaller neighborhood. In particular the "standard" neighborhood where all possible flips are tried is sufficient.

With a suitable generalization the above result can be extended: LS-NOB achieves a performance ratio $1 - \frac{1}{2^k}$ for *MAX–k–SAT* . The oblivious function for *MAX–k–SAT* is of the form:

$$f_{NOB}(U) = \sum_{i=1}^{k} c_i |\text{Cov}_i|$$

and the above given performance ratio is obtained if the quantities $\Delta_i = c_{i+1} - c_i$ satisfy:

$$\Delta_i = \frac{1}{(k-i+1)\begin{pmatrix} k \\ i-1 \end{pmatrix}} \left[\sum_{j=0}^{k-i} \begin{pmatrix} k \\ j \end{pmatrix} \right]$$

Because the positive factors c_i that multiply $|\text{Cov}_i|$ in the function f_{NOB} are strictly increasing with i, the approximations obtained through f_{NOB} tend to be characterized by a "redundant" satisfaction of many clauses. Better approximations, at the price of a limited number of additional iterations, can be obtained by a two-phase local search algorithm (NOB&OB): after a random start f_{NOB} guides the search until a local optimum is encountered [34]. As soon as this happens a second phase of LS is started where the move evaluation is based on f. A further reduction in the number of unsatisfied clauses can be obtained by a "plateau search" phase following NOB&OB: the search is continued for a certain number of iterations after the local optimum of OB is encountered, by using LS$^+$, with f as guiding function [34].

An example of non-oblivious search

Let us consider the following task with number of variables $n = 5$, and clauses $m = m^* = 4$, see also Fig. 35.13:

$$(\overline{u}_1 \vee \overline{u}_2 \vee u_3) \wedge (\overline{u}_1 \vee \overline{u}_2 \vee u_4) \wedge (\overline{u}_1 \vee \overline{u}_2 \vee u_5) \wedge (\overline{u}_3 \vee \overline{u}_4 \vee \overline{u}_5)$$

Let us assume that the assignment $U = (11111)$ is reached by OB local search. It is immediate to check that $U = (11111)$ is an oblivious local optimum with one unsatisfied clause (clause-4). While OB stops here, a possible sequence to reach the global optimum starting from U is the following: i) u_1 is set to **false**, ii) u_3 is set to **false**. Now, the first move does not change the number of satisfied clauses, but it changes the "amount of redundancy" (in clause-1 two literals are now satisfied, i.e., clause-1 enters Cov_2) and the move *is* a possible choice for a selection based on the *non-oblivious* function. The *oblivious* plateau has been eliminated and the search can continue toward the globally optimal point $U = (01011)$.

35.5.3 Local search satisfies most *3–SAT* formulae

An intriguing result by Koutsoupias and Papadimitriou [239] shows that, for the vast majority of satisfiable *3–SAT* formulae, the local search heuristic that starts at a random truth assignments and repeatedly flips a variable that improves the number of satisfied clauses, almost always succeeds in discovering a satisfying truth assignment.

Let us consider all clauses that are satisfied by a given truth assignment $\hat{U}$ and let us pick each of them with probability $p = 1/2$ to build a *3–SAT* formula. The following theorem [239] is demonstrated:

Theorem 35.5.3 *Let* $0 < \varepsilon < 1/2$. *Then there exists c,* $c \approx \left(1 - \sqrt{1 - (1/2 - \varepsilon)^2}\right)^2/6$, *such that for all but a fraction of at most* $n 2^n e^{-cn^2/2}$ *satisfiable 3–SAT formulae with* n *variables, the probability that local search succeeds in discovering a truth assignment in each independent trial from a random start is at least* $1 - e^{-\varepsilon^2 n}$.

Proof. Let us focus on the structure of the proof, without giving the technical details. One assumes that there is an assignment $\hat{U}$ that satisfies all clauses and shows that, if one starts from a *good* initial assignment, i.e., one that agrees with $\hat{U}$ in at least $(1/2 - \varepsilon)$ variables, the probability that the local search is ever *mislead* is small. By "*mislead*" one means that, when a variable is flipped, the Hamming distance between $U^{(t)}$ and $\hat{U}$ increases. The Hamming distance between two binary strings is given by the number of differing bits.

In detail, the quantity $1 - e^{-\varepsilon^2 n}$ in the theorem is the probability that the initial random truth assignment is *good* (use Chernoff bound). Then one demonstrates that, if the initial assignment is good, the probability that one does not reduce the Hamming distance between $U^{(t)}$ and $\hat{U}$ when an improving neighbor is chosen is at most $2e^{-cpn^2}$, the

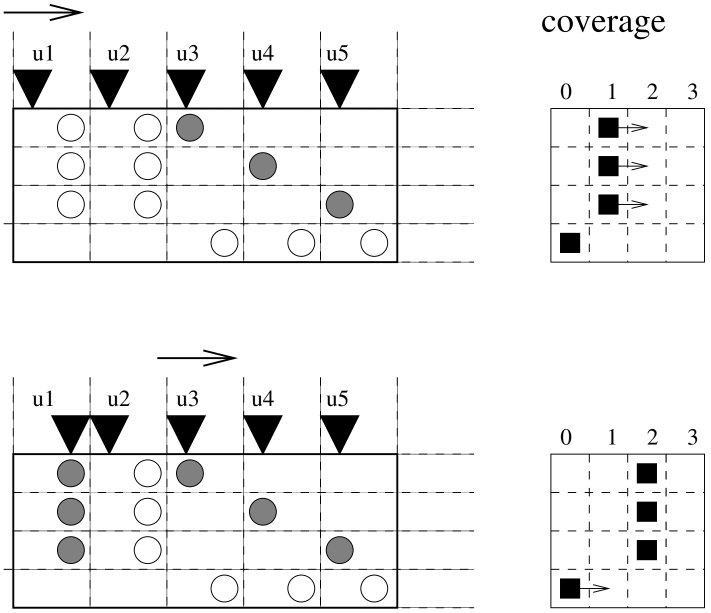


Figure 35.13: Non-oblivious search takes the different coverage into account.

probability being measured with respect to the random choice of the clauses to build the original formula ($p = 1/2$ for the above theorem).

Finally, the probability that local search starting from a good assignment will ever be misled by flipping a variable during the entire search trajectory is at most $n2^n e^{-cpn^2}$, since there are at most $n2^{n-1}$ such possible flippings – the number of edges of the n-hypercube.

□

The original formulation of the above theorem is for a *greedy* version of local search, using the function BEST-NEIGHBOR described in eqn. 35.9, but the authors note that greediness is not required for the theorem to hold, although it may be important in practice.

Let us finally note that the result, while of theoretical interest, is valid for formulae with many clauses (p must be such that the expected number of clauses is $\Omega(n^2)$), while the most difficult formulae have a number of clauses that is linear in n, see also Sec 35.8.1.

35.5.4 Randomized search for *2–SAT* (Markov processes)

A "natural" polynomial-time *randomized* search algorithm for *2–SAT* is presented in [288]. While it has long been known that *2–SAT* is a polynomially solvable problem, the algorithm is of interest because of its simplicity and is summarized here also because it motivated the GSAT-WITH-WALK algorithm of [325], see also Sec. 35.6.2.

In its "standard" form, local search is guided by the number of satisfied clauses and the basic criterion is that of accepting a neighbor only if more clauses are satisfied. The paper by Papadimitriou [288] changes the perspective by concentrating the attention to the *unsatisfied* clauses.

The algorithm for *2–SAT* , is extremely simple:

Let us note that worsening moves, leading to a lower number of satisfied clause, can be accepted during the search.

One can prove that:

Theorem 35.5.4 *The* MARKOVSEARCH *randomized algorithm for 2–SAT , if the instance is satisfiable, finds a satisfying assignment in $O(n^2)$ expected number of steps.*

```
MARKOVSEARCH
Start with any truth assignment
while there are unsatisfied clauses do
    pick one of them and flip a random literal in it
```

Figure 35.14: The MARKOVSEARCH randomized algorithm for *2–SAT* .

Proof. The proof involves an aggregation of the states of the Markov chain so that the chain is mapped to the *gambler's ruin* chain. A sketch of the proof is derived from [276]. Given an instance with a satisfying assignment $\hat{U}$, and the current assignment $U^{(t)}$, the progress of the algorithm can be represented by a particle moving between the integers $\{0, 1, ..., n\}$ on the real line. The position of the particle indicates how many variables in $U^{(t)}$ agree with those of $\hat{U}$. At each iteration the particle's position can change only by one, from the current position i to $i + 1$ or $i - 1$ for $0 < i < n$. A particle at 0 can move only to 1, and the algorithm terminates when the particle reaches position n, although it may terminate at some other position with a satisfying assignment different from $\hat{U}$. The crucial fact is that, in an unsatisfied clause, at least one of the *two* literals has an incorrect value and therefore, with probability at least $1/2$, the number of correct variables increases by one when a randomized step is executed.

The random walk on the line is one of the most extensively studied stochastic processes. In particular, the above process is a version of the "gambler's ruin" chain with reflecting barrier (that is, the house cannot lose its last dollar). Average number of steps for the gambler to be ruined is $O(n^2)$.
□

35.6 Memory-less Local Search Heuristics

State-of-the-art heuristics for *MAX–SAT* are obtained by complementing local search with schemes that are capable of producing better approximations beyond the locally optimal points. In some cases, these schemes generate a sequence of points in the set of admissible solutions in a way that is fixed before the search starts. An example is given by *multiple runs* of local search starting from different random points. The algorithm does not take into account the *history* of the previous phase of the search when the next points are generated. The term *memory-less* denotes this lack of feedback from the search history.

In addition to the cited *multiple-run* local search, these techniques are based on Markov processes (Simulated Annealing), see Sec. 35.6.1, "plateau" search and "random noise" strategies, see Sec. 35.6.2, or combinations of randomized constructions and local search, see Sec. 35.6.3.

35.6.1 Simulated Annealing

Simulated Annealing has been described in Seciton 25.5. The use of a Markov process (Simulated Annealing or SA for short) to generate a stochastic search trajectory is illustrated in Fig. 35.15, adapted from [343].

For a certain number of tries, a random truth assignment is generated (line 2) and the $temperature$ parameter is set to MAX-TEMP. In the inner loop, new assignments are generated by probabilistically flipping each variable based on the improvement δ in the number of satisfied clauses that would occur after the flip. Of course, the improvement can be negative. The probability to flip is given by a logistic function that penalizes smaller or negative improvements (line 9). The inner loop controls the *annealing schedule*: when $iter$ increases the $temperature$ slowly decreases (line 5) until a minimum of MIN-TEMP is reached and the control exits the loop (line 6) Let us note that, when the $temperature$ is large, the moves are similar to those produced by a random walk, while, when the $temperature$ is low the acceptance criterion of the moves is that of local search and the algorithm resembles GSAT, that will be introduced in Sec. 35.6.2. Implementation details, the addition of a "random walk" modification inspired by [325], and experimental results are described in the cited paper.

```
SA
for $tries \leftarrow 1$ to MAX-TRIES
    $U \leftarrow$ random truth assignment ; $iter \leftarrow 0$
    forever
        if $U$ satisfies all clause then return $U$
        $temperature \leftarrow$ MAX-TEMP $\times\ e^{-iter \times decay\_rate}$
        if $temperature <$ MIN-TEMP then exit loop
        for $i \leftarrow 1$ to $n$
            $\delta \leftarrow$ increase of satisfied clauses if $u_i$ is flipped
            FLIP$(u_i)$with probability$1/(1 + e^{-\frac{\delta}{temperature}})$
        $iter \leftarrow iter + 1$
```

Figure 35.15: The Simulated Annealing algorithm for *SAT* .

35.6.2 GSAT with "random noise" strategies

SAT is of special concern to Artificial Intelligence because of its connection to *reasoning*. In particular, deductive reasoning is the complement of satisfiability: from a collection of base facts A one should deduce a sentence F if and only if $A \cup \overline{F}$ is *not* satisfiable, see also Sec. 35.2.2. The popular and effective algorithm GSAT was proposed in [324] as a *model-finding* procedure, i.e., to find an interpretation of the variables under which the formula comes out **true**. GSAT consists of multiple runs of LS$^+$, each run consisting of a number of iterations that is typically proportional to the problem dimension n. The experiments in [324] show that GSAT can be used to solve hard (see sec. 35.8.1) randomly generated problems that are an order of magnitude larger than those that can be solved by more traditional approaches like Davis-Putnam or resolution. Of course, GSAT is an incomplete procedure: it could fail to find an optimal assignment. An extensive empirical analysis of GSAT is presented in [145, 144].

Different "noise" strategies to escape from attraction basins are added to GSAT in [325, 323]. In particular, the GSAT-WITH-WALK algorithm has been tested in [323] on the Hansen-Jaumard benchmark of [172], where a better performance with respect to SAMD is demonstrated, although requiring much longer CPU times. See Sec. 35.7.1 for the definition of SAMD.

```
GSAT-WITH-WALK
for $i \leftarrow 1$ to MAX-TRIES
    $U \leftarrow$ random truth assignment
    for $j \leftarrow 1$ to MAX-FLIPS
        if RANDOMNUMBER $< p$ then
            $u \leftarrow$ any variable occurring in some unsat. clause
        else
            $u \leftarrow$ any variable with largest$\Delta f$
        FLIP$(u)$
```

Figure 35.16: The GSAT-WITH-WALK algorithm. RANDOMNUMBER generates random numbers in the range $[0, 1]$.

The algorithm is briefly summarized in Fig. 35.16. A certain number of tries (MAX-TRIES) is executed, where each try consists of a number of iterations (MAX-FLIPS). At each iteration a variable is chosen by two possible criteria and then flipped by the function FLIP, i.e., U_i becomes equal to $(1 - U_i)$. One criterion, active with "noise" probability p, selects a variable occurring in some unsatisfied clause with uniform probability over these variables, the other one is the standard method based on the function f given by the number of satisfied clauses. The first criterion was motivated by [288], see also Sec. 35.5.4. For a generic move μ, the quantity $\Delta_\mu f$ (or Δf for short) is defined as $f(\mu\ U^{(t)}) - f(U^{(t)})$. The straightforward book-keeping part of the algorithm is not shown. In particular, the best assignment found during all trials is saved and reported at the end of the run. In addition, the run is terminated immediately if an assignment is found that satisfies all clauses. The original Gsat algorithm can be obtained by setting $p = 0$ in the Gsat-with-walk algorithm of Fig. 35.16.

35.6.3 Randomized Greedy and Local Search (Grasp)

A hybrid algorithm that combines a randomized greedy construction phase to generate initial candidate solutions, followed be a local improvement phase is the Grasp scheme proposed in [304] for the *SAT* and generalized for the *MAX W–SAT* problem in [305], a work that is briefly summarized in this section.

Grasp is an iterative process, with each iteration consisting of two phases, a construction phase and a local search phase.

During each construction, all possible choices are ordered in a candidate list with respect to a greedy function measuring the (myopic) benefit of selecting it. The algorithm is randomized because one picks in a random way one of the best candidates in the list, not necessarily the top candidate. In this way different solutions are obtained at the end of the construction phase.

Because these solutions are not guaranteed to be locally optimal with respect to simple neighborhoods, it is usually beneficial to apply a local search to attempt to improve each constructed solution.

```
Grasp($RCLSize, MaxIter, RandomSeed$)
1    △ Input instance and initialize data structures
2    for $i \leftarrow 1$ to $MaxIter$
3        $U \leftarrow$ ConstructGreedyRand($RCLSize, RandomSeed$)
4        $U \leftarrow$ LocalSearch($U$)
```

```
ConstructGreedyRand($RCLSize, RandomSeed$)
for $k \leftarrow 1$ to $n$
    MakeRCL($RCLSize$)
    $s \leftarrow$ SelectIndex($RandomSeed$)
    AssignVariable($s$)
    AdaptGreedyFunction($s$)
```

Figure 35.17: The Grasp algorithm (above) and the randomized greedy construction (below).

A high-level description of the Grasp algorithm is presented in Fig. 35.17, a summarized version of the more detailed description in [305]. After reading the instance and initializing the data structures one repeats for $MaxIter$ iterations the construction of an assignment U and the application of local search starting from U to produce a possibly better assignment (lines 2–4). Of course, the best assignment found during all iterations is saved and reported at the end. In addition to $MaxIter$, the parameters are $RCLSize$, the size of the restricted candidate list of moves out of which a random selection is executed, and a random seed used by the random number generator. In detail, see function ConstructGreedyRand in Fig. 35.17, the restricted candidate list of assignments is created by MakeRCL, the index of the next variable to be assigned a truth value is chosen by SelectIndex, the truth value is assigned by AssignVariable and the greedy function that guides the construction is changed by AdaptGreedyFunction to reflect the assignment just made.

The remaining details about the greedy function (designed to maximize the total weight of yet-unsatisfied clauses that become satisfied after a given assignment), the creation of the restricted candidate list, and local search (based on the *1-flip* neighborhood) are presented in [305], together with experimental results.

35.7 History-sensitive Heuristics

Different history-sensitive heuristics have been proposed to continue local search schemes beyond local optimality. These schemes aim at intensifying the search in promising regions and at diversifying the search into uncharted territories by using the information collected from the previous phase (the *history*) of the search. The *history* at iteration t is formally defined as the set of ordered couples (U, s) such that $0 \leq s \leq t$ and $U = U^{(s)}$.

Because of the internal feedback mechanism, some algorithm parameters can be modified and tuned in an *on-line* manner, to reflect the characteristics of the *task* to be solved and the *local* properties of the configuration space in the neighborhood of the current point. This tuning has to be contrasted with the *off-line* tuning of an algorithm, where some parameters or choices are determined for a given problem in a preliminary phase and they remain fixed when the algorithm runs on a specific instance.

35.7.1 Prohibition-based Search: TS and SAMD

Tabu Search (TS) is a *history-sensitive* heuristic proposed by F. Glover [148] and, independently, by Hansen and Jaumard, that used the term SAMD ("steepest ascent mildest descent") and applied it to the *MAX–SAT* problem in [172]. The main mechanism by which the history influences the search in TS is that, at a given iteration, some neighbors are *prohibited*, only a non-empty subset $N_A(U^{(t)}) \subset N(U^{(t)})$ of them is *allowed*. The general way of generating the search trajectory that we consider is given by:

$$N_A(U^{(t)}) \quad = \quad \text{ALLOW}(N(U^{(t)}), U^{(0)}, ..., U^{(t)}) \qquad (35.20)$$

$$U^{(t+1)} \quad = \quad \text{BEST-NEIGHBOR}(\ N_A(U^{(t)})\ ) \qquad (35.21)$$

The set-valued function ALLOW selects a non-empty subset of $N(U^{(t)})$ in a manner that depends on the entire previous history of the search $U^{(0)}, ..., U^{(t)}$. Let us note that worsening moves *can* be produced by eqn. 35.21, as it must be in order to exit local optima.

The introduction of algorithm SAMD is motivated in [172] by contrasting the technique with Simulated Annealing (SA) [234] for maximization. The directions of local changes are little explored by SA: for example, if the objective function increases, the change is always accepted however small it may be. On the contrary, it is desirable to exploit the information on the direction of *steepest* ascent and yet to retain the property of not being blocked at the first local optimum found. SAMD performs local changes in the direction of steepest ascent until a local optimum is encountered, then a local change along the direction of mildest descent takes place and the reverse move is *forbidden* for a given number of iterations to avoid cycling with a high probability. The details of the SAMD technique as well as additional specialized devices for detecting and breaking cycles are outlined in [172]. A computational comparison with SA and with Johnson's two algorithms is also presented. A specialized Tabu Search heuristic is used in [215] to speed up the search for a solution (if the problem is satisfiable) as part of a branch-and-bound algorithm for *SAT* , that adopts both a relaxation and a decomposition scheme by using polynomial instances, i.e., *2–SAT* and Horn *SAT* .

35.7.2 HSAT and "clause weighting"

In addition to the already cited SAMD [172] heuristic that uses the temporary prohibitions of recently executed moves, let us mention two variations of GSAT that make use of the previous history.

HSAT [145] introduces a tie-breaking rule into GSAT: if more moves produce the same (best) Δf, the preferred move is the one that has not been applied for the longest span. HSAT can be seen as a "soft" version of Tabu Search: while TS prohibits recently-applied moves, HSAT discourages recent moves if the same Δf can be obtained with moves that have been "inactive" for a longer time. It is remarkable to see how this innocent variation of GSAT can increase its performance on some *SAT* benchmark tasks [145].

Clause–weighting has been proposed in [321] in order to increase the effectiveness of GSAT for problems characterized by strong asymmetries. In this algorithm a positive weight is associated to each clause to determine how often the clause should be counted when determining which variable to flip. The weights are dynamically modified during problem solving and the qualitative effect is that of “filling in” local optima while the search proceeds. Clause–weighting can be considered as a “reactive” technique where a repulsion from a given local optimum is generated in order to induce an escape from a given attraction basin.

35.7.3 The Hamming-Reactive Tabu Search (H-RTS) algorithm

The Reactive Search Optimization (RSO) principles of “learning while searching” have been introduced in Chapter 27.

An algorithm that combines the previously described techniques of local search (oblivious and non-oblivious), the use of prohibitions (see TS and SAMD), and a reactive scheme to determine the prohibition parameter is presented in [33]. The algorithm is called HAMMING-REACTIVE-TS algorithm, and its core is illustrated in Fig. 35.18.

```
HAMMING-REACTIVE-TS
1   repeat
2       $t_r \leftarrow t$
3       $U \leftarrow$ random truth assignment
4       $T \leftarrow \lfloor T_f \, n \rfloor$

5       repeat                              { NOB local search }
6           $U \leftarrow$ BEST-MOVE$(LS, f_{NOB})$
7       until largest $\Delta f_{NOB}$ = 0

8       repeat
9           repeat                          { local search }
10              $U \leftarrow$ BEST-MOVE$(LS, f_{OB})$
11          until largest $\Delta f_{OB}$ = 0
12          $U_I \leftarrow U$

13          for $2(T+1)$ iterations         { reactive tabu search }
14              $U \leftarrow$ BEST-MOVE$(TS, f_{OB})$
15          $U_F \leftarrow U$

16          $T \leftarrow$ REACT$(T_f, U_F, U_I)$
17      until $(t - t_r) > 10\, n$
18  until solution is acceptable or max. number of iterations reached
```

Figure 35.18: The *H-RTS* algorithm.

The initial truth assignment is generated in a random way, and non-oblivious local search (LS-NOB) is applied until the first local optimum of f_{NOB} is encountered. LS-NOB obtains local minima of better average quality than LS-OB, but then the guiding function becomes the standard oblivious one. This choice was motivated by the success of the NOB & OB combination [34] and by the poor diversification properties of NOB alone, see [33].

The search proceeds by repeating phases of local search followed by phases of TS (lines 8–17 in Fig. 35.18), until a suitable number of iterations are accumulated after starting from the random initial truth assignment (see line 17 in Fig. 35.18). A single elementary move is applied at each iteration. The variable t, initialized to zero, identifies the current iteration and increases after a local move is applied, while t_r identifies the iteration when the last random assignment was generated. Some trivial bookkeeping details (like the increase of t) are not shown in the figure.

During each combined phase, first the local optimum of f is reached, then $2(T+1)$ moves of Tabu Search are executed. The design principle underlying this choice is that prohibitions are necessary for diversifying the search only after LS reaches a local optimum. The fractional prohibition T_f is changed during the run by the function REACT to obtain a proper balance of diversification and bias [33].

The random restart executed after $10\ n$ moves guarantees that the search trajectory is not confined in a localized portion of the search space.

Being an heuristic algorithm, there is not a natural termination criterion. In its practical application, the algorithm is therefore run until either the solution is acceptable, or a maximum number of moves (and therefore CPU time) has elapsed. What is demonstrated in the computational experiments in [33] is that, given a fixed number of iterations, HAMMING-REACTIVE-TS achieves much better average results with respect to competitive algorithms (GSAT and GSAT-WITH-WALK). Because, to a good approximation, the actual running time is proportional to the number of iterations, HAMMING-REACTIVE-TS should therefore be used to obtain better approximations in a given allotted number of iterations, or equivalent approximations in a much smaller number of iterations.

35.8 Models of hardness and threshold effects

Given the hardness of the problem and the relevancy for applications in different fields, the emphasis on the experimental analysis of algorithms for the *MAX–SAT* problem has been growing in recent years.

In some cases the experimental comparisons have been executed in the framework of "challenges," with support of electronic collection and distribution of software, problem generators and test instances. Practical and industrial *MAX–SAT* problems and benchmarks, with significant case studies are also presented in [120], see also the contained review [163].

In some cases it is of interest to model the hardness of instances with appropriate models. Let us describe some basic problem models that are considered both in theoretical and in experimental studies of *MAX–SAT* algorithms [163].

- **k-SAT model**, also called **fixed length clause model**. A randomly generated CNF formula consists of independently generated random clauses, where each clause contains exactly k literals. Each literal is chosen uniformly from $U = \{u_1, ..., u_n\}$ without replacement, and negated with probability p. The default value for p is $1/2$.
- **average k-SAT model**, also called **random clause model**. A randomly generated CNF formula consists of independently generated random clauses. Each literal has ha probability p of being part of a clause. In detail, each of the n variables occurs positively with probability $p(1-p)$, negatively with probability $p(1-p)$, both positively and negatively with probability p^2, and is absent with probability $(1-p)^2$.

Both models have many variations depending on whether the clauses are required to be different, whether a variable and its negation can be present in the same clause, etc.

Although superficially similar, the two models differ in the *difficulty* to solve the obtained formulae and in the mathematical analysis. In particular, when the initial formula comes from the average k-SAT model, a step that fixes the value of a variable produces a set of clauses from the same model, while if the same step is executed in the k-SAT model, the resulting clauses do not necessarily have the same length and therefore do not come from the k-SAT model.

Other *structured* problem models are derived from the mapping of instances of different problems, like *coloring*, n-queens, etc. [207]. The performance of algorithms on these more structured models tend to have little correlation with the performance tested on the above introduced random problems. Unfortunately, the theoretical analysis of these more structured problems is very hard. The situation worsens if one considers "real-world" practical applications, where one is typically confronted with a few instances and little can be derived about the "average" performance, both because the probability distribution is not known and because the number of instances tends to be very small.

A compromise can be reached by having parametrized generators that capture some of the relevant structure of the "real-world" problems of interest.

35.8.1 Hardness and threshold effects

Different algorithms demonstrate a different degree of effort, measured by number of elementary steps or CPU time, when solving different kinds of instances. For example, Mitchell et al. [272] found that some distributions used in past experiments are of little interest because the generated formulae are almost always very easy to satisfy. They also reported that one can generate very hard instances of k-SAT, for $k \geq 3$. In addition, they report the following observed behavior for random fixed length *3–SAT* formulae: if r is the ratio r of clauses to variables ($r = m/n$), almost all formulae are satisfiable if $r < 4$, almost all formulae are unsatisfiable if $r > 4.5$. A rapid transition seems to appear for $r \approx 4.2$, the same point where the computational complexity for solving the generated instances is maximized, see [235, 99] for reviews of experimental results.

A series of theoretical analyses aim at approximating the unsatisfiability threshold of random formulae. Let us define the notation and summarize some results obtained.

Let **C** be a random k-SAT formula. The research problem that has been considered, see for example [236], is to compute the least real number κ such that, if r is larger than κ, then the probability of **C** being satisfiable converges to 0 as n tends to infinity. In this case one says that **C** is asymptotically almost certainly satisfiable. Experimentally, κ is a threshold value marking a "sudden" change from probabilistically certain satisfiability to probabilistically certain unsatisfiability. More precisely [5], given a sequence of events $\mathcal{E}_i$, one says that $\mathcal{E}_n$ occurs almost surely (a.s.) if $\lim_{n\to\infty} \mathbf{Pr}\left[\mathcal{E}_n\right] = 1$, where $\mathbf{Pr}\left[event\right]$ denotes the probability of an event. The behavior observed in experiments with random k-SAT leads to the following conjecture:
For every $k \geq 2$, there exist r_k such that for any $\varepsilon > 0$, random instances of k-SAT with $(r_k - \varepsilon)n$ clauses are a.s. satisfiable and random instances with $(r_k + \varepsilon)n$ clauses are a.s. unsatisfiable

For $k = 2$ (i.e., for the polynomially solvable *2–SAT*) the conjecture was proved [89, 156], in fact showing that $r_2 = 1$. For $k = 3$ much less progress has been made: neither the existence of r_3 nor its value has been determined.

In the fixed-length *3–SAT* model, the total number of all possible clauses is $8\binom{n}{3}$ and the probability that a random clause is satisfied by a truth assignment U is $7/8$.

Let $\mathcal{U}_n$ be the set of all truth assignments on n variables, and let $\mathcal{S}_n$ be the set of assignments that satisfy the random formula **C**. Therefore the cardinality $|\mathcal{S}_n|$ is a random variable. Given **C**, let $|\mathcal{S}_n(\mathbf{C})|$ be the number of assignments satisfying **C**.

The expected value of the number of satisfying truth assignments of a random formula, $\mathbf{E}\left[|\mathcal{S}_n|\right]$, is defined as:

$$\mathbf{E}\left[|\mathcal{S}_n|\right] = \sum_{\mathbf{C}} (\mathbf{Pr}\left[\mathbf{C}\right] |\mathcal{S}_n(\mathbf{C})|) \tag{35.22}$$

The probability that a random formula is satisfiable is:

$$\mathbf{Pr}\left[\text{the random formula is satisfiable}\right] = \sum_{\mathbf{C}} (\mathbf{Pr}\left[\mathbf{C}\right] I_{\mathbf{C}}) \tag{35.23}$$

where $I_{\mathbf{C}}$ is 1 if **C** is satisfiable, 0 otherwise.

From equations (35.22) and (35.23) the following Markov's inequality follows:

$$\mathbf{Pr}\left[\text{the random formula is satisfiable}\right] \leq \mathbf{E}\left[|\mathcal{S}_n|\right] \tag{35.24}$$

Let us now consider the "first moment" argument to obtain an upper bound for κ in the *3–SAT* model. First one observes that the expected number of truth assignments that satisfy **C** is $2^n(7/8)^{rn}$, then one lets this expected value converge to zero and uses the above Markov's inequality. From this one obtains

$$\kappa \leq \log_{8/7} 2 = 5.191$$

This result has been found independently by many people, including [129] and [90]. More refined studies are present for example in [77, 236, 226, 5]

Gist

SAT and *MAX–SAT* deal with assigning truth values to variables in Boolean formulas to make them true ("satisfied"). They are interesting and extremely relevant optimization problems, easy to define and visualize, for which most algorithmic ideas have been tried with success in creative combinations.

These include branch-and-bound, integer linear programming, continuous approaches, approximation algorithms, randomized algorithms, perturbative local search and greedy constructions, reactive search optimization, experimental studies of hardness.

A full grasp of the approaches for solving *SAT* and *MAX–SAT* is therefore beneficial to fully understand how to apply these principles for a very concrete simple problem, before considering more complicated versions like constraint programming (CP).

The satisfaction of studying and using *SAT* and *MAX–SAT* is never ending.

Chapter 36

Design of experiments, query learning, and surrogate model-based optimization

Scientists and engineers study the behavior of systems to find improving or optimal configurations. Consider for example the fuel consumption of a motor; it will depend on various parameters, including the motor geometry, the temperature of operation, the kind of fuel, etc. To minimize it, one needs a model of how the consumption depends on the design parameters.

In abstract terms, one deals with a system transforming a vector of inputs X into an output Y. Only in some very rare cases an explicit and exact analytic model is available. In other and more frequent cases, deriving the output Y requires running a simulator or even building prototypes. The two operations can be very costly in terms of time or money. Minimizing the number of simulator runs or experiments is a therefore a critical issue. Building a surrogate (approximated) model based on the executed experiments can be a way, if the model evaluation is much faster than the real system. When an initial model is available, it can be used to make predictions of to identify optimal configurations by optimization. If calculating $Y(\mathbf{x})$ for different $\mathbf{x}$ values is very costly, all evaluations done are collected to build initial models, useful to guide the generation of the future input configurations to be evaluated. This is a paradigmatic case of "learning while optimizing", also known as **surrogate optimization**, or **optimization based on response surfaces** (Response Surface Methodology or RSM), and related to Kriging (Section 1.2), to locally-weighted regression (Section 9.2), and to global optimization schemes based on memory and statistical inference (Section 25.4).

In this chapter we focus on data-driven models for which **experimental data is not available at the beginning and needs to be acquired in a strategic and intelligent manner**. In medicine, one may want to understand if a medical treatment is successful or not. Experiments imply treating patients with different medicines in a carefully controlled context, to avoid *placebo* effects, or effects caused by different populations of patients. Some patients may have dangerous side-effects during the tests, some may even die. As one can imagine, these experiments are incredibly costly and slow, causing years of delay between the invention of new treatments and their commercialization. In manufacturing, one may want to fine-tune a casting process. Through casting a liquid material is poured into a mold, which contains a hollow cavity of the desired shape, and then allowed to solidify. It is the main method to produce most of our physical goods, but also very complex and fragile. Variations of temperature, pressure, speed of injection, composition of the metal, may lead to defective parts which need to be discarded. In manufacturing, simulating a specific setting or - even worse - running a production facility just to accumulate data can be very time-consuming and costly.

