Introduction to Python for Econometrics, Statistics and Data Analysis

4th Edition

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Solutions and Other Material

Solutions

Solutions for exercises and some extended examples are available on GitHub.
`https://github.com/bashtage/python-for-econometrics-statistics-data-analysis`

Introductory Course

A self-paced introductory course is available on GitHub in the course/introduction folder. Solutions are available in the solutions/introduction folder.
`https://github.com/bashtage/python-introduction/`

Video Demonstrations

The introductory course is accompanied by video demonstrations of each lesson on YouTube.
`https://www.youtube.com/playlist?list=PLVR_rJLcetzkqoeuhpIXmG9uQCtSoGBz1`

Using Python for Financial Econometrics

A self-paced course that shows how Python can be used in econometric analysis, with an emphasis on financial econometrics, is also available on GitHub in the course/autumn and course/winter folders.
`https://github.com/bashtage/python-introduction/`

Changes

Changes since the Fourth Edition

- Added a discussion of context managers using the `with` statement.

- Switched examples to prefer the context manager syntax to reflect best practices.

Notes to the Fourth Edition

Changes in the Fourth Edition

- Python 3.8 is the recommended version. The notes require Python 3.6 or later, and all references to Python 2.7 have been removed.

- Removed references to NumPy's `matrix` class and clarified that it should not be used.

- Verified that all code and examples work correctly against 2020 versions of modules. The notable packages and their versions are:

  - Python 3.8 (Preferred version), 3.6 (Minimum version)
  - NumPy: 1.19.1
  - SciPy: 1.5.3
  - pandas: 1.1
  - matplotlib: 3.3

- Expanded description of model classes and statistical tests in statsmodels that are most relevant for econometrics. TODO

- Expanded the list of packages of interest to researchers working in statistics, econometrics and machine learning. TODO

- Introduced f-Strings in Section 21.3.3 as the preferred way to format strings using modern Python.

- Added `minimize` as the preferred interface for non-linear function optimization in Chapter 20. TODO

Changes since the Third Edition

- Verified that all code and examples work correctly against 2019 versions of modules. The notable packages and their versions are:

  - Python 3.7 (Preferred version)
  - NumPy: 1.16
  - SciPy: 1.3
  - pandas: 0.25
  - matplotlib: 3.1

- Python 2.7 support has been officially dropped, although most examples continue to work with 2.7. **Do not Python 2.7 in 2019 for numerical code**.

- Small typo fixes, thanks to Marton Huebler.

- Fixed direct download of FRED data due to API changes, thanks to Jesper Termansen.

- Thanks for Bill Tubbs for a detailed read and multiple typo reports.

- Updated to changes in line profiler (see Ch. 23)

- Updated deprecations in pandas.

- Removed `hold` from plotting chapter since this is no longer required.

- Thanks for Gen Li for multiple typo reports.

- Tested all code on Pyton 3.6. Code has been tested against the current set of modules installed by conda as of February 2018. The notable packages and their versions are:

    - NumPy: 1.13
    - Pandas: 0.22

Notes to the Third Edition

This edition includes the following changes from the second edition (August 2014).

Changes in the Third Edition

- Rewritten installation section focused exclusively on using Continuum's Anaconda.

- Python 3.5 is the default version of Python instead of 2.7. Python 3.5 (or newer) is well supported by the Python packages required to analyze data and perform statistical analysis, and bring some new useful features, such as a new operator for matrix multiplication (`@`).

- Removed distinction between integers and longs in built-in data types chapter. This distinction is only relevant for Python 2.7.

- `dot` has been removed from most examples and replaced with `@` to produce more readable code.

- Split Cython and Numba into separate chapters to highlight the improved capabilities of Numba.

- Verified all code working on current versions of core libraries using Python 3.5.

- pandas

  - Updated syntax of pandas functions such as `resample`.
  - Added pandas `Categorical`.
  - Expanded coverage of pandas `groupby`.
  - Expanded coverage of date and time data types and functions.

- New chapter introducing statsmodels, a package that facilitates statistical analysis of data. statsmodels includes regression analysis, Generalized Linear Models (GLM) and time-series analysis using ARIMA models.

Changes since the Second Edition

- Fixed typos reported by a reader – thanks to Ilya Sorvachev

- Code verified against Anaconda 2.0.1.

- Added diagnostic tools and a simple method to use external code in the Cython section.

- Updated the Numba section to reflect recent changes.

- Fixed some typos in the chapter on Performance and Optimization.

- Added examples of joblib and IPython's cluster to the chapter on running code in parallel.

- New chapter introducing object-oriented programming as a method to provide structure and organization to related code.

- Added seaborn to the recommended package list, and have included it be default in the graphics chapter.

- Based on experience teaching Python to economics students, the recommended installation has been simplified by removing the suggestion to use virtual environment. The discussion of virtual environments as been moved to the appendix.

- Rewrote parts of the pandas chapter.

- Changed the Anaconda install to use both create and install, which shows how to install additional packages.

- Fixed some missing packages in the direct install.

- Changed the configuration of IPython to reflect best practices.

- Added subsection covering IPython profiles.

- Small section about Spyder as a good starting IDE.

Notes to the Second Edition

This edition includes the following changes from the first edition (March 2012).

Changes in the Second Edition

- The preferred installation method is now Continuum Analytics' Anaconda. Anaconda is a complete scientific stack and is available for all major platforms.

- New chapter on pandas. pandas provides a simple but powerful tool to manage data and perform preliminary analysis. It also greatly simplifies importing and exporting data.

- New chapter on advanced selection of elements from an array.

- Numba provides just-in-time compilation for numeric Python code which often produces large performance gains when pure NumPy solutions are not available (e.g. looping code).

- Dictionary, set and tuple comprehensions

- Numerous typos

- All code has been verified working against Anaconda 1.7.0.

Contents

Chapter 1

Introduction

1.1 Background

These notes are designed for someone new to statistical computing wishing to develop a set of skills necessary to perform original research using Python. They should also be useful for students, researchers or practitioners who require a versatile platform for econometrics, statistics or general numerical analysis (e.g. numeric solutions to economic models or model simulation).

Python is a popular general–purpose programming language that is well suited to a wide range of problems.[1] Recent developments have extended Python's range of applicability to econometrics, statistics, and general numerical analysis. Python – with the right set of add-ons – is comparable to domain-specific languages such as R, MATLAB or Julia. If you are wondering whether you should bother with Python (or another language), an incomplete list of considerations includes:

You might want to consider R if:

- You want to apply statistical methods. The statistics library of R is second to none, and R is clearly at the forefront of new statistical algorithm development – meaning you are most likely to find that new(ish) procedure in R.

- Performance is of secondary importance.

- Free is important.

You might want to consider MATLAB if:

- Commercial support and a clear channel to report issues is important.

- Documentation and organization of modules are more important than the breadth of algorithms available.

- Performance is an important concern. MATLAB has optimizations, such as Just-in-Time (JIT) compilation of loops, which is not automatically available in most other packages.

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[1] According to the ranking on `http://www.tiobe.com/tiobe-index/`, Python is the 5th most popular language. `http://langpop.corger.nl/` ranks Python as 4th or 5th.

You might want to consider Julia if:

- Performance in an interactive based language is your most important concern.

- You don't mind learning enough Python to interface with Python packages. The Julia ecosystem is less complete than Python and a bridge to Python is used to provide missing features.

- You like to do most things yourself or you are on the bleeding edge and so existing libraries do not exist with the features you require.

Having read the reasons to choose another package, you may wonder why you should consider Python.

- You need a language which can act as an end-to-end solution that allows access to web-based services, database servers, data management and processing and statistical computation. Python can even be used to write server-side apps such as a dynamic website (see e.g. http://stackoverflow.com), apps for desktop-class operating systems with graphical user interfaces, or apps for tablets and phones apps (iOS and Android).

- Data handling and manipulation – especially cleaning and reformatting – is an important concern. Python is substantially more capable at data set construction than either R or MATLAB.

- Performance is a concern, but not at the top of the list.[2]

- Free is an important consideration – Python can be freely deployed, even to 100s of servers in on a cloud-based cluster (e.g. Amazon Web Services, Google Compute or Azure).

- Knowledge of Python, as a general purpose language, is complementary to R/MATLAB/Julia/Ox/-GAUSS/Stata.

1.2 Conventions

These notes will follow two conventions.

1. Code blocks will be used throughout.

```python
"""A docstring
"""

# Comments appear in a different color

# Reserved keywords are highlighted
and as assert break class continue def del elif else
except exec finally for from global if import in is
lambda not or pass print raise return try while with yield

# Common functions and classes are highlighted in a
# different color. Note that these are not reserved,
# and can be used although best practice would be
# to avoid them if possible
array range list True False None

# Long lines are indented
some_text = 'This is a very, very, very, very, very, very, very, very, very, very,
    very, very long line.'
```

---

[2]Python performance can be made arbitrarily close to C using a variety of methods, including numba (pure python), Cython (C/Python creole language) or directly calling C code. Moreover, recent advances have substantially closed the gap with respect to other Just-in-Time compiled languages such as MATLAB.

2. When a code block contains >>>, this indicates that the command is running an interactive IPython session. Output will often appear after the console command, and will *not* be preceded by a command indicator.

```
>>> x = 1.0
>>> x + 2
3.0
```

If the code block does not contain the console session indicator, the code contained in the block is intended to be executed in a standalone Python file.

```python
import numpy as np

x = np.array([1,2,3,4])
y = np.sum(x)
print(x)
print(y)
```

1.3 Important Components of the Python Scientific Stack

1.3.1 Python

Python 3.6 (or later) is required, and Python 3.8 (the latest release) is recommended. This provides the core Python interpreter.

1.3.2 NumPy

NumPy provides a set of array data types which are essential for statistics, econometrics and data analysis.

1.3.3 SciPy

SciPy contains a large number of routines needed for analysis of data. The most important include a wide range of random number generators, linear algebra routines, and optimizers. SciPy depends on NumPy.

1.3.4 Jupyter and IPython

IPython provides an interactive Python environment which enhances productivity when developing code or performing interactive data analysis. Jupyter provides a generic set of infrastructure that enables IPython to be run in a variety of settings including an improved console (QtConsole) or in an interactive web-browser based notebook.

1.3.5 matplotlib and seaborn

matplotlib provides a plotting environment for 2D plots, with limited support for 3D plotting. seaborn is a Python package that improves the default appearance of matplotlib plots without any additional code.

1.3.6 pandas

pandas provides high-performance data structures and is essential when working with data.

1.3.7   statsmodels

statsmodels is pandas-aware and provides models used in the statistical analysis of data including linear regression, Generalized Linear Models (GLMs), and time-series models (e.g., ARIMA).

1.3.8   Performance Modules

A number of modules are available to help with performance. These include Cython and Numba. Cython is a Python module which facilitates using a Python-like language to write functions that can be compiled to native (C code) Python extensions. Numba uses a method of just-in-time compilation to translate a subset of Python to native code using Low-Level Virtual Machine (LLVM).

1.4   Setup

The recommended method to install the Python scientific stack is to use Continuum Analytics' Anaconda. Appendix **??** describes a more complex installation procedure with instructions for directly installing Python and the required modules when it is not possible to install Anaconda.

Continuum Analytics' Anaconda

Anaconda, a free product of Continuum Analytics (www.continuum.io), is a virtually complete scientific stack for Python. It includes both the core Python interpreter and standard libraries as well as most modules required for data analysis. Anaconda is free to use and modules for accelerating the performance of linear algebra on Intel processors using the Math Kernel Library (MKL) are provided. Continuum Analytics also provides other high-performance modules for reading large data files or using the GPU to further accelerate performance for an additional, modest charge. Most importantly, installation is extraordinarily easy on Windows, Linux, and OS X. Anaconda is also simple to update to the latest version using

```
conda update conda
conda update anaconda
```

Windows

Installation on Windows requires downloading the installer and running. Anaconda comes in both Python 2.7 and 3.x flavors, and the latest Python 3.x is required. These instructions use ANACONDA to indicate the Anaconda installation directory (e.g., the default is C:\Anaconda). Once the setup has completed, open a PowerShell command prompt and run

```
cd ANACONDA\Scripts
conda init powershell
conda update conda
conda update anaconda
conda install html5lib seaborn jupyterlab
```

which will first ensure that Anaconda is up-to-date. `conda install` can be used later to install other packages that may be of interest. Note that if Anaconda is installed into a directory other than the default, the full path should not contain Unicode characters or spaces.

Notes

The recommended settings for installing Anaconda on Windows are:

- Install for all users, which requires admin privileges. If these are not available, then choose the "Just for me" option, but be aware of installing on a path that contains non-ASCII characters which can cause issues.

- Run `conda init powershell` to ensure that Anaconda commands can be run from the PowerShell prompt.

- Register Anaconda as the system Python unless you have a specific reason not to (unlikely).

Linux and OS X

Installation on Linux requires executing

```
bash Anaconda3-x.y.z-Linux-ISA.sh
```

where `x.y.z` will depend on the version being installed and `ISA` will be either x86 or more likely x86_64. Anaconda comes in both Python 2.7 and 3.x flavors, and the latest Python 3.x is required. The OS X installer is available either in a GUI installed (pkg format) or as a bash installer which is installed in an identical manner to the Linux installation. It is strongly recommended that the anaconda/bin is prepended to the path. This can be performed in a session-by-session basis by entering `conda init bash` and then restarting your terminal. Note that other shells such as zsh are also supported, and can be initialized by replacing bash with the name of your preferred shell.

After installation completes, execute

```
conda update conda
conda update anaconda
conda install html5lib seaborn jupyterlab
```

which will first ensure that Anaconda is up-to-date and then install some optional modules. `conda install` can be used later to install other packages that may be of interest.

Notes

All instructions for OS X and Linux assume that `conda init bash` has been run. If this is not the case, it is necessary to run

```
cd ANACONDA
cd bin
```

and then all commands must be prepended by a `.` as in

```
./conda update conda
```

1.5 Using Python

Python can be programmed using an interactive session using IPython or by directly executing Python scripts – text files that end with the extension .py – using the Python interpreter.

1.5.1 Python and IPython

Most of this introduction focuses on interactive programming, which has some distinct advantages when learning a language. The standard Python interactive console is very basic and does not support useful features such as tab completion. IPython, and especially the QtConsole version of IPython, transforms the console into a highly productive environment which supports a number of useful features:

- Tab completion - After entering 1 or more characters, pressing the tab button will bring up a list of functions, packages, and variables which match the typed text. If the list of matches is large, pressing tab again allows the arrow keys can be used to browse and select a completion.

- "Magic" function which make tasks such as navigating the local file system (using `%cd ~/directory/` or just `cd ~/directory/` assuming that `%automagic` is on) or running other Python programs (using `run program.py`) simple. Entering `%magic` inside and IPython session will produce a detailed description of the available functions. Alternatively, `%lsmagic` produces a succinct list of available magic commands. The most useful magic functions are

  - `cd` - change directory
  - `edit` *filename* - launch an editor to edit *filename*
  - `ls` or `ls` *pattern* - list the contents of a directory
  - `run` filename - run the Python file *filename*
  - `timeit` - time the execution of a piece of code or function
  - `history` - view commands recently run. When used with the `-1` switch, the history of previous sessions can be viewed (e.g., `history -1 100` will show the most recent 100 commands irrespective of whether they were entered in the current IPython session of a previous one).

- Integrated help - When using the QtConsole, calling a function provides a view of the top of the help function. For example, entering `mean (` will produce a view of the top 20 lines of its help text.

- Inline figures - Both the QtConsole and the notebook can also display figure inline which produces a tidy, self-contained environment. This can be enabled by entering `%matplotlib inline` in an IPython session.

- The special variable _ contains the last result in the console, and so the most recent result can be saved to a new variable using the syntax `x = _`.

- Support for profiles, which provide further customization of sessions.

1.5.2 Launching IPython

OS X and Linux

IPython can be started by running

```
ipython
```

in the terminal. IPython using the QtConsole can be started using

```
jupyter qtconsole
```

A single line launcher on OS X or Linux can be constructed using

```
bash -c "jupyter qtconsole"
```
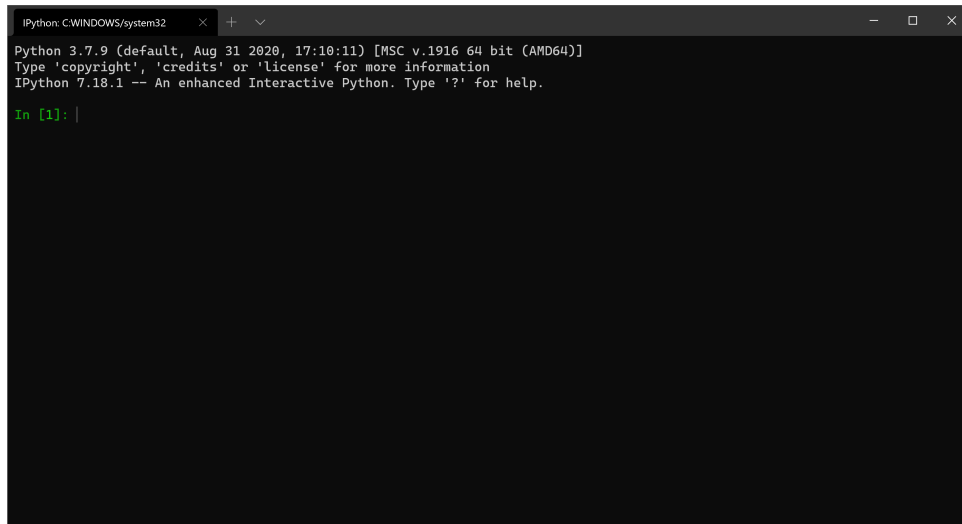
Figure 1.1: IPython running in the Windows Terminal app.

This single line launcher can be saved as *filename*.command where *filename* is a meaningful name (e.g. IPython-Terminal) to create a launcher on OS X by entering the command

```
chmod 755 /FULL/PATH/TO/filename.command
```

The same command can to create a Desktop launcher on Ubuntu by running

```
sudo apt-get install --no-install-recommends gnome-panel
gnome-desktop-item-edit ~/Desktop/ --create-new
```

and then using the command as the Command in the dialog that appears.

Windows (Anaconda)

To run IPython open PowerShell and enter IPython in the start menu. Starting IPython using the QtConsole is similar and is simply called QtConsole in the start menu. Launching IPython from the start menu should create a window similar to that in figure 1.1.

Next, run

```
jupyter qtconsole --generate-config
```

in the terminal or command prompt to generate a file named jupyter_qtconsole_config.py. This file contains settings that are useful for customizing the QtConsole window. A few recommended modifications are

```
c.ConsoleWidget.font_size = 12
c.ConsoleWidget.font_family = "Bitstream Vera Sans Mono"
c.JupyterWidget.syntax_style = "monokai"
```

These commands assume that the Bitstream Vera fonts have been locally installed, which are available from http://ftp.gnome.org/pub/GNOME/sources/ttf-bitstream-vera/1.10/. Opening Qt-Console should create a window similar to that in figure 1.2 (although the appearance might differ) if you did not use the recommendation configuration.
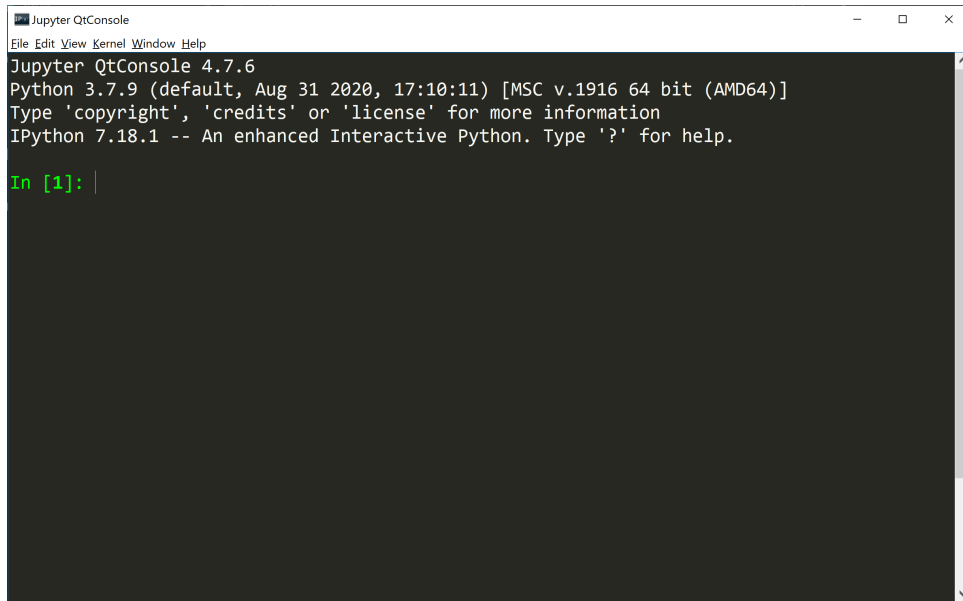
Figure 1.2: IPython running in a QtConsole session.

1.5.3 Getting Help

Help is available in IPython sessions using `help` (*function*) . Some functions (and modules) have very long help files. When using IPython, these can be paged using the command `?`*function* or *function*`?` so that the text can be scrolled using page up and down and q to quit. `??`*function* or *function*`??` can be used to type the entire function including both the docstring and the code.

1.5.4 Running Python programs

While interactive programming is useful for learning a language or quickly developing some simple code, complex projects require the use of complete programs. Programs can be run either using the IPython magic work `%run program.py` or by directly launching the Python program using the standard interpreter using `python program.py`. The advantage of using the IPython environment is that the variables used in the program can be inspected after the program run has completed. Directly calling Python will run the program and then terminate, and so it is necessary to output any important results to a file so that they can be viewed later.[3]

To test that you can successfully execute a Python program, input the code in the block below into a text file and save it as `firstprogram.py`.

```python
# First Python program
import time

print("Welcome to your first Python program.")
input("Press enter to exit the program.")
print("Bye!")
time.sleep(2)
```

Once you have saved this file, open the console, navigate to the directory you saved the file and enter `python firstprogram.py`. Finally, run the program in IPython by first launching IPython, and the using `%cd` to

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[3]Programs can also be run in the standard Python interpreter using the command:
`exec(compile(open('filename.py').read(),'filename.py','exec'))`

change to the location of the program, and finally executing the program using `%run firstprogram.py`.

1.5.5 `%pylab` and `%matplotlib`

When writing Python code, only a small set of core functions and variable types are available in the interpreter. The standard method to access additional variable types or functions is to use `import`s, which explicitly allow access to specific packages or functions. While it is best practice to only `import` required functions or packages, there are many functions in multiple packages that are commonly encountered in these notes. Pylab is a collection of common NumPy, SciPy and Matplotlib functions that can be easily imported using a single command in an IPython session, `%pylab`. This is nearly equivalent to calling `from pylab import *`, since it also sets the *backend* that is used to draw plots. The backend can be manually set using `%pylab` *backend* where *backend* is one of the available backends (e.g., `qt5` or `inline`). Similarly `%matplotlib` *backend* can be used to set just the backend without importing all of the modules and functions come with `%pylab`.

Most chapters assume that `%pylab` has been called so that functions provided by NumPy can be called without explicitly importing them.

1.5.6 Testing the Environment

To make sure that you have successfully installed the required components, run IPython using shortcut or by running `ipython` or `jupyter qtconsole` run in a terminal window. Enter the following commands, one at a time (the meaning of the commands will be covered later in these notes).

```
>>> %pylab qt5
>>> x = randn(100,100)
>>> y = mean(x,0)
>>> import seaborn
>>> plot(y)
>>> import scipy as sp
```

If everything was successfully installed, you should see something similar to figure 1.3.

1.5.7 jupyterlab notebooks

A jupyter notebook is a simple and useful method to share code with others. Notebooks allow for a fluid synthesis of formatted text, typeset mathematics (using LaTeX via MathJax) and Python. The primary method for using notebooks is through a web interface, which allows creation, deletion, export and interactive editing of notebooks.

To launch the jupyterlab server, open a command prompt or terminal and enter

```
jupyter lab
```

This command will start the server and open the default browser which should be a modern version of Chrome (preferable), Chromium, Firefox or Edge. If the default browser is Safari or Internet Explorer, the URL can be copied and pasted into Chrome. The first screen that appears will look similar to figure 1.4, except that the list of notebooks will be empty. Clicking on New Notebook will create a new notebook, which, after a bit of typing, can be transformed to resemble figure 1.5. Notebooks can be imported by dragging and dropping and exported from the menu inside a notebook.

1.5.8 Integrated Development Environments

As you progress in Python and begin writing more sophisticated programs, you will find that using an Integrated Development Environment (IDE) will increase your productivity. Most contain productivity enhancements
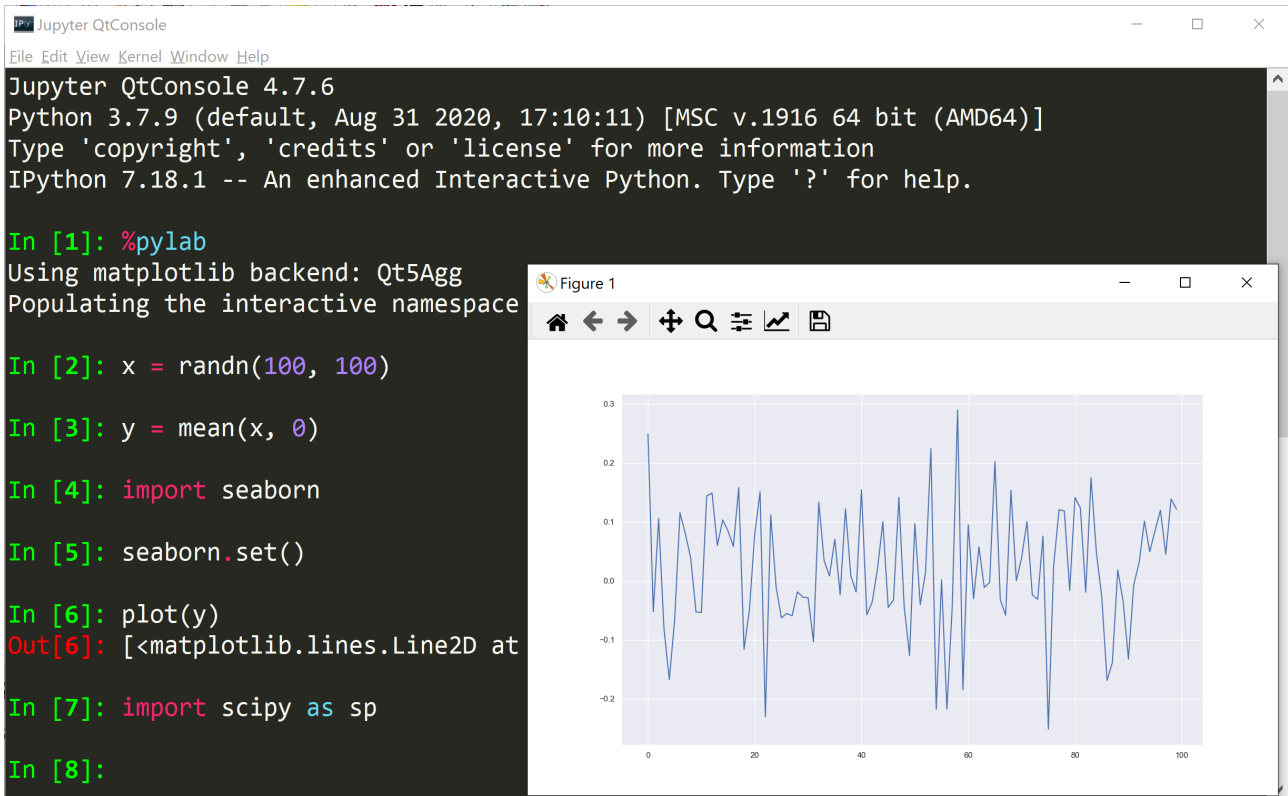
Figure 1.3: A successful test that matplotlib, IPython, NumPy and SciPy were all correctly installed.
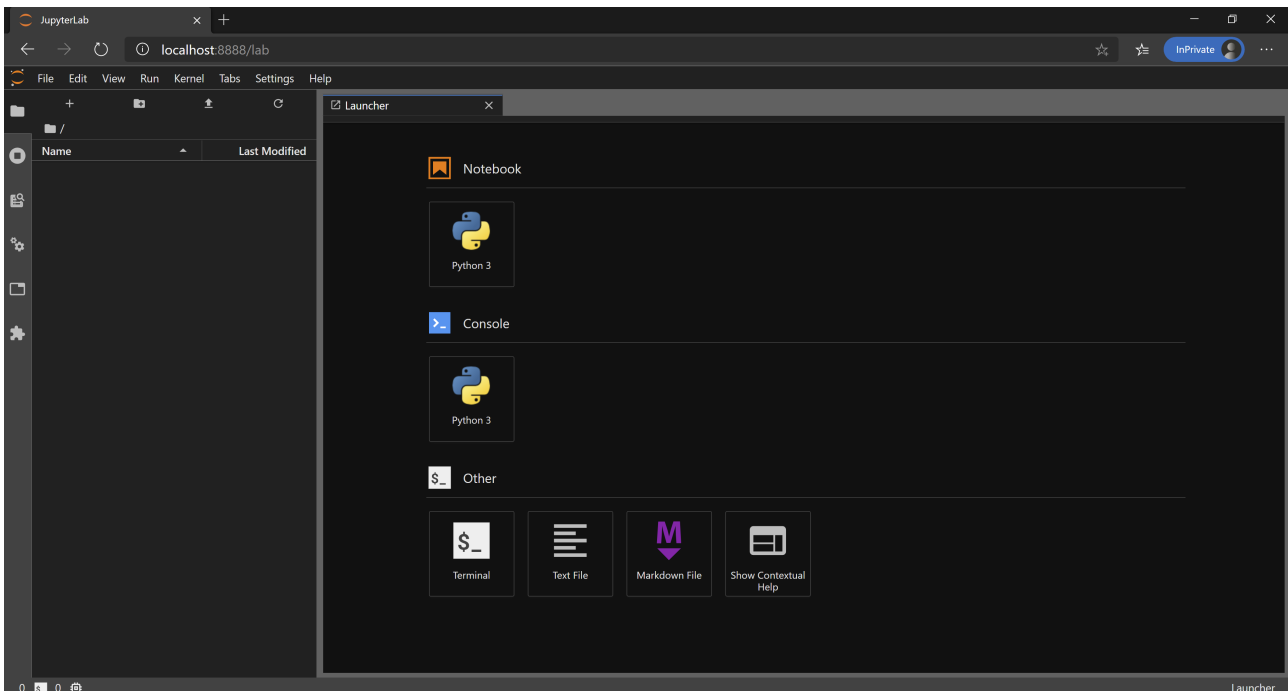
Figure 1.4: The default IPython Notebook screen showing two notebooks.
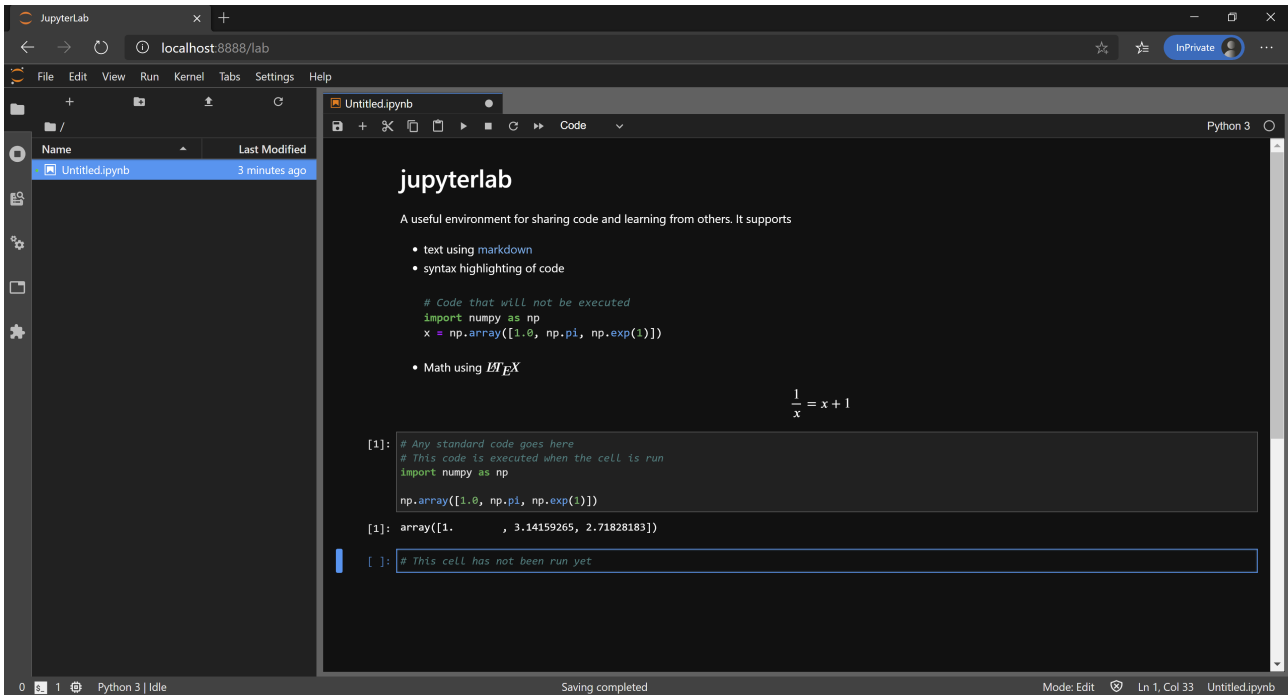
Figure 1.5: A jupyterlab notebook showing formatted markdown, LaTeX math and cells containing code.

such as built-in consoles, code completion (or IntelliSense, for completing function names) and integrated debugging. Discussion of IDEs is beyond the scope of these notes, although Spyder is a reasonable choice (free, cross-platform). Visual Studio Code is an excellent alternative. My preferred IDE is PyCharm, which has a community edition that is free for use (the professional edition is low cost for academics).

spyder

spyder is an IDE specialized for use in scientific applications of Python rather than for general purpose application development. This is both an advantage and a disadvantage when compared to a full featured IDE such as PyCharm or VS Code. The main advantage is that many powerful but complex features are not integrated into Spyder, and so the learning curve is much shallower. The disadvantage is similar - in more complex projects, or if developing something that is not straight scientific Python, Spyder is less capable. However, netting these two, Spyder is almost certainly the IDE to use when starting Python, and it is always relatively simple to migrate to a sophisticated IDE if needed.

Spyder is started by entering `spyder` in the terminal or command prompt. A window similar to that in figure 1.6 should appear. The main components are the editor (1), the object inspector (2), which dynamically will show help for functions that are used in the editor, and the console (3). By default, Spyder opens a standard Python console, although it also supports using the more powerful IPython console. The object inspector window, by default, is grouped with a variable explorer, which shows the variables that are in memory and the file explorer, which can be used to navigate the file system. The console is grouped with an IPython console window (needs to be activated first using the Interpreters menu along the top edge), and the history log which contains a list of commands executed. The buttons along the top edge facilitate saving code, running code and debugging.
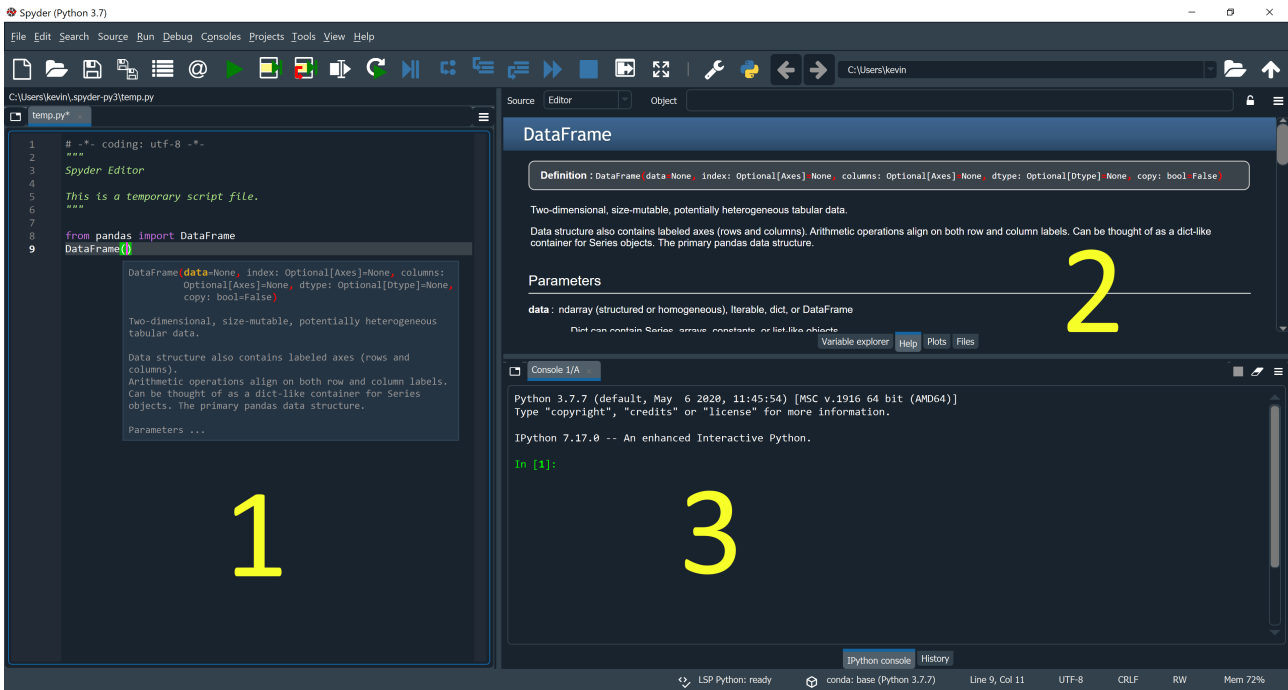
Figure 1.6: The default Spyder IDE on Windows.

1.6   Exercises

1. Install Python.

2. Test the installation using the code in section 1.5.6.

3. Customize IPython QtConsole using a font or color scheme. More customization options can be found by running `ipython -h`.

4. Explore tab completion in IPython by entering `a<TAB>` to see the list of functions which start with a and are loaded by pylab. Next try `i<TAB>`, which will produce a list longer than the screen – press ESC to exit the pager.

5. Launch IPython Notebook and run code in the testing section.

6. Open Spyder and explore its features.

1.A   Additional Installation Issues

1.A.1   Frequently Encountered Problems

All

Whitespace sensitivity

Python is whitespace sensitive and so indentation, either spaces or tabs, affects how Python interprets files. The configuration files, e.g. ipython_config.py, are plain Python files and so are sensitive to whitespace. Introducing white space before the start of a configuration option will produce an error, so ensure there is no whitespace before active lines of a configuration .

Windows

Spaces in path

Python may work when directories have spaces.

Unicode in path

Python does not always work well when a path contains Unicode characters, which might occur in a user name. While this isn't an issue for installing Python or Anaconda, it is an issue for IPython which looks in c:\user*username*\\.ipython for configuration files. The solution is to define the HOME variable before launching IPython to a path that has only ASCII characters.

```
mkdir c:\anaconda\ipython_config
set HOME=c:\anaconda\ipython_config
c:\Anaconda\Scripts\activate econometrics
ipython profile create econometrics
ipython --profile=econometrics
```

The `set HOME=c:\anaconda\ipython_config` can point to any path with directories containing only ASCII characters, and can also be added to any batch file to achieve the same effect.

OS X

Installing Anaconda to the root of the partition

If the user account used is running as root, then Anaconda may install to /anaconda and not ~/anaconda by default. Best practice is not to run as root, although in principle this is not a problem, and /anaconda can be used in place of ~/anaconda in any of the instructions.

1.A.2   Setup using Virtual Environments

The simplest method to install the Python scientific stack is to use directly Continuum Analytics' Anaconda. These instructions describe alternative installation options using *virtual environments*, which allow alternative configurations to simultaneously co-exist on a single system. The primary advantage of a virtual environment is that it allows package versions to be frozen so that code that upgrading a module or all of Anaconda does not upgrade the packages in a particular virtual environment.

Windows

Installation on Windows requires downloading the installer and running. These instructions use ANACONDA to indicate the Anaconda installation directory (e.g. the default is C:\Anaconda). Once the setup has completed, open a PowerShell prompt and run

```
cd ANACONDA\Scripts
conda init powershell
conda update conda
conda update anaconda
conda create -n econometrics qtconsole notebook matplotlib numpy pandas scipy spyder
    statsmodels
conda install -n econometrics cython lxml nose numba numexpr pytables sphinx xlrd xlwt
    html5lib seaborn
```

which will first ensure that Anaconda is up-to-date and then create a virtual environment named econometrics. Using a virtual environment is a best practice and is important since component updates can lead to errors in otherwise working programs due to backward incompatible changes in a module. The long list of modules in the `conda create` command includes the core modules. `conda install` contains the remaining packages and is shown as an example of how to add packages to an existing virtual environment after it has been created. It is also possible to install all available Anaconda packages using the command `conda create -n econometrics anaconda`.

The econometrics environment must be activated before use. This is accomplished by running

```
conda activate econometrics
```

from the command prompt, which prepends [econometrics] to the prompt as an indication that virtual environment is active. Activate the econometrics environment and then run

```
cd c:\
ipython
```

which will open an IPython session using the newly created virtual environment.

Virtual environments can also be created using specific versions of packages using pinning. For example, to create a virtual environment names old using Python 3.6 and NumPy 1.16,

```
conda create -n old python=3.6 numpy=1.16 scipy pandas
```

which will install the requested versions of Python and NumPy as well as the latest version of SciPy and pandas that are compatible with the pinned versions.

Linux and OS X

Installation on Linux requires executing

```
bash Anaconda3-x.y.z-Linux-ISA.sh
```

where `x.y.z` will depend on the version being installed and `ISA` will be either x86 or more likely x86_64. The OS X installer is available either in a GUI installed (pkg format) or as a bash installer which is installed in an identical manner to the Linux installation. After installation completes, change to the folder where Anaconda installed (written here as ANACONDA, default ~/anaconda) and execute

```
cd ANACONDA
cd bin
./conda init bash
./conda update conda
./conda update anaconda
./conda create -n econometrics qtconsole notebook matplotlib numpy pandas scipy spyder
    statsmodels
./conda install -n econometrics cython lxml nose numba numexpr pytables sphinx xlrd xlwt
    html5lib seaborn
```

which will first ensure that Anaconda is up-to-date and then create a virtual environment named econometrics with the required packages. `conda create` creates the environment and `conda install` installs additional packages to the existing environment. `conda install` can be used later to install other packages that may be of interest. To activate the newly created environment, run

```
conda activate econometrics
```

and then run the command

```
ipython
```

to launch IPython using the newly created virtual environment.

Chapter 2

Built-in Data Types

Before diving into Python for analyzing data or running Monte Carlos, it is necessary to understand some basic concepts about the core Python data types. Unlike domain-specific languages such as MATLAB or R, where the default data type has been chosen for numerical work, Python is a general purpose programming language which is also well suited to data analysis, econometrics, and statistics. For example, the basic numeric type in MATLAB is an array (using double precision, which is useful for *floating point* mathematics), while the basic numeric data type in Python is a 1-dimensional scalar which may be either an integer or a double-precision floating point, depending on the formatting of the number when input.

2.1 Variable Names

Variable names can take many forms, although they can only contain numbers, letters (both upper and lower), and underscores (_). They must begin with a letter or an underscore and are `CaSe SeNsItIve`. Additionally, some words are reserved in Python and so cannot be used for variable names (e.g. `import` or `for`). For example,

```
x = 1.0
X = 1.0
X1 = 1.0
X1 = 1.0
x1 = 1.0
dell = 1.0
dellreturns = 1.0
dellReturns = 1.0
_x = 1.0
x_ = 1.0
```

are all legal and distinct variable names. Note that names which begin or end with an underscore, while legal, are not normally used since by convention these convey special meaning.[1] Illegal names do not follow these rules.

```
# Not allowed
x: = 1.0
1X = 1
X-1 = 1
for = 1
```

---

[1]Variable names with a single leading underscore, for example `_some_internal_value`, indicate that the variable is for internal use by a module or class. While indicated to be private, this variable will generally be accessible by calling code. Double leading underscores, for example `__some_private_value`, indicate that a value is actually private and is not accessible. Variable names with trailing underscores are used to avoid conflicts with reserved Python words such as `class_` or `lambda_`. Double leading and trailing underscores are reserved for "magic" variable (e.g. `__init__`) , and so should be avoided except when specifically accessing a feature.

Multiple variables can be assigned on the same line using commas,

```
x, y, z = 1, 3.1415, 'a'
```

2.2 Core Native Data Types

2.2.1 Numeric

Simple numbers in Python can be either integers, floats or complex. This chapter does not cover all Python data types and instead focuses on those which are most relevant for numerical analysis, econometrics, and statistics. The `byte`, `bytearray` and `memoryview` data types are not described.

2.2.1.1 Floating Point (float)

The most important (scalar) data type for numerical analysis is the float. Unfortunately, not all non-complex numeric data types are floats. To input a floating data type, it is necessary to include a `.` (period, dot) in the expression. This example uses the function type() to determine the data type of a variable.

```
>>> x = 1
>>> type(x)
int

>>> x = 1.0
>>> type(x)
float

>>> x = float(1)
>>> type(x)
float
```

This example shows that using the expression that `x = 1` produces an integer-valued variable while `x = 1.0` produces a float-valued variable. Using integers can produce unexpected results and so it is important to include ".0" when expecting a float.

2.2.1.2 Complex (complex)

Complex numbers are also important for numerical analysis. Complex numbers are created in Python using `j` or the function `complex()`.

```
>>> x = 1.0
>>> type(x)
float

>>> x = 1j
>>> type(x)
complex

>>> x = 2 + 3j
>>> x
(2+3j)

>>> x = complex(1)
>>> x
(1+0j)
```

Note that $a+b$j is the same as `complex(`a,b`)`, while `complex(`a`)` is the same as $a+0$j.

2.2.1.3 Integers (int)

Floats use an approximation to represent numbers which may contain a decimal portion. The integer data type stores numbers using an exact representation, so that no approximation is needed. The cost of the exact representation is that the integer data type cannot express anything that isn't an integer, rendering integers of limited use in most numerical work.

Basic integers can be entered either by excluding the decimal (see float), or explicitly using the `int()` function. The `int()` function can also be used to convert a float to an integer by round towards 0.

```
>>> x = 1
>>> type(x)
int

>>> x = 1.0
>>> type(x)
float

>>> x = int(x)
>>> type(x)
int
```

Python integers support have unlimited range since the amount of bits used to store an integer is dynamic.

```
>>> x = 1
>>> x
1

>>> type(x)
int

>>> x = 2 ** 127 + 2 ** 65  # ** is denotes exponentiation, y^64 in TeX
>>> x
170141183460469231768580791863303208960
```

2.2.2 Boolean (bool)

The Boolean data type is used to represent true and false, using the reserved keywords `True` and `False`. Boolean variables are important for program flow control (see Chapter 12) and are typically created as a result of logical operations (see Chapter 10), although they can be entered directly.

```
>>> x = True
>>> type(x)
bool

>>> x = bool(1)
>>> x
True

>>> x = bool(0)
>>> x
False
```

Non-zero, non-empty values generally evaluate to true when evaluated by `bool()`. Zero or empty values such as `bool(0)`, `bool(0.0)`, `bool(0.0j)`, `bool(None)`, `bool('')` and `bool([])` are all false.

2.2.3 Strings (str)

Strings are not usually important for *numerical* analysis, although they are frequently encountered when dealing with data files, especially when importing or when formatting output for human consumption. Strings are delimited using single quotes (`''`) or double quotes (`""`) but not using combination of the two delimiters (i.e., do not use `'"`) in a single string, except when used to express a quotation.

```
>>> x = 'abc'
>>> type(x)
str

>>> y = '"A quotation!"'
>>> print(y)
"A quotation!"
```

String manipulation is further discussed in Chapter 21.

2.2.3.1 Slicing Strings

Substrings within a string can be accessed using *slicing*. Slicing uses `[]` to contain the indices of the characters in a string, where the first index is 0, and the last is $n-1$ (assuming the string has n letters). The following table describes the types of slices which are available. The most useful are `s[i]`, which will return the character in position i, `s[:i]`, which return the leading characters from positions 0 to $i-1$, and `s[i:]` which returns the trailing characters from positions i to $n-1$. The table below provides a list of the types of slices which can be used. The second column shows that slicing can use negative indices which essentially index the string backward.

Slice	Behavior
`s[:]`	Entire string
`s[i]`	Characters i
`s[i:]`	Characters $i,\ldots,n-1$
`s[:i]`	Characters $0,\ldots,i-1$
`s[i:j]`	Characters $i,\ldots,j-1$
`s[i:j:m]`	Characters $i, i+m, \ldots i+m\lfloor \frac{j-i-1}{m} \rfloor$
`s[-i]`	Characters $n-i$
`s[-i:]`	Characters $n-i,\ldots,n-1$
`s[:-i]`	Characters $0,\ldots,n-i-1$
`s[-j:-i]`	Characters $n-j,\ldots,n-i-1,\ -j<-i$
`s[-j:-i:m]`	Characters $n-j, n-j+m,\ldots,n-j+m\lfloor \frac{j-i-1}{m} \rfloor$

```
>>> text = 'Python strings are sliceable.'
>>> text[0]
'P'

>>> text[10]
'i'

>>> L = len(text)
>>> text[L] # Error
IndexError: string index out of range

>>> text[L-1]
```

```
'.'

>>> text[:10]
'Python str'

>>> text[10:]
'ings are sliceable.'
```

2.2.4   Lists (list)

Lists are a built-in container data type which hold other data. A list is a collection of other *objects* – floats, integers, complex numbers, strings or even other lists. Lists are essential to Python programming and are used to store collections of other values. For example, a list of floats can be used to express a vector (although the NumPy data type `array` is better suited to working with collections of numeric values). Lists also support *slicing* to retrieve one or more elements. Basic lists are constructed using square braces, `[]`, and values are separated using commas.

```
>>> x = []
>>> type(x)
builtins.list

>>> x=[1,2,3,4]
>>> x
[1,2,3,4]

# 2-dimensional list (list of lists)
>>> x = [[1,2,3,4], [5,6,7,8]]
>>> x
[[1, 2, 3, 4], [5, 6, 7, 8]]

# Jagged list, not rectangular
>>> x = [[1,2,3,4] , [5,6,7]]
>>> x
[[1, 2, 3, 4], [5, 6, 7]]

# Mixed data types
>>> x = [1,1.0,1+0j,'one',None,True]
>>> x
[1, 1.0, (1+0j), 'one', None, True]
```

These examples show that lists can be regular, nested and can contain any mix of data types including other lists.

2.2.4.1   Slicing Lists

Lists, like strings, can be sliced. Slicing is similar, although lists can be sliced in more ways than strings. The difference arises since lists can be multi-dimensional while strings are always $1 \times n$. Basic list slicing is identical to slicing strings, and operations such as `x[:]`, `x[1:]`, `x[:1]` and `x[-3:]` can all be used. To understand slicing, assume x is a 1-dimensional list with n elements and $i \geq 0, j > 0, i < j, m \geq 1$. Python uses 0-based indices, and so the n elements of x can be thought of as $x_0, x_1, \ldots, x_{n-1}$.

Slice	Behavior,	Slice	Behavior
x[:]	Return all x	x[$-i$]	Returns x_{n-i} except when $i = -0$
x[i]	Return x_i	x[$-i$:]	Return $x_{n-i},\ldots,x_{n-1}$
x[i:]	Return $x_i,\ldots x_{n-1}$	x[:$-i$]	Return $x_0,\ldots,x_{n-i-1}$
x[:i]	Return $x_0,\ldots,x_{i-1}$	x[$-j$:$-i$]	Return $x_{n-j},\ldots,x_{n-i-1}$
x[i:j]	Return $x_i,x_{i+1},\ldots x_{j-1}$	x[$-j$:$-i$:m]	Returns $x_{n-j},x_{n-j+m},\ldots,x_{n-j+m\lfloor\frac{j-i-1}{m}\rfloor}$
x[i:j:m]	Returns $x_i,x_{i+m},\ldots x_{i+m\lfloor\frac{j-i-1}{m}\rfloor}$		

The default list slice uses a unit stride (step size of one) . It is possible to use other strides using a third input in the slice so that the slice takes the form `x[i:j:m]` where `i` is the index to start, `j` is the index to end (exclusive) and `m` is the stride length. For example `x[::2]` will select every second element of a list and is equivalent to `x[0:n:2]` where `n = len(x)`. The stride can also be negative which can be used to select the elements of a list in reverse order. For example, `x[::-1]` will reverse a list and is equivalent to `x[0:n:-1]` .

Examples of accessing elements of 1-dimensional lists are presented below.

```
>>> x = [0,1,2,3,4,5,6,7,8,9]
>>> x[0]
0
>>> x[5]
5
>>> x[10] # Error
IndexError: list index out of range
>>> x[4:]
[4, 5, 6, 7, 8, 9]
>>> x[:4]
[0, 1, 2, 3]
>>> x[1:4]
[1, 2, 3]
>>> x[-0]
0
>>> x[-1]
9
>>> x[-10:-1]
[0, 1, 2, 3, 4, 5, 6, 7, 8]
```

List can be multidimensional, and slicing can be done directly in higher dimensions. For simplicity, consider slicing a 2-dimensional list `x = [[1,2,3,4], [5,6,7,8]]`. If single indexing is used, `x[0]` will return the first (inner) list, and `x[1]` will return the second (inner) list. Since the list returned by `x[0]` is sliceable, the inner list can be directly sliced using `x[0][0]` or `x[0][1:4]`.

```
>>> x = [[1,2,3,4], [5,6,7,8]]
>>> x[0]
[1, 2, 3, 4]
>>> x[1]
[5, 6, 7, 8]
>>> x[0][0]
1
>>> x[0][1:4]
[2, 3, 4]
>>> x[1][-4:-1]
[5, 6, 7]
```

2.2.4.2   List Functions

A number of functions are available for manipulating lists. The most useful are

Function	Method	Description
`list`.append(x, *value*)	`x`.append(*value*)	Appends *value* to the end of the list.
`len`(x)	–	Returns the number of elements in the list.
`list`.extend(x, *list*)	`x`.extend(*list*)	Appends the values in *list* to the existing list.[2]
`list`.pop(x, *index*)	`x`.pop(*index*)	Removes the value in position *index* and returns the value.
`list`.remove(x, *value*)	`x`.remove(*value*)	Removes the first occurrence of *value* from the list.
`list`.count(x, *value*)	`x`.count(*value*)	Counts the number of occurrences of *value* in the list.
`del` x[*slice*]		Deletes the elements in *slice*.

```
>>> x = [0,1,2,3,4,5,6,7,8,9]
>>> x.append(0)
>>> x
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0]

>>> len(x)
11

>>> x.extend([11,12,13])
>>> x
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 0, 11, 12, 13]

>>> x.pop(1)
1

>>> x
[0, 2, 3, 4, 5, 6, 7, 8, 9, 0, 11, 12, 13]

>>> x.remove(0)
>>> x
[2, 3, 4, 5, 6, 7, 8, 9, 0, 11, 12, 13]
```

Elements can also be deleted from lists using the keyword `del` in combination with a slice.

```
>>> x = [0,1,2,3,4,5,6,7,8,9]
>>> del x[0]
>>> x
[1, 2, 3, 4, 5, 6, 7, 8, 9]

>>> x[:3]
[1, 2, 3]

>>> del x[:3]
>>> x
[4, 5, 6, 7, 8, 9]

>>> del x[1:3]
>>> x
[4, 7, 8, 9]

>>> del x[:]
>>> x
[]
```

2.2.5   Tuples (tuple)

A tuple is virtually identical to a list with one important difference – *tuples are immutable*. Immutability means that a tuple cannot be changed once created. It is not possible to add, remove, or replace elements in a tuple.

However, if a tuple contains a mutable data type, for example a tuple that contains a list, the contents mutable data type can be altered.

Tuples are constructed using parentheses (`()`) in place of the square brackets (`[]`) used to create lists. Tuples can be sliced in an identical manner as lists. A list can be converted into a tuple using `tuple()` (Similarly, a tuple can be converted to list using `list()`).

```
>>> x =(0,1,2,3,4,5,6,7,8,9)
>>> type(x)
tuple

>>> x[0]
0

>>> x[-10:-5]
(0, 1, 2, 3, 4)

>>> x = list(x)
>>> type(x)
list

>>> x = tuple(x)
>>> type(x)
tuple

>>> x= ([1,2],[3,4])
>>> x[0][1] = -10
>>> x # Contents can change, elements cannot
([1, -10], [3, 4])
```

Note that tuples containing a single element must contain a comma when created, so that `x = (2,)` is assign a tuple to `x`, while `x=(2)` will assign 2 to `x`. The latter interprets the parentheses as if they are part of a mathematical formula rather than being used to construct a tuple. `x = tuple([2])` can also be used to create a single element tuple. Lists do not have this issue since square brackets do not have this ambiguity.

```
>>> x =(2)
>>> type(x)
int

>>> x = (2,)
>>> type(x)
tuple

>>> x = tuple([2])
>>> type(x)
tuple
```

2.2.5.1 Tuple Functions

Tuples are immutable, and so only have the methods `index` and `count`, which behave in an identical manner to their list counterparts.

2.2.6 Dictionary (dict)

Dictionaries are encountered far less frequently than then any of the previously described data types in numerical Python. They are, however, commonly used to pass options into other functions such as optimizers, and so familiarity with dictionaries is important. Dictionaries in Python are composed of keys (words) and values

(definitions). Dictionaries keys must be unique immutable data types (e.g. strings, the most common key, integers, or tuples containing immutable types), and values can contain any valid Python data type.[3] Values are accessed using keys.

```
>>> data = {'age': 34, 'children' : [1,2], 1: 'apple'}
>>> type(data)
dict

>>> data['age']
34
```

Values associated with an existing key can be updated by making an assignment to the key in the dictionary.

```
>>> data['age'] = 'xyz'
>>> data['age']
'xyz'
```

New key-value pairs can be added by defining a new key and assigning a value to it.

```
>>> data['name'] = 'abc'
>>> data
{1: 'apple', 'age': 'xyz', 'children': [1, 2], 'name': 'abc'}
```

Key-value pairs can be deleted using the reserved keyword `del`.

```
>>> del data['age']
>>> data
{1: 'apple', 'children': [1, 2], 'name': 'abc'}
```

2.2.7 Sets (set, frozenset)

Sets are collections which contain all *unique* elements of a collection. `set` and `frozenset` only differ in that the latter is immutable (and so has higher performance), and so `set` is similar to a unique `list` while `frozenset` is similar to a unique `tuple` . While sets are generally not important in numerical analysis, they can be very useful when working with messy data – for example, finding the set of unique tickers in a long list of tickers.

2.2.7.1 Set Functions

A number of methods are available for manipulating sets. The most useful are

Function	Method	Description
`set.add(x,`*element*`)`	`x.add(`*element*`)`	Appends *element* to a set.
`len(x)`	–	Returns the number of elements in the set.
`set.difference(x,`*set*`)`	`x.difference(`*set*`)`	Returns the elements in `x` which are not in *set*.
`set.intersection(x,`*set*`)`	`x.intersection(`*set*`)`	Returns the elements of `x` which are also in *set*.
`set.remove(x,`*element*`)`	`x.remove(`*element*`)`	Removes *element* from the set.
`set.union(x,`*set*`)`	`x.union(`*set*`)`	Returns the set containing all elements of `x` and *set*.

The code below demonstrates the use of `set`. Note that `'MSFT'` is repeated in the list used to initialize the set, but only appears once in the set since all elements must be unique.

```
>>> x = set(['MSFT','GOOG','AAPL','HPQ','MSFT'])
>>> x
{'AAPL', 'GOOG', 'HPQ', 'MSFT'}
```

---

[3] Formally dictionary keys must support the `__hash__` function, equality comparison and it must be the case that different keys have different hashes.

```
>>> x.add('CSCO')
>>> x
{'AAPL', 'CSCO', 'GOOG', 'HPQ', 'MSFT'}

>>> y = set(['XOM', 'GOOG'])
>>> x.intersection(y)
{'GOOG'}

>>> x = x.union(y)
>>> x
{'AAPL', 'CSCO', 'GOOG', 'HPQ', 'MSFT', 'XOM'}

>>> x.remove('XOM')
{'AAPL', 'CSCO', 'GOOG', 'HPQ', 'MSFT'}
```

A `frozenset` supports the same methods except `add` and `remove`.

2.2.8 `range`

A `range` is most commonly encountered in a `for` loop. `range(a,b,i)` creates the sequences that follows the pattern $a, a+i, a+2i, \ldots, a+(m-1)i$ where $m = \lceil \frac{b-a}{i} \rceil$. In other words, it find all integers x starting with a such $a \le x < b$ and where two consecutive values are separated by i. `range` can be called with 1 or two parameters – `range(a,b)` is the same as `range(a,b,1)` and `range(b)` is the same as `range(0,b,1)`.

```
>>> x = range(10)
>>> type(x)
range

>>> print(x)
range(0, 10)

>>> list(x)
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]

>>> x = range(3,10)
>>> list(x)
[3, 4, 5, 6, 7, 8, 9]

>>> x = range(3,10,3)
>>> list(x)
[3, 6, 9]
```

`range` is not technically a list, which is why the statement `print(x)` returns `range(0,10)`. Explicitly converting with `list` produces a list which allows the values to be printed. `range` is technically an iterator which does not actually require the storage space of a list.

2.3 Additional Container Data Types in the Standard Library

Python includes an extensive standard library that provides many features that extend the core Python language. Data types in the standard library are always installed alongside the Python interpreter. However, they are not "built-in" since using one requires an explicit `import` statement to make a particular data type available. The standard library is vast and some examples of the included functionality are support for working with dates (provided by the `datetime` module, see Chapter 13), functional programming tools (`itertools`, `functools` and `operator`), tools for accessing the file system (`os.path` and `glob` *inter alia.*, see Chapter 22), and support for interacting with resources on the the internet (`urllib` and `ftplib` *inter alia.*). One of the more useful modules included in the standard library is the `collections` module. This module provides a set of specialized

container data types that extend the built-in data container data types. Two are particularly useful when working with data: `OrderedDict` and `defaultdict`. Both of these extend the built-in dictionary `dict` with useful features.

2.3.1 OrderedDict

When using a standard Python dict, items order is not guaranteed. `OrderedDict` addresses this frequent shortcoming by retaining a list of the keys inserted into the dictionary in the order in which they have been inserted. The order is also preserved when deleting keys from an `OrderedDict`.

```
>>> from collections import OrderedDict
>>> od = OrderedDict()
>>> od['key1'] = 1
>>> od['key2'] = 'a'
>>> od['key3'] = 'alpha'
>>> plain = dict(od)
>>> print(list(od.keys()))
['key1', 'key2', 'key3']

>>> print(list(plain.keys()))
['key2', 'key1', 'key3']

>>> del od['key1']
>>> print(list(od.keys()))
['key2', 'key3']

>>> od['key1'] = 'some other value'
print(list(od.keys()))
['key2', 'key3', 'key1']
```

This functionality is particularly useful when iterating over the keys in a dictionary since it guarantees a predictable order when accessing the keys (see Chapter 12). Recent versions of pandas also respect the order in an `OrderedDict` when adding columns to a `DataFrame` (see Chapter 15).

2.3.2 defaultdict

By default attempting to access a key in a dictionary that does not exist will produce an error. There are circumstances where this is undesirable, and when a key is encountered that doesn't exist, a default value should be added to the dictionary and returns. One particularly useful example of this behavior is when making keyed lists – that is, grouping like elements according to a key in a list. If the key exists, the elements should be appended to the existing list. If the key doesn't exist, the key should be added and a new list containing the new element should be inserted into the disctionary. `defaultdict` enables this exact scenario by accepting a callable function as an argument. When a key is found, it behaved just like a standard dictionary. When a key isn't found, the output of the callable function is assigned to the key. This example uses `list` to add a new list whenever a key is not found.

```
>>> d = {}
>>> d['one'].append('an item') # Error
KeyError: 'one'

>>> from collections import defaultdict
>>> dd = defaultdict(list)
>>> dd['one'].append('first')
>>> dd['one'].append('second')
>>> dd['two'].append('third')
>>> print(dd)
```

```
defaultdict(<class 'list'>, {'one': ['first', 'second'], 'two': ['third']})
```

The callable argument provided to `defaultdict` can be anything that is useful including other containers, objects that will be initialized the first time called, or an anonymous function (i.e. a function defined using `lambda`, see Section 17.4).

2.4 Python and Memory Management

Python uses a highly optimized memory allocation system which attempts to avoid allocating unnecessary memory. As a result, when one variable is assigned to another (e.g. to $y = x$), these will actually point to the same data in the computer's memory. To verify this, `id()` can be used to determine the unique identification number of a piece of data.[4]

```
>>> x = 1
>>> y = x
>>> id(x)
82970264

>>> id(y)
82970264

>>> x = 2.0
>>> id(x)
93850568

>>> id(y)
82970264
```

In the above example, the initial assignment of $y = x$ produced two variables with the same ID. However, once `x` was changed, its ID changed while the ID of `y` did not, indicating that the data in each variable was stored in different locations. This behavior is both safe and efficient and is common to the basic Python *immutable* types: int, float, complex, string, tuple, frozenset and range.

2.4.1 Example: Lists

Lists are mutable and so assignment does not create a copy , and so changes to either variable affect both.

```
>>> x = [1, 2, 3]
>>> y = x
>>> y[0] = -10
>>> y
[-10, 2, 3]

>>> x
[-10, 2, 3]
```

Slicing a list creates a copy of the list and *any immutable* types in the list – but not mutable elements in the list.

```
>>> x = [1, 2, 3]
>>> y = x[:]
>>> id(x)
86245960

>>> id(y)
86240776
```

---

[4]The ID numbers on your system will likely differ from those in the code listing.

To see that the inner lists are not copied, consider the behavior of changing one element in a nested list.

```
>>> x=[[0,1],[2,3]]
>>> y = x[:]
>>> y
[[0, 1], [2, 3]]

>>> id(x[0])
117011656

>>> id(y[0])
117011656

>>> x[0][0]
0.0

>>> id(x[0][0])
30390080

>>> id(y[0][0])
30390080

>>> y[0][0] = -10.0
>>> y
[[-10.0, 1], [2, 3]]

>>> x
[[-10.0, 1], [2, 3]]
```

When lists are nested or contain other mutable objects (which do not copy), slicing copies the outermost list to a new ID, but the inner lists (or other objects) are still linked. In order to copy nested lists, it is necessary to explicitly call `deepcopy()`, which is in the module `copy`.

```
>>> import copy as cp
>>> x=[[0,1],[2,3]]
>>> y = cp.deepcopy(x)
>>> y[0][0] = -10.0
>>> y
[[-10.0, 1], [2, 3]]

>>> x
[[0, 1], [2, 3]]
```

2.5 Exercises

1. Enter the following into Python, assigning each to a unique variable name:

    (a) `4`
    (b) `3.1415`
    (c) `1.0`
    (d) `2+4j`
    (e) `'Hello'`
    (f) `'World'`

2. What is the type of each variable? Use `type` if you aren't sure.

3. Which of the 6 types can be:

    (a) Added `+`
    (b) Subtracted `–`
    (c) Multiplied `*`
    (d) Divided `/`

4. What are the types of the output (when an error is not produced) in the above operations?

5. Input the variable

    ```
    ex = 'Python is an interesting and useful language for numerical computing!'
    ```

    Using slicing, extract the text strings below. Note: There are multiple answers for all of the problems.

    (a) `Python`
    (b) `!`
    (c) `computing`
    (d) `in`
    (e) `!gnitupmoc laciremun rof egaugnal lufesu dna gnitseretni na si nohtyP'` (Reversed)
    (f) `nohtyP`
    (g) `Pto sa neetn n sfllnug o ueia optn!`

6. What are the direct 2 methods to construct a tuple that has only a single item? How many ways are there to construct a list with a single item?

7. Construct a nested list to hold the array

    $$\begin{bmatrix} 1 & .5 \\ .5 & 1 \end{bmatrix}$$

    so that item `[i][j]` corresponds to the position in the array (Remember that Python uses 0 indexing).

8. Assign the array you just created first to `x`, and then assign `y=x`. Change `y[0][0]` to `1.61`. What happens to `x`?

9. Next assign `z=x[:]` using a simple slice. Repeat the same exercise using `y[0][0] = 1j`. What happens to `x` and `z` ? What are the `id`s of `x`, `y` and `z`? What about `x[0]`, `y[0]` and `z[0]`?

10. How could you create `w` from `x` so that `w` can be changed without affecting `x`?

11. Initialize a list containing `4`, `3.1415`, `1.0`, `2+4j`, `'Hello'`, `'World'`. How could you:

    (a) Delete `1.0` if you knew its position? What if you didn't know its position?
    (b) How can the list `[1.0, 2+4j, 'Hello']` be added to the existing list?
    (c) How can the list be reversed?
    (d) In the extended list, how can you count the occurrence of `'Hello'`?

12. Construct a dictionary with the keyword-value pairs: `'alpha'` and `1.0`, `'beta'` and `3.1415`, `'gamma'` and `-99`. How can the value of `alpha` be retrieved?

13. Convert the final list at the end of problem 11 to a `set`. How is the set different from the list?

Chapter 3

Arrays

NumPy provides the core data type for numerical analysis – arrays. NumPy arrays are widely used through the Python econsystem and are extended by other key libraries including pandas, an essential library for data analysis.

3.1 Array

Arrays are the base data type in NumPy, are in similar to lists or tuples since they both contain collections of elements. The focus of this section is on homogeneous arrays containing numeric data – that is, an array where all elements have the same numeric type (heterogeneous arrays are covered in Chapters 16 and 15). Additionally, arrays, unlike lists, are always rectangular so that all dimensions have the same number of elements.

Arrays are initialized from lists (or tuples) using `array`. Two-dimensional arrays are initialized using lists of lists (or tuples of tuples, or lists of tuples, etc.), and higher dimensional arrays can be initialized by further nesting lists or tuples.

```
>>> from numpy import array
>>> x = [0.0, 1, 2, 3, 4]
>>> y = array(x)
>>> y
array([ 0.,  1.,  2.,  3.,  4.])

>>> type(y)
numpy.ndarray
```

Two (or higher) -dimensional arrays are initialized using nested lists.

```
>>> y = array([[0.0, 1, 2, 3, 4], [5, 6, 7, 8, 9]])
>>> y
array([[ 0.,  1.,  2.,  3.,  4.],
       [ 5.,  6.,  7.,  8.,  9.]])

>>> shape(y)
(2, 5)

>>> y = array([[[1,2],[3,4]],[[5,6],[7,8]]])
>>> y
array([[[1, 2],
        [3, 4]],

       [[5, 6],
        [7, 8]]])
```

```
>>> shape(y)
(2, 2, 2)
```

3.1.1 Array dtypes

Homogeneous arrays can contain a variety of numeric data types. The most common data type is `float64` (or `double`), which corresponds to the python built-in data type of float (and C/C++ double). By default, calls to `array` will preserve the type of the input, if possible. If an input contains all integers, it will have a dtype of `int32` (similar to the built-in data type `int`). If an input contains integers, floats, or a mix of the two, the array's data type will be `float64`. If the input contains a mix of integers, floats and complex types, the array will be initialized to hold complex data.

```
>>> x = [0, 1, 2, 3, 4] # Integers
>>> y = array(x)
>>> y.dtype
dtype('int32')

>>> x = [0.0, 1, 2, 3, 4] # 0.0 is a float
>>> y = array(x)
>>> y.dtype
dtype('float64')

>>> x = [0.0 + 1j, 1, 2, 3, 4] # (0.0 + 1j) is a complex
>>> y = array(x)
>>> y
array([ 0.+1.j,  1.+0.j,  2.+0.j,  3.+0.j,  4.+0.j])

>>> y.dtype
dtype('complex128')
```

NumPy attempts to find the smallest data type which can represent the data when constructing an array. It is possible to force NumPy to select a particular dtype by using the keyword argument dtype=*datatype* when initializing the `array`.

```
>>> x = [0, 1, 2, 3, 4] # Integers
>>> y = array(x)
>>> y.dtype
dtype('int32')

>>> y = array(x, dtype='float64') # String dtype
>>> y.dtype
dtype('float64')

>>> y = array(x, dtype=float32) # NumPy type dtype
>>> y.dtype
dtype('float32')
```

3.2 1-dimensional Arrays

A vector

$$x = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 \end{bmatrix}$$

is entered as a 1-dimensional array using

```
>>> x=array([1.0, 2.0, 3.0, 4.0, 5.0])
array([ 1.,   2.,   3.,   4.,   5.])

>>> ndim(x)
1
```

If an array with 2-dimensions is required, it is necessary to use a trivial nested list.

```
>>> x=array([[1.0,2.0,3.0,4.0,5.0]])
array([[ 1.,   2.,   3.,   4.,   5.]])

>>> ndim(x)
2
```

Notice that the output representation uses nested lists (`[[ ]]`) to emphasize the 2-dimensional structure of the array. The column vector,

$$
x = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}
$$

is entered as a 2-dimensional array using a set of nested lists

```
>>> x = array([[1.0],[2.0],[3.0],[4.0],[5.0]])
>>> x
array([[ 1.],
       [ 2.],
       [ 3.],
       [ 4.],
       [ 5.]])
```

3.3   2-dimensional Arrays

Two-dimensional arrays are rows of columns, and so

$$
x = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix},
$$

is input by enter the array one row at a time, each in a list, and then encapsulate the row lists in another list.

```
>>> x = array([[1.0,2.0,3.0],[4.0,5.0,6.0],[7.0,8.0,9.0]])
>>> x
array([[ 1.,   2.,   3.],
       [ 4.,   5.,   6.],
       [ 7.,   8.,   9.]])
```

3.4   Multidimensional Arrays

Higher dimensional arrays have a number of uses, for example when modeling a time-varying covariance. Multidimensional (*N*-dimensional) arrays are available for *N* up to about 30, depending on the size of each dimension. Manually initializing higher dimension arrays is tedious and error prone, and so it is better to use functions such as `zeros((2, 2, 2))` or `empty((2, 2, 2))`.

Matrix

Matrices are essentially a subset of arrays and behave in a virtually identical manner. The matrix class is deprecated and so should not be used. While NumPy is likely to support the matrix class for the forseeable future, its use is discouraged. In practice, there is no good reason to not use 2-dimensional arrays.
The two important differences are:

- Matrices always have 2 dimensions

- Matrices follow the rules of linear algebra for *

1- and 2-dimensional arrays can be copied to a matrix by calling `matrix` on an array. Alternatively, `mat` or `asmatrix` provides a faster method to coerce an array to behave like a matrix without copying any data.

```
>>> x = [0.0, 1, 2, 3, 4] # Any float makes all float
>>> y = array(x)
>>> type(y)
numpy.ndarray

>>> y * y # Element-by-element
array([  0.,   1.,   4.,   9.,  16.])

>>> z = asmatrix(x)
>>> type(z)
numpy.matrixlib.defmatrix.matrix

>>> z * z # Error
ValueError: matrices are not aligned
```

3.5 Concatenation

Concatenation is the process by which one array is appended to another. Arrays can be concatenation horizontally or vertically. For example, suppose

$$x = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \text{ and } y = \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} \text{ and } z = \begin{bmatrix} x \\ y \end{bmatrix}$$

needs to be constructed. This can be accomplished by treating `x` and `y` as elements of a new array and using the function `concatenate` to join them. The inputs to `concatenate` must be grouped in a tuple and the keyword argument `axis` specifies whether the arrays are to be vertically (`axis = 0`) or horizontally (`axis = 1`) concatenated.

```
>>> x = array([[1.0,2.0],[3.0,4.0]])
>>> y = array([[5.0,6.0],[7.0,8.0]])
>>> z = concatenate((x,y),axis = 0)
>>> z
array([[ 1.,   2.],
       [ 3.,   4.],
       [ 5.,   6.],
       [ 7.,   8.]])

>>> z = concatenate((x,y),axis = 1)
>>> z
array([[ 1.,   2.,   5.,   6.],
```

```
        [ 3.,   4.,   7.,   8.]])
```

Concatenating is the code equivalent of block forms in linear algebra. Alternatively, the functions `vstack` and `hstack` can be used to vertically or horizontally stack arrays, respectively.

```
>>> z = vstack((x,y)) # Same as z = concatenate((x,y),axis = 0)
>>> z = hstack((x,y)) # Same as z = concatenate((x,y),axis = 1)
```

3.6   Accessing Elements of an Array

Four methods are available for accessing elements contained within an array: scalar selection, slicing, numerical indexing and logical (or Boolean) indexing. Scalar selection and slicing are the simplest and so are presented first. Numerical indexing and logical indexing both depends on specialized functions and so these methods are discussed in Chapter 11.