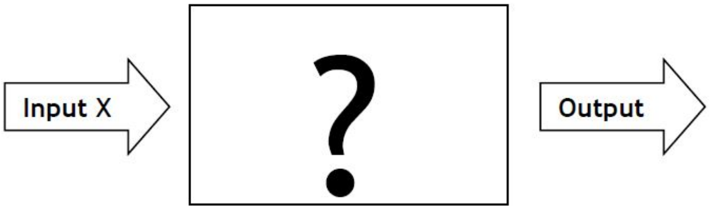


Figure 36.1: Design of Experiments (DOE): how to generate appropriate inputs to study and model an unknown system.

When one needs experimental data to study a system or to **generate training examples in machine learning**, the objectives are to limit costs, while getting informative data, sufficient to build precise models. The topic is not recent, being deeply related with the scientific method. In science and engineering it is known as **design of experiments**. In ML, with a different but related context, it is known as **active or query learning**.

36.1 Design of experiments (DOE)

Experimentation is a goal-directed activity. In spite of stories of apples falling on sleeping scientists leading to elegant theories of gravitation, most experiments need to be **designed** with precise objectives and with a careful allocation of physical or computational resources. Inspiration and creativity are crucial to define the initial goals but sterile without the 90% "perspiration" in the experimental work.

If the objective is to model a system and understand which inputs are relevant to predict the output, the questions (the input points $\mathbf{x}$) have to be produced in order to derive accurate models, and to identify the *factors of variation*. The concept of factors of variations is related to the concept of *informative features* in ML. Inputs that do not influence the output in a significant manner can be eliminated from the model. **Design of experiments** refers to a systematic and principled manner to generate examples to characterize, predict, and then improve the behavior of any system or process.

All experimental activity is usually accompanied by **experimental noise** in the form of measurement errors, hidden and uncontrollable factors affecting the experiments, and by the **possibility to be fooled by chance** into deriving wrong conclusions.

Because physical measurements are subject to errors, one often assumes that the measured output $Y(X)$ is equal to a "true" response $Y_t(X)$ plus a random error term ϵ : $Y(X) = Y_t(X) + \epsilon$, ϵ being a random variable chracterized by a given distribution (usually, a Gaussian with a given standard deviation σ).

We will first introduce some DOE methods popular with engineers and then (in Section 36.3) present the different but related concept of active and query learning.

In DOE, inputs are usually called "design variables" or "factors", output is called "response". Let's note that no simple receipt exists to apply DOE and response surfaces. All techniques depend on assumptions that can be easily violated in real systems, so that the focused attention by the experimenter and the critical use of more than one technique are required to avoid the most obvious mistakes. Let's just make a motivating example. Imagine that we want to measure the effect of a medication on cholesterol level and let's assume that the cholesterol levels depend both on taking the medication but also on age. If the original experimental data are not generated with a careful DOE, it can happen – by chance, or by having two different hospitals with patients of different age collecting the data - that the patients receiving the medication are much older, so that cholesterol levels are higher in spite of the medication. The effect of the medication can be canceled or reversed by the effect of age. To separate the medication effect, the sample of people should have their age randomized (no statistically significant age distribution should be present in the two groups).

In many engineering applications, a simulator can be used to generate example outputs Y corresponding to user-chosen inputs X. The situation can be different if examples require running a physical system, or observing a process in action. But if one is in the lucky case, designing an experiment means deciding the appropriate number of examples to generate and where they are generated in the input space. The overall DOE objective of getting a surrogate model is clear, but the devil is in the details, and one must consider the assumptions and how the model is going to be used. Selection of a proper DOE is a matter that requires expert advice, knowledge of the problem, and estimates of the time-budget allocated to the generation of sample output values, which usually is the most time-consuming part.

A simple constraint on the input can be given by specifying a design space, usually by setting separate upper and lower bounds on each x variable. Without loss of generality, if n is the input dimension, we can think about the hypercube $[-1, 1]^n$ or $[0, 1]^n$. The original range can then be recovered by appropriately scaling the individual variables. If one has reasons to believe that the form of the model is correct (for example, that the real physical process is described by a low-order polynomial), placing the examples near or on the boundaries of the design space makes sense because this choice will minimize the effect of the random error ϵ on the determination of the model parameters. Think about fitting a line with two points, the more separated they are in the x direction, the more stable will be the line with respect to random noise in the y position. On the contrary, if the model is a rough approximation, and one aims at using the model in the interior part of the design space, for example for finding an optimal configuration, a good fraction of the points should be placed also in the interior part of the design space. In other words, one could aim at minimizing the average model discrepancy (called generalization error in the language of machine learning) more than at determining individual coefficients with a high precision. Another critical parameter is the total number of examples. In general, the more examples the better (provided that they are well distributed), but the computational cost of running the simulator can be very large and one must settle for the minimal number which is sufficient to identify a workable model. A second possibility is to use multiple iterations, by first running an exploratory analysis in the entire design space, and then additional investigations in more concentrated areas of the design space.

As a rule of thumb, the number of examples has to be larger than the number of parameters in the model (i fpossible much larger). Otherwise the model will easily fit the examples but produce wildly-oscillating "nonsense" results in regions of the design space far from the chosen examples. As an overall advice, randomization will avoid the most serious faults inherent in advanced DOE methods based on specific assumptions. The popular design of experiment techniques are summarized in the following sections.

36.1.1 Full factorial design

In spite of the sophisticated name, this is the most obvious (and naive) way to proceed. It is based on determining the number of levels (i.e. different values) for each variables and then generating sample points on a **regular grid**. For two levels the points are placed at the left and right boundary of the design space variable. For three levels, an additional point is added in the middle, and so on.

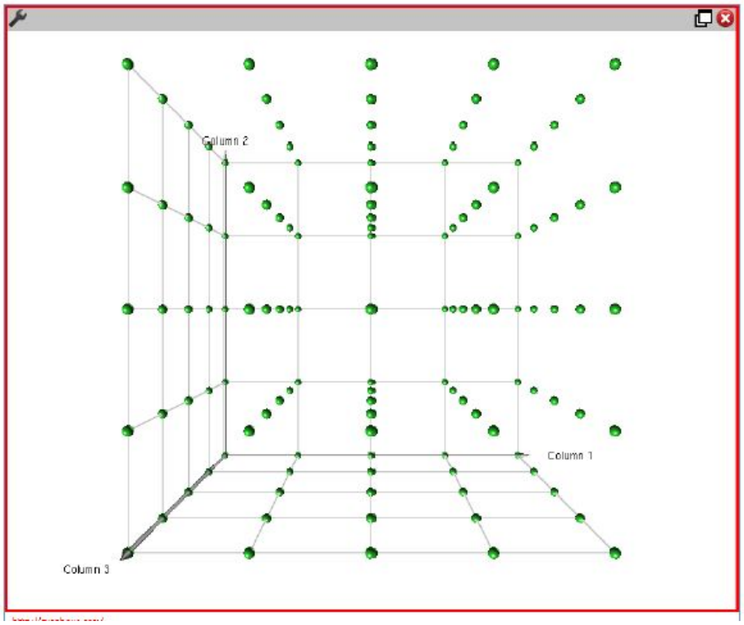


Figure 36.2: A full factorial design.

The figure shows a full-factorial DOE with 5 levels for each factor, in three dimensions. The advantage of the full factorial design is its simplicity; its disadvantage lies in its regular grid-like nature. The generated samples may miss some relevant effect between the sample points. The number of points generated, if the number of levels L is the same for all variables, is equal to L^n, a number which will explode very rapidly to make this method applicable only to problems with a small number of input variables. Full factorial designs are very expensive: the number of samples grows exponentially when the input dimension grows. It is not surprising that reduced factorial designs using only a subset of the full factorial design points are considered.

36.1.2 Randomized design: pseudo Montecarlo sampling

A full factorial design ie very expensive. In spite of its cost it can be fragile. If the interesting areas of parameters lie between the regularly-spaced points, they will never be identified. A more robust design, which can generate more points if more time is available, is based on a simple randomization. A randomized design will a uniform probability generates points in every area with a probability different from zero.

Pseudo-random number generators can be used to generate random numbers uniformly distributed in an interval, for example [0,1]. By repeated calls of a good-quality pseudo-random number generator, one can create random vectors uniformly distributed in the design space. $X = \{rand(), rand(), rand(), \ldots\}$

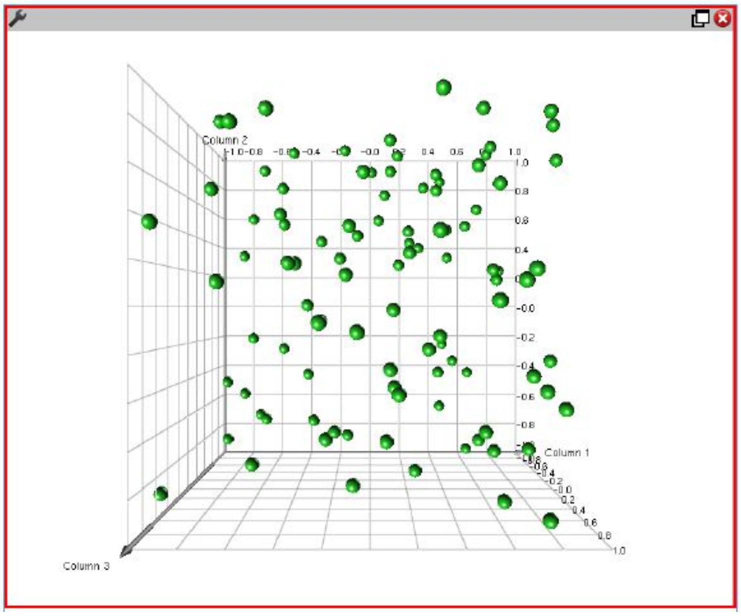


Figure 36.3: A randomized design.

Fig. 36.3 shows a pseudo-Monte Carlo DOE with 100 points in three dimensions. The distribution of points along the three different factors is shown in the parallel coordinates plot in Fig. 36.4 (the parallel coordinate plot is explained in Section 18.3). Two rather large gaps in the factor corresponding to the first coordinate are highlighted with an arrow. By chance, Some large areas can remain empty of sample points.

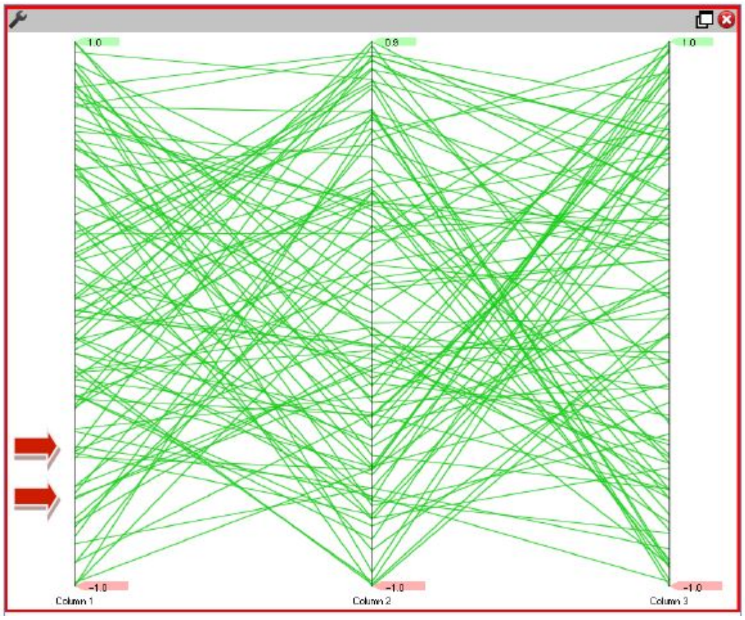


Figure 36.4: Parallel coordinates plot: a randomized design may leave some holes.

By suitable transformations, one can easily generate random samples for simple design spaces, like circles, circular regions, triangles, etc. In the absence of detailed and trusted information about the physical system under analysis, it is difficult to beat the simplicity and the robustness of the pseudo-random design. The more advanced techniques must be used with care and with more competence, and it is not guaranteed that they will add a lot of information with respect to what can be gained by simple randomization. Another advantage of a randomized design is that it works for any number of samples, and that it can be immediately repeated (by using a different random number seed and therefore a different sequence of random numbers) to check for the robustness or fragility of the first DOE. A weakness of the basic pseudo-random design is that, because of the random and independent nature of the samples, it will often leave large regions of the design space unexplored. The **stratified Monte Carlo sampling** was developed to cure the above problem, provided that one can afford the required number of samples. The idea is to divide each interval into subintervals (or "bins") of equal probability. Once the bins are defined, a sample position is then randomly selected within each bin. This trivially guarantees that at least a sample will be present in each interval. The drawback is that, if the minimum of two intervals is generated for each input dimension, the number of samples grows at best like 2^n.

36.1.3 Latin hypercube sampling

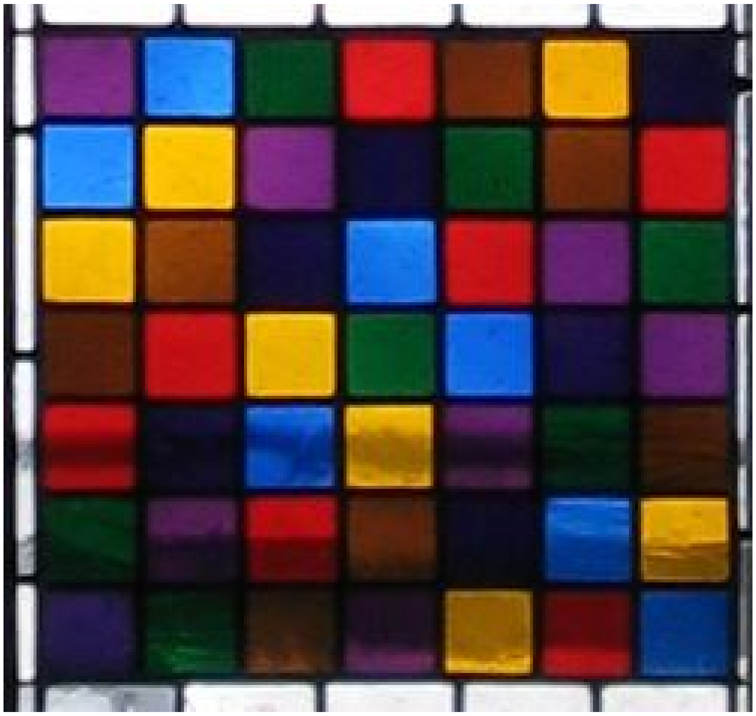


Figure 36.5: Stained glass window in the dining hall of Caius College, in Cambridge, commemorating Ronald Fisher and representing a Latin square.

Latin Hypercube sampling (LHS)[266, 204] is a modern and popular randomized DOE method than can work with any user-selected number of samples k. Under certain assumptions, LHS provides a more accurate estimate of the mean value of the Y function than the standard Monte Carlo sampling. Its motivation is to ensure that, for a given number of samples k, and k equally-spaced bins, for all one-dimensional projections of the samples there will be one and only one sample in each bin. A square grid containing sample positions is a Latin square if (and only if) there is only one sample in each row and each column. A Latin hypercube is the generalisation of this concept to an arbitrary number of dimensions, whereby each sample is the only one in each axis-aligned hyperplane containing it.

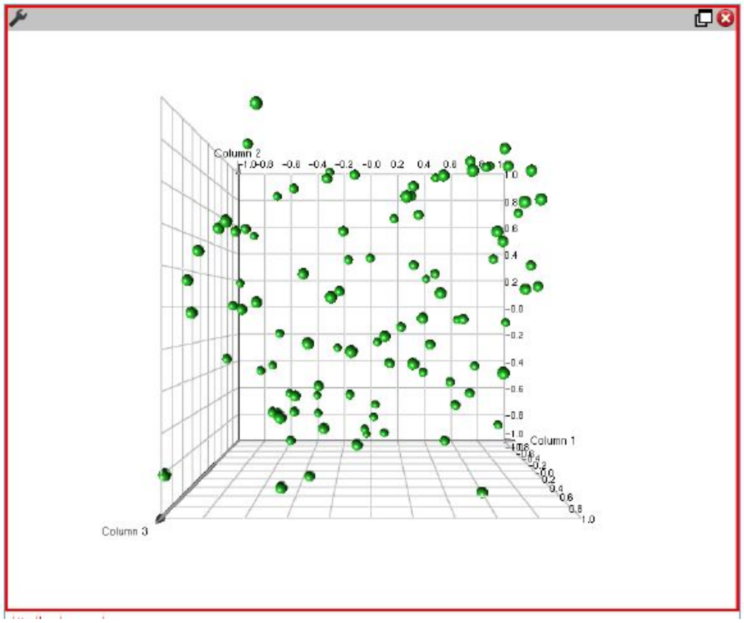


Figure 36.6: A Latin hypercube sampling.

Fig. 36.6 shows a LHS DOE with 100 samples, in three dimensions. The parallel coordinates visualization in Fig. 36.7 shows the uniform distribution of points along each factor: each one of the 100 bins is covered by one and only one point.

The method to generate LHS samples is the following. In one dimension x_1, partition the range into k bins and then generate one sample per bin with uniform probability. In two dimensions, x_1 and x_2, after generating the x_1 values, pick the bin in the x_2 direction according to a permutation of the x_1 bin index. The permutation will ensure that all vertical bins will be covered by one and only one sample. After generalizing, and picking a separate random permutation of the bins for each input variable, one obtains the complete LHS design. In detail, in the $[0,1]^n$ hypercube, if p is the number of samples and $x_j^{(i)}$ is the j-th component of the i-th sample, for $1 \leq j \leq n$ and $1 \leq i \leq k$, and $\pi_j^{(i)}$ is the permutation for variable j, permuting integers $0, 1, .., k-1$, evaluated at i, the coordinates are obtained as:

$$x_j^{(i)} = (x_j^{(i)} + U_j^{(i)})/k$$

where U is a uniform random value on $[0,1]$.

36.2 Surrogate model-based optimization

A **surrogate model** is an engineering method used when an outcome of interest cannot be easily directly measured, so a model of the outcome is used instead. Most engineering design problems require experiments and/or simulations to evaluate design objective and constraint functions as function of design variables. For example, in order to find the optimal airfoil shape for an aircraft wing, an engineer simulates the air flow around the wing for different shape variables (length, curvature, material, ..). For many real-world problems, however, a single simulation can take many minutes, hours, or even days to complete. As a result, routine tasks such as design optimization, design space exploration, sensitivity analysis and what-if analysis become impossible since they require thousands or even millions of simulation evaluations. To alleviate this burden on can use approximated models, known as **surrogate models, response surface models, meta-models or emulators**, that mimic the behavior of the system as closely as possible

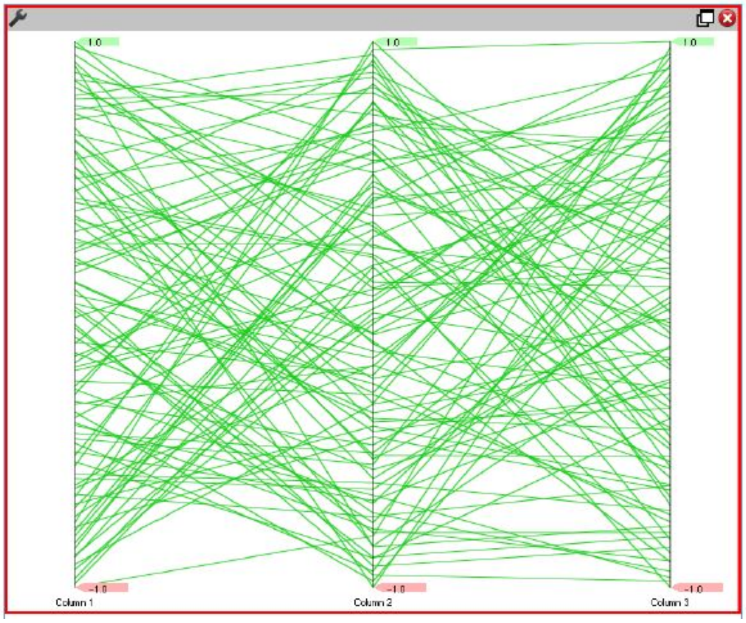


Figure 36.7: A Latin hypercube sampling: The parallel coordinates visualization shows the uniform distribution of points along each factor.

while being computationally cheaper to evaluate. Surrogate models are constructed by using a data-driven, bottom-up approach. The exact, inner working of the simulation code is not assumed to be known (or even understood), solely the input-output behavior is available (the system is considered as a **black box**). A surrogate model is constructed based on measuring the response of the simulator to a limited number of intelligently chosen data points obtained by a careful design of experiments. The surrogate model can be called "approximation model" "DACE model" (DACE stays for design and analysis of computer experiments), or "response surface approximation", leading to the term of **Response Surface Methodology (RSM)** in the optimization o fsystems. The main goal of response surface methodology is to create a predictive model of the relationship between the inputs and the outputs and then using the model to determine optimal operating settings for the system.

The surrogate models need to be determined ("trained") by considering a set of example pairs (X_e, Y_e), giving input and the corresponding output for a set of example values, used to fix the model parameters.

Let's consider a single input and output parameter: if the models of the relationship between input and output is given by a polynomial function with M parameters $a_0, a_1, \dots, a_{(M-1)}$ then $Y(X) = a_0 + a_1 X + ... + a_{(M-1)} X^{(M-1)}$. The model parameters can be fixed by requiring that some measure of the average difference, on the examples, between the Y values of the polynomial and the corresponding Y_e values of the examples, is minimized. This amounts to asking that the model approximately reproduces the desired input-output relationships on the examples. A widely used and statistically motivated way can be to find the values of the parameters $a_0, a_1, \dots, a_{(M-1)}$ which minimizes the average quadratic error on the examples as described in Section 5.1-5.2 (*least-squares fit* and *maximum-likelihood* estimation).

An alternative when the functional form is not known is to consider non-parametric models in machine learning.

Because the model is approximated, in Response Surface Methodology (RSM) for optimization, care must be taken to ensure that the optimal point determined by using the response surface indeed corresponds to the optimal point of the real system. In practice, this requires an iterative process, where a first model is built and used to determine a first candidate optimal X value, and then a second more localized model is built in the neighborhood of this first candidate optimizer for additional checking and refinement.

An example of a model (in this particular case Bayesian Locally-Weighted Regression (Section 9.2.1) applied to

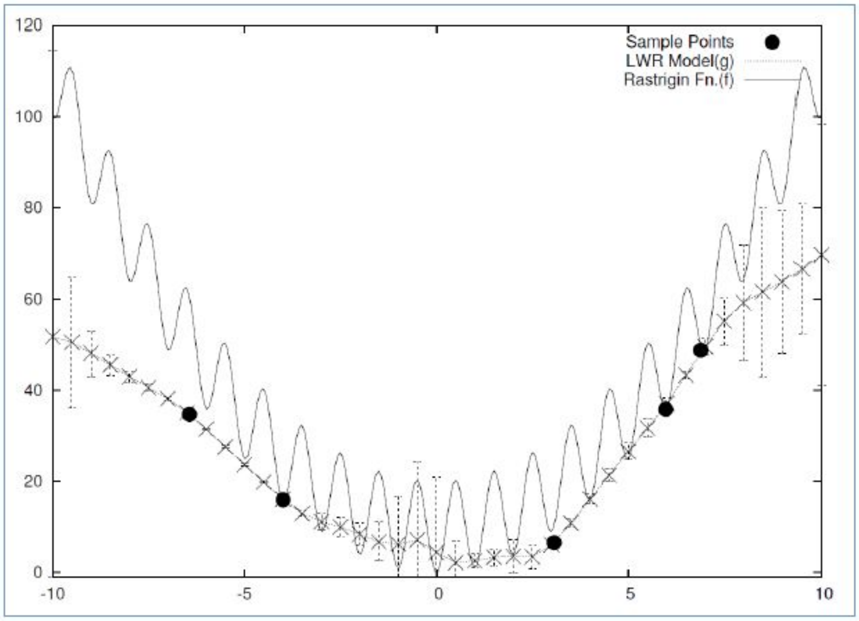


Figure 36.8: A response surface obtained by fitting the generated experimental points (black circles). The oscillating curve shows the original Rastrigin benchmark function. The surrogate model (crosses) in this case filters out the rapid oscillations and extracts the large-scale behavior of the system.

the Rastrigin benchmark function) is shown in Fig. 36.8. The sample points are used to build the model which in this case "irons out" the small oscillations and is therefore very useful to identify the area of x values corresponding to the optimal configurations.

36.3 Active or query learning

Acquiring training examples for supervised learning tasks is typically an expensive and time-consuming process. **Active learning** approaches attempt to reduce this cost by actively suggesting inputs for which supervision should be collected, in an iterative process **alternating learning and feedback elicitation**. At each iteration, active learning methods select the inputs maximizing an informativeness measure, which estimates how much an input would improve the current model if it was added to the current training set. The **informativeness of the query** inputs can be defined in different ways, and several active learning techniques exist [330].

The **uncertainty sampling (US)** principle [330] considers the input with highest predictive uncertainty as the most informative training example for the current model. This requires a learning model that can quantify its predictive uncertainty. The ability of **Gaussian Process Regression GPR** in estimating the confidence for individual predictions enables a suitable application of the uncertainty sampling principle. A Gaussian process is a statistical distribution X_t, $t \in T$, for which any finite linear combination of samples has a joint Gaussian distribution. This property permits the analytic calculation of relevant quantities, like the uncertainty in the prediction. A large variance σ^2 of the predictive distribution for a single test input $\mathbf{x}$ means that the test sample is not represented by the Gaussian Process (GP) model learned from the training data. The predictive variance quantifies the predictive uncertainty of the GP model. Therefore the input maximizing the predictive variance is selected by the uncertainty sampling principle. With GPR, the predictive uncertainty grows in regions away from training inputs. Active learning strategies more sophisticated than the US principle exist, but they usually demand more expensive computation.

The **query-by-committee strategy** maintains a committee of models, trained on the current set of examples and representing competing hypotheses. Each committee member votes on the output value of the candidate inputs, and the input considered most informative is the one on which they disagree most.

The **expected model change** principle considers as the most informative query the input that, when added to the training set would yield the greatest change in the current model (i.e., that has the greatest influence on the model parameters).

The **expected error reduction** criterion selects the input that is expected to yield the greatest reduction in the generalization error of the current model. Computing the expected generalization error is, however, computationally expensive, and, in general, it cannot be expressed analytically.

To overcome this limitation, the **variance reduction** approach queries the input that minimizes the model variance. The generalization error can in fact be decomposed into three components, refereed to as the noise, the bias, and the model variance. The noise component defines the variance of the output distribution given the input and is independent of the model and the training set. The bias error is introduced by the model class (e.g., a linear model class adopted to approximate a nonlinear function). The model variance estimates how much the model predictions vary when changing the training set. Because the model parameters can influence neither the noise nor the bias, the only way to reduce the future generalization error consists of minimizing the model variance. An effective application of the variance reduction approach is possible only under the assumption that the bias error is negligible.

An application of active learning principles in the area of multi-objective optimization, for the active learning of Pareto fronts, is presented in [74].

Gist

Contrary to some popular stories, the **experimental activity combines abundant creativity with a strategic focus on a goal to be reached**. If the focus is to model a system, often to identify improving configurations via automated optimization, sample input points need to be chosen carefully, depending on the goal and without wasting computational or real resources.

Samples generated by DOE can be used as *starting points* for explorations by optimization techniques based on local search.

Picking the appropriate design of experiments is not trivial and has consider carefully the type of model and the problem. If the form of the model is known and the model is parametric (e.g., the model is a polynomial of degree three), the experimental points can be generated to reduce the uncertainty in the estimated parameters, usually at the boundary of the admissible region. If the form is not known, like in the "non-parametric" modeling characterizing machine learning, a **randomized design** can be the most robust choice.

Chapter 37

Measuring problem difficulty in local search

A pessimist sees the difficulty in every opportunity; an optimist sees the opportunity in every difficulty.
(Winston Churchill)

37.1 Measuring and modeling problem difficulty

When using machine learning strategies in the area of heuristics, finding appropriate features to measure and appropriate metrics is a precious guide for the design of effective methods and for explaining and understanding.

Some challenging questions for the design of heuristics are:

- How can one predict *the future evolution of an optimization algorithm*? E.g., the running time to completion, the probability of finding a solution within given time bounds, etc.

- What is is *the most effective heuristic* for a given problem, or for a specific instance?
- What are the *intrinsically more difficult problems or instances* for a given search technique?

In this chapter we mention some interesting research issues related to measuring problem difficulty, measuring individual algorithm components, and selecting them through a diversification and bias metric.

Let us consider the issue of *understanding* why a problem is more difficult to solve for a stochastic local search method. One aims at discovering relationships between problem characteristics and problem difficulty. Because the focus is on local search methods, one would like to characterize statistical properties of the solution *landscape* causing poor or slow results by local search.

The effectiveness of a stochastic local search method is determined by how *microscopic local decisions* made at each search step interact to determine the *macroscopic global behavior* of the system. In particular, one studies how the function value f depends on the input configuration and changes after small and local modifications. **Statistical mechanics** has been very successful in the past at relating local and global behaviors of systems [184], for example starting from the molecule-molecule interaction to derive macroscopic quantities like pressure and temperature. Statistical mechanics builds upon statistics, by identifying appropriate statistical *ensembles* (configurations with their probabilities of occurrence) and deriving typical global behaviors of the ensemble members. When the number of system components is very large, the variance in the behavior is very small: most members of the ensemble will behave in a similar way. As an example in Physics, if one has two communicating containers of one liter and a gas with five flying molecules, the probability to find all molecules in one container is not negligible. On the other hand, if the containers are filled with air at normal pressure, the probability to observe more than 51% of the molecules in one container is very close to zero : even if the individual motion is very complex, the macroscopic behavior will produce a 50% subdivision with a very small and hardly measurable random deviation.

Unfortunately, the situation for combinatorial search problems is much more complicated than the situations for physics-related problems, so that the precision of theoretical results is more limited. Nonetheless, a growing body of literature exists, which sheds light onto different aspects of combinatorial problems and permits *a level of understanding and explanation which goes beyond the simple empirical models* derived from massive experimentation.

37.2 Phase transitions in combinatorial problems

Models inspired by statistical mechanics have been proposed for some well known combinatorial problems. An extensive review of models applied to constraint satisfaction problems, in particular the graph coloring problem, is present in [184]. The SAT problem, in particular the 3-SAT, has been the playground for many investigations [94, 104, 292, 334].

Phase-transitions have been identified as a mechanism to study and explain problem difficulty. A phase transition in a physical system is characterized by the abrupt change of its macroscopic properties at certain values of the defining parameters. For example, consider the transitions from ice to water to steam at specific values of temperature and pressure. Phenomena analogous to phase transitions have been studied for random graphs [125, 60]: as a function of the average node degree, some macroscopic property like connectivity change in a very rapid manner. The work in [198] predicts that large-scale artificial intelligence systems and cognitive models will undergo sudden phase transitions from disjointed parts into coherent structures as their topological connectivity increases beyond a critical value. Citing from the paper: "this phenomenon, analogous to phase transitions in nature, provides a new paradigm with which to analyze the behavior of large-scale computation and determine its generic features."

Phase transitions in Constraint Satisfaction and SAT problems have been widely analyzed [82, 272, 326, 235, 337, 292]. A clear introduction to phase transitions and the search problem is present in [185]. A surprising result is that hard problem instances are concentrated near the same parameter values for a wide variety of common search heuristics. This location also corresponds to a **transition between solvable and unsolvable instances**. For example, when the control parameter that is changed is the number of clauses in SAT instances, different schemes like complete backtracking and local search show very long computing times in the same transition region.

For backtracking, this is due to a competition between two factors: number of solutions and facility of pruning many subtrees. A small number of clauses (*under-constrained* problem) implies many solutions, it is easy to find one of them. At the other extreme, a large number of clauses (*over-constrained* problem) implies that any tentative solution is quickly ruled out (pruned from the tree). It is fast to rule out all possibilities and conclude that there is no solution. The *critically constrained* instances in between are the hardest ones.

The local search method is not complete and one must limit the experimentation to solvable instances. One may naïvely expect that the search becomes harder with a smaller *number of solutions* but the situation is not so simple. At the limit, if only one solution is available but the attraction basin is very large, local search will easily find it. Not only the number of solutions but also the number and depth of *sub-optimal local minima* play a role. A large number of deep local minima is causing a waste of search time in a similar way to tentative solutions in backtracking, which fail only after descending very deeply in the search tree. Among a growing body of experimental research, [94] presents results on CSP and SAT, [104] results on the crossover point in random 3-SAT.

In addition to being of high scientific interest, identifying zones where the most difficult problems are is relevant for **generating difficult instances to challenge algorithms**. As strange as it may sound at the beginning, it is not so easy to identify difficult instances of NP-hard problems [326]. Computational complexity classes are defined through a *worst-case* analysis: in practice the worst cases may be very difficult to encounter or to generate.

37.3 Empirical models of fitness surfaces

More empirical *descriptive cost models* of problem difficulty aim at identifying measurable *instance characteristics (features) influencing the search cost*. A good descriptive model should account for a significant portion of the variance in search cost [94, 292, 334, 377].

The performance of search algorithms depends on the features of the search space. In particular, a useful measure of variability of the search landscape is given by the correlation between the values of the objective function f over all pairs of configurations at distance d. The proper distance to be used depends on the nature of the solving technique. In local search the distance between two configurations X and X' can be measured measured as the minimum number of local steps to transform one into the other. After choosing the distance function, one defines the **Landscape Correlation Function** [378]:

$$R(d) = \frac{\mathrm{E}_{\mathrm{dist}(X,X')=d}[(f(X)-\mu)(f(X')-\mu)]}{\sigma^2}, \tag{37.1}$$

where $\mu = \mathrm{E}[X]$ and $\sigma^2 = \mathrm{Var}[X]$. This measure captures the idea of *ruggedness* of a surface: a low correlation function implies high statistical independence between points at distance d. While it is expectable that for large values of d the correlation $R(d)$ goes to zero (unless the search landscape is very smooth), the value of $R(1)$ can be meaningful.

Intuitively, $R(1)$ tells us whether a local move from the current configuration changes the f value in a manner which is significantly different from a random restart. $R(1) \approx 0$ means that, on average, there is little correlation between the objective value at a given configuration and the value of its neighbors. This can signal of a poor choice of the neighborhood structure, or that the problem is particularly hard for local search. On the other hand, $R(1) \approx 1$ is a clear indication that the neighborhood structure produces a *smooth* fitness surface.

Computing equation (37.1) for large search spaces can be difficult. A common estimation technique uses random walks. In particular, Big-Valley models [59] (a.k.a. *massif central* models) have been considered to explain the success of local search, and the preference for continuing from a given local optimum instead of restarting from scratch. These models measure the **autocorrelation of the time-series of f values produced by a random walk**. The autocorrelation function (ACF) of a random process describes the correlation between the process at different points in time. Let $X^{(t)}$ be the search configuration at time t. If $f(X^{(t)})$ has mean μ and variance σ^2 then the ACF can be defined as

$$R'(d) = \frac{E_t[(f(X^{(t)})-\mu)(f(X^{(t+d)})-\mu)]}{\sigma^2}. \tag{37.2}$$

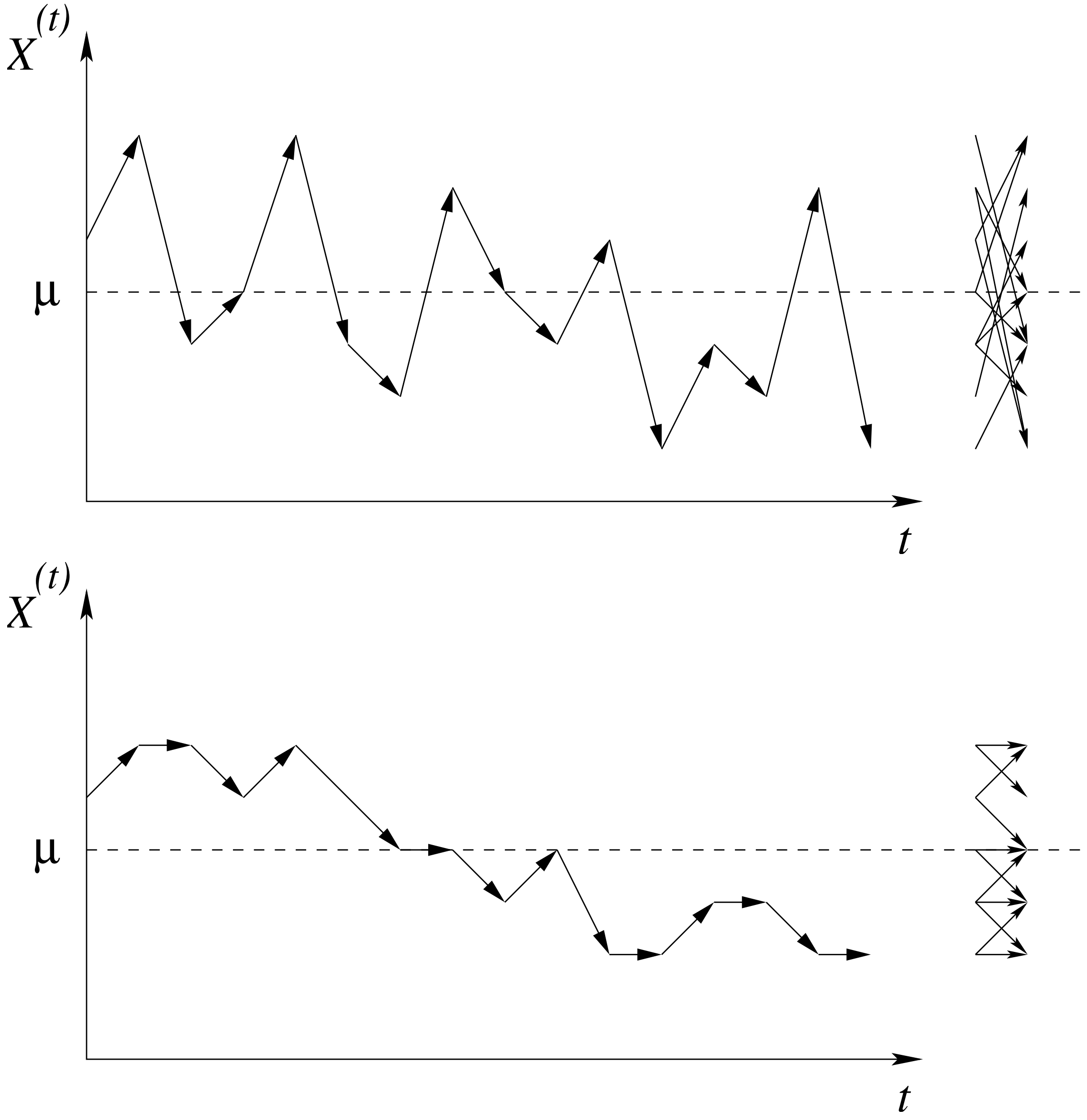


Figure 37.1: Estimating autocorrelation on a rugged (top) and a smooth (bottom) landscape by means of a random walk. Vectors between fitness values at subsequent steps are shown on the right; in particular, $R'(1)$ is determined as the correlation between the endpoints of these arrows with respect to the mean value (dashed line).

Fig. 37.1 provides a pictorial view of autocorrelation estimation by means of a random walk. In particular, the right side of each plot shows how subsequent moves are correlated: every arrow shows one step, so that correlation is computed between the head and the tail of each arrow with respect to the mean value (dashed line). It is apparent that the bottom walk represents a smoother landscape, and this translates to correlated arrow endpoints.

As noted above, it is expected that both $R(d)$ and $R'(d)$ become smaller and smaller as long as d increases: points separated by a small path are more correlated than separated ones. Empirical measurements show that $R'(d)$ often follows an exponential decay law:

$$R'(d) \approx e^{-\frac{d}{\lambda}}. \tag{37.3}$$

The value of λ that best approximates the $R'(\cdot)$ sequence is called the **correlation length**, and it measures the range over which fluctuations of f in one region of space are correlated. An approximation of λ can be obtained by solving (37.3) when $d = 1$:

$$\lambda \approx -\frac{1}{\ln R'(1)}.$$

Clearly, we are assuming that correlation between nearby configurations is positive: otherwise, no significant approximation can be obtained and the whole correlation analysis loses its meaning.

Equation (37.3) defines the correlation length as the distance where autocorrelation decreases by a factor of e, so that the definition is somewhat arbitrary. Moreover, for many problems the correlation length is a function of the problem's size and it does not explain the variance in computational cost among instances of the same size [377]. However, it is possible to normalize it with respect to some measure of the problem's instance (e.g., number of dimensions, size of the neighborhood) in order to make it a useful tool for comparisons.

An example of fitness landscape analysis for the Quadratic Assignment Problem is presented in [267], where autocorrelation analysis and fitness-distance correlation analysis [223] are adopted for choosing suitable evolutionary operators.

A **fitness distance correlation** (FDC) c an be calculated by measuring the Hamming distances between sets of bit-strings and the global optimum, and comparing with their fitness. Of course, the technique can be generalized to deal with different distance measures. An instructive counterexample is presented in [9].

37.4 Tunable landscapes

The *NK landscape model* [230], proposed in the field of computational biology, provides a parametric and tunable landscape for the generation of problem instances. *NK* landscapes capture the intuition that every coordinate in the search space contributes to the overall fitness in a complex way, often by enabling or disabling the contribution of other variables in a process that is known in biology as *epistasis*.

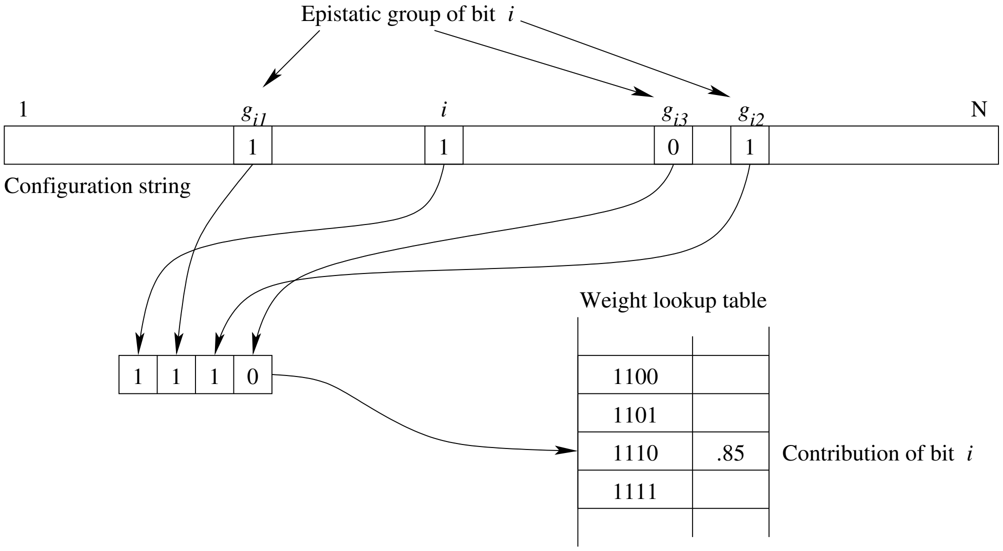


Figure 37.2: Epistatic contribution of bit i in an NK model for $K = 3$.

An NK system is defined by N binary components (e.g., bits in the configuration string) and by the number K of other components that interact with each component. In other words, each bit identifies a $(K+1)$-bit interaction group. A uniform random-distributed mapping from $\{0,1\}^{K+1}$ to $[0,1]$ determines the contribution of each interaction group to the total fitness, which is computed as the average of all contributions.

In mathematical terms, let the configuration space be the N-bit strings $\{0,1\}^N$. The current configuration is $S = s_1 \dots s_N$, $s_i \in \{0,1\}$. For every position $i = 1, \dots, N$, let us define its interaction group as a set of $K+1$ different indices $G_i = (g_{i0}, g_{i1}, \dots, g_{iK})$ so that $g_{i0} = i$, $g_ij \in \{1, \dots, N\}$ and if $l \neq m$ then $g_{il} \neq g_{im}$. Let $w : \{0,1\}^{K+1} \to [0,1]$, defined by random uniform distribution, represent the contribution of each interaction group. Then

$$f(S) = \frac{1}{N} \sum_{i=1}^{N} w(s_{g_{i0}} s_{g_{i1}} \dots s_{g_{iK}}).$$

Fig. 37.2 shows how every bit contributes to the fitness value by means of its epistatic interaction group as defined before. For small values of K the contribution function w can be encoded as a (2^{K+1})-entry lookup table.

The parameter K controls the so-called "ruggedness" of the landscape: $K = 0$ means that no bitwise interaction is present, so that every bit independently contributes to the overall fitness, leading to an embarrassingly simple optimization task. On the other hand, if $K = N-1$, then changing a single bit modifies all contributions to the overall fitness value: the ruggedness of the surface is maximized.

NK systems have been used as problem generators in the study of various combinatorial optimization algorithms [224, 175, 338].

37.5 Measuring local search components: diversification and bias

To ensure progress in algorithmic research it is not sufficient to have a horse-race of different algorithms on a set of instances and declare winners and losers. Actually, very little information can be obtained by these kinds of comparisons. In fact, if the number of instances for the benchmark is limited and if sufficient time is given to an intelligent researcher (...and very motivated to get publication!) be sure that some promising results will be eventually obtained, via a careful tuning of algorithm parameters.

A better method is to design a *generator of random instances* so that it can produce instances used during the development and tuning phase, while a different set of instances extracted from the same generator is used for the final test. This method mitigates the effect of "intelligent tuning done by the researcher on a finite set of instances," but still it does not explain *why* a method is better than another one. Explaining *why* is related to the **generality and prediction power** of the model. If one can predict the performance of a technique on a problem (or on a single instance) – of course before the run is finished, predicting the past is always easy! – then he takes some steps towards understanding.

This exercise takes different forms depending on what one is predicting, what are the starting data, what is the computational effort spent on the prediction, etc. The work in [33] dedicated to solving the MAX-SAT problem with non-oblivious local search aims at **relating the final performance to measures obtained after short runs of a method**. In particular, the average f value (*bias*) and the average speed in Hamming distance from a starting configuration (*diversification*) is monitored and related to the final algorithm performance.

Let us focus onto local-search based heuristics: it is well known that the basic compromise to be reached is that between **diversification and bias**. Given the obvious fact that only a negligible fraction of the admissible points can be visited for a non-trivial task, the search trajectory $X^{(t)}$ should be generated to visit preferentially points with large f values (*bias*) and to avoid the confinement of the search in a limited and localized portion of the search space (*diversification*). The two requirements are conflicting: as an extreme example, random search is optimal for diversification but not for bias. Diversification can be associated with different metrics. Here we adopt the *Hamming distance* as a measure of the distance between points along the search trajectory. The Hamming distance $H(X,Y)$ between two binary strings X and Y is given by the number of bits that are different.

The investigation follows this scheme:

- After selecting the metric (diversification is measured with the Hamming distance and bias with mean f values visited), the diversification of simple *random walk* is analyzed to provide a basic system against which more complex components are evaluated.
- The **diversification-bias plots (D-B plots)** of different basic components are investigated and a conjecture is formulated that the best components for a given problem are the *maximal elements* in the diversification-bias (D-B) plane for a suitable partial ordering (Section 37.5.1).
- The conjecture is validated by a competitive analysis of the components on a benchmark.

Let us now consider the **diversification properties of Random Walk**. Random Walk generates a Markov chain by selecting at each iteration a random move, with uniform probability:

$$X^{(t+1)} = \mu_{r(t)} X^{(t)} \ \text{ where } \ r(t) = \text{Rand}\{1, \ldots, n\}$$

Without loss of generality, let us assume that the search starts from the zero string: $X^{(0)} = (0, 0, ..., 0)$. In this case the Hamming distance at iteration t is:

$$H(X^{(t)}, X^{(0)}) = \sum_{i=1}^{n} x_i^{(t)}$$

and therefore the expected value of the Hamming distance at time t, defined as $\widehat{H}^{(t)} = \widehat{H}(X^{(t)}, X^{(0)})$, is:

$$\widehat{H}^{(t)} = \sum_{i=1}^{n} \widehat{x_i}^{(t)} = n\, \widehat{x}^{(t)} \tag{37.4}$$

The equation for $\widehat{x}^{(t)}$, the probability that a bit is equal to 1 at iteration t, is derived by considering the two possible events that i) the bit remains equal to 1 and ii) the bit is set to 1. In detail, after defining as $p = 1/n$ the probability that a given bit is changed at iteration t, one obtains:

$$\widehat{x}^{(t+1)} = \widehat{x}^{(t)}\ (1-p)\ +\ (1-\widehat{x}^{(t)})\, p = \widehat{x}^{(t)}\ +\ p\,(1 - 2\widehat{x}^{(t)}) \tag{37.5}$$

It is straightforward to derive the following theorem:

Theorem 4 *If $n > 2$ (and therefore $0 < p < \frac{1}{2}$) the difference equation (37.5) for the evolution of the probability $\widehat{x}^{(t)}$ that a bit is equal to one at iteration t, with initial value $\widehat{x}^{(0)} = 0$, is solved for t integer, $t \geq 0$ by:*

$$\widehat{x}^{(t)} \ = \ \frac{1 - (1-2p)^t}{2} \tag{37.6}$$

The qualitative behavior of the average Hamming distance can be derived from the above. At the beginning $\widehat{H}^{(t)}$ has a linear growth in time:

$$\widehat{H}^{(t)} \approx t \tag{37.7}$$

For large t the expected Hamming distance $\widehat{H}^{(t)}$ tends to its asymptotic value of $n/2$ in an exponential way, with a “time constant” $\tau = n/2$

Let us now compare the evolution of the mean Hamming distance for different algorithms. The analysis is started as soon as the first local optimum is encountered by LS, when diversification becomes crucial. LS$^+$ has the same evolution as LS with the only difference that it *always* moves to the best neighbor, even if the neighbor has a worse solution value f. LS$^+$, and Fixed-TS with fractional prohibition T_f equal to 0.1, denoted as TS(0.1), are then run for 10 n additional iterations. Fig. 37.3 shows the average Hamming distance as a function of the additional iterations after reaching the LS optimum, see [33] for experimental details.

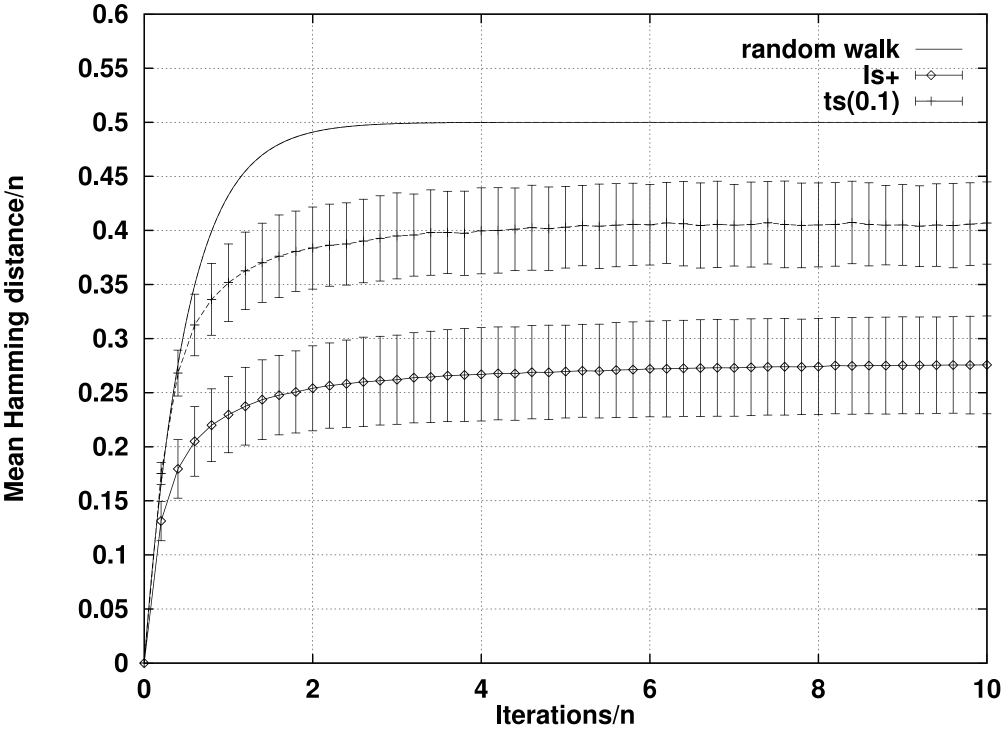


Figure 37.3: Average Hamming distance reached by Random Walk, LS^+ and TS(0.1) from the first local optimum of LS, with standard deviation (MAX-3-SAT). Random walk evolution is also reported for reference.

Although the initial linear growth is similar to that of Random Walk, the Hamming distance does not reach the asymptotic value $n/2$ and a remarkable difference is present for the two algorithms. The fact that the asymptotic value is not reached even for large iteration numbers implies that all visited strings tend to lie in a confined region of the search space, with bounded Hamming distance from the starting point.

Let's note that, for large n values, most binary strings are at distance of approximately $n/2$ from a given string. In detail, the Hamming distances are distributed with a binomial distribution with the same probability of success and failure ($p = q = 1/2$): the fraction of strings at distance H is equal to

$$\binom{n}{H} \times \frac{1}{2^n} \tag{37.8}$$

It is well known that the mean is $n/2$ and the standard deviation is $\sigma = \sqrt{n}/2$. The above coefficients increase up to the mean $n/2$ and then decrease. Because the ratio σ/n tends to zero for n tending to infinity, for large n values most strings are clustered in a narrow peak at Hamming distance $H = n/2$. As an example, one can use the Chernoff bound [168]:

$$Pr[H \leq (1-\theta)pn] \leq e^{-\theta^2 np/2} \tag{37.9}$$

the probability to find a point at a distance less than $np = n/2$ decreases in the above exponential way ($\theta \geq 0$). The distribution of Hamming distances for $n = 500$ is shown in Fig. 37.4.

Clearly, if better local optima are located in a cluster that is not reached by the trajectory, they will never be found. In other words, a robust algorithm demands that some stronger diversification action is executed. For example, an option is to activate a restart after a number of iterations that is a small multiple of the time constant $n/2$.

When a local search component is started, new configurations are obtained at each iteration until the first local optimum is encountered, because the number of satisfied clauses increases by at least one. During this phase additional

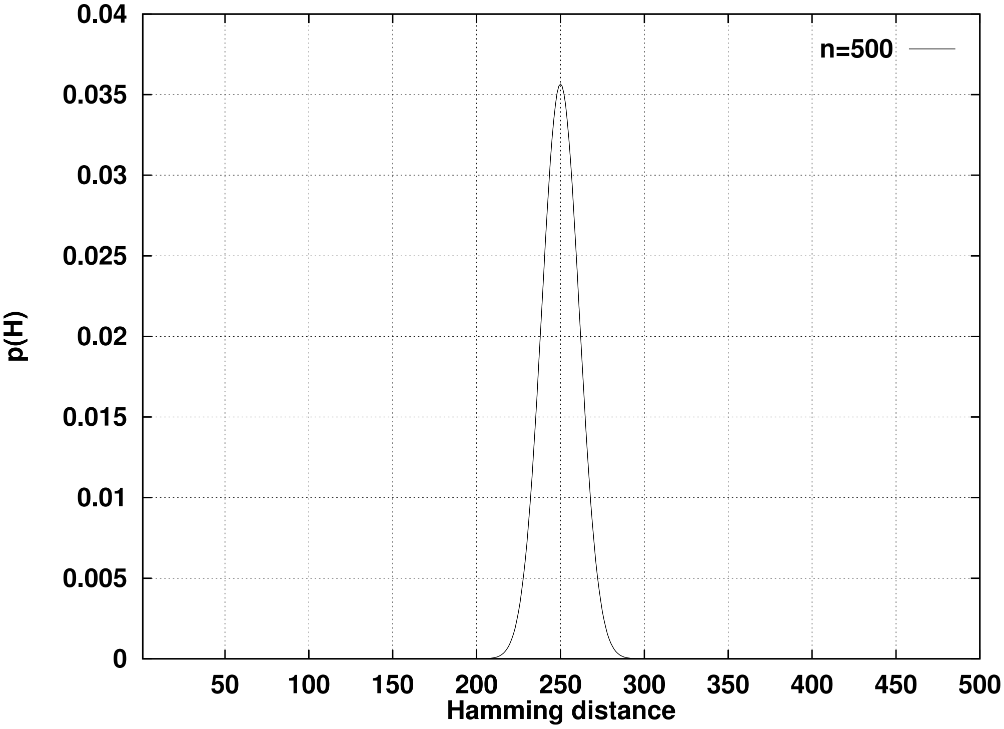


Figure 37.4: Probability of different Hamming distances for n = 500.

diversification schemes are not necessary and potentially dangerous, because they could lead the trajectory astray, away from the local optimum.

The compromise between bias and diversification becomes critical after the first local optimum is encountered. In fact, if the local optimum is strict, the application of a move will worsen the f value, and an additional move could be selected to bring the trajectory back to the starting local optimum.

The mean bias and diversification depend on the value of the internal parameters of the different components. All runs proceed as follows: as soon as the first local optimum is encountered by LS, it is stored and the selected component is then run for additional $4n$ iterations. The final Hamming distance H from the stored local optimum and the final value of the number of unsatisfied clauses u are collected. The values are then averaged over different tasks and different random number seeds.

Different diversification-bias (D-B) plots are shown in Fig. 40.3. Each point gives the D-B coordinates $(\widehat{H_n}, \widehat{u})$, i.e., average Hamming distance divided by n and average number of unsatisfied clauses, for a specific parameter setting in the different algorithms. The Hamming distance is normalized with respect to the problem dimension n, i.e., $\widehat{H_n} \equiv \widehat{H}/n$. Three basic algorithms are considered: GSAT-with-walk, Fixed-TS, and HSAT. For each of these, two options about the guiding functions are studied: one adopts the "standard" oblivious function, the other the non-oblivious f_{NOB} introduced in Section 35.5.2. Finally, for GSAT-with-walk one can change the probability parameter p, while for Fixed-TS one can change the fractional prohibition T_f: parametric curves as a function of a single parameter are therefore obtained.

GSAT, Fixed-TS(0.0), and GSAT-with-walk(0.0) coincide: no prohibitions are present in TS and no stochastic choice is present in GSAT-with-walk. The point is marked with "0.0" in Fig. 40.3. By considering the parametric curve for GSAT-with-walk(p) (label "gsat" in Fig. 40.3) one observes a gradual increase of $\widehat{u}$ for increasing p, while the mean Hamming distance reached at first decreases and then increases. The initial decrease is unexpected because it contradicts the intuitive argument that more stochasticity implies more diversification. The reason for the above result

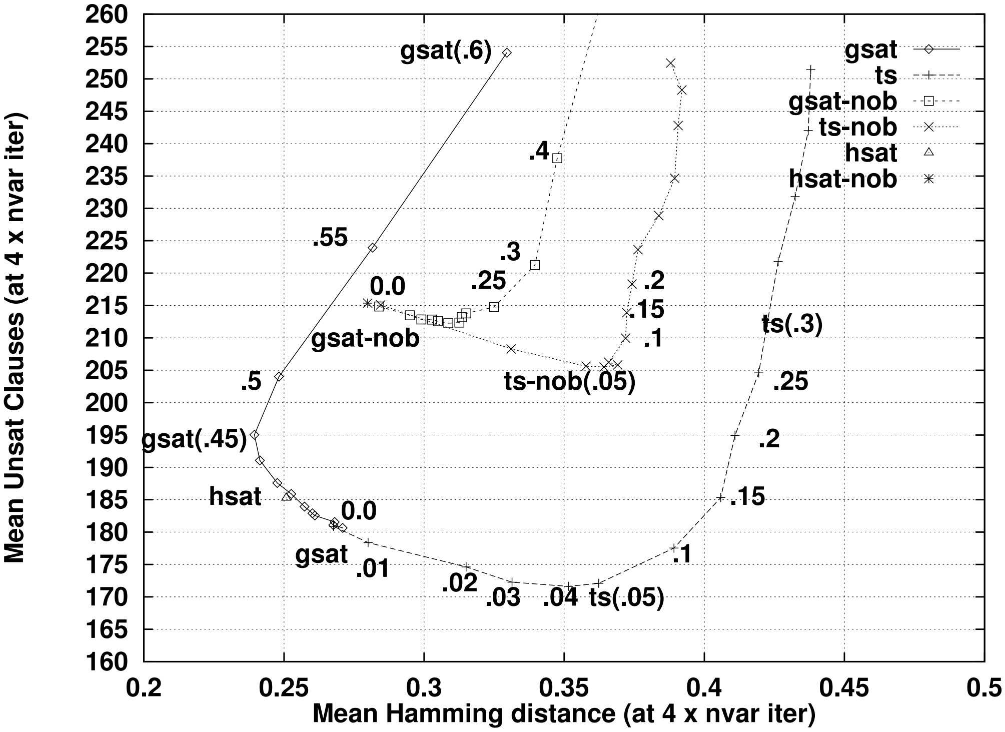


Figure 37.5: Diversification-bias plane. Mean number of unsatisfied clauses after $4\ n$ iterations versus mean Hamming distance. MAX-3-SAT tasks. Each run starts from GSAT local optimum, see [33].

is that there are two sources of “randomness” in the GSAT-with-walk algorithm (see Fig. 35.16), one deriving from the random choice among variables in unsatisfied clauses, active with probability p, the other one deriving from the random breaking of ties if more variables achieve the largest Δf.

Because the first randomness source increases with p, the decrease in $\widehat{H_n}$ could be explained if the second source decreases. This conjecture has been tested and confirmed [33]. The larger amount of stochasticity implied by a larger p keeps the trajectory on a rough terrain at higher values of f, where flat portions tend to be rare. *Vice versa*, almost no tie is present when the non-oblivious function is used. The algorithm on the optimal frontier of Fig. 40.3 is Fixed-TS(T_f), and the effect of a simple **aspiration criterion** [148], and a **tie-breaking rule** for it is studied in [33].

The advantage of the D-B plot analysis is clear: it suggests possible causes for the behavior of different algorithms, leading to a more focused investigation.

37.5.1 A conjecture: better algorithms are Pareto-optimal in D-B plots

A conjecture about the relevance of the diversification-bias metric is proposed in [33]. A relation of partial order, denoted by the symbol $\geq$ and called “domination,” is introduced in a set of algorithms in the following way: given two component algorithms A and B, *A dominates B* ($A \geq B$) if and only if it has a larger or equal diversification and bias: $\widehat{f}_A \geq \widehat{f}_B$ and $\widehat{H_n}_A \geq \widehat{H_n}_B$.

By definition, component A is a *maximal element* of the given relation if the other components in the set *do not* possess both a higher diversification, and a better bias. In the graph one plots the number of *un*satisfied clauses versus the Hamming distance, therefore the *maximal* components are in the lower–right corner of the set of $(\widehat{H_n}, \widehat{u})$ points. The points are characterized by the fact that no other point has both a larger diversification and a smaller number of satisfied clauses.

Conjecture
If local-search based components are used in heuristic algorithms for optimization, the components producing the best f values during a run, on the average, are the maximal elements *in the diversification-bias plane for the given partial order.*

The conjecture produces some "falsifiable" predictions that can be tested experimentally. In particular, a partial ordering of the different components is introduced: component A is better than component B if $\widehat{H}_{nA} \geq \widehat{H}_{nB}$ *and* $\widehat{u}_A \leq \widehat{u}_B$. The ordering is partial because no conclusions can be reached if, for example, A has better diversification but worse bias when compared with B.

Clearly, when one applies a technique for optimization, one wants to maximize the best value found during the run. This value is affected by both the *bias* and the *diversification*. The search trajectory must visit preferentially points with large f values but, as soon as one of this point is visited, the search must proceed to visit new regions. The above conjecture is tested experimentally in [33], with fully satisfactory results. We do not expect this conjecture to be always valid but it is a useful guide when designing and understanding component algorithms.

A definition of three metrics is used in [318] [342] for studying algorithms for SAT and CSP. The first two metrics *depth* (average unsatisfied clauses) and *mobility* (Hamming distance speed) correspond closely to the above used *bias* and *diversification*. The third measure (*coverage*) takes a more global view at the search progress. In fact, one may have a large mobility but nonetheless remain confined in a small portion of the search space. A two-dimensional analogy is that of bird flying at high speed along a circular trajectory: if fresh corn is not on the trajectory it will never discover it. Coverage is intended to measure *how systematically* the search explores the entire space. In other words, coverage is what one needs to ensure that eventually the optimal solution will be identified, no matter how it is camouflaged in the search landscape. The motivation for a *speed of coverage* measure is intuitively clear, but the detailed definition and implementation is somewhat challenging. In [318] a worst-case scenario is considered and *coverage* is defined as the size of the *largest unexplored gap in the search space*. For a binary string, this is given by the maximum Hamming distance between any unexplored assignment and the nearest explored assignment.

Unfortunately, measuring the speed of coverage it is not so fast, actually it can be NP-hard for problems with binary strings, and one has to resort to approximations [318]. For an example, one can consider sample points given by the negation of the visited points along the trajectory and determine the maximum minimum distance between these points and points along the search trajectory. The rationale for this heuristic choice is that the negation of a string is the farthest point from a *given* string (one tries to be on the safe side to estimate the real coverage). After this estimate is available one divides by the number of search steps. Alternatively, one could consider how fast coverage decreases during the search (a discrete approximation of the coverage speed). Dual measures on the constraints are studied in [342].

Gist

A motivated researcher may use junk heuristics and get positive results after carefully tuning their meta-parameters on single benchmark instances. Science and technology will not advance with this kind of brutal horse-racing but they require predictive and explanatory models.

In a manner similar to machine learning, to get usable flexible algorithms, tuning should be done in an automated manner on some “training instances”, and performance should be tested on novel instances characterized by similar statistical properties.

Measures of problem difficulty are a first step in this scientific process. **Phase-transitions** can explain why some instances are very easy and other instances almost impossible to solve.

Empirical models of fitness surfaces can explain if local search will be effective and can help in selecting the proper local moves.

Tunable landscapes and problem generators are useful probes to validate different choices in algorithm design.

Diversification-bias plots (D-B plots) can measure the effectiveness of single building blocks and deliver insight on their balance of exploration versus exploitation.

For comparable results, the simplest algorithms (with less meta-parameters) should always be chosen because they are more robust and simpler to study and understand. Complexity in optimization heuristics should grow in stages, after careful motivations of each addition and demonstrations of the gained performance benefits. Less is more, also in heuristics.