3.6.1   Scalar Selection

Pure scalar selection is the simplest method to select elements from an array, and is implemented using $[i]$ for 1-dimensional arrays, $[i, j]$ for 2-dimensional arrays and $[i_1, i_2,\ldots, i_n]$ for general n-dimensional arrays. Like all indexing in Python, selection is 0-based so that $[0]$ is the first element in a 1-d array, $[0,0]$ is the upper left element in a 2-d array, and so on.

```
>>> x = array([1.0,2.0,3.0,4.0,5.0])
>>> x[0]
1.0

>>> x = array([[1.0,2,3],[4,5,6]])
>>> x
array([[ 1.,   2.,   3.],
       [ 4.,   5.,   6.]])

>>> x[1, 2]
6.0

>>> type(x[1,2])
numpy.float64
```

Pure scalar selection always returns a single element which is *not* an array. The data type of the selected element matches the data type of the array used in the selection. Scalar selection can also be used to assign values in an array.

```
>>> x = array([1.0,2.0,3.0,4.0,5.0])
>>> x[0] = -5
>>> x
array([-5.,   2.,   3.,   4.,   5.])
```

3.6.2   Array Slicing

Arrays, like lists and tuples, can be sliced. Arrays slicing is virtually identical list slicing except that a simpler slicing syntax is available when using multiple dimensions. Arrays are sliced using the syntax `[:,:,...,:]` (where the number of dimensions of the arrays determines the size of the slice).[1] Recall that the slice notation

---

[1]It is not necessary to include all trailing slice dimensions, and any omitted trailing slices are set to select all elements (the slice `:`). For example, if `x` is a 3-dimensional array, `x[0:2]` is the same as `x[0:2,:,:]` and `x[0:2,0:2]` is the same as `x[0:2,0:2,:]`.

a:*b*:*s* will select every *s*th element where the indices *i* satisfy $a \leq i < b$ so that the starting value *a* is always included in the list and the ending value *b* is always excluded. Additionally, a number of shorthand notations are commonly encountered

- `:` and `::` are the same as `0:n:1` where `n` is the length of the array (or list).

- `a:` and `a:n` are the same as `a:n:1` where `n` is the length of the array (or list).

- `:b` is the same as `0:b:1`.

- `::s` is the same as `0:n:s` where `n` is the length of the array (or list).

Basic slicing of 1-dimensional arrays is identical to slicing a simple list, and the returned type of all slicing operations matches the array being sliced.

```
>>> x = array([1.0,2.0,3.0,4.0,5.0])
>>> y = x[:]
array([ 1.,   2.,   3.,   4.,   5.])

>>> y = x[:2]
array([ 1.,   2.])

>>> y = x[1::2]
array([ 2.,   4.])
```

In 2-dimensional arrays, the first dimension specifies the row or rows of the slice and the second dimension specifies the column or columns. Note that the 2-dimensional slice syntax `y[a:b,c:d]` is the same as `y[a:b,:][:,c:d]` or `y[a:b][:,c:d]`, although the shorter form is preferred. In the case where only row slicing in needed `y[a:b]`, the equivalent of `y[a:b, :]`, is the shortest syntax.

```
>>> y = array([[0.0, 1, 2, 3, 4],[5, 6, 7, 8, 9]])
>>> y
array([[ 0.,   1.,   2.,   3.,   4.],
       [ 5.,   6.,   7.,   8.,   9.]])

>>> y[:1,:] # Row 0, all columns
array([[ 0.,   1.,   2.,   3.,   4.]])

>> y[:1] # Same as y[:1,:]
array([[ 0.,   1.,   2.,   3.,   4.]])

>>> y[:,:1] # all rows, column 0
array([[ 0.],
       [ 5.]])

>>> y[:1,0:3] # Row 0, columns 0 to 2
array([[ 0.,   1.,   2.]])

>>> y[:1][:,0:3] # Same as previous
array([[ 0.,   1.,   2.]])

>>> y[:,3:] # All rows, columns 3 and 4
array([[ 3.,   4.],
       [ 8.,   9.]])

>>> y = array([[[1.0,2],[3,4]],[[5,6],[7,8]]])
>>> y[:1,:,:] # Panel 0 of 3D y
array([[[ 1.,   2.],
        [ 3.,   4.]]])
```

In the previous examples, slice notation was always used even when only selecting 1 row or column. This was done to emphasize the difference between using slice notation, which always returns an array with the same dimension and using a scalar selector which will perform dimension reduction.

3.6.3 Mixed Selection using Scalar and Slice Selectors

When arrays have more than 1-dimension, it is often useful to mix scalar and slice selectors to select an entire row, column or panel of a 3-dimensional array. This is similar to pure slicing with one important caveat – dimensions selected using scalar selectors are eliminated. For example, if `x` is a 2-dimensional array, then `x[0,:]` will select the first row. However, unlike the 2-dimensional array constructed using the slice `x[:1,:]`, `x[0,:]` will be a 1-dimensional array.

```
>>> x = array([[1.0,2],[3,4]])
>>> x[:1,:] # Row 1, all columns, 2-dimensional
array([[ 1.,  2.]])

>>> x[0,:] # Row 1, all columns, dimension reduced
array([ 1.,  2.])
```

While these two selections appear similar, the first produces a 2-dimensional array (note the `[[ ]]` syntax) while the second is a 1-dimensional array. In most cases where a single row or column is required, using scalar selectors such as `y[0,:]` is the best practice. It is important to be aware of the dimension reduction since scalar selections from 2-dimensional arrays will not have 2-dimensions. This type of dimension reduction may matter when evaluating linear algebra expression.

The principle adopted by NumPy is that slicing should always preserve the dimension of the underlying array, while scalar indexing should always collapse the dimension(s). This is consistent with `x[0,0]` returning a scalar (or 0-dimensional array) since both selections are scalar. This is demonstrated in the next example which highlights the differences between pure slicing, mixed slicing, and pure scalar selection. Note that the function `ndim` returns the number of dimensions of an array.

```
>>> x = array([[0.0, 1, 2, 3, 4],[5, 6, 7, 8, 9]])
>>> x[:1,:] # Row 0, all columns, 2-dimensional
array([[ 0.,  1.,  2.,  3.,  4.]])

>>> ndim(x[:1,:])
2

>>> x[0,:] # Row 0, all column, dim reduction to 1-d array
array([ 0.,  1.,  2.,  3.,  4.])

>>> ndim(x[0,:])
1

>>> x[0,0] # Top left element, dim reduction to scalar (0-d array)
0.0

>>> ndim(x[0,0])
0

>>> x[:,0] # All rows, 1 column, dim reduction to 1-d array
array([ 0., 5.])
```

3.6.4 Assignment using Slicing

Slicing and scalar selection can be used to assign arrays that have the same dimension as the slice.[2]

```
>>> x = array([[0.0]*3]*3)  # *3 repeats the list 3 times
>>> x
array([[0, 0, 0],
       [0, 0, 0],
       [0, 0, 0]])

>>> x[0,:] = array([1.0, 2.0, 3.0])
>>> x
array([[ 1.,  2.,  3.],
       [ 0.,  0.,  0.],
       [ 0.,  0.,  0.]])

>>> x[::2,::2]
array([[ 1.,  3.],
       [ 0.,  0.]])

>>> x[::2,::2] =  array([[-99.0,-99],[-99,-99]]) # 2 by 2
>>> x
array([[-99.,   2., -99.],
       [  0.,   0.,   0.],
       [-99.,   0., -99.]])

>>> x[1,1] = pi
>>> x
array([[-99.        ,   2.        , -99.        ],
       [  0.        ,   3.14159265,   0.        ],
       [-99.        ,   0.        , -99.        ]])
```

NumPy attempts to automatic (silent) data type conversion if an element with one data type is inserted into an array with a different type. For example, if an array has an integer data type, placing a float into the array results in the float being truncated and stored as an integer. This is dangerous, and so in most cases, arrays should be initialized to contain floats unless a considered decision is taken to use a different data type.

```
>>> x = [0, 1, 2, 3, 4] # Integers
>>> y = array(x)
>>> y.dtype
dtype('int32')

>>> y[0] = 3.141592
>>> y
array([3, 1, 2, 3, 4])

>>> x = [0.0, 1, 2, 3, 4] # 1 Float makes all float
>>> y = array(x)
>>> y.dtype
dtype('float64')

>>> y[0] = 3.141592
>>> y
array([ 3.141592, 1.      , 2.      , 3.      , 4.      ])
```

---

[2]Formally, the array to be assigned must be broadcastable to the size of the slice. Broadcasting is described in Chapter 4, and assignment using broadcasting is discussed in Chapter 11.

3.6.5 Linear Slicing using `flat`

Data in arrays is stored in *row-major order* – elements are indexed by first counting across rows and then down columns. For example, in the 2-dimensional array

$$x = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

the first element of x is 1, the second element is 2, the third is 3, the fourth is 4, and so on.

In addition to slicing using the `[:,:,...,:]` syntax, k-dimensional arrays can be linear sliced. Linear slicing assigns an index to each element of the array, starting with the first (0), the second (1), and so on until the final element $(n-1)$. In 2-dimensions, linear slicing works by first counting across rows, and then down columns. To use linear slicing, the method or function `flat` must first be used.

```
>>> y = reshape(arange(25.0),(5,5))
>>> y
array([[  0.,   1.,   2.,   3.,   4.],
       [  5.,   6.,   7.,   8.,   9.],
       [ 10.,  11.,  12.,  13.,  14.],
       [ 15.,  16.,  17.,  18.,  19.],
       [ 20.,  21.,  22.,  23.,  24.]])

>>> y[0] # Same as y[0,:], first row
array([ 0.,  1.,  2.,  3.,  4.])

>>> y.flat[0] # Scalar slice, flat is 1-dimensional
0

>>> y[6] # Error
IndexError: index out of bounds

>>> y.flat[6] # Element 6
6.0

>>> y.flat[12:15]
array([ 12.,  13.,  14.])

>>> y.flat[:] # All element slice
array([[  0.,   1.,   2.,   3.,   4.,   5.,   6.,   7.,   8.,   9.,  10.,
        11.,  12.,  13.,  14.,  15.,  16.,  17.,  18.,  19.,  20.,  21.,
        22.,  23.,  24.]])
```

Note that `arange` and `reshape` are useful functions are described in later chapters.

3.7 Slicing and Memory Management

Unlike lists, slices of arrays do not copy the underlying data. Instead, a slice of an array returns a *view* of the array which shares the data in the sliced array. This is important since changes in slices will propagate to the original array as well as to any other slices which share the same element.

```
>>> x = reshape(arange(4.0),(2,2))
>>> x
array([[ 0.,  1.],
       [ 2.,  3.]])

>>> s1 = x[0,:] # First row
```

```
>>> s2 = x[:,0] # First column
>>> s1[0] = -3.14 # Assign first element
>>> s1
array([-3.14,  1.  ])

>>> s2
array([-3.14,  2.  ])

>>> x
array([[-3.14,  1.  ],
       [ 2.  ,  3.  ]])
```

If changes should not propagate to parent and sibling arrays, it is necessary to call copy on the slice. Alternatively, they can also be copied by calling array on an existing array.

```
>>> x = reshape(arange(4.0),(2,2))
>>> s1 = copy(x[0,:]) # Function copy
>>> s2 = x[:,0].copy() # Method copy, more common
>>> s3 = array(x[0,:]) # Create a new array
>>> s1[0] = -3.14
>>> s1
array([-3.14,  1.])

>>> s2
array([ 0.,  2.])

>>> s3
array([0.,  1.])

>>> x[0,0]
array([[ 0.,  1.],
       [ 2.,  3.]])
```

There is one notable exception to this rule – when using pure scalar selection the (scalar) value returned is always a copy.

```
>>> x = arange(5.0)
>>> y = x[0] # Pure scalar selection
>>> z = x[:1] # A pure slice
>>> y = -3.14
>>> y # y Changes
-3.14

>>> x # No propagation
array([ 0.,  1.,  2.,  3.,  4.])

>>> z  # No changes to z either
array([ 0.])

>>> z[0] = -2.79
>>> y # No propagation since y used pure scalar selection
-3.14

>>> x # z is a view of x, so changes propagate
array([-2.79,  1.  ,  2.  ,  3.  ,  4.  ])
```

Finally, assignments from functions which change values will automatically create a copy of the underlying array.

```
>>> x = array([[0.0, 1.0],[2.0,3.0]])
>>> y = x
```

```
>>> print(id(x),id(y)) # Same id, same object
 129186368 129186368
>>> y = x + 1.0
>>> y
array([[ 1.,  2.],
       [ 3.,  4.]])

>>> print(id(x),id(y)) # Different
129186368 129183104

>>> x # Unchanged
array([[ 0.,  1.],
       [ 2.,  3.]])

>>> y = exp(x)
>>> print(id(x),id(y)) # Also Different
129186368 129185120
```

Even trivial function such as `y = x + 0.0` create a copy of `x`, and so the only scenario where explicit copying is required is when `y` is directly assigned using a slice of `x`, and changes to `y` should not propagate to `x`.

3.8 `import` and Modules

Python, by default, only has access to a small number of built-in types and functions. The vast majority of functions are located in modules, and before a function can be accessed, the module which contains the function must be imported. For example, when using `%pylab` in an IPython session a large number of modules are automatically imported, including NumPy, SciPy, and matplotlib. While this style of importing useful for learning and interactive use, care is needed to make sure that the correct module is imported when designing more complex programs. For example, both NumPy and SciPy have functions called `sqrt` and so it is not clear which will be used by Pylab.

`import` can be used in a variety of ways. The simplest is to use `from` *module* `import` `*` which imports all functions in *module*. This method of using `import` can dangerous since it is possible for functions in one module to be hidden by later imports from other modeuls. A better method is to only import the required functions. This still places functions at the top level of the namespace while preventing conflicts.

```
from pylab import log2 # Will import log2 only
from scipy import log10 # Will not import the log2 from SciPy
```

The functions `log2` and `log10` can both be called in subsequent code. An alternative and more common method is to use `import` in the form

```
import pylab
import scipy
import numpy
```

which allows functions to be accessed using dot-notation and the module name, for example `scipy.log2`. It is also possible to rename modules when imported using `as`

```
import pylab as pl
import scipy as sp
import numpy as np
```

The only difference between the two types is that `import scipy` is implicitly calling `import scipy as scipy`. When this form of import is used, functions are used with the "as" name. For example, the square root provided by SciPy is accessed using `sp.sqrt`, while the pylab square root is `pl.sqrt`. Using this form of import allows both to be used where appropriate.

3.9   Calling Functions

Functions calls have different conventions than most other expressions. The most important difference is that functions can take more than one input and return more than one output. The generic structure of a function call is *out1*, *out2*, *out3*, ... = `functionname`(*in1*, *in2*, *in3*, ...). The important aspects of this structure are

- If multiple outputs are returned, but only one output variable is provided, the output will (generally) be a tuple.

- If more than one output variable is given in a function call, the number of output must match the number of output provided by the function. It is not possible to ask for two output if a function returns three – using an incorrect number of outputs results in `ValueError: too many values to unpack`.

- Both inputs and outputs must be separated by commas (,)

- Inputs can be the result of other functions. For example, the following are equivalent,

```
>>> y = var(x)
>>> mean(y)
```

and

```
>>> mean(var(x))
```

Required Arguments

Most functions have required arguments. For example, consider the definition of `array` from `help(array)`,

```
array(object, dtype=None, copy=True, order=None, subok=False, ndmin=0)
```

Array has 1 required input, `object`, which is the list or tuple which contains values to use when creating the array. Required arguments can be determined by inspecting the function signature since all of the input follow the pattern *keyword=default* except `object` – required arguments will not have a default value provided. The other arguments can be called in order (`array` accepts at most 2 non-keyword arguments).

```
>>> array([[1.0,2.0],[3.0,4.0]])
array([[ 1.,   2.],
       [ 3.,   4.]])

>>> array([[1.0,2.0],[3.0,4.0]], 'int32')
array([[1, 2],
       [3, 4]])
```

Keyword Arguments

All of the arguments to `array` can be called by the keyword that appears in the help file definition.

```
array(object=[[1.0,2.0],[3.0,4.0]])
array([[1.0,2.0],[3.0,4.0]], dtype=None, copy=True, order=None, subok=False)
```

Keyword arguments have two important advantages. First, they do not have to appear in any order (Note: randomly ordering arguments is not good practice, and this is only an example), and second, keyword arguments can be used only when needed since a default value is always given.

```
>>> array(dtype='complex64', object = [[1.0,2.0],[3.0,4.0]], copy=True)
array([[ 1.+0.j,   2.+0.j],
       [ 3.+0.j,   4.+0.j]], dtype=complex64)
```

Default Arguments

Functions have defaults for optional arguments. These are listed in the function definition and appear in the help in the form *keyword=default*. Returning to `array`, all inputs have default arguments except `object` – the only required input.

Multiple Outputs

Some functions can have more than 1 output. These functions can be used in a single output mode or in multiple output mode. For example, `shape` can be used on an array to determine the size of each dimension.

```
>>> x = array([[1.0,2.0],[3.0,4.0]])
>>> s = shape(x)
>>> s
(2, 2)
```

Since shape will return as many outputs as there are dimensions, it can be called with 2 outputs when the input is a 2-dimensional array.

```
>>> x = array([[1.0,2.0],[3.0,4.0]])
>>> M, N = shape(x)
>>> M
2

>>> N
2
```

Requesting more outputs than are required will produce an error.

```
>>> M, N, P = shape(x) # Error
ValueError: need more than 2 values to unpack
```

Similarly, providing two few output can also produce an error. Consider the case where the argument used with shape is a 3-dimensional array.

```
>>> x = randn(10,10,10)
>>> shape(x)
(10, 10, 10)
>>> M, N = shape(x) # Error
ValueError: too many values to unpack
```

3.10 Exercises

1. Input the following mathematical expressions into Python as arrays.

$$u = \begin{bmatrix} 1 & 1 & 2 & 3 & 5 & 8 \end{bmatrix}$$

$$v = \begin{bmatrix} 1 \\ 1 \\ 2 \\ 3 \\ 5 \\ 8 \end{bmatrix}$$

$$x = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$y = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

$$z = \begin{bmatrix} 1 & 2 & 1 & 2 \\ 3 & 4 & 3 & 4 \\ 1 & 2 & 1 & 2 \end{bmatrix}$$

$$w = \begin{bmatrix} x & x \\ y & y \end{bmatrix}$$

Note: A column vector must be entered as a 2-dimensional array.

2. What command would select x from w? (Hint: `w[?,?]` is the same as x.)

3. What command would select $[x' \, y']'$ from w? Is there more than one? If there are, list all alternatives.

4. What command would select y from z? List all alternatives.

5. Explore the options for creating an array using keyword arguments. Create an array containing

$$y = \begin{bmatrix} 1 & -2 \\ -3 & 4 \end{bmatrix}$$

with combination of keyword arguments in:

   (a) `dtype` in `float`, `float64`, `int32` (32-bit integers), `uint32` (32-bit unsigned integers) and `complex128` (double precision complex numbers).
   (b) `copy` either `True` or `False`.
   (c) `ndim` either 3 or 4. Use `shape(y)` to see the effect of this argument.

6. Enter $y = [1.6180 \; 2.7182 \; 3.1415]$ as an array. Define `x = mat(y)`. How is x different from y?

Chapter 4

Basic Math

Note: Python contains a `math` module providing functions which operate on built-in scalar data types (e.g. `float` and `complex`). This and subsequent chapters assume mathematical functions must operate on arrays, and so are imported from NumPy.

4.1 Operators

These standard operators are available:

Operator	Meaning	Example	Algebraic
+	Addition	`x + y`	$x + y$
-	Subtraction	`x - y`	$x - y$
*	Multiplication	`x * y`	xy
/	Division (Left divide)	`x/y`	$\frac{x}{y}$
//	Integer Division	`x//y`	$\left\lfloor \frac{x}{y} \right\rfloor$
**	Exponentiation	`x**y`	x^y

When `x` and `y` are scalars, the behavior of these operators is obvious. When `x` and `y` are arrays, the behavior of mathematical operations is more complex.

4.2 Broadcasting

Under the normal rules of array mathematics, addition and subtraction are only defined for arrays with the same shape or between an array and a scalar. For example, there is no obvious method to add a 5-element vector and a 5 by 4 2-dimensional array. NumPy uses a technique called broadcasting to allow element-by-element mathematical operations on arrays which would not be compatible under the standard rules of array mathematics.

Arrays can be used in element-by-element mathematics if `x` is broadcastable to `y`. Suppose `x` is an m-dimensional array with dimensions $d = [d_1, d_2 \ldots d_m]$, and `y` is an n-dimensional array with dimensions $f = [f_1, f_2 \ldots f_n]$ where $m \geq n$. Formally, two arrays are broadcastable if the following two conditions hold.

1. If $m > n$, then treat `y` as a m-dimensional array with size $g = [1, 1, \ldots, 1, f_1, f_2 \ldots f_n]$ where the number of 1s prepended is $m - n$. The dimensions are $g_i = 1$ for $i = 1, \ldots m - n$ and $g_i = f_{i-m+n}$ for $i > m - n$.

2. For $i = 1, \ldots, m$, $\max(d_i, g_i) / \min(d_i, g_i) \in \{1, \max(d_i, g_i)\}$.

The first rule specified that if one array has fewer dimensions, it is treated as having the same number of dimensions as the larger array by prepending 1s. The second rule specifies that arrays will only be broadcastable if either (a) they have the same dimension along axis i or (b) one has dimension 1 along axis i. When 2 arrays are broadcastable, the dimension of the output array is $\max(d_i, g_i)$ for $i = 1, \ldots n$.

Consider the following examples where m, n, and p are assumed to have different values.

x	y	Broadcastable	Output Size	x Operation	y Operation
Any	Scalar	✓	Same as x	x	`tile(y,shape(x))`
$m, 1$	$1, n$ or n	✓	m, n	`tile(x,(1,n))`	`tile(y,(m,1))`
$m, 1$	$n, 1$	✗			
m, n	$1, n$ or n	✓	m, n	x	`tile(y,(m,1))`
$m, n, 1$	$1, 1, p$ or $1, p$ or p	✓	m, n, p	`tile(x,(1,1,p))`	`tile(y,(m,n,1))`
m, n, p	$1, 1, p$ or $1, p$ or p	✓	m, n, p	x	`tile(y,(m,n,1))`
$m, n, 1$	$p, 1$	✗			
$m, 1, p$	$1, n, 1, 1, n, p$ or $n, 1$	✓	m, n, p	`tile(x,(1,n,1))`	`tile(y,(m,1,p))`

One simple method to visualize broadcasting is to use an add and subtract operation where the addition causes the smaller array to be broadcast, and then the subtract removes the values in the larger array. This will produce a replicated version of the smaller array which shows the nature of the broadcasting.

```
>>> x = array([[1,2,3.0]])
>>> x
array([[ 1.,   2.,   3.]])

>>> y = array([[0],[0],[0.0]])
>>> y
array([[ 0.],
       [ 0.],
       [ 0.]])

>>> x + y   # Adding 0 produces broadcast
array([[ 1.,   2.,   3.],
       [ 1.,   2.,   3.],
       [ 1.,   2.,   3.]])
```

In the next example, x is 3 by 5, so y must be either scalar or a 5-element array or a 1×5 array to be broadcastable. When y is a 3-element array (and so matches the *leading* dimension), an error occurs.

```
>>> x = reshape(arange(15),(3,5))
>>> x
array([[ 0,   1,   2,   3,   4],
       [ 5,   6,   7,   8,   9],
       [10, 11, 12, 13, 14]])
>>> y = 5
>>> x + y - x
array([[5, 5, 5, 5, 5],
       [5, 5, 5, 5, 5],
       [5, 5, 5, 5, 5]])

>>> y = arange(5)
>>> y
array([0, 1, 2, 3, 4])

>>> x + y - x
```

```
array([[0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4]])

>>> y = arange(3)
>>> y
array([0, 1, 2])

>>> x + y - x # Error
ValueError: operands could not be broadcast together with shapes (3,5) (3)
```

4.3 Addition (+) and Subtraction (−)

Subject to broadcasting restrictions, addition and subtraction operate element-by-element.

4.4 Multiplication (∗)

The standard multiplication operator, ∗, performs *element-by-element* multiplication and so inputs must be broadcastable.

4.5 Matrix Multiplication (@)

The matrix multiplication operator @ was introduced in Python 3.5. It can only be used to two arrays and cannot be used to multiply an array and a scalar. If x is N by M and y is K by L and both are non-scalar matrices, x @ y requires $M = K$. Similarly, y @ x requires $L = N$. When x and y are both arrays, z = x @ y produces an array with $z_{ij} = \sum_{k=1}^{M} x_{ik} y_{kj}$. **Note**s: The rules for @ conform to the standard rules of matrix multiplication except that scalar multiplication is not allowed. Multiplying an array by a scalar requires using ∗ or dot. x @ y is identical to x.dot(y) or np.dot(x, y).

```
>>> x = array([[1.0, 2],[ 3, 2], [3, 4]])
>>> y = array([[9.0, 8],[7, 6]])
>>> x @ y
array([[ 23.,  20.],
       [ 41.,  36.],
       [ 55.,  48.]])

>>> x.dot(y)
array([[ 23.,  20.],
       [ 41.,  36.],
       [ 55.,  48.]])

>>> 2 @ x # Error
ValueError: Scalar operands are not allowed, use '*' instead

>>> 2 * x
array([[ 2.,  4.],
       [ 6.,  4.],
       [ 6.,  8.]])
```

@ supports broadcasting in the sense that multiplying a 1-d array and a 2-d array will promote the 1-d array to be a 2-d array using the rules of broadcasting so that the *m* element array is created as a 1 by *m* element array.

4.6   Array and Matrix Division (/)

Division is always element-by-element, and the rules of broadcasting are used.

4.7   Exponentiation (**)

Array exponentiation operates element-by-element.

4.8   Parentheses

Parentheses can be used in the usual way to control the order in which mathematical expressions are evaluated, and can be nested to create complex expressions. See section 4.10 on Operator Precedence for more information on the order mathematical expressions are evaluated.

4.9   Transpose

Matrix transpose is expressed using either `.T` or the `transpose` function. For instance, if `x` is an *M* by *N* array, `transpose(x)`, `x.transpose()` and `x.T` are all its transpose with dimensions *N* by *M*. In practice, using the `.T` is the preferred method and will improve readability of code. Consider

```
>>> x = randn(2,2)
>>> xpx1 = x.T @ x
>>> xpx2 = x.transpose() @ x
>>> xpx3 = transpose(x) @ x
```

Transpose has no effect on 1-dimensaional arrays. In 2-dimensions, transpose switches indices so that if `z=x.T`, `z[j,i]` is that same as `x[i,j]`. In higher dimensions, transpose reverses the order or the indices. For example, if `x` has 3 dimensions and `z=x.T`, then `x[i,j,k]` is the same as `z[k,j,i]`. Transpose takes an optional second argument to specify the axis to use when permuting the array.

4.10   Operator Precedence

Computer math, like standard math, has operator precedence which determined how mathematical expressions such as

$$2**3+3**2/7*13$$

are evaluated. Best practice is to always use parentheses to avoid ambiguity in the order or operations. The order of evaluation is:

Operator	Name	Rank
( ), [ ], (,)	Parentheses, Lists, Tuples	1
**	Exponentiation	2
~	Bitwise NOT	3
+,-	Unary Plus, Unary Minus	3
*, /, //, %	Multiply, Divide, Modulo	4
+,-	Addition and Subtraction	5
&	Bitwise AND	6
^	Bitwise XOR	7
	Bitwise OR	8
<, <=, >, >=	Comparison operators	9
==, !=	Equality operators	9
in, not in	Identity Operators	9
is, is not	Membership Operators	9
not	Boolean NOT	10
and	Boolean AND	11
or	Boolean OR	12
=,+=,-=,/=,*=,**=	Assignment Operators	13

Note that some rows of the table have the same precedence, and are only separated since they are conceptually different. In the case of a tie, operations are executed left-to-right. For example, `x**y**z` is interpreted as `(x**y)**z`. This table has omitted some operators available in Python which are not generally useful in numerical analysis (e.g. shift operators).

Note: Unary operators are + or - operations that apply to a single element. For example, consider the expression `(-4)`. This is an instance of a unary negation since there is only a single operation and so `(-4)**2` produces 16. On the other hand, `-4**2` produces -16 since `**` has higher precedence than unary negation and so is interpreted as `-(4**2)`. `-4 * -4` produces `16` since it is interpreted as `(-4) * (-4)` since unary negation has higher precedence than multiplication.

4.11 Exercises

1. Using the arrays entered in exercise 1 of chapter 3, compute the values of $u + v'$, $v + u'$, vu, uv and xy (where the multiplication is as defined as linear algebra).

2. Which of the arrays in exercise 1 are broadcastable with:

$$a = [3\,2],$$

$$b = \begin{bmatrix} 3 \\ 2 \end{bmatrix},$$

$$c = [3\,2\,1\,0],$$

$$d = \begin{bmatrix} 3 \\ 2 \\ 1 \\ 0 \end{bmatrix}.$$

3. Is `x/1` legal? If not, why not. What about `1/x`?

4. Compute the values `(x+y)**2` and `x**2+x*y+y*x+y**2`. Are they the same when x and y are arrays?

5. Is `x**2+2*x*y+y**2` the same as any of the above?

6. For conformable arrays, is `a*b+a*c` the same as `a*b+c`? If so, show with an example. If not, how can the second be changed so they are equal?

7. Suppose a command `x**y*w+z` was entered. What restrictions on the dimensions of `w`, `x`, `y` and `z` must be true for this to be a valid statement?

8. What is the value of `-2**4`? What about `(-2)**4`? What about `-2*-2*-2*-2`?

Chapter 5

Basic Functions and Numerical Indexing

5.1 Generating Arrays

linspace

linspace(l, u, n) generates a set of n points uniformly spaced between l, a lower bound (inclusive) and u, an upper bound (inclusive).

```
>>> x = linspace(0, 10, 11)
>>> x
array([  0.,   1.,   2.,   3.,   4.,   5.,   6.,   7.,   8.,   9.,  10.])
```

logspace

logspace(l, u, n) produces a set of logarithmically spaced points between 10^l and 10^u. It is identical to `10**linspace(l,u,n)`.

arange

arange(l, u, s) produces a set of points spaced by s between l, a lower bound (inclusive) and u, an upper bound (exclusive). arange can be used with a single parameter, so that arange(n) is equivalent to arange(0,n,1). Note that arange will return integer data type if all inputs are integer.

```
>>> x = arange(11)
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10])

>>> x = arange(11.0)
array([  0.,   1.,   2.,   3.,   4.,   5.,   6.,   7.,   8.,   9.,  10.])

>>> x = arange(4, 10, 1.25)
array([ 4.  ,  5.25,  6.5 ,  7.75,  9.  ])
```

meshgrid

meshgrid broadcasts two vectors to produce two 2-dimensional arrays, and is a useful function when plotting 3-dimensional functions.

```
>>> x = arange(5)
>>> y = arange(3)
>>> X,Y = meshgrid(x,y)
>>> X
```

```
array([[0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4],
       [0, 1, 2, 3, 4]])

>>> Y
array([[0, 0, 0, 0, 0],
       [1, 1, 1, 1, 1],
       [2, 2, 2, 2, 2]])
```

r_

r_ is a convenience function which generates 1-dimensional arrays from slice notation. While r_ is highly flexible, the most common use it r_[*start* : *end* : *stepOrCount*] where *start* and *end* are the start and end points, and *stepOrCount* can be either a step size, if a real value, or a count, if complex.

```
>>> r_[0:10:1] # arange equiv
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

>>> r_[0:10:.5] # arange equiv
array([ 0. ,  0.5,  1. ,  1.5,  2. ,  2.5,  3. ,  3.5,  4. ,  4.5,  5. ,
        5.5,  6. ,  6.5,  7. ,  7.5,  8. ,  8.5,  9. ,  9.5])

>>> r_[0:10:5j] # linspace equiv, includes end point
array([ 0. ,  2.5,  5. ,  7.5,  10. ])
```

r_ can also be used to concatenate slices using commas to separate slice notation blocks.

```
>>> r_[0:2, 7:11, 1:4]
array([ 0,  1,  7,  8,  9, 10,  1,  2,  3])
```

Note that r_ is *not* a function and that is used with [].

c_

c_ is virtually identical to r_ except that column arrays are generates, which are 2-dimensional (second dimension has size 1)

```
>>> c_[0:5:2]
array([[0],
       [2],
       [4]])

>>> c_[1:5:4j]
array([[ 1.        ],
       [ 2.33333333],
       [ 3.66666667],
       [ 5.        ]])
```

c_, like r_, is not a function and is used with [].

ix_

ix_(*a, b*) constructs an *n*-dimensional open mesh from *n* 1-dimensional lists or arrays. The output of ix_ is an *n*-element tuple containing 1-dimensional arrays. The primary use of ix_ is to simplify selecting slabs inside an array. Slicing can also be used to select elements from an array as long as the slice pattern is regular. ix_ is particularly useful for selecting elements from an array using indices which are not regularly spaced, as in the final example.

```
>>> x = reshape(arange(25.0),(5,5))
>>> x
array([[  0.,   1.,   2.,   3.,   4.],
       [  5.,   6.,   7.,   8.,   9.],
       [ 10.,  11.,  12.,  13.,  14.],
       [ 15.,  16.,  17.,  18.,  19.],
       [ 20.,  21.,  22.,  23.,  24.]])

>>> x[ix_([2,3],[0,1,2])] # Rows 2 & 3, cols 0, 1 and 2
array([[ 10.,  11.,  12.],
       [ 15.,  16.,  17.]])

>>> x[2:4,:3] # Same, standard slice
array([[ 10.,  11.,  12.],
       [ 15.,  16.,  17.]])

>>> x[ix_([0,3],[0,1,4])] # No slice equiv
```

mgrid

mgrid is very similar to meshgrid but behaves like r_ and c_ in that it takes slices as input, and uses a real valued variable to denote step size and complex to denote number of values. The output is an $n+1$ dimensional vector where the first index of the output indexes the meshes.

```
>>> mgrid[0:3,0:2:.5]
array([[[ 0. ,  0. ,  0. ,  0. ],
        [ 1. ,  1. ,  1. ,  1. ],
        [ 2. ,  2. ,  2. ,  2. ]],

       [[ 0. ,  0.5,  1. ,  1.5],
        [ 0. ,  0.5,  1. ,  1.5],
        [ 0. ,  0.5,  1. ,  1.5]]])

>>> mgrid[0:3:3j,0:2:5j]
array([[[ 0. ,  0. ,  0. ,  0. ,  0. ],
        [ 1.5,  1.5,  1.5,  1.5,  1.5],
        [ 3. ,  3. ,  3. ,  3. ,  3. ]],

       [[ 0. ,  0.5,  1. ,  1.5,  2. ],
        [ 0. ,  0.5,  1. ,  1.5,  2. ],
        [ 0. ,  0.5,  1. ,  1.5,  2. ]]])
```

ogrid

ogrid is identical to mgrid except that the arrays returned are always 1-dimensional. ogrid output is generally more appropriate for looping code, while mgrid is usually more appropriate for vectorized code. When the size of the arrays is large, then ogrid uses much less memory.

```
>>> ogrid[0:3,0:2:.5]
[array([[ 0.],
        [ 1.],
        [ 2.]]), array([[ 0. ,  0.5,  1. ,  1.5]])]
>>> ogrid[0:3:3j,0:2:5j]
[array([[ 0. ],
        [ 1.5],
        [ 3. ]]),
 array([[ 0. ,  0.5,  1. ,  1.5,  2. ]])]
```

5.2   Rounding

around, round

around rounds to the nearest integer, or to a particular decimal place when called with two arguments.

```
>>> x = randn(3)
array([ 0.60675173, -0.3361189 , -0.56688485])

>>> around(x)
array([ 1.,  0., -1.])

>>> around(x, 2)
array([ 0.61, -0.34, -0.57])
```

around can also be used as a method on an ndarray – except that the method is named round. For example, x.round(2) is identical to around(x, 2). The change of names is needed to avoid conflicting with the Python built-in function round.

floor

floor rounds to the next smallest integer.

```
>>> x = randn(3)
array([ 0.60675173, -0.3361189 , -0.56688485])

>>> floor(x)
array([ 0., -1., -1.])
```

ceil

ceil rounds to the next largest integer.

```
>>> x = randn(3)
array([ 0.60675173, -0.3361189 , -0.56688485])

>>> ceil(x)
array([ 1., -0., -0.])
```

Note that the values returned are still floating points and so -0. is the same as 0..

5.3   Mathematics

sum, cumsum

sum sums elements in an array. By default, it will sum all elements in the array, and so the second argument is normally used to provide the axis to use – 0 to sum down columns, 1 to sum across rows. cumsum produces the cumulative sum of the values in the array, and is also usually used with the second argument to indicate the axis to use.

```
>>> x = randn(3,4)
>>> x
array([[-0.08542071, -2.05598312,  2.1114733 ,  0.7986635 ],
       [-0.17576066,  0.83327885, -0.64064119, -0.25631728],
       [-0.38226593, -1.09519101,  0.29416551,  0.03059909]])

>>> sum(x) # all elements
```

```
-0.62339964288008698

>>> sum(x, 0) # Down rows, 4 elements
array([-0.6434473 , -2.31789529,  1.76499762,  0.57294532])

>>> sum(x, 1) # Across columns, 3 elements
array([ 0.76873297, -0.23944028, -1.15269233])

>>> cumsum(x,0) # Down rows
array([[-0.08542071, -2.05598312,  2.1114733 ,  0.7986635 ],
       [-0.26118137, -1.22270427,  1.47083211,  0.54234622],
       [-0.6434473 , -2.31789529,  1.76499762,  0.57294532]])
```

`sum` and `cumsum` can both be used as function or as methods. When used as methods, the first input is the axis so that `sum(x,0)` is the same as `x.sum(0)`.

prod, cumprod

`prod` and `cumprod` behave similarly to `sum` and `cumsum` except that the product and cumulative product are returned. `prod` and `cumprod` can be called as function or methods.

diff

`diff` computes the finite difference of a vector (also array) and returns *n*-1 an element vector when used on an *n* element vector. `diff` operates on the last axis by default, and so `diff(x)` operates across columns and returns `x[:,1:size(x,1)]-x[:,:size(x,1)-1]` for a 2-dimensional array. `diff` takes an optional keyword argument `axis` so that `diff(x, axis=0)` will operate across rows. `diff` can also be used to produce higher order differences (e.g. double difference).

```
>>> x= randn(3,4)
>>> x
array([[-0.08542071, -2.05598312,  2.1114733 ,  0.7986635 ],
       [-0.17576066,  0.83327885, -0.64064119, -0.25631728],
       [-0.38226593, -1.09519101,  0.29416551,  0.03059909]])

>>> diff(x) # Same as diff(x,1)
-0.62339964288008698

>>> diff(x, axis=0)
array([[-0.09033996,  2.88926197, -2.75211449, -1.05498078],
       [-0.20650526, -1.92846986,  0.9348067 ,  0.28691637]])

>>> diff(x, 2, axis=0) # Double difference, column-by-column
array([[-0.11616531, -4.81773183,  3.68692119,  1.34189715]])
```

exp

`exp` returns the element-by-element exponential (e^x) for an array.

log

`log` returns the element-by-element natural logarithm ($\ln(x)$) for an array.

log10

`log10` returns the element-by-element base-10 logarithm ($\log_{10}(x)$) for an array.

sqrt

`sqrt` returns the element-by-element square root ($\sqrt{x}$) for an array.

square

`square` returns the element-by-element square (x^2) for an array, and is equivalent to calling `x**2.0` when `x` is an `array`.

absolute, abs

`abs` and `absolute` returns the element-by-element absolute value for an array. Complex modulus is returned when the input is complex valued ($|a+bi| = \sqrt{a^2 + b^2}$).

sign

`sign` returns the element-by-element sign function, defined as 0 if $x = 0$, and $x/|x|$ otherwise.

5.4 Complex Values

real

`real` returns the real elements of a complex array. `real` can be called either as a function `real(x)` or as an attribute `x.real`.

imag

`imag` returns the complex elements of a complex array. `imag` can be called either as a function `imag(x)` or as an attribute `x.imag`.

conj, conjugate

`conj` returns the element-by-element complex conjugate for a complex array. `conj` can be called either as a function `conj(x)` or as a method `x.conj()`. `conjugate` is identical to `conj`.

5.5 Set Functions

unique

`unique` returns the unique elements in an array. It only operates on the entire array. An optional second argument can be returned which contains the original indices of the unique elements.

```
>>> x = repeat(randn(3),(2))
array([ 0.11335982,  0.11335982,  0.26617443,  0.26617443,  1.34424621,
        1.34424621])

>>> unique(x)
array([ 0.11335982,  0.26617443,  1.34424621])

>>> y,ind = unique(x, True)
>>> ind
array([0, 2, 4], dtype=int64)
```

```
>>> x.flat[ind]
array([ 0.11335982,  0.26617443,  1.34424621])
```

in1d

in1d returns a Boolean array with the same size as the first input array indicating the elements which are also in a second array.

```
>>> x = arange(10.0)
>>> y = arange(5.0,15.0)
>>> in1d(x,y)
array([False, False, False, False, False,  True,  True,  True,  True,  True])
```

intersect1d

intersect1d is similar to in1d, except that it returns the elements rather than a Boolean array, and only unique elements are returned. It is equivalent to unique(x.flat[in1d(x,y)]).

```
>>> x = arange(10.0)
>>> y = arange(5.0,15.0)
>>> intersect1d(x,y)
array([ 5.,  6.,  7.,  8.,  9.])
```

union1d

union1d returns the unique set of elements in 2 arrays.

```
>>> x = arange(10.0)
>>> y = arange(5.0,15.0)
>>> union1d(x,y)
array([  0.,   1.,   2.,   3.,   4.,   5.,   6.,   7.,   8.,   9.,  10.,
        11.,  12.,  13.,  14.])
```

setdiff1d

setdiff1d returns the set of the elements which are only in the first array but not in the second array.

```
>>> x = arange(10.0)
>>> y = arange(5.0,15.0)
>>> setdiff1d(x,y)
array([ 0.,  1.,  2.,  3.,  4.])
```

setxor1d

setxor1d returns the set of elements which are in one (and only one) of two arrays.

```
>>> x = arange(10.0)
>>> y = arange(5.0,15.0)
>>> setxor1d(x,y)
array([  0.,   1.,   2.,   3.,   4.,  10.,  11.,  12.,  13.,  14.])
```

5.6 Sorting and Extreme Values

sort

`sort` sorts the elements of an array. By default, it sorts using the last axis of x. It uses an optional second argument to indicate the axis to use for sorting (i.e. 0 for column-by-column, `None` for sorting all elements). `sort` does not alter the input when called as function, unlike the method version of `sort`.

```
>>> x = randn(4,2)
>>> x
array([[ 1.29185667,  0.28150618],
       [ 0.15985346, -0.93551769],
       [ 0.12670061,  0.6705467 ],
       [ 2.77186969, -0.85239722]])

>>> sort(x)
array([[ 0.28150618,  1.29185667],
       [-0.93551769,  0.15985346],
       [ 0.12670061,  0.6705467 ],
       [-0.85239722,  2.77186969]])

>>> sort(x, 0)
array([[ 0.12670061, -0.93551769],
       [ 0.15985346, -0.85239722],
       [ 1.29185667,  0.28150618],
       [ 2.77186969,  0.6705467 ]])

>>> sort(x, axis=None)
array([-0.93551769, -0.85239722,  0.12670061,  0.15985346,  0.28150618,
        0.6705467 ,  1.29185667,  2.77186969])
```

ndarray.sort, argsort

`ndarray.sort` is a method for `ndarrays` which performs an in-place sort. It economizes on memory use, although `x.sort()` is different from x after the function, unlike a call to `sort(x)`. `x.sort()` sorts along the last axis by default, and takes the same optional arguments as `sort(x)`. `argsort` returns the indices necessary to produce a sorted array, but does not actually sort the data. It is otherwise identical to `sort`, and can be used either as a function or a method.

```
>>> x = randn(3)
>>> x
array([ 2.70362768, -0.80380223, -0.10376901])

>>> sort(x)
array([-0.80380223, -0.10376901,  2.70362768])

>>> x
array([ 2.70362768, -0.80380223, -0.10376901])

>>> x.sort() # In-place, changes x
>>> x
array([-0.80380223, -0.10376901,  2.70362768])
```

max, amax, argmax, min, amin, argmin

`max` and `min` return the maximum and minimum values from an array. They take an optional second argument which indicates the axis to use.

```
>>> x = randn(3,4)
>>> x
array([[-0.71604847,  0.35276614, -0.95762144,  0.48490885],
       [-0.47737217,  1.57781686, -0.36853876,  2.42351936],
       [ 0.44921571, -0.03030771,  1.28081091, -0.97422539]])

>>> amax(x)
2.4235193583347918

>>> x.max()
2.4235193583347918

>>> x.max(0)
array([ 0.44921571,  1.57781686,  1.28081091,  2.42351936])

>>> x.max(1)
array([ 0.48490885,  2.42351936,  1.28081091])
```

max and min can only be used on arrays as methods. When used as a function, amax and amin must be used to avoid conflicts with the built-in functions max and min. This behavior is also seen in around and round. argmax and argmin return the index or indices of the maximum or minimum element(s). They are used in an identical manner to max and min, and can be used either as a function or method.

minimum, maximum

maximum and minimum can be used to compute the maximum and minimum of two arrays which are broadcastable.

```
>>> x = randn(4)
>>> x
array([-0.00672734,  0.16735647,  0.00154181, -0.98676201])

>>> y = randn(4)
array([-0.69137963, -2.03640622,  0.71255975, -0.60003157])

>>> maximum(x,y)
array([-0.00672734,  0.16735647,  0.71255975, -0.60003157])
```

5.7 Nan Functions

NaN function are convenience function which act similarly to their non-NaN versions, only ignoring NaN values (rather than propagating) when computing the function.

nansum

nansum is identical sum, except that NaNs are ignored. nansum can be used to easily generate other NaN-functions, such as nanstd (standard deviation, ignoring nans) since variance can be implemented using 2 sums.

```
>>> x = randn(4)
>>> x[1] = nan
>>> x
array([-0.00672734,         nan,  0.00154181, -0.98676201])

>>> sum(x)
nan
```

```
>>> nansum(x)
-0.99194753275859726

>>> nansum(x) / sum(x[logical_not(isnan(x))])
1.0

>>> nansum(x) / sum(1-isnan(x)) # nanmean
-0.33064917999999999
```

nanmax, nanargmax, nanmin, nanargmin

nanmax, nanmin, nanargmax and nanargmin are identical to their non-NaN counterparts, except that NaNs are ignored.

5.8 Functions and Methods/Properties

Many operations on NumPy arrays can be performed using a function or as a method of the array. For example, consider reshape.

```
>>> x = arange(25.0)
>>> y = x.reshape((5,5))
>>> y
array([[  0.,   1.,   2.,   3.,   4.],
       [  5.,   6.,   7.,   8.,   9.],
       [ 10.,  11.,  12.,  13.,  14.],
       [ 15.,  16.,  17.,  18.,  19.],
       [ 20.,  21.,  22.,  23.,  24.]])

>>> z = reshape(x,(5,5))
>>> z
array([[  0.,   1.,   2.,   3.,   4.],
       [  5.,   6.,   7.,   8.,   9.],
       [ 10.,  11.,  12.,  13.,  14.],
       [ 15.,  16.,  17.,  18.,  19.],
       [ 20.,  21.,  22.,  23.,  24.]])
```

Both the function and method produce the same output and the choice of which to use is ultimately a personal decision. I use both and the choice primarily depends on the context. For example, to get the shape of an array, my preference is for x.shape over shape(x) since shape appears to be integral to x.[1] On the other hand, I prefer shape(y+z) over (y+z).shape due to the presence of the mathematical operation.

5.9 Exercises

1. Construct each of the following sequences using linspace, arange and r_:

$$0, 1, \ldots, 10$$

$$4, 5, 6, \ldots, 13$$

$$0, .25, .5, .75, 1$$

$$0, -1, -2, \ldots, -5$$

---

[1]Formally shape is a property of an array, not a method since it does not require a function call.

2. Show that `logspace(0,2,21)` can be constructed using `linspace` and `10` (and `**`). Similarly, show how `linsapce(2,10,51)` can be constructed with `logspace` and `log10`.

3. Determine the differences between the rounding by applying `round` (or `around`), `ceil` and `floor` to

$$y = [0, 0.5, 1.5, 2.5, 1.0, 1.0001, -0.5, -1, -1.5, -2.5]$$

4. Prove the relationship that $\sum_{j=1}^{n} j = n(n+1)/2$ for $0 \leq n \leq 10$ using `cumsum` and directly using math on an array.

5. `randn(20)` will generate an array containing draws from a standard normal random variable. If `x=randn(20)`, which element of `y=cumsum(x)` is the same as `sum(x)`?

6. `cumsum` computes the cumulative sum while `diff` computes the difference. Is `diff(cumsum(x))` the same as `x`? If not, how can a small modification be made to the this statement to recover `x`?

7. Compute the `exp` of
$$y = [\ln 0.5 \ \ln 1 \ \ln e]$$

Note: You should use `log` and the constant `numpy.e` to construct `y`.

8. What is `absolute` of `0.0`, `-3.14`, and `3+4j`?

9. Suppose $x = [-42 - 9 - 8 \ 10]$. What is the difference between `y = sort(x)` and `x.sort()`?

10. Using the same x as in the previous problem, find the `max`. Also, using `argmax` and a slice, retrieve the same value.

11. Show that `setdiff1d` could be replaced with `in1d` and `intersect1d` using $x = [1\,2\,3\,4\,5]$ and $y = [1\,2\,4\,6]$? How could `setxor1d` be replaced with `union1d`, `intersect1d` and `in1d`?

12. Suppose $y = [\text{nan} \ 2.2 \ 3.9 \ 4.6 \ \text{nan} \ 2.4 \ 6.1 \ 1.8]$. How can `nansum` be used to compute the variance or the data? Note: `sum(1-isnan(y))` will return the count of non-NaN values.

Chapter 6

Special Arrays

Functions are available to construct a number of useful, frequently encountered arrays.

ones

`ones` generates an array of 1s and is generally called with one argument, a tuple, containing the size of each dimension. `ones` takes an optional second argument (`dtype`) to specify the data type. If omitted, the data type is float.

```
>>> M, N = 5, 5
>>> x = ones((M,N)) # M by N array of 1s
>>> x =  ones((M,M,N)) # 3D array
>>> x =  ones((M,N), dtype='int32') # 32-bit integers
```

`ones_like` creates an array with the same shape and data type as the input. Calling `ones_like(x)` is equivalent to calling `ones(x.shape,x.dtype)`.

zeros

`zeros` produces an array of 0s in the same way `ones` produces an array of 1s, and commonly used to initialize an array to hold values generated by another procedure. `zeros` takes an optional second argument (`dtype`) to specify the data type. If omitted, the data type is float.

```
>>> x = zeros((M,N)) # M by N array of 0s
>>> x = zeros((M,M,N)) # 3D array of 0s
>>> x = zeros((M,N),dtype='int64') # 64 bit integers
```

`zeros_like` creates an array with the same size and shape as the input. Calling `zeros_like(x)` is equivalent to calling `zeros(x.shape,x.dtype)`.

empty

`empty` produces an empty (uninitialized) array to hold values generated by another procedure. `empty` takes an optional second argument (`dtype`) which specifies the data type. If omitted, the data type is float.

```
>>> x = empty((M,N)) # M by N empty array
>>> x = empty((N,N,N,N)) # 4D empty array
>>> x = empty((M,N),dtype='float32') # 32-bit floats (single precision)
```

Using `empty` is slightly faster than calling zeros since it does not assign 0 to all elements of the array – the "empty" array created will be populated with (essential random) non-zero values. `empty_like` creates an array with the same size and shape as the input. Calling `empty_like(x)` is equivalent to calling `empty(x.shape,x.dtype)`.

eye, identity

`eye` generates an identity array – an array with ones on the diagonal, zeros everywhere else. Normally, an identity array is square and so usually only 1 input is required. More complex zero-padded arrays containing an identity matrix can be produced using optional inputs.

```
>>> In = eye(N)
```

`identity` is a virtually identical function with similar use, `In = identity(N)`.

6.1 Exercises

1. Produce two arrays, one containing all zeros and one containing only ones, of size 10×5.

2. Multiply (linear algebra) these two arrays in both possible ways.

3. Produce an identity matrix of size 5. Take the exponential of this matrix, element-by-element.

4. How could `ones` and `zeros` be replaced with `tile`?

5. How could `eye` be replaced with `diag` and `ones`?

6. What is the value of `y=empty((1,))`? Is it the same as any element in `y=empty((10,))`?

Chapter 7

Array Functions

Many functions operate exclusively on array inputs, including functions which are mathematical in nature, for example computing the eigenvalues and eigenvectors and functions for manipulating the elements of an array.

7.1 Shape Information and Transformation

shape

`shape` returns the size of all dimensions or an array as a tuple. `shape` can be called as a function or an attribute. `shape` can also be used to reshape an array by entering a tuple of sizes. Additionally, the new shape can contain -1 which indicates to expand along this dimension to satisfy the constraint that the number of elements cannot change.

```
>>> x = randn(4,3)
>>> x.shape
(4, 3)

>>> shape(x)
(4, 3)

>>> M,N = shape(x)
>>> x.shape = 3,4
>>> x.shape
(3, 4)

>>> x.shape = 6,-1
>>> x.shape
(6, 2)
```

reshape

`reshape` transforms an array with one set of dimensions and to one with a different set, preserving the number of elements. Arrays with dimensions M by N can be reshaped into an array with dimensions K by L as long as $MN = KL$. The most useful call to reshape switches an array into a vector or vice versa.

```
>>> x = array([[1,2],[3,4]])
>>> y = reshape(x,(4,1))
>>> y
array([[1],
       [2],
       [3],
```

```
        [4]])

>>> z=reshape(y,(1,4))
>>> z
array([[1, 2, 3, 4]])

>>> w = reshape(z,(2,2))
array([[1, 2],
       [3, 4]])
```

The crucial implementation detail of `reshape` is that arrays are stored using row-major notation. Elements in arrays are counted first across rows and then then down columns. `reshape` will place elements of the old array into the same position in the new array and so after calling `reshape`, $x(1) = y(1)$, $x(2) = y(2)$, and so on.

size

`size` returns the total number of elements in an array. `size` can be used as a function or an attribute.

```
>>> x = randn(4,3)
>>> size(x)
12

>>> x.size
12
```

ndim

`ndim` returns the number of dimensions of an array. `ndim` can be used as a function or an attribute .

```
>>> x = randn(4, 3)
>>> ndim(x)
2

>>> x.ndim
2
```

tile

`tile`, along with `reshape`, are two of the most useful non-mathematical functions. `tile` replicates an array according to a specified size vector. To understand how `tile` functions, imagine forming an array composed of blocks. The generic form of `tile` is `tile(X, (M, N) )` where X is the array to be replicated, M is the number of rows in the new block array, and N is the number of columns in the new block array. For example, suppose X was an array

$$X = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$$

and the block array

$$Y = \begin{bmatrix} X & X & X \\ X & X & X \end{bmatrix}$$

was required. This could be accomplished by manually constructing y using `hstack` and `vstack`.

```
>>> x = array([[1,2],[3,4]])
>>> z = hstack((x,x,x))
>>> y = vstack((z,z))
```

However, `tile` provides a much easier method to construct `y`

```
>>> w = tile(x,(2,3))
>>> y - w
array([[0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0],
       [0, 0, 0, 0, 0, 0]])
```

`tile` has two clear advantages over manual allocation: First, `tile` can be executed using parameters determined at run-time, such as the number of explanatory variables in a model and second `tile` can be used for arbitrary dimensions. Manual array construction becomes tedious and error prone with as few as 3 rows and columns. `repeat` is a related function which copies data in a less useful manner.

ravel

`ravel` returns a flattened view (1-dimensional) of an array. `ravel` does not copy the underlying data (when possible), and so it is very fast.

```
>>> x = array([[1,2],[3,4]])
>>> x
array([[ 1,  2],
       [ 3,  4]])

>>> x.ravel()
array([1, 2, 3, 4])

>>> x.T.ravel()
array([1, 3, 2, 4])
```

flatten

`flatten` works like `ravel` except that it copies the array when producing the flattened version. In most cases, `ravel` should be used.

flat

`flat` produces a `numpy.flatiter` object (flat iterator) which is an iterator over a flattened view of an array. Because it is an iterator, it is especially fast and memory friendly. `flat` can be used as an iterator in a for loop or with slicing notation.

```
>>> x = array([[1,2],[3,4]])
>>> x.flat
<numpy.flatiter at 0x6f569d0>

>>> x.flat[2]
3

>>> x.flat[1:4] = -1
>>> x
array([[ 1, -1],
       [-1, -1]])
```

broadcast, broadcast_arrays

broadcast can be used to broadcast two broadcastable arrays without actually copying any data. It returns a broadcast object, which works like an iterator.

```
>>> x = array([[1,2,3,4]])
>>> y = reshape(x,(4,1))
>>> b = broadcast(x,y)
>>> b.shape
(4, 4)

>>> for u,v in b:
...     print('x: ', u, ' y: ',v)
x:  1  y:  1
x:  2  y:  1
x:  3  y:  1
x:  4  y:  1
x:  1  y:  2
 ... ... ...
```

broadcast_arrays works similarly to broadcast, except that it copies the broadcast arrays into new arrays. broadcast_arrays is generally slower than broadcast, and should be avoided if possible.

```
>>> x = array([[1,2,3,4]])
>>> y = reshape(x,(4,1))
>>> b = broadcast_arrays(x,y)
>>> b[0]
array([[1, 2, 3, 4],
       [1, 2, 3, 4],
       [1, 2, 3, 4],
       [1, 2, 3, 4]])

>>> b[1]
array([[1, 1, 1, 1],
       [2, 2, 2, 2],
       [3, 3, 3, 3],
       [4, 4, 4, 4]])
```

vstack, hstack

vstack, and hstack stack compatible arrays vertically and horizontally, respectively. Arrays are vstack compatible if they have the same number of columns, and are hstack compatible if they have the same number of rows. Any number of arrays can be stacked by placing the input arrays in a list or tuple, e.g. (x,y,z).

```
>>> x = reshape(arange(6),(2,3))
>>> y = x
>>> vstack((x,y))
array([[0, 1, 2],
       [3, 4, 5],
       [0, 1, 2],
       [3, 4, 5]])

>>> hstack((x,y))
array([[0, 1, 2, 0, 1, 2],
       [3, 4, 5, 3, 4, 5]])
```

concatenate

`concatenate` generalizes `vstack` and `hsplit` to allow concatenation along any axis using the keyword argument `axis`.

split, vsplit, hsplit

`vsplit` and `hsplit` split arrays vertically and horizontally, respectively. Both can be used to split an array into *n* equal parts or into arbitrary segments, depending on the second argument. If scalar, the array is split into *n* equal sized parts. If a 1 dimensional array, the array is split using the elements of the array as break points. For example, if the array was `[2,5,8]`, the array would be split into 4 pieces using `[:2]` , `[2:5]`, `[5:8]` and `[8:]`. Both `vsplit` and `hsplit` are special cases of `split`, which can split along an arbitrary axis.

```
>>> x = reshape(arange(20),(4,5))
>>> y = vsplit(x,2)
>>> len(y)
2

>>> y[0]
array([[0, 1, 2, 3, 4],
       [5, 6, 7, 8, 9]])

>>> y = hsplit(x,[1,3])
>>> len(y)
3

>>> y[0]
array([[ 0],
       [ 5],
       [10],
       [15]])

>>> y[1]
array([[ 1,  2],
       [ 6,  7],
       [11, 12],
       [16, 17]])
```

delete

`delete` removes values from an array, and is similar to splitting an array, and then concatenating the values which are not deleted. The form of delete is `delete(x, rc, axis)` where *rc* are the row or column indices to delete, and *axis* is the axis to use (0 or 1 for a 2-dimensional array). If *axis* is omitted, `delete` operated on the flattened array.

```
>>> x = reshape(arange(20),(4,5))
>>> delete(x,1,0) # Same as x[[0,2,3]]
array([[ 0,  1,  2,  3,  4],
       [10, 11, 12, 13, 14],
       [15, 16, 17, 18, 19]])

>>> delete(x,[2,3],1) # Same as x[:,[0,1,4]]
array([[ 0,  1,  4],
       [ 5,  6,  9],
       [10, 11, 14],
       [15, 16, 19]])
```

```
>>> delete(x,[2,3]) # Same as hstack((x.flat[:2],x.flat[4:]))
array([ 0,  1,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16, 17, 18,
       19])
```

squeeze

squeeze removes singleton dimensions from an array, and can be called as a function or a method.

```
>>> x = ones((5,1,5,1))
>>> shape(x)
(5, 1, 5, 1)

>>> y = x.squeeze()
>>> shape(y)
(5, 5)

>>> y = squeeze(x)
```

fliplr, flipud

fliplr and flipud flip arrays in a left-to-right and up-to-down directions, respectively. flipud reverses the elements in a 1-dimensional array, and flipud(x) is identical to x[::-1]. fliplr cannot be used with 1-dimensional arrays.

```
>>> x = reshape(arange(4),(2,2))
>>> x
array([[0, 1],
       [2, 3]])

>>> fliplr(x)
array([[1, 0],
       [3, 2]])

>>> flipud(x)
array([[2, 3],
       [0, 1]])
```

diag

The behavior of diag differs depending on the shape of the input. If the input is a square array, it will return a column vector containing the elements of the diagonal. If the input is an vector, it will return an array containing the elements of the vector along its diagonal. Consider the following example:

```
>>> x = array([[1,2],[3,4]])
>>> x
array([[1, 2],
       [3, 4]])

>>> y = diag(x)
>>> y
array([1, 4])

>>> z = diag(y)
>>> z
array([[1, 0],
       [0, 4]])
```

triu, tril

triu and tril produce upper and lower triangular arrays, respectively.

```
>>> x = array([[1,2],[3,4]])
>>> triu(x)
array([[1, 2],
       [0, 4]])

>>> tril(x)
array([[1, 0],
       [3, 4]])
```

7.2 Linear Algebra Functions

matrix_power

matrix_power raises a 2-dimensional square array to an integer power, and matrix_power(x,n) is identical to x**n.

svd

svd computes the singular value decomposition of an 2-dimensional array X, defined as

$$X = U\Sigma V$$

where Σ is diagonal, and U and V are unitary arrays (orthonormal if real valued). SVDs are closely related to eigenvalue decompositions when X is a real, positive definite array. The returned value is a tuple containing (U,s,V) where $\Sigma = \mathrm{diag}\,(s)$.

cond

cond computes the condition number of a 2-dimensional array, which measures how close to singular a matrix is. Lower numbers indicate that the input is better conditioned (further from singular).

```
>>> x = array([[1.0,0.5],[.5,1]])
>>> cond(x)
3
>>> x = array([[1.0,2.0],[1.0,2.0]]) # Singular
>>> cond(x)
inf
```

slogdet

slogdet computes the sign and log of the absolute value of the determinant. slogdet is useful for computing determinants which may be very large or small to avoid numerical problems.

solve

solve solves the system $X\beta = y$ when X is square and invertible so that the solution is exact.

```
>>> X = array([[1.0,2.0,3.0],[3.0,3.0,4.0],[1.0,1.0,4.0]])
>>> y = array([[1.0],[2.0],[3.0]])
>>> solve(X,y)
array([[ 0.625],
       [-1.125],
       [ 0.875]])
```

lstsq

lstsq solves the system $X\beta = y$ when X is n by k, $n > k$ by finding the least squares solution. lstsq returns a 4-element tuple where the first element is β and the second element is the sum of squared residuals. The final two outputs are diagnostic – the third is the rank of X and the fourth contains the singular values of X.

```
>>> X = randn(100, 2)
>>> y = randn(100)
>>> lstsq(X, y, rcond=None)
(array([ 0.03414346,  0.02881763]),
 array([ 3.59331858]),
 2,
 array([ 3.045516  ,  1.99327863]))array([[ 0.625],
       [-1.125],
       [ 0.875]])
```

Note: The rcond=None line is used to suppress a NumPy warning. Calling lstsq(X, y) produces a warning about future changes to how singular regressor arrays X are checked.

cholesky

cholesky computes the Cholesky factor of a 2-dimensional positive definite array. The Cholesky factor is a lower triangular matrix and is defined as C in

$$CC' = \Sigma$$

where Σ is a positive definite matrix.

```
>>> x = array([[1,.5],[.5,1]])
>>> c = cholesky(x)
>>> c@c.T - x
array([[ 0.00000000e+00,  0.00000000e+00],
       [ 0.00000000e+00, -1.11022302e-16]])
```

det

det computes the determinant of a square array.

```
>>> x = array([[1,.5],[.5,1]])
>>> det(x)
0.75
```

eig

eig computes the eigenvalues and eigenvectors of a square array. When used with one output, the eigenvalues and eigenvectors are returned as a tuple.

```
>>> x = array([[1,.5],[.5,1]])
>>> val,vec = eig(x)
>>> vec@diag(val)@vec.T
array([[ 1. ,   0.5],
       [ 0.5,   1. ]])
```

`eigvals` can be used if only eigenvalues are needed.

eigh

`eigh` computes the eigenvalues and eigenvectors of a symmetric array. When used with one output, the eigenvalues and eigenvectors are returned as a tuple. `eigh` is faster than `eig` for symmetrix inputs since it exploits the symmetry of the input. `eigvalsh` can be used if only eigenvalues are needed from a symmetric array.

inv

`inv` computes the inverse of an array.

```
>>> x = array([[1,.5],[.5,1]])
>>> xInv = inv(x)
>>> dot(x,xInv)
array([[ 1.,   0.],
       [ 0.,   1.]])
```

kron

`kron` computes the Kronecker product of two arrays,

$$z = x \otimes y$$

and is written as `z = kron(x,y)`.

trace

`trace` computes the trace of a square array (sum of diagonal elements). `trace(x)` equals `sum(diag(x))`.

matrix_rank

`matrix_rank` computes the rank of an array using a SVD.

```
>>> x = array([[1,.5],[1,.5]])
>>> x
array([[ 1. ,   0.5],
       [ 1. ,   0.5]])
>>> matrix_rank(x)
1
```

7.3 Views

Views are computationally efficient methods to produce objects of one type which behave as other objects of another type *without* copying data.

view

`view` can be used to produce a representation of an array as another type without copying the data. Using `view` is faster than copying data into a new class.

```
>>> x = arange(5)
>>> type(x)
numpy.ndarray

>>> x.view(recarray)
rec.array([0, 1, 2, 3, 4])
```

asarray

`asarray` is commonly used to ensure that a value is a NumPy `array`. It will create a new array if its input is not an array. If its input is an array, it defaults to returning the array without copying.

```
>>> from pandas import DataFrame
>>> x = DataFrame([[1,2],[3,4]])
>>> type(x)   # not an array
pandas.core.frame.DataFrame

>>> asarray(x)
array([[1, 2],
       [3, 4]], dtype=int64)
```

7.4 Exercises

1. Let `x = arange(12.0)`. Use both `shape` and `reshape` to produce 1×12, 2×6, 3×4, 4×3, 6×2 and $2 \times 2 \times 3$ versions or the array. Finally, return `x` to its original size.

2. Let `x = reshape(arange(12.0),(4,3))`. Use `ravel`, `flatten` and `flat` to extract elements 1, 3, ..., 11 from the array (using a 0 index).

3. Let x be 2 by 2 array, y be a 1 by 1 array, and z be a 3 by 2 array. Construct

$$
w = \begin{bmatrix} x & y & y & y \\ & y & y & y \\ & & z' & \\ z & y & y & y \end{bmatrix}
$$

   using `hstack`, `vstack`, and `tile`.

4. Let `x = reshape(arange(12.0),(2,2,3))`. What does `squeeze` do to x?

5. How can a diagonal array containing the diagonal elements of

$$
y = \begin{bmatrix} 2 & .5 \\ .5 & 4 \end{bmatrix}
$$

   be constructed using only `diag`?

6. Using the y array from the previous problem, verify that `cholesky` work by computing the Cholesky factor, and then multiplying to get y again.

7. Using the y array from the previous problem, verify that the sum of the eigenvalues is the same as the trace, and the product of the eigenvalues is the determinant.

8. Using the y array from the previous problem, verify that the inverse of y is equal to $VD^{-1}V'$ where V is the array containing the eigenvectors, and D is a diagonal array containing the eigenvalues.

9. Simulate some data where x = randn(100,2), e = randn(100,1), B = array([[1],[0.5]]) and $y = x\beta + \varepsilon$. Use lstsq to estimate β from x and y.

10. Suppose
$$y = \begin{bmatrix} 5 & -1.5 & -3.5 \\ -1.5 & 2 & -0.5 \\ -3.5 & -0.5 & 4 \end{bmatrix}$$

use matrix_rank to determine the rank of this array. Verify the results by inspecting the eigenvalues using eig and check that the determinant is 0 using det.

11. Let x = randn(100,2). Use kron to compute
$$I_2 \otimes \Sigma_X$$

where Σ_X is the 2 by 2 covariance matrix of x.

Chapter 8

Importing and Exporting Data

8.1 Importing Data using pandas

pandas is an increasingly important component of the Python scientific stack, and a complete discussion of its main features is included in Chapter 15. All of the data readers in pandas load data into a pandas DataFrame (see Section 15.1.2), and so these examples all make use of the `values` property to extract a NumPy array. In practice, the DataFrame is much more useful since it includes useful information such as column names read from the data source. In addition to the three formats presented here, pandas can also read json, SQL, html tables or from the clipboard, which is particularly useful for interactive work since virtually any source that can be copied to the clipboard can be imported.

8.1.1 CSV and other formatted text files

Comma-separated value (CSV) files can be read using `read_csv`. When the CSV file contains mixed data, the default behavior will read the file into an array with an `object` data type, and so further processing is usually required to extract the individual series.

```
>>> from pandas import read_csv
>>> csv_data = read_csv('FTSE_1984_2012.csv')
>>> csv_data = csv_data.to_numpy()  # As a NumPy array
>>> csv_data[:4]
array([['2012-02-15', 5899.9, 5923.8, 5880.6, 5892.2, 801550000, 5892.2],
       ['2012-02-14', 5905.7, 5920.6, 5877.2, 5899.9, 832567200, 5899.9],
       ['2012-02-13', 5852.4, 5920.1, 5852.4, 5905.7, 643543000, 5905.7],
       ['2012-02-10', 5895.5, 5895.5, 5839.9, 5852.4, 948790200, 5852.4]],
      dtype=object)

>>> open_price = csv_data[:,1]
```

When the entire file is numeric, the data will be stored as a homogeneous array using one of the numeric data types, typically float64. In this example, the first column contains Excel dates as numbers, which are the number of days past January 1, 1900.

```
>>> csv_data = read_csv('FTSE_1984_2012_numeric.csv')
>>> csv_data = csv_data.to_numpy()
>>> csv_data[:4,:2]
array([[ 40954. ,    5899.9],
       [ 40953. ,    5905.7],
       [ 40952. ,    5852.4],
       [ 40949. ,    5895.5]])
```

8.1.2 Excel files

Excel files, both 97/2003 (xls) and 2007/10/13 (xlsx), can be imported using `read_excel`. Two inputs are required to use `read_excel`, the filename and the sheet name containing the data. In this example, pandas makes use of the information in the Excel workbook that the first column contains dates and converts these to `datetimes`. Like the mixed CSV data, the array returned has `object` data type.

```
>>> from pandas import read_excel
>>> excel_data = read_excel('FTSE_1984_2012.xls','FTSE_1984_2012')
>>> excel_data = excel_data.values
>>> excel_data[:4,:2]
array([[datetime.datetime(2012, 2, 15, 0, 0), 5899.9],
       [datetime.datetime(2012, 2, 14, 0, 0), 5905.7],
       [datetime.datetime(2012, 2, 13, 0, 0), 5852.4],
       [datetime.datetime(2012, 2, 10, 0, 0), 5895.5]], dtype=object)

>>> open_price = excel_data[:,1]
```

8.1.3 STATA files

pandas also contains a method to read STATA files.

```
>>> from pandas import read_stata
>>> stata_data = read_stata('FTSE_1984_2012.dta')
>>> stata_data = stata_data.values
>>> stata_data[:4,:2]
array([[  0.00000000e+00,   4.09540000e+04],
       [  1.00000000e+00,   4.09530000e+04],
       [  2.00000000e+00,   4.09520000e+04],
       [  3.00000000e+00,   4.09490000e+04]])
```

8.2 Importing Data without pandas

Importing data without pandas ranges from easy to difficult depending on whether the files contain only numbers, the data size and the regularity of the format of the data. A few principles can simplify this task:

- The file imported should contain numbers *only*, with the exception of the first row which may contain the variable names.

- Use another program, such as Microsoft Excel, to manipulate data before importing.

- Each column of the spreadsheet should contain a single variable.

- Dates should be converted to YYYYMMDD, a numeric format, before importing. This can be done in Excel using the formula:
  `=10000*YEAR(A1)+100*MONTH(A1)+DAY(A1)+(A1-FLOOR(A1,1))`

- Store times separately from dates using a numeric format such as seconds past midnight or HHmmSS.sss.

8.2.1 CSV and other formatted text files

A number of importers are available for regular (e.g. all rows have the same number of columns) comma-separated value (CSV) data. The choice of which importer to use depends on the complexity and size of the file. Purely numeric files are the simplest to import, although most files which have a repeated structure can be directly imported (unless they are very large).

loadtxt

loadtxt is a simple, fast text importer. The basic use is loadtxt(*filename*), which will attempt to load the data in file name as floats. Other useful named arguments include delim, which allow the file delimiter to be specified, and skiprows which allows one or more rows to be skipped.

loadtxt requires the data to be numeric and so is only useful for the simplest files.

```
>>> data = loadtxt('FTSE_1984_2012.csv',delimiter=',') # Error
ValueError: could not convert string to float: Date

# Fails since CSV has a header
>>> data = loadtxt('FTSE_1984_2012_numeric.csv',delimiter=',') # Error
ValueError: could not convert string to float: Date

>>> data = loadtxt('FTSE_1984_2012_numeric.csv',delimiter=',',skiprows=1)
>>> data[0]
array([ 4.09540000e+04, 5.89990000e+03, 5.92380000e+03, 5.88060000e+03,
5.89220000e+03, 8.01550000e+08, 5.89220000e+03])
```

genfromtxt

genfromtxt is a slightly slower, more robust importer. genfromtxt is called using the same syntax as loadtxt, but will not fail if a non-numeric type is encountered. Instead, genfromtxt will return a NaN (not-a-number) for fields in the file it cannot read.

```
>>> data = genfromtxt('FTSE_1984_2012.csv',delimiter=',')
>>> data[0]
array([ nan,   nan,   nan,   nan,   nan,   nan,   nan])
>>> data[1]
array([ nan, 5.89990000e+03, 5.92380000e+03, 5.88060000e+03, 5.89220000e+03, 8.01550000e+08,
5.89220000e+03])
```

Tab delimited data can be read in a similar manner using delimiter='\t'.

```
>>> data = genfromtxt('FTSE_1984_2012_numeric_tab.txt',delimiter='\t')
```

csv2rec

csv2rec has been removed from matplotlib. pandas is the preferred method to import csv data.

8.2.2 Excel Files

xlrd

Reading Excel files in Python is more involved, and it is simpler to convert the xls to CSV. Excel files can be read using xlrd (which is part of xlutils).

```python
import xlrd

wb = xlrd.open_workbook('FTSE_1984_2012.xls')
# To read xlsx change the filename
# wb = xlrd.open_workbook('FTSE_1984_2012.xlsx')
sheetNames = wb.sheet_names()
# Assumes 1 sheet name
sheet = wb.sheet_by_name(sheetNames[0])
excelData = [] # List to hold data
for i in range(sheet.nrows):
```

```
        excelData.append(sheet.row_values(i))

# Subtract 1 since excelData has the header row
open_price = empty(len(excelData) - 1)
for i in range(len(excelData) - 1):
    open_price[i] = excelData[i+1][1]
```

The listing does a few things. First, it opens the workbook for reading (`open_workbook`), then it gets the sheet names (`wb.sheet_names()`) and opens a sheet (`wb.sheet_by_name` using the first sheet name in the file, `sheetNames[0]`). From the sheet, it gets the number of rows (`sheet.nrows`), and fills a list with the values, row-by-row. Once the data has been read-in, the final block fills an array with the opening prices. This is substantially more complicated than importing from a CSV file, although reading Excel files is useful for automated work (e.g. you have no choice but to import from an Excel file since it is produced by some other software).

openpyxl

openpyxl reads and writes the modern Excel file format (.xlsx) that is the default in Office 2007 or later. openpyxl also supports a reader and writer which is optimized for large files, a feature not available in xlrd. Unfortunately, openpyxl uses a different syntax from xlrd, and so some modifications are required when using openpyxl.

```
import openpyxl

wb = openpyxl.load_workbook('FTSE_1984_2012.xlsx')
sheetNames = wb.sheetnames
# Assumes 1 sheet name
sheet = wb[sheetNames[0]]
rows = sheet.rows

# rows is a generator, so it is directly iterable
open_price = [row[1].value for row in rows]
```

The strategy with 2007/10/13 xlsx files is essentially the same as with 97/2003 files. The main difference is that the command `sheet.rows()` returns a tuple containing the all of the rows in the selected sheet. Each row is itself a tuple which contains `Cells` (which are a type created by openpyxl), and each cell has a `value` (Cells also have other useful attributes such as `data_type` and methods such as `is_date()`).

Using the optimized reader is similar. The primary differences are:

- The rows are sequentially accessible using `iter_rows()`.

- `value` is not available, and so `internal_value` must be used.

- The number of rows is not known, and so it isn't possible to pre-allocate the storage variable with the correct number of rows.

```
import openpyxl

wb = openpyxl.load_workbook('FTSE_1984_2012.xlsx')
sheetNames = wb.sheetnames
# Assumes 1 sheet name
sheet = wb[sheetNames[0]]

# Use list to store data
open_price = []
```

```
# Changes since access is via memory efficient iterator
# Note () on iter_rows
for row in sheet.iter_rows():
    # Must use internal_value
    open_price.append(row[1].internal_value)

# Burn first row and convert to array
open_price = array(open_price[1:])
```

8.2.3 MATLAB Data Files (.mat)

Modern mat files

MATLAB stores data in a standard format known as Hierarchical Data Format, of HDF. HDF is a generic storage technology that provides fast access to stored data as well as on-the-fly compression. Starting in MATLAB 7.3, mat files are stored using HDF version 5, and so can be read in using the PyTables package.

```
>>> import tables
>>> matfile = tables.open_file('FTSE_1984_2012_v73.mat')
>>> matfile.root
/ (RootGroup) ''
  children := ['volume' (CArray), 'high' (CArray), 'adjclose' (CArray), 'low' (CArray), '
      close' (CArray), 'open' (CArray)]

>>> matfile.root.open
/open (CArray(1, 7042), zlib(3)) ''
  atom := Float64Atom(shape=(), dflt=0.0)
  maindim := 0
  flavor := 'numpy'
  byteorder := 'little'
  chunkshape := (1, 7042)

>>> open_price = matfile.root.open.read()
>>> open_price
array([[5899.9, 5905.7, 5852.4, ..., 1095.4, 1095.4, 1108.1]])

>>> matfile.close() # Close the file
```

Legacy mat files

SciPy enables legacy MATLAB data files (mat files) to be read. The most recent file format, V7.3, is not supported but can be read using PyTables or h5py. Data from compatible mat files can be loaded using loadmat. The data is loaded into a dictionary, and individual variables are accessed using the keys of the dictionary.

```
>>> import scipy.io as sio
>>> mat_data = sio.loadmat('FTSE_1984_2012.mat')
>>> type(mat_data)
dict

>>> mat_data.keys()
['volume',
 '__header__',
 '__globals__',
 'high',
 'adjclose',
 'low',
 'close',
```

```
'__version__',
'open']

>>> open_price = mat_data['open']
```

8.2.4 Reading Complex Files

Python can be programmed to read any text file format since it contains functions for directly accessing files and parsing strings. Reading poorly formatted data files is an advanced technique and should be avoided if possible. However, some data is only available in formats where reading in data line-by-line is the only option. For example, the standard import methods fail if the raw data is very large (too large for Excel) and is poorly formatted. In this case, the only possibility may be to write a program to read the file line-by-line (or in blocks) and to directly process the raw text.

The file *IBM_TAQ.txt* contains a simple example of data that is difficult to import. This file was downloaded from Wharton Research Data Services and contains all prices for IBM from the TAQ database between January 1, 2001, and January 31, 2001. It is too large to use in Excel and has both numbers, dates, and text on each line. The following code block shows one method for importing this data set.

```python
from numpy import array

f = open('IBM_TAQ.txt', 'r')
line = f.readline()
# Burn the first list as a header
line = f.readline()

date = []
time = []
price = []
volume = []
while line:
    data = line.split(',')
    date.append(int(data[1]))
    price.append(float(data[3]))
    volume.append(int(data[4]))
    t = data[2]
    time.append(int(t.replace(':','')))
    line = f.readline()

# Convert to arrays, which are more useful than lists
# for numeric data
date = array(date)
price = array(price)
volume = array(volume)
time = array(time)

all_data = array([date, price, volume, time])

f.close()
```

This block of code does a few things:

- Open the file directly using `open`[1]

- Reads the file line by line using `readline`

---

[1]See Section 22.4 for information on context managers, the preferred way to use `open`.

- Initializes lists for all of the data

- Rereads the file parsing each line by the location of the commas using `split(',')` to split the line at each comma into a list

- Uses `replace(':','')` to remove colons from the times

- Uses `int()` and `float()` to convert strings to numbers

- Closes the file directly using `close()`

8.3 Saving or Exporting Data using pandas

pandas supports writing to CSV, other delimited text formats, Excel files, json, html tables, HDF5 and STATA. An understanding of the pandas' DataFrame is required prior to using pandas file writing facilities, and Chapter 15 provides further information.

8.4 Saving or Exporting Data without pandas

Native NumPy Format

A number of options are available for saving data. These include using native npz data files, MATLAB data files, CSV or plain text. Multiple NumPy arrays can be saved using NumPy's `savez_compressed`.

```
x = arange(10)
y = zeros((100,100))
savez_compressed('test',x,y)
data = load('test.npz')
# If no name is given, arrays are generic names arr_1, arr_2, etc
x = data['arr_1']

savez_compressed('test',x=x,otherData=y)
data = load('test.npz')
# x=x provides the name x for the data in x
x = data['x']
# otherDate = y saves the data in y as otherData
y = data['otherData']
```

A version which does not compress data but is otherwise identical is `savez`. Compression is usually a good idea and is very helpful for storing arrays which have repeated values and are large.

8.4.1 Writing MATLAB Data Files (.mat)

SciPy enables MATLAB data files to be written. Data can be written using `savemat`, which takes two inputs, a file name and a dictionary containing data, in its simplest form.

```
import scipy.io as sio

x = array([1.0,2.0,3.0])
y = zeros((10,10))
# Set up the dictionary
saveData = {'x':x, 'y':y}
sio.savemat('test',saveData,do_compression=True)
# Read the data back in
mat_data = sio.loadmat('test.mat')
```

savemat uses the optional argument do_compression = True, which compresses the data, and is generally a good idea on modern computers and/or for large datasets.

8.4.2 Exporting Data to Text Files

Data can be exported to a tab-delimited text files using savetxt. By default, savetxt produces tab delimited files, although then can be changed using the names argument delimiter.

```
x = randn(10,10)
# Save using tabs
savetxt('tabs.txt',x)
# Save to CSV
savetxt('commas.csv',x,delimiter=',')
# Reread the data
x_data = loadtxt('commas.csv',delimiter=',')
```

8.5 Exercises

Note: There are no exercises using pandas in this chapter. For exercises using pandas to read or write data, see Chapter 15.

1. The file *exercise3.xls* contains three columns of data, the date, the return on the S&P 500, and the return on XOM (ExxonMobil). Using Excel, convert the date to YYYYMMDD format and save the file.

2. Save the file as both CSV and tab delimited. Use the three text readers to read the file, and compare the arrays returned.

3. Parse loaded data into three variables, dates, SP500 and XOM.

4. Save NumPy, compressed NumPy and MATLAB data files with all three variables. Which files is the smallest?

5. Construct a new variable, sumreturns as the sum of SP500 and XOM. Create another new variable, outputdata as a horizontal concatenation of dates and sumreturns.

6. Export the variable outputdata to a new CSV file using savetxt.

7. (Difficult) Read in *exercise3.xls* directly using xlrd.

8. (Difficult) Save *exercise3.xls* as *exercise3.xlsx* and read in directly using openpyxl.

Chapter 9

`Inf`, `NaN` and Numeric Limits

9.1 `inf` and `NaN`

`inf` represents infinity and `inf` is distinct from `-inf`. `inf` can be constructed in a number for ways, for example or `exp(710)`. `nan` stands for Not a Number, and `nan`s are created whenever a function produces a result that cannot be clearly evaluated to produce a number or infinity. For example, `inf`/`inf` results in `nan`. `nan`s often cause problems since most mathematical operations involving a `nan` produce a `nan`.

```
>>> x = nan
>>> 1.0 + x
nan

>>> 1.0 * x
nan

>>> 0.0 * x
nan

>>> mean(x)
nan
```

9.2 Floating point precision

All numeric software has limited precision; Python is no different. The easiest to understand the upper and lower limits, which are 1.7976×10^{308} (see `finfo(float).max`) and -1.7976×10^{308} (`finfo(float).min`). Numbers larger (in absolute value) than these are `inf`. The smallest positive number that can be expressed is 2.2250×10^{-308} (see `finfo(float).tiny`). Numbers between -2.2251×10^{-308} and 2.2251×10^{-308} are numerically 0.

However, the hardest concept to understand about numerical accuracy is the limited *relative* precision which is 2.2204×10^{-16} on most x86 and x86_64 systems. This value is returned from the command `finfo(float).eps` and may vary based on the type of CPU and/or the operating system used. Numbers which differ by less than 2.2204×10^{-16} are numerically the same. To explore the role of precision, examine the results of the following:

```
>>> x = 1.0
>>> eps = finfo(float).eps
>>> x = x+eps/2
>>> x == 1
True

>>> x-1
```

```
0.0

>>> x = 1 + 2*eps
>>> x == 1
False

>>> x-1
ans = 4.4408920985006262e-16
```

Moreover, any number y where $y < (x \times 2.2204 \times 10^{-16})$ is treated as 0 when added or subtracted. This is referred to as the relative range.

```
>>> x=10
>>> x+2*eps
>>> x-10
0

>>> (x-10) == 0
True

>>> (1e120 - 1e103) == 1e120
True

>>> 1e103 / 1e120
1e-17
```

In the first example, `eps/2<eps` *when compared to 1* so it has no effect while `2*eps>eps` and so this value is different from 1. In the second example, `2*eps/10<eps`, it has no effect when added. The final example subtracts 10^{103} from 10^{120} and shows that this is numerically the same as 10^{120} – again, this occurs since $10^{103}/10^{120} = 10^{-17} <$`eps`. While numeric limits is a tricky concept to understand, failure to understand these limits can produce unexpected results in code that appears to be otherwise correct. The practical usefulness of limited precision is to consider data scaling since many variables have natural scales which differ by many orders of magnitude.

9.3 Exercises

Let `eps = finfo(float).eps` in the following exercises.

1. What is the value of `log(exp(1000))` both analytically and in Python? Why do these differ?

2. Is `eps/10` different from 0? If `x = 1 + eps/10 - 1`, is x different from 0?

3. Is `1-eps/10-1` difference from `0`? What about `1-1-eps/10`?

4. Is `.1` different from `.1+eps/10`?

5. Is x = `10.0**120` (1×10^{120}) different from y = `10.0**120 + 10.0**102`? (Hint: Test with `x == y`)

6. Why is x = `10**120` (1×10^{120}) different from y = `10**120 + 10**102`?

7. Suppose x = `2.0`. How many times (n) can x = `1.0 + (x-1.0)/2.0` be run before `x==1` shows `True`? What is the value of `2.0**(-n)`. Is this value surprising?

Chapter 10

Logical Operators and Find

Logical operators are useful when writing batch files or custom functions. Logical operators, when combined with flow control, allow for complex choices to be compactly expressed.

10.1 >, >=, <, <=, ==, !=

The core logical operators are

Symbol	Function	Definition
>	greater	Greater than
>=	greater_equal	Greater than or equal to
<	less	Less than
<=	less_equal	Less than or equal to
==	equal	Equal to
!=	not_equal	Not equal to

Logical operators can be used on scalars, arrays or matrices. All comparisons are done element-by-element and return either `True` or `False`. For example, suppose x and y are arrays which are broadcastable. `z= x < y` will be an array of the same size as `broadcast(x,y).shape` composed of `True` and `False`. Alternatively, if one is scalar, say y, then the elements of z are `z[i,j] = x[i,j] < y`. For instance, suppose `z = ` xLy where L is one of the logical operators above such as `<` or `==`. The following table examines the behavior when x and/or y are scalars or arrays. Suppose `z = x < y`:

		y	
		Scalar	Array
x	Scalar	Any	Any
		$z = x < y$	$z_{ij} = x < y_{ij}$
	Array	Any	Broadcastable
		$z_{ij} = x_{ij} < y$	$z_{ij} = \tilde{x}_{ij} < \tilde{y}_{ij}$

where $\tilde{x}$ and $\tilde{y}$ are the post-broadcasting versions of x and y. Logical operators are frequently used in portions of programs known as flow control (e.g. `if ... else ...` blocks) which are be discussed in Chapter 12. It is important to remember that array logical operations return arrays and that flow control blocks *require scalar logical expressions*.

```
>>> x = array([[1,2],[-3,-4]])
>>> x > 0
array([[ True,  True],
```

```
        [False, False]])

>>> x == -3
array([[False, False],
       [ True, False]])

>>> y = array([1,-1])
>>> x < y # y broadcast to be (2,2)
array([[False, False],
       [ True,  True]])

>>> z = array([[1,1],[-1,-1]]) # Same as broadcast y
>>> x < z
array([[False, False],
       [ True,  True]])
```

10.2   and, or, not and xor

Logical expressions can be combined using four logical devices,

Keyword (Scalar)	Function	Bitwise	True if …
and	logical_and	&	Both True
or	logical_or		Either or Both True
not	logical_not	~	Not True
	logical_xor	^	One True and One False

There are three versions of all operators except XOR. The keyword version (e.g. `and`) can only be used with scalars and so it not useful when working with NumPy. Both the function and bitwise operators can be used with NumPy arrays, although care is required when using the bitwise operators. Bitwise operators have high priority – higher than logical comparisons – and so parentheses are required around comparisons. For example, `(x>1) & (x<5)` is a valid statement, while `x>1 & x<5`, which is evaluated as `(x>(1 & x))<5`, produces an error.

```
>>> x = arange(-2.0,4)
>>> y = x >= 0
>>> z = x < 2
>>> logical_and(y, z)
array([False, False,  True,  True, False, False])

>>> y & z
array([False, False,  True,  True, False, False])

>>> (x > 0) & (x < 2)
array([False, False,  True,  True, False, False])

>>> x > 0 & x < 4 # Error
TypeError: ufunc 'bitwise_and' not supported for the input types, and the inputs could
    not be safely coerced to any supported types according to the casting rule ''safe''

>>> ~(y & z) # Not
array([ True,  True, False, False,  True,  True])
```

These operators follow the same rules as most mathematical operators on arrays, and so require the broadcastable input arrays.

10.3   Multiple tests

`all` and `any`

The commands `all` and `any` take logical input and are self-descriptive. `all` returns `True` if all logical elements in an array are 1. If `all` is called without any additional arguments on an array, it returns `True` if all elements of the array are logical true and 0 otherwise. `any` returns `logical(True)` if any element of an array is `True`. Both `all` and `any` can be also be used along a specific dimension using a second argument or the keyword argument `axis` to indicate the axis of operation (0 is column-wise and 1 is row-wise). When used column- or row-wise, the output is an array with one less dimension than the input, where each element of the output contains the truth value of the operation on a column or row.

```
>>> x = array([[1, 2], [3, 4]])
>>> y = x <= 2
>>> y
array([[ True,  True],
       [False, False]])

>>> any(y)
True

>>> any(y,0)
array([[ True,  True]])

>>> any(y,1)
array([[ True],
       [False]])
```

`allclose`

`allclose` can be used to compare two arrays for near equality. This type of function is important when comparing floating point values which may be effectively the same although not identical.

```
>>> eps = np.finfo(np.float64).eps
>>> eps
2.2204460492503131e-16

>>> x = randn(2)
>>> y = x + eps
>>> x == y
array([False, False])

>>> allclose(x,y)
True
```

The tolerance for being close can be set using keyword arguments either relatively (`rtol`) or absolutely (`atol`).

`array_equal`

`array_equal` tests if two arrays have the same shape and elements. It is safer than comparing arrays directly since comparing arrays which are not broadcastable produces an error.

`array_equiv`

`array_equiv` tests if two arrays are equivalent, even if they do not have the exact same shape. Equivalence is defined as one array being broadcastable to produce the other.

```
>>> x = randn(10,1)
>>> y = tile(x,2)
>>> array_equal(x,y)
False

>>> array_equiv(x,y)
True
```

10.4 `is*`

A number of special purpose logical tests are provided to determine if an array has special characteristics. Some operate element-by-element and produce an array of the same dimension as the input while other produce only scalars. These functions all begin with `is`.

Operator	True if …	Method of operation
isnan	1 if nan	element-by-element
isinf	1 if inf	element-by-element
isfinite	1 if not inf and not nan	element-by-element
isposfin,isnegfin	1 for positive or negative inf	element-by-element
isreal	1 if not complex valued	element-by-element
iscomplex	1 if complex valued	element-by-element
isreal	1 if real valued	element-by-element
is_string_like	1 if argument is a string	scalar
is_numlike	1 if is a numeric type	scalar
isscalar	1 if scalar	scalar
isvector	1 if input is a vector	scalar

```
>>> x=array([4,pi,inf,inf/inf])
>>> x
array([4.      ,  3.14159265,       inf,       nan])

>>> isnan(x)
array([False, False, False,  True])

>>> isinf(x)
array([False, False,  True, False])

>>> isfinite(x)
array([ True,  True, False, False])

>>> isnan(x)  isinf(x)  isfinite(x)
array([ True,  True,  True,  True])
```

isnan(x) *isinf(x)* isfinite(x) always equals True for elements of a numeric array, implying any element falls into one (and only one) of these categories.

10.5 Exercises

1. Using the data file created in Chapter 8, count the number of negative returns in both the S&P 500 and ExxonMobil.

2. For both series, create an indicator variable that takes the value 1 if the return is larger than 2 standard deviations or smaller than -2 standard deviations. What is the average return conditional on falling each range for both returns.

3. Construct an indicator variable that takes the value of 1 when both returns are negative. Compute the correlation of the returns conditional on this indicator variable. How does this compare to the correlation of all returns?

4. What is the correlation when at least 1 of the returns is negative?

5. What is the relationship between `all` and `any`. Write down a logical expression that allows one or the other to be avoided (i.e. write `def` `myany(x)` and `def` `myall(y)`).

Chapter 11

Advanced Selection and Assignment

Elements from NumPy arrays can be selected using four methods: scalar selection, slicing, numerical (or list-of-locations) indexing and logical (or Boolean) indexing. Chapter 3 described scalar selection and slicing, which are the basic methods to access elements in an array. Numerical indexing and logical indexing are closely related and allow for more flexible selection. Numerical indexing uses lists or arrays of locations to select elements while logical indexing uses arrays containing Boolean values to select elements.

11.1   Numerical Indexing

Numerical indexing, also called list-of-location indexing, is an alternative to slice notation. The fundamental idea underlying numerical indexing is to use coordinates to select elements, which is similar to the underlying idea behind slicing. Numerical indexing differs from standard slicing in three important ways:

- Arrays created using numerical indexing are copies of the underlying data, while slices are views (and so do not copy the data). This means that while changing elements in a slice also changes elements in the slice's parent, changing elements in an array constructed using numerical indexing does not. This also can create performance concerns and slicing should generally be used whenever it is capable of selecting the required elements.

- Numerical indices can contain repeated values and are not required to be monotonic, allowing for more flexible selection. The sequences produced using slice notation are always monotonic with unique values.

- The shape of the array selected is determined by the shape of the numerical indices. Slices are similar to 1-dimensional arrays but the shape of the slice is determined by the slice inputs.

Numerical indexing in 1-dimensional arrays uses the numerical index values as locations in the array (0-based indexing) and returns an array with the same dimensions as the numerical index. To understand the core concept behind numerical indexing, consider the case of selecting 4 elements form a 1-dimensional array with locations $i_1, \ldots, i_4$. Numerical indexing uses the four indices and arranges them to determine the shape (and order) of the output. For example, if the order was

$$\begin{bmatrix} i_3 & i_2 \\ i_4 & i_1 \end{bmatrix}$$

then the array selected would be 2 by 2 with elements

$$\begin{bmatrix} x_{i_3} & x_{i_2} \\ x_{i_4} & x_{i_1} \end{bmatrix}.$$

Numerical indexing allows for arbitrary shapes and repetition, and so the selection matrix

$$\begin{bmatrix} i_3 & i_2 & i_3 & i_2 \\ i_4 & i_1 & i_3 & i_2 \\ i_4 & i_1 & i_4 & i_1 \end{bmatrix}$$

could be used to produce a 4 by 2 array containing the corresponding elements of x. In these examples the indices are not used in any particular order and are repeated to highlight the flexibility of numerical indexing.

Note that the numerical index can be either a list or a NumPy array and *must contain integer data*.

```
>>> x = 10 * arange(5.0)
>>> x[[0]] # List with 1 element
array([ 0.])

>>> x[[0,2,1]] # List
array([ 0.,   20.,   10.])

>>> sel = array([4,2,3,1,4,4]) # Array with repetition
>>> x[sel]
array([ 40.,   20.,   30.,   10.,   40.,   40.])

>>> sel = array([[4,2],[3,1]]) # 2 by 2 array
>>> x[sel] # Selection has same size as sel
array([[ 40.,   20.],
       [ 30.,   10.]])

>>> sel = array([0.0,1]) # Floating point data
>>> x[sel] # Error
IndexError: arrays used as indices must be of integer (or boolean) type

>>> x[sel.astype(int)] # No error
array([ 10.,   20.])

>>> x[0] # Scalar selection, not numerical indexing
1.0
```

These examples show that the numerical indices determine the element location and the shape of the array used to index determines the output shape. The final three examples show slightly different behavior. The first two of these demonstrate that only integer arrays can be used in numerical indexing, while the final example shows that there is a subtle difference between `x[[0]]` (or `x[array([0])]`), which is using numerical indexing and `x[0]` which is using a scalar selector. `x[[0]]` returns a 1-dimensional array since the list has 1 dimension while `x[0]` returns a non-array (or scalar or 0-dimensional array) since the input is not a list or array.

Numerical indexing in 2- or higher-dimensional arrays uses numerical index arrays for each dimension. The fundamental idea behind numerical indexing in 2-dimensional arrays is to format coordinate pairs of the form (i_k, j_k) into separate arrays. The size of the arrays will determine the shape of the array selected. For example, if the two selection arrays were

$$[i_1, i_3, i_2, i_4] \text{ and } [j_1, j_3, j_2, j_4]$$

then a 1-dimensional array would be selected containing the elements

$$[x(i_i, j_i), x(i_3, j_3), x(i_2, j_2), x(i_4, j_4)].$$

In practice multidimensional indexing is more flexible that this simple example since the arrays used as selectors can have either the same shape *or* can be broadcastable (see Section 4.2).

Consider the following four examples.

```
>>> x = reshape(arange(10.0), (2,5))
>>> x
array([[ 0.,  1.,  2.,  3.,  4.],
       [ 5.,  6.,  7.,  8.,  9.]])

>>> sel = array([0,1])
>>> x[sel,sel] # 1-dim arrays, no broadcasting
array([ 0.,  6.])

>>> x[sel, sel+1]
array([ 1.,  7.])

>>> sel_row = array([[0,0],[1,1]])
>>> sel_col = array([[0,1],[0,1]])
>>> x[sel_row,sel_col] # 2 by 2, no broadcasting
array([[ 0.,  1.],
       [ 5.,  6.]])

>>> sel_row = array([[0],[1]])
>>> sel_col = array([[0,1]])
>>> x[sel_row,sel_col] # 2 by 1 and 1 by 2 - difference shapes, broadcasted as 2 by 2
array([[ 0.,  1.],
       [ 5.,  6.]])
```

In the first example, `sel` is a 1-dimensional array containing `[0,1]`, and so the returned value is also a 1-dimensional array containing the $(0,0)$ and $(1,1)$ elements of `x`. Numerical indexing uses the array in the first position to determine row locations and the array in the second position to determine column locations. The first element of the row selection is paired with the first element of column selection (as is the second element). This is why `x[sel,sel+1]` selects the elements in the $(0,1)$ and $(1,2)$ positions (1 and 7, respectively). The third example uses 2-dimensional arrays and selects the elements $(0,0)$, $(0,1)$, $(1,0)$ and $(1,1)$. The final example also uses 2-dimensional arrays but with different sizes – 2 by 1 and 1 by 2 – which are broadcastable to a common shape of 2 by 2 arrays.

Next, consider what happens when non-broadcastable arrays are used in as numerical indexing.

```
>>> sel_row = array([0,1]) # 1-dimensional with shape (2,)
>>> sel_col = array([1,2,3]) # 1-dimensional with shape (3,)
>>> x[sel_row,sel_col] # Error
ValueError: shape mismatch: objects cannot be broadcast to a single shape
```

An error occurs since these two 1-dimensional arrays are not broadcastable. `ix_` can be used to easily select rows and columns using numerical indexing by translating the 1-dimesnional arrays to be the correct size for broadcasting.

```
>>> x[ix_([0,1],[1,2,3])]
array([[ 2.,  3.,  4.],
       [ 7.,  8.,  9.]])
```

11.1.1 Mixing Numerical Indexing with Scalar Selection

NumPy permits using difference types of indexing in the same expression. Mixing numerical indexing with scalar selection is trivial since any scalar can be broadcast to any array shape.

```
>>> sel=array([[1],[2]]) # 2 by 1
>>> x[0,sel] # Row 0, elements sel
array([[ 1.],
       [ 2.]])

>>> sel_row = array([[0],[0]])
```

```
>>> x[sel_row,sel] # Identical
array([[ 1.],
       [ 2.]])
```

11.1.2 Mixing Numerical Indexing with Slicing

Mixing numerical indexing and slicing allow for entire rows or columns to be selected.

```
>>> x[:,[1]]
array([[ 2.],
       [ 7.]])

>>> x[[1],:]
array([[  6.,   7.,   8.,   9.,  10.]])
```

Note that the mixed numerical indexing and slicing uses a list (`[1]`) so that it is not a scalar. This is important since using a scalar will result in dimension reduction.

```
>>> x[:,1] # 1-dimensional
array([ 2.,   7.])
```

Numerical indexing and slicing can be mixed in more than 2-dimensions, although some care is required. In the simplest case where only one numerical index is used which is 1-dimensional, then the selection is equivalent to calling `ix_` where the slice $a:b:s$ is replaced with `arange(a,b,s)`.

```
>>> x = reshape(arange(3**3), (3,3,3)) # 3-d array
>>> sel1 = x[::2,[1,0],:1]
>>> sel2 = x[ix_(arange(0,3,2),[1,0],arange(0,1))]
>>> sel1.shape
(2, 2, 1)

>>> sel2.shape
(2, 2, 1)

>>> amax(abs(sel1-sel2))
0
```

When more than 1 numerical index is used, the selection can be viewed as a 2-step process.

1. Select using only slice notation where the dimensions using numerical indexing use the slice `:`.

2. Apply the numerical indexing to the array produced in step 1.

```
>>> sel1 = x[[0,0],[1,0],:1]
>>> step1 = x[:,:,:1]
>>> step2 = x[[0,0],[1,0],:]
>>> step2.shape
(2, 1)

>>> amax(abs(sel1-step2))
0
```

In the previous example, the shape of the output was `(2, 1)` which may seem surprising since the numerical indices where both 1-dimensional arrays with 2 elements. The "extra" dimension comes from the slice notation which always preserves its dimension. In the next example, the output is 3-dimensional since the numerical indices are 1-dimensional and the 2 slices preserve their dimension.

```
>>> x = reshape(arange(4**4), (4,4,4,4))
>>> sel = x[[0,1],[0,1],:2,:2] # 1-dimensional numerical and 2 slices
>>> sel.shape
(2, 2, 2)
```

It is possible to mix multidimensional numerical indexing with slicing and multidimensional arrays. This type of selection is not explicitly covered since describing the output is complicated and this type of selection is rarely encountered.

11.1.3   Linear Numerical Indexing using `flat`

Like slicing, numerical indexing can be combined with `flat` to select elements from an array using the row-major ordering of the array. The behavior of numerical indexing with `flat` is identical to that of using numerical indexing on a flattened version of the underlying array.

```
>>> x.flat[[3,4,9]]
array([  4.,    5.,   10.])

>>> x.flat[[[3,4,9],[1,5,3]]]
array([[  4.,    5.,   10.],
       [  2.,    6.,    4.]])
```

11.1.4   Mixing Numerical Indexing with Slicing and Scalar Selection

Mixing the three is identical to using numerical indexing and slicing since the scalar selection is always broadcast to be compatible with the numerical indices.

11.2   Logical Indexing

Logical indexing differs from slicing and numeric indexing by using logical indices to select elements, rows or columns. Logical indices act as light switches and are either "on" (`True`) or "off" (`False`). Pure logical indexing uses a logical indexing array with the same size as the array being used for selection and always returns a 1-dimensional array.

```
>>> x = arange(-3,3)
>>> x < 0
array([ True,   True,   True, False, False, False])

>>> x[x < 0]
array([-3, -2, -1])

>>> x[abs(x) >= 2]
array([-3, -2,  2])

>>> x = reshape(arange(-8, 8), (4,4))
>>> x[x < 0]
array([-8, -7, -6, -5, -4, -3, -2, -1])
```

It is tempting to use two 1-dimensional logical arrays to act as row and column masks on a 2-dimensional array. This does not work, and it is necessary to use `ix_` if interested in this type of indexing.

```
>>> x = reshape(arange(-8,8),(4,4))
>>> cols = any(x < -6, 0)
>>> rows = any(x < 0, 1)
>>> cols
array([ True,   True, False, False])

>>> rows
array([ True,   True, False, False])

>>> x[cols,rows] # Not upper 2 by 2
```

```
array([-8, -3])

>>> x[ix_(cols,rows)] # Upper 2 by 2
array([[-8, -7],
       [-4, -3]])
```

The difference between the final 2 commands is due to the implementation of logical indexing when more than one logical index is used. When using 2 or more logical indices, they are first transformed to numerical indices using `nonzero` which returns the locations of the non-zero elements (which correspond to the `True` elements of a Boolean array).

```
>>> cols.nonzero()
(array([0, 1], dtype=int64),)

>>> rows.nonzero()
(array([0, 1], dtype=int64),)
```

The corresponding numerical index arrays have compatible sizes – both are 2-element, 1-dimensional arrays – and so numeric selection is possible. Attempting to use two logical index arrays which have non-broadcastable dimensions produces the same error as using two numerical index arrays with non-broadcastable sizes.

```
>>> cols = any(x < -6, 0)
>>> rows = any(x < 4, 1)
>>> rows
array([ True,  True,  True, False])

>>> x[cols,rows] # Error
ValueError: shape mismatch: objects cannot be broadcast to a single shape
```

11.2.1   Mixing Logical Indexing with Scalar Selection

Logical indexing can be combined with scalar selection to select elements from a specific row or column in a 2-dimensional array. Combining these two types of indexing is no different from first applying the scalar selection to the array and then applying the logical indexing.

```
>>> x = reshape(arange(-8,8), (4,4))
>>> x
array([[-8, -7, -6, -5],
       [-4, -3, -2, -1],
       [ 0,  1,  2,  3],
       [ 4,  5,  6,  7]])

>>> sum(x, 0)
array([-8, -4,  0,  4])

>>> sum(x, 0) >= 0
array([False, False,  True,  True])

>>> x[0,sum(x, 0) >= 0]
array([-6, -5])
```

11.2.2   Mixing Logical Indexing with Slicing

Logical indexing can be freely mixed with slices by using 1-dimensional logical index arrays which act as selectors for columns or rows.

```
>>> sel = sum(x < -1, 0) >= 2
>>> sel
```

```
array([ True,   True,   True, False])

>>> x[:,sel] # All rows, sel selects columns
array([[-8, -7, -6],
       [-4, -3, -2],
       [ 0,  1,  2],
       [ 4,  5,  6]])

>>> x[1:3,sel] # Rows 1 and 2, sel selects columns
array([[-4, -3, -2],
       [ 0,  1,  2]])

>>> x[sel,2:] # sel selects rows, columns 2 and 3
array([[-6, -5],
       [-2, -1],
       [ 2,  3]])
```

11.2.3   Mixing Logical Indexing with Numerical Indexing

Mixing numerical indexing and logical indexing behaves identically to numerically indexing where the logical index is converted to a numerical index using `nonzero`. It must be the case that the array returned by `nonzero` and the numerical index arrays are broadcastable.

```
>>> sel = array([True,True,False,False])
>>> sel.nonzero()
(array([0, 1], dtype=int64),)

>>> x[[2,3],sel] # Elements (2,0) and (3,1)
array([0, 5])

>>> x[[2,3],[0,1]] # Identical
array([0, 5])
```

11.2.4   Logical Indexing Functions

`nonzero` and `flatnonzero`

`nonzero` is a useful function for working with multiple data series. `nonzero` takes logical inputs and returns a tuple containing the indices where the logical statement is true. This tuple is suitable for indexing so that the corresponding elements can be accessed using `x[indices]`.

```
>>> x = array([[1,2],[3,4]])
>>> sel = x <= 3
>>> indices = nonzero(sel)
>>> indices
(array([0, 0, 1], dtype=int64), array([0, 1, 0], dtype=int64))

>>> x[indices]
array([[1, 2, 3]])
```

`flatnonzero` is similar to `nonzero` except that the indices returned are for the flattened version of the input.

```
>>> flatnonzero(sel)
array([0, 1, 2], dtype=int64)

>>> x.flat[flatnonzero(sel)]
array([1, 2, 3])
```

argwhere

`argwhere` returns an array containing the locations of elements where a logical condition is `True`. It is the same as `transpose(nonzero(x))`

```
>>> x = randn(3)
>>> x
array([-0.5910316 ,  0.51475905,  0.68231135])

>>> argwhere(x<0.6)
array([[0],
       [1]], dtype=int64)

>>> argwhere(x<-10.0) # Empty array
array([], shape=(0, 1), dtype=int64)

>>> x = randn(3,2)
>>> x
array([[ 0.72945913,  1.2135989 ],
       [ 0.74005449, -1.60231553],
       [ 0.16862077,  1.0589899 ]])

>>> argwhere(x<0)
array([[1, 1]], dtype=int64)

>>> argwhere(x<1)
array([[0, 0],
       [1, 0],
       [1, 1],
       [2, 0]], dtype=int64)
```

extract

`extract` is similar to `argwhere` except that it returns the values where the condition is true rather than the indices.

```
>>> x = randn(3)
>>> x
array([-0.5910316 ,  0.51475905,  0.68231135])

>>> extract(x<0, x)
array([-0.5910316])

>>> extract(x<-10.0, x) # Empty array
array([], dtype=float64)

>>> x = randn(3,2)
>>> x
array([[ 0.72945913,  1.2135989 ],
       [ 0.74005449, -1.60231553],
       [ 0.16862077,  1.0589899 ]])

>>> extract(x>0,x)
array([ 0.72945913,  1.2135989 ,  0.74005449,  0.16862077,  1.0589899 ])
```

11.3 Performance Considerations and Memory Management

Arrays constructed using any numerical indexing and/or logical indexing are *always* copies of the underlying array. This is different from the behavior of slicing and scalar selection which returns a view, not a copy, of an array. This is easily verified by selecting the same elements using different types of selectors.

```
>>> x = reshape(arange(9), (3,3))
>>> s_slice = x[:1,:] # Pure slice
>>> s_scalar = x[0] # Scalar selection
>>> s_numeric = x[[0],:] # Numeric indexing
>>> s_logical = x[array([True,False,False]),:] # Logical indexing
>>> s_logical[0,0] = -40
>>> s_numeric[0,0] = -30
>>> s_numeric # -30
array([[-10,   1,   2]])

>>> s_logical # -40, not -30
array([[-40,   1,   2]])

>>> s_scalar[0] = -10
>>> s_scalar
array([-10,   1,   2])

>>> x # Has a -10
array([[-10,   1,   2],
       [  3,   4,   5],
       [  6,   7,   8]])

>>> s_slice # Has a -10
array([[-10,   1,   2]])
```

Since both numerical and logical indexing produce copies, some care is needed when using these selectors on large arrays.

11.4 Assignment with Broadcasting

Any of the selection methods can be used for assignment. When the shape of the array to be assigned is the same as the selection, the assignment simply replaces elements using an element-by-element correspondence.

```
>>> x = arange(-2,2.0)
>>> x
array([-2., -1.,  0.,  1.])

>>> x[0] = 999 # Scalar
>>> x
array([999., -1.,  0.,  1.])
>>> x[:2] = array([99.0,99]) # Slice
>>> x
array([ 99.,  99.,   0.,   1.])

>>> x[[0,1,2]] = array([-3.14,-3.14,-3.14]) # Numerical indexing
>>> x
array([-3.14, -3.14, -3.14,  1.  ])

>>> x[x<0] = zeros(3) # Logical indexing
array([ 0.,  0.,  0.,  1.])
```

Assignment is not limited to arrays with exact shape matches, and any assignment where two conditions are met is allowed:

- Each dimension of the array to be assigned is either 1 or matches the selection.

- The array to be assigned and the selection are broadcastable.

These two conditions ensure that the array to be assigned can be broadcast up to the shape of the selection – it is not sufficient that the selection and the array to be assigned are simply broadcastable. The simplest form of broadcasting assigns a scalar to a selection, and since a scalar can always be broadcast to any shape this is always possible.

```
>>> x = array([99.0, 99.0, nan, nan])
>>> x
array([ 99.,   99.,    nan,   nan])

>>> x[isnan(x)] = 0   # Logical indexing
>>> x
array([ 99.,   99.,    0.,    0.])

>>> x.shape = (2,2)
>>> x[:,:] = 3.14   # Could also use x[:]
>>> x
array([[ 3.14,   3.14],
       [ 3.14,   3.14]])
```

While broadcasting a scalar is the most frequently encountered case, there are useful applications of vector (or 1-dimensional array) to 2-dimensional array assignment. For example, it may be necessary to replace all rows in an array where some criteria are satisfied in the row.

```
>>> x = reshape(arange(-10,10.0),(4,5))
array([[-10.,   -9.,   -8.,   -7.,   -6.],
       [ -5.,   -4.,   -3.,   -2.,   -1.],
       [  0.,    1.,    2.,    3.,    4.],
       [  5.,    6.,    7.,    8.,    9.]])

>>> x[sum(x,1)<0,:] = arange(5.0) # Replace rows w/ negative sum
>>> x = reshape(arange(-10,10.0),(4,5))
>>> # Replace columns with negative sum
>>> x[:, sum(x,0)<0] = arange(4.0) # Error
 ValueError: shape mismatch: value array of shape (4,) could not be broadcast to
indexing result of shape (3,4)

>>> x[:, sum(x,0)<0] = reshape(arange(4.0),(4,1)) # Broadcastable col replacement
>>> x
array([[ 0.,   0.,   0.,  -7.,  -6.],
       [ 1.,   1.,   1.,  -2.,  -1.],
       [ 2.,   2.,   2.,   3.,   4.],
       [ 3.,   3.,   3.,   8.,   9.]])
```

The error in the previous example occurs because the slice selects a 4 by 2 array, but the array to be assigned is 1-dimensional with 4 elements. The rules of broadcasting always prepend 1s when determining whether two arrays are broadcastable, and so the 1-dimensional array is considered to be a 1 by 4 array, which is not broadcastable to a 4 by 2 array. Using an explicitly 2-dimensional array with shape 4 by 1 allows for broadcasting.

11.5 Exercises

Let `x=arange(10.0)`, `y=reshape(arange(25.0),(5,5))` and `z=reshape(arange(64.0),(4,4,4))` in all exercises.

1. List all methods to select `4.0` from `x`.

2. List all methods to select the first 5 elements of `x`.

3. List all methods to select every second element of `x`.

4. List all methods to select the row 2 from `y`.

5. List all methods to select the rows 2 and 4 from `y`.

6. List all methods to select the rows 2 and 4 and columns 2, 3 and 4 from `y`.

7. Select all rows of `y` which have at least one number divisible by 5 and at least one divisible by 7.

8. List all the methods to select panel 1 from `z`.

9. List all the methods to select rows 2 and 3 from all panels of `z`.

10. Assign 0 to every second element of `z`. List the alternative methods.

11. Assign $[-1, -1, -1, -1]$ to all rows of `z` which have at least one number divisible by 4 and one divisible by 6. For example, the row containing $[16, 17, 18, 19]$ satisfies this criteria.

12. (Difficult) Define `sel = array([[0,1],[1,0]])`, What shape does `y[sel,:]` have? Can this be explained?

Chapter 12

Flow Control, Loops and Exception Handling

The previous chapter explored one use of logical variables, selecting elements from an array. Flow control also utilizes logical variables to allow different code to be executed depending on whether certain conditions are met. Flow control in Python comes in two forms - conditional statement and loops.

12.1   Whitespace and Flow Control

Python uses white space changes to indicate the start and end of flow control blocks, and so indention matters. For example, when using `if` ... `elif` ... `else` blocks, all of the control blocks must have the same indentation level and all of the statements inside the control blocks should have the same level of indentation. Returning to the previous indentation level instructs Python that the block is complete. Best practice is to only use spaces (and not tabs) and to use 4 spaces when starting a new level of indentation which represents a reasonable balance between readability and wasted space.

12.2   `if` ... `elif` ... `else`

`if` ... `elif` ... `else` blocks always begin with an `if` statement immediately followed by a *scalar* logical expression. `elif` and `else` are optional and can always be replicated using nested `if` statements at the expense of more complex logic and deeper nesting. The generic form of an `if` ... `elif` ... `else` block is

```
if logical_1:
    Code to run if logical_1
elif  logical_2:
    Code to run if logical_2 and not logical_1
elif  logical_3:
    Code to run if logical_3 and not logical_1 or logical_2
...
...
else:
    Code to run if all previous logicals are false
```

However, simpler forms are more common,

```
if logical:
    Code to run if logical true
```

or

```
if logical:
    Code to run if logical true
else:
    Code to run if logical false
```

Important: Remember that all *logical*s must be scalar logical values. While it is possible to use arrays containing a single element, attempting to use an array with more than 1 element results in an error.

A few simple examples

```
>>> x = 5
>>> if x<5:
...     x += 1
... else:
...     x -= 1

>>> x
4
```

and

```
>>> x = 5;
>>> if x<5:
...     x = x + 1
... elif x>5:
...     x = x - 1
... else:
...     x = x * 2

>>> x
 10
```

These examples have all used simple logical expressions. However, any *scalar* logical expressions, such as `(y<0 or y>1)`, `(x<0 or x>1) and (y<0 or y>1)` or `isinf(x) or isnan(x)`, can be used in `if` ... `elif` ... `else` blocks.

12.3 `for`

`for` loops begin with `for` *item* `in` *iterable*`:`, and the generic structure of a `for` loop is

```
for item in iterable:
    Code to run
```

item is an element from *iterable*, and *iterable* can be anything that is iterable in Python. The most common examples are `range`, lists, tuples, arrays or matrices. The `for` loop will iterate across all items in iterable, beginning with item `0` and continuing until the final item. When using multidimensional arrays, only the outside dimension is directly iterable. For example, if `x` is a 2-dimensional array, then the iterable elements are `x[0]`, `x[1]` and so on.

```
count = 0
for i in range(100):
    count += i

count = 0
x = linspace(0,500,50)
for i in x:
    count += i

count = 0
x = list(arange(-20,21))
```

```
for i in x:
    count += i
```

The first loop will iterate over $i = 0, 1, 2, \ldots, 99$. The second loops over the values produced by the function `linspace`, which returns an array with 50 uniformly spaced points between 0 and 500, inclusive. The final loops over x, a vector constructed from a call to `list(arange(-20,21))`, which produces a list containing the series $-20, -19, \ldots, 0, \ldots 19, 20$. All three – range, arrays, and lists – are iterable. The key to understanding `for` loop behavior is that `for` always iterates over the elements of the *iterable* in the order they are presented (i.e. *iterable[0]*, *iterable[1]*, …).

Loops can also be nested

```
count = 0
for i in range(10):
    for j in range(10):
        count += j
```

or can contain flow control variables

```
returns = randn(100)
count = 0
for ret in returns:
    if ret<0:
        count += 1
```

This `for` expression can be equivalently expressed using `range` as the iterator and `len` to get the number of items in the iterable.

```
returns = randn(100)
count = 0
for i in range(len(returns)):
    if returns[i]<0:
        count += 1
```

Finally, these ideas can be combined to produce nested loops with flow control.

```
x = zeros((10,10))
for i in range(size(x,0)):
    for j in range(size(x,1)):
        if i<j:
            x[i,j]=i+j;
        else:
            x[i,j]=i-j
```

or loops containing nested loops that are executed based on a flow control statement.

```
x = zeros((10,10))
for i in range(size(x,0)):
    if (i % 2) == 1:
        for j in range(size(x,1)):
            x[i,j] = i+j
    else:
        for j in range(int(i/2)):
            x[i,j] = i-j
```

Important: The iterable variable should not be reassigned once inside the loop. Consider, for example,

```
x = range(10)
for i in x:
    print(i)
    print('Length of x:', len(x))
    x = range(5)
```

This produces the output

```
# Output
0
Length of x: 10
1
Length of x: 5
2
Length of x: 5
3
...
8
Length of x: 5
9
Length of x: 5
```

It is not safe to modify the sequence of the *iterable* when looping over it. The means that the *iterable* should not change size, which can occur when using a list and the functions `pop()`, `insert()` or `append()` or the keyword `del`. The loop below would never terminate (except for the `if` statement that `break`s the loop) since `L` is being extended each iteration.

```
L = [1, 2]
for i in L:
    print(i)
    L.append(i+2)
    if i>5:
        break
```

Finally, `for` loops can be used with 2 *items* when the *iterable* is wrapped in `enumerate`, which allows the elements of the *iterable* to be directly accessed, as well as their index in the *iterable*.

```
x = linspace(0,100,11)
for i,y in enumerate(x):
    print('i is :', i)
    print('y is :', y)
```

12.3.1 Whitespace

Like `if ... elif ... else` flow control blocks, `for` loops are whitespace sensitive. The indentation of the line immediately below the `for` statement determines the indentation that all statements in the block must have.

12.3.2 **break**

A loop can be terminated early using `break`. `break` is usually used after an `if` statement to terminate the loop prematurely if some condition has been met.

```
x = randn(1000)
for i in x:
    print(i)
    if i > 2:
        break
```

Since for loops iterate over an iterable with a fixed size, `break` is generally more useful in `while` loops.

12.3.3 **continue**

`continue` can be used to skip an iteration of a loop, immediately returning to the top of the loop using the next item in *iterable*. `continue` is commonly used to avoid a level of nesting, such as in the following two examples.

```
x = randn(10)
for i in x:
    if i < 0:
        print(i)

for i in x:
    if i >= 0:
        continue
    print(i)
```

Avoiding excessive levels of indentation is essential in Python programming – 4 is usually considered the maximum reasonable level. `continue` is particularly useful since it can be used to in a `for` loop to avoid one level of indentation.

12.4 **while**

`while` loops are useful when the number of iterations needed depends on the outcome of the loop contents. `while` loops are commonly used when a loop should only stop if a certain condition is met, such as when the change in some parameter is small. The generic structure of a `while` loop is

```
while logical:
    Code to run
    Update logical
```

Two things are crucial when using a `while` loop: first, the *logical* expression should evaluate to true when the loop begins (or the loop will be ignored) and second, the inputs to the *logical* expression must be updated inside the loop. If they are not, the loop will continue indefinitely (hit CTRL+C to break an interminable loop in IPython). The simplest while loops are (wordy) drop-in alternatives to `for` loops:

```
count = 0
i = 1
while i<10:
    count += i
    i += 1
```

which produces the same results as

```
count=0;
for i in range(0,10):
    count += i
```

`while` loops should generally be avoided when `for` loops are sufficient. However, there are situations where no `for` loop equivalent exists.

```
# randn generates a standard normal random number
mu = abs(100*randn(1))
index = 1
while abs(mu) > .0001:
    mu = (mu+randn(1))/index
    index=index+1
```

In the block above, the number of iterations required is not known in advance and since `randn` is a standard normal pseudo-random number, it may take many iterations until this criterion is met. Any finite `for` loop cannot be guaranteed to meet the criteria.

12.4.1 **break**

`break` can be used in a `while` loop to immediately terminate execution. Normally, `break` should not be used in a `while` loop – instead the logical condition should be set to `False` to terminate the loop. However, `break` can

be used to avoid running code below the `break` statement even if the logical condition is `False`.

```python
condition = True
i = 0
x = randn(1000000)
while condition:
    if x[i] > 3.0:
        break # No printing if x[i] > 3
    print(x[i])
    i += 1
```

It is better to update the logical statement which determines whether the while loop should execute.

```python
i = 0
while x[i] <= 3:
    print(x[i])
    i += 1
```

12.4.2 `continue`

`continue` can be used in a `while` loop to skip any remaining code in the loop, immediately returning to the top of the loop, which then checks the while condition, and executes the loop if it still true. Using `continue` when the logical condition in the `while` loop is `False` is the same as using `break`.

12.5 `try ... except`

Exception handling is an advanced programming technique which can be used to produce more resilient code (often at the cost of speed). `try ... except` blocks are useful for running code which may fail for reasons outside of the programmer's control. In most numerical applications, code should be deterministic and so dangerous code can usually be avoided. When it can't, for example, if reading data from a data source which isn't always available (e.g. a website), then `try ... except` can be used to attempt to execute the code, and then to do something if the code fails to execute. The generic structure of a `try ... except` block is

```python
try:
    Dangerous Code
except ExceptionType1:
    Code to run if ExceptionType1 is raised
except ExceptionType2:
    Code to run if ExceptionType1 is raised
...
...
except:
    Code to run if an unlisted exception type is raised
```

A simple example of exception handling occurs when attempting to convert text to numbers.

```python
text = ('a','1','54.1','43.a')
for t in text:
    try:
        temp = float(t)
        print(temp)
    except ValueError:
        print('Not convertable to a float')
```

12.6   List Comprehensions

List comprehensions are an optimized method of building a list which may simplify code when an iterable object is looped across and the results are saved to a list, possibly conditional on some logical test. A simple list can be used to convert a `for` loop which includes an `append` into a single line statement.

```
>>> x = arange(5.0)
>>> y = []
>>> for i in range(len(x)):
...     y.append(exp(x[i]))
>>> y
[1.0,
 2.7182818284590451,
 7.3890560989306504,
 20.085536923187668,
 54.598150033144236]

>>> z = [exp(x[i]) for i in range(len(x))]
>>> z
[1.0,
 2.7182818284590451,
 7.3890560989306504,
 20.085536923187668,
 54.598150033144236]
```

This simple list comprehension saves 2 lines of typing. List comprehensions can also be extended to include a logical test.

```
>>> x = arange(5.0)
>>> y = []
>>> for i in range(len(x)):
...     if floor(i/2)==i/2:
...         y.append(x[i]**2)
>>> y
[0.0, 4.0, 16.0]

>>> z = [x[i]**2 for i in range(len(x)) if floor(i/2)==i/2]
>>> z
[0.0, 4.0, 16.0]
```

List comprehensions can also be used to loop over multiple iterable inputs.

```
>>> x1 = arange(5.0)
>>> x2 = arange(3.0)
>>> y = []
>>> for i in range(len(x1)):
...     for j in range(len(x2)):
...         y.append(x1[i]*x2[j])
>>> y
[0.0, 0.0, 0.0, 0.0, 1.0, 2.0, 0.0, 2.0, 4.0, 0.0, 3.0, 6.0, 0.0, 4.0, 8.0]

>>> z = [x1[i]*x2[j] for i in range(len(x1)) for j in range(len(x2))]
[0.0, 0.0, 0.0, 0.0, 1.0, 2.0, 0.0, 2.0, 4.0, 0.0, 3.0, 6.0, 0.0, 4.0, 8.0]

>>> # Only when i==j
>>> z = [x1[i]*x2[j] for i in range(len(x1)) for j in range(len(x2)) if i==j]
[0.0, 1.0, 4.0]
```

While list comprehensions are powerful methods to compactly express complex operations, they are never essential to Python programming.

12.7   Tuple, Dictionary and Set Comprehensions

The other mutable Python structures, the dictionary and the set, support construction using comprehension, as does the immutable type tuple. Set and dictionary comprehensions use `{}` while tuple comprehensions require an explicit call to `tuple` since `()` has another meaning.

```
>>> x = arange(-5.0,5.0)
>>> z_set = {x[i]**2.0 for i in range(len(x))}
>>> z_set
{0.0, 1.0, 4.0, 9.0, 16.0, 25.0}

>>> z_dict = {i:exp(i) for i in x}
{-5.0: 0.006737946999085467,
 -4.0: 0.018315638888734179,
 -3.0: 0.049787068367863944,
 -2.0: 0.1353352832366127,
 -1.0: 0.36787944117144233,
 ...

>>> z_tuple = tuple(i**3 for i in x)
(-125.0, -64.0, -27.0, -8.0, -1.0, 0.0, 1.0, 8.0, 27.0, 64.0)
```

12.8   Exercises

1. Write a code block that would take a different path depending on whether the returns on two series are simultaneously positive, both are negative, or they have different signs using an `if ... elif ... else` block.

2. Simulate 1000 observations from an ARMA(2,2) where ε_t are independent standard normal innovations. The process of an ARMA(2,2) is given by

$$y_t = \phi_1 y_{t-1} + \phi_2 y_{t-2} + \theta_1 \varepsilon_{t-1} + \theta_2 \varepsilon_{t-2} + \varepsilon_t$$

   Use the values $\phi_1 = 1.4$, $\phi_2 = -.8$, $\theta_1 = .4$ and $\theta_2 = .8$. **Note**: A T vector containing standard normal random variables can be simulated using `e = randn(T)`. When simulating a process, always simulate more data than needed and throw away the first block of observations to avoid start-up biases. This process is fairly persistent, at least 100 extra observations should be computed.

3. Simulate a GARCH(1,1) process where ε_t are independent standard normal innovations. A GARCH(1,1) process is given by

$$y_t = \sigma_t \varepsilon_t$$

$$\sigma_t^2 = \omega + \alpha y_{t-1}^2 + \beta \sigma_{t-1}^2$$

   Use the values $\omega = 0.05$, $\alpha = 0.05$ and $\beta = 0.9$, and set $h_0 = \omega/(1 - \alpha - \beta)$.

4. Simulate a GJR-GARCH(1,1,1) process where ε_t are independent standard normal innovations. A GJR-GARCH(1,1) process is given by

$$y_t = \sigma_t \varepsilon_t$$

$$\sigma_t^2 = \omega + \alpha y_{t-1}^2 + \gamma y_{t-1}^2 I_{[y_{t-1}<0]} + \beta \sigma_{t-1}^2$$

Use the values $\omega = 0.05$, $\alpha = 0.02$ $\gamma = 0.07$ and $\beta = 0.9$ and set $h_0 = \omega/\left(1 - \alpha - \frac{1}{2}\gamma - \beta\right)$. Note that some form of logical expression is needed in the loop. $I_{[\bullet]}$ is an indicator variable that takes the value 1 if the expression inside the $[\,]$ is true.

5. Simulate a ARMA(1,1)-GJR-GARCH(1,1)-in-mean process,

$$y_t = \phi_1 y_{t-1} + \theta_1 \sigma_{t-1} \varepsilon_{t-1} + \lambda \sigma_t^2 + \sigma_t \varepsilon_t$$

$$\sigma_t^2 = \omega + \alpha \sigma_{t-1}^2 \varepsilon_{t-1}^2 + \gamma \sigma_{t-1}^2 \varepsilon_{t-1}^2 I_{[\varepsilon_{t-1}<0]} + \beta \sigma_{t-1}^2$$

Use the values from Exercise 4 for the GJR-GARCH model and use the $\phi_1 = -0.1$, $\theta_1 = 0.4$ and $\lambda = 0.03$.

6. Find two different methods to use a `for` loop to fill a 5×5 array with $i \times j$ where i is the row index, and j is the column index. One will use `range` as the *iterable*, and the other should directly iterate on the rows, and then the columns of the matrix.

7. Using a `while` loop, write a bit of code that will do a bisection search to invert a normal CDF. A bisection search cuts the interval in half repeatedly, only keeping the sub-interval with the target in it. Hint: keep track of the upper and lower bounds of the random variable value and use flow control. This problem requires `stats.norm.cdf`.

8. Test out the loop using by finding the inverse CDF of 0.01, 0.5 and 0.975. Verify it is working by taking the absolute value of the difference between the final value and the value produced by `stats.norm.ppf`.

9. Write a list comprehension that will iterate over a 1-dimensional array and extract the negative elements to a list. How can this be done using *only* logical functions (no explicit loop), without the list comprehension (and returning an array)?

Chapter 13

Dates and Times

pandas provides sophisticated tools for creating and manipulating dates such as the `Timestamp` object, and is the preferred method for working with dates. Section 15.3.1 builds on the content of this chapter and shows how pandas is used with dates.

Date and time manipulation is provided by a built-in Python module `datetime`. This chapter assumes that `datetime` has been imported using `import datetime as dt`.

13.1 Creating Dates and Times

Dates are created using `date` by providing integer values for year, month and day and times are created using `time` using hours, minutes, seconds and microseconds.

```
>>> import datetime as dt
>>> yr, mo, dd = 2012, 12, 21
>>> dt.date(yr, mo, dd)
datetime.date(2012, 12, 21)

>>> hr, mm, ss, ms= 12, 21, 12, 21
>>> dt.time(hr, mm, ss, ms)
dt.time(12,21,12,21)
```

Dates created using `date` do not allow times, and dates which require a time stamp can be created using `datetime`, which combine the inputs from `date` and `time`, in the same order.

```
>>> dt.datetime(yr, mo, dd, hr, mm, ss, ms)
datetime.datetime(2012, 12, 21, 12, 21, 12, 21)
```

13.2 Dates Mathematics

Date-times and dates (but not times, and only within the same type) can be subtracted to produce a `timedelta`, which consists of three values, days, seconds and microseconds. Time deltas can also be added to dates and times compute different dates – although `date` types will ignore all information in the time delta hour, minute, second and millisecond fields.

```
>>> d1 = dt.datetime(yr, mo, dd, hr, mm, ss, ms)
>>> d2 = dt.datetime(yr + 1, mo, dd, hr, mm, ss, ms)
>>> d2-d1
datetime.timedelta(365)
```

Date Unit	Common Name	Range	Time Unit	Common Name	Range
Y	Year	$\pm 9.2 \times 10^{18}$ years	h	Hour	$\pm 1.0 \times 10^{15}$ years
M	Month	$\pm 7.6 \times 10^{17}$ years	m	Minute	$\pm 1.7 \times 10^{13}$ years
W	Week	$\pm 2.5 \times 10^{16}$ years	s	Second	$\pm 2.9 \times 10^{11}$ years
D	Day	$\pm 2.5 \times 10^{16}$ years	ms	Millisecond	$\pm 2.9 \times 10^{8}$ years
			us	Microsecond	$\pm 2.9 \times 10^{5}$ years
			ns	Nanosecond	± 292 years
			ps	Picosecond	± 106 days
			fs	Femtosecond	± 2.3 hours
			as	Attosecond	± 9.2 seconds

Table 13.1: NumPy `datetime64` range. The absolute range is January 1, 1970 plus the range.

```
>>> d2 + dt.timedelta(30,0,0)
datetime.datetime(2014, 1, 20, 12, 21, 12, 20)

>>> dt.date(2012,12,21) + dt.timedelta(30,12,0)
datetime.date(2013, 1, 20)
```

If times stamps are important, `date` types can be promoted to `datetime` using `combine` and a `time`.

```
>>> d3 = dt.date(2012,12,21)
>>> dt.datetime.combine(d3, dt.time(0))
datetime.datetime(2012, 12, 21, 0, 0)
```

Values in `dates`, `times` and `datetimes` can be modified using `replace` through keyword arguments.

```
>>> d3 = dt.datetime(2012,12,21,12,21,12,21)
>>> d3.replace(month=11,day=10,hour=9,minute=8,second=7,microsecond=6)
datetime.datetime(2012, 11, 10, 9, 8, 7, 6)
```

13.3 Numpy

pandas provides a closely related format for dates and times known as a `Timestamp`, which should be preferred in most cases to direct use of NumPy's `datetime64`. See Section 15.3.1 for more information.

Version 1.7.0 of NumPy introduces a NumPy native date and time type known as `datetime64` (to distinguish it from the Python-provided `datetime` type). The NumPy date and time type is still maturing and is always fully supported in the scientific python stack at the time of writing these notes. This said, it is already widely used and should see complete support in the near future. Additionally, the native NumPy data type is generally better suited to data storage and analysis and extends the Python date and time with additional features such as business day functionality.

NumPy contains both date and time (`datetime64`) and time-difference (`timedelta64`) objects. These differ from the standard Python `datetime` since they always store the date and time or time difference using a 64-bit integer *plus* a date or time unit. The choice of the date/time unit affects both the resolution of the `datetime64` as well as the permissible range. The unit directly determines the resolution - using a date unit of a day (`'D'`) limits the resolution to days. Using a date unit of a week (`'W'`) will allow a minimum of 1 week difference. Similarly, using a time unit of a second (`'s'`) will allow resolution up to the second (but not millisecond). The set of date and time units, and their range are presented in Table 13.1.

NumPy `datetime64`s can be initialized using either human readable strings or using numeric values. The string initialization is simple and `datetime64`s can be initialized using year only, year and month, the complete date or the complete date including a time. The default time resolution is nanoseconds (10^{-9}) and `T` is used to separate the time from the date.

```
>>> datetime64('2013')
numpy.datetime64('2013')

>>> datetime64('2013-09')
numpy.datetime64('2013-09')

>>> datetime64('2013-09-01')
numpy.datetime64('2013-09-01')

>>> datetime64('2013-09-01T12:00') # Time
numpy.datetime64('2013-09-01T12:00+0100')

>>> datetime64('2013-09-01T12:00:01') # Seconds
numpy.datetime64('2013-09-01T12:00:01+0100')

>>> datetime64('2013-09-01T12:00:01.123456789') # Nanoseconds
numpy.datetime64('2013-09-01T12:00:01.123456789+0100')
```

Date or time units can be explicitly included as the second input. The final example shows that rounding can occur if the date input is not exactly representable using the date unit chosen.

```
>>> datetime64('2013-01-01T00','h')
numpy.datetime64('2013-01-01T00:00+0000','h')

>>> datetime64('2013-01-01T00','s')
numpy.datetime64('2013-01-01T00:00:00+0000')

>>> datetime64('2013-01-01T00','ms')
numpy.datetime64('2013-01-01T00:00:00.000+0000')

>>> datetime64('2013-01-01','W')
numpy.datetime64('2012-12-27')
```

NumPy `datetime64`s can also be initialized from arrays.

```
>>> dates = array(['2013-09-01','2013-09-02'],dtype='datetime64')
>>> dates
array(['2013-09-01', '2013-09-02'], dtype='datetime64[D]')

>>> dates[0]
numpy.datetime64('2013-09-01')
```

Note that `datetime64` is not timezone aware. For timezone support use pandas `Timestamp`.

Dates which are initialized using one of the shorter forms are initialized at the earliest date (and time) in the period.

```
>>> datetime64('2013')==datetime64('2013-01-01')
True

>>> datetime64('2013-09')==datetime64('2013-09-01')
True
```

A corresponding time difference class, similarly named `timedelta64`, is created when dates are differenced.

```
>>> datetime64('2013-09-02') - datetime64('2013-09-01')
numpy.timedelta64(1,'D')
```

```
>>> datetime64('2013-09-01') - datetime64('2013-09-01T00:00:00')
numpy.timedelta64(3600,'s')
```

`timedelta64` types contain two pieces of information, a number indicating the number of steps between the two dates and the size of the step.

Chapter 14

Graphics

Matplotlib is a complete plotting library capable of high-quality graphics. Matplotlib contains both high level functions which produce specific types of figures, for example a simple line plot or a bar chart, as well as a low level API for creating highly customized charts. This chapter covers the basics of producing plots and only scratches the surface of the capabilities of matplotlib. Further information is available on the matplotlib website or in books dedicated to producing print quality graphics using matplotlib.

Throughout this chapter, the following modules have been imported.

```
>>> import matplotlib.pyplot as plt
>>> import scipy.stats as stats
```

Other modules will be included only when needed for a specific plot.

A datatime converter is requried when using pandas to plot time series. The converter is installed using

```
>>> from pandas.plotting import register_matplotlib_converters
>>> register_matplotlib_converters()
```

14.1 seaborn

seaborn is a Python package which provides a number of advanced data visualized plots. It also provides a general improvement in the default appearance of matplotlib-produced plots, and so I recommend using it by default.

```
>>> import seaborn as sns
```

All figure in this chapter were produced with seaborn loaded, using the default options. The dark grid background can be swapped to a light grid or no grid using `sns.set(style='whitegrid')` (light grid) or `sns.set(style='white`
(no grid, most similar to matplotlib).

14.2 2D Plotting

14.2.1 autoscale and tight_layout

Two funciton, `plt.autoscale` and `plt.tight_layout` will generally improve the appearance of figures. `autoscale` can be used to set tight limits within a figure's axes and `tight_layout` will remove wasted space around a figure. These were used in figures that appear in this chapter, although they have been omitted the code listings (aside from the first)

14.2.2   Line Plots

The most basic, and often most useful 2D graphic is a line plot. Basic line plots are produced using `plot` using a single input containing a 1-dimensional array.

```
>>> y = randn(100)
>>> plot(y)
>>> autoscale(tight='x')
>>> tight_layout()
```

The output of this command is presented in panel (a) of figure 14.1. A more flexible form adds a format string which has 1 to 3 elements: a color, represented using a letter (e.g. g for green), a marker symbol which is either a letter of a symbol (e.g. s for square, ^ for triangle up), and a line style, which is always a symbol or series of symbols. In the next example, `'g--'` indicates green (g) and dashed line (–).

```
>>> plot(y,'g--')
```

Format strings may contain any of the elements in the next table.

Color		Marker		Line Style	
Blue	b	Point	.	Solid	–
Green	g	Pixel	,	Dashed	--
Red	r	Circle	o	Dash-dot	-.
Cyan	c	Square	s	Dotted	:
Magenta	m	Diamond	D		
Yellow	y	Thin diamond	d		
Black	k	Cross	x		
White	w	Plus	+		
		Star	⋆		
		Hexagon	H		
		Alt. Hexagon	h		
		Pentagon	p		
		Triangles	^, v, <, >		
		Vertical Line				
		Horizontal Line	_		

The default behavior is to use a blue solid line with no marker (unless there is more than one line, in which case the colors will alter, in order, through those in the Colors column, skipping white). The format string contains 1 or more or the three categories of formatting information. For example, `kx--` would produce a black dashed line with crosses marking the points, `⋆:` would produce a dotted line with the default color using stars to mark points and `yH` would produce a solid yellow line with a hexagon marker.

When `plot` is called with one array, the default x-axis values 1,2, … are used. `plot(x,y)` can be used to plot specific x values against y values. Panel (c) shows the results of running the following code.

```
>>> x = cumsum(rand(100))
>>> plot(x,y,'r-')
```

While format strings are useful for quickly adding meaningful colors or line styles to a plot, they only expose a limited range of the available customizations. The next example shows how keyword arguments are used to add customizations to a plot. Panel (d) contains the plot produced by the following code.

```
>>> plot(x,y,alpha = 0.5, color = '#FF7F00', \
...     label = 'Line Label', linestyle = '-.', \
```

```
...      linewidth = 3, marker = 'o', markeredgecolor = '#000000', \
...      markeredgewidth = 2, markerfacecolor = '#FF7F00', \
...      markersize=30)
```

Note that in the previous example, \ is used to indicate to the Python interpreter that a statement is spanning multiple lines. Some of the more useful keyword arguments are listed in the table below.

Keyword	Description
alpha	Alpha (transparency) of the plot – default is 1 (no transparency)
color	Color description for the line.[1]
label	Label for the line – used when creating legends
linestyle	A line style symbol
linewidth	A positive integer indicating the width of the line
marker	A marker shape symbol or character
markeredgecolor	Color of the edge (a line) around the marker
markeredgewidth	Width of the edge (a line) around the marker
markerfacecolor	Face color of the marker
markersize	A positive integer indicating the size of the marker

Many more keyword arguments are available for a plot. The full list can be found in the docstring or by running the following code. The functions `getp` and `setp` can be used to get the list of properties for a line (or any matplotlib object), and `setp` can also be used to set a particular property.

```
>>> h = plot(randn(10))
>>> getp(h)
    agg_filter = None
    alpha = None
    animated = False
    ...

>>> setp(h, 'alpha')
alpha: float (0.0 transparent through 1.0 opaque)

>>> setp(h, 'color')
color: any matplotlib color

>>> setp(h, 'linestyle')
linestyle: [ ``'-'`` | ``'--'`` | ``'-.'`` | ``':'`` | ``'None'`` | ``' '`` | ``''`` ]
and any drawstyle in combination with a linestyle, e.g. ``'steps--'``.

>>> setp(h, 'linestyle', '--') # Change the line style
```

Note that `setp(h, prop)` returns a description of the property and `setp(h, prop, value)` sets *prop* to *value*.

14.2.3 Scatter Plots

`scatter` produces a scatter plot between 2 1-dimensional arrays. All examples use a set of simulated normal data with unit variance and correlation of 50%. The output of the basic `scatter` command is presented in figure 14.2, panel (a).

```
>>> z = randn(100,2)
>>> z[:,1] = 0.5*z[:,0] + sqrt(0.5)*z[:,1]
>>> x=z[:,0]
>>> y=z[:,1]
>>> scatter(x,y)
```
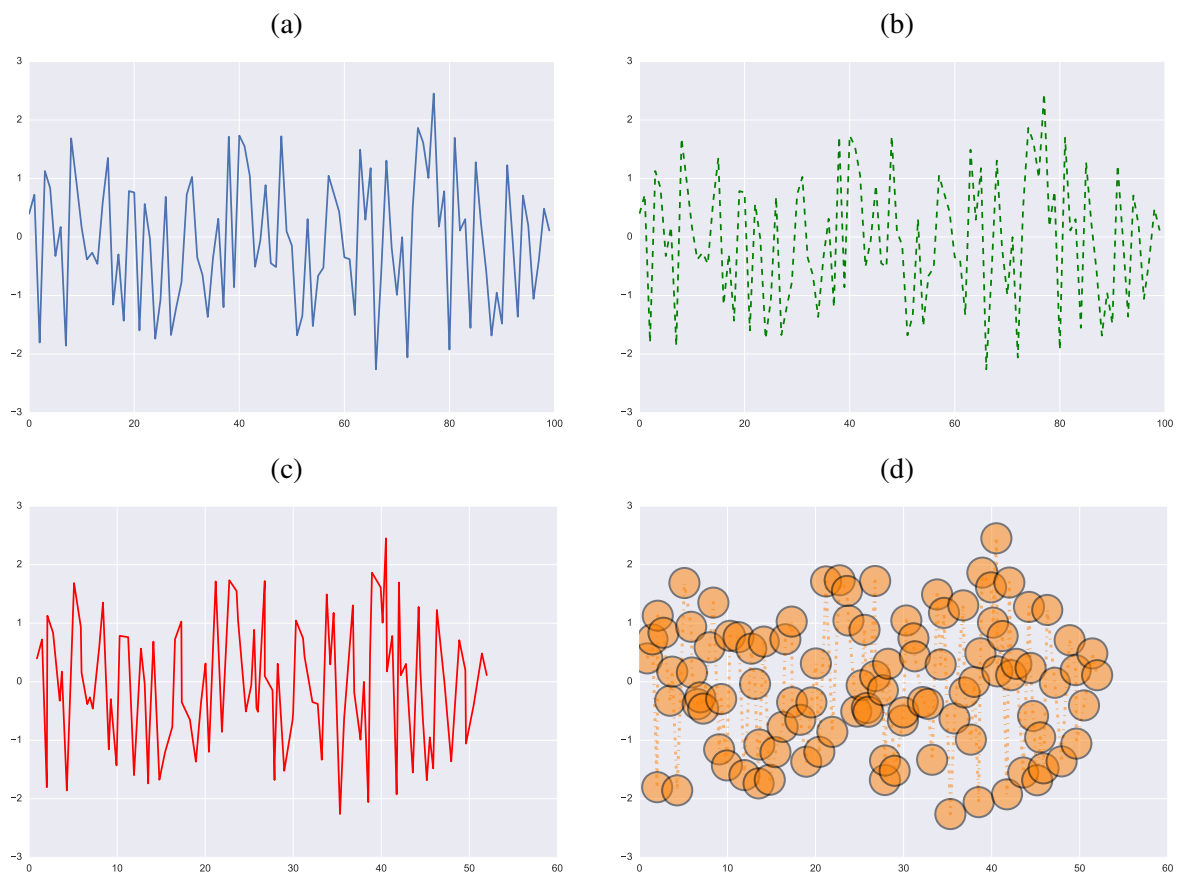
(a)

(b)

(c)

(d)

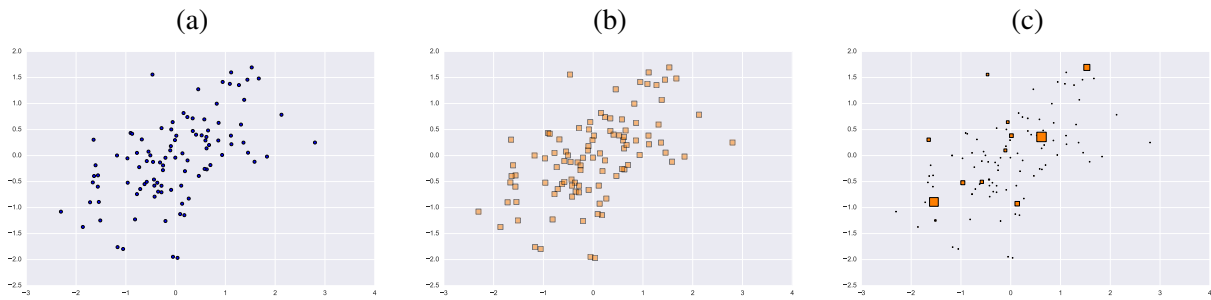Figure 14.1: Line plots produced using `plot`.