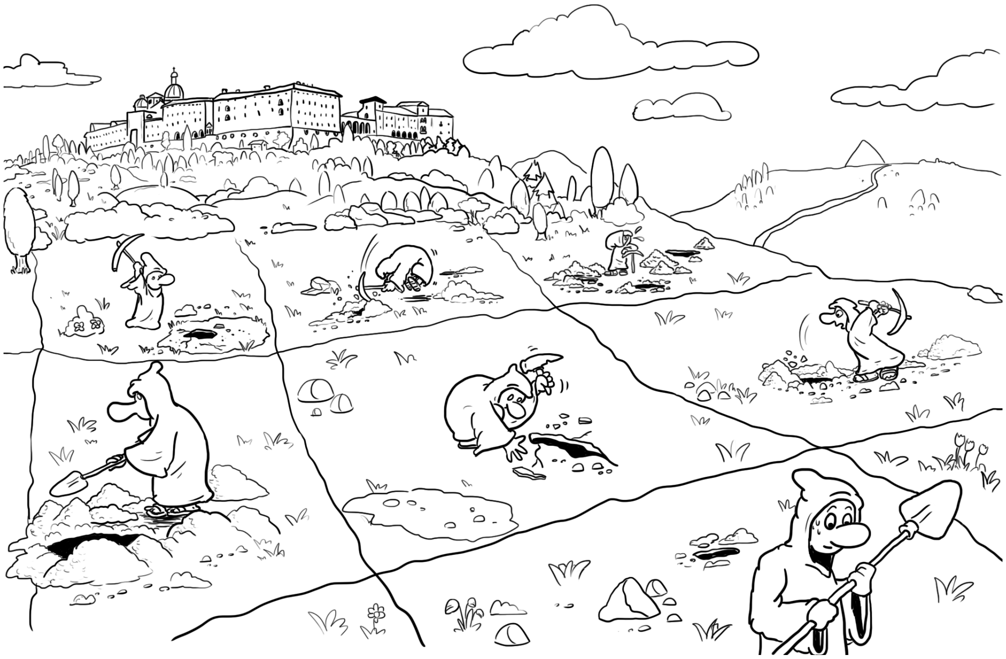
Part VI

Cooperation and multiple objectives in optimization

Chapter 38

Cooperative Learning And Intelligent Optimization (C-LION)

Whenever any important business has to be done in the monastery,
let the Abbot call together the whole community and state the matter to be acted upon.
Then, having heard the advice of the monks, let him turn the matter over in his own mind
and do what he shall judge to be most expedient.
The reason why we said that all should be consulted is that the Lord often reveals to the younger what is best.
(The Rule of Saint Benedict, 530-550, Montecassino)



As we have seen in the previous chapters, for each problem there are often **many possible algorithms** for solving it. Their effectiveness depends on the characteristics of the specific instances. Even if the performance of a single algorithm is dominating, when the algorithm has **meta-parameters or stochastic components**, there are opportunities to improve performance or to reduce the risk of suboptimal results by considering **different runs**. The objective of

C-LION is to **increase the level of automation** by designing an additional intelligent coordination layer after starting from individual algorithmic building blocks.

When considering local search (LS), we have seen that **learning from the previous phase of the stochastic search** by modifying the probabilities of generating new sample points can lead to more efficient schemes w.r.t. simple Pure Random Search, like Markov Chain Montecarlo, a.k.a. Simulated Annealing. The local minima traps can be cured by Reactive Search Optimization (RSO). Up to now the discussion was mostly dedicated to single solution schemes. One can now generalize: instead of information from a single running algorithm, one can **use information from many solution processes** running in parallel, with *complex interaction and coordination*. In particular, one can keep a sample (population) of points (current good solutions) and modify it with a generation probability that depends on all points in the population. **Population-based algorithms** do exactly this: they transform one group of points (current **generation**) to a new group of points (next generation) by probabilistic rules. Some more robustness and diversification can be obtained. The population can be seen as the concrete representation of **a probability distribution on the input space, which is dynamically changing** to reflect the accumulated knowledge and the interesting regions for future sampling.

Cooperative Learning and Intelligent Optimization (C-LION) denotes a framework for solving problems by a strategic use of memory and *cooperation* among a team of self-adaptive solution processes. Widely popular genetics and evolution-based analogies will be covered in Chapter 39. This chapter consider mostly analogies based on the organization of human society. Our species is particularly remarkable in this capability to coordinate individual human problem solvers. Our culture and civilization have a lot to do with cooperation and coordination of intelligent human beings. Coming closer to our daily work, the history of science shows a steady advancement caused by the creative interplay of many individuals, both during their lifetimes and through the continuation of work by the future generations. We are all dwarfs standing on the shoulders of giants (*nanos gigantium humeris insidentes*, Bernard of Chartres).

C-LION is a paradigm and not a single technique, so that different names have been used for specific techniques [41], but for the sake of brevity the following discussion reflects on some long-term goals of this effort, with a more focussed example for the coordination of Local Search streams. In this context, the three pillars of *C-LION* are: multiple local searchers in charge of districts (portions of input space), mutual coordination, and continuous "reactive" learning and adaptation.

C-LION adopts a **sociological/political paradigm**. Each local searcher takes care of a *district* (an input area), generates samples and decides when to fire local search in coordination with the other members. The **organized subdivision of the configuration space** is adapted in an online manner to the characteristics of the problem instance. **Coordination by use of globally collected information** is crucial to identify promising areas in configuration space and allocate search effort. Analogies are to be used only to guide intuition, the final algorithm does not have to use the terminology of the field of the analogy [341].

38.1 Intelligent and reactive solver teams

The appetite for more effective and efficient basic solvers can be satisfied by adopting more complex higher-level techniques, built on top of basic mechanisms and embodying elements of meta-optimization and self-tuning. **Meta-optimization** is the process of optimizing parameters which define a flexible optimization algorithm (e.g., the prohibition parameter in RSO based on prohibitions in Section 27.2).

When one considers the relevant issues in designing solver teams, one encounters striking analogies with sociological and behavioral theories related to human teams, with a similar presence of apparently contradictory conclusions. Let us mention some of the basic issues from a qualitative and analogical point of view, deferring more specific algorithmic implementations in the next sections.

We tend to prefer the term **solver teams** to underline that an individual solver can be an arbitrarily intelligent agent capable of collecting information, developing models, exchanging the relevant part of the obtained information with his fellow searchers, and responding in a strategic manner to the information collected. Teamwork is the concept of people working together cooperatively, as in a sports team.

Why does it make sense to consider the team members separately from the team? After all, one could design a complex entity where the boundary between the individual team members and the coordination strategy is fuzzy, a kind of Star Trek *borg hive* depicted as an amalgam of cybernetically enhanced humanoid drones of multiple species, organized as an inter-connected collective with a hive mind and assimilating the biological and technological distinctiveness of other species to their own, in pursuit of perfection.

The answer lies in the simpler design of more advanced and effective search strategies and in the better possibility to *explain* the success of a particular team by separating its members' capabilities from the coordination strategy (*divide et impera*). Let's note that alternative points of view exist and are perfectly at home in the scientific arena: for example, one may be interested in explaining how and why a collection of very simple entities manages to solve problems not solvable by the individuals. For example how simple ants manage to transport enormous weights by joining forces. In all cases, *solver team* existence cannot motivated by its sexiness or by its correspondence to poetic biological analogies [341], but only by a demonstrated superiority w.r.t. the state of the art of the individual solvers.

Individual quality of the team members. A basic issue is the relationship between the quality of the members and the collective quality of the team. If the team members are poor performers one should not expect an exceptional team. Nonetheless, it is of scientific and cultural interest to assess the potential for problem solving through the interaction of a multitude of simple members. An inspiring book [353] deals with the *wisdom of crowds*: "why the many are smarter than the few and how collective wisdom shapes business, economies, societies, and nations." Of course, acid comments go back ages, like in Nietzsche's citation "I do not believe in the collective wisdom of individual ignorance." Adapting a conclusion from the review [306], "in matters for which true expertise can be identified, one would much rather rely on the best judgments of the most knowledgeable specialists than a crowd of laymen. But in matters for which no expertise or training is genuinely involved, in dealing with fields of study whose principles are ambiguous, contentious, and rarely testable, ...then yes, there is sense to polling a group of people." In optimization, one expects a much bigger effectiveness by starting from the most competitive single-thread techniques, but some dangers lurk depending on how the team is integrated and information is shared and used.

Diversity of the team members. If all solvers act in same manner the advantage of a team is lost (see lower panes of Fig. 39.3). Diversity can be obtained in many possible ways, for example by using different solvers, or identical solvers but with different random initializations. In some cases, the effects of an initial randomization is propagated throughout a search process that shows a sensitive dependence on initial conditions that is characteristic for chaotic processes [360].

Diversity means that, in some cases, combining simpler and inferior performers with more effective ones can increase the overall performance and/or improve robustness. By the way, diversity is also crucial for ensembles of learning machines [364, 29].

Information sharing and cooperation. When designing a *solver team* one must decide about the way in which information collected by the various solvers is shared and used to modify the individual member decisions. An extreme design principle consists of **complete independence and periodic reporting** of the best solution to a coordinator. Simplicity and robustness make this extreme solution the first to try. More complex interaction schemes should always be compared against this baseline, see for example [30] where independent parallel walks of tabu search are considered.

More complex sharing schemes involve periodic collection of the best-so-far (record) values and configurations, the current configurations, more complex summaries of the entire search history of the individual solvers, for example the list of local minima encountered.

After the information is shared, a decision process modifies the individual future search in a strategic manner. Here complexities and open research issues arise. Let's consider a simple case: if a solver is informed by a team member about a new best value obtained for a configuration which is far from the current search region, is it better for it to move to the new and promising area or to keep visiting the current region? See also Fig. 39.3.

An example of the dangerous effects of interaction in the social arena is called *groupthink* [213], a mode of thinking that people engage in when they are deeply involved in a cohesive group, when the members' strivings for unanimity override their motivation to realistically appraise alternative courses of action. *Design by committee* is a second term referring to the poor results obtained by a group, particularly in the presence of poor and incompetent leadership. A camel is a horse designed by a committee.

An example of a pragmatic use of memory in cooperation is [295], where experiments highlight that "memory is useful but its use from the very beginning of the search is not recommended."

Centralized versus distributed management schemes This issue is in part related to computing hardware and communication networks, in part related to the software abstraction adopted for programming. The centralized schemes, often related to some form of synchronous communication, see a central coordinator acting in a **master-slave** relationship w.r.t. the individual solvers. The team members are given instructions (for example initialization points, parameters, detailed strategies) by the coordinator and periodically report about search progress and other parameters. The opposite design point consists of distributed computation by peers, which periodically and often asynchronously exchange information and autonomously decide about their future steps. **Gossiping optimization** schemes fall in this category. The design alternatives are related to efficiency but also to simplicity of programming and understanding. For example, a synchronous parallel machine may be handled more efficiently through a central coordination, while a collection of computers distributed in the world, connected by internet and prone to disconnections, may find a more natural coordination scheme by *gossiping*. Reviews of parallel strategies for local search and meta-heuristics are presented in [368] (see for example the *multiple walks* parallelism), in [160] ("controlled pool maintenance") and [103].

Reactive versus non-reactive schemes Last but not least comes the issue of learning on the job and self-tuning of algorithm parameters. In addition to the adaptation of individual parameters based on individual search history, which is by now familiar to the reader, new possibilities for a reactive adaptation arise by considering the search history of other team members and the overall coordination scheme. As examples, adaptation in evolutionary computation is surveyed in [178, 124]. Adaptation can act on the representation of the individuals, the evaluation function, the variation, selection and replacement operators and their probabilities, the population (size, topology, etc.). In their taxonomy, parameter tuning coincides with our "off-line tuning," while parameter control coincides with "on-line tuning," adaptive parameter control has a reactive flavor, while self-adaptive parameter control means that one want to use the same golden hammer (GA) for all nails, including meta-optimization (the parameters are encoded into chromosomes). Strategic design embodying intelligence more than randomization is also advocated in the *scatter search and path relinking approach* [151, 154]. Scatter search is a general framework to maintain a reference set of solutions, determined by their function values but also by their level of diversity, and to build new ones by "linearly interpolating and extrapolating" between subsets of these solutions. Of course, interpolation must be interpreted to work in a discrete setting (the uniform cross-over in GA is a form of interpolation) and adapted to the problem structure. *Path relinking* generalizes the concept: instead of creating a new solution from a set of two parents, an entire path between them is created by starting from one extreme and progressively modifying the solution to reduce the distance from the other point. The approach is strongly pragmatic, alternatives are tried and judged in a manner depending on the final results and not on the adherence to biological and evolutionary principles.

38.2 Portfolios and restarts

Let us consider *Las Vegas* algorithms, which always terminate with a correct solution and have a stochastic distribution of the runtime, the time required to terminate. We are interested both in the expected value of the runtime and in its standard deviation. The standard deviation is related to the **risk**; in some cases having a larger average CPU time with a small deviation is preferable to having a smaller average but with some instances requiring enormous times. There are two simple ways to combine the execution of different algorithms or of different versions of the same algorithm (with different random seeds) to obtain different expected runtimes and standard deviations: one is based on **restarting** an algorithm if it does not terminate within a given time limit, the other one is based on combining more runs in a time-sharing interleaving manner: the **portfolio** approach.

Algorithm portfolios, first proposed in [199], follow the standard practice in economics to obtain different return-risk profiles in the stock market by combining stocks characterized by individual return-risk values. Risk is related to the standard deviation of return. An algorithm portfolio runs more algorithms concurrently on a sequential computer, in a time-sharing manner, by allocating a fraction of the total CPU cycles to each of them. The first algorithm to finish determines the termination time of the portfolio, while the other algorithms are stopped immediately after one reports the solution, see Fig. 38.1.

It is intuitive that the CPU time can be radically reduced in this manner. To clarify ideas consider an extreme example where, depending on the initial random seed, the runtime can be of 1 second or of 1000 seconds, with the same probability. If one runs a single process, the expected runtime is approximately of 500 seconds. If one runs more copies, the probability that at least one of them is lucky (i.e., that it terminates in 1 second) increases very rapidly towards one. Even if termination is now longer than 1 second because more copies share the same CPU, it is intuitive that the expected time will be much shorter than 500.

A portfolio can consist of different algorithms but also of different runs of the same algorithm, with different random seeds. In the case of more runs of the same algorithm, there is a different way to have more runs share a given CPU, by terminating a run prematurely and *restarting* the algorithm.

In the above example, a run can be stopped if it does not terminate within 1 second. Because the probability to have a sequence of unlucky cases rapidly goes to zero, again the expected runtime of the restart strategy will be much less than 500 seconds.

As an example in web surfing, the response time to deliver a page can vary a lot. The customary behavior of clicking again on the same link after patience is finished can save the user from an "endless" waiting time.

38.3 Predicting the performance of a portfolio from its component algorithms

To make the above intuitive arguments precise let $T_{\mathcal{A}}$ be the random variable describing the time of arrival of process $\mathcal{A}$ when the whole CPU time is allocated to it. Let $p_{\mathcal{A}}(t)$ be its probability distribution. The *survival function* $S_{\mathcal{A}}(t)$ is the probability that process $\mathcal{A}$ takes longer that t to complete:

$$S_{\mathcal{A}}(t) = \Pr(T_{\mathcal{A}} > t) = \int_{\tau > t} p_{\mathcal{A}}(\tau)\,\mathrm{d}\tau = 1 - F_{\mathcal{A}}(t)$$

where $F_{\mathcal{A}}(t)$ is the corresponding cumulative distribution function. If only a fraction α of the total CPU time is dedicated to it in a time-sharing fashion, with arbitrarily small time quanta and no process swapping overhead, we can model the new system as a process $\mathcal{A}'$ whose time of completion is described by random variable $T_{\mathcal{A}'} = \alpha^{-1} T_{\mathcal{A}}$. Its probability distribution and cumulative distribution function are respectively:

$$p_{\mathcal{A}'}(t) = p_{\mathcal{A}}(\alpha t), \qquad F_{\mathcal{A}'}(t) = F_{\mathcal{A}}(\alpha t), \qquad S_{\mathcal{A}'}(t) = S_{\mathcal{A}}(\alpha t).$$

Consider a portfolio of two algorithms $\mathcal{A}_1$ and $\mathcal{A}_2$. To simplify the notation, let T_1 and T_2 be the random variables associated with their termination times (each being executed on the whole CPU), with survival functions S_1 and S_2. Let α_1 be the fraction of CPU time allocated to process running algorithm $\mathcal{A}_1$. Then the fraction dedicated to $\mathcal{A}_2$ is $\alpha_2 = 1 - \alpha_1$. The completion time of the two-process portfolio system is therefore described by the random variable

$$T = \min\{\alpha_1^{-1} T_1, \alpha_2^{-1} T_2\}. \tag{38.1}$$

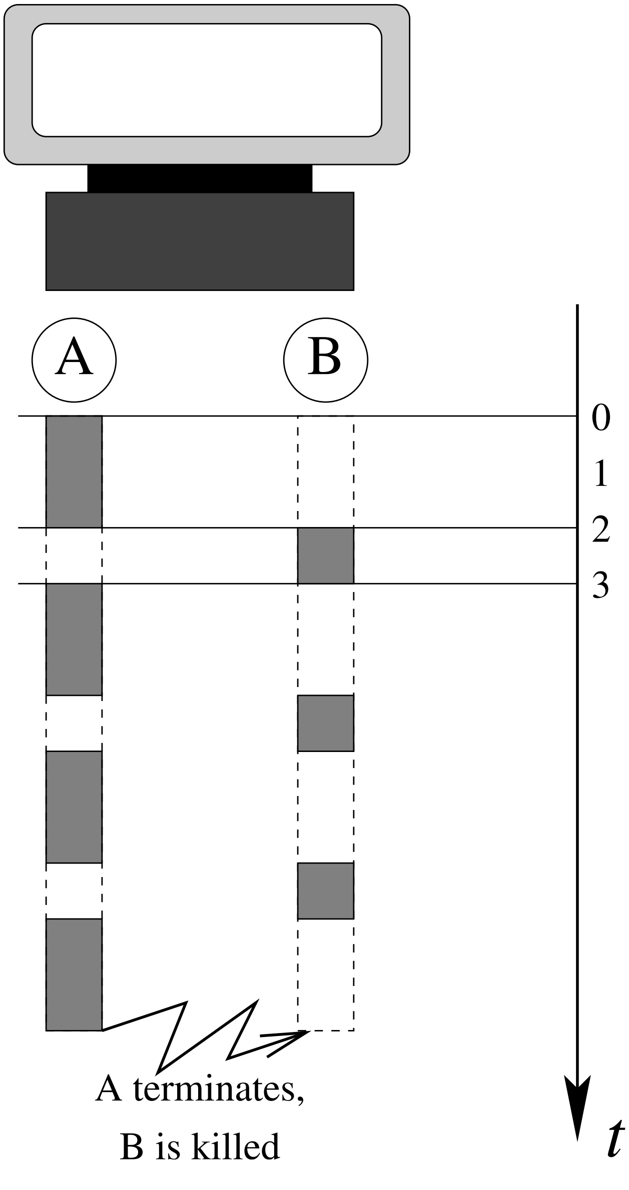


Figure 38.1: A sequential portfolio strategy.

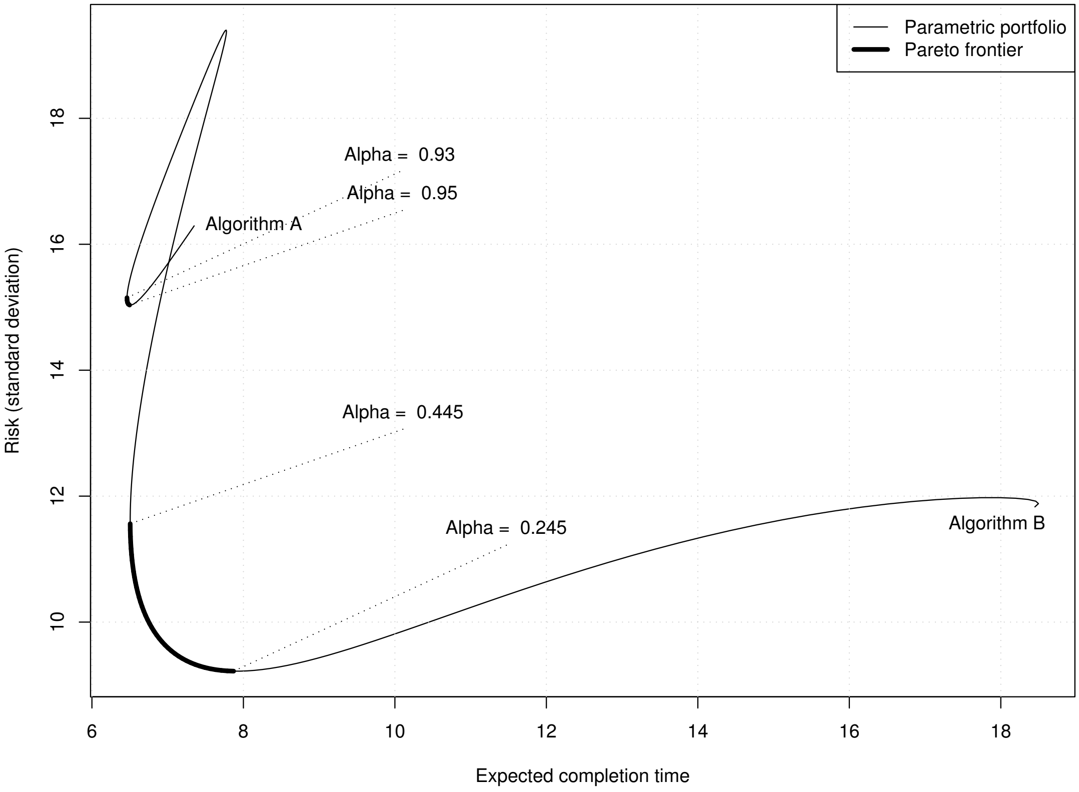


Figure 38.2: Expected runtime versus standard deviation (risk) plot. The efficient frontier contains the set of non-dominated configurations (a.k.a. Pareto-optimal or extremal points).

The survival function of the portfolio is

$$\begin{aligned}
S(t) &= \Pr(T > t) = \Pr(\min\{\alpha_1^{-1}T_1, \alpha_2^{-1}T_2\} > t) \\
&= \Pr(\alpha_1^{-1}T_1 > t \wedge \alpha_2^{-1}T_2 > t) = \Pr(\alpha_1^{-1}T_1 > t)\Pr(\alpha_2^{-1}T_2 > t) \\
&= \Pr(T_1 > \alpha_1 t)\Pr(T_2 > \alpha_2 t) \\
&= S_1(\alpha_1 t)S_2(\alpha_2 t).
\end{aligned}$$

The probability distribution of T can be obtained by differentiation:

$$p(t) = -\frac{\partial S(t)}{\partial t}.$$

Finally, the expected termination value $\mathrm{E}(T)$ and the standard deviation $\sqrt{\mathrm{Var}(T)}$ can be calculated.

By turning the α_1 knob, therefore, a series of possible combinations of expected completion time $\mathrm{E}(T)$ and risk $\sqrt{\mathrm{Var}(T)}$ becomes available. Fig. 38.2 illustrates an interesting case where two algorithms $\mathcal{A}$ and $\mathcal{B}$ are given. Algorithm $\mathcal{A}$ has a fairly low average completion time, but it suffers from a large standard deviation, because the distribution

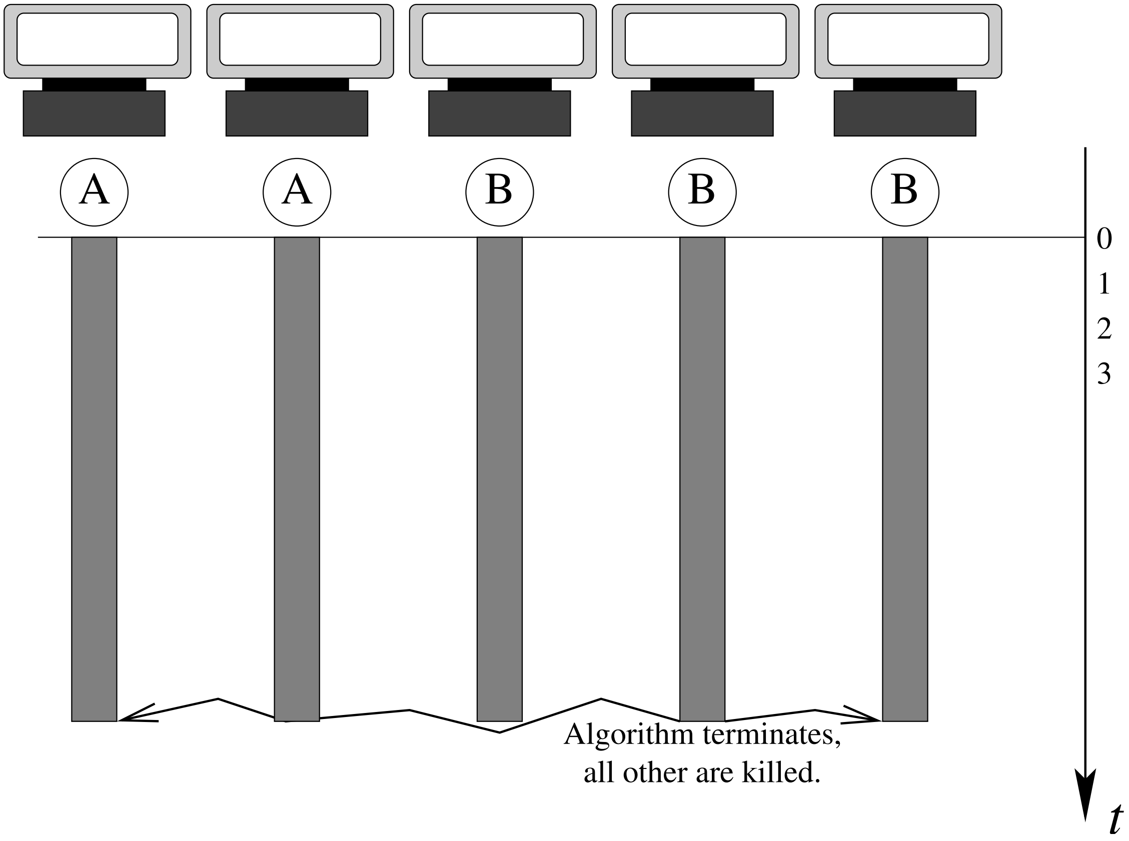


Figure 38.3: A portfolio strategy on a parallel machine.

is bimodal or heavy-tailed, while algorithm $\mathcal{B}$ has a higher expected runtime, but with the advantage of a lower risk of having a longer computation. By combining them as described above, we obtain a parametric distribution whose expected value and standard deviation are plotted against each other for α_1 going from 0 (only $\mathcal{B}$ executed) to 1 (pure $\mathcal{A}$). Some of the obtained distributions are *dominated* (there are parameter values that yield distributions with lower mean time *and* lower risk) and can be eliminated from consideration in favor of better alternatives, while the choice among the non-dominated possibilities (on the *efficient frontier* shown in black dots in the figure) has to be specified depending on the user preferences between lower expected time or lower risk. The choice along the Pareto frontier is similar when investing in the stock market: while some choices can be immediately discarded, there are no free meals and a higher return comes with a higher risk.

38.3.1 Parallel processing

Let us consider a different context [159] and assume that N equal processors and two algorithms are available so that one has to decide how many copies n_i to run of the different algorithms, as illustrated in Fig. 38.3. Of course no processor should remain idle, therefore $n_1 + n_2 = N$.

Consider time as a discrete variable (clock ticks or fractions of second), let T_i be the discrete random variable associated with the termination time of algorithm i having probability $p_i(t)$, the probability that process i halts precisely at time t. As in the previous case, we can define the corresponding cumulative probability and survival functions:

$$F_i(t) = \Pr(T \le t) = \sum_{\tau=0}^{t} p_i(\tau), \qquad S_i(t) = \Pr(T > t) = \sum_{\tau=t+1}^{\infty} p_i(\tau).$$

To calculate the probability $p(t)$ that the portfolio terminates exactly at time $T = t$, we must sum probabilities for different events: the event that one processor terminates at t while the other ones take more than t, the event that two processors terminate at t while the other ones take more than t, and so on. The different runs are independent and therefore probabilities are multiplied. If $n_1 = N$ (all processors are assigned to the same algorithm), this leads to:

$$p(t) = \sum_{i=1}^{N} \binom{N}{i} p_1(t)^i S_1(t)^{N-i} \tag{38.2}$$

The portfolio survival function $S(t)$ is easier to compute on the basis of the survival function of the single process $S_1(t)$:

$$S(t) = S_1(t)^N \tag{38.3}$$

When two algorithms are considered, the probability computation has to be modified to consider the different ways to distribute i successes at time t among the two sets of copies such that $i_1 + i_2 = i$ (i_1 and i_2 being non-negative integers).

$$p(t) = \sum_{\substack{0 \le i_1 \le n_1 \\ 0 \le i_2 \le n_2 \\ i_1 + i_2 \ge 1}} \binom{n_1}{i_1} p_1(t)^{i_1} S_1(t)^{n_1 - i_1} \binom{n_2}{i_2} p_2(t)^{i_2} S_2(t)^{n_2 - i_2}. \tag{38.4}$$

Similar although more complicated formulas hold for more algorithms. As before, the complete knowledge about $p(t)$ can then be used to calculate the mean and variance of the runtimes. **Portfolios can be effective to cure the heavy-tailed behavior** of $p_i(t)$ in many complete search methods, where very long runs occur more frequently than one may expect, in some cases leading to infinite mean or infinite variance [158]. Heavy-tailed distributions are characterized by a power-law decay, also called tails of Pareto-Lévy form, namely:

$$P(X > x) \approx C x^{-\alpha}$$

where $0 < \alpha < 2$ and C is a constant.

Experiments with the portfolio approach [199, 159] show that, in some cases, a slight **mixing of strategies** can be beneficial provided that one component has a relatively high probability of finding a solution fairly quickly. Portfolios are also particularly effective when negatively correlated strategies are combined: one algorithm tends to be good on the cases which are more difficult for the other one, and *vice versa*. In branch-and-bound applications [159] one finds that ensembles of risky strategies can outperform the more conservative best-bound strategies. In a suitable portfolio, a depth-first strategy which often quickly reaches a solution can be preferable to a breadth first strategy with lower expected time but longer time to obtain a first solution.

Portfolios can also be applied to component routines inside a single algorithm, for example to determine an acceptable move in a local-search based strategy.

38.4 Reactive portfolios

The assumption in the above analysis is that the statistical properties of the individual algorithms are known beforehand, so that the expected time and risk of the portfolio can be calculated, the efficient frontier determined and the final choice executed depending on the risk-aversion nature of the user. The strategy is therefore *off-line*: a preliminary exhaustive study of the components precedes the portfolio definition.

Variable	Scope	Meaning
$\mathcal{A}_i$	(input)	i-th algorithm ($i = 1, \dots, n$)
b_k	(input)	k-th problem instance ($k = 1, \dots, m$)
f_P	(input)	Function deciding time slice according to expected completion time
f_τ	(input)	Function estimating the expected completion time based on history
τ_i	(local)	Expected remaining time to completion of current run of algorithm $\mathcal{A}_i$
α_i	(local)	Fraction of CPU time dedicated to algorithm $\mathcal{A}_i$
history	(local)	Collection of data about execution and status of each process

```
function AOTA($\mathcal{A}_1, \dots, \mathcal{A}_n, b_1, \dots, b_m, f_P, f_\tau$)
repeat $\forall b_k$
    initialize $(\tau_1, \dots, \tau_n)$
    while ($b_k$ not solved)
        update $(\alpha_1, \dots, \alpha_n) \leftarrow f_P(\tau_1, \dots, \tau_n)$
        repeat $\forall \mathcal{A}_i$
            run $\mathcal{A}_i$ for a slot of CPU time $\alpha_i \Delta t$
            update history of $\mathcal{A}_i$
            update estimated termination $\tau_i \leftarrow f_\tau$(history)
    update model $f_\tau$ considering also the complete history of the last solved instance
```

Figure 38.4: The inter-problem AOTA framework.

If the distributions $p_i(t)$ are unknown, or if they are only partially known, one has to resort to **reactive portfolios, where the strategy is dynamically changed in an online manner** when more information is obtained about the task(s) being solved and the algorithm status. For example, one may derive a maximum-likelihood estimate of $p_i(t)$, use it to define the first values α_i of the CPU time allocations, and then refine the estimate of $p_i(t)$ when more information is received and use it to define subsequent allocations. A preliminary suggestion of dynamic online strategies is present in [199].

Dynamic strategies for search control mechanisms in a portfolio of algorithms are considered in [91, 92]. In this framework, statistical models of the quality of solutions generated by each algorithm are computed online and used as a control strategy for the algorithm portfolio, to determine how many cycles to allocate to each of the interleaved search strategies.

A "life-long learning" approach for dynamic algorithm portfolios is considered in [140]. The general approach of "dropping the artificial boundary between training and usage, exploiting the mapping *during* training, and including training time in performance evaluation," also termed Adaptive Online Time Allocation [139], is fully reactive. In the inter-problem AOTA framework, see Fig. 38.4, a set of algorithms $\mathcal{A}_i$ is given, together with a sequence of problem instances b_k, and the goal is to minimize the runtime of the whole set of instances. The model used to predict the runtime $p_i(t)$ of algorithm $\mathcal{A}_i$ is updated after each new instance b_k is solved. The portion of CPU time α_i is allocated to each algorithm $\mathcal{A}_i$ in the portfolio through a heuristic function which is decreasing for longer estimated runtimes τ_i.

An Extreme Reactive Portfolio (XRP) is proposed in [71]. It is based on simple performance indicators: record value and iterations elapsed from the last record. The two indicators are used for a combined ranking and a stochastic replacement of the worst-performing members with a new searcher with random parameters or a perturbed version of a well-performing member.

38.5 Defining an optimal restart time

Restarting an algorithm at time τ is beneficial if its expected time to convergence is less than the expected additional time to converge, given that it is still running at time τ [366]:

$$E[T] < E[T - \tau | T > \tau]. \tag{38.5}$$

Whether restart is beneficial or not depends of on the distribution of runtimes. As a trivial example, if the distribution is exponential, restarting the algorithm does not modify the expected runtime.

If the distribution is heavy-tailed, restart easily cures the problem. For example, heavy tails can be encountered if a stochastic local search algorithm like simulated annealing is trapped in the neighborhood of a local minimizer. Although eventually the probability of visiting the optimal solution will be one, an enormous number of iterations can be spent in the attraction basin around the local minimizer before escaping. Restart is a direct method to escape deep local minima!

If the algorithm is always restarted at time τ, each run corresponds to a Bernoulli trial which succeeds with probability $P_\tau = \Pr(T \leq \tau)$ — remember that T is the random variable associated with termination time of an unbounded run of the algorithm. The number of runs executed by the restart strategy before success follows a geometric distribution with parameter P_τ, in fact the probability of a success at repetition k is $(1 - P_\tau)^{k-1} P_\tau$. The distribution of the termination time T_τ of the restart strategy with restart time τ can be derived by observing that at iteration t one has had $\lfloor t/\tau \rfloor$ restarts and $(t \bmod \tau)$ remaining iterations. Therefore, the survival function of the restart strategy is

$$S_\tau(t) = \Pr(T_\tau > t) = (1 - P_\tau)^{\lfloor t/\tau \rfloor} \Pr(T > t \bmod \tau). \tag{38.6}$$

The tail decays now in an exponential manner: the restart portfolio is *not* heavy-tailed.

In general, a restart strategy consists of executing a sequence of runs of a randomized algorithm, to solve a given instance, stopping each run k after a time $\tau(k)$ if no solution is found, and restarting an independent run of the same algorithm, with a different random seed. The optimal restart strategy is uniform, i.e., one in which a constant $\tau_k = \tau$ is used to bound each run [255]. In this case, the expected value of the total runtime T_τ , i.e., the sum of runtimes of the successful run, and all previous unsuccessful runs is equal to:

$$E(T_\tau) = \frac{\tau - \displaystyle\int_0^\tau F(t)\, \mathrm{d}t}{F(\tau)} \tag{38.7}$$

where $F(\tau)$ is the cumulative distribution function of the runtime T for an unbounded run of the algorithm, i.e., the probability that the problem is solved before time τ. The demonstration is simple. For a given cutoff τ, each run succeeds with probability $F(\tau)$ (Bernoulli trials) and the mean number of trials before a successful run is encountered is $1/F(\tau)$. The expected length of each run is:

$$\int_0^\tau t p(t)\, \mathrm{d}t + \tau(1 - F(\tau))$$

Consider the cases when termination is within τ or later, so that the run is terminated prematurely. Because $p(t) = F'(t)$, this is equal to:

$$\int_0^\tau t F'(t)\, \mathrm{d}t.$$

The result follows from the fact that:

$$\frac{\mathrm{d}}{\mathrm{d}t}(tF(t)) = tF'(t) + F(t)$$

and therefore:

$$\int_0^\tau tF'(t)\, \mathrm{d}t + \int_0^\tau F(t)\, \mathrm{d}t = \tau F(\tau)$$

giving (38.7).

In the discrete case:

$$E(T_\tau) = \frac{\tau - \sum_{t<\tau} F(t)}{F(\tau)} \tag{38.8}$$

If the distribution is known, an optimal cutoff time can be determined by minimizing (38.7). If the distribution is not known, a universal non-uniform strategy, with cutoff sequence: $(1, 1, 2, 1, 1, 2, 4, 1, 1, 2, 4, 8, \dots)$ achieves a performance within a logarithmic factor of the expected runtime of the optimal policy, see [255] for details.

Calculating the runtime distribution can require large amounts of CPU time in case of heavy tails because one has to wait for the termination of very long runs. In this case the **censored sampling** approach can be used. Censored sampling allows to bound the duration of each experimental run and still exploit the information obtained from the runs which converge before the censoring threshold [280]. Let us model the probability density function as $g(t|\theta)$, θ being the parameter to be identified from the experiments. Without censoring one can determine g by maximizing the likelihood $\mathcal{L}$ of the obtained sequence of termination times $\mathcal{T} = (t_1, t_2, \dots, t_k)$ given θ:

$$\mathcal{L}(\mathcal{T}|\theta) = \prod_{i=1}^{k} \mathcal{L}(t_i|\theta) = \prod_{i=1}^{k} g(t_i|\theta) \tag{38.9}$$

With censoring, some experimental runs will exceed the cutoff time t_c. In these cases the corresponding multiplicative term in (38.9) is substituted with

$$\mathcal{L}_c(t_c|\theta) = \int_{t_c}^{\infty} g(\tau|\theta)\, \mathrm{d}\tau = 1 - G(t_c|\theta) \tag{38.10}$$

where $G(t|\theta)$ is the conditional cumulative distribution function corresponding to g.

One has to decide about a proper cutoff threshold t_c. A way to determine it is to ask for target u on the fraction of terminated runs (uncensored samples), run k experiments in parallel (or with interleaving) and stop as soon as the desired target is reached.

The final receipt is therefore: i) choose an appropriate parametric model for the runtime distribution, ii) determine the best parameters of the model by maximizing the likelihood, where some terms are substituted with the censored likelihood of (38.10), iii) use the estimated runtime distribution to determine the optimal restart time. Some examples of parametric models are considered in [141].

38.6 Reactive restarts

Up to now the assumption has been that the only observation which can be used is given by the *length of a run* and that the runs are *independent*. Let us now consider more advanced strategies where at least one of these assumptions is relaxed. Given the results mentioned in the previous section, it looks as if the problem is solved for the complete knowledge case and the zero knowledge case (within a multiplicative constant and logarithmic factor which can be large for practical applications). Actually, the most interesting case is between the two situations, when a partial knowledge is available which is increasing as soon as more data become available during a run or during a sequence of runs on related instances. Real-time observations about the characteristics of a specific instance and about the state of the solver *during a run* permit better results.

In [191, 231] features capturing the state of a solver during the initial phase of the run are used to **predict the length of a run**, so that the prediction can be used by dynamic restart policies. Bayesian models to predict the runtime starting from both structural evidence available at the beginning of the run, and execution evidence available during the run (in a reactive manner) are trained with supervised machine learning. To be more precise, the discrimination is between long and short runs, i.e., runs longer or shorter than the median. The dynamic policy considered in [191] is as follows:

1. observe a run for O steps (observation horizon)

2. if the run is not terminated predict whether it will converge in a total of L steps
3. if the prediction is negative, restart immediately, otherwise run up to a total of L steps before restarting.

Because the model is not perfect, an important parameter is the model accuracy A, the probability of a correct prediction. If p_i is the probability of a run ending within i steps, the probability of convergence during a single run is therefore $p_O + A(p_L - p_O)$ and the expected number of runs until a solution is found is $E(n) = 1/(p_O + A(p_L - p_O))$. An upper bound on the expected number of steps in a single run can be derived by assuming that runs ending within O steps take exactly O steps, while runs terminating between $O+1$ and $O+L$ steps take exactly L steps. The probability of continuation, taking the limited accuracy into account, is $Ap_L + (1-A)(1-p_L)$. An upper bound on the length of a single run is therefore $E_{\text{ub}}(R) = O + (L-O)(Ap_L + (1-A)(1-p_L))$, and an upper bound on the expected time to solve a problem with the above policy is $E(n)E_{\text{ub}}(R)$. The estimate can be now minimized by varying L and the observation horizon. The model is rude; for example, no observations during the steps after O are used, only a bound and not the exact expected number of steps is minimized. In spite of its roughness, significantly superior results of the dynamic policy w.r.t. the static one are demonstrated. Three different contexts are defined: in the *single instance* context one has to solve a specific instance as soon as possible, in the *multiple instance* context one draws cases from a distribution of instances and has to solve either *any instance* as soon as possible, or *as many instances as possible* for a given amount of time allocated (*max instances* problem) [191].

The assumption of independence among runs is relaxed in [310]. For example, independence is not valid if more runs are on the same instance picked at the beginning from one of several probability distributions. As an example, consider two distributions, one consisting of instances which are solved in 10 iterations, the other one of instances which are solved in 100 iterations. If an instance is not solved in 10 iterations we know that 100 iterations are needed and restarting would only waste computing cycles. Compare this with the situation of a single distribution with probability 0.5 of converging at iteration 10, probability 0.5 of converging at iteration 1000, with independence among the runs. Here restarting is clearly useful as shown in Section 38.5. The work in [310] considers the context where one among several RTDs is picked at the beginning - without informing the user - and a new sample is extracted at each run from the same distribution (e.g., consider two different distributions corresponding to satisfiable or unsatisfiable instances of SAT). The task is to find the optimal restart policy $(t_1, t_2, \dots)$ but now, after each unsuccessful run, the solver's belief about the source distribution can be updated. The problem of finding the optimal restart policy is formulated as a Markov decision process and solved with dynamic programming, considering both the case in which only the termination time is observed, and the case when other predictors of the distribution can be used, for example the evidence obtained during the run about the fact that a SAT instance is or is not satisfiable.

38.7 Racing: Exploration and exploitation of candidate algorithms

Portfolios and restarts are simple ways to combine more algorithms, or more runs of a given randomized strategy, to obtain either a lower expected convergence time, or a lower risk (variance), or both.

We have already seen that more advanced reactive strategies can be obtained by using a reactive learning loop *while* the portfolio or restart scheme runs. In this way, some of the portfolio parameters or the restart threshold can take fresh information into account.

A related strategy using a "life-long learning" loop to optimize the allocation of time among a set of alternative algorithms for solving a specific instance is termed **racing**. Running algorithms are like horses: after the competition is started one gets more and more information about the relative performance and periodically updates the bets on the winning horses, which are assigned a growing fraction of the available future computing cycles, see Fig. 38.5.

A racing strategy is characterized by two components: i) the estimate of the future potential given the current state of the search, i.e., given the history of the previous iterations and the corresponding results, ii) the allocation of the future CPU cycles to speedup the overall objective of minimizing a function.

Racing is related to a paradigmatic problem in machine leaning and intelligent heuristics known as the **k-armed bandit problem**. One is faced with a slot machine with k arms which, when pulled, yield a payoff from a fixed but unknown distribution. One wants to maximize the expected total payoff over a sequence of n trials. If the distribution

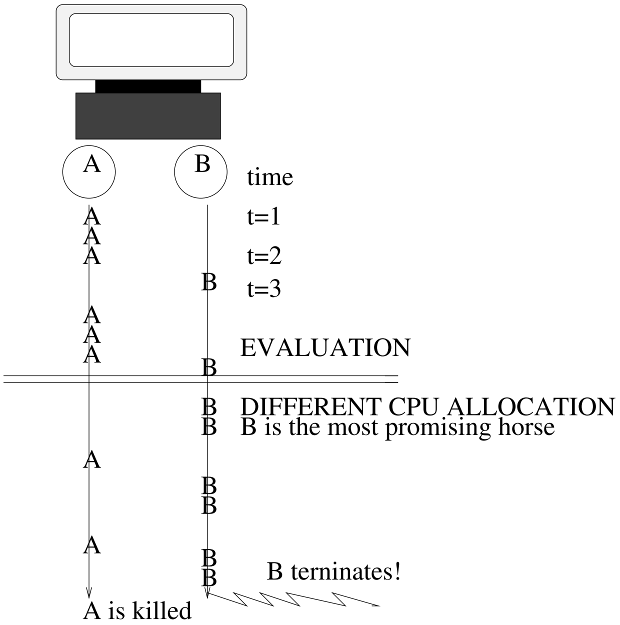


Figure 38.5: A racing strategy. The different horses (algorithms) are evaluated periodically to reallocate the CPU time shares.

is known one would immediately pull only the best performing arm. What makes the problems intriguing is that one has to split the effort between **exploration** to learn the different distributions and **exploitation** to pull the best arm, once the winner becomes clear. One is reminded of the critical exploration-versus-exploitation dilemma observed in optimization heuristics, but there is an important difference: in optimization one is not interested in maximizing the total payoff but in maximizing *the best pull* (the maximum value obtained by a pull in the sequence). The paper [128] is dedicated to determining a sufficient number of pulls to select with a high probability an arm (an hypothesis) whose *average* payoff is near-optimal. The max version of the bandit problem is considered in [93, 92]. An asymptotically optimal algorithm is presented in [350], in the assumption of a generalized extreme value (GEV) payoff distribution for each arm. Our explanation follows closely [349], which presents a simple distribution-free approach.

38.7.1 Racing to maximize cumulative reward by interval estimation

The first algorithm CHERNOFF-INTERVAL-ESTIMATION is for the classical bandit problem, which is then used as a starting point for the THRESHOLD-ASCENT algorithm dedicated to the max k-armed bandit problem. The assumption is that pulling an arm produces a random variable $X_i \in [0, 1]$. Because some effort is spent in exploration to determine (in an approximated manner) the best arm, of course the performance is less than that obtainable by knowing the best arm and pulling it all the time. What one misses by not having the information about the winning horse at the beginning is called **regret**. Precisely, regret is the difference between the payoff obtained by always pulling the best arm on a specific instance minus the cumulative payoff actually received during the racing strategy.

CHERNOFF-INTERVAL-ESTIMATION pulls arms and keeps an estimate of: the number of times n_i of pulls of the i-th arm, the expected reward $\bar{\mu}_i = \frac{x_i}{n_i}$ and an upper bound (with a specific minimum probability) on the reward $U(\bar{\mu}_i, n_i)$. At each iteration, the arm with the **highest upper bound** is pulled (Fig. 38.6 and Fig. 38.7). The upper

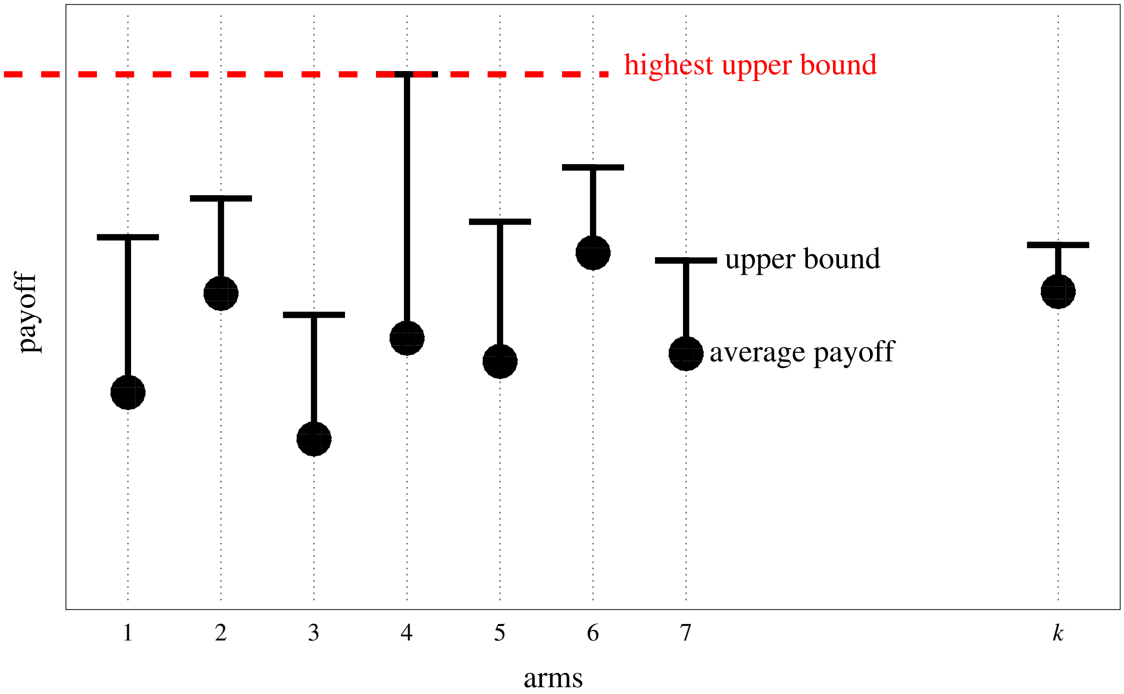


Figure 38.6: Racing with interval estimation. At each iteration an estimate of the expected payoff of each arm as well as its “error bar” are available.

```
function Chernoff_Interval_Estimation$(n, \delta)$
forall $i \in \{1, 2, ..., k\}$ Initialize $x_i \leftarrow 0,\ n_i \leftarrow 0$
repeat $n$ times:
    $\hat{\imath} \leftarrow \arg\max_i U(\bar{\mu}_i, n_i)$
    pull arm $\hat{\imath}$, receive payoff $R$
    $x_i \leftarrow x_i + R,\ n_i \leftarrow n_i + 1$
```

Figure 38.7: The CHERNOFF-INTERVAL-ESTIMATION routine.

bound is derived from Chernoff's inequality and is as follows:

$$U(\mu, n) = \begin{cases} \mu + \frac{\alpha+\sqrt{2n\mu\alpha+\alpha^2}}{n} & \text{if } n > 0 \\ \infty & \text{otherwise} \end{cases} \tag{38.11}$$

where $\alpha = \ln\left(\frac{2nk}{\delta}\right)$ and δ regulates our confidence requirements, see later.

Chernoff's inequality estimates how much the empirical average can be different from the real average. Let $X = \sum_{i=1}^{n} X_i$ be the sum of independent identically distributed random variables with $X_i \in [0, 1]$, and $\mu = E[X_i]$ be the real expected value. The probability of an error of the estimate greater than $\beta\mu$ decreases in the following exponential way:

$$P\left[\frac{X}{n} < (1-\beta)\mu\right] < e^{-\frac{n\mu\beta^2}{2}} \tag{38.12}$$

From this basic inequality, which does not depend on the particular distribution, one derives that, if arms are pulled according to the algorithm in Fig. 38.7, with probability at least $(1 - \delta/2)$, for all arms and for all n repetitions the upper bound is not wrong: $U(\bar{\mu_i}, n_i) > \mu_i$. Therefore each suboptimal arm (with $\mu_i < \mu^*$, μ^* being the best arm expected reward) is not pulled many times and the expected *regret* is limited to at most:

$$(1-\delta)2\sqrt{3\mu^* n(k-1)\alpha} + \delta\mu^* n \tag{38.13}$$

A similar algorithm based on Chernoff-Hoeffding's inequality has been presented in a previous work [12]. In their simple UCB1 deterministic policy, after pulling each arm once, one then pulls the arm with the highest bound $U(\bar{\mu}, n_i) = \bar{\mu} + \sqrt{\frac{2\ln n}{n_i}}$, see [12] for more details and experimental results.

38.7.2 Aiming at the maximum with threshold ascent

Our optimization context is characterized by a set of horses (different stochastic algorithms) aiming at discovering the maximum value for an instance of an optimization problem, for example different greedy procedures characterized by different ordering criteria, see [349] for an application to the Resource Constrained Project Scheduling Problem. The "reward" is the final result obtained by a single run of an algorithm. Racing is a way to allocate more runs to the algorithms which tend to get better results on the given instance.

We are therefore not interested in cumulative reward, but in the *maximum* reward obtained at any pull. A way to estimate the potential of different algorithms is to put a threshold $Thres$, and to estimate the probability that each algorithm produces a value above threshold. The estimate is the corresponding empirical frequency. Unfortunately, the appropriate threshold is not known at the beginning, and one may end up with a trivial threshold - so that all algorithms become indistinguishable - or with an impossible threshold, so that no algorithm will reach it. The heuristic solution presented in [349] reactively learns the appropriate threshold while the racing scheme runs (Fig. 38.9 and Fig. 38.8).

The threshold starts from zero (remember that all values are bounded in $[0, 1]$), and it is progressively raised raised until a selected number s of experimented payoffs above threshold is left. For simplicity, but it is easy to generalize, one assumes that payoffs are integer multiples of a suitably small Δ, $R \in \{0, \Delta, 2\Delta, ..., 1-\Delta, 1\}$. In the figure, $\bar{\nu_i}$ is the frequency with which arm i received a value greater than $Thres$ in the past, an estimate of the probability that it will do so in the future. This quantity is easily calculated from $n_{i,R}$, the number of payoffs equal to R received by horse i. The upper bound U is the same as before.

The parameter s controls the tradeoff between intensification and diversification. If $s = 1$ the threshold becomes so high that no algorithm reaches it: the bound is determined only by n_i and the next algorithm to run is the one with the lowest n_i (Round Robin). For larger values of s one start differentiating between the individual performance. A larger s means a more robust evaluation of the different strategies (not based on pure luck - so to speak), but a very large value means that the threshold gets lower and lower so that even poor performers have a chance of being selected. The specific setting of s is therefore not so obvious and it looks like more work is needed.

```
function Threshold_Ascent($(s, n, \delta)$)
Thres $\leftarrow 0$
forall $i \in \{1, 2, ..., k\}$
    forall $R$ values
        Initialize $n_{i,R} \leftarrow 0$
repeat $n$ times:
    while (number of payoffs received above threshold $\geq s$)
        $Thres \leftarrow Thres + \Delta$ (raise threshold)
    $\hat{i} \leftarrow \arg\max_i U(\bar{\nu}_i, n_i)$
    pull arm $\hat{i}$, receive payoff $R$
    $n_{i,R} \leftarrow n_{i,R} + 1$
```

Figure 38.8: The THRESHOLD-ASCENT routine.

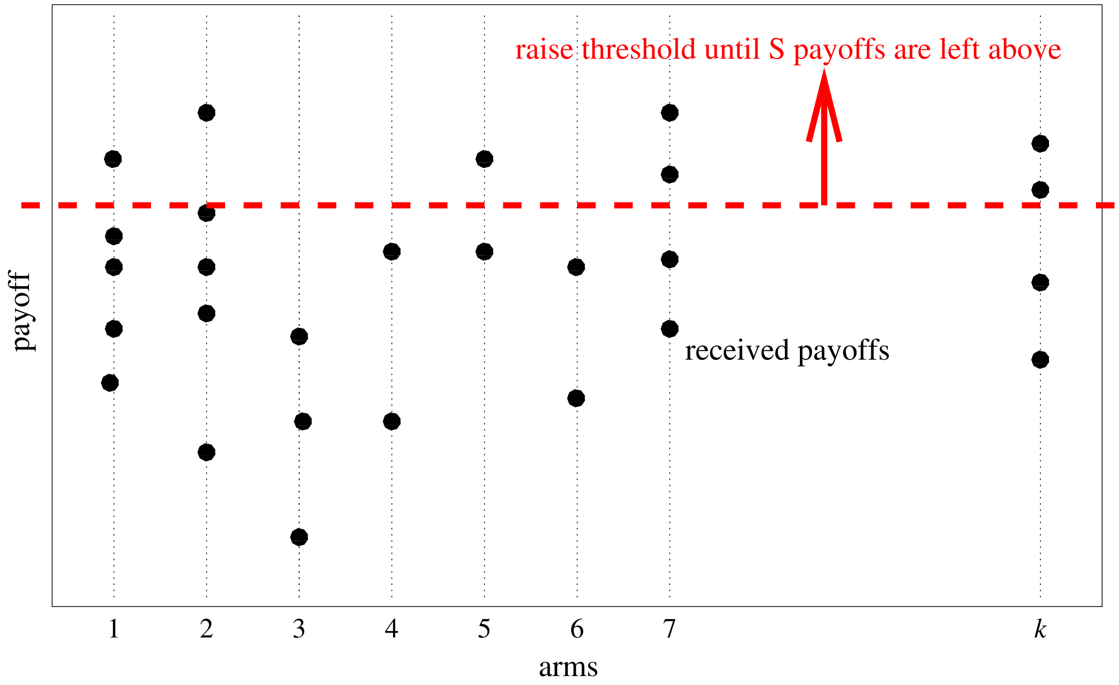


Figure 38.9: Threshold ascent: the threshold is progressively raised until a selected number of experimented payoffs is left.

38.7.3 Racing for off-line configuration of heuristics

The context here is that of selecting in an off-line manner the best configuration of parameters θ for a heuristic solving repetitive problems [54]. Let's assume that the set of possible θ values is finite. For example, a pizza delivery service receives orders and, at regular intervals, has to determine the best route to serve the last customers. In this case an off-line algorithm tuning (or "configuration"), even if expensive, is worth the effort because it is going to be used for a long time in the future.

There are two sources of randomness in the evaluation: the stochastic occurrence of an instance, with a certain probability distribution, and the intrinsic stochasticity in the randomized algorithm while solving a given instance. Given a criterion $\mathcal{C}(\theta)$ to be optimized with respect to θ, for example the average cost of the route over different instances and different runs, the ideal solution of the configuration problem is:

$$\theta^* = \arg\min_{\theta} \mathcal{C}(\theta) \tag{38.14}$$

where $\mathcal{C}(\theta)$ is the following Lebesgue integral (I is the set of instances, C is the range for the cost of the best solution found in a run, depending on the instance i and the configuration θ):

$$\mathcal{C}(\theta) = E_{I,C}\left[c(\theta,i)\right] = \int_I \int_C c(\theta,i) dP_C(c|\theta,i) dP_I(i) \tag{38.15}$$

The probability distributions are not known at the beginning. Now, to calculate the expected value for each of the finite configurations, ideally one could use a brute force approach, considering a very large number of instances and runs, tending to infinity. Unfortunately, this approach is tremendously costly, usually each run to calculate $c(\theta, i)$ implies a non-trivial CPU cost, and one has to resort to smarter methods.

Firstly, the above integral in equation (38.15) is estimated in a Monte Carlo fashion by considering a set of instances. Secondly, as soon as the first estimates become available, the manifestly poor configurations are discarded so that the **estimation effort is more concentrated onto the most promising candidates**. This process is actually a bread-and-butter issue for researchers in heuristics, with racing one aims at **a statistically sound hands-off approach**. In particular, one needs a sound criterion to determine that a candidate configuration θ_j is *significantly* worse than the current best configuration available, given the current state of the experimentation.

The situation is illustrated in Fig. 38.10, at each iteration a new test instance is generated and the surviving candidates are run on the instance. The expected performance and error bars are updated. Afterwards, if some candidates have error bars that show a clear inferior performance, they are eliminated from further consideration. Before deciding for elimination, a candidate is checked to see whether its optimistic value (top error bar) can beat the pessimistic value of the best performer.

The advantage is clear: costly evaluation cycles to get better estimates of performance are dedicated only to the most promising candidates. Racing is terminated when a single candidate emerges as the winner or when a certain maximum number of evaluations have been executed, or when a target error bar ϵ has been obtained, depending on available CPU time and application requirements.

The variations of the off-line racing technique depend on the way in which **error bars** are derived from the experimental data.

In [261], racing is used to select models in a supervised learning context, in particular for *lazy* or memory-based learning. Two methods are proposed for calculating error bars. One is based on Hoeffding's bound which makes the only assumption of independence of the samples: the probability that the true error E_{true} being more than ϵ away from the estimate E_{est} is:

$$Prob(\|E_{true} - E_{est}\| > \epsilon) < 2e^{\frac{-n\epsilon^2}{B^2}} \tag{38.16}$$

where B bound the largest possible error. In practice, this can be heuristically estimated as some multiple of the estimated standard deviation. Given the confidence parameter δ for the right-hand side of equation (38.16) (we want the probability of a large error to be less than δ), one easily solves for the error bar $\epsilon(n, \delta)$:

$$\epsilon(n,\delta) = \sqrt{\frac{B^2 \log(2/\delta)}{2n}} \tag{38.17}$$

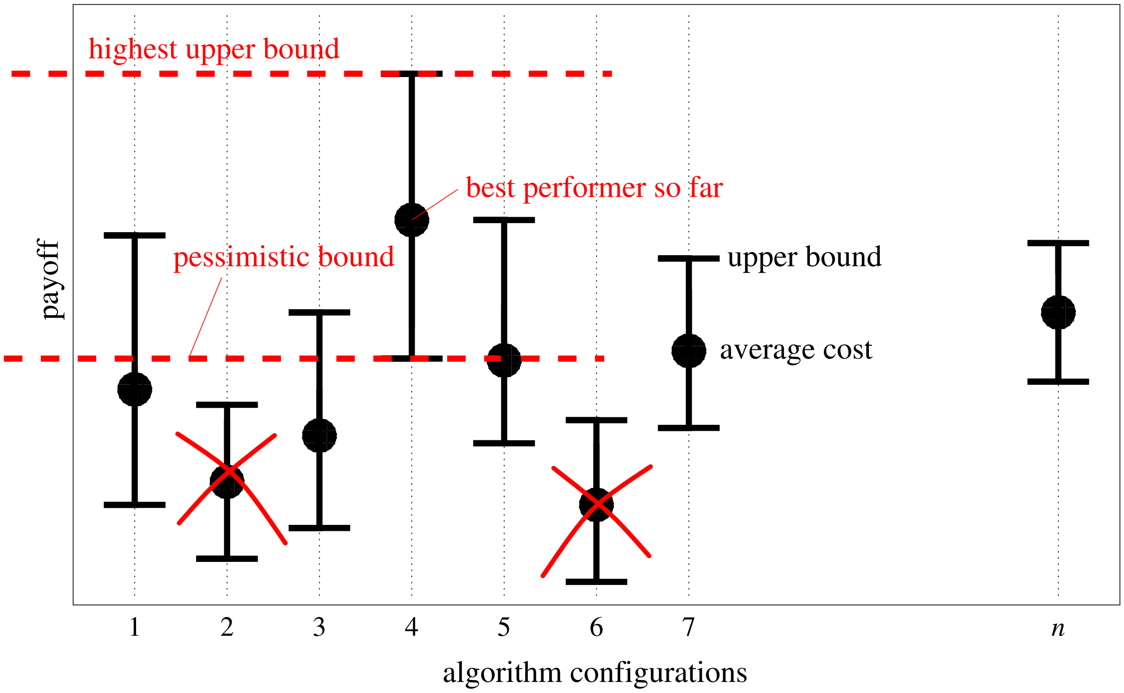


Figure 38.10: Racing for off-line optimal configuration of meta-heuristics. At each iteration an estimate of the expected performance with error bars is available. Error bars are reduced when more tests are executed, their values depend also on confidence parameter δ. In the figure, configurations 2 and 6 perform significantly worse than the best performer 4 and can be immediately eliminated from consideration: even if the real value of their performance is at the top of the error bar they cannot beat number 4.

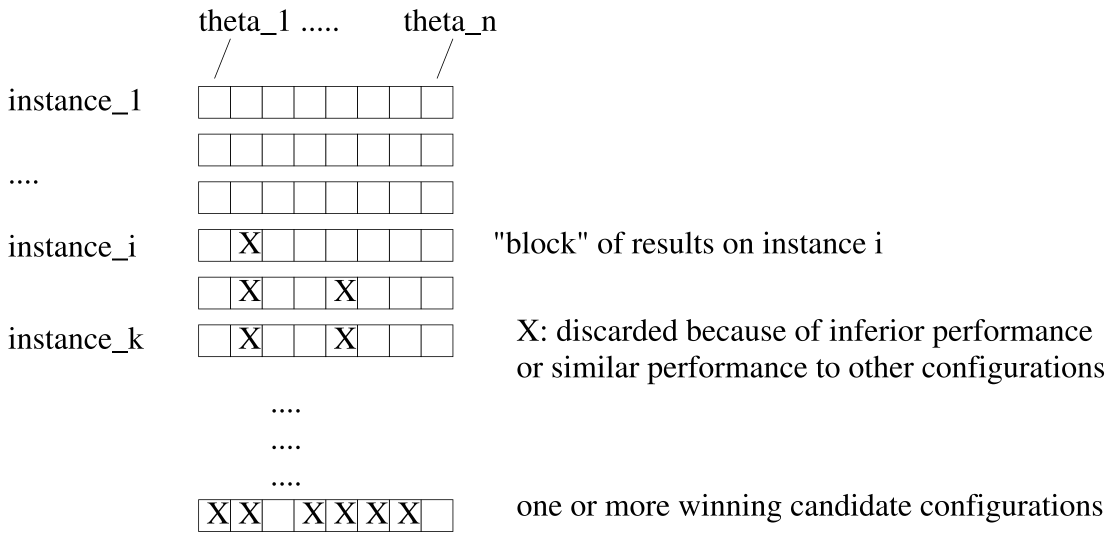

theta_1 .....
theta_n
instance_1
....
instance_i
instance_k
X
"block" of results on instance i
X: discarded because of inferior performance or similar performance to other configurations
....
one or more winning candidate configurations

Figure 38.11: Racing for off-line optimal configuration of meta-heuristics. The most promising candidate algorithm configurations are identified asap so that these can be evaluated with a more precise estimate (more test instances). Each block corresponds to results of the various configurations on the same instance.

If the accuracy ϵ and the confidence δ are fixed, one can solve for the required number of samples n. The value $(1-\delta)$ is the confidence in the bound for a single model during a single iteration, additional calculations provide a confidence $(1-\Delta)$ of selecting the best candidate after the entire algorithm is terminated [261].

Tighter error bounds can be derived by making more assumptions about the statistical distribution. If the evaluation errors are normally distributed one can use Bayesian statistics, the second method proposed in [261]. One candidate model is eliminated if the probability that a second model has a better expected performance is above the usual confidence threshold:

$$Prob(E^{j}_{true} > E^{j'}_{true} \| e_j(1), ..., e_j(n), e_{j'}(1), ..., e_{j'}(n)) > 1 - \delta \tag{38.18}$$

Additional methods for shrinking the intervals, as well as suggestions for using a statistical method known as *blocking* are explained in [261]. Model selection in continuous space is considered in [121].