Figure 14.2: Scatter plots produced using `scatter`.

Scatter plots can also be modified using keyword arguments. The most important are included in the next example, and have identical meaning to those used in the line plot examples. The effect of these keyword arguments is shown in panel (b).

```
>>> scatter(x,y, s = 60,  c = '#FF7F00', marker='s', \
...     alpha = .5, label = 'Scatter Data')
```

One interesting use of `scatter` is to add a 3rd dimension to the plot by including an array of size data which uses the shapes to convey an extra dimension of data. The use of variable size data is illustrated in the code below, which produced the scatter plot in panel (c).

```
>>> size_data = exp(exp(exp(rand(100))))
>>> size_data = 200 * size_data/amax(size_data)
>>> size_data[size_data<1]=1.0
>>> scatter(x,y, s = size_data, c = '#FF7F00', marker='s', \
...     label = 'Scatter Data')
```

14.2.4 Bar Charts

`bar` produces bar charts using two 1-dimensional arrays . The first specifies the left ledge of the bars and the second the bar heights. The next code segment produced the bar chart in panel (a) of figure 14.3.

```
>>> y = rand(5)
>>> x = arange(5)
>>> bar(x,y)
```

Bar charts take keyword arguments to alter colors and bar width. Panel (b) contains the output of the following code.

```
>>> bar(x,y, width = 0.5, color = '#FF7F00', \
...     edgecolor = '#000000', linewidth = 5)
```

Finally, `barh` can be used instead of `bar` to produce a horizontal bar chart. The next code snippet produces the horizontal bar chart in panel (c), and demonstrates the use of a list of colors to alter the appearance of the chart.

```
>>> colors = sns.color_palette('colorblind')
>>> barh(x, y, height = 0.5, color = colors, \
...     edgecolor = '#000000', linewidth = 5)
```
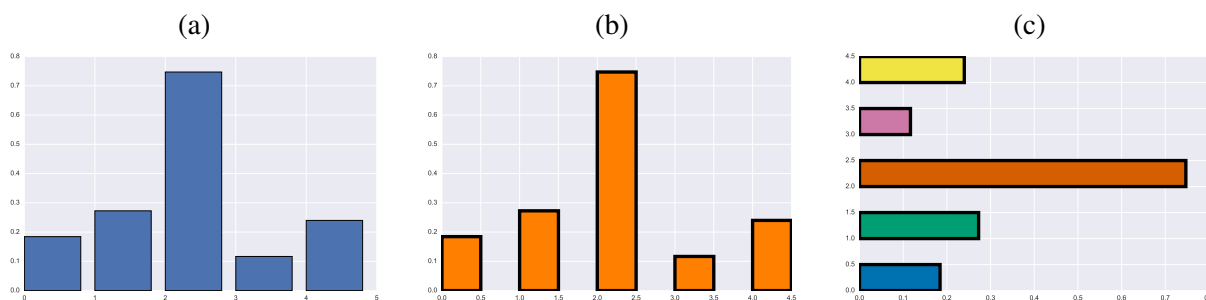
Figure 14.3: Bar charts produced using `bar` and `barh`.

14.2.5 Pie Charts

`pie` produces pie charts using a 1-dimensional array of data (the data can have any values, and does not need to sum to 1). The basic use of `pie` is illustrated below, and the figure produced appears in panel (a) of figure 14.4.

```
>>> y = rand(5)
>>> y = y/sum(y)
>>> y[y<.05] = .05
>>> pie(y)
```

Pie charts can be modified using a large number of keyword arguments, including labels and custom colors. In this example, the colors re generated using seaborn's pallate generator with 8 colors – although only the first 5 are used so that the darkest color is not too dark so that the text can be read. Exploded views of a pie chart can be produced by providing a vector of distances to the keyword argument explode. Note that `autopct = '%2.0f'` is using an old style format string to format the numeric labels. The results of running this code is shown in panel (b).

```
>>> explode = array([.2,0,0,0,0])
>>> colors = sns.dark_palette("skyblue", 8, reverse=True)
>>> labels = ['One', 'Two', 'Three', 'Four', 'Five']
>>> pie(y, explode = explode, colors = colors, \
...     labels = labels, autopct = '%2.0f', shadow = True)
```
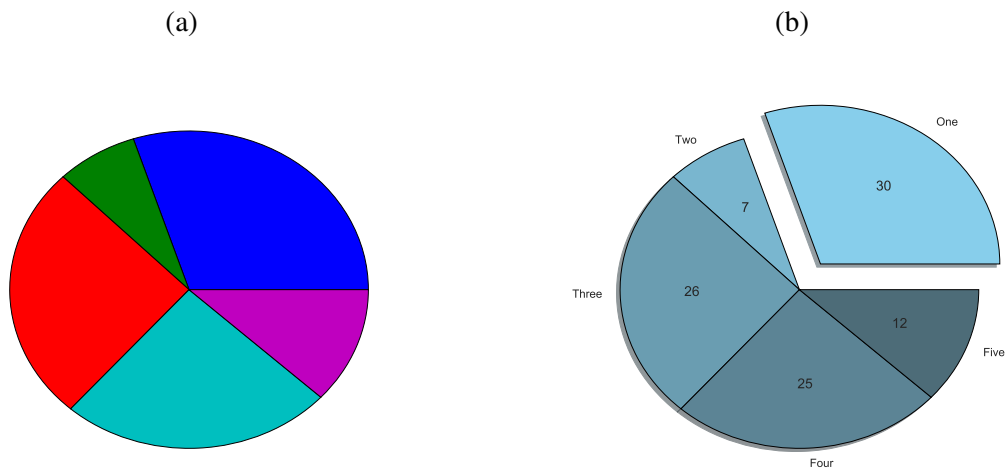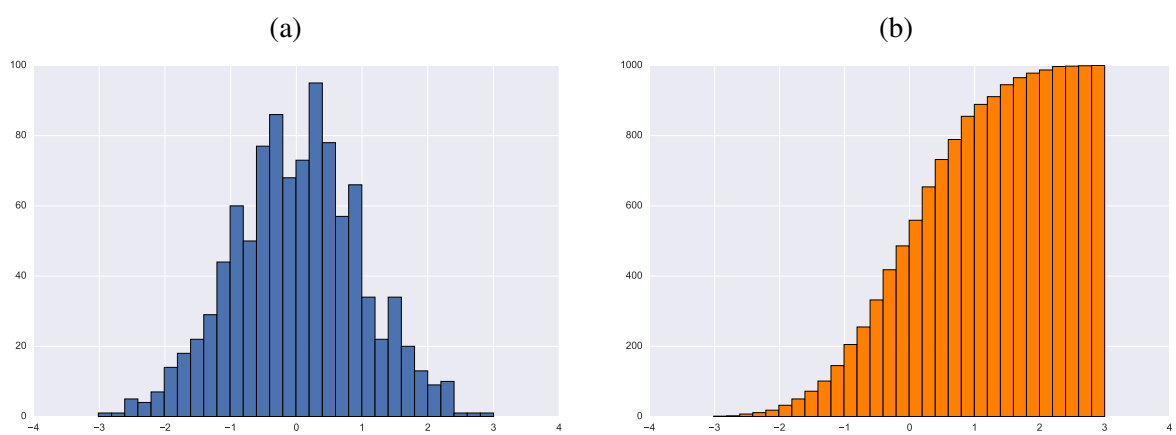
14.2.6 Histograms

Histograms can be produced using `hist`. A basic histogram produced using the code below is presented in Figure 14.5, panel (a). This example sets the number of bins used in producing the histogram using the keyword argument `bins`.

```
>>> x = randn(1000)
>>> hist(x, bins = 30)
```

Histograms can be further modified using keyword arguments. In the next example, `cumulative=True` produces the cumulative histogram. The output of this code is presented in figure (b).

```
>>> hist(x, bins = 30, cumulative=True, color='#FF7F00')
```

(a)   (b)

Figure 14.4: Pie charts produced using `pie`.

(a)   (b)

Figure 14.5: Histograms produced using `hist`.

14.3   Advanced 2D Plotting

14.3.1   Multiple Plots

In some scenarios it is advantageous to have multiple plots or charts in a single figure. Implementing this is simple using `figure` to initialize the figure window and then using `add_subplot`. Subplots are added to the figure using a grid notation with *m* rows and *n* columns where 1 is the upper left, 2 is the right of 1, and so on until the end of a row, where the next element is below 1. For example, the plots in a 3 by 2 subplot have indices

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}.$$

`add_subplot` is called using the notation `add_subplot(mni)` or `add_subplot(m,n,i)` where *m* is the number of rows, *n* is the number of columns and *i* is the index of the subplot.

Note that `add_subplot` must be called as a method from figure. Note that the next code block is sufficient long that it isn't practical to run interactively, and so `draw()` is used to force an update to the window to ensure that all plots and charts are visible. Figure 14.6 contains the result running the code below.

```python
from matplotlib.pyplot import figure, plot, bar, pie, draw, scatter
from numpy.random import randn, rand
from numpy import sqrt, arange

fig = figure()
# Add the subplot to the figure
# Panel 1
ax = fig.add_subplot(2, 2, 1)
y = randn(100)
plot(y)
ax.set_title('1')

# Panel  2
y = rand(5)
x = arange(5)
ax = fig.add_subplot(2, 2, 2)
bar(x, y)
ax.set_title('2')

# Panel 3
y = rand(5)
y = y / sum(y)
y[y < .05] = .05
ax = fig.add_subplot(2, 2, 3)
pie(y, colors=colors)
ax.set_title('3')

# Panel 4
z = randn(100, 2)
z[:, 1] = 0.5 * z[:, 0] + sqrt(0.5) * z[:, 1]
x = z[:, 0]
y = z[:, 1]
ax = fig.add_subplot(2, 2, 4)
scatter(x, y)
ax.set_title('4')
draw()
```
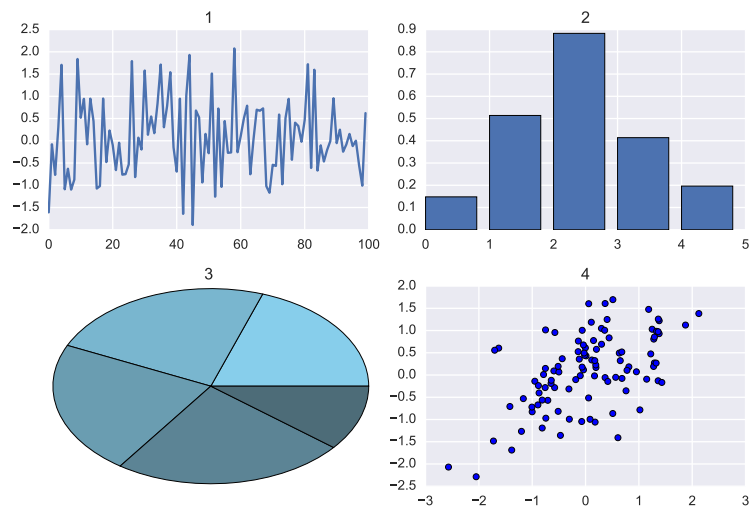
Figure 14.6: A figure containing a 2 by 2 subplot produced using `add_subplot`.

14.3.2 Multiple Plots on the Same Axes

Occasionally two different types of plots are needed in the same axes, for example, plotting a histogram and a PDF. Multiple plots can be added to the same axes by plotting the first one (e.g. a histogram) and then plotting any remaining data. By default, if a new axis is not created, additional plots will be added to the same axis.

The code in the next example begins by initializing a figure window and then adding axes. A histogram is then added to the axes and then a Normal PDF is plotted. `legend()` is called to produce a legend using the labels provided in the potting commands. `get_xlim` and `get_ylim` are used to get the limits of the axis after adding the histogram. These points are used when computing the PDF, and finally `set_ylim` is called to increase the axis height so that the PDF is against the top of the chart. Figure 14.7 contains the output of these commands.

```
from matplotlib.pyplot import figure, plot, legend, draw
from numpy import linspace
import scipy.stats as stats
from numpy.random import randn

x = randn(100)
fig = figure()
ax = fig.add_subplot(111)
ax.hist(x, bins=30, label='Empirical')
xlim = ax.get_xlim()
ylim = ax.get_ylim()
pdfx = linspace(xlim[0], xlim[1], 200)
pdfy = stats.norm.pdf(pdfx)
pdfy = pdfy / pdfy.max() * ylim[1]
plot(pdfx, pdfy, 'r-', label='PDF')
ax.set_ylim((ylim[0], 1.2 * ylim[1]))
legend()
draw()
```
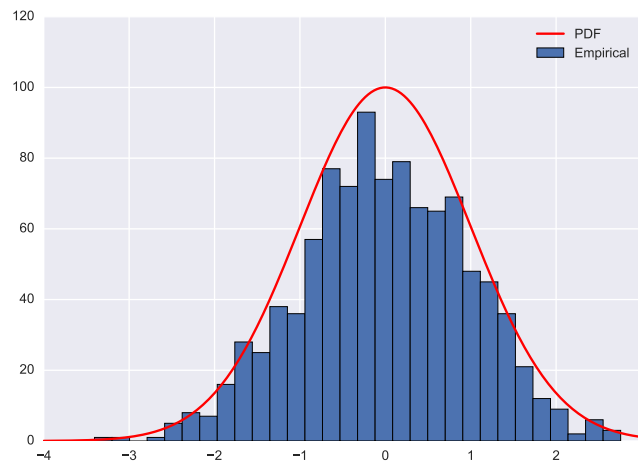
Figure 14.7: A figure containing a histogram and a line plot on the same axes.

14.3.3   Adding a Title and Legend

Titles are added with `title` and legends are added with `legend`. `legend` requires that lines have labels, which is why 3 calls are made to `plot` – each series has its own label. Executing the next code block produces a the image in figure 14.8, panel (a).

```
>>> x = cumsum(randn(100,3), axis = 0)
>>> plot(x[:,0],'b-',label = 'Series 1')
>>> plot(x[:,1],'g-.',label = 'Series 2')
>>> plot(x[:,2],'r:',label = 'Series 3')
>>> legend()
>>> title('Basic Legend')
```

`legend` takes keyword arguments which can be used to change its location (`loc` and an integer, see the docstring), remove the frame (`frameon`) and add a title to the legend box (`title`). The output of a simple example using these options is presented in panel (b).

```
>>> plot(x[:,0],'b-',label = 'Series 1')
>>> plot(x[:,1],'g-.',label = 'Series 2')
>>> plot(x[:,2],'r:',label = 'Series 3')
>>> legend(loc = 0, frameon = False, title = 'The Legend')
>>> title('Improved Legend')
```

14.3.4   Dates on Plots

Plots with date x-values on the x-axis are important when using time series data. Producing basic plots with dates is as simple as `plot(x,y)` where *x* is a list or array of dates. This first block of code simulates a random walk and constructs 2000 datetime values beginning with March 1, 2012 in a list.

```
from numpy import cumsum
from numpy.random import randn
from matplotlib.pyplot import figure, draw
import matplotlib.dates as mdates
import datetime as dt
```

(a)   (b)

Figure 14.8: Figures with titles and legend produced using `title` and `legend`.

```
# Simulate data
T = 2000
x = []
for i in range(T):
    x.append(dt.datetime(2012,3,1)+dt.timedelta(i,0,0))
y = cumsum(randn(T))
```

A basic plot with dates only requires calling `plot(x,y)` on the *x* and *y* data. The output of this code is in panel (a) of figure 14.9.

```
fig = figure()
ax = fig.add_subplot(111)
ax.plot(x,y)
draw()
```

Once the plot has been produced `autofmt_xdate()` is usually called to rotate and format the labels on the x-axis. The figure produced by running this command on the existing figure is in panel (b).

```
fig.autofmt_xdate()
draw()
```

Sometime, depending on the length of the sample plotted, automatic labels will not be adequate. To show a case where this issue arises, a shorted sample with only 100 values is simulated.

```
T = 100
x = []
for i in range(1,T+1):
    x.append(dt.datetime(2012,3,1)+dt.timedelta(i,0,0))
y = cumsum(randn(T))
```

A basic plot is produced in the same manner, and is depicted in panel (c). Note the labels overlap and so this figure is not acceptable.

```
fig = figure()
ax = fig.add_subplot(111)
ax.plot(x,y)
draw()
```

A call to `autofmt_xdate()` can be used to address the issue of overlapping labels. This is shown in panel (d).

```
fig.autofmt_xdate()
draw()
```

While the formatted x-axis dates are an improvement, they are still unsatisfactory in that the date labels have too much information (month, day and year) and are not at the start of the month. The next piece of code shows how markers can be placed at the start of the month using `MonthLocator` which is in the `matplotlib.dates` module. This idea is to construct a `MonthLocator` instance (which is a class), and then to pass this axes using `xaxis.set_major_locator` which determines the location of major tick marks (minor tick marks can be set using `xaxis.set_mijor_locator`). This will automatically place ticks on the 1st of every month. Other locators are available, including `YearLocator` and `WeekdayLocator`, which place ticks on the first day of the year and on week days, respectively. The second change is to format the labels on the x-axis to have the short month name and year. This is done using `DateFormatter` which takes a custom format string containing the desired format. Options for formatting include:

- `%Y` - 4 digit numeric year

- `%m` - Numeric month

- `%d` - Numeric day

- `%b` - Short month name

- `%H` - Hour

- `%M` - Minute

- `%D` - Named day

These can be combined along with other characters to produce format strings. For example, `%b %d, %Y` would produce a string with the format Mar 1, 2012. Finally `autofmt_xdate` is used to rotate the labels. The result of running this code is in panel (e).

```
months = mdates.MonthLocator()
ax.xaxis.set_major_locator(months)
fmt = mdates.DateFormatter('%b %Y')
ax.xaxis.set_major_formatter(fmt)
fig.autofmt_xdate()
draw()
```

Note that March 1 is not present in the figure in panel (e). This is because the plot doesn't actually include the date March 1 12:00:00 AM, but starts slightly later. To address this, simply change the axis limits using first calling `get_xlim` to get the 2-element tuple containing the limits, change the it to include March 1 12:00:00 AM using `set_xlim`. The line between these call is actually constructing the correctly formatted date. Internally, matplotlib uses serial dates which are simply the number of days past some initial date. For example March 1, 2012 12:00:00 AM is 734563.0, March 2, 2012 12:00:00 AM is 734564.0 and March 2, 2012 12:00:00 PM is 734563.5. The function `date2num` can be used to convert datetimes to serial dates. The output of running this final price of code on the existing figure is presented in panel (f)

```
xlim = list(ax.get_xlim())
xlim[0] = mdates.date2num(dt.datetime(2012,3,1))
ax.set_xlim(xlim)
draw()
```

14.3.5 Shading Areas

For a simple demonstration of the range of matplotlib, consider the problem of producing a plot of Macroeconomic time series with shaded regions to indicate business conditions. Capacity utilization data from FRED
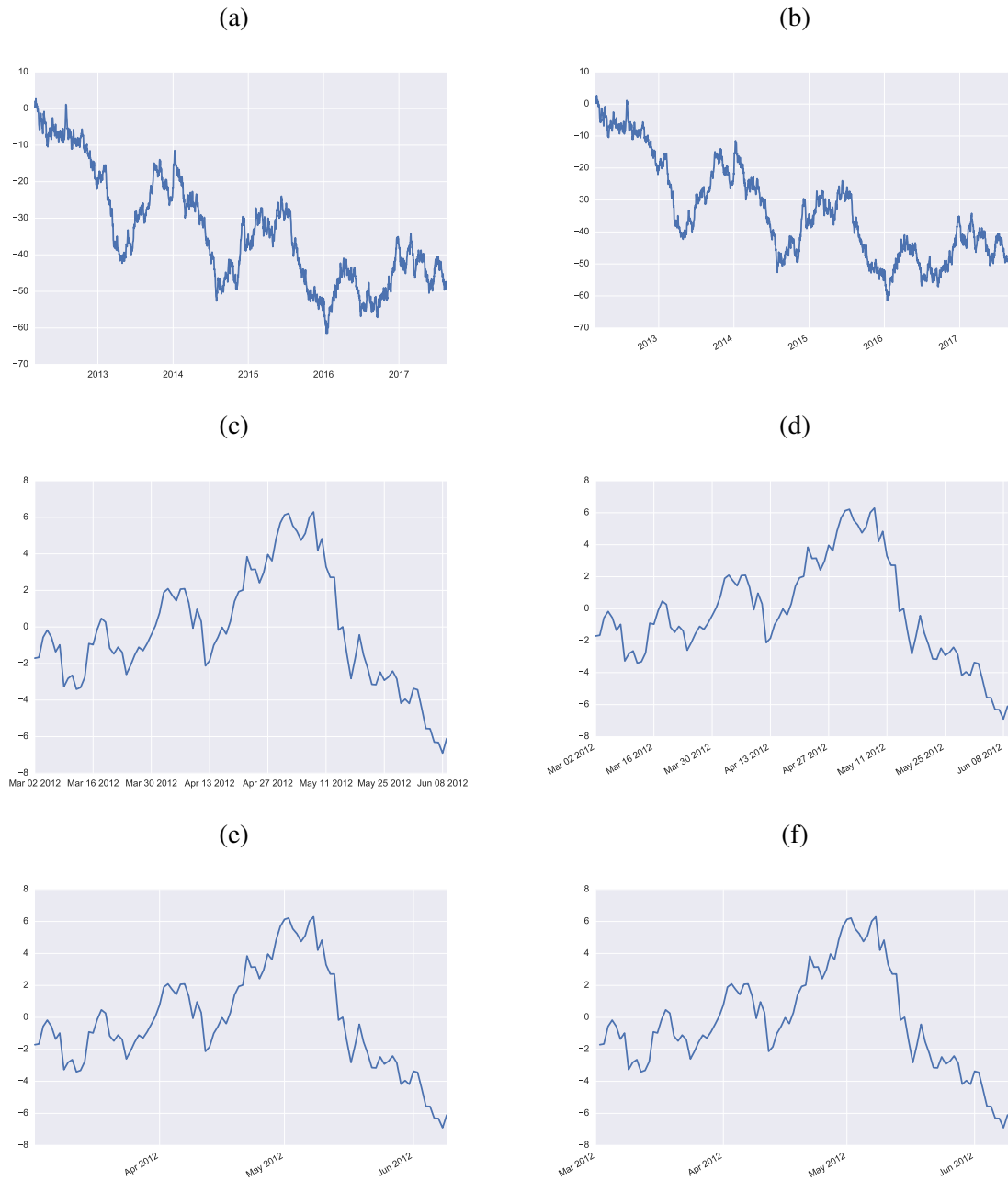
Figure 14.9: Figures with dates and additional formatting.

has been used to illustrate the steps needed to produce a plot with the time series, dates and shaded regions indicate periods classified as recessions by the National Bureau of Economic Research.

The code has been split into two parts. The first is the code needed to read the data, find the common dates, and finally format the data so that only the common sample is retained.

```python
# Reading the data
from matplotlib.pyplot import figure, plot_date, axis, draw
import matplotlib.mlab as mlab
import pandas as pd

# pd.read_csv is the best method to read csv data
recessionDates = pd.read_csv('USREC.csv', index_col='DATE', parse_dates=True)
capacityUtilization = pd.read_csv('TCU.csv', index_col='DATE', parse_dates=True)
# Merge the two data sets and keep the common rows
combined = pd.concat([recessionDates, capacityUtilization], 1).dropna()

# Find the data after the first date
plotData = capacityUtilization.loc[combined.index]
shadeData = recessionDates.loc[combined.index]
```

The second part of the code produces the plot. Most of the code is very simple. It begins by constructing a `figure`, then `add_subplot` to the figure, and the plotting the data using `plot`. `fill_between` is only one of many useful functions in matplotlib – it fills an area whenever a variable is 1, which is the structure of the recession indicator. The final part of the code adds a title with a custom font (set using a dictionary), and then changes the font and rotation of the axis labels. The output of this code is figure 14.10.

```python
# The shaded plot
x = plotData.index
y = plotData.values

# z is the shading values, 1 or 0, need to be 1-d
z = (shadeData != 0).squeeze()

# Figure
fig = figure()
ax = fig.add_subplot(111)
plot_date(x,y,'r-')
limits = axis()
font = { 'fontname':'Times New Roman', 'fontsize':14 }
ax.fill_between(x, limits[2], limits[3], where=z, edgecolor='#BBBBBB', \
    facecolor='#222222', alpha=0.3)
axis(ymin=limits[2])
ax.set_title('Capacity Utilization',font)
xl = ax.get_xticklabels()
for label in xl:
    label.set_fontname('Times New Roman')
    label.set_fontsize(14)
    label.set_rotation(45)
yl = ax.get_yticklabels()
for label in yl:
    label.set_fontname('Times New Roman')
    label.set_fontsize(14)
draw()
```
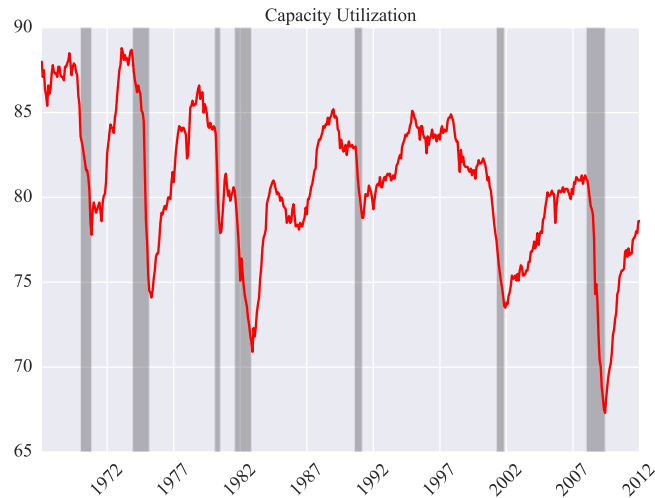
Figure 14.10: A plot of capacity utilization (US data) with shaded regions indicating NBER recession dates.

14.3.6 TEX in plots

Matplotlib supports using TEX in plots. The only steps needed are the first three lines in the code below, which configure some settings. the labels use raw mode (`r'...'`) to avoid needing to escape the \ in the TEX string. The final plot with TEX in the labels is presented in figure 14.11.

```
>>> from matplotlib import rc
>>> rc('text', usetex=True)
>>> rc('font', family='serif')
>>> y = 50*exp(.0004 + cumsum(.01*randn(100)))
>>> plot(y)
>>> xlabel(r'time ($\tau$)')
>>> ylabel(r'Price',fontsize=16)
>>> title(r'Geometric Random Walk: $d\ln p_t = \mu dt + \sigma dW_t$',fontsize=16)
>>> rc('text', usetex=False)
```

14.4 3D Plotting

The 3D plotting capabilities of matplotlib are decidedly weaker than the 2D plotting facilities, and yet the 3D capabilities are typically adequate for most application (especially since 3D graphics are rarely necessary, and often distracting).

14.4.1 Line Plots

Line plot in 3D are virtually identical to plotting in 2D, except that 3 1-dimensional vectors are needed: x, y and z (height). This simple example demonstrates how `plot` can be used with the keyword argument `zs` to construct a 3D line plot. The line that sets up the axis using `Axed3D(fig)` is essential when producing 3D graphics. The other new command, `view_init`, is used to rotate the view using code (the view can be interactive rotated in the figure window). The result of running the code below is presented in figure 14.12.

```
>>> from mpl_toolkits.mplot3d import Axes3D
```
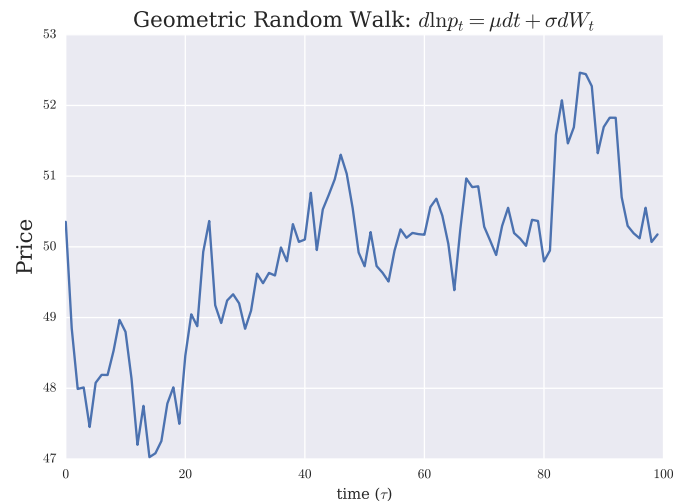
Figure 14.11: A plot that uses TEX in the labels.

```
>>> x = linspace(0,6*pi,600)
>>> z = x.copy()
>>> y = sin(x)
>>> x=  cos(x)
>>> fig = plt.figure()
>>> ax = Axes3D(fig) # Different usage
>>> ax.plot(x, y, zs=z, label='Spiral')
>>> ax.view_init(15,45)
>>> plt.draw()
```

14.4.2 Surface and Mesh (Wireframe) Plots

Surface and mesh or wireframe plots are occasionally useful for visualizing functions with 2 inputs, such as a bivariate probability density. This example produces both types of plots for a bivariate normal PDF with mean 0, unit variances and correlation of 50%. The first block of code generates the points to use in the plot with `meshgrid` and evaluates the PDF for all combinations of *x* and *y*.

```
from numpy import linspace, meshgrid, mat, zeros, shape, sqrt
import numpy.linalg as linalg

x = linspace(-3,3,100)
y = linspace(-3,3,100)
x,y = meshgrid(x,y)
z = zeros((1,2))
p = zeros(shape(x))
R = array([[1,.5],[.5,1]])
Rinv = linalg.inv(R)
for i in range(len(x)):
    for j in range(len(y)):
        z[0,0] = x[i,j]
        z[0,1] = y[i,j]
        p[i,j] = 1.0/(2*pi)*sqrt(linalg.det(R))*exp(-(z@Rinv@z.T)/2)
```
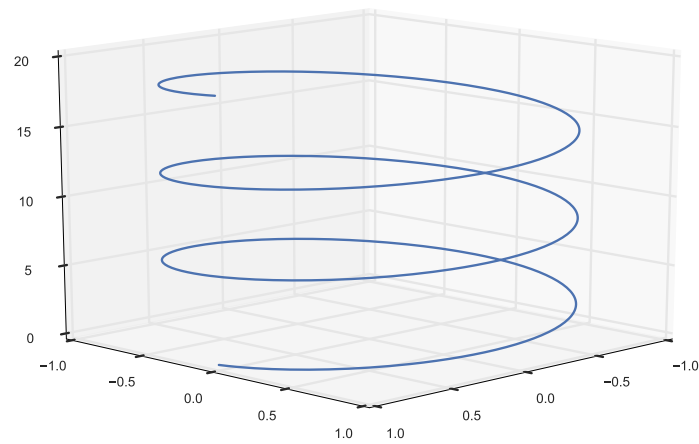
Figure 14.12: A 3D line plot constructed using `plot`.

The next code segment produces a mesh (wireframe) plot using `plot_wireframe`. The setup of the case is identical to that of the 3D line, and the call `ax = Axes3D(fig)` is again essential. The figure is drawn using the 2-dimensional arrays *x*, *y* and *p*. The output of this code is presented in panel (a) of 14.13.

```
>>> from mpl_toolkits.mplot3d import Axes3D
>>> fig = plt.figure()
>>> ax = Axes3D(fig)
>>> ax.plot_wireframe(x, y, p, rstride=5, cstride=5, color='#AD5300')
>>> ax.view_init(29,80)
>>> plt.draw()
```

Producing a surface plot is identical, only that a color map is needed from the module `matplotlib.cm` to provide different colors across the range of values. The output of this code is presented in panel (b).

```
>>> import matplotlib.cm as cm
>>> fig = plt.figure()
>>> ax = Axes3D(fig)
>>> ax.plot_surface(x, y, p, rstride=2, cstride=2, cmap=cm.coolwarm, shade='interp')
>>> ax.view_init(29,80)
>>> plt.draw()
```

14.4.3 Contour Plots

Contour plots are not technically 3D, although they are used as a 2D representation of 3D data. Since they are ultimately 2D, little setup is needed, aside from a call to `contour` using the same inputs as `plot_surface` and `plot_wireframe`. The output of the code below is in figure 14.14.

```
>>> fig = plt.figure()
>>> ax = fig.gca()
>>> ax.contour(x,y,p)
>>> plt.draw()
```
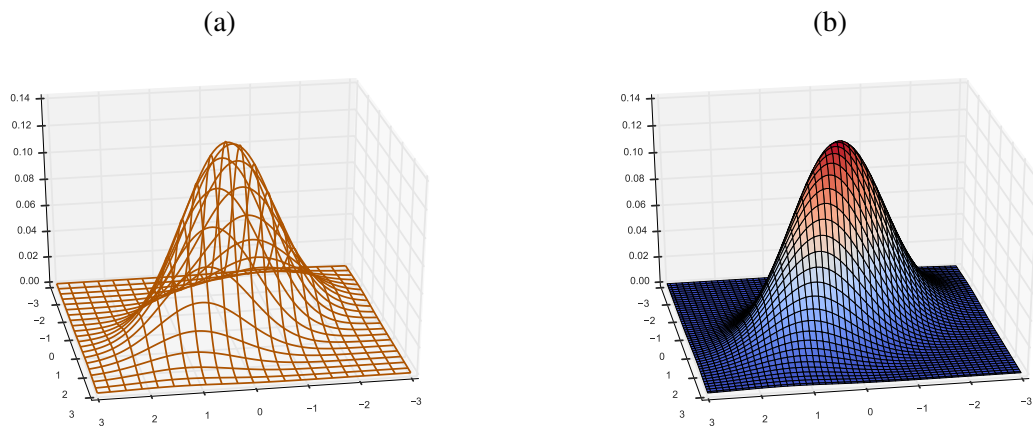
(a) (b)

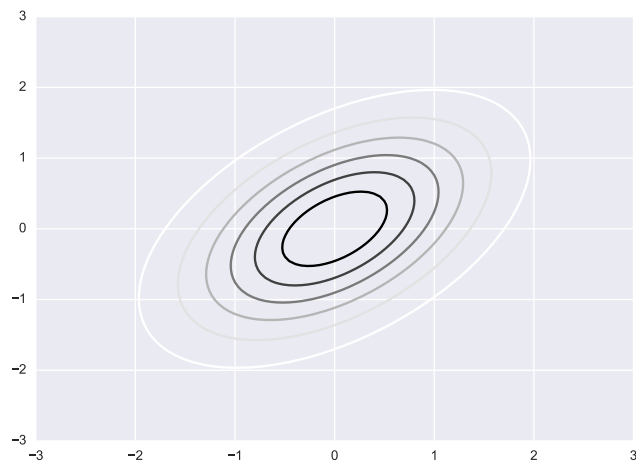Figure 14.13: 3D figures produced using `plot_wireframe` and `plot_surface`.

Figure 14.14: Contour plot produced using `contour`.

14.5 General Plotting Functions

figure

`figure` is used to open a figure window, and can be used to generate axes. `fig = figure(n)` produces a figure object with id *n*, and assigns the object to `fig`.

add_subplot

`add_subplot` is used to add axes to a figure. `ax = fig.add_subplot(111)` can be used to add a basic axes to a figure. `ax = fig.add_subplot(m,n,i)` can be used to add an axes to a non-trivial figure with a *m* by *n* grid of plots.

close

`close` closes figures. `close(n)` closes the figure with id *n*, and `close('all')` closes all figure windows.

show

`show` is used to force an update to a figure, and pauses execution if not used in an interactive console (close the figure window to resume execution). `show` should not be used in standalone Python programs – `draw` should be used instead.

draw

`draw` forces an update to a figure.

14.6 Exporting Plots

Exporting plots is simple using `savefig('`*filename.ext*`')` where *ext* determines the type of exported file to produce. *ext* can be one of png, pdf, ps, eps or svg.

```
>>> plot(randn(10,2))
>>> savefig('figure.pdf') # PDF export
>>> savefig('figure.png') # PNG export
>>> savefig('figure.svg') # Scalable Vector Graphics export
```

`savefig` has a number of useful keyword arguments. In particular, `dpi` is useful when exporting png files. The default `dpi` is 100.

```
>>> plot(randn(10,2))
>>> savefig('figure.png', dpi = 600) # High resolution PNG export
```

14.7 Exercises

1. Download data for the past 20 years for the S&P 500 from Yahoo!. Plot the price against dates, and ensure the date display is reasonable.

2. Compute Friday-to-Friday returns using the log difference of closing prices and produce a histogram. Experiment with the number of bins.

3. Compute the percentage of weekly returns and produce a pie chart containing the percentage of weekly returns in each of:

    (a) $r \leq -2\%$

    (b) $-2\% < r \leq 0\%$

    (c) $0 < r \leq 2\%$

    (d) $r > 2\%$

4. Download 20 years of FTSE data, and compute Friday-to-Friday returns. Produce a scatter plot of the FTSE returns against the S&P 500 returns. Be sure to label the axes and provide a title.

5. Repeat exercise 4, but add in the fit line showing is the OLS fit of regressing FTSE on the S&P plus a constant.

6. Compute EWMA variance for both the S&P 500 and FTSE and plot against dates. An EWMA variance has $\sigma_t^2 = (1 - \lambda) r_{t-1}^2 + \lambda \sigma_{t-1}^2$ where $r_0^2 = \sigma_0^2$ is the full sample variance and $\lambda = 0.97$.

7. Explore the chart gallery on the matplotlib website.

Chapter 15

pandas

pandas is a high-performance package that provides a comprehensive set of structures for working with data. pandas excels at handling structured data, such as data sets containing many variables, working with missing values and merging across multiple data sets. pandas is an essential component of the Python scientific stack when operating on data. pandas also provides high-performance, robust methods for importing from and exporting to a wide range of formats.

15.1 Data Structures

pandas provides a set of data structures which include Series, DataFrames and Panels. Series are the equivalent of 1-dimensional arrays. DataFrames are collections of Series and so are 2-dimensional. Panels are collections of DataFrames, and have 3 dimensions. *Note that the Panel type is scheduled for deprecation and so is not covered in this chapter.*

15.1.1 Series

Series are the primary building block of the data structures in pandas, and in many ways a Series behaves similarly to a NumPy array. A Series is initialized using a list, tuple, directly from a NumPy array or using a dictionary.

```
>>> a = array([0.1, 1.2, 2.3, 3.4, 4.5])
>>> a
array([ 0.1,  1.2,  2.3,  3.4,  4.5])

>>> from pandas import Series
>>> s = Series([0.1, 1.2, 2.3, 3.4, 4.5])
>>> s
0    0.1
1    1.2
2    2.3
3    3.4
4    4.5
dtype: float64

>>> s = Series(a) # NumPy array to Series
```

Series, like arrays, are sliceable. However, unlike a 1-dimensional array, a Series has an additional column – an index – which is a set of values which are associated with the rows of the Series. In this example, pandas has automatically generated an index using the sequence $0, 1, \ldots$ since no index was provided. It is also possible to use other values as the index when initializing the Series using a keyword argument.

```
>>> s = Series([0.1, 1.2, 2.3, 3.4, 4.5], index = ['a','b','c','d','e'])
>>> s
a    0.1
b    1.2
c    2.3
d    3.4
e    4.5
dtype: float64
```

The index is an important part of the utility of the pandas's data structures (Series and DataFrame) and allows for dictionary-like access using values in the index (in addition to both numeric slicing and logical indices).[1]

```
>>> s['a']
0.10000000000000001

>>> s[0]
0.10000000000000001

>>> s.iloc[0]
0.10000000000000001

>>> s[['a','c']]
a    0.1
c    2.3
dtype: float64

>>> s[[0,2]]
a    0.1
c    2.3
dtype: float64

>>> s[:2]
a    0.1
b    1.2
dtype: float64

>>> s[s>2]
c    2.3
d    3.4
e    4.5
dtype: float64
```

In this examples, 'a' and 'c' behave in the same manner as 0 and 2 would in a standard NumPy array. The elements of an index do not have to be unique which another way in which a Series generalizes a NumPy array.

```
>>> s = Series([0.1, 1.2, 2.3, 3.4, 4.5], index = ['a','b','c','a','b'])
>>> s
a    0.1
b    1.2
c    2.3
a    3.4
b    4.5
dtype: float64

>>> s['a']
```

---

[1]Using numeric index values other than the default sequence will break scalar selection since there is ambiguity between numerical slicing and index access. For this reason, access using numerical indices should .iloc[*slice*].

```
a    0.1
a    3.4
dtype: float64
```

Series can also be initialized directly from dictionaries.

```
>>> s = Series({'a':0.1 ,'b': 1.2, 'c': 2.3, 'd':3.4, 'e': 4.5})
>>> s
a    0.1
b    1.2
c    2.3
d    3.4
e    4.5
dtype: float64
```

Series are like NumPy arrays in that they support most numerical operations.

```
>>> s = Series({'a': 0.1, 'b': 1.2, 'c': 2.3})
>>> s * 2.0
a    0.2
b    2.4
c    4.6
dtype: float64

>>> s - 1.0
a   -0.9
b    0.2
c    1.3
dtype: float64
```

However, Series are different from arrays when math operations are performed across two Series. In particular, math operations involving two series operate by *aligning indices*. The mathematical operation is performed in two steps. First, the union of all indices is created, and then the mathematical operation is performed on matching indices. Indices that do not match are given the value NaN (not a number), and values are computed for all unique pairs of repeated indices.

```
>>> s1 = Series({'a': 0.1, 'b': 1.2, 'c': 2.3})
>>> s2 = Series({'a': 1.0, 'b': 2.0, 'c': 3.0})
>>> s3 = Series({'c': 0.1, 'd': 1.2, 'e': 2.3})
>>> s1 + s2
a    1.1
b    3.2
c    5.3
dtype: float64

>>> s1 * s2
a    0.1
b    2.4
c    6.9
dtype: float64

>>> s1 + s3
a    NaN
b    NaN
c    2.4
d    NaN
e    NaN
dtype: float64
```

Mathematical operations performed on series which have non-unique indices will broadcast the operation to all indices which are common. For example, when one array has 2 elements with the same index, and another

has 3, adding the two will produce 6 outputs.

```
>>> s1 = Series([1.0,2,3],index=['a'] * 3)
>>> s2 = Series([4.0,5],index=['a'] * 2)
>>> s1 + s2
a    5.0
a    6.0
a    6.0
a    7.0
a    7.0
a    8.0
dtype: float64
```

The underlying NumPy array is accessible through the `values` property, and the index is accessible the `index` property, which returns an `Index` type. The NumPy array underlying the index can be retrieved using `values` on the `Index` object returned.

```
>>> s1 = Series([1.0,2,3])
>>> s1.values
array([ 1.,  2.,  3.])

>>> s1.index
RangeIndex(start=0, stop=3, step=1)

>>> s1.index.values
array([0, 1, 2], dtype=int64)

>>> s1.index = ['cat','dog','elephant']
>>> s1.index
Index([u'cat', u'dog', u'elephant'], dtype='object')
```

Notable Methods and Properties

Series provide a large number of methods to manipulate data. These can broadly be categorized into mathematical and non-mathematical functions. The mathematical functions are generally very similar to those in NumPy due to the underlying structure of a Series and so do not warrant a separate discussion. In contrast, the non-mathematical methods are unique to pandas.

`head` and `tail`

`head()` shows the first 5 rows of a series, and `tail()` shows the last 5 rows. An optional argument can be used to return a different number of entries, as in `head(10)`.

`isnull` and `notnull`

`isnull()` returns a Series with the same indices containing Boolean values indicating `True` for null values which include `NaN` and `None`, among others. `notnull()` returns the negation of `isnull()` – that is, `True` for non-null values, and `False` otherwise.

`loc` and `iloc`

While Series elements can be directly accessed using bracket notation, there are cases where ambiguity can arise. For example, consider accessing element 0 from

```
>>> s = Series([1.0,2,3], index=[7,2,8])
>>> s[0]  # Error
KeyError: 0
>>> s[2]
2.0
```

This error occurs since 0 is not in the index. To access element by their position using `iloc` only provides this access.

```
>>> s.iloc[0]
1.0
>>> s.iloc[::2]
7    1.0
8    3.0
dtype: float64
```

`loc`, on the other hand, only allow access using index value or logical arrays.

```
>>> s.loc[0] # Error
KeyError: 'the label [0] is not in the [index]'
>>> s.loc[[7,8]]
7    1.0
8    3.0
dtype: float64
>>> s.loc[s.index<8]
7    1.0
2    2.0
dtype: float64
```

describe

`describe()` returns a simple set of summary statistics. The values returned is a series where the index contains the names of the statistics computed.

```
>>> s1 = Series(arange(10.0,20.0))
>>> s1.describe()
count    10.00000
mean     14.50000
std       3.02765
min      10.00000
25%      12.25000
50%      14.50000
75%      16.75000
max      19.00000
dtype: float64

>>> summ = s1.describe()
>>> summ['mean']
14.5
```

unique and nunique

`unique()` returns the unique elements of a series and `nunique()` returns the number of unique values in a Series.

drop and dropna

`drop(labels)` drop elements with the selected labels from a Series.

```
>>> s1 = Series(arange(1.0,6),index=['a','a','b','c','d'])
>>> s1
a    1.0
a    2.0
b    3.0
c    4.0
d    5.0
dtype: float64

>>> s1.drop('a')
b    3.0
c    4.0
d    5.0
dtype: float64
```

`dropna()` is similar to `drop()` except that it only drops null values – `NaN` or similar.

```
>>> s1 = Series(arange(1.0,4.0),index=['a','b','c'])
>>> s2 = Series(arange(1.0,4.0),index=['c','d','e'])
>>> s3 = s1 + s2
>>> s3
a    NaN
b    NaN
c      4
d    NaN
e    NaN
dtype: float64

>>> s3.dropna()
c      4
dtype: float64
```

Both return Series and so it is necessary to assign the values to have a series with the selected elements dropped.

fillna

`fillna(value)` fills all null values in a series with a specific value.

```
>>> s1 = Series(arange(1.0,4.0),index=['a','b','c'])
>>> s2 = Series(arange(1.0,4.0),index=['c','d','e'])
>>> s3 = s1 + s2
>>> s3.fillna(-1.0)
a    -1.0
b    -1.0
c     4.0
d    -1.0
e    -1.0
dtype: float64
```

append

`append(series)` appends one series to another, and is similar to `list.append`.

replace

`replace(list, values)` replaces a set of values in a Series with a new value. `replace` is similar to `fillna` except that `replace` also replaces non-null values.

update

update(*series*) replaces values in a series with those in another series, matching on the index, and is similar to an update operation in SQL.

```
>>> s1 = Series(arange(1.0,4.0),index=['a','b','c'])
>>> s1
a    1.0
b    2.0
c    3.0
dtype: float64

>>> s2 = Series(-1.0 * arange(1.0,4.0),index=['c','d','e'])
>>> s1.update(s2)
>>> s1
a    1.0
b    2.0
c   -1.0
dtype: float64
```

15.1.2 DataFrame

While the Series class is the building block of data structures in pandas, the DataFrame is the work-horse. DataFrames collect multiple series in the same way that a spreadsheet collects multiple columns of data. In a simple sense, a DataFrame is like a 2-dimensional NumPy array – and when all data is numeric and of the same type (e.g. float64), it is virtually indistinguishable. However, a DataFrame is composed of Series and each Series has its own data type, and so not all DataFrames are representable as homogeneous NumPy arrays.

A number of methods are available to initialize a DataFrame. The simplest method uses a homogeneous NumPy array.

```
>>> from pandas import DataFrame
>>> a = array([[1.0,2],[3,4]])
>>> df = DataFrame(a)
>>> df
   0  1
0  1  2
1  3  4
```

Like a Series, a DataFrame contains the input data as well as row labels. However, since a DataFrame is a collection of columns, it also contains column labels (located along the top edge). When none are provided, the numeric sequence $0, 1, \ldots$ is used.

Column names are entered using a keyword argument or later by assigning to columns.

```
>>> df = DataFrame(array([[1,2],[3,4]]),columns=['a','b'])
>>> df
   a  b
0  1  2
1  3  4

>>> df = DataFrame(array([[1,2],[3,4]]))
>>> df.columns = ['dogs','cats']
>>> df
   dogs  cats
```

```
0    1    2
1    3    4
```

Index values are similarly assigned using either the keyword argument index or by setting the `index` property.

```
>>> df = DataFrame(array([[1,2],[3,4]]), columns=['dogs','cats'],
... index=['Alice','Bob'])
>>> df
       dogs  cats
Alice     1     2
Bob       3     4
```

DataFrames can also be created from NumPy arrays with structured data.

```
>>> import datetime as dt
>>> t = dtype([('datetime', 'O8'), ('value', 'f4')])
>>> x = zeros(1,dtype=t)
>>> x[0][0] = dt.datetime(2013,1,1)
>>> x[0][1] = -99.99
>>> x
array([(dt.datetime(2013, 1, 1, 0, 0), -99.98999786376953)],
      dtype=[('datetime', 'O'), ('value', '<f4')])

>>> df = DataFrame(x)
>>> df
    datetime      value
0 2013-01-01 -99.989998
```

In the previous example, the DataFrame has automatically pulled the column names and column types from the NumPy structured data.

The final method to create a DataFrame uses a dictionary containing Series, where the keys contain the column names. The DataFrame will automatically align the data using the common indices.

```
>>> s1 = Series(arange(0.0,5))
>>> s2 = Series(arange(1.0,3))
>>> DataFrame({'one': s1, 'two': s2})
   one  two
0  0.0  1.0
1  1.0  2.0
2  2.0  NaN
3  3.0  NaN
4  4.0  NaN

>>> s3 = Series(arange(0.0,3))
>>> DataFrame({'one': s1, 'two': s2, 'three': s3})
   one  three  two
0  0.0    0.0  1.0
1  1.0    1.0  2.0
2  2.0    2.0  NaN
3  3.0    NaN  NaN
4  4.0    NaN  NaN
```

In the final example, the third series (`s3`) has fewer values and the DataFrame automatically fills missing values as `NaN`. Note that is possible to create DataFrames from Series which do not have unique index values, although in these cases the index values of the two series must match *exactly* – that is, have the same index values in the same order.

Manipulating DataFrames

The use of DataFrames will be demonstrated using a data set containing a mix of data types using state-level GDP data from the US. The data set contains both the GDP level between 2009 and 2012 (constant 2005 US$)

and the growth rates for the same years as well as a variable containing the region of the state. The data is loaded directly into a DataFrame using `read_excel`, which is described in Section 15.4.

```
>>> from pandas import read_excel
>>> state_gdp = read_excel('US_state_GDP.xls','Sheet1')
>>> state_gdp.head()
  state_code        state  gdp_2009  gdp_2010  gdp_2011  gdp_2012  \
0         AK       Alaska     44215     43472     44232     44732
1         AL      Alabama    149843    153839    155390    157272
2         AR     Arkansas     89776     92075     92684     93892
3         AZ      Arizona    221405    221016    224787    230641
4         CA   California   1667152   1672473   1692301   1751002

   gdp_growth_2009  gdp_growth_2010  gdp_growth_2011  gdp_growth_2012 region
0              7.7             -1.7              1.7              1.1     FW
1             -3.9              2.7              1.0              1.2     SE
2             -2.0              2.6              0.7              1.3     SE
3             -8.2             -0.2              1.7              2.6     SW
4             -5.1              0.3              1.2              3.5     FW
```

Selecting Columns

Single columns are selectable using the column name, as in `state_gdp['state']`, and the value returned in a Series. Multiple columns are similarly selected using a list of column names as in

```
state_gdp[['state_code', 'state']]
```

or equivalently using an Index object. Note that these two methods are slightly different – selecting a single column returns a Series while selecting multiple columns returns a DataFrame. This is similar to how NumPy's scalar selection returns an array with a lower dimension. Use a list of column names containing a single name to return a DataFrame with a single column.

```
>>> state_gdp['state_code'].head() # Series
0    AK
1    AL
2    AR
3    AZ
4    CA
Name: state_code, dtype: object

>>> state_gdp[['state_code']].head() # DataFrame
  state_code
0         AK
1         AL
2         AR
3         AZ
4         CA

>>> state_gdp[['state_code','state']].head()
  state_code        state
0         AL      Alabama
1         AK       Alaska
2         AZ      Arizona
3         AR     Arkansas
4         CA   California

>>> cols = state_gdp.columns
>>> state_gdp[cols[1:3]].head()  # Elements 1 and 2 (0-based counting)
        state  gdp_2009
```

```
0      Alabama     149843
1       Alaska      44215
2      Arizona     221405
3     Arkansas      89776
4   California    1667152
```

Finally, single columns can also be selected using dot-notation and the column name.[2] This is identical to using `df['column']` and so the value returned is a Series.

```
>>> state_gdp.state_code.head()
0    AL
1    AK
2    AZ
3    AR
4    CA
Name: state_code, dtype: object

>>> type(state_gdp.state_code)
pandas.core.series.Series
```

Selecting Rows

Rows can be selected using standard numerical slices.

```
>>> state_gdp[1:3]
  state_code      state   gdp_2009   gdp_2010   gdp_2011   gdp_2012  \
1         AL    Alabama     149843     153839     155390     157272
2         AR   Arkansas      89776      92075      92684      93892


   gdp_growth_2009  gdp_growth_2010   gdp_growth_2011   gdp_growth_2012 region
1             -3.9              2.7               1.0               1.2     SE
2             -2.0              2.6               0.7               1.3     SE
```

A function version is also available using `iloc[rows]` which is identical to the standard slicing syntax. Labeled rows can also be selected using the method `loc[label]` or `loc[list of labels]` to elect multiple rows using their label .

Finally, rows can also be selected using logical selection using a Boolean array with the same number of elements as the number of rows as the DataFrame.

```
>>> state_long_recession = state_gdp['gdp_growth_2010']<0
>>> state_gdp[state_long_recession].head()
   state_code      state   gdp_2009   gdp_2010   gdp_2011   gdp_2012  \
0          AK     Alaska      44215      43472      44232      44732
3          AZ    Arizona     221405     221016     224787     230641
33         NV     Nevada     110001     109610     111574     113197
50         WY    Wyoming      32439      32004      31231      31302


    gdp_growth_2009  gdp_growth_2010   gdp_growth_2011   gdp_growth_2012 region
0               7.7             -1.7               1.7               1.1     FW
3              -8.2             -0.2               1.7               2.6     SW
33             -8.2             -0.4               1.8               1.5     FW
50              3.4             -1.3              -2.4               0.2     RM
```

Selecting Rows and Columns

Since the behavior of slicing depends on whether the input is text (selects columns) or numeric/Boolean (selects rows), it isn't possible to use standard slicing to select both rows and columns. Instead, the selector method

---

[2]The column name must be a legal Python variable name, and so cannot contain spaces or reserved notation.

ix[*rowselector*, *colselector*] allows joint selection where *rowselector* is either a scalar selector, a slice selector, a Boolean array, a numeric selector or a row label or list of row labels and *colselector* is a scalar selector, a slice selector, a Boolean array, a numeric selector or a column name or list of column names.

```
>>> state_gdp.loc[state_long_recession,'state']
1       Alaska
2       Arizona
28      Nevada
50      Wyoming
Name: state, dtype: object

>>> state_gdp.loc[state_long_recession,
... ['state','gdp_growth_2009','gdp_growth_2010']]
        state  gdp_growth_2009  gdp_growth_2010
1     Alaska              7.7             -1.7
2     Arizona            -8.2             -0.2
28    Nevada             -8.2             -0.4
50    Wyoming             3.4             -1.3

>>> state_gdp.iloc[10:15,0] # Slice and scalar
10    GA
11    HI
12    IA
13    ID
14    IL
15    IN

>>> state_gdp.iloc[10:15,:2] # Slice and slice
   state_code      state
10         GA    Georgia
11         HI     Hawaii
12         IA       Iowa
13         ID      Idaho
14         IL   Illinois
15         IN    Indiana
```

Adding Columns

Columns are added using one of three methods. The most natural method adds a Series using a dictionary-like syntax. Here .copy() is used to ensure state_gdp_2012 contains its own copy of the original data and is not sharing with state_gdp

```
>>> state_gdp_2012 = state_gdp[['state','gdp_2012']].copy()
>>> state_gdp_2012.head()
        state  gdp_2012
0     Alabama    157272
1      Alaska     44732
2     Arizona    230641
3    Arkansas     93892
4  California   1751002

>>> state_gdp_2012['gdp_growth_2012'] = state_gdp['gdp_growth_2012']
>>> state_gdp_2012.head()
        state  gdp_2012  gdp_growth_2012
0     Alabama    157272              1.2
1      Alaska     44732              1.1
2     Arizona    230641              2.6
3    Arkansas     93892              1.3
```

This syntax always adds the column at the end. `insert(`*location*`,`*column_name*`,`*series*`)` inserts a Series at a specific location, where *location* uses 0-based indexing (i.e. 0 places the column first, 1 places it second, etc.), *column_name* is the name of the column to be added and *series* is the series data. *series* is either a Series or another object that is readily convertible into a Series such as a NumPy array.

```
>>> state_gdp_2012 = state_gdp[['state','gdp_2012']].copy()
>>> state_gdp_2012.insert(1,'gdp_growth_2012',state_gdp['gdp_growth_2012'])
>>> state_gdp_2012.head()
        state  gdp_growth_2012  gdp_2012
0     Alabama              1.2    157272
1      Alaska              1.1     44732
2     Arizona              2.6    230641
3    Arkansas              1.3     93892
4  California              3.5   1751002
```

Formally this type of join performs a *left join* which means that only index values in the base DataFrame will appear in the combined DataFrame, and so inserting columns with different indices or fewer items than the DataFrame results in a DataFrame with the *original indices* with NaN-filled missing values in the new Series.

```
>>> state_gdp_2012 = state_gdp[['state','gdp_2012']].head(3)
>>> state_gdp_2012
     state  gdp_2012
0  Alabama    157272
1   Alaska     44732
2  Arizona    230641

>>> gdp_2011 = state_gdp['gdp_2011']
>>> state_gdp_2012['gdp_2011'] = gdp_2011
>>> state_gdp_2012.head(3)
     state  gdp_2012  gdp_2011
0  Alabama    157272       NaN
1   Alaska     44732     44232
2  Arizona    230641    224787
```

Deleting Columns

Columns are deleted using the `del` keyword, using `pop(`*column*`)` on the DataFrame or by calling `drop(`*list of column*s`,axis=1)` . The behavior of these differs slightly: `del` will simply delete the Series from the DataFrame. `pop()` will both delete the Series and return the Series as an output, and `drop()` will return a DataFrame with the Series dropped without modify the original DataFrame.

```
>>> state_gdp_copy = state_gdp.copy()
>>> columns = ['state_code','gdp_growth_2011','gdp_growth_2012']
>>> state_gdp_copy = state_gdp_copy[columns]
>>> state_gdp_copy.index = state_gdp['state_code']
>>> state_gdp_copy.head()
            gdp_growth_2011  gdp_growth_2012
state_code
AK                      1.7              1.1
AL                      1.0              1.2
AR                      0.7              1.3
AZ                      1.7              2.6
CA                      1.2              3.5

>>> gdp_growth_2012 = state_gdp_copy.pop('gdp_growth_2012')
>>> gdp_growth_2012.head()
state_code
AK              1.1
```

```
AL          1.2
AR          1.3
AZ          2.6
CA          3.5
Name: gdp_growth_2012, dtype: float64

>>> state_gdp_copy.head()
          gdp_growth_2011
state_code
AK                    1.7
AL                    1.0
AR                    0.7
AZ                    1.7
CA                    1.2

>>> del state_gdp_copy['gdp_growth_2011']
>>> state_gdp_copy.head()
Empty DataFrame
Columns: []
Index: [AK, AL, AR, AZ, CA]

>>> state_gdp_copy = state_gdp.copy()
>>> state_gdp_copy = state_gdp_copy[columns]
>>> state_gdp_dropped = state_gdp_copy.drop(['state_code','gdp_growth_2011'],
... axis=1)
>>> state_gdp_dropped.head()
   gdp_growth_2012
0             1.1
1             1.2
2             1.3
3             2.6
4             3.5
```

Notable Properties and Methods

`drop`, `dropna` and `drop_duplicates`

`drop()`, `dropna()` and `drop_duplicates()` can all be used to drop rows or columns from a DataFrame. `drop(`*labels*`)` drops rows based on the row labels in a label or list *labels*. `drop(`*column_name*`,axis=1)` drops columns based on a column name or list *column names*.

    `dropna()` drops rows with any NaN (or null) values. It can be used with the keyword argument `dropna(how='all')` to only drop rows which have missing values for all variables. It can also be used with the keyword argument `dropna(axis=1)` to drop columns with missing values. Finally, `drop_duplicates()` removes rows which are duplicates or other rows, and is used with the keyword argument `drop_duplicates(cols=`*col_list*`)` to only consider a subset of all columns when checking for duplicates.

`values` and `index`

`values` retrieves a the NumPy array (structured if the data columns are heterogeneous) underlying the DataFrame, and `index` returns the index of the DataFrame or can be assigned to set the index.

`fillna`

`fillna()` fills NaN or other null values with other values. The simplest use fill all NaNs with a single value and is called `fillna(value=`*value* `)`. Using a dictionary allows for more sophisticated na-filling with column

names as the keys and the replacements as the values.

```
>>> df = DataFrame(array([[1, nan],[nan, 2]]))
>>> df.columns = ['one','two']
>>> replacements = {'one':-1, 'two':-2}
>>> df.fillna(value=replacements)
   one  two
0    1   -2
1   -1    2
```

T and `transpose`

`T` and `transpose` are identical – both swap rows and columns of a DataFrame. `T` operates like a property, while `transpose` is used as a method.

`sort` and `sort_index`

`sort_values` and `sort_index` provide methods to sort a `DataFrame`. `sort_values` sorts the contents of the `DataFrame` along either axis using the contents of a single column or row. Passing a list of coumns names or index values implements lexicographic search. `sort_index` will sort a `DataFrame` by the values in the index. Both support the keyword argument `ascending` to determine the direction of the sort (ascending by default). `ascending` can be used with a list to allow sorting in different directions for different sort variables.

```
>>> df = DataFrame(array([[1, 3],[1, 2],[3, 2],[2,1]]), columns=['one','two'])
>>> df.sort_values(by='one')
   one  two
0    1    3
1    1    2
3    2    1
2    3    2

>>> df.sort_values(by=['one','two'])
   one  two
1    1    2
0    1    3
3    2    1
2    3    2

>>> df.sort_values(by=['one','two'], ascending=[0,1])
   one  two
2    3    2
3    2    1
1    1    2
0    1    3
```

The default behavior is to *not* sort in-place and so it is necessary to assign the output of a sort. Using the keyword argument `inplace=True` will change the default behavior.

`pivot`

`pivot` reshapes a table using column values when reshaping. `pivot` takes three inputs. The first, `index`, defines the column to use as the index of the pivoted table. The second, `columns`, defines the column to use to form the column names, and `values` defines the columns to for the data in the constructed DataFrame. The following example shows how a flat `DataFrame` with repeated values is transformed into a more meaningful representation.

```
>>> prices = [101.0,102.0,103.0]
>>> tickers = ['GOOG','AAPL']
>>> import itertools
>>> data = [v for v in itertools.product(tickers,prices)]
>>> import pandas as pd
>>> dates = pd.date_range('2013-01-03',periods=3)
>>> df = DataFrame(data, columns=['ticker','price'])
>>> df['dates'] = dates.append(dates)
>>> df
  ticker  price       dates
0   GOOG  101.0  2013-01-03
1   GOOG  102.0  2013-01-04
2   GOOG  103.0  2013-01-05
3   AAPL  101.0  2013-01-03
4   AAPL  102.0  2013-01-04
5   AAPL  103.0  2013-01-05

>>> df.pivot(index='dates',columns='ticker',values='price')
ticker        AAPL   GOOG
dates
2013-01-03  101.0  101.0
2013-01-04  102.0  102.0
2013-01-05  103.0  103.0
```

stack and unstack

stack and unstack transform a `DataFrame` to a Series (stack) and back to a DataFrame (unstack). The stacked DataFrame (a Series) uses an index containing both the original row and column labels.

concat and append

append appends rows of another `DataFrame` to the end of an existing `DataFrame`. If the data appended has a different set of columns, missing values are NaN-filled. The keyword argument `ignore_index=True` instructs append to ignore the existing index in the appended DataFrame. This is useful when index values are not meaningful, such as when they are simple numeric values.

pd.concat is a core function which concatenates two or more `DataFrame`s using an *outer join* by default. An outer join is a method of joining `DataFrame`s which will return a `DataFrame` using the union of the indices of input DataFrames. This differs from the *left join* that is used when adding a Series to an existing `DataFrame` using dictionary syntax. The keyword argument `join='inner'` can be used to perform an *inner join*, which will return a `DataFrame` using the intersection of the indices in the input `DataFrame`s. Be default pd.concat will concatenate using column names, and the keyword argument `axis=1` can be used to join using index labels.

```
>>> df1 = DataFrame([1,2,3],index=['a','b','c'],columns=['one'])
>>> df2 = DataFrame([4,5,6],index=['c','d','e'],columns=['two'])
>>> pd.concat((df1,df2), axis=1)
   one  two
a  1.0  NaN
b  2.0  NaN
c  3.0  4.0
d  NaN  5.0
e  NaN  6.0

>>> pd.concat((df1,df2), axis=1, join='inner')
   one  two
c    3    4
```

`reindex` and `reindex_like`

`reindex` changes the labels while null-filling any missing values, which is useful for selecting subsets of a DataFrame or re-ordering rows. `reindex_like` behaves similarly but instead uses the index from another DataFrame. The keyword argument `axis` directs `reindex` to alter either rows or columns.

```
>>> original = DataFrame([[1,1],[2,2],[3.0,3]],
...                       index=['a','b','c'],
...                       columns=['one','two'])
>>> original.reindex(index=['b','c','d'])
   one  two
b  2.0  2.0
c  3.0  3.0
d  NaN  NaN

>>> different = DataFrame([[1,1],[2,2],[3.0,3]],
...                       index=['c','d','e'],
...                       columns=['one','two'])
>>> original.reindex_like(different)
   one  two
c  3.0  3.0
d  NaN  NaN
e  NaN  NaN

>>> original.reindex(['two','one'], axis = 1)
   two  one
a    1  1.0
b    2  2.0
c    3  3.0
```

`merge` and `join`

`merge` and `join` provide SQL-like operations for merging the DataFrames using row labels or the contents of columns. The primary difference between the two is that `merge` defaults to using column contents while `join` defaults to using index labels. Both commands take a large number of optional inputs. The important keyword arguments are:

- `how`, which must be one of `'left'`, `'right'`, `'outer'`, `'inner'` describes which set of indices to use when performing the join. `'left'` uses the indices of the DataFrame that is used to call the method and `'right'` uses the DataFrame input into `merge` or `join`. `'outer'` uses a union of all indices from both DataFrames and `'inner'` uses an intersection from the two DataFrames.

- `on` is a single column name or list of column names to use in the merge. `on` assumes the names are common. If no value is given for `on` or `left_on`/`right_on`, then the common column names are used.

- `left_on` and `right_on` allow for a merge using columns with different names. When `left_on` and `right_on` contains the same column names, the behavior is the same as `on`.

- `left_index` and `right_index` indicate that the index labels are the join key for the left and right DataFrames.

```
>>> left = DataFrame([[1,2],[3,4],[5,6]],columns=['one','two'])
>>> right = DataFrame([[1,2],[3,4],[7,8]],columns=['one','three'])
>>> left.merge(right,on='one') # Same as how='inner'
   one  two  three
0    1    2      2
```

```
1    3    4       4

>>> left.merge(right,on='one', how='left')
   one  two  three
0    1    2    2.0
1    3    4    4.0
2    5    6    NaN

>>> left.merge(right,on='one', how='right')
   one  two  three
0    1  2.0      2
1    3  4.0      4
2    7  NaN      8

>>> left.merge(right,on='one', how='outer')
   one  two  three
0    1  2.0    2.0
1    3  4.0    4.0
2    5  6.0    NaN
3    7  NaN    8.0
```

update

`update` updates the values in one DataFrame using the non-null values from another DataFrame, using the index labels to determine which records to update.

```
>>> left = DataFrame([[1,2],[3,4],[5,6]],columns=['one','two'])
>>> left
   one  two
0    1    2
1    3    4
2    5    6

>>> right = DataFrame([[nan,12],[13,nan],[nan,8]],
...                   columns=['one','two'],
...                   index=[1,2,3])
>>> right
   one  two
1  NaN   12
2   13  NaN
3  NaN    8

>>> left.update(right) # Updates values in left
>>> left
    one   two
0   1.0   2.0
1   3.0  12.0
2  13.0   6.0
```

apply

`apply` executes a function along the columns or rows of a DataFrame. The following example applies the mean function both down columns and across rows, which is trivial example since `mean` could be executed on the DataFrame directly. `apply` is more general since it allows custom functions to be applied to a DataFrame.

```
>>> cols = ['gdp_growth_2009', 'gdp_growth_2010', 'gdp_growth_2011']
>>> subset = state_gdp[cols]
```

```
>>> subset.index = state_gdp['state_code'].to_numpy()
>>> subset.head()
    gdp_growth_2009  gdp_growth_2010  gdp_growth_2011
AK              7.7             -1.7              1.7
AL             -3.9              2.7              1.0
AR             -2.0              2.6              0.7
AZ             -8.2             -0.2              1.7
CA             -5.1              0.3              1.2

>>> subset.apply(mean) # Same as subset.mean()
gdp_growth_2009   -2.313725
gdp_growth_2010    2.462745
gdp_growth_2011    1.590196
dtype: float64

>>> subset.apply(mean, axis=1).head() # Same as subset.mean(axis=1)
AK     2.200
AL     0.250
AR     0.650
AZ    -1.025
CA    -0.025
dtype: float64
```

applymap

applymap is similar to apply, only that it applies element-by-element rather than column- or row-wise.

pivot_table

pivot_table provides a method to summarize data by groups. A pivot table first forms groups based using the keyword argument index and then returns an aggregate of all values within the group (using mean by default). The keyword argument aggfun allows for other aggregation function.

```
>>> subset = state_gdp[['gdp_growth_2009','gdp_growth_2010','region']]
>>> subset.head()
   gdp_growth_2009  gdp_growth_2010 region
0             7.7             -1.7     FW
1            -3.9              2.7     SE
2            -2.0              2.6     SE
3            -8.2             -0.2     SW
4            -5.1              0.3     FW

>>> subset.pivot_table(index='region')
        gdp_growth_2009  gdp_growth_2010
region
FW            -2.483333         1.550000
GL            -5.400000         3.660000
MW            -1.250000         2.433333
NE            -2.350000         2.783333
PL            -1.357143         2.900000
RM            -0.940000         1.380000
SE            -2.633333         2.850000
SW            -2.175000         1.325000
```

pivot_table differs from pivot since an aggregation function is used when transforming the data.

15.1.3 Split-Apply-Combine using `groupby`

`groupby` produces a `DataFrameGroupBy` object which is a grouped DataFrame, and is useful when a DataFrame has columns containing group data (e.g., sex or race in cross-sectional data). The basic construction of a `DataFrameGroupBy` uses syntax of the form *DataFrame*`.groupby(`*key*`)` to group by a single column *key* or *DataFrame*`.groupby([`*key*$_1$`, `*key*$_2$`, ...])` to group by multiple columns. When grouping by multiple keys, `groupby` will find all unique combinations of the key values.