In [54] the focus is explicitly on meta-heuristics configuration. Blocking through ranking is used in the F-RACE algorithm, based on the Friedman test, in addition to an aggregate test over all candidates performed before considering pairwise comparisons. Each block (Fig. 38.11) consists of the results obtained by the different candidate configurations θ_j on an additional instance i. From the results one gets a ranking R_{lj} of θ_j within block l, from the smallest to the largest, and $R_j = \sum_{l=1}^{k} R_{lj}$ the sum of the ranks over all instances. The Friedman test [98] considers the statistics T:

$$T = \frac{(n-1)\sum_{j=1}^{n}\left(R_j - \frac{k(n+1)}{2}\right)^2}{\sum_{l=1}^{k}\sum_{j=1}^{n} {R_{lj}}^2 - \frac{kn(n+1)^2}{4}} \tag{38.19}$$

Under the null hypothesis that the candidates are equivalent so that all possible rankings are equally likely, T is χ^2 distributed with $(n-1)$ degrees of freedom. If the observed t value exceeds the $(1-\delta)$ quantile of the distribution, the null hypothesis is rejected in favor of the hypothesis that at least one candidate tends to perform better than at least another one. In this case one proceed with a pairwise comparison of candidates. Configurations θ_j and θ_h are

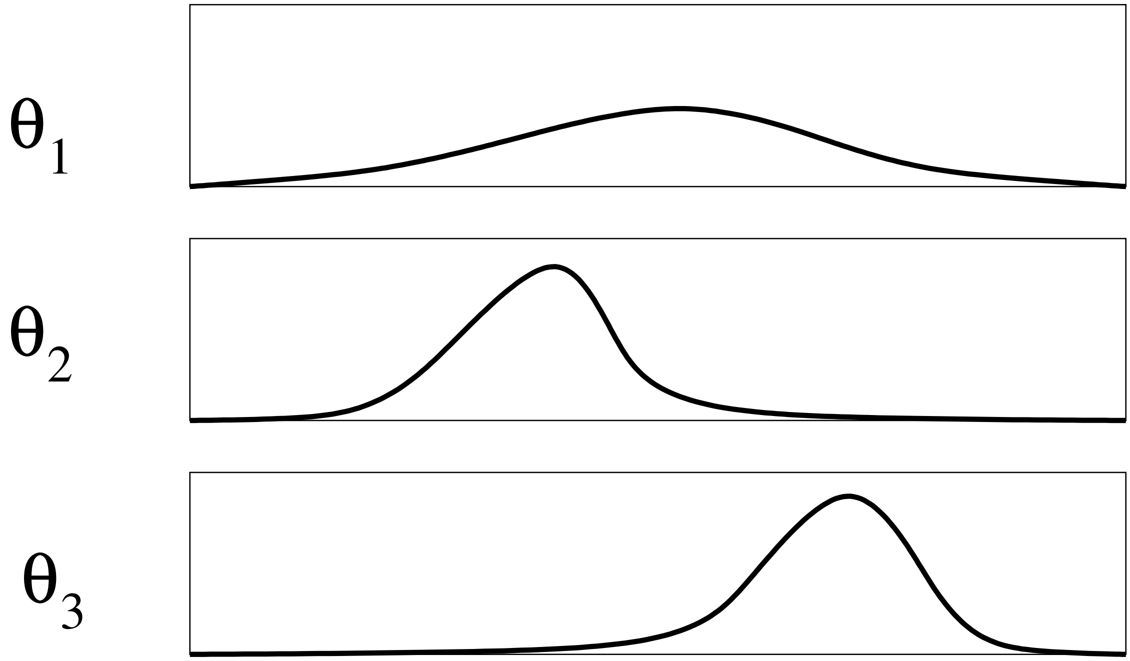


Figure 38.12: Bayesian elimination of inferior models, from the posterior distribution of costs of the different models one can eliminate the models which are inferior in a statistically significant manner, for example model θ_3 in the figure, in favor of model θ_2, while the situation is still undecided for model θ_1.

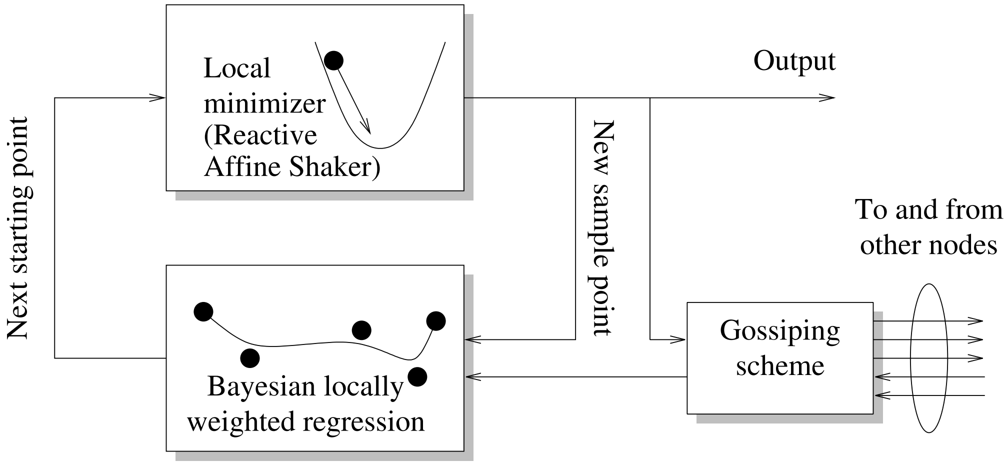


Figure 38.13: The distributed setting for the memory-based Reactive Affine Shaker.

considered different if:

$$\frac{\|R_j - R_h\|}{\sqrt{\frac{2k(1-\frac{T}{k(n-1)})\left(\sum_{l=1}^{k}\sum_{j=1}^{n} R_{ij}{}^2 - \frac{kn(n+1)^2}{4}\right)}{(k-1)(n-1)}}} > t_{1-\delta/2} \tag{38.20}$$

where $t_{1-\delta/2}$ is the $(1-\delta/2)$ quantile of the Student's t distribution. In this case the worse configuration is eliminated from further consideration.

38.8 Gossiping Optimization

Let's consider the following scenario: a set of intelligent searchers is spread on a number of computers, possibly throughout the world. While every searcher executes a local search heuristic, it takes advantage from the occasional injection of new information coming from its partners on other machines.

For instance, let's consider the field of continuous optimization, for which the RAS heuristic has been introduced in Section 32.1. In memory-based RAS [72] a fast local minimizer, the Reactive Affine Shaker, interacts with a model of the search space by feeding it with new data about the search and retrieving suggestions about the best starting point for a new run.

While MRAS has been devised as a sequential heuristic [72], it can be extended to a distributed one as described in Fig. 38.13: a gossiping component, described below, communicates model information to other nodes, and feeds information coming from other nodes to the model.

Sharing information among nodes is a delicate issue. The algorithm aims at function optimization, so it should spend most of its time doing actual optimization, not just broadcasting information to other nodes. Let's now discuss some communications issues arising in this context.

38.8.1 Epidemic communication for optimization

The use of parallel and distributed computing for solving complex optimization tasks has been investigated extensively in the last decades [356, 30]. Most works assume the availability of either a dedicated parallel computing facility or of a specialized clusters of networked machines that are coordinated in a centralized fashion (master-slave, coordinator-cohort, etc.). While these approaches simplify management, they have limitations with respect to scalability and robustness and require a dedicated investment in hardware.

Recently, the **peer-to-peer (P2P)** paradigm for distributed computing has demonstrated that networked applications can scale far beyond the limits of traditional distributed systems without sacrificing efficiency and robustness.

A well known problem with P2P systems is their high level of dynamism: nodes join and leave the system continuously, in many cases unexpectedly and without following any "exit protocol." This phenomenon, called *churn*, together with the large number of computational nodes, are the two most prominent research challenges posed by P2P systems: no node has an up-to-date knowledge of the entire system, and the maintenance of consistent distributed information may as well be impossible.

On the other hand, a clear advantage of P2P architectures is the exploitation of unused computational resources, such as personal desktop machines, volunteered by people who keep using their computers while participating to a shared optimization effort. The systems based on a central coordinator repeat a simple loop: every involved machine receives from a central server a subset of the search space (samples, parameter intervals), performs an exhaustive coverage of the subset and reports the results, receiving another search subset.

More distributed schemes originated in the context of databases [114], where **epidemic protocols** have been able to deal with the high levels of unpredictability associated with P2P systems. Apart from the original goal of information dissemination (messages are "broadcasted" through random exchanges between nodes), epidemic protocols are now used to solve several different problems, from membership and topology management to resource sharing.

We focus our attention onto stochastic local search schemes based on memory, where little or no information about the function to be optimized is available at beginning of the search. In this context, the knowledge acquired from function evaluations at different input points during the search can be mined to build models so that the future steps of the search process can be optimized. An example is the online adaptive self-tuning of parameters while solving a specific instance proposed by Reactive Search Optimization (RSO). Recent developments of interest consider the integration of multiple techniques and the feedback obtained by preliminary phases of the execution for a more efficient allocation of the future effort.

In the P2P scenario the crucial issues and tradeoffs to be considered when designing distributed optimization strategies are:

Coordination and interaction One has a choice of possibilities ranging from independent search processes reporting the end results, to fully coordinated "teams" of searchers exchanging new information after each step of the search process.

Synchronization In a peer-to-peer environment the synchronization must be very loose to avoid wasting computational cycles while waiting for synchronization events.

Type and amount of exchanged information It ranges from the periodic exchange of current configurations and related function values, see for example particle swarm [95] and genetic algorithms, to the exchange of more extensive data about past evaluations, possibly condensed into local heuristic models of the function [72].

Frequency of gossiping, convergence issues We consider a simple basic interaction where a node picks a random neighbor, exchanges some information and updates its internal state (memory). The spreading of the information depends both on the gossiping frequency and on the interconnection topology. Tradeoffs between a more rapid information exchange and a more rapid advancement of each individual search process are of interest.

Effects of delays on "distributed snapshots" Because of communication times, congestion and possible temporary disconnections, the received information originated from a node may not reflect accurately the current state, so that decisions are made in a suboptimal manner.

The distributed realization of a gossiping optimization scheme ranges between two extremes:

- **Independent execution of stochastic processes** — Some global optimization algorithms are stochastic by nature; in particular, the first evaluation is not driven by prior information, so the earliest stages of the search often require some random decision. Different runs of the same algorithm can evolve in a very different way, so that the parallel independent execution of identical algorithms with different random seeds permits to explore the tail of the outcome distribution towards lower values.

- **Complete synchronization and sharing of information** — Some optimization algorithms can be modeled as parallel processes with shared memory. Processes can be coordinated in such a way that every single step of each process, i.e., decision on the next point to evaluate, is performed while considering information about all processes.

Between the two extremal cases, a wide spectrum of algorithms can be designed to perform individual searches with some form of loose coordination. An example is the “GOSH!” paradigm (Gossiping Optimization Search Heuristics) proposed in [52]. In this proposal, in order to distribute the Memory-Based Affine Shaker (MRAS) algorithm, every node maintains its own past history and uses it to model the function landscape and locate the best suitable starting point. Occasionally, pairs of nodes communicate and share relevant information about their past history in order to build a better common model.

38.9 Intelligent coordination of local search processes

Models of cultural evolution inspire a set of powerful optimization techniques known as **Memetic Algorithms (MAs)**. According to a seminal paper [275], memetic algorithms are population-based approaches that combine a fast heuristic to improve a solution (and even reach a local minimum) with a recombination mechanism that creates new individuals.

The fast heuristic to improve a solution is some form of **local search** (LS) already explained in Chapter 24. As explained, the motivation for the effectiveness of stochastic local search for many real-world optimization tasks lies in the *correlation between function values at nearby points*. The probability to find points with lower values is larger for neighbors of points which are *already* at low function values.

Although powerful, LS finds *locally optimal* points, which are not necessarily globally optimal. The paradigm is that of starting from a **basin of attraction** around a locally optimal point (or region) and generating a trajectory in the configuration space through a discrete dynamical system which is “flowing like a drop of water towards the bottom of the basin.” Repeated LS, starting from different initial points, is a partial cure of the local minima problem but is completely *memory-less*: no information about previous searches influences future efforts.

In many cases a given optimization instance is characterized by *structure at different levels*, as explained with the big valley property of Fig. 24.7 in Chapter 24. If we reduce the initial search space to a set of attractors (the local minima), again it may be the case that nearby attractors – having an attraction basin close to each other – tend to have correlated values. This means that *knowledge* of previously found local optima can be used to direct the future investigation efforts. Starting from initial points close to promising attractors favors the discovery of other good quality local optima, provided of course that a sufficient diversification mechanism avoids falling back to previously visited ones.

In sequential local search the knowledge accumulated about the fitness surface flows from past to future searches, while in parallel processes with more local searchers active at the same time, knowledge is transferred by mutual sharing of partial results. We argue that the relevant subdivision is not between sequential and parallel processes (one can easily simulate a parallel process on a sequential machine) but between different ways of **using the knowledge accumulated by set of local search streams to influence the strategic allocation of computing resources** to the different LS streams, which will be activated, terminated, or modified depending on a shared knowledge base, either accumulated in a central storage, or in a distributed form but with a periodic exchange of information.

MAs fit in this picture, a set of individuals described by genes and subjected to genetic evolution scouts the fitness surface to search for successful initial points, while LS mechanisms (analogous to life-time learning) lead selected individuals to express their full potential by reaching local optima through local search. The **Genetic Algorithms** used in standard MAs follow the biological paradigms of selection/reproduction, cross-over and mutation. While GAs are effective for many problems, there is actually no guarantee that specific biologically-motivated genetic operators must be superior to **human-made direct mechanisms to share the knowledge accumulated** about the fitness surface by a set of parallel search streams (a.k.a. population). Alternative coordination mechanisms have been proposed for example in [363].

38.10 *C-LION*: a political analogy

We like analogies derived from the human experience more that analogies based on animals or genetics. Politics is a process by which groups of people make collective decisions. Groups can be governments, but also corporate, academic, and religious institutions. The issue is one of finding deliberate plans of action to guide decisions and achieve rational outcome(s). In politics one aims at making important organizational decisions, including the identification of spending priorities, and choosing among them on the basis of the impact they will have.

Local search is an effective building block for starting from an initial configuration of a problem instance and progressively building better solutions by moving to neighboring configurations. In an organized institution, like a corporation composed of individuals with intelligent problem-solving capabilities, each expert, when working on a tentative solution in his competence area, will after some time come up with an improved solution. The objective is to strategically allocate the work so that, depending on the accumulated performance of the different experts and competencies, superior solutions are obtained.

Memetic Algorithms start from local search and consider a hybridized genetic mechanism to implicitly accumulate knowledge about past local search performance by the traditional biologically-motivated mechanisms of selection/reproduction, mutation and cross-over. The first observation is that an individual can exploit its initial genetic content (its initial position) in a more directed and determined way. This is effected by considering the initial string as a *starting point* and by initiating a run of local search from this initial point, for example scouting for a local optimum. The term **memetic algorithms** [241, 275] has been introduced for models which combine the evolutionary adaptation of a population with individual learning within the lifetime of its members. The term derives from Dawkins' concept of a *meme* which is a unit of cultural evolution that can exhibit local refinement [112]. Actually, there are two obvious ways in which individual learning can be integrated: a first way consists of replacing the initial genotype with the better solution identified by local search (*Lamarckian evolution*), a second way can consist of modifying the fitness function by taking into account not the initial value but the final one obtained through local search. In other words, the fitness does not evaluate the initial state but the value of the "learning potential" of an individual, measured by the result obtained after local search. This evaluation changes the fitness landscape, while the evolution is still Darwinian in nature.

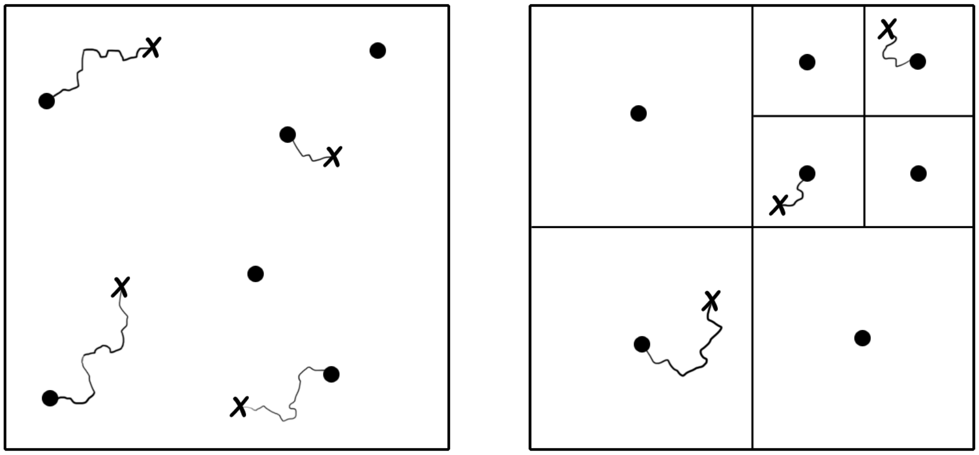


Figure 38.14: Different ways of allocating local searchers: by Memetic Algorithms (left) and by a political analogy (right). Crosses represent starting points, circles local optima reached after running local search. In the second case each individual is responsible for an area of configuration space. The political analogy is with territorial subdivisions given by electoral districts, or areas assigned to different marketing managers in a business example. Some local search streams are shown.

When the road of cultural paradigms is followed, it is natural to consider models derived from organizations of intelligent individuals equipped with individual learning and social interaction capabilities also in the **strategic allocation of resources** to the different search streams. In particular, the work in [41] presents a hybrid algorithm for the global optimization of functions (called continuous reactive tabu search), in which a fast combinatorial component (the Reactive Search Optimization based on prohibitions) identifies promising *districts* (boxes) in a tree-like partition of the initial search space, and a stochastic local search minimizer (the Reactive Affine Shaker — RAS — algorithm) finds the local minimum in a promising attraction basin. The social analogy can be that of organizing a marketing effort in a large company, see also Fig. 38.14: each individual (in the analogy a marketing manager) is responsible for a geographical area, the size of the geographical area is adapted to the interest of the different regions and the budget allocated to the different individuals is related to results obtained during their previous campaigns. A second political analogy is with a territorial subdivision given by electoral districts, again adapted to the interest of the different areas (population density) and again fighting for resources according to the area potentials.

But now it is time to stop with analogies and to consider the algorithms. The development of the *C-LION* framework is guided by the following design principles.

- **General-purpose optimization:** no requirements of differentiability or continuity are placed on the function f to be optimized.

- **Global optimization:** while the local search component identifies a local optimum in a given attraction basin, the combinatorial component favors jumps between different basins, with a *bias* toward regions that plausibly contain good local optima.

- **Multi-scale search:** the use of grids at different scales in a tree structure is used to spare CPU time in slowly-varying regions of the search space and to intensify the search in critical regions.

- **Simplicity, reaction and adaptation:** the algorithmic structure of *C-LION* is simple, the few parameters of the method are adapted in an automated way during the search, by using the information derived from memory. The dilemma between intensification and diversification is solved by using intensification until there is evidence that diversification is needed (when too many districts are repeated excessively often along the search trajectory). The tree-like discretization of the search space in districts is activated by evidence that the current district contains more than one attraction basin.

- **Tunable precision:** the global optimum can be located with high precision both because of the local adaptation of the grid size and because of the decreasing sampling steps of the stochastic RAS when it converges.

C-LION is characterized by an efficient use of *memory* during the search, as advocated by the Reactive Search Optimization (RSO). In addition, simple *adaptive* (*feedback*) mechanisms are used to tune the space discretization, by growing a *tree* of search districts, and to adapt the prohibition period of RSO acting on prohibitions. This adaptation limits the amount of user intervention to the definition of an initial search region, by setting upper and lower bounds on each variable, no parameters need to be tuned.

The *C-LION* framework based on Local Search **fuses Reactive Search Optimization with a problem-specific Local Search component**. An instance of an optimization problem is a pair $(\mathcal{X}, f)$, where $\mathcal{X}$ is a set of feasible points and f is the cost function to be *minimized*: $f : \mathcal{X} \rightarrow \mathbb{R}$. In the following we consider *continuous optimization* tasks where $\mathcal{X}$ is a compact subset of $\mathbb{R}^N$, defined by bounds on the N independent variables x_i, where $B_{Li} \leq x_i \leq B_{Ui}$ (B_L and B_U are the lower and upper bounds, respectively).

In many popular algorithms for continuous optimization one identifies a “local minimizer” that locates a local minimum by descending from a starting point, and a “global” component that is used to diversify the search and to reach the global optimum. We define as *attraction basin* of a local minimum X_l the set of points that will lead to X_l when used as starting configurations for the local minimizer.

In some cases, as we noted in our starting assumptions, an effective problem-specific local search component is available for the problem at hand, and one is therefore motivated to consider a **hybrid strategy**, whose local minimizer has the purpose of finding the local minimum with adequate precision, and whose combinatorial component has the duty of discovering promising attraction basins for the local minimizer to be activated. Because the local minimizer is costly, it is activated only when the plausibility that a region contains a good local optimum is high. On the contrary, a fast evaluation of the search districts is executed by the combinatorial component, and the size of the candidate districts is adapted so that it is related to that of a single attraction basin. A district is split when there is evidence that at least two different local minima are located in the same district.

38.11 A C-LION example: RSO cooperating with RAS

We now briefly summarize a concrete example of the *C-LION* framework based on Local Search, called *continuous reactive tabu search (C-RTS)* in the original publication [41].

As local minimizer, the Reactive Affine Shaker described in Section 32.1 is used in this case, although the *C-LION* method can of course be developed with other local searchers with demonstrated efficiency on the problem at hand. In the hybrid scheme, *RSO* identifies promising regions for the local minimizer to be activated.

The initial search region is specified by bounds on each independent variable x_i, where $B_{Li} \leq x_i \leq B_{Ui}$, for $i = 1, ..., N$. The basic structure through which the initial search region is partitioned consists of a *tree of districts* (boxes with axes parallel to the coordinate axes). The tree is born with 2^N equal-size leaves, obtained by dividing in half the initial range on each variable. Each district is then subdivided into 2^N equally-sized children, as soon as two different local minima are found in it. Because the subdivision process is triggered by the local properties of f, after some iterations of *C-RTS* the tree will be of varying depth in the different regions, with districts of smaller sizes being present in regions that require an intensification of the search. Only the *leaves* of the tree are admissible search points for the combinatorial component of *C-RTS*. The leaves partition the initial region: the intersection of two leaves is empty, the union of all leaves coincides with the initial search space. A typical configuration for a two-dimensional task is shown in Fig. 38.15, where each leaf-district is identified by thick borders and a bold binary string.

Each existing district for a problem of dimension N is identified by a unique binary string B_S with $n \times N$ bits: $B_S = [g_{11}, ..., g_{1n}, ..., g_{N1}, ..., g_{Nn}]$. The value n is the depth of the district in the tree: $n = 0$ for the *root* district, $n = 1$ for the leaves of the initial tree (and therefore the initial string has N bits), n increases by one when a given district is subdivided. The length of the district edge along the i-th coordinate is therefore equal to $(B_{Ui} - B_{Li})/2^n$. The position of the district origin B_{Oi} along the i-th coordinate is

$$B_{Oi} = B_{Li} + (B_{Ui} - B_{Li}) \sum_{j=1}^{n} \frac{g_{ij}}{2^j}.$$

The evaluated neighborhood of a given district consists only of existing leaf-districts: no new districts are created during the neighborhood evaluation. Now, after applying the elementary moves to the identifying binary string B_S of a given district B, one obtains $N \times n$ districts of the same size distributed over the search space as illustrated in Fig. 38.15, for the case of $B_S = (1010, 1011)$. Because the tree can have different depth in different regions, it can happen that some of the obtained strings do *not* correspond to leaf-districts, others can cover *more* than a single leaf-district. In the first case one evaluates the smallest *enclosing* leaf-district, in the second case one evaluates a randomly-selected *enclosed* leaf-district. The random selection is executed by generating a point with uniform probability in the original district, and by selecting the leaf that contains the point. This assures that the probability for a leaf to be selected is proportional to its volume.

Evaluating opportunities for the different districts

While the RSO algorithm for combinatorial optimization generates a search trajectory consisting of points $X^{(t)}$, *C-RTS* generates a trajectory consisting of *leaf-districts* $B^{(t)}$. There are two important changes to be underlined: firstly, the function $f(X)$ must be substituted with a routine measuring the potential that the current district contains good local optima, secondly, the tree is *dynamic* and the number of existing districts grows during the search.

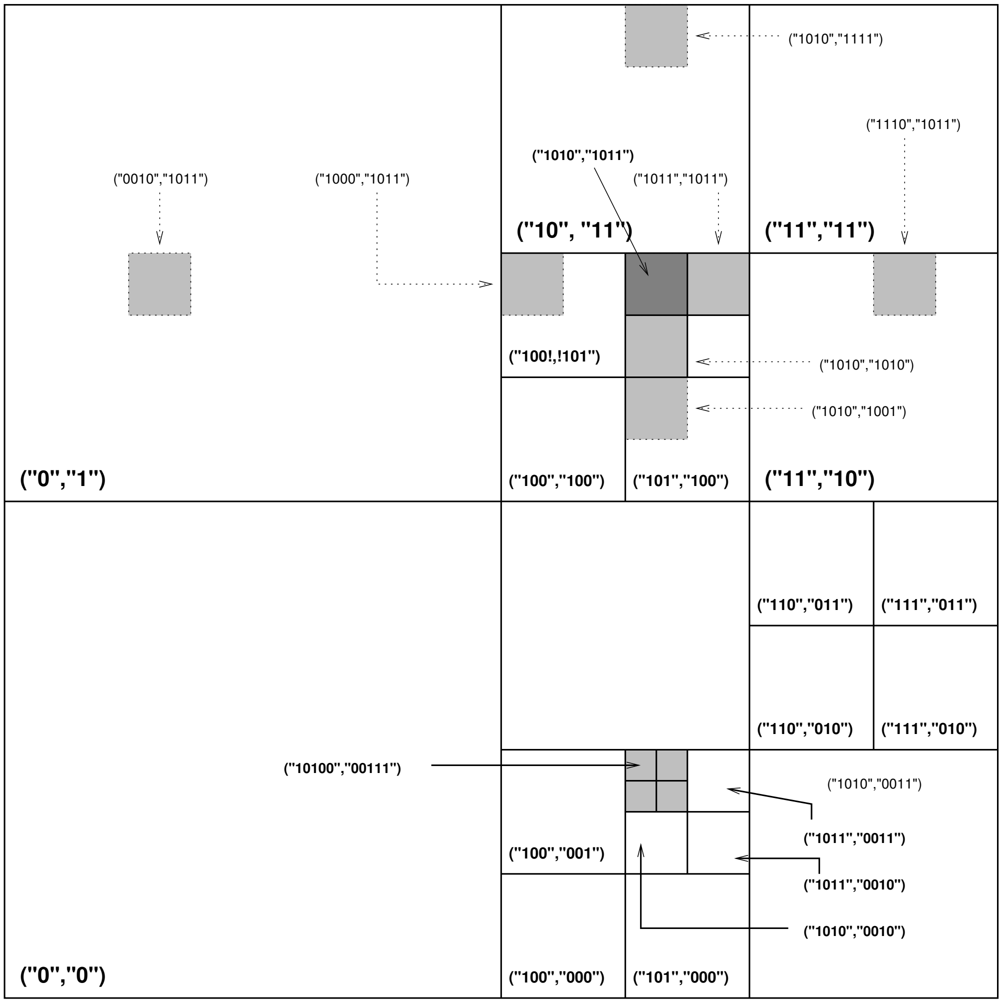


Figure 38.15: *C-RTS*: tree of search *districts*. Thick borders and bold strings identify existing leaf-districts, hatched districts show the neighborhood of district (1010,1011).

The combinatorial component must identify promising districts quickly. In the absence of detailed models about the function f to be minimized, a simple evaluation of a district B can be obtained by generating a point X with a uniform probability distribution inside its region and by evaluating the function $f(X)$ at the obtained point. Let us use the same function symbol, the difference being evident from its argument: $f(B) \equiv f(rand\ X \in B)$. The potential drawback of this simple evaluation is that the search can be strongly biased in favor of a district in the case of a "lucky" evaluation (e.g., $f(X)$ close to the minimum in the given district), or away from a district in the opposite case. To avoid this drawback, when a district is encountered again during the search, a *new* point X is generated and evaluated and some collective information is returned. The value $f(B)$ returned is then the *average* of the evaluated X_i: $f(B) \equiv (1/N_B) \sum_{i=1}^{N_B} f(X_i)$, where N_B is the number of points.

Let us consider the example of Fig. 38.15. The current district (1010,1011) has the neighbors shown with a hatched pattern. The neighbor (0010,1011) in the upper left part is not an existing leaf-district, it is therefore transformed into the enclosing existing leaf-district (0,1). *Vice versa* the neighbor (1010,0011) in the lower right part contains four leaves, one of them (10100,00111) is the output of a random selection. Fig. 38.16 specifies the complete final

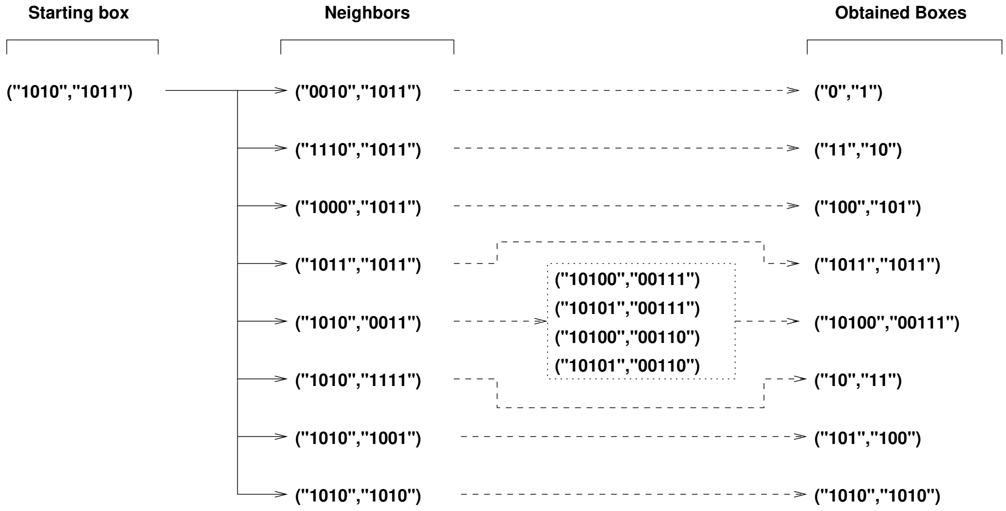


Figure 38.16: *C-RTS*: Evaluation of the neighborhood of district (1010,1011).

neighborhood obtained for the given example.

Decision about activating Local Search in a given region

According to the RSO dynamics the neighborhood districts obtained starting from a current district are evaluated only if the corresponding basic move from the current point is not prohibited. Only if the evaluation $f(B^{(t)})$ of the current district is less than all evaluations executed in the neighborhood, a decision is taken about the possible triggering of the Local Search component (the Reactive Affine Shaker). In other words, a necessary condition for activating high-precision and expensive searches with Local Search is that there is a high plausibility — measured by $f(B)$ — that the current region can produce local minima that are better with respect to the given neighborhood of candidate districts. Given the greedy nature of the combinatorial component, the current district $B^{(t)}$ on the search trajectory moves toward non-tabu locally optimal districts, therefore it will eventually become locally optimal and satisfy the conditions for triggering RAS. Let us note that, if a given district B loses the above contest (i.e., it is not locally optimal for RSO), it *maintains* the possibility to win when it is encountered again during the search, because the evaluation of a different random point X can produce a better $f(B)$ value. Thanks to the evaluation method *C-RTS* is *fast in optimal conditions*, when the f surface is smooth and $f(B)$ is a reliable indicator of the local minimum that can be obtained in region B, but it is *robust in harder cases*, when the $f(B)$ values have a high standard deviation or when they are unreliable indicators of good local minima obtainable with the Reactive Affine Shaker.

The local optimality of the current district B is necessary for activating RAS but it is not sufficient, unless B is locally optimal for the first time, a case in which RAS is always triggered. Otherwise, if $r > 1$ is the number of times that district B has been locally optimal during the search, an additional RAS run must be justified by a sufficient probability to find a *new* local minimum in B. Bayesian rules to estimate the probability that all local optima have been visited can be applied in the context of a single district, where a multi-start technique is realized with repeated activations of RAS from uniformly distributed starting points. Because of our splitting criterion, at most one local optimum will be associated to a given district (a district is split as soon as two different local optima are found, see Section 38.11). In addition, some parts of the district can be such that RAS will exit the borders if the initial point belongs to these portions. One can therefore partition the district region into W components, the attraction basins of the local minima contained in the district and a possible basin that leads RAS outside, so that the probabilities of the basins sum up to one ($\sum_{w=1}^{W} P_w = 1$).