Aggregation (`aggregate`)

The simplest application of `groupby` is to aggregate statistics such as group means or extrema. All aggregation functions will return a single value per column for each group. Many common aggregation functions have optimized versions provided by pandas. For example, `mean`, `sum`, `min`, `std`, and `count` can all be directly used on a `DataFrameGroupBy` object.

```
>>> grouped_data = subset.groupby('region')
>>> grouped_data.mean()
        gdp_growth_2009   gdp_growth_2010
region
FW           -2.483333          1.550000
GL           -5.400000          3.660000
MW           -1.250000          2.433333
NE           -2.350000          2.783333
PL           -1.357143          2.900000
RM           -0.940000          1.380000
SE           -2.633333          2.850000
SW           -2.175000          1.325000


>>> grouped_data.std()   # Can use other methods
        gdp_growth_2009   gdp_growth_2010
region
FW            5.389403          2.687564
GL            2.494995          1.952690
MW            2.529624          1.358921
NE            0.779102          1.782601
PL            2.572196          2.236068
RM            2.511573          1.522170
SE            2.653071          1.489051
SW            4.256270          1.899781
```

If these are not sufficient, the method `aggregate` can be used to apply a user-provided function to each group. The function provided to `aggregate` must operate both column-by-column (as if used on the original with the `.apply` method) and across the entire subframe.

```
>>> grouped_data.aggregate(lambda x: x.max() - x.min())
        gdp_growth_2009   gdp_growth_2010
region
FW                15.9               7.4
GL                 6.3               4.6
MW                 7.4               3.7
NE                 2.0               4.6
PL                 7.3               7.2
RM                 6.2               3.6
SE                 9.1               5.5
SW                 9.9               4.3
```

Transformation (`transform`)

Unlike `aggregate` which returns a single value for each column using some forms of aggregation function, `transform` returns a [DataFrame](#) where each subframe has transformed using a user provided function. For example, `transform` can be used to fill values in the subframe of a particular group based on other values in the group.

```
>>> subset_copy = subset.copy()
>>> subset_copy.iloc[::3,:2] = np.nan
>>> subset_copy.head()
   gdp_growth_2009  gdp_growth_2010 region
0             NaN              NaN     FW
1            -3.9              2.7     SE
2            -2.0              2.6     SE
3             NaN              NaN     SW
4            -5.1              0.3     FW

>>> filled_data = grouped_data.transform(lambda x:x.fillna(x.mean()))
>>> filled_data.head()
   gdp_growth_2009  gdp_growth_2010
0            -3.6             2.85
1            -3.9             2.70
2            -2.0             2.60
3             0.6             2.45
4            -5.1             0.30
```

Filtration (filter)

`filter` allows groups to be selected based on some function. The function input is the group subframe and it must return either `True` or `False`. This example selects any regions with a single growth rate over 3.3%.

```
>>> grouped_data = subset.groupby(by='region')
>>> grouped_data.filter(lambda x: x.gdp_growth_2009.max() > 3.3)
    gdp_growth_2009  gdp_growth_2010 region
0              7.7             -1.7     FW
4             -5.1              0.3     FW
5             -2.2              2.2     RM
11            -3.7              3.1     FW
13            -2.8              1.6     RM
26            -2.1              2.1     RM
33            -8.2             -0.4     FW
37            -3.2              5.7     FW
44            -1.0              2.3     RM
47            -2.4              2.3     FW
50             3.4             -1.3     RM
```

Iteration and Selection of a Group

`groupby` supports iteration across groups if the desired result cannot be computed using one of the direct methods – aggregation, transformation or filtration. Iteration returns two values, the group key and the subset of data in the group. This example makes use of the state GDP data and groups the data by the region.

```
>>> subset = state_gdp[['gdp_growth_2009','gdp_growth_2010','region']]
>>> subset.head()
   gdp_growth_2009  gdp_growth_2010 region
0              7.7             -1.7     FW
1             -3.9              2.7     SE
```

```
2              -2.0              2.6     SE
3              -8.2             -0.2     SW
4              -5.1              0.3     FW

>>> grouped_data = subset.groupby(by='region')
>>> for group_name, group_data in grouped_data:
...     if group_name == 'SW':
...         print(group_data)
    gdp_growth_2009  gdp_growth_2010 region
103             -8.2             -0.2     SW
132              1.7              0.8     SW
136             -1.7              0.6     SW
143             -0.5              4.1     SW
```

groupby also exposes a property, groups, which will return a dictionary containing the group name and the index values of the group members.

```
>>> grouped_data.groups # Lists group names and index labels
{'FW': Int64Index([0, 4, 11, 33, 37, 47], dtype='int64'),
 'GL': Int64Index([14, 15, 22, 35, 48], dtype='int64'),
 'MW': Int64Index([7, 8, 20, 31, 34, 38], dtype='int64'),
 'NE': Int64Index([6, 19, 21, 30, 39, 46], dtype='int64'),
 'PL': Int64Index([12, 16, 23, 24, 28, 29, 41], dtype='int64'),
 'RM': Int64Index([5, 13, 26, 44, 50], dtype='int64'),
 'SE': Int64Index([1, 2, 9, 10, 17, 18, 25, 27, 40, 42, 45, 49], dtype='int64'),
 'SW': Int64Index([3, 32, 36, 43], dtype='int64')}
```

15.1.4 Categorical

Categoricals are a special type of Series optimized to efficiently store repeated values. In most relevant cases the underlying data will be a string, although this is not a requirement. For example, genders or state codes can be efficiently stored as a Categorical. Categoricals map the inputs onto integer values and use a lookup table to map the original values to the integer values used to represent the categorical data. In practice, Categoricals should only be used when values are repeated – using a Categorical on a string Series containing only unique values will require more storage than the original string Series. This example shows the gain to used a Categorical to represent 1,000,000 gender values coded as strings. A DataFrame containing the string version requires about 7.6 MiB, which a DataFrame containing the Categorical requires less than 1 MiB. Savings can be substantially larger when the original string values are larger.

```
>>> from numpy.random import choice
>>> from pandas import Categorical
>>> gender = Series(choice(['M','F'], 1000000))
>>> df = DataFrame(gender)
>>> df.info(memory_usage=True)
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1000000 entries, 0 to 999999
Data columns (total 1 columns):
0    1000000 non-null object
dtypes: object(1)
memory usage: 7.6+ MB

>>> gender_cat = Categorical(gender)
>>> df = DataFrame([gender_cat])
```

```
>>> df.info(memory_usage=True)
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 1000000 entries, 0 to 999999
Data columns (total 1 columns):
0    1000000 non-null category
dtypes: category(1)
memory usage: 976.7 KB
```

15.2 Statistical Functions

pandas Series and DataFrame are derived from NumPy arrays and so the vast majority of simple statistical functions are available. This list includes sum, mean, std, var, skew, kurt, prod, median, quantile, abs, cumsum, and cumprod. DataFrame also supports cov and corr – the keyword argument axis determines the direction of the operation (0 for down columns, 1 for across rows). Novel statistical routines are described below.

count

count returns number of non-null values – that is, those which are not NaN or another null value such as None or NaT (not a time, for datetimes).

describe

describe provides a summary of the Series or DataFrame.

```
>>> state_gdp.describe()
           gdp_2009       gdp_2010     gdp_2011       gdp_2012  \
count   5.100000e+01   5.100000e+01  5.100000e+01   5.100000e+01
mean    2.468670e+05   2.528407e+05  2.569956e+05   2.633273e+05
std     2.991342e+05   3.044468e+05  3.096895e+05   3.198425e+05
min     2.210800e+04   2.334100e+04  2.363900e+04   2.391200e+04
25%     6.407050e+04   6.522900e+04  6.571400e+04   6.628800e+04
50%     1.498430e+05   1.538390e+05  1.553900e+05   1.572720e+05
75%     3.075225e+05   3.187485e+05  3.274885e+05   3.370160e+05
max     1.667152e+06   1.672473e+06  1.692301e+06   1.751002e+06


        gdp_growth_2009  gdp_growth_2010  gdp_growth_2011  gdp_growth_2012
count        51.000000        51.000000        51.000000        51.000000
mean         -2.313725         2.462745         1.590196         2.103922
std           3.077663         1.886474         1.610497         1.948944
min          -9.100000        -1.700000        -2.600000        -0.100000
25%          -3.900000         1.450000         0.900000         1.250000
50%          -2.400000         2.300000         1.700000         1.900000
75%          -1.050000         3.300000         2.200000         2.500000
max           7.700000         7.200000         7.800000        13.400000
```

value_counts

value_counts performs histogramming of a Series or DataFrame.

```
>>> state_gdp.region.value_counts()
SE    12
PL     7
NE     6
FW     6
```

```
MW      6
GL      5
RM      5
SW      4
dtype: int64
```

15.3   Time-series Data

The pandas TimeSeries object is currently limited to a span of about 585 years centered at 1970. While this is unlikely to create problems, it may not be appropriate for some applications.

pandas includes a substantial number of routines which are primarily designed to work with time-series data. A TimeSeries is basically a series where the index contains datetimes index values (more formally the class TimeSeries inherits from Series), and Series constructor will automatically promote a Series with datetime index values to a TimeSeries. The TimeSeries examples all make use of US real GDP data from the Federal Reserve Economic Database (FRED).

```
>>> GDP_data = read_excel('GDP.xls','GDP',skiprows=19)
>>> GDP_data.head()
        DATE   VALUE
0 1947-01-01  243.1
1 1947-04-01  246.3
2 1947-07-01  250.1
3 1947-10-01  260.3
4 1948-01-01  266.2

>>> type(GDP_data.VALUE)
pandas.core.series.Series

>>> gdp = GDP_data.VALUE
>>> gdp.index = GDP_data.DATE
>>> gdp.head()
DATE
1947-01-01    243.1
1947-04-01    246.3
1947-07-01    250.1
1947-10-01    260.3
1948-01-01    266.2
Name: VALUE, dtype: float64

>>> type(gdp.index)
pandas.tseries.index.DatetimeIndex
```

TimeSeries have some useful indexing tricks. For example, all of the data for a particular year can retrieved using gdp['*yyyy*'] syntax where *yyyy* is a year.

```
>>> gdp['2009']
DATE
2009-01-01    14381.2
2009-04-01    14342.1
2009-07-01    14384.4
2009-10-01    14564.1
Name: VALUE, dtype: float64

>>> gdp['2009-04'] # All for a particular month
DATE
2009-04-01    14342.1
Name: VALUE, dtype: float64
```

Dates can also be used for slicing using the notation `gdp['d1:d2:']` where *d1* and *d2* are both valid date formats (e.g `'2009'` or `'2009-01-01'`)

```
>>> gdp['2009':'2010']
DATE
2009-01-01    14381.2
2009-04-01    14342.1
2009-07-01    14384.4
2009-10-01    14564.1
2010-01-01    14672.5
2010-04-01    14879.2
2010-07-01    15049.8
2010-10-01    15231.7
Name: VALUE, dtype: float64

>>> gdp['2009-06-01':'2010-06-01']
DATE
2009-07-01    14384.4
2009-10-01    14564.1
2010-01-01    14672.5
2010-04-01    14879.2
Name: VALUE, dtype: float64
```

Slicing indexing can also be accomplished using datetime, for example `gdp[datetime(2009,01, 01):datetime(2011,12,31)]` where `datetime` has been imported using `from pandas import datetime`.

pct_change

Growth rates are computed using `pct_change`. The keyword argument `periods` constructs overlapping growth rates which are useful when using seasonal data.

```
>>> gdp.pct_change().tail()
DATE
2012-04-01    0.007406
2012-07-01    0.012104
2012-10-01    0.003931
2013-01-01    0.007004
2013-04-01    0.008019
Name: VALUE, dtype: float64

>>> gdp.pct_change(periods=4).tail() # Quarterly data, annual difference
DATE
2012-04-01    0.045176
2012-07-01    0.047669
2012-10-01    0.038031
2013-01-01    0.030776
2013-04-01    0.031404
Name: VALUE, dtype: float64
```

15.3.1 Dates and Times

pandas provides its own date and time functionality that extends NumPy's `datetime64`. There are two main types to represent dates and times. The first, pandas `Timestamps` are directly based on NumPy's `datetime64` and add time zone support. `Timestamps` always use `datetime64` with nano-second resolution, indicated by `[ns]`, and so only support dates and times in the between 1677 and 2262 (1970 ± 292 years). The second, `Periods`, is a custom pandas data type that can be used to express dates and times over a wider interval. The conceptual difference between the two is that a `Timestamp` represents a point in time which a `Period` represents

a range. For example, January 2010 when represented as a `Timestamp` has to be some specific point in time in January 2010, while represented as a `Period` is it just January 2010 (with no day, hour, etc.).

`Timestamp` and `Timedelta`

`Timestamp`s and `Timedelta`s are the pandas analogs of NumPy's `datetime64`s and `timedelta64`s. The primary difference is that pandas continues to support time zone information using the timezone information provided by either the pytz or dateutil packages (pytz is preferred and dateutil will only be used if pytz is not installed).

   `Timestamp`s can be created from strings, NumPy `datetime64`s or Python native `datetime`s.

```
>>> from pandas import Timestamp, Timedelta
>>> from numpy import datetime64
>>> import datetime as dt
>>> Timestamp('1960-1-1')
Timestamp('1960-01-01 00:00:00')

>>> Timestamp(datetime64('1960-01-01'))
Timestamp('1960-01-01 00:00:00')

>>> Timestamp(dt.datetime(1960, 1, 1))
Timestamp('1960-01-01 00:00:00')
```

`to_datetime`

The simplest method to create arrays of `Timestamp`s is to use `to_datetime` which accepts iterable inputs containing dates in any of the convertible formats: strings, `datetime` or `datetime64`. `to_datetime` also provides additional options for parsing string dates include a format string which allow non-standard date formats to be parsed.

```
>>> from pandas import to_datetime
>>> to_datetime(['1960-1-1', '1970-1-1', '1980-1-1'])
DatetimeIndex(['1960-01-01', '1970-01-01', '1980-01-01'],
              dtype='datetime64[ns]', freq=None)
```

`Period`

`Period`s are an alternative format to `Timestamp`s that represent an interval of time rather than a point in time. `Period`s are only specified up to the required resolution. For example, when using quarterly data, a `Period` will only have a year and quarter while a `Timestamp` will always be specified up to the nanosecond. Using a `Period` avoids choices such as using quarter start or end dates, as well as choosing an arbitrary time of day. `Period`s can be specified using a string or through inputs that accept numeric values representing the year, month, day, hour, minute and second. When using a string the frequency is inferred. When using numeric inputs, the frequency must also be specified.

```
>>> from pandas import Period
>>> Period('1980')
Period('1980', 'A-DEC')

>>> Period(year=1980, freq='A')
Period('1980', 'A-DEC')

>>> Period(year=1980, month=1, freq='Q')
Period('1980Q1', 'Q-DEC')

>>> Period(year=1980, month=5, freq='Q')
Period('1980Q2', 'Q-DEC')
```

Periods can be used to represent dates outside the range supported by Timestampss. The supported range is years between 1 and 9999.

date_range and bdate_range

date_range is a very useful function provided by pandas to generate ranges of dates. The basic use is either date_range(*beginning_date*, *ending_date*) which will produce a daily series between the two dates (inclusive) or date_range(*beginning_date*, periods=*numperiods*) which will produce a daily series starting at *beginning_date* with *numperiods* periods.

```
>>> from pandas import date_range, bdate_range
>>> date_range('2013-01-03','2013-01-05')
DatetimeIndex(['2013-01-03', '2013-01-04', '2013-01-05'],
              dtype='datetime64[ns]', freq='D')

>>> date_range('2013-01-03', periods = 3)
DatetimeIndex(['2013-01-03', '2013-01-04', '2013-01-05'],
              dtype='datetime64[ns]', freq='D')
```

The keyword argument freq changes the frequency, and common choices include

'S'	seconds	'U'	micro-second
'T'	minutes	'L'	millisecond
'H'	hourly	'B'	daily (business)
'D'	daily	'W'	weekly
'M'	monthly (end)	'Q'	quarterly (end)
'A'	annual (end)		

Many of the frequency choices can be modified to produce only business dates (e.g., Monday to Friday) or start of period dates. For example, 'MS' will produce the first day in the month, 'BQ' will produce the last business day in a quarter, and 'BMS' will produce the first business day in the month.

```
>>> date_range('2013-01-03',periods=2, freq='Q')
DatetimeIndex(['2013-03-31', '2013-06-30'],dtype='datetime64[ns]',freq='Q-DEC')

>>> date_range('2013-01-03',periods=2, freq='BQ')
DatetimeIndex(['2013-03-29', '2013-06-28'],dtype='datetime64[ns]',freq='BQ-DEC')
```

Scaling the frequency produces skips that are a multiple of the default, such as in 2D which uses every other day. Combining multiple frequencies produces less regular skips, e.g. 2H10T.

```
>>> date_range('2013-01-03',periods=4, freq='Q')
DatetimeIndex(['2013-03-31', '2013-06-30', '2013-09-30', '2013-12-31'],
              dtype='datetime64[ns]', freq='Q-DEC')

>>> date_range('2013-01-03',periods=4, freq='7D4H')
DatetimeIndex(['2013-01-03 00:00:00', '2013-01-10 04:00:00',
               '2013-01-17 08:00:00', '2013-01-24 12:00:00'],
              dtype='datetime64[ns]', freq='172H')
```

bdate_range is identical to date_range except the defult frequency is business days.

```
>>> date_range('2013-01-03', periods=4)
DatetimeIndex(['2013-01-03', '2013-01-04', '2013-01-05', '2013-01-06'],
              dtype='datetime64[ns]', freq='D')

>>> bdate_range('2013-01-03', periods=4)
DatetimeIndex(['2013-01-03', '2013-01-04', '2013-01-07', '2013-01-08'],
              dtype='datetime64[ns]', freq='B')
```

period_range

period_range is the analogue function to date_range for generating Periods. It is normally called with three arguments, either start, end, and frequency or start, periods, and frequency.

```
>>> from pandas import period_range
>>> period_range('2013-01-03', periods=4, freq='M')
PeriodIndex(['2013-01', '2013-02', '2013-03', '2013-04'],
            dtype='period[M]', freq='M')

>>> period_range('2013-01-03', periods=4, freq='A')
PeriodIndex(['2013', '2014', '2015', '2016'],
            dtype='period[A-DEC]', freq='A-DEC')

>>> period_range('2013-01-03', '2019-01-01', freq='A')
PeriodIndex(['2013', '2014', '2015', '2016', '2017', '2018', '2019'],
            dtype='period[A-DEC]', freq='A-DEC')
```

15.3.2 `resample`

pandas supports sophisticated resampling which is useful for aggregating from a higher frequency to a lower one using resample. resample is similar to groupby and so requires calling an aggregation function on the output of the resample call. This example resamples from quarterly to annual (`'A'`) and shows alternative aggregation functions.

```
>>> gdp.resample('A').mean().tail() # Annual average
DATE
2009-12-31    14417.950
2010-12-31    14958.300
2011-12-31    15533.825
2012-12-31    16244.575
2013-12-31    16601.600
Freq: A-DEC, Name: VALUE, dtype: float64

>>> gdp.resample('A').max().tail() # Maximum
DATE
2009-12-31    14564.1
2010-12-31    15231.7
2011-12-31    15818.7
2012-12-31    16420.3
2013-12-31    16667.9
gdp.resample('A').max().tail() # Maximum
```

15.4   Importing and Exporting Data

In addition to providing data management tools, pandas also excels at importing and exporting data. pandas supports reading and Excel, csv and other delimited files, Stata files, fixed-width text, html, json, HDF5 and

from SQL databases. The functions to read follow the common naming convention `read_`*type* where type is the file type, e.g. `excel` or `csv`. The writers are all methods of Series or DataFrame and follow the naming convention `to_`*type*.

Reading Data

`read_excel`

`read_excel` supports reading data from both xls (Excel 2003) and xlsx (Excel 2007/10/13) formats. Reading these formats depends on the Python package xlrd. The basic usage required two inputs, the file name and the sheet name. Other notable keyword arguments include:

- `header`, an integer indicating which row to use for the column labels. The default is 0 (top) row, and if `skiprows` is used, this value is relative.

- `skiprows`, typically an integer indicating the number of rows at the top of the sheet to skip before reading the file. The default is 0.

- `skip_footer`, typically an integer indicating the number of rows at the bottom of the sheet to skip when reading the file. The default is 0.

- `index_col`, an integer or column name indicating the column to use as the index. If not provided, a basic numeric index is generated.

- `parse_cols`, `None`, an integer, a list of integers or strings, tells pandas whether to attempt to parse a column. The default is `None` which will parse all columns. Alternatively, if an integer is provided then the value is interpreted as the last column to parse. Finally, if a list of integers is provided, the values are interpreted as the columns to parse (0-based, e.g. `[0,2,5]`). The string version takes one of the forms `'A'`, `'A,C,D'`, `'A:D'` or a mix of the latter two (`'A,C:D,G,W:Z'`).

`read_csv`

`read_csv` reads comma separated value files. The basic use only requires one input, a file name. `read_csv` also accepts valid URLs (HTTP, FTP, or S3 (Amazon) if the boto package is available) or any object that provides a `read` method in places of the file name. A huge range of options are available, and so only the most relevant are presented in the list below.

- `delimiter`, the delimiter used to separate values. The default is `','`. Complicated delimiters are matched using a regular expression.

- `delim_whitespace`, Boolean indicating that the delimiter is white space (space or tab). This is preferred to using a regular expression to detect white space.

- `header`, an integer indicating the row number to use for the column names. The default is 0.

- `skiprows`, similar to `skiprows` in `read_excel`.

- `skip_footer`, similar to `skip_footer` in `read_excel`.

- `index_col`, similar to `index_col` in `read_excel`.

- `names`, a list of column names to use in-place of any found in the file Must use `header=0` (the default value).

- `parse_dates`, either a Boolean indicating whether to parse dates encountered or a list of integers or strings indicating which columns to parse. Supports more complicated options to combine columns (see `read_csv`).

- `date_parser`, a function to use when parsing dates. The default parser is `dateutil.parser`.

- `dayfirst`, a Boolean indicating whether to use European date format (DD/MM, `True`) or American date format (MM/DD `False`) when encountering dates. The default is `False`.

- `error_bad_lines`, when `True` stops processing on a bad line. If `False`, continues skipping any bad lines encountered.

- `encoding`, a string containing the file encoding (e.g. `'utf-8'` or `'latin-1'`).

- `converters`, a dictionary of functions for converting values in certain columns, where keys can either integers (column-number) or column labels.

- `nrows`, an integer, indicates the maximum number of rows to read. This is useful for reading a subset of a file.

- `usecols`, a list of integers or column names indicating which column to retain.

- `dtype` A data type to use for the read data or a dictionary of data types using the column names as keys. If not provided, the type is inferred.

read_table

`read_table` is similar to `read_csv` and both are wrappers around a private read function provided by pandas.

read_hdf

`read_hdf` is primarily for reading pandas DataTables which were written using `DataTable.to_hdf`

read_stata

`read_stata` can be used to import Stata DTA files into Python.

Writing Data

Writing data from a Series or DataFrame is much simpler since the starting point (the Series or the DataFrame) is well understood by pandas. While the file writing methods all have a number of options, most can safely be ignored.

```
>>> state_gdp.to_excel('state_gdp_from_dataframe.xls')
>>> state_gdp.to_excel('state_gdp_from_dataframe_sheetname.xls', sheet_name='State GDP')
>>> state_gdp.to_excel('state_gdp_from_dataframe.xlsx')
>>> state_gdp.to_csv('state_gdp_from_dataframe.csv')
>>> from io import StringIO
>>> sio = StringIO()
>>> state_gdp.to_json(sio)
>>> sio.seek(0)
>>> sio.read(50)
'{"state_code":{"0":"AK","1":"AL","2":"AR","3":"AZ"'

>>> state_gdp.to_string()[:50]
u'   state_code                    state  gdp_2009  gdp'
```

Stata DTA files can be exported using `to_stata`. One writer, `to_hdf` is worth special mention. `to_hdf` writes pandas DataFrames to HDF5 files which are binary files which support compression. HDF5 files can achieve fantastic compression ratios when data are regular, and so are often much more useful than CSV or xlsx (which is also compressed). The usage of `to_hdf` is not meaningfully different from the other writers except that:

- In addition to the filename, an argument is required containing the key, which is usually the variable name.

- Two additional arguments must be passed to compressed the output file. These two keyword arguments are `complib` and `complevel`, which I recommend to setting to 'zlib' and 6, respectively.

```
>>> df = DataFrame(zeros((1000,1000)))
>>> df.to_csv('size_test.csv')
>>> df.to_hdf('size_test.h5','df') # h5 is the usual extension for HDF5
# h5 is the usual extension for HDF5
>>> df.to_hdf('size_test_compressed.h5','df',complib='zlib',complevel=6)
>>> ls size_* # Ignore
09/19/2013  04:16 PM           4,008,782 size_test.csv
09/19/2013  04:16 PM           8,029,160 size_test.h5
09/19/2013  04:16 PM              33,812 size_test_compressed.h5

>>> df.to_csv('size_test.csvz', compression='gzip')
>>> ls size_test.csvz # Ignore
09/19/2013  04:18 PM              10,544 size_test.csvz
>>> from pandas import read_csv
>>> df_from_csvz = read_csv('size_test.csvz',compression='gzip')
```

The final block of lines shows how a CSV with gzip compression is written and directly read using pandas. This method also achieves a very high level of compression.

Any NumPy array is easily written to a file using a single, simple line using pandas.

```
>>> x = randn(100,100)
>>> DataFrame(x).to_csv('numpy_array.csv',header=False,index=False)
```

15.4.1 `HDFStore`

`HDFStore` is the Class that underlies `to_hdf`, and is useful for storing multiple Series or DataFrames to a single HDF file. Its use is similar to that of any generic file writing function in Python – it must be opened, data can be read or written, and then it must be closed. Storing data is as simple as inserting objects into a dictionary.

The basic use of a HDFStore for saving data is

```
>>> from pandas import HDFStore
>>> store = HDFStore('store.h5',mode='w',complib='zlib',complevel=6)
```

which opens the `HDFStore` named `store` for writing (`mode='w'`) with compression. Stores can also be opened for reading (`mode='r'`) or appending (`mode='a'`). When opened for reading, the compression options are not needed. Data can then be stored in the `HDFStore` using dictionary syntax.

```
>>> store['a'] = DataFrame([[1,2],[3,4]])
>>> store['b'] = DataFrame(np.ones((10,10)))
```

and finally, the store must be closed.

```
>>> store.close()
```

The data can then be read using similar commands,

```
>>> store = HDFStore('store.h5',mode='r')
>>> a = store['a']
>>> b = store['b']
>>> store.close()
```

which will read the data with key `'a'` in a variable named `a`, and similarly for `b`.

A slightly better method for using a store is to use the Python keyword `with` and `HDFStore`. When `HDFStore` is used in the manner, it is called a context manager. Context managers automatically call `close()` when the `with` block exists, and so ensures that files are always closed.[3]

```
with HDFStore('store.h5') as store:
    a = store['a']
    b = store['b']
```

is equivalent to the previous code block, only the `close()` is called implicitly after the variables are read. The context manager usage of `HDFStore` can also be used to write HDF files and accepts the usual keyword arguments to, e.g., enable compression or set the mode for opening the file.

15.5   Graphics

pandas provides a set of useful plotting routines based on matplotlib which makes use of the structure of a DataFrame. Everything in pandas plot library is reproducible using matplotlib, although often at the cost of additional typing and code complexity (for example, axis labeling).

plot

`plot` is the main plotting method, and by default will produce a line graph of the data in a DataFrame. Calling `plot` on a DataFrame will plot all series using different colors and generate a legend. A number of keyword argument are available to affect the contents and appearance of the plot.

- `style`, a list of matplotlib styles, one for each series plotted. A dictionary using column names as keys and the line styles as values allows for further customization.

- `title`, a string containing the figure title.

- `subplots`, a Boolean indicating whether to plot using one subplot per series (`True`). The default it `False`.

- `legend`, a Boolean indicating whether to show a legend

- `secondary_y`, a Boolean indicating whether to plot a series on a secondary set of axis values. See the example below.

- `ax`, a matplotlib axis object to use for the plot. If no axis is provided, then a new axis is created.

- `kind`, a string, one of:

    - `'line'`, the default
    - `'bar'` to produce a bar chart. Can also use the keyword argument `stacked=True` to produce a stacked bar chart.
    - `'barh'` to produce a horizontal bar chart. Also support `stacked=True`.
    - `'kde'` or `'density'` to produce a kernel density plot.

---

[3]See Section 22.4 for further details on context managers.

hist

`hist` produces a histogram plot, and is similar to producing a bar plot using the output of `value_count`.

boxplot

`boxplot` produces box plots of the series in a DataFrame.

scatter_plot

`scatter_plot` produce a scatter plot from two series in a DataFrame. Three inputs are required: the DataFrame, the column name for the x-axis data and the column name for the y-axis data. `scatter_plot` is located in `pandas.tools.plotting`.

scatter_matrix

`scatter_matrix` produces a *n* by *n* set of subplots where each subplot contains the bivariate scatter of two series. One input is required, the DataFrame. `scatter_matrix` is located in `pandas.tools.plotting`. By default, the diagonal elements are histograms, and the keyword argument `diagonal='kde'` produces a kernel density plot.

lag_plot

`lag_plot` produces a scatter plot of a series against its lagged value. The keyword argument `lag` chooses the lag used in the plot (default is 1).

15.6 Examples

15.6.1 FRED Data

The Federal Reserve Economics Database is a comprehensive database of US, and increasingly global, macroeconomics data. This example will directly download a small macroeconomics data set from FRED and merge it into a single DataFrame. The data in FRED is available in CSV using the url pattern `https://fred.stlouisfed.org/graph/fredgraph.csv?id=CODE` where CODE is the series code. This example will make use of Real GDP, Industrial Production, Core CPI the Unemployment Rate, the Treasury yield slope (10-year yield minus 1-year yield) and the default premium, based on the difference between BAA and AAA rated bonds. The list of series is in table 15.1.

The initial block of code imports the future functions, `read_csv`, `DataFrame` and `scatter_matrix`, the only pandas functions directly used in this example. It also sets up lists containing the codes and nice names for the series and contains the URL root for fetching the data

```python
from pandas import read_csv
from pandas.plotting import scatter_matrix

codes = ['GDPC1','INDPRO','CPILFESL','UNRATE','GS10','GS1','BAA','AAA']
names = ['Real GDP','Industrial Production','Core CPI','Unemployment Rate',\
   '10 Year Yield','1 Year Yield','Baa Yield','Aaa Yield']

# r to disable escape
base_url = r'https://fred.stlouisfed.org/graph/fredgraph.csv?id={code}'
```

The next piece of code starts with an empty list to hold the DataFrames produced by `read_csv`. The codes are then looped over and directly used in the CSV reader.

Series	Code	Frequency
Real GDP	GDPC1	Quarterly
Industrial Production	INDPRO	Quarterly
Core CPI	CPILFESL	Monthly
Unemployment Rate	UNRATE	Monthly
10 Year Yield	GS10	Monthly
1 Year Yield	GS1	Monthly
Baa Yield	BAA	Monthly
Aaa Yield	AAA	Monthly

Table 15.1: The series, codes and their frequencies used in the FRED example.

```python
data = []
for code in codes:
    print(code)
    url = base_url.format(code=code)
    data.append(read_csv(url))
```

Next, the data is merged into a single DataFrame by building a dictionary where the keys are the codes and the values are the Series from each downloaded DataFrame. This block makes use of `zip` to quickly concatenate two lists into a single iterable.

```python
time_series = {}
for code, d in zip(codes,data):
    d.index = d.DATE
    time_series[code] = d[code]

merged_data = DataFrame(time_series)
# Unequal length series
print(merged_data)
```

The next step is to construct the Term and Default premia series using basic math on the series. The resulting Series are given a name, which is required for the join operation. Finally, the non-required columns are dropped.

```python
term_premium = merged_data['GS10'] - merged_data['GS1']
term_premium.name = 'Term'
merged_data = merged_data.join(term_premium,how='outer')
default_premium = merged_data['BAA'] - merged_data['AAA']
default_premium.name = 'Default'
merged_data = merged_data.join(default_premium,how='outer')
merged_data = merged_data.drop(['AAA','BAA','GS10','GS1'],axis=1)
print(merged_data.tail())
```

The next block forms a quarterly data set by dropping the rows with any null values.

```python
quarterly = merged_data.dropna()
print(quarterly.tail())
```

Finally, it is necessary to transform some of the series to be growth rates since the data contains both $I(0)$ and $I(1)$ series. This is done using `pct_change` on a subset of the quarterly data.

```python
growth_rates_selector = ['GDPC1','INDPRO','CPILFESL']
growth_rates = 100 * quarterly[growth_rates_selector].pct_change()
final = quarterly.drop(growth_rates_selector, axis=1).join(growth_rates)
```

Series	Description
Treated	Dummy indicating whether the candidate received the treatment
Age	Age in years
Education (years)	Years of Education
Black	Dummy indicating African-American
Hispanic	Dummy indicating Hispanic
Married	Dummy indicating married
Real income Before ($)	Income before program
Real income After ($)	Income after program

Table 15.2: The series, codes and their frequencies used in the FRED example.

The last step is to rename some of the columns using `rename` with the keyword argument `columns`. The names are changed using a dictionary where the key is the old name and the value is the new name. The last two lines save the final version of the data to HDF5 and to an excel file.

```
new_names = {'GDPC1':'GDP_growth',   \
             'INDPRO':'IP_growth',   \
             'CPILFESL':'Inflation', \
             'UNRATE':'Unemp_rate'}
final = final.rename(columns = new_names ).dropna()
final.to_hdf('FRED_data.h5','FRED',complevel=6,complib='zlib')
final.to_excel('FRED_data.xlsx')
```

The plots provide a simple method to begin exploring the data. Both plots are shown in Figure 15.1.

```
ax = final[['GDP_growth','IP_growth','Unemp_rate']].plot(subplots=True)
fig = ax[0].get_figure()
fig.savefig('FRED_data_line_plot.pdf')

columns = ['GDP_growth','IP_growth','Unemp_rate']
ax = scatter_matrix(final[columns], diagonal='kde')
fig = ax[0,0].get_figure()
fig.savefig('FRED_data_scatter_matrix.pdf')
```

15.6.2 NSW Data

The National Supported Work Demonstration was a program to determine whether giving disadvantaged workers useful job skills would translate into increased earnings. The data set used here is a subset of the complete data set and contains the variables in table 15.2.

The first block contains the standard imports as well as the functions which are used in this example. Both `sqrt` and `stats` are used to perform a t-test.

```
from pandas import read_excel
from numpy import sqrt
import scipy.stats as stats
import seaborn
```

The data is contained in a well-formatted Excel file, and so importing the data using `read_excel` is straightforward. The second line in this block prints the standard descriptive statistics.

```
NSW = read_excel('NSW.xls','NSW')
print(NSW.describe())
```
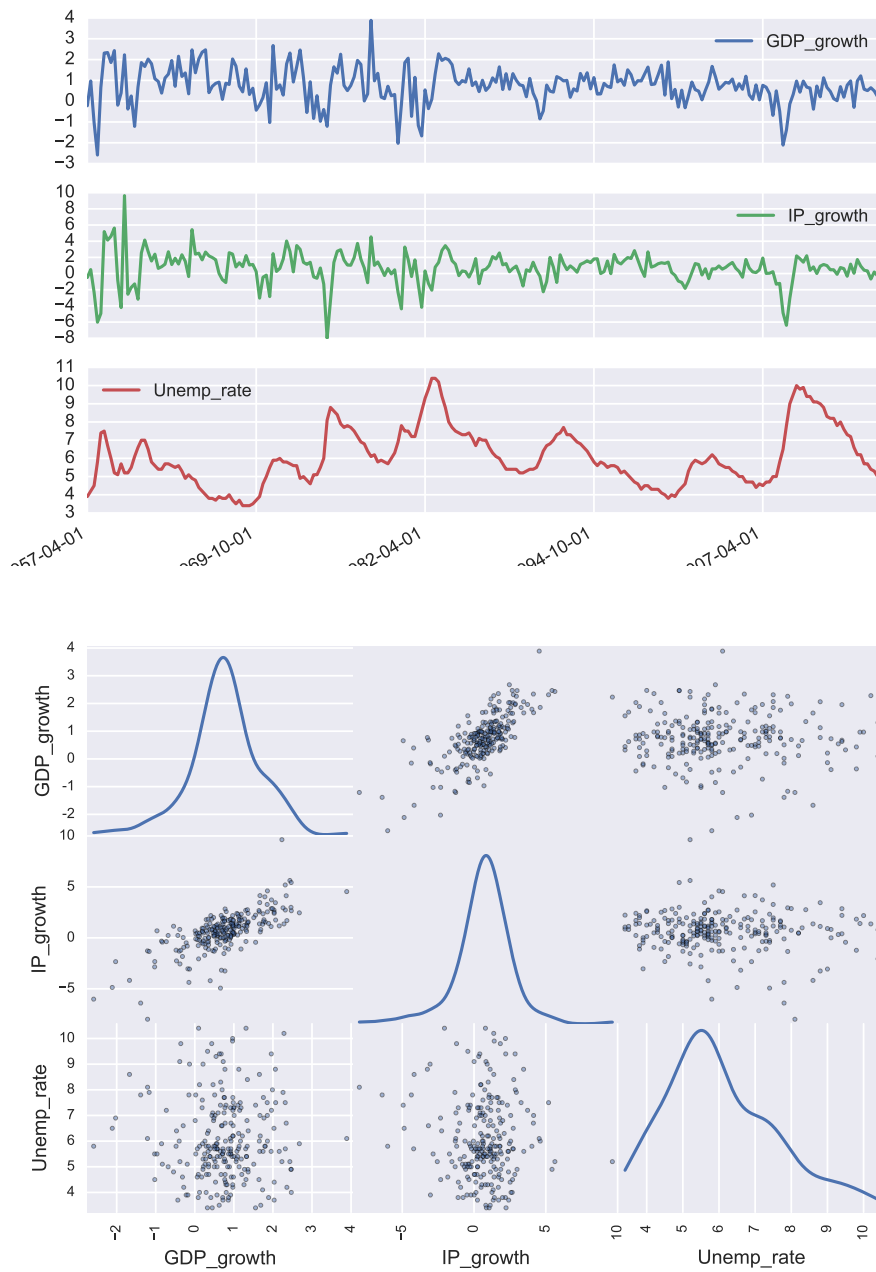
Figure 15.1: The top panel contains line plots of the FRED data. The bottom panel shows the output of `scatter_matrix` using kernel density plots along the diagonal.

rename is then used to give the columns some more useful names – names with spaces cannot be directly accessed using dot notation (i.e. NSW.Income_after works, but there is no method to do the same using NSW.'Real income After ($)'.

```python
NSW = NSW.rename(columns={'Real income After ($)':'Income_after',
                          'Real income Before ($)':'Income_before',
                          'Education (years)':'Education'})
NSW['Minority'] = NSW['Black']+NSW['Hispanic']
```

Next, pivot_table is used to look at the variable means using some of the groups. The third call uses two indices and a double sort.

```python
print(NSW.pivot_table(index='Treated'))

print(NSW.pivot_table(index='Minority'))

print(NSW.pivot_table(index=['Minority','Married']))
```

Next, density plots of the income before and after are plotted. Figure 15.2 shows the plots.

```python
ax = NSW[['Income_before','Income_after']].plot(kind='kde',subplots=True)
fig = ax[0].get_figure()
fig.savefig('NSW_density.pdf')
```

Finally a t-test of equal incomes using the before and after earnings for the treated and non-treated is computed. The t-stat has a one-sided p-val of .9%, indicating rejection of the null of no impact at most significance levels.

```python
income_diff = NSW['Income_after']-NSW['Income_before']
t = income_diff[NSW['Treated']==1]
nt = income_diff[NSW['Treated']==0]
tstat = (t.mean() - nt.mean())/sqrt(t.var()/t.count() - nt.var()/nt.count())
pval = 1 - stats.norm.cdf(tstat)
print(f'T-stat: {tstat:.2f}, P-val: {pval:.3f}')
```
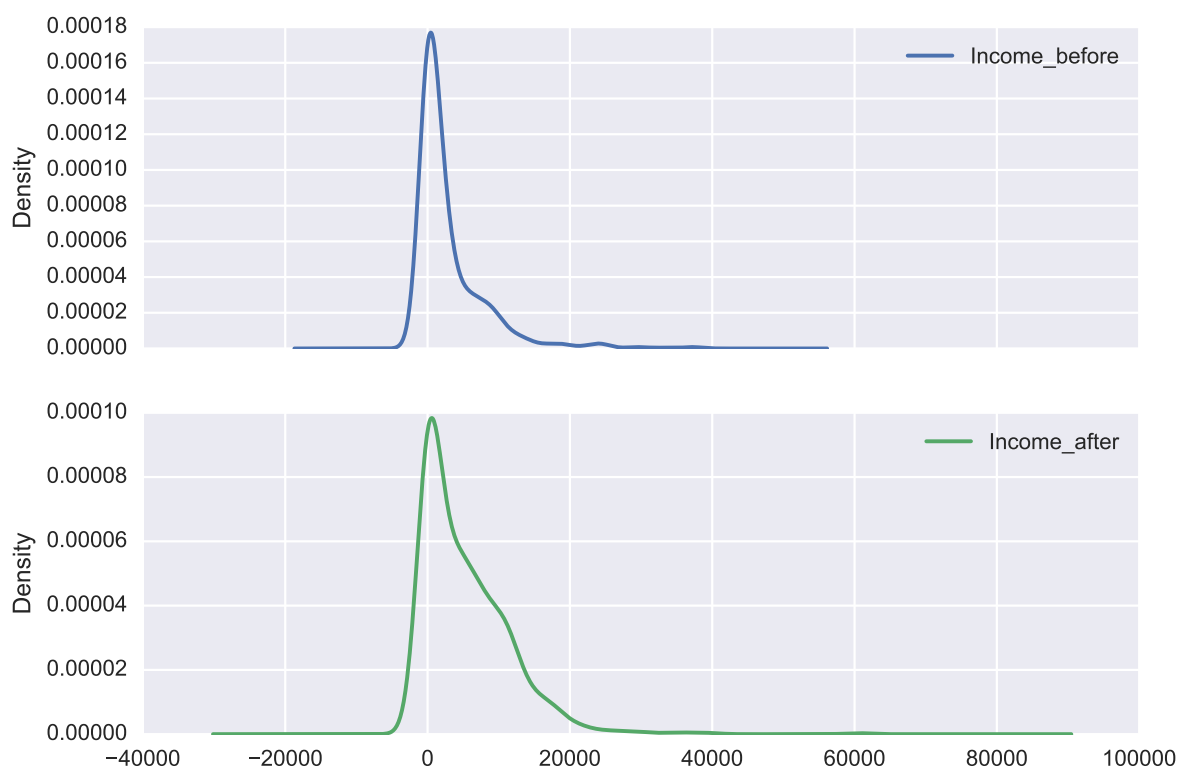
Figure 15.2: Density plot of the before and after income.

Chapter 16

Structured Arrays

pandas, the topic of Chapter 15, has substantially augmented the structured arrays provided by NumPy. The pandas Series and DataFrame types are the preferred method to handle heterogeneous data and/or data sets which have useful metadata. This chapter has been retained since the NumPy data structures may be encountered when using some functions, or in legacy code produced by others.

The standard, homogeneous NumPy array is a highly optimized data structure where all elements have the same data type (e.g. float) and can be accessed using slicing in many dimensions. These data structures are essential for high-performance numerical computing – especially for linear algebra. Unfortunately, actual data is often heterogeneous (e.g. mixtures of dates, strings and numbers) and it is useful to track series by meaningful names, not just "column 0". These features are not available in a homogeneous NumPy array. However, NumPy also supports mixed arrays which solve both of these issues and so are a useful data structures for managing data prior to statistical analysis. Conceptually, a mixed array with named columns is similar to a spreadsheet where each column can have its own name and data type.

16.1 Mixed Arrays with Column Names

A mixed NumPy array can be initialized using `array`, `zeros` or other functions which create arrays and allow the data type to be directly specified. Mixed arrays are in many ways similar to standard NumPy arrays, except that the `dtype` input to the function is specified either using tuples of the form (*name*, *type*), or using a dictionary of the form {`'names'`:*name*s, `'formats'`:*formats*) where *names* is a tuple of column names and *formats* is a tuple of NumPy data types.

```
>>> x = zeros(4,[('date','int'),('ret','float')])
>>> x = zeros(4,{'names': ('date','ret'), 'formats': ('int', 'float')})
>>> x
array([(0, 0.0), (0, 0.0), (0, 0.0), (0, 0.0)],
      dtype=[('date', '<i4'), ('ret', '<f8')])
```

These two commands are identical, and illustrate the two methods to create arrays that contain a named column "date", for integer data, and a named column "ret" for floats. Named columns allows for access using dictionary-type syntax.

```
>>> x['date']
array([0, 0, 0, 0])

>>> x['ret']
array([0.0, 0.0, 0.0, 0.0])
```

Standard multidimensional slice notation is not available since heterogeneous arrays behave like nested lists and not homogeneous NumPy arrays.

```
>>> x[0] # Data tuple 0
(0, 0.0)

>>> x[:3] # Data tuples 0, 1 and 2
array([(0, 0.0), (0, 0.0), (0, 0.0)],
      dtype=[('date', '<i4'), ('ret', '<f8')])

>>> x[:,1] # Error
IndexError: too many indices
```

The first two commands show that the array is composed of tuples and so differs from standard homogeneous NumPy arrays. The error in the third command occurs since columns are accessed using names and not multi-dimensional slices.

16.1.1 Data Types

A large number of primitive data types are available in NumPy.

Type	Syntax	Description
Boolean	b	True/False
Integers	i1,i2,i4,i8	1 to 8 byte signed integers $(-2^{B-1}, \ldots 2^{B-1} - 1)$
Unsigned Integers	u1,u2,u4,u8	1 to 8 byte signed integers $(0, \ldots 2^B)$
Floating Point	f4,f8	Single (4) and double (8) precision float
Complex	c8,c16	Single (8) and double (16) precision complex
Object	On	Generic n-byte object
String	Sn, an	n-letter string
Unicode String	Un	n-letter unicode string

The majority of data types are for numeric data, and are simple to understand. The n in the string data type indicates the maximum length of a string. Attempting to insert a string with more than n characters will truncate the string. The object data type is somewhat abstract, but allows for storing Python objects such as datetimes.

Custom data types can be built using dtype. The constructed data type can then be used in the construction of a mixed array.

```
>>> type = dtype([('var1','f8'), ('var2','i8'), ('var3','u8')])
>>> type
dtype([('var1', '<f8'), ('var2', '<i8'), ('var3', '<u8')])
```

Data types can even be nested to create a structured environment where one of the "variables" has multiple values. Consider this example which uses a nested data type to contain the bid and ask price of a stock, along with the time of the transaction.

```
>>> ba_type = dtype([('bid','f8'), ('ask','f8')])
>>> t = dtype([('date', 'O8'), ('prices', ba_type)])
>>> data = zeros(2,t)
>>> data
array([(0, (0.0, 0.0)), (0, (0.0, 0.0))],
      dtype=[('date', 'O'), ('prices', [('bid', '<f8'), ('ask', '<f8')])])

>>> data['prices']
array([(0.0, 0.0), (0.0, 0.0)],
      dtype=[('bid', '<f8'), ('ask', '<f8')])

>>> data['prices']['bid']
array([ 0.,   0.])
```

In this example, data is an array where each item has 2 elements, the date and the price. Price is also an array with 2 elements. Names can also be used to access values in nested arrays (e.g. `data['prices']['bid']` returns an array containing all bid prices). In practice nested arrays can almost always be expressed as a non-nested array without loss of fidelity.

Determining the size of object NumPy arrays can store objects which are anything which fall outside of the usual data types. One example of a useful, but abstract, data type is `datetime`. One method to determine the size of an object is to create a plain array containing the object – which will automatically determine the data type – and then to query the size from the array.

```
>>> import datetime as dt
>>> x = array([dt.datetime.now()])
>>> x.dtype.itemsize # The size in bytes
>>> x.dtype.descr # The name and description
```

16.1.2 Example: TAQ Data

TAQ is the NYSE Trade and Quote database which contains all trades and quotes of US listed equities which trade on major US markets (not just the NYSE). A record from a trade contains a number of fields:

- Date - The Date in YYYYMMDD format stored as a 4-byte unsigned integer

- Time - Time in HHMMSS format, stored as a 4-byte unsigned integer

- Size - Number of shares trades, stores as a 4 byte unsigned integer

- G127 rule indicator - Numeric value, stored as a 2 byte unsigned integer

- Correction - Numeric indicator of a correction, stored as a 2 byte unsigned integer

- Condition - Market condition, a 2 character string

- Exchange - The exchange where the trade occurred, a 1-character string

First consider a data type which stores the data in an identical format.

```
>>> t = dtype([('date', 'u4'), ('time', 'u4'),
...            ('size', 'u4'), ('price', 'f8'),
...            ('g127', 'u2'), ('corr', 'u2'),
...            ('cond', 'S2'), ('ex', 'S2')])
>>> taqData = zeros(10, dtype=t)
>>> taqData[0] = (20120201,120139,1,53.21,0,0,'','N')
```

An alternative is to store the date and time as a `datetime`, which is an 8-byte object.

```
>>> import datetime as dt
>>> t = dtype([('datetime', 'O8'), ('size', 'u4'), ('price', 'f8'), \
...            ('g127', 'u2'), ('corr', 'u2'), ('cond', 'S2'), ('ex', 'S2')])
>>> taqData = zeros(10, dtype=t)
>>> taqData[0] = (dt.datetime(2012,2,1,12,1,39),1,53.21,0,0,'','N')
```

16.2 Record Arrays

The main feature of record arrays, that the series can be accessed by series name as a property of a variable, is also available in a pandas' DataFrame.

Record arrays are closely related to mixed arrays with names. The primary difference is that elements record arrays can be accessed using *variable.name* format.

```
>>> x = zeros((4,1),[('date','int'),('ret','float')])
>>> y = rec.array(x)
>>> y.date
array([[0],
       [0],
       [0],
       [0]])

>>> y.date[0]
array([0])
```

In practice record arrays may be slower than standard arrays, and unless the *variable.name* is really important, record arrays are not compelling.

Chapter 17

Custom Function and Modules

This chapter uses `@` to multiply arrays. If using Python 3.4 or earlier, or if using a version of NumPy that does not support `@`, these commands should be replaced with `dot`. For example, `X @ X.T` would be `X.dot(X.T)` or `np.dot(X,X.T)`.

Python supports a wide range of programming styles including procedural (imperative), object oriented and functional. While object oriented programming and functional programming are powerful programming paradigms, especially in large, complex software, procedural is often both easier to understand and a direct representation of a mathematical formula. The basic idea of procedural programming is to produce a function or set of function (generically) of the form

$$y = f(x).$$

That is, the functions take one or more inputs and produce one or more outputs.

17.1 Functions

Python functions are very simple to declare and can occur in the same file as the main program or a standalone file. Functions are declared using the `def` keyword, and the value produced is returned using the `return` keyword. Consider a simple function which returns the square of the input, $y = x^2$.

```python
def square(x):
    return x**2

# Call the function
x = 2
y = square(x)
print(x,y)
```

In this example, the same Python file contains the main program – the final 3 lines – as well as the function. More complex function can be crafted with multiple inputs.

```python
def l2distance(x,y):
    return (x-y)**2

# Call the function
x = 3
y = 10
z = l2distance(x,y)
print(x,y,z)
```

Function can also be defined using NumPy arrays and matrices.

```python
import numpy as np

def l2_norm(x,y):
    d = x - y
    return np.sqrt(d @ d)

# Call the function
x = np.random.randn(10)
y = np.random.randn(10)
z = l2_norm(x,y)
print(x-y)
print("The L2 distance is ",z)
```

When multiple outputs are returned but only a single variable is available for assignment, all outputs are returned in a tuple. Alternatively, the outputs can be directly assigned when the function is called with the same number of variables as outputs.

```python
import numpy as np

def l1_l2_norm(x,y):
    d = x - y
    return sum(np.abs(d)),np.sqrt(d @ d)

# Call the function
x = np.random.randn(10)
y = np.random.randn(10)
# Using 1 output returns a tuple
z = l1_l2_norm(x,y)
print(x-y)
print("The L1 distance is ",z[0])
print("The L2 distance is ",z[1])

# Using 2 output returns the values
l1,l2 = l1_l2_norm(x,y)
print("The L1 distance is ",l1)
print("The L2 distance is ",l2)
```

All of these functions have been placed in the same file as the main program. Placing functions in modules allows for reuse in multiple programs, and will be discussed later in this chapter.

17.1.1 Keyword Arguments

All input variables in functions are automatically keyword arguments, so that the function can be accessed either by placing the inputs in the order they appear in the function (positional arguments), or by calling the input by their name using *keyword=value*.

```python
import numpy as np

def lp_norm(x,y,p):
    d = x - y
    return sum(abs(d)**p)**(1/p)

# Call the function
x = np.random.randn(10)
y = np.random.randn(10)
z1 = lp_norm(x,y,2)
z2 = lp_norm(p=2,x=x,y=y)
print("The Lp distances are ",z1,z2)
```

Because variable names are automatically keywords, it is important to use meaningful variable names when possible, rather than generic variables such as `a`, `b`, `c` or `x`, `y` and `z`. In some cases, `x` may be a reasonable default, but in the previous example which computed the L_p norm, calling the third input `z` would be bad idea.

17.1.2 Default Values

Default values are set in the function declaration using the syntax *input=default*.

```
import numpy as np

def lp_norm(x,y,p = 2):
    d = x - y
    return sum(abs(d)**p)**(1/p)

# Call the function
x = np.random.randn(10)
y = np.random.randn(10)
# Inputs with default values can be ignored
l2 = lp_norm(x,y)
l1 = lp_norm(x,y,1)
print("The l1 and l2 distances are ",l1,l2)
print("Is the default value overridden?", sum(abs(x-y))==l1)
```

Default values should not normally be mutable (e.g. lists or arrays) since they are only initialized the first time the function is called. Subsequent calls will use the same value, which means that the default value could change every time the function is called.

```
import numpy as np

def bad_function(x = zeros(1)):
    print(x)
    x[0] = np.random.randn(1)

# Call the function
bad_function()
bad_function()
bad_function()
```

Each call to `bad_function` shows that `x` has a different value – despite the default being 0. The solution to this problem is to initialize mutable objects to `None`, and then the use an `if` to check and initialize only if the value is `None`. Note that tests for `None` use the `is` keyword rather the testing for equality using `==`.

```
import numpy as np

def good_function(x = None):
    if x is None:
        x = zeros(1)
    print(x)
    x[0] = np.random.randn(1)


# Call the function
good_function()
good_function()
```

Repeated calls to `good_function()` all show `x` as 0.

17.1.3 Variable Number of Inputs

Most function written as an "end user" have an known (*ex ante*) number of inputs. However, functions which evaluate other functions often must accept variable numbers of input. Variable inputs can be handled using the `*args` (arguments) or `**kwargs` (keyword arguments) syntax. The `*args` syntax will generate tuple a containing all inputs past the required input list. For example, consider extending the L_p function so that it can accept a set of p values as extra inputs (Note: in practice it would make more sense to accept an array for p).

```python
import numpy as np

def lp_norm(x,y,p = 2, *args):
    d = x - y
    print('The L' + str(p) + ' distance is :', sum(abs(d)**p)**(1/p))
    out = [sum(abs(d)**p)**(1/p)]

    print('Number of *args:', len(args))
    for p in args:
        print('The L' + str(p) + ' distance is :', sum(abs(d)**p)**(1/p))
        out.append(sum(abs(d)**p)**(1/p))

    return tuple(out)


# Call the function
x = np.random.randn(10)
y = np.random.randn(10)
# x & y are required inputs and so are not in *args
lp = lp_norm(x,y)
# Function takes 3 inputs, so no *args
lp = lp_norm(x,y,1)
# Inputs with default values can be ignored
lp = lp_norm(x,y,1,2,3,4,1.5,2.5,0.5)
```

The alternative syntax, `**kwargs`, generates a dictionary with all keyword inputs which are not in the function signature. One reason for using `**kwargs` is to allow a long list of optional inputs without having to have an excessively long function definition. This is how this input mechanism operates in many `matplotlib` functions such as `plot`.

```python
import numpy as np

def lp_norm(x,y,p = 2, **kwargs):
    d = x - y
    print('Number of *kwargs:', len(kwargs))
    for key in kwargs:
        print('Key :', key, ' Value:', kwargs[key])

    return sum(abs(d)**p)

# Call the function
x = np.random.randn(10)
y = np.random.randn(10)
# Inputs with default values can be ignored
lp = lp_norm(x,y,kword1=1,kword2=3.2)
# The p keyword is in the function def, so not in **kwargs
lp = lp_norm(x,y,kword1=1,kword2=3.2,p=0)
```

It is possible to use both `*args` and `**kwargs` in a function definition and their role does not change – `*args` appears in the function as a tuple that contains all extraneous non-keyword inputs, and `**kwargs` appears inside the function as a dictionary that contains all keyword arguments not appearing in the function definition.

Functions with both often have the simple signature `y = f(*args, **kwargs)` which allows for any set of inputs.

17.1.4 The Docstring

The docstring is one of the most important elements of any function – especially a function written for use by others. The docstring is a special string, enclosed with triple-quotation marks, either `'''` or `"""`, which is available using `help()`. When `help(fun)` is called (or `fun?`/`?fun` in IPython), Python looks for the docstring which is placed immediately below the function definition.

```python
import numpy as np

def lp_norm(x,y,p = 2):
    """ The docstring contains any available help for
        the function.  A good docstring should explain the
        inputs and the outputs, provide an example and a list
        of any other related function.
    """
    d = x - y
    return sum(abs(d)**p)
```

Calling `help(lp_norm)` produces

```python
>>> help(lp_norm)
Help on function lp_norm in module __main__:

lp_norm(x, y, p=2)
    The docstring contains any available help for
    the function.  A good docstring should explain the
    inputs and the outputs, provide an example and a list
    of any other related function.
```

This docstring is not a good example. I suggest following the NumPy guidelines, currently available at the NumPy source repository (or search for *numpy docstring*). Also see NumPy example.py These differ from and are more specialized than the standard Python docstring guidelines, and are more appropriate for numerical code. A better docstring for `lp_norm` would be

```python
import numpy as np

def lp_norm(x,y,p = 2):
    r""" Compute the distance between vectors.

    The Lp normed distance is sum(abs(x-y)**p)**(1/p)

    Parameters
    ----------
    x : ndarray
        First argument
    y : ndarray
        Second argument
    p : float, optional
        Power used in distance calculation, >=0

    Returns
    -------
    output : scalar
        Returns the Lp normed distance between x and y

    Notes
```

```
    -----

    For p>=1, returns the Lp norm described above.  For 0<=p<1,
    returns sum(abs(x-y)**p).  If p<0, p is set to 0.

    Examples
    --------
    >>> x=[0,1,2]
    >>> y=[1,2,3]

    L2 norm is the default

    >>> lp_norm(x,y)

    Lp can be computed using the optional third input

    >>> lp_norm(x,y,1)

    """

    if p<0: p=0
    d = x - y

    if p == 0:
        return sum(d != 0)
    elif p < 1:
        return sum(abs(d)**p)
    else:
        return sum(abs(d)**p)**(1/p)
```

Convention is to use triple double-quotes in docstrings, with `r"""` used to indicate "raw" strings, which will ignore backslashes rather than treating them like an escape character (use `u"""` if the docstring contains Unicode text, which is not usually necessary). A complete docstring may contain, in order:

- Parameters - a description of key inputs

- Returns - a description of outputs

- Other Parameters - a description of seldom used inputs

- Raises - an explanation of any exceptions raised. See Section 12.5.

- See also - a list of related functions

- Notes - details of the algorithms or assumptions used

- References - any bibliographic information

- Examples - demonstrates use form console

17.2   Variable Scope

Variable scope determines which functions can access, and possibly modify a variable. Python determines variable scope using two principles: where the variable appears in the file, and whether the variable is inside a function or in the main program. Variables declared inside a function are local variables and are only available to that function. Variables declared outside a function are global variables, and can be accessed but not modified (unless using `global`) . Consider the example which shows that variables at the root of the program that have been declared before a function definition can be printed by that function.

```python
import numpy as np

a, b, c = 1, 3.1415, 'Python'

def scope():
    print(a)
    print(b)
    print(c)
    # print(d) #Error, d has not be declared yet

scope()
d = np.array(1)

def scope2():
    print(a)
    print(b)
    print(c)
    print(d) # Ok now

scope2()

def scope3():
    a = 'Not a number' # Local variable
    print('Inside scope3, a is ', a)

print('a is ',a)
scope3()
print('a is now ',a)
```

Using the name of a global variable inside a function does produce any changes outside of the function. In `scope3`, a is given a different value. That value is specific to the function `scope3` and outside of the function, a will have its global value. Generally, global variables can be accessed, but not modified inside a function. The only exception is when a variable is declared inside the function using the keyword `global`.

```python
import numpy as np

a = 1

def scope_local():
    a = -1
    print('Inside scope_local, a is ',a)

def scope_global():
    global a
    a = -10
    print('Inside scope_global, a is ',a)

print('a is ',a)
scope_local()
print('a is now ',a)
scope_global()
print('a is now ',a)
```

One word of caution: a variable name cannot be used as a local and global variable in the same function. Attempting to access the variable as a global (e.g. for printing) and then locally assign the variable produces an error.

17.3   Example: Least Squares with Newey-West Covariance

Estimating cross-section regressions using time-series data is common practice. When regressors are persistent, and errors are not white noise, standard inference, including White standard errors, is no longer consistent. The most common solution is to use a long-run covariance estimator, and the most common long-run covariance estimator is known as the Newey-West covariance estimator which uses a Bartlett kernel applied to the auto-covariances of the scores. This example produces a function which returns parameter estimates, the estimated asymptotic covariance matrix of the parameters, the variance of the regression error, the R^2, and adjusted R^2 and the fit values (or errors, since actual is equal to fit plus errors). These are computed using a T-vector for the regressand (dependent variable), a T by k matrix for the regressors, an indicator for whether to include a constant in the model (default True), and the number of lags to include in the long-run covariance (default behavior is to automatically determine based on sample size). The steps required to produce the function are:

1. Determine the size of the variables

2. Append a constant, if needed

3. Compute the regression coefficients

4. Compute the errors

5. Compute the covariance or the errors

6. Compute the covariance of the parameters

7. Compute the R^2 and $\bar{R}^2$

The function definition is simple and allows for up to 4 inputs, where 2 have default values: `def olsnw(y, X, constant=True, lags=None):`. The size of the variables is then determined using `size` and the constant is prepended to the regressors, if needed, using `hstack`. The regression coefficients are computed using `lstsq`, and then the Newey-West covariance is computed for both the errors and scores. The covariance of the parameters is then computed using the NW covariance of the scores. Finally the R^2 and $\bar{R}^2$ are computed. A complete code listing is presented in the appendix to this chapter.

17.4   Anonymous Functions

Python supports anonymous functions using the keyword `lambda`. Anonymous functions are usually encountered when another function expects a function as an input *and* a simple function will suffice. Anonymous function take the generic form `lambda` $a,b,c,\ldots:code\ using\ a,b,c$. The key elements are the keyword `lambda`, a list of comma separated inputs, a colon between the inputs and the actual function code. For example `lambda x,y:x+y` would return the sum of the variables `x` and `y`.

   Anonymous functions are simple but useful. For example, when lists contain other lists it isn't directly possible to sort on an arbitrary element of the nested list. Anonymous functions allow sorting through the keyword argument `key` by returning the element Python should use to sort. In this example, a direct call to `sort()` will sort on the first element (first name). Using the anonymous function `lambda x:x[1]` to return the second element of the tuple allows for sorting on the last name. `lambda x:x[2]` would allow for sorting on the University.

```
>>> nested = [('John','Doe','Oxford'),\
...           ('Jane','Dearing','Cambridge'),\
...           ('Jerry','Dawn','Harvard')]
```

```
>>> nested.sort()
>>> nested
[('Jane', 'Dearing', 'Cambridge'),
 ('Jerry', 'Dawn', 'Harvard'),
 ('John', 'Doe', 'Oxford')]

>>> nested.sort(key=lambda x:x[1])
>>> nested
[('Jerry', 'Dawn', 'Harvard'),
 ('Jane', 'Dearing', 'Cambridge'),
 ('John', 'Doe', 'Oxford')]
```

17.5 Modules

The previous examples all included the function in the same Python as the main program. While this is conve-
nient, especially when coding the function, it hinders use in other code. Modules allow multiple functions to be
combined in a single Python file and accessed using `import` *module* and then *module.function* syntax. Suppose
a file named core.py contains the following code:

```
r"""Demonstration module.
This is the module docstring.
"""

def square(x):
    r"""Returns the square of a scalar input
    """
    return x*x

def cube(x):
    r"""Returns the cube of a scalar input
    """
    return x*x*x
```

The functions `square` and `cube` can be accessed by other files in the same directory using

```
import core

y = -3
print(core.square(y))
print(core.cube(y))
```

The functions in core.py can be imported using any of the standard import methods: `import core as c`,
`from core import square` or `from core import *` in which case both functions could be directly accessed.

17.5.1 __main__

Normally modules should only have code required for the module to run, and other code should reside in a
different function. However, it is possible that a module could be both directly importable and also directly
runnable. If this is the case, it is important that the directly runnable code should not be executed when the
module is imported by other code. This can be accomplished using a special construct, `if __name__ ==`
`"__main__":` before any code that should execute when the module is run as a standalone program. Consider
the following simple example in a module named `test.py`.

```
def square(x):
    return x**2

if __name__ == "__main__":
```

```
    print('Program called directly.')
else:
    print('Program called indirectly using name: ', __name__)
```

Running and importing `test` cause the different paths to be executed.

```
>>> %run test.py
Program called directly.

>>> import test
Program called indirectly using name:  test
```

17.6 Packages

As a modules grows, organizing large amounts of code a single file – especially code that serve very different purposes – becomes difficult. Packages solve this problem by allowing multiple files to exist in the same namespace, as well as sub-namespaces. Python packages are constructed using directory structures using a special file name: __init__.py. A Python package begins with a file folder using the name of the package. For example, consider developing a package called metrics which will contain common econometrics routines. The minimal package structure would have

```
metrics/
    __init__.py
```

The __init__.py file instructs Python to treat this directory as part of a package. __init__.py is a standard Python file, although it is not necessary to include any code in this file. However, code included in __init__.py will appear in the root of the package namespace. Suppose __init__.py contained a function with the name `reg`. Assuming `import core` was used to import the module, this function would be accessible as `core.reg`. Next, suppose other Python files are included in the directory under core, so that the directory structure looks like

```
core/
    __init__.py
    crosssection.py
    timeseries.py
```

This would allow functions to be directly included the core namespace by including the function in __init__.py. Functions that resided in crosssection.py would be accessible using `import core.crosssection as cs` and then `cs.reg`.

Finally, suppose that crosssection.py was replaced with a directory where the directory contained other Python files, including __init__.py.

```
core/
    __init__.py
    crosssection/
        __init__.py
        regression.py
        limdep.py
    timeseries/
        __init__.py
        arma.py
        var.py
```

This structure allows functions to be accessible directly from `core` using the __init__.py file, accessible from `core.crosssection` using the __init__.py located in the directory crosssection or accessible using `core.crosssection.re` for functions inside the file regression.py.

__init__.py is useful in Python packages beyond simply instructing Python that a directory is part of a package. It can be used to initialize any common information required by functions in the module or to "fake" the

location of a deeply nested functions. __init__.py is executed whenever a package is imported, and since it can contain standard Python code, it is possible define variables in the package namespace or execute code which will be commonly used by functions in the module (e.g. reading a config file). Suppose that the __init__.py located in the directory core contains

```
from core.crosssection.regression import *
```

This single import will make all functions in the file regression.py available directly after running `import core`. For example, suppose regression.py contains the function `leastsquares`. Without the import statement in __init__.py, `leastsquares` would only be available through `core.crosssection.regression`. However, after including the `import` statement in __init__.py, `leastsquares` is directly accessible from `core`. Using __init__.py allows for a flexible file and directory structure that reflects the code's function while avoiding complex import statements.

17.7 PYTHONPATH

While it is simple to reference files in the same current working directory, this behavior is undesirable for code shared between multiple projects. The PYTHONPATH allows directories to be added so that they are automatically searched if a matching module cannot be found in the current directory. The current path can be checked by running

```
>>> import sys
>>> sys.path
```

Additional directories can be added at runtime using

```
import sys

# New directory is first to be searched
sys.path.insert(0, 'c:\\path\\to\add')
# New directory is last to be searched
sys.path.append('c:\\path\\to\add')
```

Directories can also be added permanently by adding or modifying the environment variable PYTHONPATH. On Windows, the System environment variables can be found in My Computer > Properties > Advanced System Settings > Environment Variables. PYTHONPATH should be a System Variable. If it is present, it can be edited, and if not, added. The format of PYTHONPATH is

```
c:\dir1;c:\dir2;c:\dir2\dir3;
```

which will add 3 directories to the path. On Linux, PYTHONPATH is stored in either ~/.bash_rc or ~/.bash_profile, and it should resemble

```
PYTHONPATH="${PYTHONPATH}:/dir1/:/dir2/:/dir2/dir3/"
export PYTHONPATH
```

after three directories have been added, using : as a separator between directories. On OSX the PYTHONPATH is stored in ~/.profile.

17.8 Python Coding Conventions

There are a number of common practices which can be adopted to produce Python code which looks more like code found in other modules:

1. Use 4 spaces to indent blocks – avoid using tab, except when an editor automatically converts tabs to 4 spaces

2. Avoid more than 4 levels of nesting, if possible

3. Limit lines to 79 characters. The \ symbol can be used to break long lines

4. Use two blank lines to separate functions, and one to separate logical sections in a function.

5. Use ASCII mode in text editors, not UTF-8

6. One module per import line

7. Avoid `from` *module* `import` `*` (for any module). Use either `from` *module* `import` *func1, func2* or `import` *module* `as` *shortname*.

8. Follow the NumPy guidelines for documenting functions

More suggestions can be found in PEP8.

17.9 Exercises

1. Write a function which takes an array with T elements contains categorical data (e.g. 1,2,3), and returns a T by C array of indicator variables where C is the number of unique values of the categorical variable, and each column of the output is an indicator variable (0 or 1) for whether the input data belonged to that category. For example, if $x = [1\,2\,1\,1\,2]$, then the output is

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The function should provide a second output containing the categories (e.g. $[1\,2]$ in the example).

2. Write a function which takes a T by K array X, a T by 1 array y, and a T by T array Ω are computes the GLS parameter estimates. The function definition should be
   `def gls(X, y, Omega = None)`
   and if Ω is not provided, an identity matrix should be used.

3. Write a function which will compute the partial correlation. Lower partial correlation is defined as

$$\frac{\sum_{\mathcal{S}} (r_{i,1} - \bar{r}_{1,\mathcal{S}})(r_{i,2} - \bar{r}_{2,\mathcal{S}})}{\sum_{\mathcal{S}} (r_{j,1} - \bar{r}_{1,\mathcal{S}})^2 \sum_{\mathcal{S}} (r_{k,2} - \bar{r}_{2,\mathcal{S}})^2}$$

where $\mathcal{S}$ is the set where $r_{1,i}$ and $r_{2,i}$ are both less than their (own) quantile q. Upper partial correlation uses returns greater than quantile q. The function definition should have definition
   `def partial_corr(x, y=None, quantile = 0.5, tail = 'Lower')`
   and should take either a T by K array for x, or T by 1 arrays for x and y. If x is T by K, then y is ignored and the partial correlation should be computed pairwise. `quantile` determines the quantile to use for the cut off. Note: if $\mathcal{S}$ is empty or has 1 element, `nan` should be returned. `tail` is either `'Lower'` or `'Upper'`, and determined whether the lower or upper tail is used. The function should return both the partial correlation matrix (K by K), and the number of observations used in computing the partial correlation.

17.A   Listing of econometrics.py

The complete code listing of `econometrics`, which contains the function `olsnw`, is presented below.

```python
from numpy import mat, asarray, mean, size, shape, hstack, ones, ceil, \
    zeros, arange
from numpy.linalg import inv, lstsq

def olsnw(y, X, constant=True, lags=None):
    r""" Estimation of a linear regression with Newey-West covariance

    Parameters
    ----------
    y : array_like
        The dependent variable (regressand).  1-dimensional with T elements.
    X : array_like
        The independent variables (regressors). 2-dimensional with sizes T
        and K.  Should not include a constant.
    constant: bool, optional
        If true (default) includes model includes a constant.
    lags: int or None, optional
        If None, the number of lags is set to 1.2*T**(1/3), otherwise the
        number of lags used in the covariance estimation is set to the value
        provided.

    Returns
    -------
    b : ndarray, shape (K,) or (K+1,)
        Parameter estimates.  If constant=True, the first value is the
        intercept.
    vcv : ndarray, shape (K,K) or (K+1,K+1)
        Asymptotic covariance matrix of estimated parameters
    s2 : float
        Asymptotic variance of residuals, computed using Newey-West variance
        estimator.
    R2 : float
        Model R-square
    R2bar : float
        Adjusted R-square
    e : ndarray, shape (T,)
        Array containing the model errors

    Notes
    -----
    The Newey-West covariance estimator applies a Bartlett kernel to estimate
    the long-run covariance of the scores.  Setting lags=0 produces White's
    Heteroskedasticity Robust covariance matrix.

    See also
    --------
    np.linalg.lstsq

    Example
    -------
    >>> X = randn(1000,3)
    >>> y = randn(1000)
    >>> b,vcv,s2,R2,R2bar = olsnw(y, X)

    Exclude constant:
```

```python
>>> b,vcv,s2,R2,R2bar = olsnw(y, X, False)

Specify number of lags to use:

>>> b,vcv,s2,R2,R2bar = olsnw(y, X, lags = 4)

"""

T = y.size
if size(X, 0) != T:
    X = X.T

T,K = shape(X)
if constant:
    X = copy(X)
    X = hstack((ones((T,1)),X))
    K = size(X,1)

if lags is None:
    lags = int(ceil(1.2 * float(T)**(1.0/3)))

# Parameter estimates and errors

out = lstsq(X,y)
b = out[0]
e = y - X @ b

# Covariance of errors
gamma = zeros((lags+1))
for lag in range(lags+1):
    gamma[lag] = (e[:T-lag] @ e[lag:]) / T

w = 1 - arange(0,lags+1)/(lags+1)
w[0] = 0.5
s2 = gamma @ (2*w)

# Covariance of parameters
Xe = mat(zeros(shape(X)))
for i in range(T):
    Xe[i] = X[i] * float(e[i])

Gamma = zeros((lags+1,K,K))
for lag in range(lags+1):
    Gamma[lag] = Xe[lag:].T*Xe[:T-lag]

Gamma = Gamma/T

S = Gamma[0].copy()
for i in range(1,lags+1):
    S = S + w[i]*(Gamma[i]+Gamma[i].T)

XpX = (X.T @ X)/T
XpXi = inv(XpX)
vcv = mat(XpXi)*S*mat(XpXi)/T
vcv = asarray(vcv)

# R2, centered or uncentered
if constant:
```

```
        R2 = (e @ e) / (y-mean(y) @ y-mean(y))
    else:
        R2 = (e @ e) / (y @ y)

    R2bar = 1-R2*(T-1)/(T-K)
    R2 = 1 - R2

    return b,vcv,s2,R2,R2bar,e
```

Chapter 18

Probability and Statistics Functions

This chapter is divided into two main parts, one for NumPy and one for SciPy. Both packages contain important functions for simulation, probability distributions and statistics.

NumPy

18.1   Simulating Random Variables

18.1.1   Core Random Number Generators

NumPy random number generators are all stored in the module `numpy.random`. These can be imported with using `import numpy as np` and then calling `np.random.rand`, for example, or by importing `import numpy.random as rnd` and using `rnd.rand`.[1]

rand, random_sample

`rand` and `random_sample` are uniform random number generators which are identical except that `rand` takes a variable number of integer inputs – one for each dimension – while `random_sample` takes a *n*-element tuple. `random_sample` is the preferred NumPy function, and `rand` is a convenience function primarily for MATLAB users.

```
>>> x = rand(3,4,5)
>>> y = random_sample((3,4,5))
```

randn, standard_normal

`randn` and `standard_normal` are standard normal random number generators. `randn`, like `rand`, takes a variable number of integer inputs, and `standard_normal` takes an *n*-element tuple. Both can be called with no arguments to generate a single standard normal (e.g. `randn()`). `standard_normal` is the preferred NumPy function, and `randn` is a convenience function primarily for MATLAB users .

```
>>> x = randn(3,4,5)
>>> y = standard_normal((3,4,5))
```

---

[1]Other import methods can also be used, such as `from numpy.random import rand` and then calling `rand`.

`randint`

`randint` is a uniform integer random number generators which take 3 inputs, low, high and size. Low is the lower bound of the integers generated, high is the upper and size is a *n*-element tuple. `randint` and differ in that `randint` generates integers exclusive of the value in high (as do most Python functions, e.g., `range` and `np.arange`).

```
>>> x = randint(0,10,(100))
>>> x.max() # Is 9 since range is [0,10)
9
```

`random_integers` is a similar function that treats the upper end point differently. It has been deprecated and so should not be used as an alternative to `randint`.

18.1.2 Random Array Functions

`shuffle`

`shuffle` randomly reorders the elements of an array *in place*.

```
>>> x = arange(10)
>>> shuffle(x)
>>> x
array([4, 6, 3, 7, 9, 0, 2, 1, 8, 5])
```

`permutation`

`permutation` returns randomly reordered elements of an array as a copy while not directly changing the input.

```
>>> x = arange(10)
>>> permutation(x)
array([2, 5, 3, 0, 6, 1, 9, 8, 4, 7])

>>> x
array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

18.1.3 Select Random Number Generators

NumPy provides a large selection of random number generators for specific distribution. All take between 0 and 2 required inputs which are parameters of the distribution, plus a tuple containing the size of the output. All random number generators are in the module `numpy.random`.

Bernoulli

There is no Bernoulli generator. Instead use `binomial(1,p)` to generate a single draw or `binomial(1,p,(10,10))` to generate an array where `p` is the probability of success.

beta

`beta(a,b)` generates a draw from the Beta(a,b) distribution. `beta(a,b,(10,10))` generates a 10 by 10 array of draws from a Beta(a,b) distribution.

binomial

`binomial(n,p)` generates a draw from the Binomial(n, p) distribution. `binomial(n,p,(10,10))` generates a 10 by 10 array of draws from the Binomial(n, p) distribution.

chisquare

`chisquare(nu)` generates a draw from the χ^2_ν distribution, where ν is the degree of freedom. `chisquare(nu, (10,10))` generates a 10 by 10 array of draws from the χ^2_ν distribution.

exponential

`exponential()` generates a draw from the Exponential distribution with scale parameter $\lambda = 1$. `exponential(lambda, (10,10))` generates a 10 by 10 array of draws from the Exponential distribution with scale parameter λ.

f

`f(v1,v2)` generates a draw from the distribution F_{v_1, v_2} distribution where v_1 is the numerator degree of freedom and v_2 is the denominator degree of freedom. `f(v1,v2,(10,10))` generates a 10 by 10 array of draws from the F_{v_1, v_2} distribution.

gamma

`gamma(a)` generates a draw from the Gamma$(\alpha, 1)$ distribution, where α is the shape parameter. `gamma(a, theta, (10,10))` generates a 10 by 10 array of draws from the Gamma(α, θ) distribution where θ is the scale parameter.

laplace

`laplace()` generates a draw from the Laplace (Double Exponential) distribution with centered at 0 and unit scale. `laplace(loc, scale, (10,10))` generates a 10 by 10 array of Laplace distributed data with location `loc` and scale `scale`. Using `laplace(loc, scale)` is equivalent to calling `loc + scale*laplace()`.

lognormal

`lognormal()` generates a draw from a Log-Normal distribution with $\mu = 0$ and $\sigma = 1$. `lognormal(mu, sigma, (10,10))` generates a 10 by 10 array or Log-Normally distributed data where the underlying Normal distribution has mean parameter μ and scale parameter σ.

multinomial

`multinomial(n, p)` generates a draw from a multinomial distribution using n trials and where each outcome has probability p, a k-element array where $\Sigma_{i=1}^{k} p = 1$. Note that p must be an array or other iterable value. The output is a k-element array containing the number of successes in each category. `multinomial(n, p, (10,10))` generates a 10 by 10 by k array of multinomially distributed data with n trials and probabilities p.

multivariate_normal

`multivariate_normal(mu, Sigma)` generates a draw from a multivariate Normal distribution with mean μ (k-element array) and covariance Σ (k by k array). `multivariate_normal(mu, Sigma, (10,10))` generates a 10 by 10 by k array of draws from a multivariate Normal distribution with mean μ and covariance Σ.

negative_binomial

`negative_binomial(n, p)` generates a draw from the Negative Binomial distribution where n is the number of failures before stopping and p is the success rate. `negative_binomial(n, p, (10, 10))` generates a 10 by 10 array of draws from the Negative Binomial distribution where n is the number of failures before stopping and p is the success rate.

normal

`normal()` generates draws from a standard Normal (Gaussian). `normal(mu, sigma)` generates draws from a Normal with mean μ and standard deviation σ. `normal(mu, sigma, (10,10))` generates a 10 by 10 array of draws from a Normal with mean μ and standard deviation σ. `normal(mu, sigma)` is equivalent to `mu + sigma * standard_normal()`.

poisson

`poisson()` generates a draw from a Poisson distribution with $\lambda = 1$. `poisson(lambda)` generates a draw from a Poisson distribution with expectation λ. `poisson(lambda, (10,10))` generates a 10 by 10 array of draws from a Poisson distribution with expectation λ.

standard_t

`standard_t(nu)` generates a draw from a Student's t with shape parameter ν. `standard_t(nu, (10,10))` generates a 10 by 10 array of draws from a Student's t with shape parameter ν.

uniform

`uniform()` generates a uniform random variable on $(0,1)$. `uniform(low, high)` generates a uniform on (l,h). `uniform(low, high, (10,10))` generates a 10 by 10 array of uniforms on (l,h).

18.2   Simulation and Random Number Generation

Computer simulated random numbers are usually constructed from very complex but ultimately deterministic functions. Because they are not actually random, simulated random numbers are generally described to as pseudo-random. All pseudo-random numbers in NumPy use one core random number generator based on the Mersenne Twister, a generator which can produce a very long series of pseudo-random data before repeating (up to $2^{19937} - 1$ non-repeating values).

RandomState

`RandomState` is the class used to control the random number generators. Multiple generators can be initialized by `RandomState`.

```
>>> gen1 = np.random.RandomState()
>>> gen2 = np.random.RandomState()
>>> gen1.uniform() # Generate a uniform
0.6767614077579269

>>> state1 = gen1.get_state()
>>> gen1.uniform()
0.6046087317893271

>>> gen2.uniform() # Different, since gen2 has different seed
0.04519705909244154

>>> gen2.set_state(state1)
>>> gen2.uniform() # Same uniform as gen1 after assigning state
0.6046087317893271
```

18.2.1 State

Pseudo-random number generators track a set of values known as the state. The state is usually a vector which has the property that if two instances of the same pseudo-random number generator have the same state, the sequence of pseudo-random numbers generated will be identical. The state of the default random number generator can be read using `numpy.random.get_state` and can be restored using `numpy.random.set_state`.

```
>>> st = get_state()
>>> randn(4)
array([ 0.37283499,  0.63661908, -1.51588209, -1.36540624])

>>> set_state(st)
>>> randn(4)
array([ 0.37283499,  0.63661908, -1.51588209, -1.36540624])
```

The two sequences are identical since they the state is the same when `randn` is called. The state is a 5-element tuple where the second element is a 625 by 1 vector of unsigned 32-bit integers. In practice the state should only be stored using `get_state` and restored using `set_state`.

get_state

`get_state()` gets the current state of the random number generator, which is a 5-element tuple. It can be called as a function, in which case it gets the state of the default random number generator, or as a method on a particular instance of `RandomState`.

set_state

`set_state(state)` sets the state of the random number generator. It can be called as a function, in which case it sets the state of the default random number generator, or as a method on a particular instance of `RandomState`. `set_state` should generally only be called using a state tuple returned by `get_state`.

18.2.2 Seed

`numpy.random.seed` is a more useful function for initializing the random number generator, and can be used in one of two ways. `seed()` will initialize (or reinitialize) the random number generator using some actual random data provided by the operating system.[2] `seed(s)` takes a vector of values (can be scalar) to initialize

---

[2]All modern operating systems collect data that is effectively random by collecting noise from device drivers and other system monitors.

the random number generator at particular state. `seed(s)` is particularly useful for producing simulation studies which are reproducible. In the following example, calls to `seed()` produce different random numbers, since these reinitialize using random data from the computer, while calls to `seed(0)` produce the same (sequence) of random numbers.

```
>>> seed()
>>> randn()
array([ 0.62968838])

>>> seed()
>>> randn()
array([ 2.230155])

>>> seed(0)
>>> randn()
array([ 1.76405235])

>>> seed(0)
>>> randn()
array([ 1.76405235])
```

NumPy always calls `seed()` when the first random number is generated. As a result. calling `standard_normal()` across two "fresh" sessions will not produce the same random number.

seed

`seed(value)` uses *value* to seed the random number generator. `seed()` takes actual random data from the operating system when initializing the random number generator (e.g. /dev/random on Linux, or CryptGenRandom in Windows).

18.2.3 Replicating Simulation Data

It is important to have reproducible results when conducting a simulation study. There are two methods to accomplish this:

1. Call `seed()` and then `state = get_state()`, and save `state` to a file which can then be loaded in the future when running the simulation study.

2. Call `seed(s)` at the start of the program (where *s* is a constant).

Either of these will allow the same sequence of random numbers to be used.

Warning: Do not *over-initialize* the pseudo-random number generators. The generators should be initialized once per session and then allowed to produce the pseudo-random sequence. Repeatedly re-initializing the pseudo-random number generators will produce a sequence that is decidedly less random than the generator was designed to provide.

Considerations when Running Simulations on Multiple Computers

Simulation studies are ideally suited to parallelization, although parallel code makes reproducibility more difficult. There are 2 methods which can ensure that a parallel study is reproducible.

1. Have a single process produce all of the random numbers, where this process has been initialized using one of the two methods discussed in the previous section. Formally this can be accomplished by pre-generating all random numbers, and then passing these into the simulation code as a parameter, or equivalently by pre-generating the data and passing the state into the function. Inside the simulation

function, the random number generator will be set to the state which was passed as a parameter. The latter is a better option if the amount of data per simulation is large.

2. Seed each parallel worker independently, and then return the state from the simulation function along with the simulation results. Since the state is saved for each simulation, it is possible to use the same state if repeating the simulation using, for example, a different estimator.

18.3 Statistics Functions

mean

mean computes the average of an array. An optional second argument provides the axis to use (default is to use entire array). mean can be used either as a function or as a method on an array.

```
>>> x = arange(10.0)
>>> x.mean()
4.5

>>> mean(x)
4.5

>>> x= reshape(arange(20.0),(4,5))
>>> mean(x,0)
array([ 7.5,   8.5,   9.5,  10.5,  11.5])

>>> x.mean(1)
array([ 2.,   7.,  12.,  17.])
```

median

median computed the median value in an array. An optional second argument provides the axis to use (default is to use entire array).

```
>>> x= randn(4,5)
>>> x
array([[-0.74448693, -0.63673031, -0.40608815,  0.40529852, -0.93803737],
       [ 0.77746525,  0.33487689,  0.78147524, -0.5050722 ,  0.58048329],
       [-0.51451403, -0.79600763,  0.92590814, -0.53996231, -0.24834136],
       [-0.83610656,  0.29678017, -0.66112691,  0.10792584, -1.23180865]])

>>> median(x)
-0.45558017286810903

>>> median(x, 0)
 array([-0.62950048, -0.16997507,  0.18769355, -0.19857318, -0.59318936])
```

Note that when an array or axis dimension contains an even number of elements (n), median returns the average of the 2 inner elements.

std

std computes the standard deviation of an array. An optional second argument provides the axis to use (default is to use entire array). std can be used either as a function or as a method on an array.

var

var computes the variance of an array. An optional second argument provides the axis to use (default is to use entire array). var can be used either as a function or as a method on an array.

corrcoef

corrcoef(x) computes the correlation between the rows of a 2-dimensional array x. corrcoef(x, y) computes the correlation between two 1- dimensional vectors. An optional keyword argument rowvar can be used to compute the correlation between the columns of the input – this is corrcoef(x, rowvar=False) and corrcoef(x.T) are identical.

```
>>> x= randn(3,4)
>>> corrcoef(x)
array([[ 1.        ,  0.36780596,  0.08159501],
       [ 0.36780596,  1.        ,  0.66841624],
       [ 0.08159501,  0.66841624,  1.        ]])

>>> corrcoef(x[0],x[1])
array([[ 1.        ,  0.36780596],
       [ 0.36780596,  1.        ]])

>>> corrcoef(x, rowvar=False)
array([[ 1.        , -0.98221501, -0.19209871, -0.81622298],
       [-0.98221501,  1.        ,  0.37294497,  0.91018215],
       [-0.19209871,  0.37294497,  1.        ,  0.72377239],
       [-0.81622298,  0.91018215,  0.72377239,  1.        ]])

>>> corrcoef(x.T)
array([[ 1.        , -0.98221501, -0.19209871, -0.81622298],
       [-0.98221501,  1.        ,  0.37294497,  0.91018215],
       [-0.19209871,  0.37294497,  1.        ,  0.72377239],
       [-0.81622298,  0.91018215,  0.72377239,  1.        ]])
```

cov

cov(x) computes the covariance of an array x. cov(x,y) computes the covariance between two 1-dimensional vectors. An optional keyword argument rowvar can be used to compute the covariance between the columns of the input – this is cov(x, rowvar=False) and cov(x.T) are identical.

histogram

histogram can be used to compute the histogram (empirical frequency, using k bins) of a set of data. An optional second argument provides the number of bins. If omitted, $k = 10$ bins are used. histogram returns two outputs, the first with a k-element vector containing the number of observations in each bin, and the second with the $k + 1$ endpoints of the k bins.

```
>>> x = randn(1000)
>>> count, binends = histogram(x)
>>> count
array([  7,  27,  68, 158, 237, 218, 163,  79,  36,   7])

>>> binends
array([-3.06828057, -2.46725067, -1.86622077, -1.26519086, -0.66416096,
       -0.06313105,  0.53789885,  1.13892875,  1.73995866,  2.34098856,
        2.94201846])
```

```
>>> count, binends = histogram(x, 25)
```

histogram2d

`histogram2d(x,y)` computes a 2-dimensional histogram for 1-dimensional vectors. An optional keyword argument `bins` provides the number of bins to use. `bins` can contain either a single scalar integer or a 2-element list or array containing the number of bins to use in each dimension.

SciPy

SciPy provides an extended range of random number generators, probability distributions and statistical tests.

```
import scipy
import scipy.stats as stats
```

18.4 Continuous Random Variables

SciPy contains a large number of functions for working with continuous random variables. Each function resides in its own class (e.g. `norm` for Normal or `gamma` for Gamma), and classes expose methods for random number generation, computing the PDF, CDF and inverse CDF, fitting parameters using MLE, and computing various moments. The methods are listed below, where *dist* is a generic placeholder for the distribution name in SciPy. While the functions available for continuous random variables vary in their inputs, all take 3 generic arguments:

1. `*args` a set of distribution specific non-keyword arguments. These must be entered in the order listed in the class docstring. For example, when using a *F*-distribution, two arguments are needed, one for the numerator degree of freedom, and one for the denominator degree of freedom.

2. `loc` a location parameter, which determines the center of the distribution.

3. `scale` a scale parameter, which determine the scaling of the distribution. For example, if *z* is a standard normal, then $s \times z$ is a scaled standard normal.

dist.rvs

Pseudo-random number generation. Generically, `rvs` is called using *dist*`.rvs(*args, loc=0, scale=1, size=size)` where `size` is an *n*-element tuple containing the size of the array to be generated.

dist.pdf

Probability density function evaluation for an array of data (element-by-element). Generically, `pdf` is called using *dist*`.pdf(x, *args, loc=0, scale=1)` where `x` is an array that contains the values to use when evaluating PDF.

dist.logpdf

Log probability density function evaluation for an array of data (element-by-element). Generically, `logpdf` is called using *dist*`.logpdf(x, *args, loc=0, scale=1)` where `x` is an array that contains the values to use when evaluating log PDF.

dist.cdf

Cumulative distribution function evaluation for an array of data (element-by-element). Generically, cdf is called using *dist*.cdf(x, *args, loc=0, scale=1) where x is an array that contains the values to use when evaluating CDF.

dist.ppf

Inverse CDF evaluation (also known as percent point function) for an array of values between 0 and 1. Generically, ppf is called using *dist*.ppf(p, *args, loc=0, scale=1) where p is an array with all elements between 0 and 1 that contains the values to use when evaluating inverse CDF.

dist.fit

Estimate shape, location, and scale parameters from data by maximum likelihood using an array of data. Generically, fit is called using *dist*.fit(data, *args, floc=0, fscale=1) where data is a data array used to estimate the parameters. floc forces the location to a particular value (e.g. floc=0). fscale similarly forces the scale to a particular value (e.g. fscale=1) . It is necessary to use floc and/or fscale when computing MLEs if the distribution does not have a location and/or scale. For example, the gamma distribution is defined using 2 parameters, often referred to as shape and scale. In order to use ML to estimate parameters from a gamma, floc=0 must be used.

dist.median

Returns the median of the distribution. Generically, median is called using *dist*.median(*args, loc=0, scale=1).

dist.mean

Returns the mean of the distribution. Generically, mean is called using *dist*.mean(*args, loc=0, scale=1).

dist.moment

n^{th} non-central moment evaluation of the distribution. Generically, moment is called using *dist*.moment(r, *args, loc=0, scale=1) where r is the order of the moment to compute.

dist.varr

Returns the variance of the distribution. Generically, var is called using *dist*.var(*args, loc=0, scale=1).

dist.std

Returns the standard deviation of the distribution. Generically, std is called using *dist*.std(*args, loc=0, scale=1).

18.4.1 Example: gamma

The gamma distribution is used as an example. The gamma distribution takes 1 shape parameter *a* (*a* is the only element of *args), which is set to 2 in all examples.

```
>>> import scipy.stats as stats
>>> gamma = stats.gamma
>>> gamma.mean(2), gamma.median(2), gamma.std(2), gamma.var(2)
 (2.0, 1.6783469900166608, 1.4142135623730951, 2.0)

>>> gamma.moment(2,2) - gamma.moment(1,2)**2 # Variance
2

>>> gamma.cdf(5, 2), gamma.pdf(5, 2)
(0.95957231800548726, 0.033689734995427337)

>>> gamma.ppf(.95957231800548726, 2)
5.0000000000000018

>>> log(gamma.pdf(5, 2)) - gamma.logpdf(5, 2)
0.0

>>> gamma.rvs(2, size=(2,2))
array([[ 1.83072394,  2.61422551],
       [ 1.31966169,  2.34600179]])

>>> gamma.fit(gamma.rvs(2, size=(1000)), floc = 0) # a, 0, shape
(2.209958533078413, 0, 0.89187262845460313)
```

18.4.2   Important Distributions

SciPy provides classes for a large number of distribution. The most important are listed in the table below, along with any required arguments (shape parameters). All classes can be used with the keyword arguments `loc` and `scale` to set the location and scale, respectively. The default location is 0 and the default scale is 1. Setting `loc` to something other than 0 is equivalent to adding `loc` to the random variable. Similarly setting `scale` to something other than 0 is equivalent to multiplying the variable by `scale`.

Distribution Name	SciPy Name	Required Arguments	Notes
Normal	`norm`		Use `loc` to set mean (μ), `scale` to set std. dev. (σ)
Beta(a,b)	`beta`	a: a, b: b	
Cauchy	`cauchy`		
χ^2_ν	`chi2`	ν: df	
Exponential(λ)	`expon`		Use `scale` to set shape parameter (λ)
Exponential Power	`exponpow`	shape: b	Nests normal when b=2, Laplace when b=1
F(ν_1, ν_2)	`f`	ν_1: dfn, ν_2: dfd	
Gamma(a,b)	`gamma`	a: a	Use `scale` to set scale parameter (b)
Laplace, Double Exponential	`laplace`		Use `loc` to set mean (μ), `scale` to set std. dev. (σ)
Log Normal(μ, σ^2)	`lognorm`	σ: s	Use `scale` to set μ where `scale`=`exp(mu)`
Student's-t_ν	`t`	ν: df	

18.4.3   Frozen Random Variable Object

Random variable objects can be used in one of two ways:

1. Calling the class along with any shape, location and scale parameters, simultaneously with the method. For example `gamma(1, scale=2).cdf(1)`.

2. Initializing the class with any shape, location and scale arguments and assigning a variable name. Using the assigned variable name with the method. For example:

```
>>> g = scipy.stats.gamma(1, scale=2)
>>> g.cdf(1)
0.39346934028736652
```

The second method is known as using a frozen random variable object. If the same distribution (with fixed parameters) is repeatedly used, frozen objects can be used to save typing potentially improve performance since frozen objects avoid re-initializing the class.

18.5 Select Statistics Functions

mode

`mode` computes the mode of an array. An optional second argument provides the axis to use (default is to use entire array). Returns two outputs: the first contains the values of the mode, the second contains the number of occurrences.

```
>>> x=randint(1,11,1000)
>>> stats.mode(x)
(array([ 4.]), array([ 112.]))
```

moment

`moment` computed the rth central moment for an array. An optional second argument provides the axis to use (default is to use entire array).

```
>>> x = randn(1000)
>>> moment = stats.moment
>>> moment(x,2) - moment(x,1)**2
0.94668836546169166

>>> var(x)
0.94668836546169166

>>> x = randn(1000,2)
>>> moment(x,2,0) # axis 0
array([ 0.97029259,  1.03384203])
```

skew

`skew` computes the skewness of an array. An optional second argument provides the axis to use (default is to use entire array).

```
>>> x = randn(1000)
>>> skew = stats.skew
>>> skew(x)
0.027187705042705772

>>> x = randn(1000,2)
>>> skew(x,0)
array([ 0.05790773, -0.00482564])
```

kurtosis

`kurtosis` computes the *excess* kurtosis (actual kurtosis minus 3) of an array. An optional second argument provides the axis to use (default is to use entire array). Setting the keyword argument `fisher=False` will compute the actual kurtosis.

```
>>> x = randn(1000)
>>> kurtosis = stats.kurtosis
>>> kurtosis(x)
 -0.2112381820194531

>>> kurtosis(x, fisher=False)
2.788761817980547

>>> kurtosis(x, fisher=False) - kurtosis(x) # Must be 3
3.0

>>> x = randn(1000,2)
>>> kurtosis(x,0)
array([-0.13813704, -0.08395426])
```

pearsonr

`pearsonr` computes the Pearson correlation between two 1-dimensional vectors. It also returns the 2-tailed p-value for the null hypothesis that the correlation is 0.

```
>>> x = randn(10)
>>> y = x + randn(10)
>>> pearsonr = stats.pearsonr
>>> corr, pval = pearsonr(x, y)
>>> corr
0.40806165708698366

>>> pval
0.24174029858660467
```

spearmanr

`spearmanr` computes the Spearman correlation (rank correlation). It can be used with a single 2-dimensional array input, or 2 1-dimensional arrays. Takes an optional keyword argument `axis` indicating whether to treat columns (0) or rows (1) as variables. If the input array has more than 2 variables, returns the correlation matrix. If the input array as 2 variables, returns only the correlation between the variables.

```
>>> x = randn(10,3)
>>> spearmanr = stats.spearmanr
>>> rho, pval = spearmanr(x)
>>> rho
array([[ 1.        , -0.02087009, -0.05867387],
       [-0.02087009,  1.        ,  0.21258926],
       [-0.05867387,  0.21258926,  1.        ]])

>>> pval
array([[ 0.        ,  0.83671325,  0.56200781],
       [ 0.83671325,  0.        ,  0.03371181],
       [ 0.56200781,  0.03371181,  0.        ]])

>>> rho, pval = spearmanr(x[:,1],x[:,2])
```

```
>>> corr
-0.020870087008700869

>>> pval
0.83671325461864643
```

`kendalltau`

`kendalltau` computed Kendall's τ between 2 1-dimensonal arrays.

```
>>> x = randn(10)
>>> y = x + randn(10)
>>> kendalltau = stats.kendalltau
>>> tau, pval = kendalltau(x,y)
>>> tau
0.46666666666666673

>>> pval
0.06034053974834707
```

`linregress`

`linregress` estimates a linear regression between 2 1-dimensional arrays. It takes two inputs, the independent variables (regressors) and the dependent variable (regressand). Models always include a constant.

```
>>> x = randn(10)
>>> y = x + randn(10)
>>> linregress = stats.linregress
>>> slope, intercept, rvalue, pvalue, stderr = linregress(x,y)
>>> slope
1.6976690163576993

>>> rsquare = rvalue**2
>>> rsquare
0.59144988449163494

>>> x.shape = 10,1
>>> y.shape = 10,1
>>> z = hstack((x,y))
>>> linregress(z) # Alternative form, [x y]
(1.6976690163576993,
 -0.79983724584931648,
 0.76905779008578734,
 0.0093169560056056751,
 0.4988520051409559)
```

18.6   Select Statistical Tests

`normaltest`

`normaltest` tests for normality in an array of data. An optional second argument provides the axis to use (default is to use entire array). Returns the test statistic and the p-value of the test. This test is a small sample modified version of the Jarque-Bera test statistic.

kstest

kstest implements the Kolmogorov-Smirnov test. Requires two inputs, the data to use in the test and the distribution, which can be a string or a frozen random variable object. If the distribution is provided as a string, then any required shape parameters are passed in the third argument using a tuple containing these parameters, in order.

```
>>> x = randn(100)
>>> kstest = stats.kstest
>>> stat, pval = kstest(x, 'norm')
>>> stat
0.11526423481470172

>>> pval
0.12963296757465059

>>> ncdf = stats.norm().cdf # No () on cdf to get the function
>>> kstest(x, ncdf)
 (0.11526423481470172, 0.12963296757465059)

>>> x = gamma.rvs(2, size = 100)
>>> kstest(x, 'gamma', (2,)) # (2,) contains the shape parameter
(0.079237623453142447, 0.54096739528138205)

>>> gcdf = gamma(2).cdf
>>> kstest(x, gcdf)
(0.079237623453142447, 0.54096739528138205)
```

ks_2samp

ks_2samp implements a 2-sample version of the Kolmogorov-Smirnov test. It is called ks_2samp(x,y) where both inputs are 1-dimensonal arrays, and returns the test statistic and p-value for the null that the distribution of *x* is the same as that of *y*.

shapiro

shapiro implements the Shapiro-Wilk test for normality on a 1-dimensional array of data. It returns the test statistic and p-value for the null of normality.

18.7 Exercises

1. For each of the following distributions, simulate 1000 pseudo-random numbers:

    (a) $N(0, 1^2)$

    (b) $N\left(3, 3^2\right)$

    (c) $Unif\left(0, 1\right)$

    (d) $Unif\left(-1, 1\right)$

    (e) $Gamma\left(1, 2\right)$

    (f) $LogN\left(.08, .2^2\right)$

2. Use kstest to compute the p-value for each set of simulated data.

3. Use `seed` to re-initialize the random number generator.

4. Use `get_state` and `set_state` to produce the same set of pseudo-random numbers.

5. Write a custom function that will take a T vector of data and returns the mean, standard deviation, skewness and kurtosis (not excess) as a 4-element array.

6. Generate a 100 by 2 array of normal data with covariance matrix

$$\begin{bmatrix} 1 & -.5 \\ -.5 & 1 \end{bmatrix}$$

and compute the Pearson and Spearman correlation and Kendall's τ.

7. Compare the analytical median of a Gamma$(1,2)$ with that of 10,000 simulated data points. (You will need a `hist`, which is discussed in the graphics chapter to finish this problem.)

8. For each of the sets of simulated data in exercise 1, plot the sorted CDF values to verify that these lie on a 45° line. (You will need `plot`, which is discussed in the graphics chapter to finish this problem.)

Chapter 19

Statistical Analysis with `statsmodels`

> **Note**: This chapter provides an short introduction to statsmodels. There are many models, statistical procedures and diagnostics that are not covered. See statsmodel's documentation for more information on the available models and statistics.

statsmodels provides a large range of cross-sectional models as well as some time-series models. statsmodels uses a model descriptive language (provided via the Python package patsy) to formulate the model when working with pandas DataFrames. Models supported include linear regression, generalized linear models, limited dependent variable models, ARMA and VAR models.

19.1 Regression

Basic linear regression is provided by OLS. Estimating a model requires specifying the model and then calling a method to estimate the parameters (named `fit` in most models). This example will make use of one of the data sets provided with statsmodels named `statecrime` which contains data from the American National Elections Study of 1996.

```
>>> import statsmodels.api as sm
>>> data = sm.datasets.statecrime.load_pandas()
```

The dataset contains a number of variables, including

- state – State name (51 including Washington, DC)

- violent – Rate of violent crimes / 100,000 population. Includes murder, forcible rape, robbery, and aggravated assault.

- murder – Rate of murders / 100,000 population.

- hs_grad – Percent of the population having graduated from high school or higher.

- poverty – Percent of individuals below the poverty line.

- white – Percent of population that is one race - white only.

- single – Percent of family households that have a single parent.

- urban - Percent of population in urbanized areas.

The dataset includes attributes that list the exogeneous and endogenous variables, `endog_name` and `exog_name`, respectively. The variables can be directly accessed as pandas structures using the attributes `endog` and `exog`.

```
>>> data.endog_name
'murder'
>>> data.exog_name
['urban', 'poverty', 'hs_grad', 'single']
```

The model measures the murder rate using four explanatory variables. Models can be expressed using one of two equivalent formats. The first simply inputs the endogenous variable (y-variable, left-hand-side variable) as a 1-dimensional vector and the exogenous variables (x-variables, right-hand-side variables) as a 2-d array. When using this form it is necessary to explicitly include a column containing 1s as the constant in the model. Here this is column is added using the convenience function `add_constant`.

The standard pattern in statsmodels is to specify the model and then to call `fit` to estimate parameters. The allows the same specification to be estimated using different options when calling `fit`. Here the model is specified using `OLS` and then the parameters and other quantities are estimated by a parameter-less call to `fit` which return a class containing results. While the various quantities computed can be directly accessed by attribute from the result class (`res` in this example), `summary` is a useful method for printing a formatted summary of the estimation results.

```
>>> mod = sm.OLS(data.endog, sm.add_constant(data.exog))
>>> res = mod.fit()
>>> print(res.summary())
                        OLS Regression Results
==============================================================================
Dep. Variable:                  murder   R-squared:                       0.813
Model:                             OLS   Adj. R-squared:                  0.797
Method:                  Least Squares   F-statistic:                     50.08
Date:                 Fri, 04 Nov 2016   Prob (F-statistic):           3.42e-16
Time:                         22:32:08   Log-Likelihood:                -95.050
No. Observations:                   51   AIC:                             200.1
Df Residuals:                       46   BIC:                             209.8
Df Model:                            4
Covariance Type:             nonrobust
==============================================================================
                 coef     std err          t      P>t      [0.025      0.975]
------------------------------------------------------------------------------
const         -44.1024      12.086     -3.649      0.001     -68.430     -19.774
urban           0.0109       0.015      0.707      0.483      -0.020       0.042
poverty         0.4121       0.140      2.939      0.005       0.130       0.694
hs_grad         0.3059       0.117      2.611      0.012       0.070       0.542
single          0.6374       0.070      9.065      0.000       0.496       0.779
==============================================================================
Omnibus:                         1.618   Durbin-Watson:                   2.507
Prob(Omnibus):                   0.445   Jarque-Bera (JB):                0.831
Skew:                           -0.220   Prob(JB):                        0.660
Kurtosis:                        3.445   Cond. No.                     5.80e+03
==============================================================================
```

The result class has a large number of attributes which can be listed using `dir`.

```
# All attributed directly available
>>> print(sorted([v for v in dir(res) if not v.startswith('_')]))
['HC0_se', 'HC1_se', 'HC2_se', 'HC3_se', 'aic', 'bic', 'bse', 'centered_tss',
 'compare_f_test', 'compare_lm_test', 'compare_lr_test', 'condition_number',
 'conf_int', 'conf_int_el', 'cov_HC0', 'cov_HC1', 'cov_HC2', 'cov_HC3',
 'cov_kwds', 'cov_params', 'cov_type', 'df_model', 'df_resid', 'eigenvals',
 'el_test', 'ess', 'f_pvalue', 'f_test', 'fittedvalues', 'fvalue',
 'get_influence', 'get_prediction', 'get_robustcov_results', 'initialize',
```

```
'k_constant', 'llf', 'load', 'model', 'mse_model', 'mse_resid', 'mse_total',
'nobs', 'normalized_cov_params', 'outlier_test', 'params', 'predict',
'pvalues', 'remove_data', 'resid', 'resid_pearson', 'rsquared', 'rsquared_adj',
'save', 'scale', 'ssr', 'summary', 'summary2', 't_test', 'tvalues',
'uncentered_tss', 'use_t', 'wald_test', 'wald_test_terms', 'wresid']
```

A detailed description of the regression result outputs is available using the help for
`sm.regression.linear_model.RegressionResults`.

The `fit` method allows estimation options to be specified. The most useful option in OLS is the specification of the parameter covariance. The default uses the classical covariance which assumes that the model errors are homoskedastic. Using the option `cov_type='HC0'` will instead use White's heteroskedasticity-consistent covariance estimator.

```
>>> res_white = mod.fit(cov_type='HC0')
>>> import pandas as pd
>>> se = pd.concat([res.bse, res_white.bse],1)
>>> se.columns = ['No option', 'HC0']
>>> print(se)
          No option        HC0
const     12.086045  11.873042
urban      0.015397   0.013380
poverty    0.140220   0.114653
hs_grad    0.117179   0.110730
single     0.070314   0.082418
```

The previous results were constructed be specifying the model by explicitly inputting arrays containing the endogenous and exogenous data. Models can alternatively be specified using formulas similar to R through the method `from_formula`. Two inputs are required. The first is the formula to fit where the exogenous (left-hand-side) variable is listed first, a tilde (~) is used to separate this variable from the exogenous variables which are specified using a list. The formula is a string. The second input is a `DataFrame` which should have column names that match the formula. Here the `1` in the formula indicates that a constant should be included in the model. Here the murder rate is modeled using a constant, the percent urban and the percent single.

```
>>> df = pd.concat([data.endog, data.exog],1)
>>> mod = sm.OLS.from_formula('murder ~ 1 + urban + single', data=df)
>>> res = mod.fit()
```

The primary advantage of formulas is that extending the model is simple and direct. This next example extends the previous to include the percent that graduated high school.

```
>>> new_mod = sm.OLS.from_formula('murder ~ 1 + urban + single + hs_grad', data=df)
>>> new_res = new_mod.fit()
```

Related estimators for weighted least squares (WLS), generalized least squares (GLS) and generalized least squares with autoregressive errors (GLSAR). These are virtually identical to OLS except that they allow weights (WLS) or error variances (GLS) to be specified to improve the model estimation.

19.1.1   Weighted Least Squares (WLS)

19.1.2   Generalized Least Squares (WLS)

19.1.3   Diagnostics and Graphics

19.2   Generalized Linear Models

19.3   Other Notable Models

19.4   Time-series Analysis

19.4.1   Models

19.4.2   Statistics

19.4.3   Graphics

19.5   Generalized Linear Models

Chapter 20

Non-linear Function Optimization

SciPy contains a number of routines to the find extremum of a user-supplied objective function located in `scipy.optimize`. Most of these implement a version of the Newton-Raphson algorithm which uses the gradient to find the *minimum* of a function. However, this is not a limitation since if f is a function to be maximized, $-1 \times f$ is a function with the minimum located at the same point as the maximum of f.

A custom function that returns the function value at a set of parameters – for example a log-likelihood or a GMM quadratic form – is required to use one an optimizer. All optimization targets must have the parameters as the first argument. For example, consider finding the minimum of x^2. A function which allows the optimizer to work correctly has the form

```python
def optim_target1(x):
    return x**2
```

When multiple parameters (a parameter vector) are used, the objective function must take the form

```python
def optim_target2(params):
    x, y = params

    return x**2-3*x+3+y*x-3*y+y**2
```

Optimization targets can also have additional inputs that are not parameters of interest such as data or hyperparameters.

```python
def optim_target3(params,hyperparams):
    x, y = params
    c1, c2, c3=hyperparams

    return x**2+c1*x+c2+y*x+c3*y+y**2
```

This form is especially useful when optimization targets require both parameters and data. Once an optimization target has been specified, the next step is to use one of the optimizers find the minimum. The remainder of this chapter assumes that the following import is used to import the SciPy optimizers.

```python
import scipy.optimize as opt
```

20.1   Unconstrained Optimization

A number of functions are available for unconstrained optimization using derivative information. Each uses a different algorithm to determine the best direction to move and the best step size to take in the direction. The basic structure of all of the unconstrained optimizers is

```python
optimizer(f, x0)
```

where *optimizer* is one of `fmin_bfgs`, `fmin_cg`, `fmin_ncg` or `fmin_powell`, `f` is a callable function and `x0` is an initial value used to start the algorithm. All of the unconstrained optimizers take the following keyword arguments, except where noted:

Keyword	Description	Note
`fprime`	Function returning derivative of `f`. Must take same inputs as `f`	(1)
`args`	Tuple containing extra parameters to pass to `f`	
`gtol`	Gradient norm for terminating optimization	(1)
`norm`	Order of norm (e.g. inf or 2)	(1)
`epsilon`	Step size to use when approximating f'	(1)
`maxiter`	Integer containing the maximum number of iterations	
`disp`	Boolean indicating whether to print convergence message	
`full_output`	Boolean indicating whether to return additional output	
`retall`	Boolean indicating whether to return results for each iteration.	
`callback`	User supplied function to call after each iteration.	

(1) Except `fmin`, `fmin_powell`.

fmin_bfgs

`fmin_bfgs` is a classic optimizer which uses information in the 1st derivative to estimate the second derivative, an algorithm known as BFGS (after the initials of the creators). This should usually be the first option explored when optimizing a function without constraints. A function which returns the first derivative of the problem can also be provided, and if not provided, the first derivative is numerically approximated. The basic use of `fmin_bfgs` for finding the minimum of `optim_target1` is shown below.

```
>>> opt.fmin_bfgs(optim_target1, 2)
Optimization terminated successfully.
        Current function value: 0.000000
        Iterations: 2
        Function evaluations: 12
        Gradient evaluations: 4
array([ -7.45132576e-09])
```

This is a very simple function to minimize and the solution is accurate to 8 decimal places. `fmin_bfgs` can also use first derivative information, which is provided using a function which *must have the same inputs are the optimization target*. In this simple example, $f'(x) = 2x$.

```
def optim_target1_grad(x):
    return 2*x
```

The derivative information is used through the keyword argument `fprime`. Using analytic derivatives typically improves both the accuracy of the solution and the time required to find the optimum.

```
>>> opt.fmin_bfgs(optim_target1, 2, fprime = optim_target1_grad)
Optimization terminated successfully.
        Current function value: 0.000000
        Iterations: 2
        Function evaluations: 4
        Gradient evaluations: 4
array([  2.71050543e-20])
```

Multivariate optimization problems are defined using an array for the starting values, but are otherwise identical.

```
>>> opt.fmin_bfgs(optim_target2, array([1.0,2.0]))
Optimization terminated successfully.
```

```
        Current function value: 0.000000
        Iterations: 3
        Function evaluations: 20
        Gradient evaluations: 5
array([ 1.       ,  0.99999999])
```

Additional inputs are can be passed to the optimization target using the keyword argument `args` and a tuple containing the input arguments in the correct order. Note that since there is a single additional input, the comma is necessary in `(hyperp,)` to let Python know that this is a tuple.

```
>>> hyperp = array([1.0,2.0,3.0])
>>> opt.fmin_bfgs(optim_target3, array([1.0,2.0]), args=(hyperp,))
Optimization terminated successfully.
        Current function value: -0.333333
        Iterations: 3
        Function evaluations: 20
        Gradient evaluations: 5
array([ 0.33333332, -1.66666667])
```

Derivative functions can be produced in a similar manner, although the derivative of a scalar function with respect to an *n*-element vector is an *n*-element vector. It is important that the derivative (or gradient) returned has the same order as the input parameters. Note that the inputs must both be present, even when not needed, and in the same order.

```
def optim_target3_grad(params,hyperparams):
    x, y = params
    c1, c2, c3=hyperparams

    return array([2*x+c1+y, x+c3+2*y])
```

Using the analytical derivative reduces the number of function evaluations and produces the same solution.

```
>>> optimum = opt.fmin_bfgs(optim_target3, array([1.0,2.0]),
...                         fprime=optim_target3_grad,
...                         args=(hyperp ,))
Optimization terminated successfully.
        Current function value: -0.333333
        Iterations: 3
        Function evaluations: 5
        Gradient evaluations: 5
>>> optimum
array([ 0.33333333, -1.66666667])
>>> optim_target3_grad(optimum, hyperp) # Numerical zero
array([ -2.22044605e-16,   0.00000000e+00])
```

fmin_cg

`fmin_cg` uses a nonlinear conjugate gradient method to minimize a function. A function which returns the first derivative of the problem can be provided, and when not provided, the gradient is numerically approximated.

```
>>> opt.fmin_cg(optim_target3, array([1.0,2.0]),
...             args=(hyperp ,))
Optimization terminated successfully.
        Current function value: -0.333333
        Iterations: 7
        Function evaluations: 59
        Gradient evaluations: 12
array([ 0.33333334, -1.66666666])
```

fmin_ncg

`fmin_ncg` use a Newton conjugate gradient method. `fmin_ncg` *requires* a function which can compute the first derivative of the optimization target, and can also take a function which returns the second derivative (Hessian) of the optimization target. It not provided, the Hessian will be numerically approximated.

```
>>> opt.fmin_ncg(optim_target3,
...              array([1.0,2.0]),
...              optim_target3_grad, args=(hyperp,))
Optimization terminated successfully.
        Current function value: -0.333333
        Iterations: 5
        Function evaluations: 6
        Gradient evaluations: 21
        Hessian evaluations: 0
array([ 0.33333333, -1.66666666])
```

The hessian can optionally be provided to `fmin_ncg` using the keyword argument `fhess`. The hessian returns $\partial^2 f/\partial x \partial x'$, which is an *n* by *n* array of derivatives. In this simple problem, the hessian does not depend on the hyper-parameters, although the Hessian function *must* take the same inputs are the optimization target.

```
def optim_target3_hess(params,hyperparams):
    x, y = params
    c1, c2, c3=hyperparams

    return(array([[2, 1],[1, 2]]))
```

Using an analytical Hessian can reduce the number of function evaluations. While in theory an analytical Hessian should produce better results, it may not improve convergence, especially if the Hessian is nearly singular for some parameter values (for example, near a saddle point which is not a minimum).

```
>>> opt.fmin_ncg(optim_target3, array([1.0,2.0]), optim_target3_grad, \
... fhess = optim_target3_hess, args=(hyperp ,))
Optimization terminated successfully.
        Current function value: -0.333333
        Iterations: 5
        Function evaluations: 6
        Gradient evaluations: 5
        Hessian evaluations: 5
array([ 0.33333333, -1.66666667])
```

In addition to the keyword argument outlined in the main table, `fmin_ncg` can take the following additional arguments.

Keyword	Description	Note
fhess_p	Function returning second derivative of `f` times a vector *p*. Must take same inputs as `f`	Only `fmin_ncg`
fhess	Function returning second derivative of `f`. Must take same inputs as `f`	Only `fmin_ncg`
avestol	Average relative error to terminate optimizer.	Only `fmin_ncg`

20.2 Derivative-free Optimization

Derivative free optimizers do not use gradients and so can be used in a wider variety of problems such as functions which are not continuously differentiable. They can also be used for functions which are continuously

differentiable, although they are likely to be slower than derivative-based optimizers. Derivative free optimizers take some alternative keyword arguments.

Keyword	Description	Note
`xtol`	Change in x to terminate optimization	
`ftol`	Change in function to terminate optimization	
`maxfun`	Maximum number of function evaluations	
`direc`	Initial direction set, same size as x_0 by m	Only `fmin_powell`

fmin

`fmin` uses a simplex algorithm to minimize a function. The optimization in a simplex algorithm is often described as an amoeba which crawls around on the function surface expanding and contracting while looking for lower points. The method is derivative free, and so optimization target need not be continuously differentiable(e.g. the "tick" loss function used in estimation of quantile regression).

```python
def tick_loss(quantile, data, alpha):
    e = data - quantile

    return (alpha - (e<0)) @ e
```

The tick loss function is used to estimate the median by using $\alpha = 0.5$. This loss function is not continuously differential and so standard derivative-based optimizers cannot be used.

```python
>>> data = randn(1000)
>>> opt.fmin(tick_loss, 0, args=(data, 0.5))
Optimization terminated successfully.
        Current function value: -0.333333
        Iterations: 48
        Function evaluations: 91
array([-0.00475])
>>> median(data)
-0.0047118168472319406
```

The estimate is close to the sample median, as expected.

fmin_powell

`fmin_powell` used Powell's method, which is derivative free, to minimize a function. It is an alternative to `fmin` which uses a different algorithm.

```python
>>> opt.fmin_powell(tick_loss, 0, args=(data, 0.5))
Optimization terminated successfully.
        Current function value: 396.760642
        Iterations: 1
        Function evaluations: 17
array(-0.004673123552046776)
```

`fmin_powell` converged quickly and requires far fewer function calls.

20.3   Constrained Optimization

Constrained optimization is frequently encountered in economic problems where parameters are only meaningful in some particular range – for example, a variance which must be weakly positive. The relevant class

constrained optimization problems can be formulated

$$
\begin{aligned}
\min_\theta f(\theta) \quad & \text{subject to} \\
g(\theta) = 0 \quad & \text{(equality)} \\
h(\theta) \geq 0 \quad & \text{(inequality)} \\
\theta_L \leq \theta \leq \theta_H \quad & \text{(bounds)}
\end{aligned}
$$

where the bounds constraints are redundant if the optimizer allows for general inequality constraints since when a scalar x satisfies $x_L \leq x \leq x_H$, then $x - x_L \geq 0$ and $x_H - x \geq 0$. The optimizers in SciPy allow for different subsets of these constraints.

fmin_slsqp

`fmin_slsqp` is the most general constrained optimizer and allows for equality, inequality and bounds constraints. While bound constraints are redundant, constraints which take the form of bounds should be implemented using bounds since this provides more information directly to the optimizer. Constraints are provided either as list of callable functions or as a single function which returns an array. The latter is simpler if there are multiple constraints, especially if the constraints can be easily calculated using linear algebra. Functions which compute the derivative of the optimization target, the derivative of the equality constraints, and the derivative of the inequality constraints can be optionally provided. If not provided, these are numerically approximated.

As an example, consider the problem of optimizing a CRS Cobb-Douglas utility function of the form $U(x_1, x_2) = x_1^\lambda x_2^{1-\lambda}$ subject to a budget constraint $p_1 x_1 + p_2 x_2 \leq 1$. This is a nonlinear function subject to a linear constraint (note that is must also be that case that $x_1 \geq 0$ and $x_2 \geq 0$). First, specify the optimization target

```
def utility(x, p, alpha):
    # Minimization, not maximization so -1 needed
    return -1.0 * (x[0]**alpha)*(x[1]**(1-alpha))
```

There are three constraints, $x_1 \geq 0$, $x_2 \geq 0$ and the budget line.[1] All constraints must take the form of ≥ 0 constraint, so that the budget line can be reformulated as $1 - p_1 x_1 - p_2 x_2 \geq 0$. Note that the arguments in the constraint must be identical to those of the optimization target, which is why the utility function takes prices as an input, even though the prices are not required to compute the utility. Similarly the constraint function takes α as an unnecessary input.

```
def utility_constraints(x, p, alpha):
    return array([x[0] - 1e-8, x[1] - 1e-8, 1 - p[0]*x[0] - p[1]*x[1]])
```

The optimal combination of goods can be computed using `fmin_slsqp` once the starting values and other inputs for the utility function and budget constraint are constructed.

```
>>> p = array([1.0,1.0])
>>> alpha = 1.0/3
>>> x0 = array([.4,.4])
>>> opt.fmin_slsqp(utility, x0, f_ieqcons=utility_constraints, args=(p, alpha))
Optimization terminated successfully.    (Exit mode 0)
            Current function value: -0.529133683989
            Iterations: 2
            Function evaluations: 8
            Gradient evaluations: 2
array([ 0.33333333,  0.66666667])
```

---

[1] The code imposes the constraints that $x_j \geq 10^{-8}$ to ensure that the the values are always slightly positive.

`fmin_slsqp` can also take functions which compute the gradient of the optimization target, as well as the gradients of the constraint functions (both inequality and equality). The gradient of the optimization function should return a *n*-element vector, one for each parameter of the problem.

```
def utility_grad(x, p, alpha):
    grad = zeros(2)
    grad[0] = -1.0 * alpha * (x[0]**(alpha-1))*(x[1]**(1-alpha))
    grad[1] = -1.0 * (1-alpha) * (x[0]**(alpha))*(x[1]**(-alpha))
    return grad
```

The gradient of the constraint function returns a *m* by *n* array where *m* is the number of constraints. When both equality and inequality constraints are used, the number of constraints will be m_{eq} and m_{in} which will generally not be the same.

```
def utility_constraint_grad(x, p, alpha):
    grad = zeros((3,2)) # 3 constraints, 2 variables
    grad[0,0] = 1.0
    grad[0,1] = 0.0
    grad[1,0] = 0.0
    grad[1,1] = 1.0
    grad[2,0] = -p[0]
    grad[2,1] = -p[1]
    return grad
```

The two gradient functions can be passed using keyword arguments.

```
>>> opt.fmin_slsqp(utility, x0, f_ieqcons=utility_constraints, args=(p, alpha), \
... fprime = utility_grad, fprime_ieqcons = utility_constraint_grad)
Optimization terminated successfully.    (Exit mode 0)
            Current function value: -0.529133683989
            Iterations: 2
            Function evaluations: 2
            Gradient evaluations: 2
array([ 0.33333333,  0.66666667])
```

Like in other problems, gradient information reduces the number of iterations and/or function evaluations needed to find the optimum.

`fmin_slsqp` also accepts bounds constraints. Since two of the three constraints are $x_1 \geq 0$ and $x_2 \geq 0$, these can be easily specified as a bound. Bounds are given as a list of tuples, where there is a tuple for each variable with an upper and lower bound. It is not always possible to use `np.inf` as the upper bound, even if there is no implicit upper bound since this may produce a `nan`. In this example, 2 was used as the upper bound since it was outside of the possible range given the constraint. Using bounds also requires reformulating the budget constraint to only include the budget line.

```
def utility_constraints_alt(x, p, alpha):
    return array([1 - p[0]*x[0] - p[1]*x[1]])
```

Bounds are used with the keyword argument `bounds`.

```
>>> opt.fmin_slsqp(utility, x0, f_ieqcons=utility_constraints_alt, args=(p, alpha), \
... bounds = [(0.0,2.0),(0.0,2.0)])
Optimization terminated successfully.    (Exit mode 0)
            Current function value: -0.529133683989
            Iterations: 2
            Function evaluations: 8
            Gradient evaluations: 2
array([ 0.33333333,  0.66666667])
```

The use of non-linear constraints can be demonstrated by formulating the dual problem of cost minimization subject to achieving a minimal amount of utility. In this alternative formulation, the optimization problems becomes

$$\min_{x_1,x_2} p_1 x_1 + p_2 x_2 \text{ subject to } U(x_1,x_2) \geq \bar{U}$$

```
def total_expenditure(x,p,alpha,Ubar):
    return x @ p
```

```
def min_utility_constraint(x,p,alpha,Ubar):
    x1,x2 = x
    u=x1**(alpha)*x2**(1-alpha)
    return array([u - Ubar]) # >= constraint, must be array, even if scalar
```

The objective and the constraint are used along with a bounds constraint to solve the constrained optimization problem.

```
>>> x0 = array([1.0,1.0])
>>> p = array([1.0,1.0])
>>> alpha = 1.0/3
>>> Ubar = 0.529133683989
>>> opt.fmin_slsqp(total_expenditure, x0, f_ieqcons=min_utility_constraint, \
...     args=(p, alpha, Ubar), bounds =[(0.0,2.0),(0.0,2.0)])
Optimization terminated successfully.    (Exit mode 0)
        Current function value: 0.999999999981
        Iterations: 6
        Function evaluations: 26
        Gradient evaluations: 6
Out[84]: array([ 0.33333333,  0.66666667])
```

As expected, the solution is the same.

fmin_tnc

`fmin_tnc` supports only bounds constraints.

fmin_l_bfgs_b

`fmin_l_bfgs_b` supports only bounds constraints.

fmin_cobyla

`fmin_cobyla` supports only inequality constraints, which must be provided as a list of functions. Since it supports general inequality constraints, bounds constraints are included as a special case, although these must be included in the list of constraint functions.

```
def utility_constraints1(x, p, alpha):
    return x[0] - 1e-8
```

```
def utility_constraints2(x, p, alpha):
    return x[1] - 1e-8
```

```
def utility_constraints3(x, p, alpha):
    return (1 - p[0]*x[0] - p[1]*x[1])
```

Note that `fmin_cobyla` takes a list rather than an array for the starting values. Using an array produces a warning, but otherwise works.

```
>>> p = array([1.0,1.0])
>>> alpha = 1.0/3
>>> x0 = array([.4,.4])
>>> cons = [utility_constraints1, utility_constraints2, utility_constraints3]
>>> opt.fmin_cobyla(utility, x0, cons, args=(p, alpha), rhoend=1e-7)
array([ 0.33333326,  0.66666674])
```

20.3.1 Reparameterization

Many constrained optimization problems can be converted into an unconstrained program by reparameterizing from the space of unconstrained variables into the space where the parameters must reside. For example, the constraints in the utility function optimization problem require $0 \leq x_1 \leq 1/p_1$ and $0 \leq x_2 \leq 1/p_2$. Additionally the budget constraint must be satisfied so that if $x_1 \in [0, 1/p_1]$, $x_2 \in [0, (1 - p_1 x_1)/p_2]$. These constraints can be implemented using a "squasher" function which maps x_1 into its domain, and x_2 into its domain and is one-to-one and onto (i.e. a bijective relationship). For example,

$$x_1 = \frac{1}{p_1} \frac{e^{z_1}}{1 + e^{z_1}}, \ x_2 = \frac{1 - p_1 x_1}{p_2} \frac{e^{z_2}}{1 + e^{z_2}}$$

will always satisfy the constraints, and so the constrained utility function can be mapped to an unconstrained problem, which can then be optimized using an unconstrained optimizer.

```
def reparam_utility(z,p,alpha,printX = False):
    x = exp(z)/(1+exp(z))
    x[0] = (1.0/p[0]) * x[0]
    x[1] = (1-p[0]*x[0])/p[1] * x[1]
    if printX:
        print(x)
    return -1.0 * (x[0]**alpha)*(x[1]**(1-alpha))
```

The unconstrained utility function can be minimized using `fmin_bfgs`. Note that the solution returned is in the transformed space, and so a special call to `reparam_utility` is used to print the actual values of `x` at the solution (which are virtually identical to those found using the constrained optimizer).

```
>>> x0 = array([.4,.4])
>>> optX = opt.fmin_bfgs(reparam_utility, x0, args=(p,alpha))
Optimization terminated successfully.
        Current function value: -0.529134
        Iterations: 24
        Function evaluations: 104
        Gradient evaluations: 26
>>> reparam_utility(optX, p, alpha, printX=True)
[ 0.33334741  0.66665244]
```

20.4 Scalar Function Minimization

SciPy provides a number of scalar function minimizers. These are very fast since additional techniques are available for solving scalar problems which are not applicable when the parameter vector has more than 1 element. A simple quadratic function will be used to illustrate the scalar solvers. Scalar function minimizers do not require starting values, but may require bounds for the search.

```
def optim_target5(x, hyperparams):
    c1,c2,c3 = hyperparams

    return c1*x**2 + c2*x + c3
```

fminbound

`fminbound` finds the minimum of a scalar function between two bounds.

```
>>> hyperp = array([1.0, -2.0, 3])
>>> opt.fminbound(optim_target5, -10, 10, args=(hyperp,))
1.0000000000000002
>>> opt.fminbound(optim_target5, -10, 0, args=(hyperp,))
-5.3634455116374429e-06
```

golden

`golden` uses a golden section search algorithm to find the minimum of a scalar function. It can optionally be provided with bracketing information which can speed up the solution.

```
>>> hyperp = array([1.0, -2.0, 3])
>>> opt.golden(optim_target5, args=(hyperp,))
0.999999992928981
>>> opt.golden(optim_target5, args=(hyperp,), brack=[-10.0,10.0])
0.9999999942734483
```

brent

`brent` uses Brent's method to find the minimum of a scalar function.

```
>>> opt.brent(optim_target5, args=(hyperp,))
0.99999998519
```

    '

20.5   Nonlinear Least Squares

Non-linear least squares (NLLS) is similar to general function minimization. In fact, a generic function minimizer can (attempt to) minimize a NLLS problem. The main difference is that the optimization target returns a vector of errors rather than the sum of squared errors.

```
def nlls_objective(beta, y, X):
    b0 = beta[0]
    b1 = beta[1]
    b2 = beta[2]

    return y - b0 - b1 * (X**b2)
```

A simple non-linear model is used to demonstrate `leastsq`, the NLLS optimizer in SciPy.

$$y_i = \beta_1 + 2\beta_2 x^{\beta_3} + e_i$$

where x and e are i.i.d. standard normal random variables. The true parameters are $\beta_1 = 10$, $\beta_2 = 2$ and $\beta_3 = 1.5$.

```
>>> X = 10 *rand(1000)
>>> e = randn(1000)
>>> y = 10 + 2 * X**(1.5) + e
>>> beta0 = array([10.0,2.0,1.5])
>>> opt.leastsq(nlls_objective, beta0, args = (y, X))
(array([ 10.08885711,   1.9874906 ,   1.50231838]), 1)
```

`leastsq` returns a tuple containing the solution, which is very close to the true values, as well as a flag indicating that convergence was achieved. `leastsq` takes many of the same additional keyword arguments as other optimizers, including `full_output`, `ftol`, `xtol`, `gtol`, `maxfev` (same as `maxfun`). It has the additional keyword argument:

Keyword	Description	Note
`Ddun`	Function to compute the Jacobian of the problem. Element i, j should be $\partial e_i / \partial \beta_j$	
`col_deriv`	Direction to use when computing Jacobian numerically	
`epsfcn`	Step to use in numerical Jacobian calculation.	
`diag`	Scalar factors for the parameters. Used to rescale if scale is very different.	
`factor`	used to determine the initial step size.	Only `fmin_powell`

20.6 Exercises

1. The MLE for μ in a normal random variable is the sample mean. Write a function which takes a scalar parameter μ (1st argument) and a T vector of data and computes the negative of the log-likelihood, assuming the data is random and the variance is 1. Minimize the function (starting from something other than the same mean) using `fmin_bfgs` and `fmin`.

2. Extend to previous example where the first input is a 2-element vector containing μ and σ^2, and compute the negative log-likelihood. Use `fmin_slsqp` along with a lower bound of 0 for σ^2.

3. Repeat the exercise in problem 2, except using reparameterization so that σ is input (and then squared).

4. Verify that the OLS β is the MLE by writing a function which takes 3 inputs: K vector β, T by K array X and T by 1 array y, and computes the negative log-likelihood for these values. Minimize the function using `fmin_bfgs` starting at the OLS estimates of β.

Chapter 21

String Manipulation

Strings are usually less interesting than numerical values in econometrics and statistics. There are, however, some important uses for strings:

- Reading complex data formats

- Outputting formatted results to screen or file

Recall that strings are sliceable, but unlike arrays, are immutable, and so it is not possible to replace part of a string.

21.1   String Building

21.1.1   Adding Strings (+)

Strings are concatenated using +.

```
>>> a = 'Python is'
>>> b = 'a rewarding language.'
>>> a + ' ' + b
'Python is a rewarding language.'
```

While + is a simple method to join strings, the modern method is to use `join`. `join` is a string method which joins a list of strings (the input) using the object calling the string as the separator.

```
>>> a = 'Python is'
>>> b = 'a rewarding language.'
>>> ' '.join([a,b])
'Python is a rewarding language.'
```

Alternatively, the same output may be constructed using an empty string `''`.

```
>>> a = 'Python is'
>>> b = 'a rewarding language.'
>>> ''.join([a,' ',b])
'Python is a rewarding language.'
```

`join` is also useful for producing comma separated lists.

```
>>> words = ['Python','is','a','rewarding','language']
>>> ','.join(words)
'Python,is,a,rewarding,language'
```

21.1.2 Multiplying Strings (*)

Strings, like lists, can be repeated using `*`.

```
>>> a = 'Python is '
>>> 2*a
'Python is Python is '
```

21.1.3 Using StringIO

While adding strings using + or `join` is extremely simple, concatenation is slow for large strings. The module `io` provides an optimized class, `StringIO`, for performing string operations, including buffering strings for fast string building. This example shows how `write(`*string*`)` fills a `StringIO` buffer. Before reading the contents `seek(0)` is called to return to cursor to the beginning of the buffer, and then `read()` returns the entire string from the buffer.

```
>>> from io import StringIO
>>> sio = StringIO()
>>> for i in range(10000):
...     sio.write('cStringIO is faster than +! ')

>>> sio.seek(0)
>>> sio.read()
```

Note that this example is trivial since `*` could have been used instead.

21.2 String Functions

21.2.1 `split` and `rsplit`

`split` splits a string into a list based on a character, for example a comma. An optional third argument `maxsplit` can be used to limit the number of outputs in the list. `rsplit` works identically to split, only scanning from the end of the string – `split` and `rsplit` only differ when `maxsplit` is used.

```
>>> s = 'Python is a rewarding language.'
>>> s.split(' ')
['Python', 'is', 'a', 'rewarding', 'language.']

>>> s.split(' ',3)
['Python', 'is', 'a', 'rewarding language.']

>>> s.rsplit(' ',3)
['Python is', 'a', 'rewarding', 'language.']
```

21.2.2 `join`

`join` concatenates a list or tuple of strings using the first argument `sep` to specify a separator. The more common form directly calls `join` on the string to use as the separator.

```
>>> import string
>>> a = 'Python is'
>>> b = 'a rewarding language.'
>>> str.join(' ', (a,b))
'Python is a rewarding language.'

>>> str.join(':', (a,b))
```

```
'Python is:a rewarding language.'

>>> ' '.join((a,b)) # Preferred version
'Python is a rewarding language.'
```

21.2.3 `strip`, `lstrip`, and `rstrip`

`strip` removes leading and trailing whitespace from a string. An optional input `char` removes leading and trailing occurrences of the input value (instead of space). `lstrip` and `rstrip` work identically, only stripping from the left and right, respectively.

```
>>> s = '    Python is a rewarding language.    '
>>> s=s.strip()
'Python is a rewarding language.'

>>> s.strip('P')
'ython is a rewarding language.'
```

21.2.4 `find` and `rfind`

`find` locates the lowest index of a substring in a string and returns -1 if not found. Optional arguments limit the range of the search, and `s.find('i',10,20)` is identical to `s[10:20].find('i')`. `rfind` works identically, only returning the highest index of the substring.

```
>>> s = 'Python is a rewarding language.'
>>> s.find('i')
7

>>> s.find('i',10,20)
18

>>> s.rfind('i')
18
```

`find` and `rfind` are commonly used in flow control.

```
>>> words = ['apple','banana','cherry','date']
>>> words_with_a = []
>>> for word in words:
...     if word.find('a')>=0:
...         words_with_a.append(word)

>>> words_with_a
['apple', 'banana', 'date']
```

21.2.5 `index` and `rindex`

`index` returns the lowest index of a substring, and is identical to `find` except that an error is raised if the substring does not exist. As a result, `index` is only safe to use in a `try` … `except` block.

```
>>> s = 'Python is a rewarding language.'
>>> s.index('i')
7

>>> s.index('q') # Error
ValueError: substring not found
```

21.2.6 `count`

`count` counts the number of occurrences of a substring, and takes optional arguments to limit the search range.

```
>>> s = 'Python is a rewarding language.'
>>> s.count('i')
2

>>> s.count('i', 10, 20)
1
```

21.2.7 `lower` and `upper`

`lower` and `upper` convert strings to lower and upper case, respectively. They are useful to remove case when comparing strings.

```
>>> s = 'Python is a rewarding language.'
>>> s.upper()
'PYTHON IS A REWARDING LANGUAGE.'

>>> s.lower()
'python is a rewarding language.'
```

21.2.8 `ljust`, `rjust` and `center`

`ljust`, `rjust` and `center` left justify, right justify and center, respectively, a string while expanding its size to a given length. If the desired length is smaller than the string, the unchanged string is returned.

```
>>> s = 'Python is a rewarding language.'
>>> s.ljust(40)
'Python is a rewarding language.         '

>>> s.rjust(40)
'         Python is a rewarding language.'

>>> s.center(40)
'    Python is a rewarding language.     '
```

21.2.9 `replace`

`replace` replaces a substring with an alternative string, which can have different size. An optional argument limits the number of replacement.

```
>>> s = 'Python is a rewarding language.'
>>> s.replace('g','Q')
'Python is a rewardinQ lanQuaQe.'

>>> s.replace('is','Q')
'Python Q a rewarding language.'

>>> s.replace('g','Q',2)
'Python is a rewardinQ lanQuage.'
```

21.2.10 `textwrap.wrap`

The module `textwrap` contains a function `wrap` which reformats a long string into a fixed width paragraph stored line-by-line in a list. An optional argument changes the width of the output paragraph form the default of 70 characters.

```
>>> import textwrap
>>> s = 'Python is a rewarding language. '
>>> s = 10*s
>>> textwrap.wrap(s)
['Python is a rewarding language. Python is a rewarding language. Python',
'is a rewarding language. Python is a rewarding language. Python is a',
'rewarding language. Python is a rewarding language. Python is a',
'rewarding language. Python is a rewarding language. Python is a',
'rewarding language. Python is a rewarding language.']

>>> textwrap.wrap(s,50)
['Python is a rewarding language. Python is a',
'rewarding language. Python is a rewarding',
'language. Python is a rewarding language. Python',
'is a rewarding language. Python is a rewarding',
'language. Python is a rewarding language. Python',
'is a rewarding language. Python is a rewarding',
'language. Python is a rewarding language.']
```

21.3   Formatting Numbers

Formatting numbers when converting to a string allows for automatic generation of tables and well formatted screen output. Numbers are formatted using the `format` function, which is used in conjunction with a format specifier. For example, consider these examples which format π.

```
>>> pi
3.141592653589793

>>> '{:12.5f}'.format(pi)
'     3.14159'

>>> '{:12.5g}'.format(pi)
'      3.1416'

>>> '{:12.5e}'.format(pi)
' 3.14159e+00'
```

These all provide alternative formats and the difference is determined by the letter in the format string. The generic form of a format string is $\{n{:}faswc.pt\}$ or $\{n{:}faswcmt\}$. To understand the alternative choices, consider the output produced by the basic output string `'{0:}'`

```
>>> '{0:}'.format(pi)
'3.14159265359'
```

  • n is a number 0,1,... indicating which value to take from the format function

```
>>> '{0:}, {1:} and {2:} are all related to pi'.format(pi,pi+1,2*pi)
'3.14159265359, 4.14159265359 and 6.28318530718 are all related to pi'

>>> '{2:}, {0:} and {1:} reorder the output.'.format(pi,pi+1,2*pi)
'6.28318530718, 3.14159265359 and 4.14159265359 reorder the output.
```

- *fa* are fill and alignment characters, typically a 2 character string. Fill may be any character except },
  although space is the most common choice. Alignment can < (left) ,> (right), ^ (center) or = (pad to the
  right of the sign). Simple left 0-fills can omit the alignment character so that *fa* = 0.

```
>>> '{0:0<20}'.format(pi) # Left, 0 padding, precion 20
'3.141592653590000000'

>>> '{0:0>20}'.format(pi) # Right, 0 padding, precion 20
'00000003.14159265359'

>>> '{0:0^20}'.format(pi) # Center, 0 padding, precion 20
'0003.141592653590000'

>>> '{0: >20}'.format(pi) # Right, space padding, precion 20
'       3.14159265359'

>>> '{0:$^20}'.format(pi) # Center, dollar sign padding, precion 20
'$$$3.14159265359$$$$'
```

- *s* indicates whether a sign should be included. + indicates always include sign, – indicates only include if
  needed, and a blank space indicates to use a blank space for positive numbers, and a − sign for negative
  numbers – this format is useful for producing aligned tables.

```
>>> '{0:+}'.format(pi)
'+3.14159265359'

>>> '{0:+}'.format(-1.0 * pi)
'-3.14159265359'

>>> '{0:-}'.format(pi)
'3.14159265359'

>>> '{0: }'.format(pi)
' 3.14159265359'

>>> '{0: }'.format(-1.0 * pi)
'-3.14159265359'
```

- *m* is the minimum total size of the formatted string

```
>>> '{0:10}'.format(pi)
'3.14159265359'

>>> '{0:20}'.format(pi)
'       3.14159265359'

>>> '{0:30}'.format(pi)
'                 3.14159265359'
```

- *c* may be , or omitted. , produces numbers with 1000s separated using a ,. In order to use *c* it is
  necessary to include the . before the precision.

```
>>> '{0:.10}'.format(1000000 * pi)
'3141592.654'

>>> '{0:,.10}'.format(1000000 * pi)
'3,141,592.654'
```

- *p* is the precision. The interpretation of precision depends on *t*. In order to use *p*, it is necessary to include a . (dot). If not included, *p* will be interpreted as *m*.

```
>>> '{0:.1}'.format(pi)
'3e+00'

>>> '{0:.2}'.format(pi)
'3.1'

>>> '{0:.5}'.format(pi)
'3.1416'
```

- *t* is the type. Options include:

Type	Description
e, E	Exponent notation, e produces e+ and E produces E+ notation
f, F	Display number using a fixed number of digits
g, G	General format, which uses f for smaller numbers, and e for larger. G is equivalent to switching between F and E. g is the default format if no presentation format is given
n	Similar to g, except that it uses locale specific information.
%	Multiplies numbers by 100, and inserts a % sign

```
>>> '{0:.5e}'.format(pi)
'3.14159e+00'

>>> '{0:.5g}'.format(pi)
'3.1416'

>>> '{0:.5f}'.format(pi)
'3.14159'

>>> '{0:.5%}'.format(pi)
'314.15927%'

>>> '{0:.5e}'.format(100000 * pi)
'3.14159e+05'

>>> '{0:.5g}'.format(100000 * pi)
'3.1416e+05'

>>> '{0:.5f}'.format(100000 * pi)
'314159.26536'
```

Combining all of these features in a single format string produces complexly presented data.

```
>>> '{0: > 20.4f}, {1: > 20.4f}'.format(pi,-pi)
'              3.1416,              -3.1416'

>>> '{0: >+20,.2f}, {1: >+20,.2f}'.format(100000 * pi,-100000 * pi)
'        +314,159.27,         -314,159.27'
```

In the first example, reading from left to right after the colon, the format string consists of:

1. Space fill (the blank space after the colon)

2. Right align (>)

3. Use no sign for positive numbers, − sign for negative numbers (the blank space after >)

4. Minimum 20 digits

5. Precision of 4 fixed digits

The second is virtually identical to the first, except that it includes a , to show the 1000s separator and a + to force the sign to be shown.

21.3.1 Formatting Strings

`format` outputs formatted strings using a similar syntax to number formatting, although some options such as precision, sign, comma and type are not relevant.

```
>>> s = 'Python'
>>> '{0:}'.format(s)
'Python'

>>> '{0: >20}'.format(s)
'              Python'

>>> '{0:!>20}'.format(s)
'!!!!!!!!!!!!!!Python'

>>> 'The formatted string is: {0:!<20}'.format(s)
'The formatted string is: Python!!!!!!!!!!!!!!'
```

21.3.2 Formatting Multiple Objects

`format` also formats multiple objects in the same string output. There are three methods to do this:

- No position arguments, in which case the objects are matched to format strings in order

- Numeric positional arguments, in which case the first object is mapped to `'{0:}'`, the second to `'{1:}'`, and so on.

- Named arguments such as `'{price:}'` and volume `'{volume:}'`, which match keyword arguments inside format.

```
>>> price = 100.32
>>> volume = 132000
>>> 'The price yesterday was {:} with volume {:}'.format(price,volume)
'The price yesterday was 100.32 with volume  132000'

>>> 'The price yesterday was {0:} and the volume was {1:}'.format(price,volume)
'The price yesterday was 100.32 with volume 132000'

>>> 'The price yesterday was {1:} and the volume was {0:}'.format(volume,price)
'The price yesterday was 100.32 with volume 132000'

>>> 'The price yesterday was {price:} and the volume was {volume:}'.format(price=price,volume=volume
'The price yesterday was 100.32 with volume 132000'
```

21.3.3 f-Strings

f-Strings were introduced in Python 3.6 and provide a compact method to produce formatted strings using a special syntax. f-Strings allow variables to be directly included in the string which save appending `format` mathod to the string. the All f-Strings being with the character `f` followed by one of the quotation marks. Variables in f-Strings are included by enclosing them in braces, e.g., `{some_variable}`. To appreciate the elegance of f-Strings, consider the previous example:

```
>>> price = 100.32
>>> volume = 132000
>>> 'The price yesterday was {price:} and the volume was {volume:}'.format(price=price,volume=volume
'The price yesterday was 100.32 with volume 132000'
```

When written using an f-String, the simpler version is:

```
>>> f'The price yesterday was {price} and the volume was {volume}'
'The price yesterday was 100.32 with volume 132000'
```

This allows the variable to be directly included in the string. The default behavior is equivalent to calling `str` on each variable and then replacing the variable expressions with their `str` version. Formatting information can be provided using a `:`. For example, to format both `price` and volume `volume` using exponent notation:

```
>>> f'The price yesterday was {price:4.4e} and the volume was {volume:10.1e}'
'The price yesterday was 1.0032e+02 and the volume was    1.3e+05'
```

f-Strings are increasingly common and are the preferred way to format text in most cases. The main limitation of f-Strings is that the variable must be defined when the f-String is created. If the variable is not known, then it is still necessary to use the `format` method. For example

```
>>> f'The new price of {new_price} is not known'  # Error
NameError: name 'new_price' is not defined

>>> txt = 'The new price of {new_price} is now known'
>>> new_price = price + 1
>>> txt.format(new_price=new_price)
'The new price of 101.32 is now known'
```

21.3.4 Old style format strings

Some Python code still uses an older style format string. Old style format strings have $\%(map)flm.pt$, where:

- (map) is a mapping string containing a name, for example `(price)`

- fl is a flag which may be one or more of:

    - `0`: Zero pad
    - (blank space)
    - – Left adjust output
    - + Include sign character

- m, p and t are identical to those of the new format strings.

In general, the old format strings should only be used when required by other code (e.g. matplotlib). Below are some examples of their use in strings.

```
>>> price = 100.32
>>> volume = 132000
>>> 'The price yesterday was %0.2f with volume %d' % (price, volume)
'The price yesterday was 100.32 with volume  132000'

>>> 'The price yesterday was %(price)0.2f with volume %(volume)d' \
...     % {'price': price, 'volume': volume}
'The price yesterday was 100.32 with volume 132000'

>>> 'The price yesterday was %+0.3f and the volume was %010d' % (price, volume)
'The price yesterday was +100.320 and the volume was 0000132000'
```

21.4   Regular Expressions

Regular expressions are powerful tools for matching patterns in strings. While reasonable coverage of regular expressions is beyond the scope of these notes – there are 500 page books dedicated to constructing regular expressions – they are sufficiently useful to warrant an introduction. There are many online regular expression generators which can assist in finding the pattern to use, and so they are accessible to even casual users working with unformatted text.

Using regular expression requires the `re` module. The most useful functions for regular expression matching are `findall`, `finditer` and `sub`. `findall` and `finditer` work in similar manners, except that `findall` returns a list while `finditer` returns an iterable. `finditer` is preferred if a large number of matches is possible. Both search through a string and find all non-overlapping matches of a regular expression.

```
>>> import re
>>> s = 'Find all numbers in this string: 32.43, 1234.98, and 123.8.'
>>> re.findall('[\s][0-9]+\.\d*',s)
[' 32.43', ' 1234.98', ' 123.8']

>>> matches = re.finditer('[\s][0-9]+\.\d*',s)
>>> for m in matches:
...     print(s[m.span()[0]:m.span()[1]])
 32.43
 1234.98
 123.8
```

`finditer` returns `MatchObject`s which contain the method `span`. `span` returns a 2 element tuple which contains the start and end position of the match.

`sub` replaces all matched text with another text string (or a function which takes a `MatchObject`).

```
>>> s = 'Find all numbers in this string: 32.43, 1234.98, and 123.8.'
>>> re.sub('[\s][0-9]+\.\d*',' NUMBER',s)
'Find all numbers in this string: NUMBER, NUMBER, and NUMBER.'

>>> def reverse(m):
...     """Reverse the string in the MatchObject group"""
...     s = m.group()
...     s = s.rstrip()
...     return ' ' + s[::-1]

>>> re.sub('[\s][0-9]+\.\d*',reverse,s)
'Find all numbers in this string: 34.23, 89.4321, and 8.321.'
```

21.4.1   Compiling Regular Expressions

When repeatedly using a regular expression, for example running it on all lines in a file, it is better to compile the regular expression, and then to use the resulting `RegexObject`.