According to [58], if $r > W + 1$ restarts have been executed and W different cells have been identified, the total relative volume of the "observed region" (i.e., the posterior expected value of the relative volume Ω) can be estimated by

$$E(\Omega|r, W) = \frac{(r - W - 1)\ (r + W)}{r\ (r - 1)}\ ; \qquad\qquad r > W + 1. \tag{38.21}$$

The Reactive Affine Shaker is always triggered if $r \leq W + 1$, because the above estimate is not valid in this case, otherwise the RAS is executed again with probability equal to $1 - E(\Omega|r, W)$. In this way, additional runs of RAS tend to be spared if the above estimate predicts a small probability to find a new local optimum, but a new run is never completely prohibited for the sake of robustness: it can happen that the Bayesian estimate of equation (38.21) is unreliable, or that the unseen portion $(1 - E(\Omega|r, W))$ contains a very good minimum with a small attraction basin.

The initial conditions for RAS (described in Fig. 32.1) are that the initial search point is extracted from the uniform distribution inside B, the initial search frame is $\vec{b}_i = \vec{e}_i \times (1/4) \times (B_{U\,i} - B_{L\,i})$ where $\vec{e}_i$ are the canonical basis vectors of $\mathbb{R}^N$. The Reactive Affine Shaker generates a trajectory that must be contained in the district B enlarged by a border region of width $(1/2) \times (B_{U\,i} - B_{L\,i})$, and it must converge to a point contained in B. If RAS exits the enlarged district or the root-district, it is terminated, the function evaluations executed by RAS are discarded. If it converges to a point outside the original district but inside the enlarged district, the point location is saved. In both cases the *C-RTS* combinatorial component continues in the normal way: the next district $B^{(t+1)}$ is the best one in the admissible neighborhood of $B^{(t)}$. In any case the "best so far" value is always updated by considering all admissible points evaluated (those that are inside of the root-district).

A possible exception to the normal *C-RTS* evolution can happen only in the event that RAS converges inside $B^{(t)}$ to a local minimum X_l. If X_l is the first local minimum found, it is saved in a memory structure associated to the district. If a local minimum Y_l was already present, and X_l corresponds to the same point, it is discarded, otherwise the current district is *split* until the "siblings" in the tree divide the two points. After the splitting is completed, the current district $B^{(t)}$ does not correspond to an existing leaf anymore: to restore legality a point is selected at random with uniform distribution in $B^{(t)}$ and the legal $B^{(t)}$ becomes the leaf-district that contains the random point. Therefore each leaf-district in the partition of the initial district has a probability of being selected that is proportional to its volume. The splitting procedure is explained in the following section.

Adapting the district area to the local fitness surface

As soon as two different local minima X_l and Y_l are identified in a given district B, the current district is subdivided into 2^N equal-sized boxes. If X_l and Y_l belong to two different leaf-districts of the new partition, the splitting is terminated, otherwise the splitting is applied to the district containing X_l and Y_l, until their separation is obtained.

In all cases the old district ceases to exist and it is substituted with the collection obtained through the splitting. The local minima X_l and Y_l are associated with their new boxes. Numerically, the criterion used in the tests for considering *different* two local minima X_l and Y_l is that $\|X_l - Y_l\| < \epsilon$, where ϵ is a user-defined precision requirement.

All local minima identified are saved and reported when *C-RTS* terminates.

An example of the tree structure produced during a run of *C-RTS* is shown in Fig. 38.17, for the case of a two-dimensional function (a "Strongin" function described in [41]). The local optima are clearly visible as "mountain tops." One notices that the points evaluated (the points used to calculate $f(B)$) are distributed quasi-uniformly over the search space: this is a result of the volume-proportional selection, and it guarantees that all regions of the search space are treated in a fair manner. The RAS trajectories either converge to a local minimum (bullet) or are terminated when they exit from the enlarged district, as explained in Section 38.11. Because of our splitting criterion, each district contains at most one local minimum. Although it is not visible from the figure, most points (about 85% in the example) are evaluated during the local search phases, that are the most expensive parts of the *C-RTS* algorithm.

38.12 Other C-LION algorithms

C-LION is **a paradigm to increase automation**, by using different optimization building blocks (or different instances of randomized algorithms), and by coordinating and managing them in an intelligent adaptive manner.

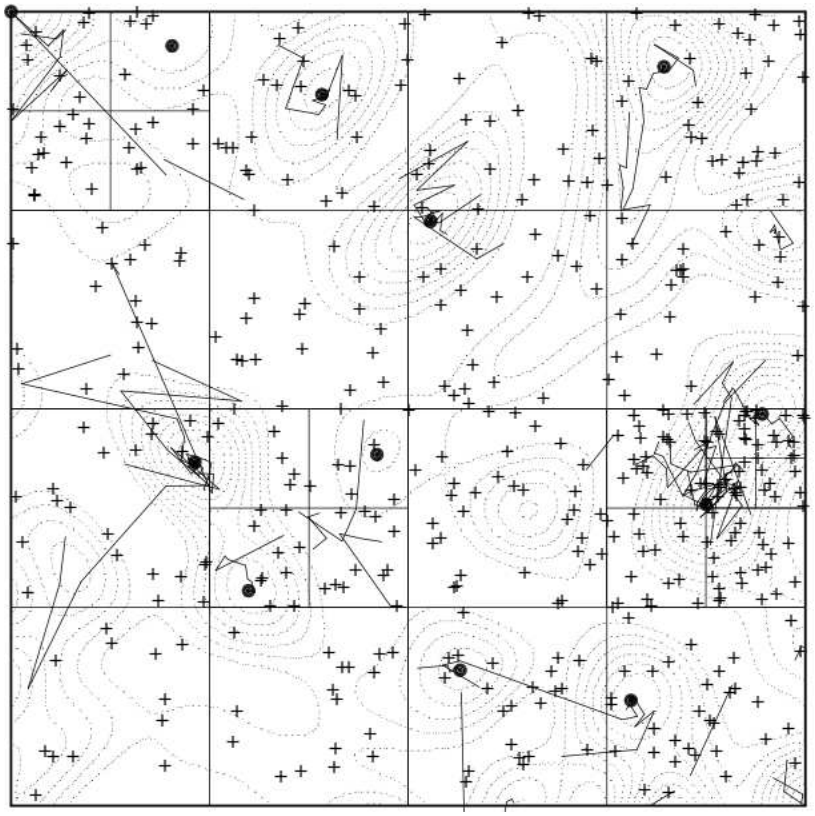


Figure 38.17: A *C-RTS* tree structure adapted to a fitness surface and calculated points. Evaluated points (crosses), local minima (bullets), LS trajectories (jagged lines). Figure derived from [41].

The cooperation structure exemplified by C-RTS can be used with different local search components, or different details about splitting the original space and firing local searches.

The work [70] proposes a variation of C-RTS (called *CoRSO*)in which the Inertial Shaker method generates candidate points in an adaptive search box and a moving average of the steps filters out evaluation noise and high-frequency oscillations. Finally, a portfolio of independent search streams (*P-CoRSO*) is proposed to increase the robustness of the algorithm.

Other notable examples are strategies like the '**Divide-the-Best**' algorithms based on Lipschitz assumptions and on efficient diagonal partitions and the **P-algorithm with simplicial partitioning** [390].

If $f(x)$ satisfies the Lipschitz condition over the search hyper-interval with an unknown Lipschitz constant K, a deterministic 'Divide-the-Best' algorithm based on efficient diagonal partitions of the search domain and smooth auxiliary functions is proposed in [329]. The method adaptively estimates the unknown Lipschitz constant K and the objective function and its gradient are evaluated only at two vertices corresponding to the main diagonal of the generated hyperintervals.

The second case assumes that the functions satisfies some statistical model, so that theoretically justified methods can be developed, in the framework of rational decision making under uncertainty, to generate new sample points based on information derived from previous samples, and to study convergence properties [390]. The P-algorithm [393] generates the next point to be evaluated as the one maximizing the probability to improve the current record, given the previously observed samples. In multiple dimensions, if y_{on} is the current record value and (x_i, y_i) are the previous evaluated points and corresponding values, the next $(n+1)$-th optimization step is defined as:

$$x_{n+1} = \operatorname*{argmax}_{x} \Pr\Big\{ \xi(x) \leqslant (y_{on} - \epsilon) \mid \xi(x_1) = y_1, ..., \xi(x_n) = y_n \Big\}.$$

The P-algorithm with simplicial partitioning is proposed in [394] to obtain a practical algorithm. The observation points coincide with the vertices of the simplices and different strategies for defining an initial covering and subdividing the interesting simplices are proposed and considered. The P^*-algorithm, combining the P-algorithm with local search, is related to the algorithm presented in this paper, which is also based on a combination of global models and efficient local searches when the current area is deemed sufficiently interesting.

Gist

Many optimization problems of real-world interest are complex and need enormous computing times for their solution. Luckily, there are often **many different algorithms** to try, different by their design or by the value of their meta-parameters. In addition, the use of many **computers working in parallel** (maybe living in the cloud, rented when they are needed) comes to the rescue to reduce the clock time to produce acceptable solutions.

In some cases, one can consider **independent search streams**, periodically reporting the best solutions found so far to some central coordinator. You should never ever underestimate the power of simple solutions!

In other cases, more **intelligent schemes of coordination** among the various running algorithms lead to higher automation, and better efficiency and effectiveness. The C-LION paradigm proposes to coordinate and manage a team of interacting optimization algorithms through adaptation based on intelligent reflection on their current and past results.

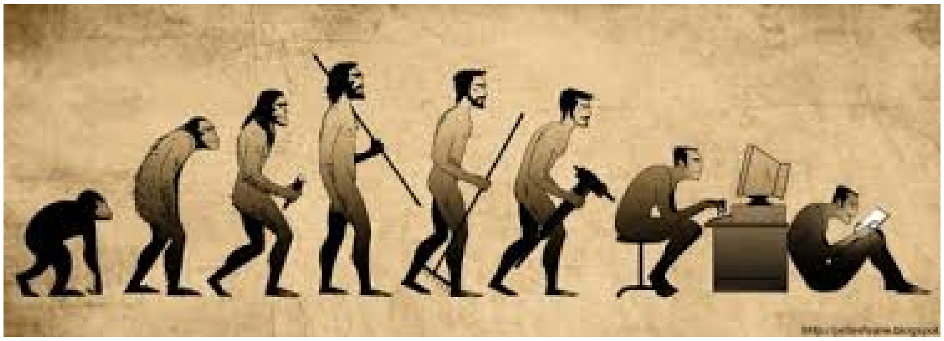
Paradigms derived from human organizations, characterized by "learning on the job" capabilities, can lead to superior results with respect to paradigms derived from simpler living organisms or genetic principles.

Sane human people solve complex problems better than viruses, normally with less deadly consequences. Flies do not learn a lot during their lives, and easily end up burnt by incandescent light bulbs. Kids need to touch a hot bulb once to become aware and avoid doing that again in the future.

Chapter 39

Genetics, evolution and nature-inspired analogies

What a book a devil's chaplain might write on the clumsy, wasteful,
blundering, low, and horribly cruel work of nature!
(Charles Darwin)



Population-based algorithms using multiple search streams became popular by using analogies derived from genetics, nature, and evolution. This emphasis on the imitation of very simple living organism is not always justified and more effective schemes can be developed by considering more explicit learning and self-tuning schemes. But if you are selling optimization, be aware of the surprising effect of nature-inspired analogies. In this area, biological analogies derived from the behavior of different species abound [341]. Elegant flocks of birds search for food or migrate in effective manners, herds of sheep get better guidance and protection than isolated members. Groups of hunting animals can often prevail over much bigger and powerful but isolated ones.

Analogies from nature can be inspiring but also misleading when they are translated directly into procedures for problem solving and optimization. Let's consider a flock of birds or an ant colony searching for food. If an individual finds food, it makes perfect sense for the survival of the species to inform other members so that they can also get their share of nutrients. The analogy between food and good solutions of an optimization problems is not only far-fetched but quite simply wrong. If one searcher already found a good suboptimal solution, attracting other searchers in the same attraction basin around the locally optimal point only means wasting precious computational resources which could be spent by exploring different regions of the search space. One encounters here the basic tradeoff between intensification and diversification.

The adoption of a set of interacting search streams has a long history, not only when considering natural evolution, but also heuristics and learning machines. It is not surprising to find very similar ideas under different names, including ensembles, pools, agents, committees, multiple threads, mixture of experts, genetic algorithms, particle swarms, evolutionary strategies. The terms are not synonymous because each parish church has specific strong beliefs and true believers.

39.1 Genetic algorithms and evolution strategies

A rich source of inspiration for adopting a set of evolving candidate solutions is derived from the theory natural evolution of the species, dating back to the original book by Charles Darwin [108] "On the Origin of Species by Means of Natural Selection, or the preservation of favored races in the struggle for life." It introduced the theory that populations evolve over the course of generations through a process of **natural selection**: individuals more suited to the environment are more likely to survive and more likely to reproduce, leaving their inheritable traits to future generations. After the more recent discovery of the genes, the connection with optimization is as follows: each individual is a candidate solution described by its genetic content (genotype). The genotype is randomly changed by mutations, the suitability for the environment is described by a *fitness function*, which is related to the function to be optimized. Fitter individuals in the current population produce a larger offspring (new candidate solutions), whose genetic material is a recombination of the genetic material of their parents.

Seminal works include [17, 303, 131, 319, 186]. A complete presentation of different directions in this huge area is out of the scope of this section, let's concentrate on some basic ideas, and on the relationships between GA and intelligent search strategies.

Let's consider an optimization problem where the configuration is described by a binary string, mutation consists of randomly changing bit values with a fixed probability Π_{mute} and recombination consists of the so called *uniform cross-over*: starting from two binary strings X and Y a third string Z is derived where each individual bit is copied from X with probability $1/2$, from Y otherwise

The pseudo-code for a slightly more general version of a genetic algorithm, with an additional parameter for cross-over probability Π_{cross} is shown in Fig. 39.1, and illustrated in Fig. 39.2. After the generation of an initial population P, the algorithm iterates through a sequence of basic operations: first the fitness of each individual is computed and, if goals are met, the algorithm stops. Some individuals are chosen by a random selection process that favors elements with a high fitness function; a crossover is applied to randomly selected pairs in order to combine their features, then some individuals undergo a random mutation. The algorithm is then repeated on the new population.

Let the population of candidate solutions be a set of configurations scattered on the fitness surface. Such configurations explore their neighborhoods through the mutation mechanism: usually the mutation probability is very low, so that in the above example a small number of bits is changed. After this very primitive form of local (perturbative) search move the population is substituted by a new one, where the better points have a larger probability to survive and a larger probability to generate offspring points. With a uniform cross-over the offspring is generated through a kind of "linear interpolation" between the two parents. Because a real interpolation is excluded for binary values, this combination is obtained by the random mechanism described: if two bits at corresponding positions in X and Y have the same value, this value is maintained in Z - as it is in a linear interpolation of real-valued vectors - otherwise a way to define a point in between is to pick randomly from either X or Y if they are different.

There are at least three critical issues when adopting biological mechanisms for solving optimization problems: first one should demonstrate that they are effective - not so easy because defining the function that biological organisms are optimizing is far from trivial. One risks a circular argument: survival of the fittest means that the fittest are the ones who survived. Second, one should demonstrate that they are efficient. Just consider how many generations were needed to adapt our species to the environment. Third, even assuming that GA are effective, one should ask whether natural evolution proceeds in a Darwinian way because it is intrinsically superior or because of **hard biological constraints**, which may be masochistic to keep in a human-designed algorithm.

For example, it is now believed that Lamarck was wrong in assuming that the experience of an individual could be passed to his descendants: **genes do not account for modifications caused by lifelong learning**. Airplanes do not flap their wings and, in a similar manner, when a technological problem has to be solved, one is free to depart from the biological analogy and to design the most effective method with complete freedom.

Initialization — Compute a random population with M members $P = \{s^{(j)} \in S^{\ell}, j = 0, \ldots, M-1\}$, where each string is built by randomly choosing ℓ symbols of S.

Repeat :

Evaluation — Evaluate the fitness $f^{(i)} = f(s^{(i)})$; compute the rescaled fitness $\bar{f}^{(j)}$:

$$f_{\text{min}} = \min_j f^{(j)}; \quad f_{\text{max}} = \max_j f^{(j)}; \quad \bar{f}^{(j)} = \frac{f^{(j)} - f_{\text{min}}}{f_{\text{max}} - f_{\text{min}}}$$

Test — If the population P contains one or more individuals achieving the optimization goal within the requested tolerance, stop the execution.

Stochastic selection — Build a new population $Q = \{q^{(j)}, j = 0, \ldots, N-1\}$ such that the probability that an individual $q \in P$ is member of Q is given by $f(q)/\sum_{p \in P} f(p)$:

Reproduction — Choose $N/2$ distinct pairs $(q^{(i)}, q^{(j)})$ using the N individuals of Q. For each pair build, with probability Π_{cross}, a new pair of offsprings mixing the parents' genes, otherwise copy the original genes:

```
for $i \leftarrow 0, \ldots, (M-1)/2$
    if Rand(1) < $\Pi_{\text{cross}}$
        for $j \leftarrow 0, \ldots, l-1$
            if Rand(1) < .5
                $\bar{q}_j^{(2i)} \leftarrow q_j^{(2i)}$; $\bar{q}_j^{(2i+1)} \leftarrow q_j^{(2i+1)}$
            else
                $\bar{q}_j^{(2i)} \leftarrow q_j^{(2i+1)}$; $\bar{q}_j^{(2i+1)} \leftarrow q_j^{(2i)}$
    else
        $\bar{q}^{(2i)} \leftarrow q^{(2i)}$; $\bar{q}^{(2i+1)} \leftarrow q^{(2i+1)}$
```

Mutation — In each new individual $\bar{q}^{(j)}$ change, with probability Π_{mutate}, each gene $\bar{q}_i^{(j)}$ with a randomly chosen gene of S. Let us denote the new population Q'.

Replacement — Replace the population P with the newly computed one Q'.

Figure 39.1: Pseudocode for a popular version of GA.

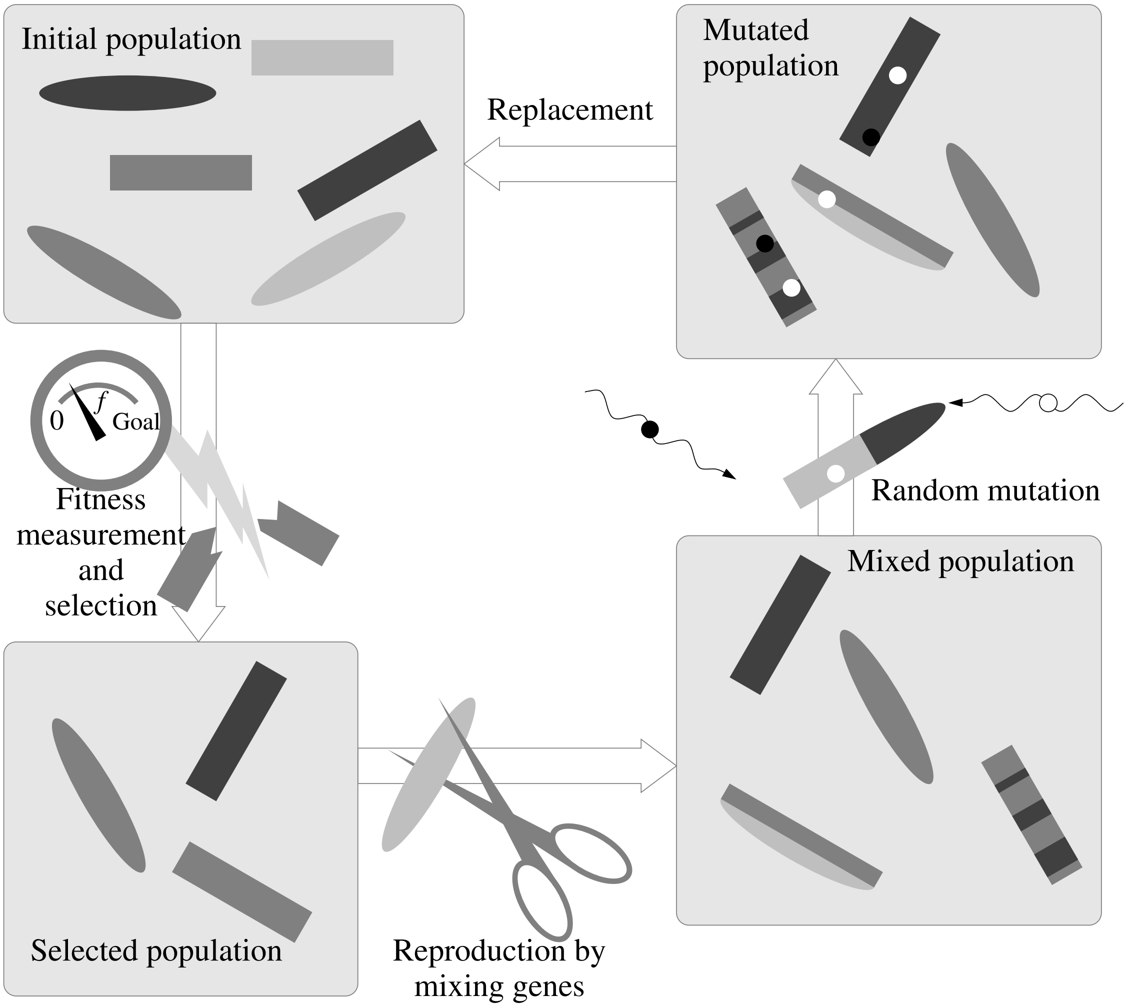


Figure 39.2: Representation of a genetic algorithm framework. Counter-clockwise from top left: starting from an initial population, stochastic selection is applied, then genes are mixed and random mutations occur to form a new population.

A second departure from the biological world is as follows: in biology one is interested in the convergence of the entire population/species to a high fitness value, in optimization one aims at having at least *one* high-fitness solutions *during* the search, not necessarily at the end, and one could not care less whether most individuals are far from the best when the search is terminated.

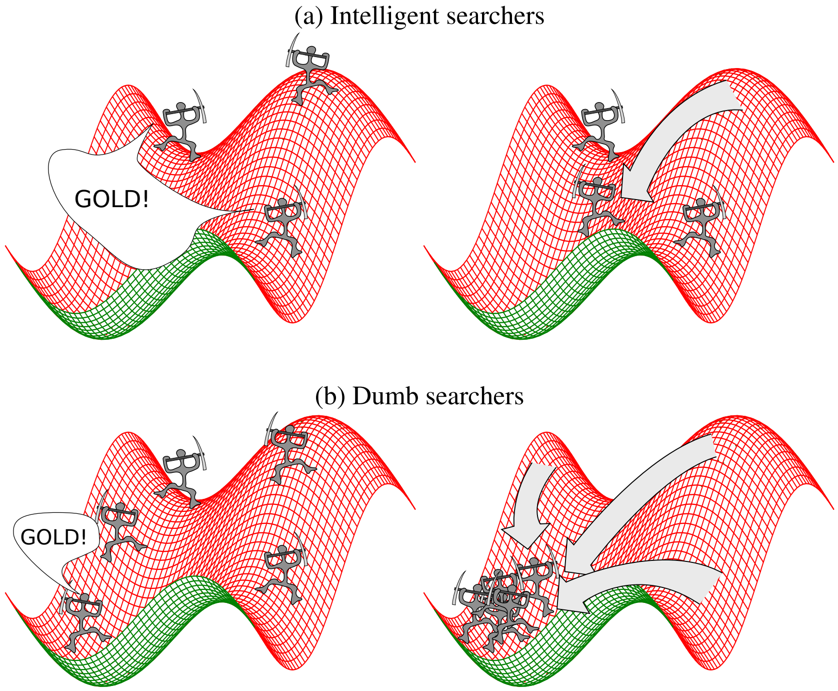
When using the stochastic local search language adopted in this book, the role of the mutation/selection and recombination operators cannot be explained in a clear-cut manner. When the mutation rate is small, the effect of the combined **mutation and selection of the fittest** can be interpreted as searching in the neighborhood of a current point, and accepting (selecting) the new point in a manner proportional to the novel fitness value. The behavior is of intensification/exploitation provided that the mutation rate is small, otherwise one ends up with a random restart, but not too small, otherwise one is stuck with the starting solution. The explanation of **cross-over** is more dubious. Let's consider uniform cross-over: if the two parents are very different, the distance between parents and offspring is large so that cross-over has the effect of moving the points rapidly on the fitness surface, while keeping the most stable bits constant and concentrating the exploration on the most undecided bits, the ones varying the most between members of the population. But if the similarity between parents is large, the cross-over will have little effect on the offspring, the final danger being that of a *premature convergence* of the population to a suboptimal point. The complexity inherent in explaining Darwinian metaphors for optimization makes one think whether more direct terms and definitions should be used [107] ("metaphors are not always rhetorically innocent").

At this point, you may wonder whether the term "team member" is justified in a basic GA algorithm. After all, each member is a very simple individual indeed, it comes to life through some randomized recombination of its parents and does a little exploration of its neighborhood. If it is lucky by encountering a better fitness value in the neighborhood, it has some probability to leave some of its genetic material to its offspring, otherwise it is terminated. No memory is kept of the individuals, only **a collective form of history is kept through the population**. Yes, "team member" *is* exaggerated. But now let's come back to the issue "airplanes do not flap their wings" to remember that as computer scientists and problem solvers our design freedom is limited only by our imagination.

We may imagine at least two different forms of *hybridized genetic algorithms*. The first observation is that, in order to deserve its name, a team member can execute a more directed and determined exploitation of its initial genetic content (its initial position). This is effected by considering the initial string as a *starting point* and by initiating a run of local search from this initial point, for example scouting for a local optimum. Lamarck can have his revenge here, now nobody prohibits substituting the initial individual with its ameliorated version after the local search. The term **memetic algorithms** [275, 241] has been introduced for models which combine the evolutionary adaptation of a population with individual learning within the lifetime of its members. The term derives from Dawkins' concept of a *meme* which is a unit of cultural evolution that can exhibit local refinement [112].

Actually, there are two obvious ways in which individual learning can be integrated: a first way consists of replacing the initial genotype with the better solution identified by local search (**Lamarckian evolution**), a second way can be of modifying the fitness by taking into account not the initial value but the final one obtained through local search. In other words, the fitness does not evaluate the initial state but the value of the "learning potential" of an individual, measured by the result obtained after the local search. This has the effect of changing the fitness landscape, while the resulting form of evolution is still Darwinian in nature. This and related forms of combinations of learning and evolution are known as the **Baldwin effect** [179, 381].

An interesting observation in [390] is that having two parents to generate a descendant may actually lead to less efficient algorithms with respect to simple versions of population-based algorithms in which each descendant has only one parent. Airplaned do not flap their wings to fly, in a similar manner efficient population-based algorithms do not need to imitate nature for the sake of imitating it, therefore leaving more freedom to the algorithm designer to experiment with effective novel ideas.



(a) Intelligent searchers

(b) Dumb searchers

Figure 39.3: Opportunities and pitfalls of teams of searchers: an intelligent searcher may decide to move between two successful ones (top panes), while dumb searchers (bottom) swarm to the same place, so that diversification can be lost. If you were a 49er, which model would you choose (and, besides, would you scream your findings)?

Gist

There is little doubt that considering **more search processes during optimization with some form of coordination** is a useful higher level, going beyond a single search process.

There are more **doubts on the intrinsic usefulness of specific analogies from nature**, genetics and evolution to develop effective state-of-the-art algorithms.

For sure, these analogies have a positive effect on the marketing of optimization and may help in converting new researchers to the growing area of optimization heuristics.

On the other hand, if one cares about scientific progress, one should be completely free to abandon analogies - based on nature or culture - in order to design the most effective algorithms.

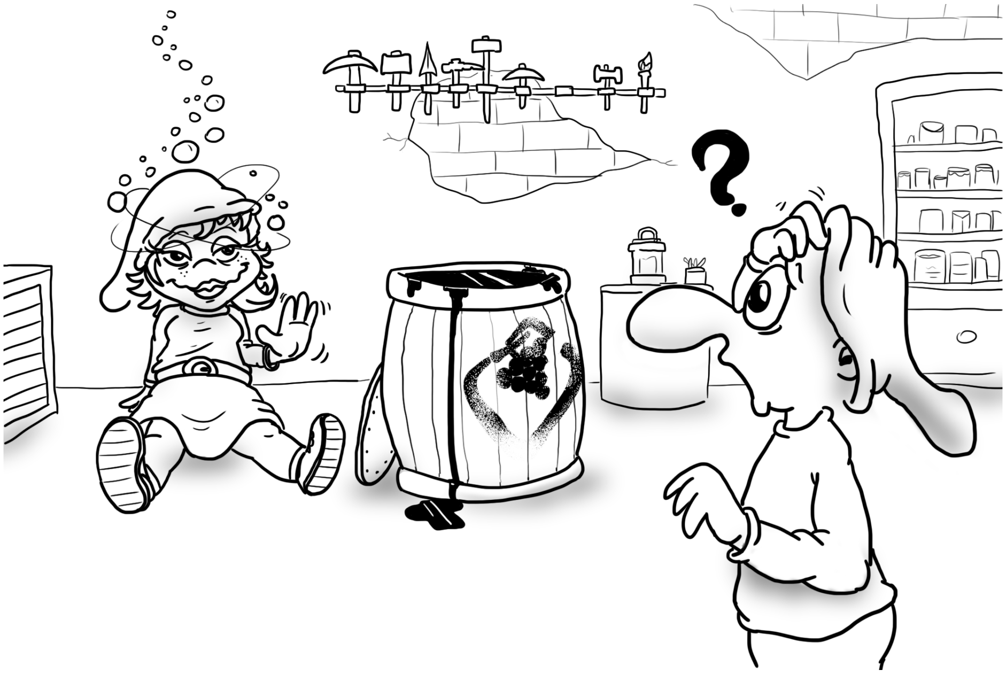
In particular, one should remember that viruses do not learn a lot while they are living, and that by using memory and machine learning strategies, one can greatly improve most primitive techniques, even if the final method does not use sex for mating individuals and is therefore less sexy.

Everybody would like that math studied during lifetime could be passed to his children via genes, but biological constraints so far failed to implement a Lamarckian mechanism: the passage occurs by more direct training mechanisms! Feel free to improve this sad state of affairs in your algorithms.

Chapter 40

Multi-Objective Optimization

Non si può avere la botte piena e la moglie ubriaca.
One cannot have a full wine-barrel and a drunk wife.
(Italian proverb)



Life is full of compromises, popular wisdom says that one cannot "ride two horses with one ass." Most of the real-world problem cannot be cast into the simple and mathematically crystal-clear form of minimizing a function $f(x)$.

There are two crucial difficulties. First, most problems have **more than one objective** to reach, to be maximized. This is the case in **multi-objective optimization problems** (**MOOP**), for which many *conflicting* objectives have to be traded off in selecting the preferred choice. Most real-world problems are of this kind. When you buy a car, you have different objectives in mind: speed, cost, size, etc. and you have your own way of weighing the different objectives. If you bought a Ferrari, your preferences are probably different from someone who bought a city car. If you are searching for a partner, different combinations of beauty and intelligence are available for the possible candidates

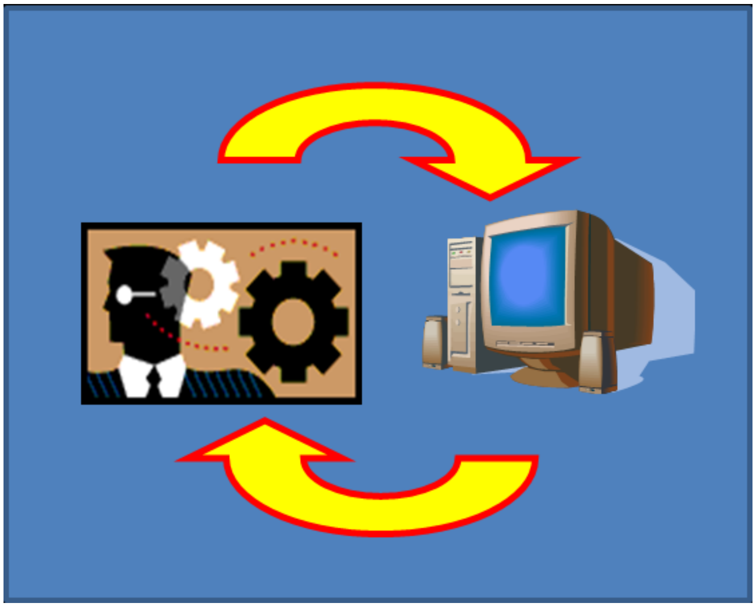


Figure 40.1: Problem solving and optimization frequently involves an iterative process with crucial learning steps.

(agreed, this is a coarse simplification!). Unfortunately, it is rare that a candidate simultaneously maximizes both parameters, **compromises and tradeoffs** must be accepted.

Even if an optimal abstract combination of two or more objectives into an overall *utility function* to be maximized exists, **obtaining a function in a closed mathematical form can be very difficult**, if not impossible. Try asking your best friend (better not to ask directly your partner): “Can you give me the utility function describing your best combination of beauty and intelligence?”, or, if you limit your model to linear combinations, “Can you tell me your weights to combine beauty and intelligence?” Problem solving and optimization techniques often deliver a large number of potential solutions. Design process innovation, virtual prototyping, business process engineering are some examples. The decision maker is left with the crucial task of identifying a preferred solution, taking into account explicitly defined objectives (one or more mathematical functions to maximize), hard and soft constraints, and **preferences which are not explicit but often crucial for an intelligent decision**.