```
>>> import re
>>> s = 'Find all numbers in this string: 32.43, 1234.98, and 123.8.'
>>> numbers = re.compile('[\s][0-9]+\.\d*')
>>> numbers.findall(s)
[' 32.43', ' 1234.98', ' 123.8']
```

Parsing the regular expression text is relatively expensive, and compiling the expression avoids this cost.

21.5   Safe Conversion of Strings

When reading data into Python using a mixed format, blindly converting text to integers or floats is dangerous. For example, `float('a')` returns a `ValueError` since Python doesn't know how to convert `'a'` to a string. The simplest method to safely convert potentially non-numeric data is to use a `try` ... `except` block.

```
S = ['1234','1234.567','a','1234.a34','1.0','a123']
for s in S:
    try:
        # If integer, use int
        int(s)
        print(s, 'is an integer.')
    except:
        try:
            # If not integer, may be float
            float(s)
            print(s, 'is a float.')
        except:
            print('Unable to convert', s)
```

Chapter 22

File System Operations

Manipulating files and directories is surprising useful when undertaking complex projects. The most important file system commands are located in the modules `os` and `shutil`. This chapter assumes that

```python
import os
import shutil
```

have been included.

22.1 Changing the Working Directory

The working directory is where files can be created and accessed without any path information. `os.getcwd()` can be used to determine the current working directory, and `os.chdir(`*path*`)` can be used to change the working directory, where *path* is a directory, such as /temp or c:\\temp.[1] Alternatively, *path* can can be .. to more up the directory tree.

```python
pwd = os.getcwd()
os.chdir('c:\\temp')
os.chdir(r'c:\temp') # Raw string, no need to escape \
os.chdir('c:/temp')  # Identical
os.chdir('..')       # Walk up the directory tree
os.getcwd()          # Now in 'c:\\'
```

22.2 Creating and Deleting Directories

Directories can be created using `os.mkdir(`*dirname*`)`, although it must be the case that the higher level directories exist (e.g. to create /temp/Python/new , it /temp/Python already exists). `os.makedirs(`*dirname*`)` works similar to `os.mkdir(`*dirname*`)`, except that is will create any higher level directories needed to create the target directory.

Empty directories can be deleted using `os.rmdir(`*dirname*`)` – if the directory is not empty, an error occurs. `shutil.rmtree(`*dirname*`)` works similarly to `os.rmdir(`*dirname*`)`, except that it will delete the directory, and any files or other directories contained in the directory.

```python
os.mkdir('c:\\temp\\test')
os.makedirs('c:/temp/test/level2/level3')  # mkdir will fail
os.rmdir('c:\\temp\\test\\level2\\level3')
shutil.rmtree('c:\\temp\\test')  # rmdir fails, since not empty
```

---

[1]On Windows, directories use the backslash, which is used to escape characters in Python, and so an escaped backslash – \\ – is needed when writing Windows' paths. Alternatively, the forward slash can be substituted, so that c:\\temp and c:/temp are equivalent.

22.3   Listing the Contents of a Directory

The contents of a directory can be retrieved in a list using `os.listdir`(*dirname*), or simply `os.listdir('.')` to list the current working directory. The list returned contains all files and directories. `os.path.isdir(`*name*`)` can be used to determine whether a value in the list is a directory, and `os.path.isfile`(*name*) can be used to determine if it is a file. `os.path` contains other useful functions for working with directory listings and file attributes.

```python
os.chdir('c:\\temp')
files = os.listdir('.')
for f in files:
    if os.path.isdir(f):
        print(f, ' is a directory.')
    elif os.path.isfile(f):
        print(f, ' is a file.')
    else:
        print(f, ' is a something else.')
```

A more sophisticated listing which accepts wildcards and is similar to `dir` (Windows) and `ls` (Linux) can be constructed using the glob module.

```python
import glob
files = glob.glob('c:\\temp\\*.txt')

for file in files:
    print(file)
```

22.4   Copying, Moving and Deleting Files

File contents can be copied using `shutil.copy(`*src*, *dest*`)`, `shutil.copy2(`*src*, *dest*`)` or `shutil.copyfile(`*src*, *dest*`)`. These functions are all similar, and the differences are:

- `shutil.copy` will accept either a filename or a directory as *dest*. If a directory is given, the a file is created in the directory with the same name as the original file

- `shutil.copyfile` requires a filename for *dest*.

- `shutil.copy2` is identical to `shutil.copy` except that metadata, such as last access times, is also copied.

Finally, `shutil.copytree(`*src*, *dest*`)` will copy an entire directory tree, starting from the directory *src* to the directory *dest*, which must *not* exist. `shutil.move(`*src*, *dest*`)` is similar to `shutil.copytree`, except that it moves a file or directory tree to a new location. If preserving file metadata (such as permissions or file streams) is important, it is better use system commands (copy or move on Windows, cp or mv on Linux) as an external program.

```python
os.chdir('c:\\temp\\python')
# Make an empty file
f = open('file.ext','w')
f.close()
# Copies file.ext to 'c:\temp\'
shutil.copy('file.ext','c:\\temp\\')
# Copies file.ext to 'c:\temp\\python\file2.ext'
shutil.copy('file.ext','file2.ext')
# Copies file.ext to 'c:\\temp\\file3.ext', plus metadata
shutil.copy2('file.ext','file3.ext')
shutil.copytree('c:\\temp\\python\\','c:\\temp\\newdir\\')
shutil.move('c:\\temp\\newdir\\','c:\\temp\\newdir2\\')
```

Context Managers

Context managers are the preferred method to use when opening and closing files. A context manager always begins with the keyword `with` and uses the syntax `with` *command* `as` *variable*. *command* is the command you are using (e.g., `open`) and *variable* is the name of the variable you with to assign the output of the command to. A context manager will keep the file open while the code in the `with` block is executed. It will then automatically close the file when the block finishes. The following two blocks of commands are equivalent:

```python
f = open('file.txt','w')
f.write("Some text in the file")
f.close()
```

and

```python
with open('file.txt','w') as f:
    f.write("Some text in the file")
```

The second block is shorter and less error-prone since there is no need to call `close()` directly.

Beyond File Operations

While context managers are most commonly encountered in file I/O operations, they are more flexible. Whenever you initialize a context manager, Python calls the method __enter__(). This function performs any initialization such as opening a file handle and returns the object that is assigned using the `as` statement. When the context manager completes, the companion method __exit__() is automatically called. This method performs any clean-up operations such as closing open file handles. The previous examples could be equivalently written as:

```python
f = open('file.txt','w').__enter__()
f.write("Some text in the file")
f.__exit__()
```

Note that __enter__() and __exit__() should not usually be directly called and so should only be (silently) used in conjunction with a `with` statement.

22.5 Executing Other Programs

Occasionally it is necessary to call other programs, for example to decompress a file compressed in an unusual format or to call system copy commands to preserve metadata and file ownership. Both `os.system` and `subprocess.call` (which requires `import subprocess`) can be used to execute commands as if they were executed directly in the shell.

```python
import subprocess

# Copy using xcopy
os.system('xcopy /S /I c:\\temp c:\\temp4')
subprocess.call('xcopy /S /I c:\\temp c:\\temp5',shell=True)
# Extract using 7-zip
subprocess.call('"C:\\Program Files\\7-Zip\\7z.exe" e -y c:\\temp\\zip.7z')
```

22.6 Creating and Opening Archives

Creating and extracting files from archives often allows for further automation in data processing. Python has native support for zip, tar, gzip and bz2 file formats using `shutil.make_archive(` *archivename* `,` *format*, *root*`)` where *archivename* is the name of the archive to create, without the extension, *format* is one of the supported formats (e..g `'zip'` for a zip archive or `'gztar'`, for a gzipped tar file) and *root* is the root directory which can be `'.'` for the current working directory.

```python
# Creates files.zip
shutil.make_archive('files','zip','c:\\temp\\folder_to_archive')
# Creates files.tar.gz
shutil.make_archive('files','gztar','c:\\temp\\folder_to_archive')
```

Creating a standard gzip from an existing file is slightly more complicated, and requires using the `gzip` module.[2] This example makes use of context managers to open and close both the CSV and the gzip files.

```python
import gzip

# Create file.csv.gz from file.csv
with open('file.csv','rb') as csvin:
    with gzip.GzipFile('file.csv.gz','wb') as gz:
        gz.writelines(csvin.read())
```

Zip files can be extracted using the module `zipfile`, gzip files can be extracted using `gzip`, and gzipped tar files can be extracted using `tarfile`.

```python
import zipfile
import gzip
import tarfile

# Extract zip
with zipfile.ZipFile('files.zip') as zip:
    zip.extractall('c:\\temp\\zip\\')

# Extract gzip tar 'r:gz' indicates read gzipped
with tarfile.open('file.tar.gz', 'r:gz') as gztar:
    gztar.extractall('c:\\temp\\gztar\\')

# Extract csv from gzipped csv
with gzip.GzipFile('file.csv.gz','rb') as gz:
    with open('file.csv','wb') as csvout:
        csvout.writelines(gz.read())
```

22.7 Reading and Writing Files

Occasionally it may be necessary to directly read or write a file, for example to output a formatted LATEX table. Python contains low level file access tools which can be used to generate files with any structure. Writing text files begins by using `file` to create a new file or to open an existing file. Files can be opened in different modes: 'r' for reading, 'w' for writing, and 'a' for appending ('w' will overwrite an existing file). An additional modifier 'b' can be be used if the file is binary (not text), so that 'rb', 'wb' and 'ab' allow reading, writing and appending binary files.

Reading text files is usually implemented using `readline()` to read a single line, `readlines(` *n*`)` to reads approximately *n* bytes or `readlines()` to read all lines in a file. `readline` and `readlines(` *n*`)` are usually used

---

[2]A gzip can only contain 1 file, and is usually used with a tar file to compress a directory or set of files.

inside a while loop which terminates if the value returned is an empty string (`''`, `readline`) or an empty list (`[]`, `readlines`). Note that both `''` and `[]` are false, and so can be directly used in a while statement.

```python
# Read all lines using readlines()
with open('file.csv','r') as f:
    lines = f.readlines()
    for line in lines:
        print(line)

# Using blocking via readline()
with open('file.csv','r') as f:
    line = f.readline()
    while line:
        print(line)
        line = f.readline()

# Using larger blocks via readlines(n)
with open('file.csv','r') as f
    lines = f.readlines(2)
    while lines:
        for line in lines:
            print(line)
        lines = f.readline(2)
```

Writing text files is similar, and begins by using `file` to create a file and then `fwrite` to output information. `fwrite` is conceptually similar to using print, except that the output will be written to a file rather than printed on screen. The next example show how to create a LATEX table from an array.

```python
import numpy as np
import scipy.stats as stats

x = np.random.randn(100,4)
mu = np.mean(x,0)
sig = np.std(x,0)
sk = stats.skew(x,0)
ku = stats.kurtosis(x,0)

summaryStats = np.vstack((mu,sig,sk,ku))
rowHeadings = ['Var 1','Var 2','Var 3','Var 4']
colHeadings = ['Mean','Std Dev','Skewness','Kurtosis']

# Build table, then print
latex = []
latex.append('\\begin{tabular}{r|rrrr}')
line = ' '
for i in range(len(colHeadings)):
    line += ' & ' + rowHeadings[i]

line += ' \\ \hline'
latex.append(line)

for i in range(size(summaryStats,0)):
    line = rowHeadings[i]
    for j in range(size(summaryStats,1)):
        line += ' & ' + str(summaryStats[i,j])

    latex.append(line)

latex.append('\\end{tabular}')
```

```python
# Output using write()
with open('latex_table.tex','w') as f:
    for line in latex:
        f.write(line + '\n')
```

22.8 Exercises

1. Create a new directory, *chapter22*.

2. Change into this directory.

3. Create a new file names *tobedeleted.py* a text editor in this new directory (It can be empty).

4. Create a zip file *tobedeleted.zip* containing *tobedeleted.py*.

5. Get and print the directory listing.

6. Delete the newly created file, and then delete this directory.

Chapter 23

Performance and Code Optimization

> *We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil.*

<div align="right">

Donald Knuth

</div>

23.1 Getting Started

Occasionally the performance of a direct implementation of a statistical algorithm will not execute quickly enough be applied to interesting data sets. When this occurs, there are a number of alternatives ranging from improvements possible using only NumPy and Python to using native code through a Python module.

Note that before any code optimization, it is *essential* that a clean, working implementation is available. This allows for both measuring performance improvements and to ensure that optimizations have not introduced any bugs. The famous quote of Donald Knuth should also be heeded, and in practice code optimization is only needed for a very small amount of code – code that is frequently executed.

23.2 Timing Code

Timing code is an important step in measuring performance. IPython contains the magic keywords `%timeit` and `%time` which can be used to measure the execution time of a block of code. `%time` simply runs the code and reports the time needed. `%timeit` is smarter in that it will vary the number of iterations to increase the accuracy of the timing. Both are used with the same syntax, `%timeit` *code to time*.[1]

```
>>> x = randn(1000,1000)
>>> %timeit inv(x.T @ x)
1 loops, best of 3: 387 ms per loop

>>> %time inv(x.T @ x)
Wall time: 0.52 s

>>> x = randn(100,100)
>>> %timeit inv(x.T @ x)
1000 loops, best of 3: 797 us per loop
```

---

[1] All timings were performed using Anaconda version 2.0.1.

23.3   Vectorize to Avoid Unnecessary Loops

Vectorization is the key to writing high performance code in Python. Code that is vectorized run *insides* NumPy and so executes as quickly as possible (with some small technical caveats, see NumExpr). Consider the difference between manually multiplying two matrices and using `@`.

```python
def pydot(a, b):
    M,N = shape(a)
    P,Q = shape(b)
    c = zeros((M,Q))
    for i in range(M):
        for j in range(Q):
            for k in range(N):
                c[i,j] += a[i,k] * b[k,j]
    return c
```

Timing the difference shows that NumPy is about 10000x faster than looping Python.

```python
>>> a = randn(100,100)
>>> b = randn(100,100)
>>> %timeit pydot(a,b)
1 loops, best of 3: 830 ms per loop

>>> %timeit a @ b
10000 loops, best of 3: 53.4 us per loop

>>> f'The speed-up is {0.83/0.0000534 - 1.0:.1f} times'
'The speed-up is 15542.1 times'
```

A less absurd example is to consider computing a weighted moving average across *m* consecutive values of a vector.

```python
def naive_weighted_avg(x, w):
    T = x.shape[0]
    m = len(w)
    m12 = int(ceil(m/2))
    y = zeros(T)
    for i in range(len(x)-m+1):
        y[i+m12] = x[i:i+m].T @ w

    return y
```

```python
>>> w = array(r_[1:11,9:0:-1],dtype=float64)
>>> w = w/sum(w)
>>> x = randn(10000)
>>> %timeit naive_weighted_avg(x,w)
100 loops, best of 3: 13.3 ms per loop
```

An alternative method which completely avoids loops can be constructed by carefully constructing an array containing the data. This array allows `@` to be used with the weights.

```python
def clever_weighted_avg(x,w):
    T = x.shape[0]
    m = len(w)
    wc = copy(w)
    wc.shape = m,1
    T = x.size
    xc = copy(x)
    xc.shape=T,1
    y = vstack((xc,zeros((m,1))))
    y = tile(y,(m,1))
```

```
    y = reshape(y[:len(y)-m],(m,T+m-1))
    y = y.T
    y = y[m-1:T,:]

    return y @ flipud(wc)
```

```
>>> %timeit clever_weighted_avg(x,w)
1000 loops, best of 3: 1.03 ms per loop
```

The loop-free method which uses copying and slicing is about 12 times faster than the simple looping specification.

23.4   Alter the loop dimensions

In many applications, it may be natural to loop over the long dimension in a time series. This is especially common if the mathematical formula underlying the program has a sum from $t = 1$ to T. In some cases, it is possible to replace a loop over time, which is assumed to be the larger dimension, with an alternative loop across another iterable. For example, in the moving average, it is possible to loop over the weights rather than the data, and if the moving windows length is much smaller than the length of the data, the code should run much faster.

```
def sideways_weighted_avg(x, w):
    T = x.shape[0]
    m = len(w)
    y = zeros(T)
    m12 = int(ceil(m/2))
    for i in range(m):
        y[m12:T-m+m12] = x[i:T+i-m] * w[i]

    return y
```

```
>>> %timeit sideways_weighted_avg(x,w)
1000 loops, best of 3: 262 us per loop
```

In this example, the "sideways" loop is much faster than fully vectorized version since it avoids allocating a large amount of memory.

23.5   Utilize Broadcasting

NumPy uses broadcasting for virtually all primitive mathematical operations (and for some more complicated functions). Broadcasting avoids unnecessary data replication and memory allocation, and so improves performance.

```
>>> x = randn(1000,1)
>>> y = randn(1,1000)
>>> %timeit x*y
100 loops, best of 3: 2.66 ms per loop
```

```
>>> %timeit (x @ ones((1,1000))) * (ones((1000,1)) @ y)
100 loops, best of 3: 13.1 ms per loop
```

In this example, broadcasting is about 4 times faster than manually expanding the arrays.

23.6 Use In-place Assignment

In-place assignment uses the save variable and avoids unnecessary memory allocation. The in-place operators use a syntax similar to `x += 0.0` or `x *= 1.0` instead of `x = x + 0.0`.

```
>>> x = zeros(1000000)
>>> %timeit global x; x += 0.0
1000 loops, best of 3: 613 us per loop

>>> %timeit global x; x = x + 0.0
100 loops, best of 3: 2.74 ms per loop
```

The gains to in-place allocation are larger as the dimension of `x` increases.

23.7 Avoid Allocating Memory

Memory allocation is relatively expensive, especially if it occurs inside a for loop. It is often better to pre-allocate storage space for computed values, and also to reuse existing space. Similarly, prefer slices and views to operations which create copies of arrays.

23.8 Inline Frequent Function Calls

Function calls are fast but not completely free. Simple functions, especially inside loops, should be in-lined to avoid the cost of calling functions.

23.9 Consider Data Locality in Arrays

Arrays are stored using row major format, and so data is stored across a row first, and then down columns second. This means that in an m by n array, element i, j is stored next to elements $i, j+1$ and $i, j-1$ (except when j is the first (previous is $i-1, n$) or last element in a row (next is $i+1, 1$)). Spatial location matters for performance, and it is faster to access data which is stored physically adjacent. The simplest method to understand array storage is to use:

```
>>> x = arange(16.0)
>>> x.shape = 4,4
>>> x
array([[  0.,   1.,   2.,   3.],
       [  4.,   5.,   6.,   7.],
       [  8.,   9.,  10.,  11.],
       [ 12.,  13.,  14.,  15.]])
```

23.10 Profile Long Running Functions

Profiling provides detailed information about the number of times a line is executed as well as the execution time spent on each line. The default Python profiling tools are not adequate to address all performance measurement issues in NumPy code, and so a third party library known as line_profiler is needed. line_profiler is not currently available in Anaconda and so it must be installed before use. line_profiler is available through conda and so can be installed using

```
conda install line_profiler
```

IPython Magic Keyword for Line Profiling

The simplest method to profile function is to use IPython. This requires a small amount of setup to define a new magic word, `%lprun`.

```
>>> import IPython
>>> ip = IPython.get_ipython()
>>> import line_profiler
>>> ip.register_magics(line_profiler.LineProfilerMagics)
```

Note that the final two of these fours lines can also be incorporated into startup.py (see Chapter 1) so that the magic word `%lprun` is available in all IPython sessions.

To demonstrate the use of line_profiler, the three moving average functions where combined into a single python file moving_avgs.py. line_profiler is used with the syntax `%lprun -f` *function command* where *function* is the function to profile and *command* is a command which will cause the function to run. *command* can be either a simple call to the function or a call to some other code that will run the function.

```
>>> from moving_avgs import naive_weighted_avg
>>> w = array(r_[1:11,9:0:-1],dtype=float64)
>>> w = w/sum(w)
>>> x = randn(100000)
>>> %lprun -f naive_weighted_avg naive_weighted_avg(x,w)
Timer unit: 3.94742e-07 s

File: moving_avgs.py
Function: naive_weighted_avg at line 16
Total time: 1.04589 s

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
    16                                            def naive_weighted_avg(x, w):
    17         1           27     27.0      0.0       T = x.shape[0]
    18         1           13     13.0      0.0       m = len(w)
    19         1          120    120.0      0.0       m12 = int(ceil(m/2))
    20         1          755    755.0      0.0       y = zeros(T)
    21     99983       505649      5.1     19.1       for i in range(len(x)-m+1):
    22     99982      2142994     21.4     80.9           y[i+m12] = x[i:i+m].T @ w
    23
    24         1            6      6.0      0.0       return y
```

The first attempt at a weighted average, `naive_weighted_average`, spent all of the time in the loop and most of this on the matrix multiplication.

```
>>> from moving_avgs import clever_weighted_avg
>>> %lprun -f clever_weighted_avg clever_weighted_avg(x,w)
Timer unit: 3.94742e-07 s

File: moving_avgs.py
Function: clever_weighted_avg at line 27
Total time: 0.0302076 s

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
    27                                            def clever_weighted_avg(x,w):
    28         1           33     33.0      0.0       T = x.shape[0]
    29         1           11     11.0      0.0       m = len(w)
    30         1           98     98.0      0.1       wc = copy(w)
    31         1           33     33.0      0.0       wc.shape = m,1
    32         1            9      9.0      0.0       T = x.size
    33         1          738    738.0      1.0       xc = copy(x)
```

```
   34          1           42      42.0       0.1        xc.shape=T,1
   35          1         1605    1605.0       2.1        y = vstack((xc,zeros((m,1))))
   36          1        25286   25286.0      33.0        y = tile(y,(m,1))
   37
   38          1           98      98.0       0.1        y = reshape(y[:len(y)-m],(m,T+m-1))
   39          1           12      12.0       0.0        y = y.T
   40          1           38      38.0       0.0        y = y[m-1:T,:]
   41
   42          1        48522   48522.0      63.4        return y @ flipud(wc)
```

The second attempt, `clever_weighted_avg`, spends 1/3 of the time in the tile `tile` command and the remainder in the `@`.

```
>>> from moving_avgs import sideways_weighted_avg
>>> %lprun -f sideways_weighted_avg sideways_weighted_avg(x,w)
Timer unit: 3.94742e-07 s

File: moving_avgs.py
Function: sideways_weighted_avg at line 45
Total time: 0.00962302 s

Line #      Hits         Time  Per Hit   % Time  Line Contents
==============================================================
   45                                             def sideways_weighted_avg(x, w):
   46          1           25     25.0      0.1       T = x.shape[0]
   47          1           10     10.0      0.0       m = len(w)
   48          1          417    417.0      1.7       y = zeros(T)
   49          1          182    182.0      0.7       m12 = int(ceil(m/2))
   50         20          230     11.5      0.9       for i in range(m):
   51         19        23508   1237.3     96.4           y[m12:T-m+m12] = x[i:T+i-m] * w[i]
   52
   53          1            6      6.0      0.0       return y
```

The final version spends most of its time in the matrix multiplication and the only other line with meaningful time is the call to `zeros`. Note the actual time was .0096 vs 1.06 for the naive version and .030 for the loop-free version. Comparing the naive and the sideways version really highlights the cost of repeated calls to simple functions inside loops `@` as well as the loop overhead.

Directly Using the Line Profiler

Directly using line_profiler requires adding the *decorator* `@profile` to a function. Consider profiling the three weighted average functions.

```python
from numpy import ceil, zeros, copy, vstack, flipud, reshape, tile, array, float64, r_
from numpy.random import randn

# Useful block but not necessary
import builtins

try:
    builtins.profile
    print("Running with kernprof")
except AttributeError:
    # No line profiler, provide a pass-through version
    def profile(func): return func
    builtins.profile = profile
    print("Running without kernprof")

@profile
```

```python
def naive_weighted_avg(x, w):
    T = x.shape[0]
    m = len(w)
    m12 = int(ceil(m/2))
    y = zeros(T)
    for i in range(len(x)-m+1):
        y[i+m12] = x[i:i+m].T @ w

    return y

@profile
def clever_weighted_avg(x,w):
    T = x.shape[0]
    m = len(w)
    wc = copy(w)
    wc.shape = m,1
    T = x.size
    xc = copy(x)
    xc.shape=T,1
    y = vstack((xc,zeros((m,1))))
    y = tile(y,(m,1))

    y = reshape(y[:len(y)-m],(m,T+m-1))
    y = y.T
    y = y[m-1:T,:]

    return y @ flipud(wc)

@profile
def sideways_weighted_avg(x, w):
    T = x.shape[0]
    m = len(w)
    y = zeros(T)
    m12 = int(ceil(m/2))
    y = zeros(x.shape)
    for i in range(m):
        y[m12:T-m+m12] = x[i:T+i-m] * w[i]

    return y

w = array(r_[1:11,9:0:-1],dtype=float64)
w = w/sum(w)
x = randn(100000)

naive_weighted_avg(x,w)
clever_weighted_avg(x,w)
sideways_weighted_avg(x,w)
```

The decorator `@profile` specifies which functions should be profiled by line_profiler, and should only be used on functions where profiling is needed. The final lines in this file call the functions, which is necessary for the profiling.

To profile the on Windows code (saved in moving_avgs_direct.py), run the following commands from a command prompt (not inside IPython)

```
cd PATHTOFILE
ANACONDA\Scripts\kernprof.exe -l moving_avgs_direct.py
python -m line_profiler moving_avgs_direct.py.lprof > moving_avgs_direct.prof.txt
```

where PATHTOFILE is the location of moving_avgs_direct.py. The first command changes to the directory

where moving_avgs_direct.py is located. The second actually executes the file with profiling, and the final produces a report in moving_avgs_direct.prof.txt, which can then be viewed in any text editor.[2]

On Linux or OSX, run

```
cd PATHTOFILE
kernprof -l moving_avgs_direct.py
python -m line_profiler moving_avgs_direct.py.lprof > moving_avgs_direct.prof.txt
```

The file moving_avg.prof.txt will contain a line-by-line listing of the three function which includes the number to times the line was hit as well as the time spent on each line.

Modification of Code

In the direct method, the file moving_avgs_direct.py has a strange block reproduced below.

```python
# Useful block but not necessary
import builtins

try:
    builtins.profile
    print("Running with kernprof")
except AttributeError:
    # No line profiler, provide a pass-through version
    def profile(func): return func
    builtins.profile = profile
    print("Running without kernprof")
```

I like to use this block since the decorator `@profile` is only defined when running in a profile session. Attempting to run a file without this block in a standard python session will produce an `AttributeError` since `profile` is not defined. This block allows the code to be run both with and without profiling by first checking if `profile` is defined, and if not, providing a trivial definition that does nothing.

23.11 Exercises

1. Write a Python function which will accept a $p+q+1$ vector of parameters, a T vector of data, and p and q (integers, AR and MA order, respectively) and recursively computes the ARMA error beginning with observation $p+1$. If an MA index is negative it should be backcast to 0.

2. Use line_profiler to measure the performance of the ARMA written in exercise 1.

3. Use `jit` to accelerate the ARMA function written in the exercise 1. Compare the speed to the pure Python implementation.

4. [Only for the brave] Convert the ARMA function to Cython, compile it, and compare the performance against both the pure Python and the Numba versions.

---

[2]The Windows command is more complex than the Linux command to ensure that the correct Python interpreter and environment is used to execute kernprof.py.

Chapter 24

Improving Performance using Numba

Numba is a rapidly evolving project that releases new versions monthly. This chapter was written against Numba 0.50.1 and so it is recommended to check for important changes in the the Numba documentation (http://numba.pydata.org).

24.1 Quick Start

If pure Python/NumPy is slow due to the presence of loops, Numba may be useful for compiling Python to optimized machine code using LLVM. Numba is particularly attractive since in many cases the only modification required to improve code execution speed is the addition of a *decorator* immediately before the `def` *function* `():` line. Consider a generic recursion from a GARCH(P,Q) model that computes the conditional variance given parameters, data, and a backcast value. A pure Python/NumPy implementation is provided below.

```python
def garch_recursion(parameters, data, sigma2, p, q, backcast):
    T = data.shape[0]
    for i in range(T):
        sigma2[i] = parameters[0]
        for j in range(1, p + 1):
            if (i - j) < 0:
                sigma2[i] += parameters[j] * backcast
            else:
                sigma2[i] += parameters[j] * (data[i - j] * data[i - j])
        for j in range(1, q + 1):
            if (i - j) < 0:
                sigma2[i] += parameters[p + j] * backcast
            else:
                sigma2[i] += parameters[p + j] * sigma2[i - j]

    return sigma2
```

This example is simple and only involves the (slow) recursive calculation of the conditional variance, not the other portions of the log-likelihood (which can be vectorized using NumPy). The pure Python version can be tested using `%timeit`.

```python
>>> parameters = array([.1,.1,.8])
>>> data = randn(10000)
>>> sigma2 = zeros(shape(data))
>>> p, q = 1,1
>>> backcast = 1.0
>>> %timeit -r20 garch_recursion(parameters, data, sigma2, p, q, backcast)
```

```
27.5 ms +/- 1.43 ms per loop (mean +/- std. dev. of 20 runs, 10 loops each)
```

Using Numba starts with `from numba import jit`, and then decorating the function with `@jit`.

```python
from numba import jit

@jit
def garch_recursion_numba_jit(parameters, data, sigma2, p, q, backcast):
    T = data.shape[0]
    for i in range(T):
        sigma2[i] = parameters[0]
        for j in range(1, p + 1):
            if (i - j) < 0:
                sigma2[i] += parameters[j] * backcast
            else:
                sigma2[i] += parameters[j] * (data[i - j] * data[i - j])
        for j in range(1, q + 1):
            if (i - j) < 0:
                sigma2[i] += parameters[p + j] * backcast
            else:
                sigma2[i] += parameters[p + j] * sigma2[i - j]

    return sigma2
```

The Numba version can be tested by changing the function name.

```
>>> garch_recursion_numba_jit(parameters, data, sigma2, p, q, backcast) # Warmup
>>> %timeit garch_recursion_numba_jit(parameters, data, sigma2, p, q, backcast)
42.3 us +/- 1.14 us per loop (mean +/- std. dev. of 7 runs, 10000 loops each)

>>> f'The speed-up is {0.0275/0.0000423 - 1.0:.1f} times'
'The speed-up is 649.1 times'
```

Two lines of code – an import and a decorator – produce a function that runs over 400 times faster than pure Python. Alternatively, `jit` can be used as a function to produce a just-in-time compiled function. This version is an alternative to using the decorator version `@jit` but is otherwise identical. The main advantage of the function is that it is possible to easily retain both the pure Python and the JIT version for comparisons of accuracy and performance.[1]

```
>>> garch_recursion_numba_jit_command = jit(garch_recursion)
```

Numba operates by inspecting the function, and, subject to satisfying some constraints, just-in-time compiling it to machine code by translating the Python/NumPy into an LLVM intermediate representation and then using LLVM to compile the IR into executable code. Numba generates functions that have a signature which defines the inputs and the outputs. The first time a function is called, Numba inspects the function and inputs and generates machine code to execute the function. This first call can be slow since the machinery of Numba has to act before running the function. Subsequent calls just check that the inputs match an existing signature. If they do, the optimized function previously generated is called and the total execution time should be relatively small. If the function is called with a different signature, for example, if double precision vectors are swapped to single precision vectors, Numba will generate a different function these this set of inputs. Again the first call is slow but subsequent calls with the same input data types will execute without a compilation step.

Numba can generate much faster code than pure Python since it only supports a small (but important) set of data types, functions, and operators. The pure Python loop is slow since Python doesn't know anything about NumPy arrays. Each operation in the loop requires Python to perform a number of actions such as looking up

---

[1]Numba compiled functions retain the pure Python implementation as a method (`py_func`). For example, `garch_recursion_numba_jit_command.py_func` can be executed with the same arguments to run the original function `garch_recursion`.

an element in memory (without knowing anything that happened before, such as the location of the previous element), checking whether this element supports addition or multiplication, looking up the element's addition or multiplication function, and then calling this function with the arguments. This is a very general approach which is why Python can multiply virtually anything that supports multiplication including numbers, strings, and lists. The post-JIT code produced by Numba knows substantially more about the structure of the problem. For example, through inspection, it knows that `sigma2`, `parameters`, and `data` are all double precision NumPy arrays that are contiguous in memory. This means that the ith element of the array is exactly $8 \times i$ bytes away from the first and that consecutive elements are 8 bytes apart. This means that looping up elements in these arrays is much faster than in Python. There are also gains since Numba knows these are all double precision arrays and so the elements are plain double precision numbers which have native operations for addition and multiplication. When Numba adds or multiplies these numbers it doesn't waste time looking up the function to add these – it can just issue the CPU instruction to add or multiply these numbers.

In some cases, it may be desirable to give more information to Numba. This can be done by describing the inputs and outputs to `jit`. In the code below, `double[::1]` means 1-dimensional `float64` array that is contiguous in memory (`float` in Python, which corresponds to double precision in C), `double` indicates a scalar double precision number and `int64` indicates a 64-bit integer. The string tells Numba to return a 1-dimensional double precision array, and that the inputs are 3 1-dimensional arrays containing doubles followed by 2 64-bit integers and finally a scalar double.

```
>>> garch_recursion_numba_descr = jit('double[::1](double[::1], double[::1], double[::1],
    int64, int64, double)')(garch_recursion)
```

Running the timing code, there is a no gain over the automatic version. In most cases the difference between the two versions is negligible and the additional effort is usually only helpful if Numba cannot infer types on its own.

```
>>> %timeit garch_recursion_numba_descr(parameters, data, sigma2, p, q, backcast)
41.5 us +/- 693 ns per loop (mean +/- std. dev. of 7 runs, 10000 loops each)

>>> f'The speed-up is {0.0275/0.0000415 - 1.0:.1f} times'
'The speed-up is 661.7 times'
```

The pure Python dot product can also be easily converted to Numba using only the `@jit` decorator.

```
def pydot(a, b):
    M,N = shape(a)
    P,Q = shape(b)
    c = zeros((M,Q))
    for i in range(M):
        for j in range(Q):
            for k in range(N):
                c[i,j] += a[i,k] * b[k,j]
    return c


@jit
def pydot_jit(a, b):
    M,N = shape(a)
    P,Q = shape(b)
    c = zeros((M,Q))
    for i in range(M):
        for j in range(Q):
            for k in range(N):
                c[i,j] += a[i,k] * b[k,j]
    return c
```

Timing both the simple `jit` version and the `jit` with input descriptions produce large gains, although the performance of the two versions is similar. The input declaration in `jit` uses the notation `double[:,::1]`

which tells Numba to expect a 2-dimensional array using row-major ordering, which is the default in NumPy.

```
>>> a = randn(100, 100)
>>> b = randn(100, 100)
>>> %timeit pydot(a,b)
873 ms +/- 25.1 ms per loop (mean +/- std. dev. of 7 runs, 1 loop each)

>>> %timeit -r 10 pydot_jit(a,b)  # -r 10 uses 10 instead of 3
1.01 ms +/- 18.8 us per loop (mean +/- std. dev. of 10 runs, 1000 loops each)

>>> f'The speed-up is {0.873/.00101 - 1.0:.1f} times'
 'The speed-up is 863.4 times'

>>> pydot_jit_descr = jit('double[:,::1](double[:,::1],double[:,::1])')(pydot)
>>> %timeit -r 10 pydot_jit_descr(a,b)
%timeit -r 10 pydot_jit_descr(a,b)
```

24.2 Supported Python Features

Numba is continually evolving and generally releases a new version monthly. This section focuses on a subset of available features and the full, up-to-date list of available features is available in the Numba documentation (http://numba.pydata.org).

Numba has support for a small set of core Python features that are useful for numerical work. Numba supports two modes of operation: *object mode* and *nopython mode*. Object mode is slow and would normally not be any faster than Python. Nopython mode requires that every command in a function can be translated to LLVM IR so that a fast version can be compiled to machine code without interfacing with the Python runtime. The list of supported features only includes those which can be used in nopython mode.

Basic data types such as `bool`, `int`, `float`, and `complex` are all supported. `tuple`s are fairly well supported including construction, unpacking and iteration across the elements of a tuple. `list`s are supported but only if they contain a homogeneous data type. In general, it is better to use a NumPy array than a list since the generality of lists imposes additional overheads. `set`s are also supported but only if homogeneous.

Many of the built-in functions are supported including `bool`, `int`, `float`, `complex`, `len`, enumerate, and `range`. Many functions in the `cmath` and `math` modules are supported such as `abs`, `exp`, `log` and trigonometric functions. Many of the same functions are supported if imported from NumPy, and so it isn't strictly necessary to use these modules unless intentionally avoiding NumPy. Many functions from the standard library `random` are also available. However, since the same functions are also supported when imported from NumPy, there is little reason to use the standard library's random module.

24.3 Supported NumPy Features

Numba is continually evolving and generally releases a new version monthly. This section focuses on a subset of available features and the full, up-to-date list of available features is available in the Numba documentation (http://numba.pydata.org).

Numba has added support for a large swath of NumPy features including array creation, array concatenation, core mathematical functions, nearly all NumPy *ufunc*s[2], the NumPy random number generator (`numpy.random`)

---

[2]A NumPy ufunc is a function that operated element by element and supports broadcasting when called with more than one input.

and a core subset of the linear algebra module (`numpy.linalg`). While the support for NumPy is fairly pervasive, there are many caveats and it isn't reasonable to expect a complex function, even if NumPy only, to be supported. For example, many of the supported functions only support the most common inputs, linear algebra support is only available for 1- and 2-dimensional arrays containing single-precision, double-precision, or complex arrays, and in many cases automatic type promotion is not implemented (e.g. functions that accept double-prevision but return complex in certain cases).

Array Creation and Concatenation

Direct creation of arrays using `array` is supported. Creating multidimensional arrays is supported although these *must* be constructed using nested tuples rather than nested lists. Standard methods of special arrays including `empty`, `zeros`, `ones`, and `fill` are all supported. The *_`like` methods are also supported (e.g., `empty_like`). These all support only 2 input – the required input (either `object` or `shape`) and the `dtype` (`fill` also accepts the fill values). Other array creation methods supported include `arange`, `linspace`, `eye`, and `identity`. These also have limitations The common array concatenation function, `concatenate`, `column_stack`, `dstack`, `hstack`, and `vstack` are all supported.

Array Properties and Functions

Most array properties such as `ndim`, `size`, `shape`, `dtype`, and `T` (transpose) are supported, as are most array methods are supported, including

```
all, any, argmax, argmin, cumprod, cumsum, max, mean
min, nonzero, prod, std, sum, var
```

Common array functions including sorting (`argsort`, `sort`), `copy`, `diag`, reshaping (`ravel`, `flatten`, `diag`), and location lookup (`where`) are all supported.

Array Indexing

Arrays can be accessed using many of the common index methods. The most useful method to access elements in an array is scalar selection, although more complex access including slicing is permitted. One important difference to standard NumPy indexing is that list indexing is not supported. This prevents certain types of dimension-preserving selection. For example,

```
>>> def list_sel(x, i):
...     return x[[i]]

>>> nb_list_sel = jit(list_sel, nopython=True) # Error
InternalError: unsupported array index type list(int64) in [list(int64)]

>>> x = randn(4,4)
>>> list_sel(x,2)
array([[-0.46901103, -0.0850643 , -0.89310329,  0.66715405]])
```

The solution is to use slice indexing to preserve dimension.

```
>>> def slice_sel(x, i):
...     return x[i:i+1]

>>> nb_slice_sel = jit(slice_sel, nopython=True)
>>> slice_sel(x,2)
array([[-0.46901103, -0.0850643 , -0.89310329,  0.66715405]])
```

Leading examples of ufuncs include `exp`, `log`, `sqrt`, `isnan`, trigonometric functions the logical functions (e.g., `sin`, `cos`, etc.) and the logical functions (e.g., `logical_and`, `logical_or`, etc.).

```
>>> nb_slice_sel(x,2)
array([[-0.46901103, -0.0850643 , -0.89310329,  0.66715405]])
```

ufunc Support

Universal functions, or ufuncs, are NumPy functions that operate element-by-element. Since these are fundamentally scalar functions, NumPy automatically provides support for broadcasting when there are multiple inputs. There are dozens of ufuncs including basic math (e.g., `add`, `multiply`), `exp` and `log`, powers (e.g., `sqrt` and `reciprical`), trigonometric functions, bit-twiddling functions (e.g., `bitwise_and`), logical functions (e.g., `greater`, `less_than` and `logical_and`), and rounding (e.g., `ceil` and `trunc`). Numba also supports the creation of user-defined ufuncs using the `@vectorize` decorator (see Section 24.3.2).

Linear Algebra

A core set of the linear algebra library is supported including matrix multiplication (`@` in Python 3.5+, `dot`). There are important limitations to many of the supported linear algebra functions. In particular, most only operate on 1- or 2-dimensional arrays of the same type and do not support returning a type that is different from the input type (e.g. returning complex if the input is real).

Class	Supported Functions
Multiplication	`@` (Python 3.5+), `dot`, `vdot`
Eigenvalues and vectors	`eig`, `eigh`, `eigvals`, `eigvalsh`
Matrix powers	`cholesky`, `inv`, `matrix_power`, `pinv`
Rank	`cond`, `matrix_rank`, `det`, `slogdet`
Factorization	`qr`, `svd`
Estimation and solving	`lstsq`, `solve`

Random Number Generation

Numba supported a *vendorized* version of NumPy's random number generator. Numba maintains has a separate copy of the code underlying NumPy's random modules and these two may differ in subtle ways. The most important difference is that when using functions from `numpy.random` inside a just-in-time compiled function, the state of the RNG is completely independent of the state of the NumPy random number generator. The only way to get or set the state or to seed the RNG used by Numba is to wrap the corresponding function from NumPy in a `@jit` decorated function and to call this function. Direct calls to `numpy.seed` or `numpy.set_state` will not affect the Numba RNG. The next two blocks of code demonstrate this issue. The first calls show that the Numba and NumPy RNGs will generate the same sequences when both set with the same seed. The next set of calls shows that the two do not share the same underlying RNG state. In particular, after setting the seed in Numba but not NumPy, the random numbers generated differ since the state is no longer identical.

```
from numpy.random import randn

@jit
def set_nb_seed(seed):
    np.random.seed(seed)

@jit
def nb_randn(n):
    return randn(n)
```

```
>>> import numpy.random
>>> numpy.random.seed(0)
>>> set_nb_seed(0)
>>> randn(2)
array([ 1.76405235,  0.40015721])

>>> nb_randn(2)
array([ 1.76405235,  0.40015721])

>>> set_nb_seed(0)
>>> nb_randn(2)
array([ 1.76405235,  0.40015721])

>>> randn(2)
array([ 0.97873798,  2.2408932 ])
```

Other Functions

The support for NumPy is extensive and support extends to most nan-aware functions (e.g. `nanmean`, `nanstd`), `median` calculation, and differencing (`diff`). The NumPy type functions (e.g., `int32`, `uint8`, `float32`, `double` and `complex`) which can be used to cast a value are also supported using either scalar or array inputs.

24.3.1 Example: Multivariate Time-series Simulation

A simple example showing the support for NumPy function in Numba is the generation of a process driven from a hidden state. This is the type of process that the Kalman filter is frequently applied to. The mainfunction simulates a process that can be described by two equations

$$\alpha_t = T\alpha_{t-1} + \eta_t$$
$$y_t = Z\alpha_t + \varepsilon_t$$

where η_t and ε_t are i.i.d. Gaussian random variables with $\eta_t \sim N(0,R)$ and $\varepsilon_t \sim N(0,H)$ and η_t and ε_t are independent from each other.

```python
from numpy import zeros, empty
from numpy.linalg import cholesky
from numpy.random import randn

def kalman_simulate(tau,T,R,Z,H):
    H12 = cholesky(H)
    R12 = cholesky(R)
    k = H.shape[0]
    m = R.shape[0]
    eps = randn(tau,k) @ H12
    eta = randn(tau,m) @ R12
    alpha = empty((tau,m))
    y = empty((tau,k))
    alpha[0] = eta[0] @ (eye(m) - T@T)
    y[0] = alpha[0] @ Z + eps[0]
    for t in range(1, tau):
        alpha[t] = alpha[t-1] @ T + eta[t]
        y[t] = alpha[t] @ Z + eps[t]

    return alpha, y

kalman_simulate_jit = jit(kalman_simulate, nopython=True)
```

This first run simulates a trivariate system with a bivariate hidden state. The gains from using Numba are reasonable – a factor of 5 – although much smaller than in really simple scalar code.

```
>>> tau = 1000
>>> k = 3
>>> m = 2
>>> H = 0.7 * np.eye(k) + 0.3 * np.ones((k,k))
>>> R = (eye(m) - (ones((m,m)) - eye(m)) / m)
>>> T = 0.9 * eye(m)
>>> Z = 2 * (rand(m,k) - 1)
>>> kalman_simulate_jit(tau, T, R, Z, H)
>>> %timeit kalman_simulate(tau, T, R, Z, H)
5.51 ms +/- 48.4 us per loop (mean +/- std. dev. of 7 runs, 100 loops each)

>>> %timeit kalman_simulate_jit(tau, T, R, Z, H)
826 us +/- 9.45 us per loop (mean +/- std. dev. of 7 runs, 1000 loops each)
```

This second example shows that when the dimension of the problem is increased, the gains from JIT compilation are smaller. This process has a 100-dimensional observable driven by a 10-dimensional hidden process. The gains seem smaller and the performance only differs by a factor or 2. However, the actual wall time difference is virtually identical, about 4.5 seconds. This occurs since the computational effort inside the functions that multiply matrices or generate random numbers has increased when the loop overhead is constant.

```
>>> tau = 1000
>>> k = 100
>>> m = 10
>>> H = 0.7 * np.eye(k) + 0.3 * np.ones((k,k))
>>> R = (eye(m) - (ones((m,m)) - eye(m)) / m)
>>> T = 0.9 * eye(m)
>>> Z = 2 * (rand(m,k) - 1)
>>> %timeit kalman_simulate(tau, T, R, Z, H)
9.21 ms +/- 320 us per loop (mean +/- std. dev. of 7 runs, 100 loops each)

>>> %timeit kalman_simulate_jit(tau, T, R, Z, H)
4.29 ms +/- 226 us per loop (mean +/- std. dev. of 7 runs, 100 loops each)
```

24.3.2 Custom universal functions

Numba includes a decorator `@vectorize` that can turn any function that uses supported features of Python and NumPy, accepts scalar inputs, and has a scalar output into a NumPy universal function. Decorated functions will automatically broadcast inputs if broadcasting is required. Consider a simple function that computes the largest root of a 3-lag auto regression,

$$y_t = \phi_1 y_{t-1} + \phi_2 y_{t-2} + \phi_3 y_{t-3} + \varepsilon_t.$$

A scalar function that implements this is simple to write using `abs`, `max`, `array` and `roots`, which are all supported by Numba. The input types have been specified as `complex128` even though they are not complex to ensure that Numba uses a version of `roots` that supports complex-valued roots. Failure to provide forced typing results in an error.

```
from numpy import abs, reciprocal, roots
from numba import vectorize, float64, complex128

@vectorize([float64(complex128,complex128,complex128)])
def largest_root(p1,p2,p3):
    return reciprocal(abs(roots(array([-p3,-p2,-p1,1])))).max()
```

The universal function `largest_root` can now be used with vector inputs and broadcasting. The second and third show that this can be broadcast and can produce outputs that match the broadcast input dimensions.

```
>>> p1 = linspace(-3, 3, 100)
>>> p2 = linspace(-3, 3, 100)
>>> p3 = linspace(-1, 1, 100)
>>> largest_root(p1,p2,p3)
array([ 1.00000328,  1.11734959,  1.13729174,  1.14723969,  1.15234918,
        ...
        3.59560429,  3.65864182,  3.72160503,  3.78449737,  3.8473221 ])
>>> p1.shape = (100,1)
>>> absroot = largest_root(p1,p2,p3)
>>> absroot.shape
(100, 100)

>>> p1.shape = (100,1,1)
>>> p2.shape = (1,100,1)
>>> p3.shape = (1,1,100)
>>> absroot = largest_root(p1,p2,p3)
>>> absroot.shape
(100, 100, 100)

>>> %timeit largest_root(p1,p2,p3)
5.15 s +/- 128 ms per loop (mean +/- std. dev. of 7 runs, 1 loop each)
```

The `vectorize` decorator also supports execution on multiple cores or even the GPU. When the universal function is sufficiently long-running there can be large gains to using one of these modes.

```
@vectorize([float64(complex128,complex128,complex128)], target='parallel')
def largest_root(p1,p2,p3):
    return reciprocal(abs(roots(array([-p3,-p2,-p1,1])))).max()
```

Executing the ufunc in parallel on a 2 core machine shows near perfect scaling.

```
>>> absroot = largest_root(p1,p2,p3)
>>> %timeit largest_root(p1,p2,p3)
1.96 s +/- 12 ms per loop (mean +/- std. dev. of 7 runs, 1 loop each)
```

24.4   Diagnosing Performance Issues

When Numba cannot convert Python code to native code, it will make calls to standard Python. This has a negative impact on performance if it occurs inside a tight loop. To understand which lines might be problematic, first, execute the just-in-time compiled function and then call *jit_func* `.inspect_types()` to produce a line-by-line report. While this report is relatively technical, lines that might cause performance issues will contain `:: pyobject`. If these occur inside a loop, then it might be necessary to remove these Python calls and to manually replace them with simpler code that Numba can understand.

Some changes that have been helpful in producing fast Numba code include:

- When in doubt, if possible, follow the KISS principle – Keep It Simply Scalar. Scalar code support is essentially complete so nopython model compilation of scalar functions will nearly always succeed.

- Keep the code purely numeric and minimize function calls, except `range` if possible. It is possible to call other `jit` compiled functions in a Numba function.

- Avoid calling complex NumPy functions or functions from any other module.

- Start with the inner-most loop and work outward. In deeply nested loops the gains to JIT acceleration of loops further out are lower than those on the inside since they are called fewer times.

- Numpy functions that are not currently supported in Numba can often by implemented in pure Python and JIT compiled so that they are not required.

- If loops are not accelerated, add type information, as in `@jit(float64(float64[:,::1]))`.

- If, after adding type information for inputs, loops are still not accelerated, add type information about local variables. This information can be added using a dictionary where the keys are local variable names and the values are Numba types. For example,

```python
from numba import jit, double, int32
locals = {'var1': double[:], 'var2': int32}
@jit(float64(float64[:,::1]), locals = locals)
```

A continuous time stochastic volatility model will be used to illustrate some of the issues in converting a moderately complex piece of code for use with Numba. The model is described by the two equations

$$
\begin{aligned}
dp_t &= \mu dt + \exp(\beta_0 + \beta_1 v_t)\, dw_t \\
dv_t &= \alpha v_t dt + dv_t
\end{aligned}
$$

where $T = 1$ indicates 1 day. The model parameters are $\mu = 0.03$, $\alpha = -0.100$, $\beta_0 = 0$, $\beta_1 = 0.125$, $\rho = \text{Corr}[dw_t, dv_t] = -0.62$. Pure Python code to implement the model is presented below.

```python
import numpy as np

# Setup
T = 10000# 1 year
nstep = 23400   # 1 second
p0, v0 = 0.0, 0.0

# Model Parameters
mu = 0.03
b0 = 0.000
b1 = 0.125
alpha = -0.100
rho = -0.62
# Initialize daily vectors
log_closing_price = np.zeros(T, dtype=np.float64)
integrated_variance = np.zeros(T, dtype=np.float64)
# Initialize intradaily vectors
v = np.zeros(nstep + 1, dtype=np.float64)
spot_vol = np.zeros(nstep + 1, dtype=np.float64)
p = np.zeros(nstep + 1, dtype=np.float64)
p[0] = p0
v[0] = v0

R_root = np.linalg.cholesky(np.array([[1, rho], [rho, 1]])).T

dt = 1.0 / nstep #/ 252
root_dt = np.sqrt(dt)

for t in range(T):
    e = np.random.standard_normal((nstep, 2)).dot(R_root) * root_dt
    dwp = e[:, 0]
    dwv = e[:, 1]
    # Replacement function
    # innerloop_jit(mu, alpha, b0, b1, nstep, p, v, spot_vol, dt, dwv, dwp)
```

```
    # Key loop
    #for i in range(1, nstep + 1):
    #    dv = alpha * v[i - 1] * dt + dwv[i - 1]
    #    v[i] = v[i - 1] + dv
    #    spot_vol[i] = np.exp(b0 + b1 * v[i - 1])
    #    dp = mu * dt + spot_vol[i] * dwp[i - 1]
    #    p[i] = p[i - 1] + dp

    # Save data
    integrated_variance[t] = np.mean(spot_vol ** 2.0)
    log_closing_price[t] = p[-1]

    # Reset the first price for the next day
    p[0] = p[-1]
    v[0] = v[-1]
```

The first step in converting code is to extract the core loop so that it can be converted into a function.

```
for i in range(1, nstep):
    dv = alpha * v[i - 1] * dt + dwv[i]
    v[i] = v[i - 1] + dv
    spot_vol[i] = np.exp(b0 + b1 * v[i - 1])
    dp = mu * dt + spot_vol[i] * dwp[i]
    p[i] = p[i - 1] + dp
```

In this example the code in the function was already basic scalar code and so there was no need to further alter it, aside from adding the `def` line and adding the decorator `@jit`. The final step is to comment out the loop in the original code and to uncomment the function call to `innerloop_jit`.

```
from numba import jit

@jit
def innerloop(mu, alpha, b0, b1, nstep, p, v, spot_vol, dt, dwv, dwp):
    for i in range(1, nstep):
        dv = alpha * v[i - 1] * dt + dwv[i]
        v[i] = v[i - 1] + dv
        spot_vol[i] = np.exp(b0 + b1 * v[i - 1])
        dp = mu * dt + spot_vol[i] * dwp[i]
        p[i] = p[i - 1] + dp
```

It might be tempting to wrap both the inner loop and the other loop. At the time of writing, Numba cannot compile this function – however line profiling shows that 99.5% of the time is spent in the inner loop, and the other 0.5% of the time on the random number generator. Once the JIT function is included, 86.2% of the time is still spent in the inner loop and 12.9% is in generating the random numbers. Most importantly, the total run time of the program drops from 158 to 3.23 seconds when simulating 10,000 days of data, a speed up by a factor of 50. JIT compiling the entire function would be unlikely to bring further gains.

24.5   Replacing Python function with C functions

Some Python functions are not natively available in Numba, and so including these in a loop can deteriorate performance. This code uses the `ctypes` modules to import the standard C library which contains common mathematical functions, and then provides a simple interface to the exponential function. `argtypes` is a list of input argument types and `restype` contains the type of the value returned.

```
import numpy as np
from ctypes import *
from math import pi
from numba import jit, double
```

```
proc = cdll.msvcrt
# Linux/OSX
# proc = CDLL(None)

c_exp = proc.exp
c_exp.argtypes = [c_double]
c_exp.restype = c_double

@jit
def use_numpy_exp(x):
    return np.exp(x)

@jit
def use_c_exp(x):
    return c_exp(x)
```

After calling both compiled functions with a double (e.g., 1.0), `.inspect_types()` shows that neither version requires a Python call (object mode). The C version is slightly simpler since it can directly call the C function. The output of `use_numpy_exp.inspect_types()` is

```
use_numpy_exp (float64,)
@jit

def use_numpy_exp(x):

    # --- LINE 16 ---
    # label 0
    #   x = arg(0, name=x)   :: float64
    #   $4load_method.1 = getattr(value=$2load_global.0, attr=exp)   :: Function(<ufunc '
      exp'>)
    #   del $2load_global.0
    #   del x
    #   del $4load_method.1
    #   $10return_value.4 = cast(value=$8call_method.3)   :: float64
    #   del $8call_method.3
    #   return $10return_value.4

    return np.exp(x)
```

The output of `use_c_exp.inspect_types()` is

```
use_c_exp (float64,)

@jit

def use_c_exp(x):

    # --- LINE 20 ---
    # label 0
    #   x = arg(0, name=x)   :: float64
    #   $2load_global.0 = global(c_exp: <_FuncPtr>)   :: ExternalFunctionPointer((float64
      ,) -> float64)
    #   del x
    #   del $2load_global.0
    #   $8return_value.3 = cast(value=$6call_function.2)   :: float64
    #   del $6call_function.2
    #   return $8return_value.3

    return c_exp(x)
```

24.6   Other Features of Numba

Numba is too large to fully describe in a single chapter. In particular, there are a number of features that have not been described. The most important of these features is the ability to write code that executed on either the on Nvidia GPUs that is compiled using LLVM and CUDA or on Heterogeneous System Architectures (HSAs) such as some AMD CPUs. Targeting these platforms can produce huge performance gains in some applications. Another useful feature is the ability to compile function Ahead of Time (AOT) which allows both the feature to be used without the warm-up compilation as well as the possibility of distributing the function for use in Python without requiring Numba to be installed. Numba has also been extended to all JIT compilation of classes (with many restrictions) and so it is possible to use the features of OOP in conjunction with Numba.

24.7   Exercises

1. Write a Python function which will accept a $p+q+1$ vector of parameters, a T vector of data, and p and q (integers, AR and MA order, respectively) and recursively compute the ARMA error beginning with observation $p+1$. If an MA index is negative it should be backcast to 0.

2. Use `jit` to accelerate the ARMA function written in the exercise 1. Compare the speed to the pure Python implementation.

Chapter 25

Improving Performance using Cython

Cython is a powerful, but somewhat complex, solution for situations where pure NumPy or Numba cannot achieve performance targets. Cython is a creole of Python and C, and so some familiarity, mostly with C datatypes, is helpful. Cython translates its hybrid Python code into C code, which can then be compiled into a Python extension. Cython code has a number of distinct advantages over Numba's just-in-time compilation of Python code:

- Cython modules are statically compiled and so using a Cython module does not incur a "warm-up" penalty due to just-in-time compilation.

- A Python extension produced by Cython can be distributed to other users and does not require Cython to be installed. In contrast, Numba must be installed and performance gains may vary across Numba or LLVM versions.

- Numba is a relatively new, rapidly evolving project , and so code that works in one version might break in a future version.

- Cython can be used interface to existing C/C++ code.

Using Cython on Linux is relatively painless and only requires that the system compiler is installed in addition to Cython. Using Cython on OSX requires that XCode or at least the command line tools for Xcode have been installed. To use Cython in Python x64 Windows, it is necessary to have the x64 version of Cython installed along with Visual Studio 2014 or later. All editions including the free Community edition provide the required C compiler.

Using Cython can be broken down into a two-step process. The first is to write standard Python. The second is to add some special syntax and hints about the type of data used. This first example will use the same GARCH(P,Q) code as in the Numba example. Applying Cython to an existing Python function requires a number of steps (for standard numeric code):

- Save the file with the extension pyx – for Python Extension.

- Use `cimport`, which is a special version of `import` for Cython, to import both `cython` and `numpy` `as` `np`.

- Declare types for *every* variable:

  - Scalars have standard C-types, and in almost all cases should be `double` (same as `float64` in NumPy, and `float` in Python), `int` (signed integer), `uint` (unsigned integer), or `size_t` (system unsigned integer type). `size_t` would typically only be used to counter variables in loops.

- NumPy arrays should have a memory view type. These resemble C types, but also indicate the number of dimensions, the order of data in the array, and whether that data in the array is contiguous in memory. For example, a 1-dimensional array containing double (float64 in NumPy, float in Python) is indicated by `double[:]`, a 2-dimensional array is indicated `double[:, ::1]` where the `::1` indicates that the array is contiguous and in C order. Arrays containing other data types can be similarly typed, e.g. `int[:,:,::1]` for a 3-dimensional array of integers or `float[::1, :]` for a 2-d *single-precision array in Fortran order* (note the position of `::1` in the declaration). While either C or Fortran ordered arrays can be used, C ordering is the default in NumPy. It is important to specify as much as possibly about the array – using `double[:]` and `double[::1]` will produce code that runs at different speed since `double[::1]` instructs Cython that you are passing an array that is contiguous so that the elements are contiguous in memory. Iterating across arrays that are contiguous requires fewer calculations to determine the position of the next element.

- Declare all arrays as `not None`.

- Ensure that all array access uses only single item access and not more complex slicing. For example is `x` is a 2-dimensional array, `x[i,j]` must be used and not `x[i, :]` or `x[:,j]`.

- Add decorators to disable Python safety checks. Naturally, it is important to verify that these checks are not needed, and if they are, problems like memory corruption or crashes of Python may occur. The most important of these are

  - `@cython.boundscheck(False)` - Do not check for access beyond the end of an array
  - `@cython.wraparound(False)` - Do not allow negative indexing
  - `@cython.cdivision(True)` - Do not check for division by zero

The Cythonized version of the GARCH(P,Q) recursion is presented below. All arrays are declared using `double[:]` and so the inputs must all have 1 dimension (and 1 dimension only). The inputs `p` and `q` are declared to be integers, and `backcast` is declared to be a `double`. The three local variables `T`, `i` and `j` are all declared to be `int`s. Note that is crucial that the variables used as iterators are declared as `int` (or other integer type, such as `uint` or `size_t`). The remainder of the function is *unchanged*.

```python
# garch_ext.pyx
import numpy as np
cimport numpy as np
cimport cython

@cython.boundscheck(False)
@cython.wraparound(False)
def garch_recursion(double[::1] parameters not None,
                    double[::1] data not None,
                    double[::1] sigma2 not None,
                    int p,
                    int q,
                    double backcast):
    cdef int T = np.size(data, 0)
    cdef int i, j

    for i in range(T):
        sigma2[i] = parameters[0]
        for j in range(1, p + 1):
            if (i - j) < 0:
```

```
                    sigma2[i] += parameters[j] * backcast
            else:
                    sigma2[i] += parameters[j] * (data[i - j] * data[i - j])
        for j in range(1, q + 1):
            if (i - j) < 0:
                    sigma2[i] += parameters[p + j] * backcast
            else:
                    sigma2[i] += parameters[p + j] * sigma2[i - j]

    return sigma2
```

Two additional decorators were included in the Cython version of the function, `@cython.boundscheck(False)` and `@cython.wraparound(False)`. The first disables bounds checking which speeds up the final code, but is dangerous if the data used in the loop has fewer elements than expected. The second rules out the use of negative indices, which is simple to verify and enforce.

The next step is to write a `setup.py` file which is used to convert the extension to C and compile it. The code is located in a file named `garch_ext.pyx` which will be the name of the extension. The setup code for a basic Cython extension is simple and is unlikely to require altering (aside from the extension and file name).

```
# setup.py
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext
import numpy

setup(
    cmdclass = {'build_ext': build_ext},
    ext_modules = [Extension("garch_ext", ["garch_ext.pyx"])],
    include_dirs = [numpy.get_include()]
)
```

The final step is to build the extension by running `python setup.py build_ext --inplace` from the terminal. This will produce `garch_ext`*version-os*`.pyd` which contains the compiled code where *version-os* will depend on the version of Python used as well as the underlying operating system.

```
>>> parameters = array([.1,.1,.8])
>>> data = randn(10000)
>>> sigma2 = zeros(shape(data))
>>> p,q = 1,1
>>> backcast = 1.0
>>> %timeit garch_recursion(parameters, data, sigma2, p, q, backcast)
27.9 ms +/- 258 us per loop (mean +/- std. dev. of 7 runs, 10 loops each)

>>> import garch_ext
>>> %timeit garch_ext.garch_recursion(parameters, data, sigma2, p, q, backcast)
55.1 us +/- 1.08 us per loop (mean +/- std. dev. of 7 runs, 10000 loops each)

>>> f'The speed-up is {.0279/.0000551 - 1.00:.1f} times'
'The speed-up is 505.4 times'
```

The Cythonized version is about 400 times faster than the standard Python version, and only required about 3 minutes to write (after the main Python function has been written). However, it is slower than the Numba version of the same function.

The function `pydot` was similarly Cythonized. This Cython program demonstrates how arrays should be allocated within the function which use a slightly different syntax. Arrays to be output should use the buffer syntax which is *type*`[::1]` as in `double[::1]` where *type* indicates the type of the array to create (e.g. `double` for most floating point data types). Higher dimension arrays should use the appropriate shape declaration (e.g., `:, ::1` for a 2-D array, `:, :, ::1` for a 3-D array).

```python
import numpy as np
cimport numpy as np
cimport cython

@cython.boundscheck(False)
@cython.wraparound(False)
def pydot(double[:, ::1] a not None,
          double[:, ::1] b not None):
    cdef int M, N, P, Q
    M,N = np.shape(a)
    P,Q = np.shape(b)
    assert N==P
    cdef double[:, ::1] c = np.zeros((M,N), dtype=np.float64)
    for i in range(M):
        for j in range(Q):
            for k in range(N):
                c[i,j] = c[i,j] + a[i,k] * b[k,j]
    return c
```

The Cythonized function is about 350 times faster than straight Python, although it is still much slower than the native NumPy routine underlying `@`.

```python
>>> a = randn(100,100)
>>> b = randn(100,100)
>>> %timeit pydot(a,b)
907 ms +/- 29.4 ms per loop (mean +/- std. dev. of 7 runs, 1 loop each)

>>> import pydot as p
>>> %timeit p.pydot(a,b)
2.72 ms +/- 40.4 us per loop (mean  std. dev. of 7 runs, 100 loops each)

>>> f'The speed-up is {0.907/0.00272- 1.0:.1f} times'
'The speed-up is 332.5 times'

>>> %timeit a @ b
24.8 us +/- 3.55 us per loop (mean +/- std. dev. of 7 runs, 100000 loops each)

>>> f'The speed-up is {0.00272/0.0000248 - 1.0:.1f} times'
'The speed-up is 108.7 times'
```

The final example will produce a Cython version of the weighted average. Since the original Python code used slicing, this is removed and replaced with a second loop.

```python
def naive_weighted_avg(x, w):
    T = x.shape[0]
    m = len(w)
    m12 = int(ceil(m/2))
    y = zeros(T)
    for i in range(len(x)-m+1):
        for j in range(m):
            y[i+m12] += x[i+j] * w[j]

    return y
```

This makes writing the Cython version simple.

```python
import numpy as np
cimport numpy as np
cimport cython

@cython.boundscheck(False)
```

```
@cython.wraparound(False)
def cython_weighted_avg(double[::1] x,
                        double[::1] w):
    cdef int T, m, m12, i, j
    T = x.shape[0]
    m = len(w)
    m12 = int(np.ceil(float(m)/2))
    cdef double[::1] y = np.zeros(T, dtype=np.float64)
    for i in range(T-m+1):
        for j in range(m):
            y[i+m12] += x[i+j] * w[j]

    return y
```

The Cython version can be compiled using a setup function in the same way that the GARCH recursion was compiled.

```
>>> w = array(r_[1:11,9:0:-1],dtype=float64)
>>> w = w/sum(w)
>>> x = randn(10000)
>>> %timeit naive_weighted_avg(x,w)
160 ms +/- 4.01 ms per loop (mean +/- std. dev. of 7 runs, 10 loops each)

>>> import cython_weighted_avg as c
>>> %timeit c.cython_weighted_avg(x,w)
251 us +/- 5.69 us per loop (mean +/- std. dev. of 7 runs, 1000 loops each)

>>> from numba import jit
>>> weighted_avg_jit = jit(naive_weighted_avg)
>>> %timeit weighted_avg_jit(x,w)
130 us +/- 4.75 us per loop (mean +/- std. dev. of 7 runs, 10000 loops each)
```
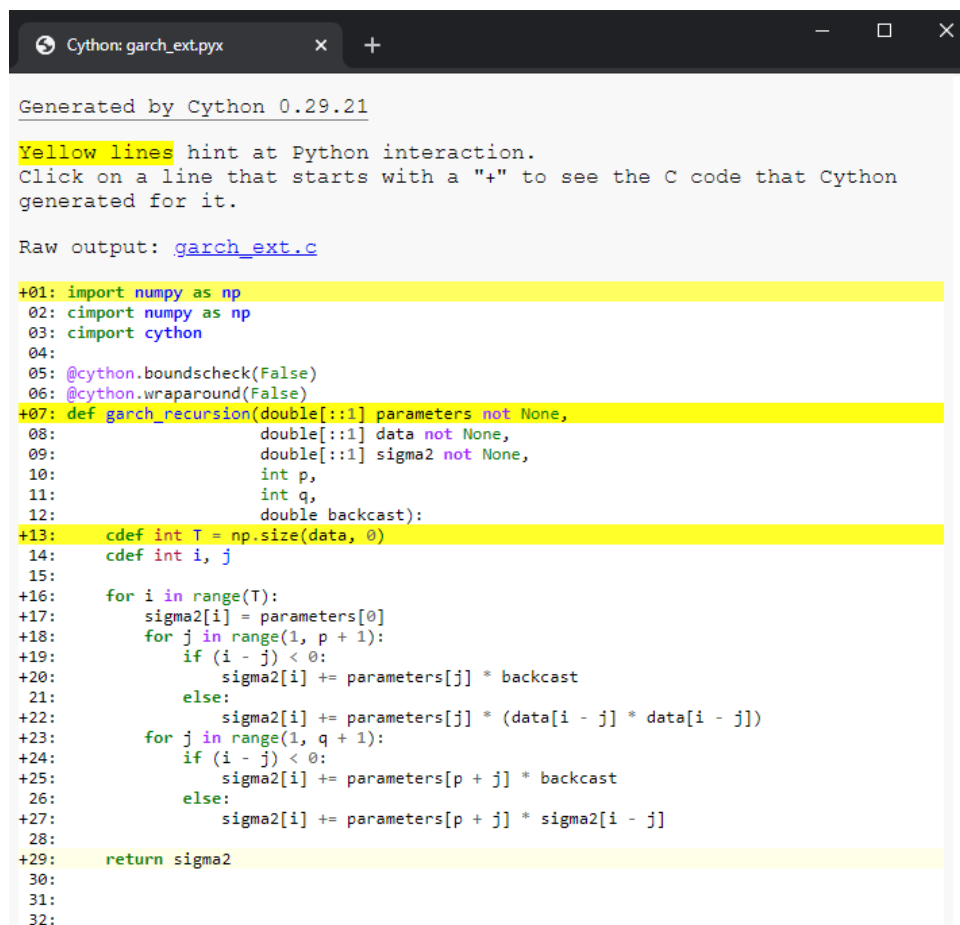
The gains are unsurprisingly large (around $500\times$) – however, the Cython code is no faster than the pure NumPy sideways version. This demonstrates that Cython is not a magic bullet and that good vectorized code, even with a small amount of looping, can be very fast. The final lines produce a Numba version of the same function, which is also much faster than the pure Python version. It is also faster than the Cython version.

25.1   Diagnosing Performance Issues

If a function contains calls to Python code which cannot be optimized by Cython, the performance of the compiled code may be similar to that in the original code. Fortunately, Cython provides a diagnostic facility to examine the Cython code for performance issues. This tool is run using the command `cython -a my_ext.pyx` which will produce a HTML report containing Cython code as well as the translated C (the C is hidden by default, double click on a line to see the translation). Highlighted lines indicate locations where the Cython interfaces with Python, which can be slow. An idealized function in Cython will have only three interface points. The first is at the top of the file, the second is the function definition line, which is required to get the data from Python and the final is in the return statement, which moves data back to Python.

Figure 25.1 shows the diagnostic output from running `cython -a garch_ext.pyx`. There are 5 highlighted lines. Three are those discussed above and are unavoidable. The remaining two are the `import numpy as np` and the call to `np.ones`, both of which require interfacing with Python. In general, the more highlighting the smaller the gains will be for converting a function to Cython. However, the most important consideration is to ensure that the core loop contains no Python calls. This important consideration is satisfied here, which is why the performance gains are large.

Figure 25.1: Diagnostic report produced by running `cython -a garch_ext.pyx`. Highlighted lines indicate performance concerns due to interfacing with Python.

25.1.1 Replacing Python function with C functions

Some algorithms require calling functions in the innermost loop. If left untreated, the Cython code will be no faster than standard Python code. To illustrate this issue, consider a simple recursion from an EGARCH model

$$\ln \sigma_t^2 = \omega + \alpha \left| r_{t-1}/\sigma_{t-1} \right| + \beta \ln \sigma_{t-1}$$

which can be expressed as a Python function

```python
import numpy as np

def egarch_recursion(parameters, data, backcast):

    T = np.size(data,0)
    lnsigma2 = np.zeros(T)
    sigma2 = np.zeros(T)
    lnsigma2[0] = backcast

    for t in range(1, T):
        sigma2[t-1] = np.exp(lnsigma2[t-1])
        lnsigma2[t] = parameters[0]
                    + parameters[1] * data[t-1] / sigma2[t]
                    + parameters[2] * lnsigma2[t-1]
    sigma2[T - 1] = np.exp(lnsigma2[t])

    return sigma2
```

A standard Cython version can be constructed using the same steps as above. This version declares an array in the function, and so it is important to declare the types of the array. This version also includes the decorator `@cython.cdivision(True)` which disables division by 0 warnings.

```python
import numpy as np
cimport numpy as np
cimport cython

@cython.boundscheck(False)
@cython.wraparound(False)
@cython.cdivision(True)
def egarch_recursion(double[::1] parameters not None,
                     double[::1] data not None,
                     double backcast):
    cdef int T = np.size(data, 0)
    cdef int t
    cdef double lnsigma2
    cdef double[::1] sigma2 = np.zeros(T, dtype=np.float64)

    lnsigma2 = backcast

    for t in range(1, T):
        sigma2[t - 1] = np.exp(lnsigma2)
        lnsigma2 = parameters[0] \
                 + parameters[1] * data[t - 1] / sigma2[t]  \
                 + parameters[2] * lnsigma2
    sigma2[T - 1] = np.exp(lnsigma2[t])

    return sigma2
```

Running `cython -a egarch_ext.pyx` produces the report in top panel of Figure 25.2, which shows that the call to `np.exp` is a performance concern since it requires interfacing with Python (dark highlighting).

Using NumPy's exp

Using the C library's exp

Figure 25.2: Diagnostic report produced by running `cython -a garch_ext.pyx`. The top panel shows high-lighted lines indicate performance concerns due to interfacing with Python. The bottom panel uses the C library's exponential and the loop will now execute quickly.

The solution to this problem is to replace the NumPy exponential with the standard math libraries exponential function which will not incur a penalty. This change is implemented using the `cdef extern` command which declares an external function that takes a float and returns a float.

```python
import numpy as np
cimport numpy as np
cimport cython

cdef extern from "math.h":
    double exp(double x)

@cython.boundscheck(False)
@cython.wraparound(False)
@cython.cdivision(True)
def egarch_recursion(double[::1] parameters not None,
                     double[::1] data not None,
                     double backcast):
    cdef int T = np.size(data, 0)
    cdef int t
    cdef double lnsigma2
    cdef double[::1] sigma2 = np.zeros(T, dtype=np.float64)

    lnsigma2 = backcast

    for t in range(1, T):
        sigma2[t - 1] = exp(lnsigma2)
        lnsigma2 = parameters[0] \
                  + parameters[1] * data[t - 1] / sigma2[t]  \
                  + parameters[2] * lnsigma2

    sigma2[T - 1] = exp(lnsigma2[t])

    return sigma2
```

The diagnostic report from this change is shown in the bottom panel of Figure 25.2.

25.2   Interfacing with External Code

The final, and most extreme, method to maximize performance is to interface with native code, usually in the form of some hand-written C/C++/Fortran or an existing DLL. There are a number of method to interface with existing code, including directly interfacing with Python using the API, wrapping code in Cython or SWIG, using ctypes to call compiled libraries (.dll on Windows, .so on Linux) and f2Py, which only works with Fortran. This section only discusses two methods – ctypes for interfacing with an existing DLL using a C interface and wraping a C file using Cython. Both examples will build on the GARCH recursion.

25.2.1   ctypes and Shared Libraries (DLL/so)

ctypes provides a simple method to call existing code in libraries that present a C interface. There are two main reasons why using a shared library might be better than directly interfacing with the code:

- The DLL/so is available but the source is not – as long as API documentation is available, the shared library can be directly used.

- The code in the DLL/so has complex dependencies – directly using the DLL, if it has been compiled to work stand-alone, does not require managing its dependencies.

- A different, higher performance compiler is required. DLLs can be compiled with any standard compliant compiler including the Intel C compiler, which allows advanced options such as autovectorization to be used. Code that is directly interfaced is usually compiled with the same compiled used to compile Python.

ctypes was previously used in the Numba example to import an external C function (`exp`). This example will show how to interface with both scalars and NumPy arrays. Two code files are required - the first is the header and the second contains the GARCH recursion that will be called from Python. First, the header,

```c
// garch_recursion.h

__declspec(dllexport) void garch_recursion(int T, double *parameters, double *data,
    double *sigma2, int p, int q, double backcast);
```

and then the main code. This function does not return anything and instead modifies the elements of `sigma2` directly.