Problem-solving is often an **iterative process with learning**, as illustrated in Fig. 40.1. A learning path occurs between two entities: the decision maker and the supporting software system. The decision maker analyzes some representative solutions, learning about concrete possibilities and updating his objectives. The software memorizes the user preferences and shifts the focus of attention to regions of the design/solution space which are deemed more relevant by the final user. The iterative process is continued until a satisfactory solution is found or patience is exhausted.

MORSO (multi-objective Reactive Search Optimization) denotes solution methods intended for **multi-objective optimization characterized by incremental and learning paths**. Learning takes places in the user mind and in the solution algorithms. A closely related term is that of interactive multi-objective optimization, but we intend to stress systematic, automated and online learning techniques in a more direct manner.

In the following sections, the concept of Pareto-optimality is formally defined in Sec. 40.1 and the main solution techniques are presented in Sec. 40.2. Finally, a way to keep the final decision maker in the loop as a provider of learning signals is illustrated in Sec. 40.4 about brain-computer optimization.

Figure 40.2: Individual objectives in Pareto-optimization are building blocks, but the preferred combination is not given (image courtesy of LEGO).

40.1 Multi-objective optimization and Pareto optimality

In the classic case of multi-objective optimization problems (MOOPs), the user specifies a set of m desirable objectives, but he does not spell out the tradeoffs, the relative importance of the different objectives, the proper combination of them into an overall utility function. A MOOP can be stated as:

$$\begin{array}{ll} \text{minimize} & \mathbf{f}(\mathbf{x}) = \{f_1(\mathbf{x}), \ldots, f_m(\mathbf{x})\} \\ \text{subject to} & \mathbf{x} \in \Omega, \end{array}$$

where $\mathbf{x} \in \mathbb{R}^n$ is a vector of n decision variables; $\Omega \subset \mathbb{R}^n$ is the *feasible region*, typically specified as a set of constraints on the decision variables. In the above example of looking for a suitable partner, Ω could be the set of all persons of a given sex (male or female) who can at least read and write. You will not even consider a partner who does not satisfy these constraints.

The vector $\mathbf{f} : \Omega \rightarrow \mathbb{R}^m$ is made of m objective functions which need to be jointly minimized[1]. Objective vectors are images of decision vectors and can be written as $\mathbf{z} = \mathbf{f}(\mathbf{x}) = \{f_1(\mathbf{x}), \ldots, f_m(\mathbf{x})\}$. The above problem is ill-posed whenever **objective functions are conflicting**, a frequent situation in real-world contexts. In these cases, an objective vector is considered optimal if none of its components can be improved without worsening at least one of the others. An objective vector $\mathbf{z}$ is said to *dominate* $\mathbf{z}'$, denoted as $\mathbf{z} \prec \mathbf{z}'$, if $z_k \leq z'_k$ for all k and there exist at least one h such that $z_h < z'_h$. A point $\hat{\mathbf{x}}$ is **Pareto-optimal** if there is no other $\mathbf{x} \in \Omega$ such that $\mathbf{f}(\mathbf{x})$ dominates $\mathbf{f}(\hat{\mathbf{x}})$. Fig. 40.3 illustrates the concept. The **Pareto frontier** (or Pareto front, **PF** for short) consists of all Pareto-optimal points. In the example, a partner is Pareto-optimal if no other partner is at the same time nicer *and* more intelligent, or nicer with the same intelligence level, etc. As you immediately recognize, considering only Pareto-optimal candidates makes sense: no rational person would ever prefer a dominated partner! By restricting attention to the Pareto frontier (the set of choices that are Pareto-efficient), a designer can make tradeoffs within this set, rather than considering the full range of every parameter. "Rob Peter to pay Paul" well expresses the concept related to modifying a solution in a way that makes some aspect better but some aspect worse, producing no net gain for all objectives.

Vilfredo Pareto had the courage to cross boundaries between disciplines. After graduating in Civil Engineering while working in Florence, he was among the first to analyze economic problems with mathematical tools [291]. In

[1] In the case of levels of beauty and intelligence, which must clearly be *maximized*, just minimize their opposites.

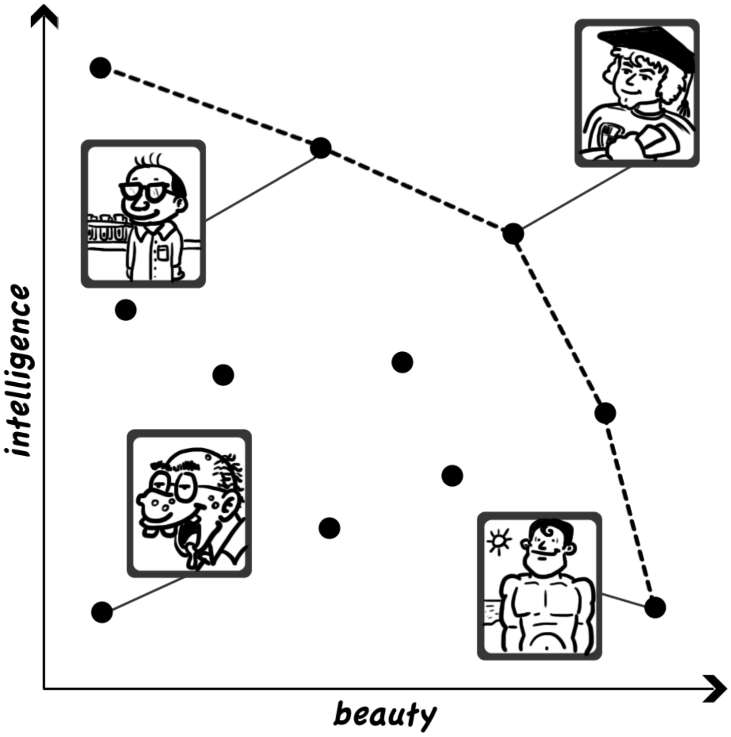


Figure 40.3: Pareto optimality. All dominated points like the persons in the middle are not considered as potential candidates for the final choice. On the Pareto frontier, shown with a dashed line, tradeoffs need to be considered.

1893, he became the Chair of Political Economy at the University of Lausanne in Switzerland, where he defined his concept of Pareto-optimality: "The optimum allocation of the resources of a society is not attained so long as it is possible to make at least one individual better off in his own estimation while keeping others as well off as before in their own estimation." After the translation of Pareto's Manual of Political Economy into English, Stadler [344] applied the notion of Pareto Optimality to the fields of engineering and science in the middle 1970's. Then the applications of multi-objective optimization in engineering design grew rapidly [123] and is now a tool used in most engineering companies.

Notable examples of Pareto-optimization are in economics (consumer demand and indifference curves, production possibilities frontier, macroeconomic policy-making), in finance (optimal portfolios maximizing return and minimizing risk, or variance of return), in engineering (engine design, controller design, product and process optimization, radio resource management, electric power systems, etc.).

40.2 Pareto-optimization: main solution techniques.

Let's mention some solution techniques to solve the MOOP defined in equation (40.1).

As mentioned, a Pareto-optimal solutions is one that cannot be improved in any of the objectives without degrading at least one of the other objectives. In mathematical terms, a feasible solution $x^1 \in \Omega$ is said to (Pareto) dominate another solution $x^2 \in \Omega$, if

$$f_i(x^1) \leq f_i(x^2) \text{for all indices} i \in \{1, 2, \ldots, k\}$$

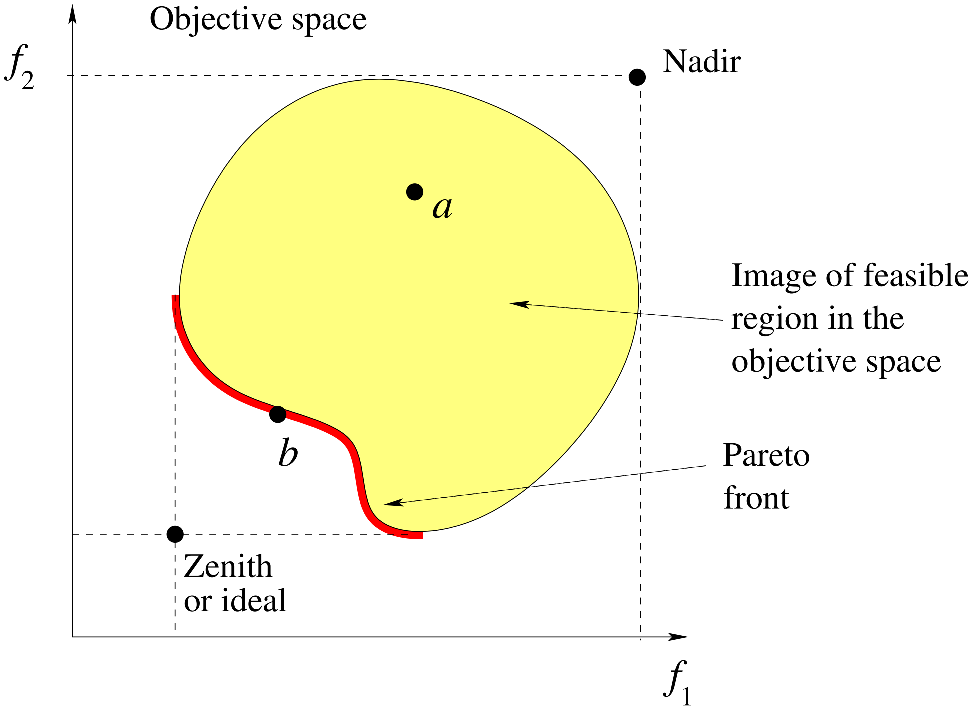


Figure 40.4: Point b belongs to the Pareto front: no other feasible solution is strictly better in one objective and at least as good for the other ones (here minimization is assumed). Point a doesn't.

and

$$f_j(x^1) < f_j(x^2)\text{for at least one index}j \in \{1, 2, \ldots, k\}\,.$$

A solution $x^1 \in \Omega$ is called Pareto optimal, if there does not exist another solution that dominates it.

The Pareto front of a multi-objective optimization problem is bounded by a so-called **nadir objective vector** z^{nad} and a **zenith** (or ideal) **objective vector** z^{zen}, defined as follows:

$$z_i^{\text{nad}} = \sup_{x \in X \text{ is Pareto optimal}} f_i(x) \text{ for all } i = 1, \ldots, k \tag{40.1}$$

$$z_i^{\text{zen}} = \inf_{x \in X} f_i(x) \text{ for all } i = 1, \ldots, k. \tag{40.2}$$

When finite, the components of a *nadir* and an *ideal* objective vector define upper and lower bounds for the objective function values of Pareto optimal solutions. The nadir objective vector can only be approximated as, typically, the whole Pareto optimal set is unknown. In addition, a **utopian objective vector** z^{utopian} can be defined because of numerical reasons as:

$$z_i^{\text{utopian}} = z_i^{\text{zen}} - \epsilon \text{ for all } i = 1, \ldots, k, \tag{40.3}$$

where $\epsilon > 0$ is a small constant.

A standard way to deal with multiple objective is to obtain a single one by combining them (this is called **aggregation by utility functions**, utility being the combined objective). **Linear scalarization** (also called **weighted-sum**) build a linear utility function. The aggregated problem to solve is defined as:

$$\min_{x \in X} \sum_{i=1}^{k} \lambda_i \, f_i(x), \tag{40.4}$$

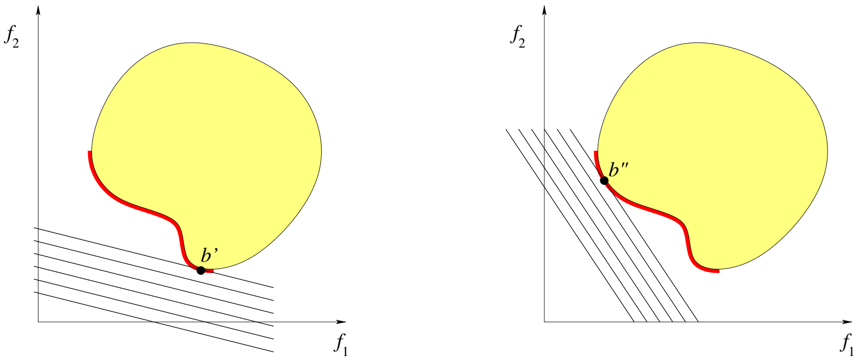


Figure 40.5: Two different scalarizations identify different preferred solutions on the PF.

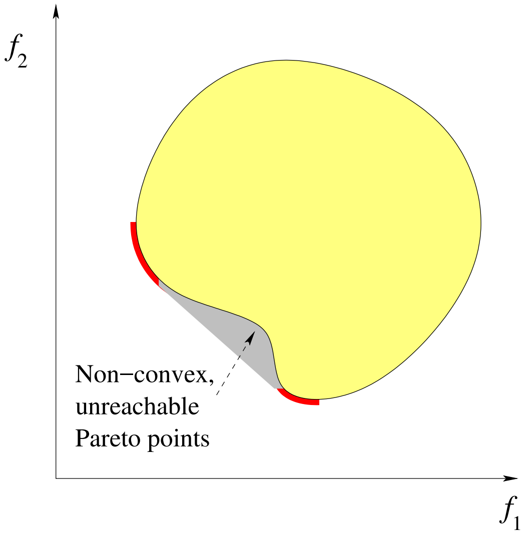


Figure 40.6: Scalarization cannot identify some Pareto-optimal solutions (unless the PF is convex).

where the weights of the objectives $\lambda_i > 0$ are the parameters ("weights") of the scalarization. Needless to say, the solution depends on the weights. Because what matters are relative sizes and not absolute values, weights are usually normalized: $\sum_{i=1}^{k} \lambda_i = 1$.

To visualize the process, one is approaching the Pareto front with a line (a plane, a hyperplane) oriented in a certain manner. When the line touches a Pareto-optimal solution, the contact point is picked as the preferred solution (Fig. 40.5). A Pareto optimal solution is called **supported-efficient** if it is an optimal solution to equation (40.4) with a particular weight vector [232]. If the Pareto-front is not convex, some Pareto-optimal solutions *cannot* be identified by solving (40.4) with some weights, so that the scalarization technique must be used with some care.

One can define a neighborhood of a locally or globally optimal solution to (40.4), and then identify more Pareto optimal solutions via some form of local search, with a reasonable amount of computational effort

In **Tchebycheff approach** [269] the scalar utility function is in the form:

$$\min_{x \in X} \max_{i=1}^{k} \{\lambda_i |f_i(x) \; - \; z^{ideal}{}_i|\}, \tag{40.5}$$

where z^{ideal} is the reference point defined above. For each Pareto-optimal point x^* there exists a weight vector such that x^* is the optimal solution of (40.5) and each optimal solution of (40.5) is a Pareto optimal solution. One weakness with this approach is that its aggregation function is not smooth for a continuous MOOP, and the simpler scalarization is often preferred.

To obtain an approximation to the PF via a certain number of Pareto-optimal points, one can solve **a set of the above single objective problems** with different carefully selected weight coefficient vectors. This **decomposition** idea has been successfully used in MOEA/D [389]. MOEA/D decomposes a multiobjective optimization problem into a number of scalar optimization subproblems, using a set of different weight vectors λ, one for each scalarized problem, and optimizes them simultaneously (Fig.40.7). By modifying local search to consider Pareto-optimality and the existence of more Pareto-optimal solutions, each subproblem can be improved in an iterative manner by using information from its several neighboring subproblems. A subproblem is a neighbor if their defining weight vectors are close.

Pareto local search (PLS) is a natural extension of single objective local search methods [290, 257]. It works with a set of mutually nondominated solutions, explores some or all of the neighbors of these solutions to find new solutions for updating this set at each iteration. PLS exploits local search algorithms for single-objective problems, and solves a multi-objective problem by **chains of related aggregations** and **chains of good solutions** for aggregations. Good solutions provide starting points for a search regarding a next aggregation. After finding an initial set of supported efficient solutions, the objective is to identify *non-supported* efficient solutions located between the supported efficient ones. In PLS, the neighborhood of every solution of a population is explored, and *if the neighbor is not dominated* by a solution of the list, the neighbor is added to the population. The exclusion of dominated neighbors is the basic modification w.r.t. standard LS.

The work [232] combines ideas from evolutionary algorithms, decomposition approaches, and **Pareto local search**. It suggests a simple yet efficient memetic algorithm for combinatorial multiobjective optimization problems: **memetic algorithm based on decomposition (MOMAD)**. It decomposes a combinatorial multiobjective problem into a number of single objective optimization problems using an aggregation method. MOMAD evolves three populations: 1) population PL for recording the current solution to each subproblem; 2) population PP for storing starting solutions for Pareto local search; and 3) an external population PE for maintaining all the nondominated solutions found so far during the search. At each generation, a Pareto local search method is first applied to search a neighborhood of each solution in PP to update PL and PE. Then a single objective local search is applied to each perturbed solution in PL for improving PL and PE, and reinitializing PP. MOMAD provides a generic hybrid multiobjective algorithmic framework in which problem specific knowledge, well developed single objective local search and Pareto local search methods can be hybridized. It is a population-based iterative method and thus an anytime algorithm.

40.3 MOOPs: how to get missing information and identify user preferences

Pareto-optimization is caused by **lack of complete information** in the definition of the problem. Some information is present, given by a set of positive objectives to reach (the individual $f_i(x)$ functions, a sort of "building blocks"), but information about how the different objectives have to be combined is missing. The tradeoffs are not yet solved, otherwise one would come up with a single combined objective.

When discussing about **the role of the final user (decision maker) in providing information to pick a preferred solution** among the Pareto front, one distinguishes the three following possibilities.

- **A priori methods** require that sufficient preference information is expressed before the solution process for example by picking weights in the the linearly-scalarized utility function method of equation (40.4), or by setting the goal in **goal programming** [251, 81]. In goal programming, a desired target is set for the solution vector, the single-objective problem associated becomes that of minimizing the deviation between the obtained solution and the target (deviation measured with a suitable metric). The drawback of *a priori* methods is that the DM often does not know before how realistic his expectations are, and that there are no subsequent learning possibilities.

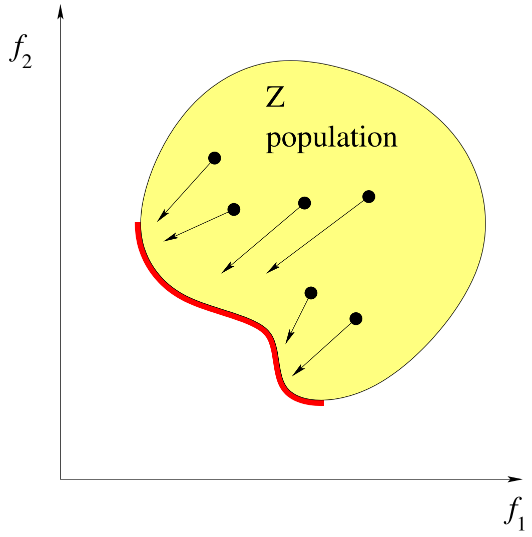


Figure 40.7: Population-based approaches (e.g., based on decomposition) can be used to obtain a set of representative solutions along the Pareto-front. The differens subproblems are iteratively improved to move them closer to the PF.

- **A posteriori methods** aim at producing all the Pareto optimal solutions or a representative subset thereof. The set is then presented to the decision maker (DM) for selecting the preferred solution. These methods demand a lot of computing and place a heavy burden on the shoulders of the DM. A human person can typically choose one among a limited set (say 10) solution, but he has difficulty in choosing one among one million of alternatives!

- In **Interactive methods**, the solution process is iterative and the decision maker continuously interacts with the method when searching for the most preferred solution. The decision maker is expected to express preferences at each iteration in order to get Pareto optimal solutions that are of interest to him and **learn what kind of solutions are attainable**.

40.4 Brain-computer optimization (BCO): the user in the loop

As mentioned, asking a user to quantify his **utility function** (for example by choosing weights of a linear combination of the different objectives) *a priori*, before seeing the actual optimization results, is challenging. If the final user is cooperating with an optimization expert, misunderstanding between the persons may arise. This problem can become dramatic when the number of the conflicting objectives in MOOP increases. As a consequence, the final user may be dissatisfied with the solutions, because some of the objectives remain hidden in his mind. Different drawbacks are present in *a posteriori* approaches, which deliver to the final user a representative set of solutions on the entire Pareto front so that he can pick his most preferred solution.

Although a user may have difficulties in providing explicit weights and mathematical formulas, for sure he can *evaluate the returned solutions*. In most cases, the situation improves with **an interactive process between the final user and the optimizer to change the definition of the problem**. The optimizer will then be run over the new version of the problem. This process may be iterated an arbitrary number of times, as shown in Fig. 40.1.

We are now entering the most advanced and exciting topic of this book: the integration of analytics, visualization and optimization. Abstract solution points are vectors of numbers which convey a specific **meaning**.

In **interactive problem-solving** sessions, the user can get information about a specific solution by calling a problem-specific routine. This routine, which has to be provided for the different applications, can be used to visualize detailed information about a specific point, e.g., through a graphical display of a solution.

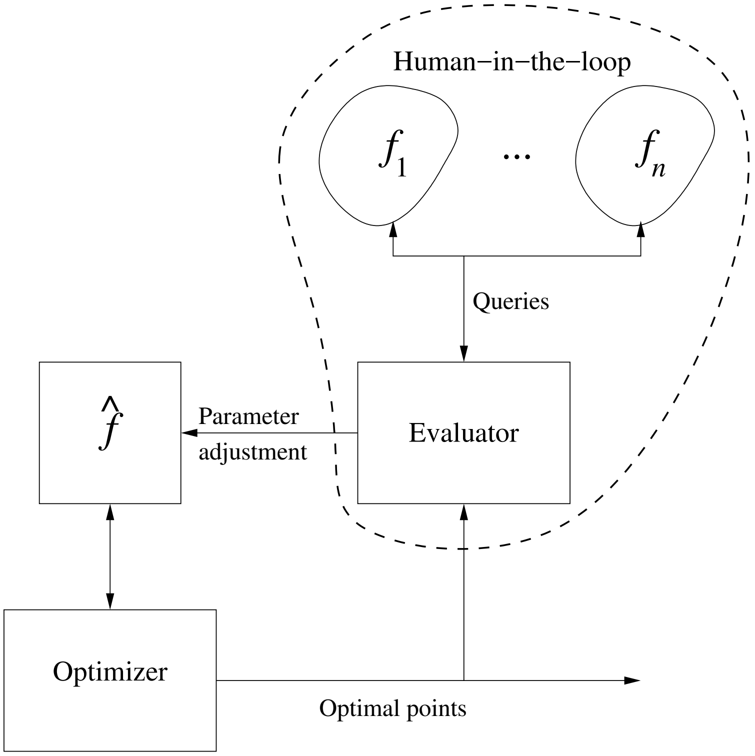


Figure 40.8: Brain-Computer Optimization: learning the problem definition from the final user in the case of interactive multi-objective optimization (adapted from [28]).

The same problem-specific routine can be used to accept **feedback** about the specific solution, such as a personal evaluation, as illustrated in Fig. 40.8.

As a rule of thumb, most of the problem-solving effort in the real world is spent on **defining the problem**, on specifying in a computable manner the function to be optimized. After this modeling work is completed, optimization becomes in certain cases a commodity. The implication for researchers and developers is that much more effort should be devoted to design supporting techniques and tools to help the final user, often without expertise in mathematics and in optimization, to define and refine the function to be optimized so that it corresponds to his real objectives. Think about defining your favorite weights for beauty versus intelligence while searching for a partner. If somebody asks you for quantitative ways to specify the tradeoff before starting the search, you may feel very embarrassed (we hope!). Only after seeing some examples you may clarify your weights and objectives.

Reactive Search Optimization is dedicated to online learning techniques to support the quest for a solution by **self-adapting a local search method in a manner depending on the previous history of the search**. The learning signals consist of data about the structural characteristics of the instance collected while the algorithm is running. For example, data about sizes of basins of attraction, entrapment of trajectories, repetitions of previously visited configurations. The algorithm learns by interacting with a previously unknown environment given by an existing (and fixed) problem definition.

We argue that there is a second interesting online learning loop, where learning signals originate from a final user and are intended to **modify and refine the problem definition** itself. This context is potentially very wide, depending on the amount of knowledge about the problem given *a priori*, on the allowed modifications, on the kind of questions asked.

An example of Interactive Multi-Objective Optimization with RSO is described in [28]. The methods share with the work in [395, 113, 346] the interaction with the final user realized via pairwise comparison of solutions, but tackle a broader class of problems with nonlinear preference functions. This case is of interest because many (maybe most) decision problems are *nonlinear*, to reflect our preference for reasonable compromise solutions. A presentation of the state of the art for learning arbitrary (*nonlinear*) models is in [32].

We focus here on the simpler and classical linear case [28] and the goal consists of **learning the non-dominated solution preferred by the final user**. Assume that the user provides the different objectives in the MOOP problem, but he cannot quantify the **weights** of the different objectives before seeing the actual optimization results. The system aims at learning the weights vector $\boldsymbol{w} = (w_1, w_2, \ldots, w_m)$ optimizing the linear combination g:

$$g(\boldsymbol{x}, \boldsymbol{w}) = w_1 f_1(\boldsymbol{x}) + w_2 f_2(\boldsymbol{x}) + \cdots + w_m f_m(\boldsymbol{x}).$$

In a more compact form:

$$g(x_1, x_2, \ldots, x_n, \boldsymbol{w}) = \boldsymbol{f}(\boldsymbol{x})^T \boldsymbol{w},$$

where $\boldsymbol{f} = (f_1, f_2, \ldots, f_m)$. Without loss of generality, assume that g must be minimized.

The feedback from the decision maker at each iteration is obtained by presenting two solutions and asking him to indicate his favorite solution between them, if any. This is the simplest question to be asked, a qualitative overall preference. If the decision maker cannot answer, he should probably get another job. The preferences stated by the final user are translated into *constraints* that the weights must satisfy. This guarantees that the obtained utility function is consistent with the user's judgments. If $\boldsymbol{a} = (a_1, a_2, \ldots, a_n)$ and $\boldsymbol{b} = (b_1, b_2, \ldots, b_n)$ are the two solutions provided by the system, the preference $\boldsymbol{a} \prec \boldsymbol{b}$ of the final user for the solution **a** with respect to the solution **b** is represented by the following constraint:

$$g(\boldsymbol{a}, \boldsymbol{w}) < g(\boldsymbol{b}, \boldsymbol{w}).$$

Therefore, a new linear constraint on the weights is generated for each question asked to the final user. The problem of learning the user preference then becomes that of finding a solution $\boldsymbol{w}$ for the set of constraints on the weights generated by the user's feedback.

The weights are initialized with random values in the interval (0,1), and then normalized so that their sum is 1. At each iteration, two non-dominated solutions $\boldsymbol{a}$ and $\boldsymbol{b}$ are compared by the final user. Both solutions are obtained by minimizing a linear combination of the objective functions of the input problem:

$$\min_{\boldsymbol{x}} g(\boldsymbol{x}, \boldsymbol{w}).$$

In particular, the first solution **a** is obtained by using the current weights vector $\boldsymbol{w}^{\text{curr}}$ found by applying the *middlemost weights* technique [297], by solving the following linear programming problem:

$$\begin{array}{ll} \max\limits_{\boldsymbol{w}} & \gamma \\ \text{subject to} & \begin{cases} g(\boldsymbol{a}, \boldsymbol{w}) \leq g(\boldsymbol{b}, \boldsymbol{w}) - \gamma & \forall \boldsymbol{a} \prec \boldsymbol{b} \\ w_i \geq \gamma & \forall i = 1, \ldots, m \\ \gamma \geq 0. \end{cases} \end{array}$$

The meaning of the above is to search for a weight which is *consistent* but also *far from the boundaries* of the consistent region. The bigger the positive γ parameter, the safer the inequalities. Even if limited noise is added (for example caused by physical quantities with measurements errors) and the g values are slightly changed, there is still a *safety margin* before the direction of the inequality is changed.

The second solution **b** can be obtained by using the weights vector $\boldsymbol{w}^{\text{pert}}$, generated by perturbing $\boldsymbol{w}^{\text{curr}}$, and by ensuring that the two generated solutions are sufficiently dissimilar. Issues related to considering possible infeasible sets of linear constraints (which can be generated by a confused decision maker, or because a linear approximation is a too rough) are considered in [28]. The more complex non-linear case is solved with machine learning techniques based on the Support Vector Machine method in [32].

A novel approach based on active learning of Pareto fronts (ALP) is presented in [74]. ALP casts the identification of the Pareto front into a supervised machine learning task. The computational effort in generating the supervised information is reduced by an active learning strategy. In particular, the model is learned from a set of informative training objective vectors.

To finish this introductory presentation, remember, if you have a challenging problem to solve, the *source of power of intelligent optimization* will help you both to *define* exactly what you want to accomplish and to actually *compute* one or more solutions.

In many cases some decisions can be, and maybe should be, deferred until some initial possible solutions are evaluated by an expert user.

Gist

When visiting a business as a consultant, a healthy carrier of the traditional math-oriented approach to optimization will ask the typical question “What is the function that you want to optimize in your business?” By “function” he means an explicit mathematical model, a formula relating inputs (decisions to be made) to output (like profit) without any ambiguity. This attitude and the lack of clearly defined models for most businesses probably explains why the power of optimization is still stifled in the real world.

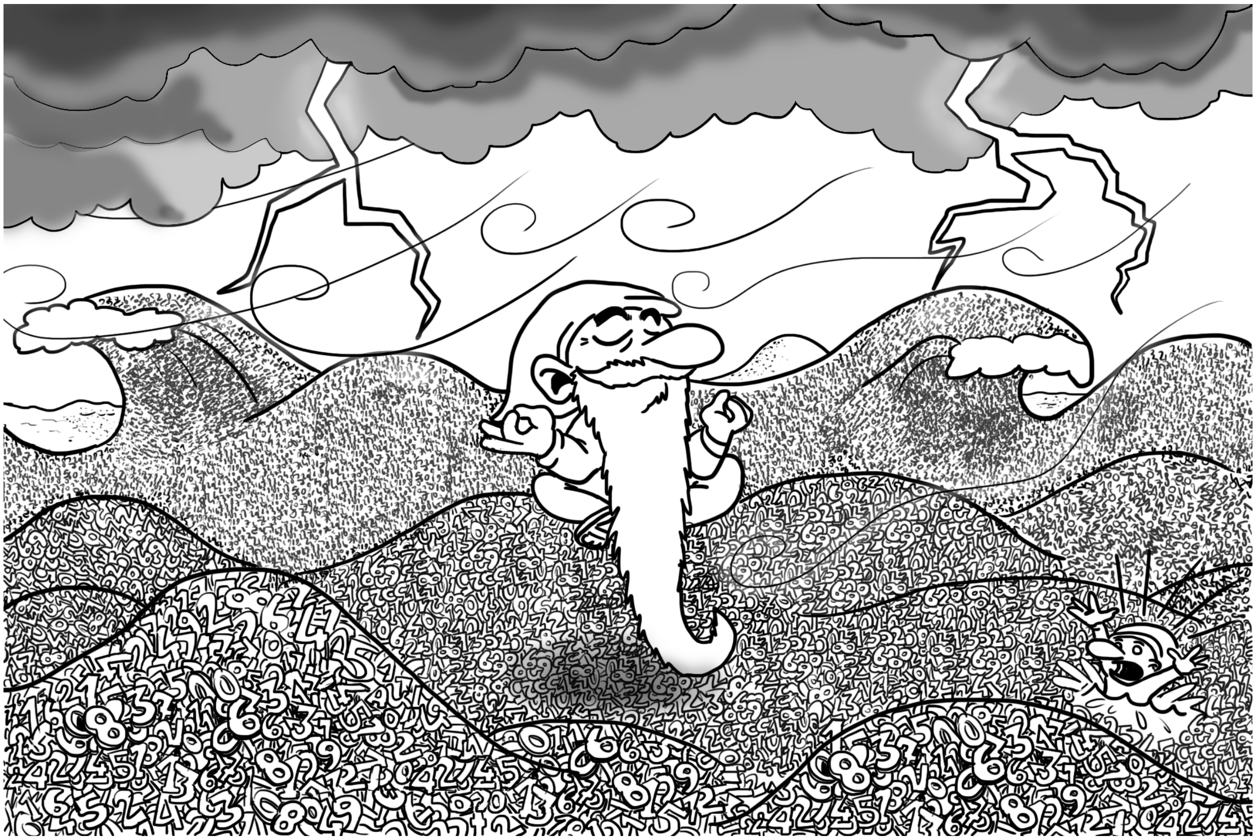
After the business owner tells him “Sorry, I have no mathematical function,” the **LION way** opens a window of hope and opportunity to unleash the power of optimization. He can reply with “Do not worry, even if you cannot give me your model, I can build it for you **from your data and your feedback**.” Using a personal computer to support decision-making should not lead you to scrap your expert personal brain.

Most problem-solving and optimization efforts are intrinsically **iterative processes with learning involved**, learning from data, and learning from the decision makers. When this is acknowledged, a bright new era of opportunities is ushered in. A lot of effort is still required, which is *good* news for data scientists, but the road ahead is mapped.

Chapter 41

Conclusion

Rem tene, verba sequentur
Master the data, verbal interpretations will follow
(attributed to Cicero and Cato)



Congratulations for reaching this point. You have now in your pockets powerful tools to build models from data, to understand and explain, to identify improvements and to create disruptive new solutions, in a never-ending loop leading to better products and better services.

It is time to read the introduction again, and check if it means something different now. Contact or visit us, we are happy to know that there are other *sane* people with a *insane* passion for data mining, building models, optimizing, and developing new ideas and business methods in the process.

Exit your building and use your knowledge to build a better world.

Figure 41.1: Ciclo dei mesi, Trento, January, circa 1397

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