```c
// garch_recursion.c
#include "garch_recursion.h"

#ifdef WIN32
#define WINAPI __declspec(dllexport)
#else
#define WINAPI
#endif

WINAPI void garch_recursion(int T, double *parameters, double *data, double *sigma2, int
    p, int q, double backcast)
{
    int i, j;
    for(i = 0; i<T; i++)
    {
        sigma2[i] = parameters[0];
        for (j=1; j<=p; j++)
        {
            if((i-j)<0)
            {
                sigma2[i] += parameters[j] * backcast;
            }
            else
            {
                sigma2[i] += parameters[j] * (data[i-j]*data[i-j]);
            }
        }
        for (j=1; j<=q; j++)
        {
            if((i-j)<0)
            {
                sigma2[i] += parameters[p+j] * backcast;
            }
            else
            {
                sigma2[i] += parameters[p+j] * sigma2[i-j];
            }
        }
    }
}
```

On Windows, the DLL can be built by running the commands

```
cl.exe -nologo -EHsc -GS -W3 -D_WIN32 -D_USRDLL -MD -Ox -c garch_recursion.c
link.exe /nologo /DLL garch_recursion.obj /OUT:garch_recursion.dll
```

On Linux, a shared library can be produced by running

```
gcc -O3 -Wall -ansi -pedantic -c -fPIC garch_recursion.c -o garch_recursion.o
gcc garch_recursion.o -shared -o garch_recursion.so
```

Once the DLL/so has been built, only the DLL/so is needed. First, the DLL/so is imported using the NumPy version of the ctypes' `load_library`. This is important when interfacing with NumPy arrays but is not required if only using scalar data. The second step is to use ctypes to import the library and declare both the argument and return types. Scalar types are obvious – they have the same name as in C. NumPy arrays use `POINTER(c_double)` (or another C type if not double precision). The final step is to write a wrapper around the imported code which simply calls the C routine, with the caveat that NumPy arrays must be called using *array*.`ctypes.data_as(ct.POINTER(ct.c_double))` (or another C type if the array contains something other than double precision floating point data) which calls the function with a pointer to the array's data rather than with the actual NumPy array.

```python
# garch_recursion_dll_wrapper.py
import ctypes as ct

import numpy as np

# Open the library
garchlib = np.ctypeslib.load_library("garch_recursion.dll", '.')
# Linux/OSX
# garchlib = np.ctypeslib.load_library("garch_recursion.so", '.')

# Define output and input types
garchlib.garch_recursion.restype = ct.c_void_p
garchlib.garch_recursion.argtypes = [ct.c_int,
                                      ct.POINTER(ct.c_double),
                                      ct.POINTER(ct.c_double),
                                      ct.POINTER(ct.c_double),
                                      ct.c_int,
                                      ct.c_int,
                                      ct.c_double]

# Wrapper function
def garch_recursion(parameters, data, sigma2, p, q, backcast):
    # Optional, but can be important if data is not contiguous
    # Will copy to temporary value, only if needed
    parameters = np.ascontiguousarray(parameters)
    data = np.ascontiguousarray(data)
    sigma2 = np.ascontiguousarray(sigma2)
    T = data.shape[0]
    return garchlib.garch_recursion(T,
                                    parameters.ctypes.data_as(ct.POINTER(ct.c_double)),
                                    data.ctypes.data_as(ct.POINTER(ct.c_double)),
                                    sigma2.ctypes.data_as(ct.POINTER(ct.c_double)),
                                    p,
                                    q,
                                    backcast)
```

Finally, it is useful to verify that the code works and to assess the performance gains, which are similar to the other compiled versions.

```
>>> import garch_recursion_dll_wrapper as dll
>>> %timeit dll.garch_recursion(parameters, data, sigma2, p, q, backcast)
60.3 us +/- 549 ns per loop (mean +/- std. dev. of 7 runs, 10000 loops each)
```

More information on using ctypes with NumPy is available in the SciPy cookbook, http://wiki.scipy.org/Cookbook/Ctypes.

25.2.2 Wrapping code with Cython

An alternative to using an existing a DLL is to directly interface the C code with Python using Cython to generate the interface. This example uses the same C and header files as in the DLL example, and so the only steps are to write the Cython file (pyx) and the setup. The Cython file has the usual header and the C function is referenced using `cdef extern from` *header file* . The function definition is identical to the previous Cython example that made use of a C function. The final step is to call the external code using a wrapper function. Best practice is to call `np.ascontiguousarray` on arrays to ensure that are contiguous – in other words, that the second element is adjacent to the first in the computer's memory. These can be omitted if the function will always be used on contiguous arrays, although the cost of using them on already contiguous arrays is very small while incorrect results will be produced if the arrays are non-contiguous. The final step is to call the C function passing NumPy arrays using a pointer to the first element &*array*[0]. Note that if passing multidimensional arrays, the pointer should be to the first element (e.g. &*array*[0, 0] for a 2-dimensional array or &*array*[0, 0, 0] for a 3-dimensional array).

```python
# garch_recursion_wrapper.pyx
import numpy as np
cimport numpy as np
cimport cython

cdef extern from "garch_recursion_standalone.h":
    void garch_recursion(int T, double * parameters, double * data, double * sigma2, int p,
               int q, double backcast)

@cython.boundscheck(False)
def garch_recursion_wrapped(double[:] parameters not None,
                            double[:] data not None,
                            double[:] sigma2 not None,
                            int p,
                            int q,
                            double backcast):
    cdef int T = np.size(data, 0)
    # Best practice is to ensure arrays are contiguous
    parameters = np.ascontiguousarray(parameters)
    data = np.ascontiguousarray(data)
    sigma2 = np.ascontiguousarray(sigma2)

    # No return, sigma2 modified in place
    garch_recursion(T, &parameters[0] , &data[0], &sigma2[0], p, q, backcast)

    return sigma2
```

The setup file is similar to the previous setup, only `sources` must be modified to include both the Cython file and the C source.

```python
# setup_garch_recursion_wrapper.py
import numpy
from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext

ext_modules = [Extension(
    name="garch_recursion_wrapper",
    sources=["garch_recursion_wrapper.pyx", "garch_recursion.c"],
    include_dirs = [numpy.get_include()])]

setup(
    name = 'garch_recursion_wrapper',
```

```
    cmdclass = {'build_ext': build_ext},
    ext_modules = ext_modules)
```

The hand-written module performs no better than any of the other methods, while it takes more time to implement the C function and wrap it. However, this example is somewhat misleading since most applications of these methods interface with *existing* C or C++ code.

```
>>> import garch_recursion_wrapper as wrapper
>>> %timeit wrapper.garch_recursion_wrapped(parameters, data, sigma2, p, q, backcast)
67.5 us +/- 2.21 us per loop (mean +/- std. dev. of 7 runs, 10000 loops each)
```

25.3 Exercises

1. Write a Python function which will accept a $p+q+1$ vector of parameters, a T vector of data, and p and q (integers, AR and MA order, respectively) and recursively computes the ARMA error beginning with observation $p+1$. If an MA index is negative it should be backcast to 0.

2. [Only for the brave] Convert the ARMA function to Cython, compile it, and compare the performance against both the pure Python and the Numba versions.

Chapter 26

Executing Code in Parallel

26.1 `map` and related functions

`map` is a built-in method to apply a function to a generic iterable. It is used as `map(` *function* , *iterable* `)`, and returns a list containing the results of applying *function* to each item of *iterable*. The list returned can be either a simple list if the function returns a single item, or a list of tuples if the function returns more than 1 value.

```
def powers(x):
    return x**2, x**3, x**4
```

This function can be called on any iterable, for example, a list.

```
>>> y = [1.0, 2.0, 3.0, 4.0]
>>> list(map(powers, y))
[(1.0, 1.0, 1.0), (4.0, 8.0, 16.0), (9.0, 27.0, 81.0), (16.0, 64.0, 256.0)]
```

`map` is a generator which defers generating results until required, and so `list` is used to force it to execute. The output is a list of tuples where each tuple contains the result of calling the function on a single input. In this case, the same result could be achieved using a list comprehension, which is the preferred syntax.

```
>>> [powers(i) for i in y]
[(1.0, 1.0, 1.0), (4.0, 8.0, 16.0), (9.0, 27.0, 81.0), (16.0, 64.0, 256.0)]
```

`map` can be used with more than 1 iterable, in which case it iterates using the length of the longest iterable. If one of the iterable is shorter than the other(s), then it is extended with `None`. It is usually best practice to ensure that all iterables have the same length before using `map`.

```
def powers(x,y):
    if x is None or y is None:
        return None
    else:
        return x**2, x*y, y**2
```

```
>>> x = [10.0, 20.0, 30.0]
>>> y = [1.0, 2.0, 3.0, 4.0]
>>> list(map(powers, x, y))
[(100.0, 10.0, 1.0), (400.0, 40.0, 4.0), (900.0, 90.0, 9.0), None]
```

A related function is `zip` which combines two or more lists into a single list of tuples. It is similar to calling `map` except that it will stop at the end of the shortest iterable, rather than extending using `None`.

```
>>> x = [10.0, 20.0, 30.0]
>>> c
>>> list(zip(x, y))
[(10.0, 1.0), (20.0, 2.0), (30.0, 3.0)]
```

26.2 `multiprocessing`

The real advantage of `map` over list comprehensions is that it can be combined with the `multiprocessing` module to run code on more than 1 (local) processor. *Note that on Windows, the* `multiprocessing` *module does not work correctly in IPython, and so it is necessary to use stand-alone Python programs.* `multiprocessing` includes a `map` function which is similar to that in the standard Python distribution except that it executes using a `Pool` rather than on a single processor. The performance gains to using a `Pool` may be large and should be close to the number of pool processes if code execution is completely independent (which should be less than or equal to the number of physical processors on a system).

   This example uses `multiprocessing` to compute critical values for a non-standard distribution and is illustrative of a Monte Carlo-like setup. The program has the standard set of imports including the `multiprocessing` module.

```
import multiprocessing as mp
import numpy as np
import matplotlib.pyplot as plt
```

   Next, a simple function is defined to compute a simulated supF test statistic which arises when testing for a structural break in a regression model when the break date is unknown. The underlying mathematical model, under the null of no structural break, is

$$y_t = \beta_0 + \beta_1' x_t + \varepsilon_t$$

and the alternative model is

$$y_t = \beta_0 + \beta_1' x_t + \gamma' x_t I_{[t>\tau]} + \varepsilon_t$$

where $I_{[t>\tau]}$ is an indicator variable that takes the value 1 when true. If τ is known, the test statistic,

$$F = \frac{\left(R_r^2 - R_u^2\right)/k}{\left(1 - R_u^2\right)/\left(T - 2k - 1\right)}$$

is a standard Chow test and follows an F distribution. When $\tau \in \left[\lfloor p_L T \rfloor, \lfloor p_H T \rfloor\right]$ where $0 < p_L < p_H < 1$ and $p_\bullet$ is suitable far from 0 or 1, then a sup version of this test can be implemented. The test is no longer distributed as an $F_{k, T-2k-1}$ where k is the number of variables in x but is based on the expected maximum value of many such tests. One method to get critical values is to simulate these, and the function `supf` can be used to produce one such test statistic from simulated x and y data. The code runs a full sample regression to compute the restricted R^2 and then run regressions with breaks across a range of possibly break dates, computing unrestricted R^2 for each break and the associated F-stat. Finally, the maximum of these is returned. `map` requires both a function and an iterable, the function can be any function located in any module and so does not need to reside in the same file as the main code. In this example, this function is stored in supf.py. An additional function `supf_wrapper` that takes a tuple input is also used for convenience.

```
# supf.py

import numpy as np
from numpy.linalg import pinv

def supf(y, x, p):
    T = y.shape[0]
    range = np.floor(np.array([T * p, T * (1 - p)]))
    range = np.arange(range[0], range[1] + 1, dtype=np.int32)
    # Demean since intercept doesn't break
    x = x - np.mean(x)
    y = y - np.mean(y)
    b = pinv(x) @ y
```

```
    e = y - x @ b
    # Compute full sample R2
    R2_r = 1 - (e @ e) / (y @ y)

    k = x.shape[1]
    F_stat = np.zeros(T)
    for t in range:
        X1 = x[:t]
        X2 = x[t:]
        # Parameters and errors before the break
        b = pinv(X1) @ y[:t]
        e[:t] = y[:t] - X1 @ b
        # Parameters and errors after the break
        b = pinv(X2) @ y[t:]
        e[t:] = y[t:] - X2 @ b
        # R2 from model with break
        R2_u = 1 - (e @ e) / (y @ y)
        # F stat for break at t
        F_stat[t] = ((R2_u - R2_r) / k) / ((1 - R2_u) / (T - 2* k - 1))

    # Only return maximum F stat
    return F_stat.max()

def supf_wrapper(args):
    # Convenience wrapper for use with map
    return supf(args[0], args[1], args[2])
```

Using `multiprocessing` requires a `__name__=='main'` block in the function. The main block does three things:

1. Compute the setup for the simulation. This is done so that the variables can be passed to the function executed in parallel.

2. Initialize the pool using `mp.Pool(processes=2)` (normally should use the same number as the number of physical cores on the system)

3. Call `map` from the `multiprocessing` module

4. Plot the results.

```
# multiprocessing_example.py
import multiprocessing as mp

import matplotlib.pyplot as plt
import numpy as np

from supf import supf_wrapper


if __name__ == '__main__':
    reps = 1000
    T = 200

    setup = []
    for i in range(reps):
        y = np.random.standard_normal(T)
        x = np.random.standard_normal((T, 1))
        p = 0.2
        setup.append((y, x, p))
```

```python
    # Non parallel map
    # res = map(surf_wrapper, setup)

    # Parallel map
    po = mp.Pool(processes=2)
    res = po.map(supf_wrapper, setup)
    print(len(res))
    po.close()

    ax = plt.hist(res)
    ax = ax[2]
    fig = ax[0].get_figure()
    fig.savefig('multiprocessing.pdf')
```

26.3 `joblib`

`joblib` is a Python package that provides a simple interface to the `multiprocessing` module with an easier to use syntax, especially for functions taking multiple arguments. This improved syntax allow for some arguments to vary according to an index but others to stay fixed, which is not simple to handle in `map`, which requires setting up a tuple with the both the dynamic and fixed parameters. `joblib` can be easily installed using `conda` from the console,

```
conda install joblib
```

Using `joblib` is a two step process:

1. Produce a delayed version of the function to be called using `delayed` (*func*)

2. Call `Parallel` with a simple loop across iterations

`Parallel` takes two sets of inputs. The first are options for use by `Parallel`, while the second is the function and loop statement. The most important options are `n_jobs` which sets the number of jobs (omit to use all cores) and `verbose` which takes a non-negative integer and instructs `joblib` to produce some output about progress and expected completion time. Reasonable values for `verbose` are typically between 5 and 10 – using 50 will produce an update on every job completion, while used 0 produces no output.

```python
# joblib_example.py
from joblib import Parallel, delayed
import numpy as np

from supf import supf_wrapper, supf


if __name__ == '__main__':
    reps = 1000
    T = 200

    setup = []
    for i in range(reps):
        y = np.random.standard_normal(T)
        x = np.random.standard_normal((T, 1))
        p = 0.2
        setup.append((y, x, p))

    # Non parallel map
    # res = map(surf_wrapper, setup)
```

```
    # joblib
    func = delayed(supf_wrapper)
    res = Parallel(n_jobs=2)(func(s) for s in setup)

    # joblib, no wrapper
    func = delayed(supf)
    res = Parallel(n_jobs=2)(func(s[0], s[1], s[2]) for s in setup)

    # joblib, no wrapper, fixed parameter
    func = delayed(supf)
    res = Parallel(n_jobs=2)(func(s[0], s[1], 0.15) for s in setup)

    # joblib, status output
    func = delayed(supf)
    res = Parallel(n_jobs=2, verbose=10)(func(s[0], s[1], s[2]) for s in setup)
```

26.4 IPython's Parallel Cluster

IPython contains a sophisticated cluster framework which allows for interactive parallel execution both locally and across a network (e.g. a supercomputer or using a cloud provider such as Amazon Web Services). IPython's parallelization framework provides both mechanisms similar to `map` in the previous example as well as more sophisticated schedulers that perform load balancing, which is useful if processing time per work unit is not deterministic. IPython parallel can be installed by running

```
conda install ipyparallel
jupyter nbextension install --sys-prefix --py ipyparallel
jupyter nbextension enable --sys-prefix --py ipyparallel
jupyter serverextension enable --sys-prefix --py ipyparallel
```

The first command installs the core module. The next threeprovide a GUI interface for starting IPython parallel sessions in the notebook interface. Using IPython parallel on a local machine is relatively simple, and a standard (local) cluster server can be initialized by running

```
ipcluster start
```

which will start a cluster with as many workers as the number of hardware threads supported on the local system. Alternatively, the format

```
ipcluster start -n=2
```

can be used to a cluster with a specific number of workers. The cluster can also be started using the Cluster tab in an IPython notebook. The cluster can be stopped by either pressing CTRL+C in the terminal or by running

```
ipcluster stop
```

in another terminal.

26.4.1 Interfaces

There are two methods to use the cluster. The first is the `DirectView` which will break up a list of tasks and run it across the cluster. The `DirectView` interface will break up jobs at the time of submission and so is well suited to jobs which are deterministic in nature. The other interface is the `LoadBalancedView` which distributes tasks when workers are ready. Since it waits for workers to be available, it is better suited to tasks that differing in their execution times, such as non-linear optimization problems. The cost of using the `LoadBalancedView` is that the scheduling takes more effort and so it is a little slower than the `DirectView`. When using the `LoadBalancedView`, it is common to use the `DirectView` to perform setup tasks prior to executing the parallel job.

26.4.1.1 `DirectView`

The `DirectView` is the natural and simplest method to execute in parallel. Using IPython parallel requires calling Client to connect to the cluster. When the cluster is local, a simple call to `Client()` is sufficient. Additional arguments can be used to select a remote cluster or provide information about how to connect to the cluster. `client.ids` can be used to see the number of workers available

```
>>> from ipyparallel import Client
>>> client = Client()
>>> client.ids  # Running on a 2 worker cluster
[0, 1]
```

The `DirectView` interface is created by slicing `client`. Normally the trivial slice is used, more complex slices will return a subset of the workers available.

```
>>> dview = client[:]
```

To begin, consider a trivial example which will square numbers using the workers in the cluster. This is done by writing a function and then calling `map`. Note that there are three versions of `map` available: `map`, `map_sync` and `map_async`. `map` and `map_async` are identical and will submit the job but then return immediately, *before the result is ready*. This means that it necessary to wait for the result to be ready by calling `.ready()` before attempting to access the function's output. `map_sync` is simpler and will wait for all jobs to be completed. For simplicity, `map_sync` is used below.

```
>>> dview = client[:]
>>> def square(x):
...     return x ** 2.0

>>> res = dview.map_sync(square, arange(10000.0))
>>> res[-5:]
[99900025.0,
 99920016.0,
 99940009.0,
 99960004.0,
 99980001.0]
```

In more complex situations, there are some important issues to be aware of when using a cluster. These all arise since cluster workers are *freshly initialized* Python instances which have no variables declared or modules imported, even those that are available in the local IPython session (or main program). Important issues include:

- Importing modules on the workers

- Pushing global variables to the workers

- Setting the Python path on the workers so they can find custom (user written) modules

Importing Modules

Workers start with no modules loaded. There are two methods to import modules on workers. The first uses `dview.execute(`*statement*`)` which can be used to execute any Python code on workers. The second, more sophisticated method is to use a `with` block,

```
>>> with dview.sync_imports():
...     import sys
...     import numpy
```

The `with` block method is more elegant, but has one important caveat – it isn't possible to rename modules, so `import numpy as np` will not work as expected and NumPy will only be available using it's full module

name (`numpy`). The following code shows two equivalent methods to import the modules on the workers with common names.

```
# Execute statement
>>> dview.execute('import numpy as np')

# With plus fix
>>> with dview.sync_imports():
...     import numpy
importing numpy on engine(s)

>>> dview.execute('np = numpy') # Equiv to as

# Show np can be used on worker
>>> dview.map_sync(lambda x: np.ones(1), range(2))
[array([ 1.]), array([ 1.])]
```

Pushing global variables

Since workers are just plain Python instances, they will not have access to global variables in the current IPython session or in the function. These can be passed using a dictionary syntax.

```
# Execute statement
>>> x = 'hello'
>>> dview['x'] = x
>>> def print_hello(i):
...     return x

>>> res = dview.map_sync(print_hello, range(2))
>>> res
['hello', 'hello']
```

Anything that can be pickled can be pushed as a global variable.

Setting the Python path

Workers are just plain Python instances and so have only the standard Python path. This will not, for example, include the current directory or other user directories. The path is simply a list containing strings, and so `extend`, `append` or `insert` can be used to modify the Python path.

```
>>> additional_path = ['c:\\temp\\one','c:\\temp\\two']
>>> dview['additional_path'] = additional_path
>>> with dview.sync_imports():
...     import sys
importing sys on engine(s)

>>> dview.execute('sys.path.extend(additional_path)')
>>> def view_path(i):
...     return sys.path
>>> res = dview.map_sync(view_path, range(2))
>>> res[0][-2:]
['c:\\temp\\one', 'c:\\temp\\two']

>>> import os
>>> cwd = os.getcwd() # Current working directory
>>> dview['cwd'] = cwd
>>> dview.execute('sys.path.insert(0,cwd)')
```

Complete Example

All of these ideas can be used to create sophisticated parallel programs. This example continues with the simulation exercise only using IPython's cluster in place `joblib` or `multiprocessing`. The program is structured in a small number of blocks:

- General imports

- Helper functions

- IPython cluster setup

- Actual code

This example executes the simulation both in serial and in parallel on a machine with 2 cores (and workers).

```python
# ipython_parallel_example.py
# General imports
import datetime as dt
import multiprocessing as mp
from ipyparallel import Client
import numpy as np
from supf import supf_wrapper
import os

# Helper functions
def print_elapsed(start):
    time_diff = dt.datetime.now() - start
    print(str(time_diff.seconds + time_diff.microseconds / 1000000.0) + ' secs')


# IPython cluster setup
client = Client()
dview = client[:]

cwd = os.getcwd()
dview['cwd'] = cwd
with dview.sync_imports():
    import sys
dview.execute('sys.path.insert(0, cwd)')

dview.execute('import numpy as np')
dview.execute('from supf import supf, supf_wrapper')

# Actual code
reps = 1000
T = 200

setup = []
for i in range(reps):
    y = np.random.standard_normal(T)
    x = np.random.standard_normal((T, 1))
    p = 0.2
    setup.append((y, x, p))

now = dt.datetime.now()
sup_F_stats = np.zeros(reps)
for b in range(reps):
    sup_F_stats[b] = supf_wrapper(setup[b])
print('Serial execution time')
```

```
print_elapsed(now)

now = dt.datetime.now()
res = dview.map_sync(supf_wrapper, setup)
print('Parallel execution time')
print_elapsed(now)
```

The program produces the following output, showing that there is a substantial gain to using the parallel interface.

```
importing sys on engine(s)
Serial execution time
17.606 secs
Parallel execution time
11.933 secs
```

26.4.1.2 `LoadBalancedView`

The `LoadBalancedView` use dynamic scheduling and is better suited to executing non-deterministic code such as non-linear optimization or various Monte Carlo algorithms that use dynamic stopping rules. This example runs the supF simulation (which is deterministic) and compares the performance of `DirectView` to `LoadBalancedView`. Unsurprisingly, the `DirectView` is (somewhat) faster.

```
# lbv_example.py
# General imports
import datetime as dt
import os

from ipyparallel import Client
import numpy as np

from supf import supf_wrapper



# Helper functions
def print_elapsed(start):
    time_diff = dt.datetime.now() - start
    print(str(time_diff.seconds + time_diff.microseconds / 1000000.0) + ' secs')


# IPython cluster setup
client = Client()
dview = client[:]

cwd = os.getcwd()
dview['cwd'] = cwd
with dview.sync_imports():
    dview.execute('sys.path.insert(0, cwd)')

dview.execute('import numpy as np')
dview.execute('from supf import supf, supf_wrapper')

# Actual code
reps = 1000
T = 200

setup = []
for i in range(reps):
```

```
    y = np.random.standard_normal(T)
    x = np.random.standard_normal((T, 1))
    p = 0.2
    setup.append((y, x, p))

now = dt.datetime.now()
res = dview.map_sync(supf_wrapper, setup)
print('DirectView execution time')
print_elapsed(now)

lbv = client.load_balanced_view()
now = dt.datetime.now()
res = lbv.map_sync(supf_wrapper, setup)
print('LoadBalancedView execution time')
print_elapsed(now)
```

The output from running this program shows that the `LoadBalancedView` is slower than serial execution here. This is due to relatively short nature of the individual simulations (around 17 ms each) and the overhead of load balancing.

```
importing os on engine(s)
DirectView execution time
11.67 secs
LoadBalancedView execution time
17.371 secs
```

Long Running Jobs

IPython's cluster controller cleverly caches results so that other workers can access them. When using the cluster on a long running job, this can lead to out-of-memory errors and so it is necessary to manually clean out the caches. This can be implemented by calling the function

```
def clear_cache(client, view):
    """Cache-clearing function from mailing list"""
    assert not rc.outstanding, "don't clear history when tasks are outstanding"
    client.purge_results('all')  # clears controller
    client.results.clear()
    client.metadata.clear()
    view.results.clear()
    client.history = []
    view.history = []
    client.session.digest_history.clear()
```

using the `client` and either `lbv` or `dview`, depending on how code is executed.[1]

26.4.2 Advanced Configuration

Many of the issues identified here such as setting the path or importing common modules can be addressed by creating a custom IPython parallel configuration. A blank profile can be created by running

```
ipython profile create --parallel --profile=parallel_profile
```

which will create a blank profile in the default profile location. There are three files relevant to the cluster: ip-controller_config.py, ipengine_config.py and ipcluster_config.py. The most important is ipengine_config.py which is used to import standard modules and set the path to a specific location each time the cluster is started.

---

[1]See https://github.com/robertnishihara/gess.

26.5   Converting a Serial Program to Parallel

The framework used to execute code in parallel makes little difference to the steps required to convert a serial program to run in parallel. This section provides some guidance on converting a serial program to run in parallel (`joblib`). The first step is to produce a *correct* serial version of the program. Naturally, simulation parameters such as the number of replications should be kept small so that the serial program completed in reasonable time. Below is a serial version of a program that would compute the critical values for a *supF* test statistic.

```python
import numpy as np
from numpy.linalg import pinv

reps = 1000
T = 200
k = 1
p = 0.2

sup_F_stat = np.zeros(reps)

for j in range(reps):
    y = np.random.standard_normal(T)
    x = np.random.standard_normal((T,k))
    range = np.floor(np.array([T * p, T * (1 - p)]))
    range = np.arange(range[0], range[1] + 1, dtype=np.int32)
    x = x - np.mean(x)
    y = y - np.mean(y)
    b = pinv(x) @ y
    e = y - x @ b
    R2_r = 1 - (e @ e) / (y @ y)

    k = x.shape[1]
    F_stat = np.zeros(T)
    for t in range:
        X1 = x[:t]
        X2 = x[t:]
        b = pinv(X1) @ y[:t]
        e[:t] = y[:t] - X1 @ b
        b = pinv(X2) @ y[t:]
        e[t:] = y[t:] - X2 @ b
        R2_u = 1 - (e @ e) / (y @ y)

        F_stat[t] = ((R2_u - R2_r) / k) / ((1 - R2_u) / (T - k))

    sup_F_stat[j] = F_stat.max()
```

The next step is to separate the key code into a function. The program should be identical at this point – it is still serial – and if given the same inputs (including the `RandomState`), it should produce identical results. Only setup code should remain in the loop.

```python
import numpy as np
from numpy.linalg import pinv

def supf(y, x, p):
    T = y.shape[0]
    range = np.floor(np.array([T * p, T * (1 - p)]))
    range = np.arange(range[0], range[1] + 1, dtype=np.int32)
    x = x - np.mean(x)
    y = y - np.mean(y)
    b = pinv(x) @ y
    e = y - x @ b
```

```python
    R2_r = 1 - (e @ e) / (y @ y)

    k = x.shape[1]
    F_stat = np.zeros(T)
    for t in range:
        X1 = x[:t]
        X2 = x[t:]
        b = pinv(X1) @ y[:t]
        e[:t] = y[:t] - X1 @ b
        b = pinv(X2) @ y[t:]
        e[t:] = y[t:] - X2 @ b
        R2_u = 1 - (e @ e) / (y @ y)

        F_stat[t] = ((R2_u - R2_r) / k) / ((1 - R2_u) / (T - k))

    return F_stat.max()

reps = 1000
T = 200
k = 1
p = 0.2

sup_F_stat = np.zeros(reps)

for j in range(reps):
    y = np.random.standard_normal(T)
    x = np.random.standard_normal((T,k))
    sup_F_stat[j] = supf(y, x, p)
```

The final step is to replace the loop by the setup block and then finally to call the main function from the parallel framework.

```python
import numpy as np
from numpy.linalg import pinv
from joblib import Parallel, delayed

# Omitted code
...

if __name__ == '__main__':
    reps = 1000
    T = 200
    k = 1
    p = 0.2

    # Setup Block
    X = []
    Y = []
    for j in range(reps):
        Y.append(np.random.standard_normal(T))
        X.append(np.random.standard_normal((T,k)))

    # Parallel block
    delayed_func = delayed(supf)
    sup_F_stat = Parallel(n_jobs=2)(delayed_func(Y[i], X[i], 0.2) for i in range(len(Y)))
```

26.6 Other Concerns when executing in Parallel

There are two important concerns that arise when executing code in parallel. The first is memory usage. While a single-threaded program can be easily monitored for excess memory use, this problem becomes acuter when executing in parallel since the amount of memory is typically *greater* than *n* times the memory of a single instance. Moreover, typical Desktop or Laptops have 8 – 32 GB of memory which can become small, on a per job basis, when running 4 – 8 parallel jobs. The second concern arises when using random numbers if replication is important. There are three options to address this:

- Generate all random numbers and save them locally and have workers read the file containing the random numbers.

- Generate all random numbers but only save the state. The state can then be passed to workers which can then set it in a new `RandomState` instance. This requires less storage and so is generally preferable to the first option.

- Ignore the issue and use a fresh random number generator in each worker using a different seed on each worker. Save the state from each worker and pass it back as part of the results. This can then be restored if results need to be exactly reproduced. Random numbers produced with method may be less random than draws produced using a single seed.

Chapter 27

Object-Oriented Programming (OOP)

27.1 Introduction

Objected-oriented programming (OOP) is an advanced programming paradigm that makes use of objects which contain both data (attributes or properties in Python) and methods (functions). The data in the object belongs to the object and the methods operate on the object's data, often changing some if it when called (but not necessarily). In Python, OOP allows for more structure than the *procedural paradigm* that has been used throughout these notes. OOP also allows code re-use through inheritance – where one class inherits the attributes, properties, and methods of a parent class – which can lead to improved long-term maintainability and shallower bugs in large code bases.

The main advantage of using OOP for most end-users is the ability to tightly couple related data and code. The example in this chapter will describe building a *class* for fitting, simulating and forecasting an autoregressive process. Note that the class based approach is not necessary – everything in this chapter can be implemented using procedural code – but can be much cleaner. For example, commands similar to those below would be used to estimate, forecast and simulate an autoregressive process in a purely procedural approach.

```
T = 500
ar_order = 2
in_sample = 250

parameters = ar_estimate(data, ar_order)
forecasts = ar_forecast(data, parameters, ar_order, in_sample)
simulated_data = ar_simulate(data, parameters, T)
```

The class-based (object-oriented) approach will use the following code to accomplish the same with somewhat cleaner code.

```
T = 500
ar_order = 2
in_sample = 250

# Initialize the object
ar = AR(data, ar_order)
ar.estimate()
forecasts = ar.forecast(in_sample)
simulated_data = ar.simulate(T)
```

The simplicity in the code above is possible since `ar` is an object which has properties `data`, `ar_order` and `parameters` and methods `estimate`, `forecast` and `simulate`.

27.2   Class basics

27.2.1   Class declaration

Classes are declared using the reserved keyword `class` and must inherit from another class. In many cases, if there is no further structure, the class should inherit from the generic class `object`.

```python
class AR(object):
    pass
```

27.2.2   `__init__`

`__init__` is a key function of a class and is implicitly called whenever the class is initialized. The `__init__` must have `self` as its first argument, and can also have positional and/or keyword arguments. `self` allows access to the object (*itself*) and is used to store attributes in the object, access properties of the object and call methods from the object.

```python
class AR(object):
    def __init__(self):
        # Do things here
        pass
```

This trivial `__init__` does nothing, but is still called whenever an object is initialized from the AR class, as in

```python
ar = AR()
```

27.2.3   Attributes

Attributes are the usual method for storing data in an object. Attributes should usually be declared in the `__init__`, although they can be added to the object at any time. The `__init__` in the next listing takes two optional (keyword) arguments. `add_an_attribute` is a *method* which adds an attribute not declared in the `__init__`, which is usually a bad idea.

```python
class AR(object):
    def __init__(self, data=None, ar_order=0):
        # Attributes
        self.data = data
        self._ar_order = ar_order

    def add_an_attribute(self):
        self.new_attribute = 'New attribute added'
```

This class can be initialized in a variety of ways, including treating keyword arguments as positional or by directly using the keyword.

```python
>>> data = np.random.standard_normal((100,1))
>>> ar = AR()
>>> ar = AR(data)
>>> ar = AR(data, 2)
>>> ar = AR(ar_order = 1)
>>> ar.__dict__ # Shows all attributed (and more usually)
{'ar_order': 1, 'data': None}

>>> ar.add_an_attribute()
>>> ar.new_attribute
'New attribute added'
>>> ar.__dict__
{'ar_order': 1, 'data': None, 'new_attribute': 'New attribute added'}
```

Attributes are easy to both get and set using their name. They are, however, completely unprotected from incorrect types or formats, and so if some protection is required (or if further processing is required) then a property is needed.

27.2.4 Properties

Properties, while superficially similar to attributes, differ since their value is set or retrieved using a function that can perform other functions. For example, it may be that a property requires a non-trivial calculation, and so it should not be computed until required. In this case, using a property allows a *private* value to be checked, and to perform the calculation before returning a value if needed. Similarly, the setter allows for arguments to be checked or other internal parameters to be changed whenever the variable's value is changed.

This example has two properties, data, and ar_order. The properties are initialized using the *decorator* @property which defaults to being read-only. When the additional .setter is defined, the property can also be used to set a value. In the code below, ar_order is read-only (it has no setter), and data can be both read and set. The data.setter checks the length of data to ensure there are sufficient observations for estimation. Note that the function immediately below the @property decorator is the "getter" method.

```python
class AR(object):
    def __init__(self, data=None, ar_order=0):
        # Attributes
        self._ar_order = ar_order
        self._data = data

    @property
    def data(self):
        return self._data

    @data.setter
    def data(self, value):
        if len(value)/2.0 < self.ar_order:
            raise ValueError('Data does not have enough elements ' /
                             'to estimate parameters.')
        self._data = value

    @property
    def ar_order(self):
        return self._ar_order
```

Properties can also have an optional .deleter this is called to remove the property, as in del ar.data. A deleter is useful when removing a property requires some internal clean-up in the object.

27.2.5 Methods

Methods are simply functions that operate on the objects attributes and properties plus possibly other variables. In this example, estimate should estimate unknown parameters (although it only raises an exception for now)

```python
class AR(object):
    def __init__(self, data=None, ar_order=0):
        # Attributes
        self._ar_order = ar_order
        self._data = data

    def estimate(self):
        raise NotImplementedError('This has not been implemented')
```

27.2.6 `self`

`self` is an important keyword inside a class and is used to refer to the object from *within* the object. For example, attributes can be set

```python
self.var = 'Some value'
```

and methods that require data from the object must reference self as their first argument

```python
class ExampleClass(object):
    def __init__(self):
        self.var = 'Hello'

    def a_method(self, var1, var2, var3='default'):
        print(self.var + var1 + var2 + var3)
        return False
```

Methods that do not include `self` as an argument cannot access data stored in an object, and are called *static*. Static methods should be decorated with the `@staticmethod` decorator.

```python
class ExampleClass(object):

    @staticmethod
    def a_static_method(var1, var2):
        print(var1 + var2)
```

27.2.7 Private Attributed and Methods

It is common for classes to have both private attributes and methods which use a leading _ to indicate that they are private. While the leading underscore is an indication to users not to directly set the value of an attribute or to call a method, private variables are *fully available* to read or assign from Python. The example below uses private variables to back properties, and private methods to perform calculations that are not directly usually of interest for someone using the AR class.

27.3 Building a class for Autoregressions

The code below builds a basic class for fitting, forecasting and simulating autoregressive processes. See `statsmodels.tsa.AR` for a complete, production-ready version of a class for estimation of Autoregressive models.

27.3.1 Imports and `__init__`

The imports include the usual packages, including seaborn (treating it as optional). The `__init__` takes 2 optional arguments, and initializes a large number of private variables, which will either act as backing for properties or hold intermediate values. The `__init__` also calls the private function `_generate_regressor_array()` if `data` is non-empty.

```python
import numpy as np
import numpy.random as rnd
from numpy import hstack, nan, tile, vstack, zeros
import matplotlib.pyplot as plt

try:
    import seaborn
except ImportError:
    pass
```

```python
class AR(object):
    def __init__(self, data=None, ar_order=1):
        self._data = data
        self._ar_order = ar_order
        self._sigma2 = 1
        self._T = None
        self._X = None
        self._y = None
        self._roots = None
        self._abs_roots = None
        self._fit_values = None
        self._parameters = None
        self._errors = None
        if data is not None:
            self._generate_regressor_array()
```

27.3.2 Properties

The class has a many properties, and most simply return the value of a private variable with the same name. The exceptions are `parameters` which estimates the model if needed and `fit_values` which computes the fit values if needed.

```python
    @property
    def data(self):
        return self._data

    @property
    def ar_order(self):
        return self._ar_order

    @property
    def parameters(self):
        return self._parameters

    @property
    def sigma2(self):
        return self._sigma2

    @property
    def roots(self):
        return self._roots

    @property
    def abs_roots(self):
        return self._abs_roots

    @property
    def fit_values(self):
        if self._fit_values is None:
            self.estimate()
        return self._fit_values
```

27.3.3 Property Setters

Most of the properties are read-only. `data`, `parameters`, and `sigma2` can be directly set. Whenever `data` is set, the regressors are updated, and, when the object has parameters, other quantities, such as the fitted values,

are computed. Setting `parameters` checks that the correct number of elements is present and then updates the characteristic equation roots. Setting `sigma2` checks that the value is positive.

```python
@data.setter
def data(self, value):
    self._data = value
    self._generate_regressor_array()
    if self._parameters is not None:
        self._update_values()

@parameters.setter
def parameters(self, value):
    if value.ndim not in (1, 2):
        raise ValueError("parameters must be a vector")
    value = value.ravel()[:, None]
    if value.shape[0] != (self._ar_order + 1):
        raise ValueError(f"parameters must have {self._ar_order + 1} elements.")

    self._parameters = value
    self._update_roots()

@sigma2.setter
def sigma2(self, value):
    if value <= 0.0:
        raise ValueError("sigma2 must be positive")
    self._sigma2 = value
```

27.3.4 Private methods

There are three private methods which:

- Generate the regressor and regressand arrays. This is called whenever data is changed.

- Update the roots and absolute roots. This is called whenever parameters are set.

- Compute fitted values, errors and estimate the variance. This is called whenever the model is estimated or the data is changed.

```python
def _generate_regressor_array(self):
    p = self._ar_order
    T = self._T = len(self._data)
    x = np.ones((T - p, p + 1))
    y = self._data[:, None]
    for i in range(p):
        x[:, [i + 1]] = y[p - i - 1:T - i - 1, :]
    self._y = self.data[p:, None]
    self._X = x

def _update_roots(self):
    if self._ar_order > 0:
        coeffs = self._parameters[1:].ravel()
        char_equation = np.concatenate(([1], -1.0 * coeffs))
        self._roots = np.roots(char_equation)
        self._abs_roots = np.absolute(self._roots)
    else:
        self._roots = None
        self._abs_roots = None
```

```python
def _update_values(self):
    fv = self._X.dot(self._parameters)
    e = self._y - fv
    self._sigma2 = np.dot(e.T, e) / len(e)
    self._errors = vstack((tile(nan, (self._ar_order, 1)), e))
    self._fit_values = vstack((tile(nan, (self._ar_order, 1)), fv))
```

27.3.5 Methods

There are 5 methods:

- `estimate` – Estimate the model parameters. Accepts an optional input `insample` to limit the amount of data that is used in the estimation.

- `forecast` – Generate h-step ahead forecast errors. The matrix returned is T by h with the h forecasts originating at time t in location t.

- `forecast_plot` – Plot the data and aligned forecasts, or the forecast errors.

- `hedgehog_plot` – A plot the original series along with multi-step forecasts originating from the series.

- `simulate` – Simulate a time series with the same parameters are the model using Gaussian shocks.

estimate

Estimation uses the already generated regressors and regressand along with `pinv` to compute OLS parameter estimates. If `insample` is specified, the size of the in-sample data is adjusted so that only the first `insample` data points are used in estimation.

```python
def estimate(self, insample=None):
    x = self._X
    y = self._y
    y = y[:, None]
    p = self._ar_order
    if insample is not None:
        x = x[:(insample - p),:]
        y = y[:(insample - p)]
    xpxi = np.linalg.pinv(x)
    self.parameters = xpxi.dot(y)
```

forecast

The forecasts are generated by *reversing* (`self._X[:, :0:-1]`) and augmenting (`hstack`) the regressors with h columns of zeros (`zeros((tau, h))`), to produce a row which look like

$$\left[y_{t-p+1} \, y_{t-p+2} \, \ldots \, y_t \, 0 \ldots 0 \right]$$

so that after the first forecast is generated, the row will look like

$$\left[y_{t-p+1} \, y_{t-p+2} \, \ldots \, y_t \, \hat{y}_{t+1|t} \, \ldots \, 0 \right]$$

and after h forecasts have been produced, the row will look like

$$\left[y_{t-p+1} \, y_{t-p+2} \, \ldots \, y_t \, \hat{y}_{t+1|t} \, \ldots \, \hat{y}_{t+h|t} \right]$$

so that the final h columns are the forecasts. Once the forecasts are generated, the final steps are to augment the forecast array to have the correct size and then to set values in the in-sample period to `nan`.

```python
def forecast(self, h=1, insample=None):
    tau = self._X[:, 1:].shape[0]
    fcasts = hstack((self._X[:, :0:-1], zeros((tau, h))))
    p = self._ar_order
    params = self._parameters
    for i in range(h):
        fcasts[:, p + i] = params[0]
        for j in range(p):
            fcasts[:, p + i] += params[j + 1] * fcasts[:, p + i - (j + 1)]

    fcasts = vstack((tile(nan, (p, p + h)), fcasts))
    if insample is not None:
        fcasts[:insample, :] = nan

    return fcasts[:, p:]
```

forecast_plot

The only non-trivial component of the forecast plot is the data alignment, which aligns the realization with the forecast, and is essentially staggering the two T-element vector by h. The plot is simple to produce using the augmented data. The output of this method is shown in panel (a) of figure 27.1 for $h = 5$.

```python
def forecast_plot(self, h=1, show=True, show_errors=False):
    fcasts = self.forecast(h=h)
    T = self._T
    p = self._ar_order
    aligned = zeros((T + h, 2))
    aligned[:T, 0] = self._data
    aligned[-T:, 1] = fcasts[:, -1]

    aligned = aligned[p:T, :]
    fig = plt.figure()
    ax = fig.add_subplot(1, 1, 1)
    if show_errors:
        ax.plot(aligned[:, 0] - aligned[:, 1])
    else:
        ax.plot(aligned)
    if show:
        plt.show(fig)

    return fig
```

hedgehog_plot

The hedgehog plot has two components, the original data and the "hairs", which are multi-step forecasts. The plot is produced by first plotting the data, then holding the plot, and iterating across all multi-step forecasts, where the data plotted are the forecasts augmented by the last value when the forecast was made. These are plotted against the index. The output of this method is shown in panel (a) of figure 27.1 for $h = 10$ with `skip` set to 5.

```python
def hedgehog_plot(self, h=1, show=True, skip=0):
    fcasts = self.forecast(h=h)
    fig = plt.figure()
    ax = fig.add_subplot(1, 1, 1)
    ax.plot(self._data)
    data = self._data
    for i in range(0, self._T, skip + 1):
```

(a)

(b)
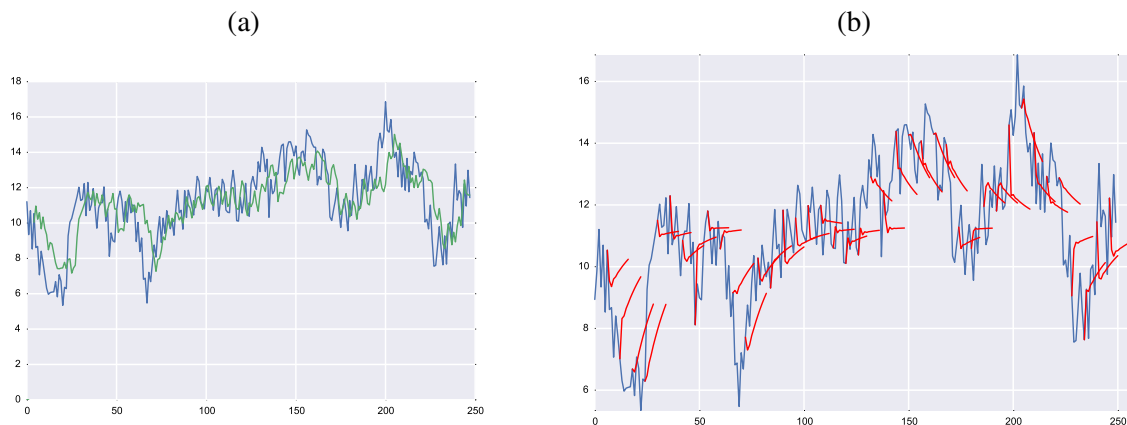
Figure 27.1: The left panel shows the forecast plot for $h = 5$ and the right panel shows a hedgehog plot with $h = 10$ where the skip parameter is set to 5.

```
        x = i + np.arange(h + 1)
        y = hstack((data[[i]], fcasts[i]))
        ax.plot(x, y, 'r')

    ax.autoscale(tight='x')
    fig.tight_layout()
    if show:
        plt.show(fig)

    return fig
```

simulate

Simulation of AR(p) models with Gaussian errors is straightforward and involves recursively computing values. This function generates T plus the burn-in size vectors of errors and allocates the output vector with the same size, and then loops across time to simulate the process.

```
def simulate(self, T=500, burnin=500):
    tau = T + burnin + self._ar_order
    e = rnd.standard_normal((tau,))
    y = zeros((tau,))
    p = self._ar_order
    for t in range(p, tau):
        y[t] = self._parameters[0]
        for i in range(p):
            y[t] += self._parameters[i + 1] * y[t - i - 1]
        y[t] += e[t]

    return y[-T:]
```

27.3.6 Improvements

There are a number of ways the AR class could be improved, including:

- Returning the log-likelihood and information criteria for a model (AIC/BIC)

- Handling "hold out" observations – those which are in the data but are not used in estimation. These are useful to ensure that models are estimated using the same number of data points when comparing models with different AR orders.

- Adding high-quality doc strings, which are essential even for your own code.

- Adding confidence intervals to the forecast plot and the forecast error plot.

- Improving the simulation code to allow errors to be directly input or other error distributions to be used.

- Compute theoretical ACF and PACF values for the model parameters.

- Initialize the simulation using the long-run variance. Note that computing the long-run variance requires the first p autocorrelations.

- The code should be tested for defects. nose or py.test are the recommended packages for writing formal tests of code.

- Make the code compatible with a pandas DataFrame or Series so that plots will show time, not just numerical indices.

These are left as an exercise.

27.4 Exercises

1. Add the log-likelihood, AIC, BIC and HQIC.

2. Allow "hold-out" observations to be specified when calling `estimate`.

3. Test the code with a Series or DataFrame containing a single column. Make any modifications required to seamlessly handle 1-d and 2-d NumPy arrays, Series and DataFrames.

4. Improve the simulation code to allow for either a $T + b$ by 1 vector of errors to be input directly or so that a function that can generate random numbers can be used.

5. Add high-quality, NumPy-style doc strings to the properties and methods. See NumPy's documentation on writing doc strings.

Chapter 28

Other Interesting Python Packages

To be completed

28.1 Statistics and Statistical Modeling

SciPy

linearmodels

pysal

pingouin

pymc

PyMC provides the tools required to fit models using Bayesian techniques, as well as to perform standard diagnostics.

pystan

pystan provides a Python interface to Stan which provides Bayesian inference using the No-U-Turn sampler.

28.2 Machine Learning

scikit-learn

scikit-learn is one of the premier in-core machine learning libraries on any platform. It contains optimized state-of-the-art algorithms suitable for many problems.

PyCaret

XGBoost

LightGBM

pdarima

28.3   Deep Learning

TensorFlow

Theano

Theano is a lower-level library that allows numerical expressions to be defined and evaluated. It support execution on the GPU as well as symbolic differentiation of expressions.

Keras

PyTorch

mlpy

mlpy is an alternative machine learning module that makes use of the GNU scientific library.

NLTK

NLTK is a complete natural language processing module for working with human langauge data.

28.4   Other Packages

pytz and babel

ptyz and babel provide extended support for time zones and formatting information.

rpy2

rpy2 provides an interface for calling R 3.0.x in Python, as well as facilities for easily moving data between the two platforms.

PyTables and h5py

PyTables and h5py both provide direct access to HDF5 files, a flexible data storage format optimized for numeric data.

Chapter 29

Examples

These examples are all actual econometric problems chosen to demonstrate the use of Python in an end-to-end manner, from importing data to presenting estimates. A reasonable familiarity with the underlying econometric models and methods is assumed and this chapter focuses on translating the mathematics to Python.

These examples all use `@` to multiply arrays. If using Python 3.4 or earlier, or if using a version of NumPy that does not support `@`, these commands should be replaced with `dot`. For example, `X @ X.T` would be `X.dot(X.T)` or `np.dot(X,X.T)`.

29.1 Estimating the Parameters of a GARCH Model

This example will highlight the steps needed to estimate the parameters of a GJR-GARCH(1,1,1) model with a constant mean. The volatility dynamics in a GJR-GARCH model are given by

$$\sigma_t^2 = \omega + \sum_{i=1}^{p} \alpha_i \varepsilon_{t-i}^2 + \sum_{j=1}^{o} \gamma_j \varepsilon_{t-j}^2 I_{[\varepsilon_{t-j}<0]} + \sum_{k=1}^{q} \beta_k \sigma_{t-k}^2.$$

Returns are assumed to be conditionally normal, $r_t|\mathcal{F}_{t-1} \sim N\left(\mu, \sigma_t^2\right)$, $\varepsilon_t = r_t - \mu$ and parameters are estimated by maximum likelihood. To estimate the parameters, it is necessary to:

1. Produce some starting values

2. Estimate the parameters using (quasi-) maximum likelihood

3. Compute standard errors using a "sandwich" covariance estimator (also known as the Bollerslev and Wooldridge (1992) covariance estimator)

The first task is to write the log-likelihood which can be used in an optimizer. The log-likelihood function will compute the volatility recursion and the log-likelihood. It will also, optionally, return the T by 1 vector of individual log-likelihoods which are useful when approximating the scores.

The first step is to import the required modules. I prefer to use the import form `from` *module* `import` *func1*, *func2* for commonly used functions. This both saves typing and increases code readability. I use `import` *module* `as` *shortname* for functions which are used less. This is a personal choice, and any combination is acceptable, although `from` *module* `import` `*` should be avoided.

```python
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
```

```
from numpy import size, log, pi, sum, array, zeros, diag, mat, asarray, sqrt, copy
from numpy.linalg import inv
from scipy.optimize import minimize
```

The conditional log-likelihood of a normal random variable is

$$\ln f\left(r_t|\mu,\sigma_t^2\right) = -\frac{1}{2}\left(\ln 2\pi + \ln \sigma_t^2 + \frac{(r_t-\mu)^2}{\sigma_t^2}\right),$$

which is negated in the code since the optimizers all minimize.

```
def gjr_garch_likelihood(parameters, data, sigma2, out=None):
    """Negative log-likelihood for GJR-GARCH(1,1,1) model"""
    mu = parameters[0]
    omega = parameters[1]
    alpha = parameters[2]
    gamma = parameters[3]
    beta = parameters[4]

    T = size(data,0)
    eps = data - mu
    # Data and sigma2 are T by 1 vectors
    for t in range(1,T):
        sigma2[t] = (omega + alpha * eps[t-1]**2
                     + gamma * eps[t-1]**2 * (eps[t-1]<0) + beta * sigma2[t-1])

    logliks = 0.5*(log(2*pi) + log(sigma2) + eps**2/sigma2)
    loglik = sum(logliks)

    if out is None:
        return loglik
    else:
        return loglik, logliks, copy(sigma2)
```

The keyword argument `out` has a default value of `None`, and is used to determine whether to return 1 output or 3. This is common practice since the optimizer requires a single output – the log-likelihood function value, but it is also useful to be able to output other useful quantities, such as $\left\{\sigma_t^2\right\}$.

The optimization is constrained so that $\alpha + \gamma/2 + \beta \leq 1$, and the constraint is provided in a separate function.

```
def gjr_constraint(parameters):
    """ Constraint that alpha+gamma/2+beta<=1"""

    alpha = parameters[2]
    gamma = parameters[3]
    beta = parameters[4]

    return array([1-alpha-gamma/2-beta])

constraint = {"type": "ineq", "fun": gjr_constraint}
```

Note that the constraint function takes the same inputs as the negative of the log-likelihood function, even though only `parameters` is required to compute the constraint.

It is necessary to discuss one other function before proceeding with the main block of code. The asymptotic variance is estimated using the "sandwich" form which is commonly expressed as

$$\mathcal{J}^{-1}\mathcal{I}\mathcal{J}^{-1}$$

where $\mathcal{J}$ is the expected Hessian and $\mathcal{I}$ is the covariance of the scores. Both are numerically approximated, and the strategy for computing the Hessian is to use the definition that

$$\mathcal{J}_{ij} \approx \frac{f\left(\theta + e_i h_i + e_j h_j\right) - f\left(\theta + e_i h_i\right) - f\left(\theta + e_j h_j\right) + f\left(\theta\right)}{h_i h_j}$$

where h_i is a scalar "step size" and e_i is a vector of 0s except for element i, which is 1. A 2-sided version of this approximation, which takes both forward and backward steps and then averages, is below. For more on numerical derivatives, see **FlanneryPressTeukolskyTeukolsky::1992**.

```python
def hessian_2sided(fun, theta, args):
    f = fun(theta, *args)
    h = 1e-5*np.abs(theta)
    thetah = theta + h
    h = thetah - theta
    K = size(theta,0)
    h = np.diag(h)

    fp = zeros(K)
    fm = zeros(K)
    for i in range(K):
        fp[i] = fun(theta+h[i], *args)
        fm[i] = fun(theta-h[i], *args)

    fpp = zeros((K,K))
    fmm = zeros((K,K))
    for i in range(K):
        for j in range(i,K):
            fpp[i,j] = fun(theta + h[i] + h[j],  *args)
            fpp[j,i] = fpp[i,j]
            fmm[i,j] = fun(theta - h[i] - h[j],  *args)
            fmm[j,i] = fmm[i,j]

    hh = (diag(h))
    hh = hh.reshape((K,1))
    hh = hh @ hh.T

    H = zeros((K,K))
    for i in range(K):
        for j in range(i,K):
            H[i,j] = (fpp[i,j] - fp[i] - fp[j] + f
                    + f - fm[i] - fm[j] + fmm[i,j])/hh[i,j]/2
            H[j,i] = H[i,j]

    return H
```

Finally, the code that does the actual work can be written. The first block imports the data, flips it using a slicing operator, and computes 100 times returns. Scaling data can be useful to improve optimizer performance, and ideally estimated parameters should have similar magnitudes (i.e. $\omega \approx .01$ and $\alpha \approx .05$).

```python
# Import data
ftse = pd.read_csv('FTSE_1984_2012.csv', parse_dates=[0])
# Set index
ftse.index = ftse.pop('Date')
# Flip upside down
ftse = ftse.iloc[::-1]
# Compute returns
ftse_price = ftse['Adj Close']
ftse_return = 100 * ftse_price.pct_change().dropna()
```

Good starting values are important. These are my guesses based on experience fitting these types of models models. An alternative is to attempt a crude grid search and use the best (smallest) log-likelihood value from the grid search.

```
# Starting values
starting_vals = array([ftse_return.mean(),
                       ftse_return.var() * .01,
                       .03, .09, .90])
```

Bounds are used in estimation to ensure that all parameters in the conditional variance are ≥ 0 and to set sensible upper bounds on the mean and ω. The vector `sigma2` is then initialized, and the arguments are placed in a tuple.

```
# Estimate parameters
finfo = np.finfo(np.float64)
bounds = [(-10*ftse_return.mean(), 10*ftse_return.mean()),
          (finfo.eps, 2*ftse_return.var() ),
          (0.0,1.0), (0.0,1.0), (0.0,1.0)]

T = ftse_return.shape[0]
sigma2 = np.ones(T) * ftse_return.var()
# Pass a NumPy array, not a pandas Series
args = (np.asarray(ftse_return), sigma2)
opt = minimize(gjr_garch_likelihood,
               starting_vals,
               constraints=constraint,
               bounds = bounds,
               args = args)
estimates = opt.x
```

The optimized log-likelihood and the time series of variances are computed by calling the objective using the keyword argument `out=True`.

```
loglik, logliks, sigma2final = gjr_garch_likelihood(estimates, ftse_return,
                                                    sigma2, out=True)
```

Next, the numerical scores and the covariance of the scores are computed. These exploit the definition of a derivative, so that for a scalar function,

$$\frac{\partial f(\theta)}{\partial \theta_i} \approx \frac{f(\theta + e_i h_i) - f(\theta)}{h_i}.$$

The covariance is computed as the outer product of the scores since the scores should have mean 0 when evaluated at the solution to the optimization problem.

```
step = 1e-5 * estimates
scores = zeros((T,5))
for i in range(5):
    h = step[i]
    delta = np.zeros(5)
    delta[i] = h

    loglik, logliksplus, sigma2 = gjr_garch_likelihood(estimates + delta, \
                            np.asarray(ftse_return), sigma2, out=True)
    loglik, logliksminus, sigma2 = gjr_garch_likelihood(estimates - delta, \
                            np.asarray(ftse_return), sigma2, out=True)

    scores[:,i] = (logliksplus - logliksminus)/(2*h)

I = (scores.T @ scores)/T
```

The next block calls `hessian_2sided` to estimate the Hessian, and then computes the asymptotic covariance.

```python
J = hessian_2sided(gjr_garch_likelihood, estimates, args)
J = J/T
Jinv = mat(inv(J))
vcv = Jinv*mat(I)*Jinv/T
vcv = asarray(vcv)
```

The penultimate step is to pretty print the results and to produce a plot of the conditional variances.

```python
output = np.vstack((estimates,sqrt(diag(vcv)),estimates/sqrt(diag(vcv)))).T
print('Parameter   Estimate       Std. Err.      T-stat')
param = ['mu','omega','alpha','gamma','beta']
for i in range(len(param)):
    print(f'{param[i]:<11} {output[i,0]:>0.6f}        {output[i,1]:0.6f}     {output[i,2]: 0.5f}')
```

This final block produces a plot of the annualized conditional standard deviations.

```python
# Register date converters
from pandas.plotting import register_matplotlib_converters
register_matplotlib_converters()

# Produce a plot
dates = ftse.index[1:]
fig = plt.figure()
ax = fig.add_subplot(111)
volatility = pd.DataFrame(np.sqrt(252 * sigma2), index=dates)
ax.plot(volatility)
ax.autoscale(tight='x')
fig.autofmt_xdate()
fig.tight_layout(pad=1.5)
ax.set_ylabel('Volatility')
ax.set_title('FTSE Annualized Volatility (GJR GARCH(1,1,1))')
plt.show()
```

29.2 Estimating the Risk Premia using Fama-MacBeth Regressions

This example highlights how to implement a Fama-MacBeth 2-stage regression to estimate factor risk premia, make inference on the risk premia, and test whether a linear factor model can explain a cross-section of portfolio returns. This example closely follows Cochrane (2001) (See also Jagannathan, Skoulakis, and Wang (2010)). As in the previous example, the first segment contains the imports.

```python
from numpy import mat, cov, mean, hstack, multiply, sqrt, diag, squeeze, ones, array, vstack, kron,
from numpy.linalg import inv
from scipy.stats import chi2
from pandas import read_csv
import statsmodels.api as sm
```

Next, the data are imported. I formatted the data downloaded from Ken French's website into an easy-to-import CSV which can be read by `pandas.read_csv`. The data is split using named columns for the small sets of variables and `ix` for the portfolios. The code uses pure NumPy arrays, and so `values` is used to retrieve the array from the DataFrame. The dimensions are determined using `shape`. Finally the risk free rate is forced to have 2 dimensions so that it will be broadcastable with the portfolio returns in the construction of the excess returns to the Size and Value-weighted portfolios. `mat` is used to return matrix views of all of the arrays. This code is linear algebra-heavy and so matrices are easier to use than arrays.

```python
data = read_csv('FamaFrench.csv')
```

```
# Split using both named colums and ix for larger blocks
dates = data['date'].values
factors = data[['VWMe', 'SMB', 'HML']].values
riskfree = data['RF'].values
portfolios = data.iloc[:, 5:].values

# Use mat for easier linear algebra
factors = mat(factors)
riskfree = mat(riskfree)
portfolios = mat(portfolios)

# Shape information
t,k = factors.shape
t,n = portfolios.shape
# Reshape rf and compute excess returns
riskfree.shape = t,1
excess_returns = portfolios - riskfree
```

The next block does 2 things:

1. Compute the time-series βs. This is done be regressing the full array of excess returns on the factors (augmented with a constant) using OLS.

2. Compute the risk premia using a cross-sectional regression of average excess returns on the estimates βs. This is a standard regression where the step 1 β estimates are used as regressors, and the dependent variable is the average excess return.

```
# Time series regressions
x = sm.add_constant(factors)
ts_res = sm.OLS(excess_returns, x).fit()
alpha = ts_res.params[0]
beta = ts_res.params[1:]
avgexcess_returns = mean(excess_returns, 0)
# Cross-section regression
cs_res = sm.OLS(avgexcess_returns.T, beta.T).fit()
risk_premia = cs_res.params
```

The asymptotic variance requires computing the covariance of the demeaned returns and the weighted pricing errors. The problem is formulated using 2-step GMM where the moment conditions are

$$
g_t(\theta) =
\begin{bmatrix}
\varepsilon_{1t} \\
\varepsilon_{1t} f_t \\
\varepsilon_{2t} \\
\varepsilon_{2t} f_t \\
\vdots \\
\varepsilon_{Nt} \\
\varepsilon_{Nt} f_t \\
\beta u_t
\end{bmatrix}
$$

where $\varepsilon_{it} = r_{it}^e - \alpha_i - \beta_i' f_t$, β_i is a K by 1 vector of factor loadings, f_t is a K by 1 set of factors, $\beta = [\beta_1 \, \beta_2 \ldots \beta_N]$ is a K by N matrix of all factor loadings, $u_t = r_t^e - \beta'\lambda$ are the N by 1 vector of pricing errors and λ is a K by 1 vector of risk premia. The collection of parameters is then $\theta = [\alpha_1 \, \beta_1' \, \alpha_2 \, \beta_2' \, \ldots \, \alpha_N \, \beta_N' \, \lambda']'$. To make inference in this problem, the derivative of the moments with respect to the parameters, $\partial g_t(\theta)/\partial \theta'$ is needed. With some work, the estimator of this matrix can be seen to be

$$
G = E\left[\frac{\partial g_t(\theta)}{\partial \theta'}\right] =
\begin{bmatrix}
-I_n \otimes \Sigma_X & 0 \\
G_{21} & -\beta\beta'
\end{bmatrix}.
$$

where $X_t = [1 \; f_t']'$ and $\Sigma_X = E[X_t X_t']$. G_{21} is a matrix with the structure

$$G_{21} = [G_{21,1} \; G_{21,2} \ldots G_{21,N}]$$

where

$$G_{21,i} = \begin{bmatrix} 0_{K,1} & \text{diag}\,(E[u_i] - \beta_i \odot \lambda) \end{bmatrix}$$

and where $E[u_i]$ is the expected pricing error. In estimation, all expectations are replaced with their sample analogues.

```
# Moment conditions
X = sm.add_constant(factors)
p = vstack((alpha, beta))
epsilon = excess_returns - x @ p
moments1 = kron(epsilon, ones((1, k + 1)))
moments1 = multiply(moments1, kron(ones((1, n)), x))
u = excess_returns - risk_premia[None,:] @ beta
moments2 = u * beta.T
# Score covariance
S = mat(cov(hstack((moments1, moments2)).T))
# Jacobian
G = mat(zeros((n * k + n + k, n * k + n + k)))
sigma_x = (x.T @ x) / t
G[:n * k + n, :n * k + n] = kron(eye(n), sigma_x)
G[n * k + n:, n * k + n:] = -beta @ beta.T
for i in range(n):
    temp = zeros((k, k + 1))
    values = mean(u[:, i]) - multiply(beta[:, i], risk_premia)
    temp[:, 1:] = diag(values)
    G[n * k + n:, i * (k + 1):(i + 1) * (k + 1)] = temp

vcv = inv(G.T) * S * inv(G) / t
```

The J-test examines whether the average pricing errors, $\hat{\alpha}$, are zero. The J statistic has an asymptotic χ^2_N distribution, and the model is badly rejected.

```
vcv_alpha = vcv[0:n * k + n:4, 0:n * k + n:4]
J = alpha @ inv(vcv_alpha) @ alpha.T
J = J[0, 0]
Jpval = 1 - chi2(25).cdf(J)
```

The final block using formatted output to present all of the results in a readable manner.

```
vcvrisk_premia = vcv[n * k + n:, n * k + n:]
annualized_rp = 12 * risk_premia
arp = list(squeeze(annualized_rp))
arp_se = list(sqrt(12 * diag(vcvrisk_premia)))
print('        Annualized Risk Premia')
print('          Market        SMB         HML')
print('--------------------------------------')
print(f'Premia    {arp[0]:0.4f}     {arp[1]:0.4f}      {arp[2]:0.4f}')
print(f'Std. Err.  {arp_se[0]:0.4f}    {arp_se[1]:0.4f}      {arp_se[2]:0.4f}')
print('\n\n')

print(f'J-test:   {J:0.4f}')
print(f'P-value:  {Jpval:0.4f}')

i = 0
beta_se = []
for j in range(5):
    for m in range(5):
```

```
        a = alpha[i]
        b = beta[:, i]
        variances = diag(vcv[(k + 1) * i:(k + 1) * (i + 1), (k + 1) * i:(k + 1) * (i + 1)])
        beta_se.append(sqrt(variances))
        s = sqrt(variances)
        c = hstack((a, b))
        t = c / s
        print(f'Size: {j+1}, Value:{m+1}    Alpha     Beta(VWM)     Beta(SMB)     Beta(HML)')
        print(f'Coefficients: {a:>10,.4f}  {b[0]:>10,.4f}  {b[1]:>10,.4f}  {b[2]:>10,.4f}')
        print(f'Std Err.      {s[0]:>10,.4f}  {s[1]:>10,.4f}  {s[2]:>10,.4f}  {s[3]:>10,.4f}')
        print(f'T-stat        {t[0]:>10,.4f}  {t[1]:>10,.4f}  {t[2]:>10,.4f}  {t[3]:>10,.4f}')
        print('')
        i += 1
```

The final block converts the standard errors of β to be an array and saves the results.

```
beta_se = array(beta_se)
savez_compressed('fama-macbeth-results', alpha=alpha, beta=beta,
                 beta_se=beta_se, arp_se=arp_se, arp=arp, J=J, Jpval=Jpval)
```

29.3 Estimating the Risk Premia using GMM

The final numeric example estimates examines the same problem, only using GMM rather than 2-stage regression. The first block imports relevant modules and functions. GMM requires non-linear optimization, and `fmin_bfgs` will be used.

```
from numpy import hstack, ones, array, mat, tile, reshape, squeeze, eye, asmatrix
from numpy.linalg import inv
from pandas import read_csv, Series
from scipy.linalg import kron
from scipy.optimize import minimize
import numpy as np
import statsmodels.api as sm
```

Before defining the problem, the next code block defines a *callback* function that can be called after each iteration of the minimizer. This function will be used to display information about the progress of the optimizer: the current function value, the iteration and the number of function calls. Because the callback only gets 1 input, the current value of the parameters used by the optimizer, it is necessary to use `global` variables to pass information between functions. Three variables have been declared: `iteration`, `last_value` and `function_count`. `iteration` is updated only by the callback function since it should report the number of completed iterations of the optimizer, and the callback is called once per iteration. `last_value` is updated each time the main GMM objective function is called, and `function_count` is incremented by 1 each time the main GMM objective is called. The variables are all initialized using `global` inside the callback so that their values can be updated.

```
iteration = 0
last_value = 0
function_count = 0

def iter_print(params):
    global iteration, last_value, function_count
    iteration += 1
    print(f'Func value: {last_value:6.6g}, Iteration: {iteration}, Function Count: {function_count}'
```

The GMM objective takes the parameters, portfolio returns, factor returns and the weighting matrix and computes the moments, average moments and the objective value. The moments used can be described as

$$\left(r_{it}^2 - \beta_i f_t\right) f_t \quad \forall i = 1, \dots N$$

and

$$r_{it} - \beta_i \lambda \quad \forall i = 1, \ldots N.$$

```python
def gmm_objective(params, p_rets, f_rets, Winv, out=False):
    global last_value, function_count
    t,n = p_rets.shape
    t,k = f_rets.shape
    beta = squeeze(array(params[:(n*k)]))
    lam = squeeze(array(params[(n*k):]))
    beta = reshape(beta, (n,k))
    lam = reshape(lam, (k,1))
    betalam = beta @ lam
    expected_ret = f_rets @ beta.T
    e = p_rets - expected_ret
    instr = tile(f_rets,n)
    moments1  = kron(e,ones((1,k)))
    moments1 = moments1 * instr
    moments2 = p_rets - betalam.T
    moments = hstack((moments1,moments2))

    avg_moment = moments.mean(axis=0)

    J = t * mat(avg_moment) * mat(Winv) * mat(avg_moment).T
    J = J[0,0]
    last_value = J
    function_count += 1
    if not out:
        return J
    else:
        return J, moments
```

The final function needed is the Jacobian of the moment conditions. Mathematically it is simply to express the Jacobian using $\otimes$(Kronecker product). This code is so literal that it is simple to reverse engineer the mathematical formulas used to implement this estimator.

$$\hat{G} = \left[\begin{array}{cc} I_N \otimes \Sigma_F & 0 \\ I_N \otimes -\lambda & -\beta \end{array} \right]$$

```python
def gmm_G(params, p_rets, f_rets):
    t,n = p_rets.shape
    t,k = f_rets.shape
    beta = squeeze(array(params[:(n*k)]))
    lam = squeeze(array(params[(n*k):]))
    beta = reshape(beta, (n,k))
    lam = reshape(lam, (k,1))
    G = np.zeros((n*k+k,n*k+n))
    ffp = (f_rets.T @ f_rets) / t
    G[:(n*k),:(n*k)]=kron(eye(n),ffp)
    G[:(n*k),(n*k):] = kron(eye(n),-lam)
    G[(n*k):,(n*k):] = -beta.T

    return G
```

The data import step is virtually identical to that in the previous example. Note that only every other portfolio is used to speed up the GMM optimization.

```python
data = read_csv('FamaFrench.csv')

# Split using both named colums and ix for larger blocks
```

```
dates = data['date'].values
factors = data[['VWMe','SMB','HML']].values
riskfree = data['RF'].values
portfolios = data.iloc[:,5:].values

t,n = portfolios.shape
portfolios = portfolios[:,np.arange(0,n,2)]
t,n = portfolios.shape
excess_ret = portfolios - np.reshape(riskfree,(t,1))
k = np.size(factors,1)
```

Starting values are important in any optimization problem. The GMM problem is closely related to Fama-MacBeth regression, and so it is sensible to use the output from a FMB regression.

```
betas = []
for i in range(n):
    res = sm.OLS(excess_ret[:,i],sm.add_constant(factors)).fit()
    betas.append(res.params[1:])

avg_return = excess_ret.mean(axis=0)
avg_return.shape = n,1
betas = array(betas)
res = sm.OLS(avg_return, betas).fit()
risk_premia = res.params
```

The GMM objective can be minimized using an identity matrix as covariance of the moment conditions along with the starting values computed using a Fama-MacBeth regression. The keyword argument `callback` is used to pass the callback function to the optimizer.

```
risk_premia.shape = 3
starting_vals = np.concatenate((betas.flatten(),risk_premia))

Winv = np.eye(n*(k+1))
args = (excess_ret, factors, Winv)
iteration = 0
function_count = 0
opt = minimize(gmm_objective, starting_vals, args=args, callback=iter_print)
step1opt = opt.x

premia = step1opt[-3:]
premia = Series(premia,index=['VWMe', 'SMB', 'HML'])
print('Annualized Risk Premia (First step)')
print(12 * premia)
```

Once the initial estimates have been computed, these can be used to estimate the covariance of the moment conditions, which is then used to estimate the optimal weighting matrix. The keyword argument `out` is used to return the moments in addition to the objective function value. Note that the variables `iteration` and `last_value` which are used in the callback are both reset to 0 so that the count will be accurate.

```
out = gmm_objective(step1opt, excess_ret, factors, Winv, out=True)
S = np.cov(out[1].T)
Winv2 = inv(S)
args = (excess_ret, factors, Winv2)

iteration = 0
function_count = 0
opt = minimize(gmm_objective, step1opt, args=args, callback=iter_print)
step2opt = opt.x
```

The final block computes estimates the asymptotic covariance of the parameters using the usual efficient GMM covariance estimator, assuming that the moments are a martingale.

```
out = gmm_objective(step2opt, excess_ret, factors, Winv2, out=True)
G = gmm_G(step2opt, excess_ret, factors)
S = np.cov(out[1].T)
vcv = inv(G @ inv(S) @ G.T)/t

premia = step2opt[-3:]
premia = Series(premia,index=['VWMe', 'SMB', 'HML'])
premia_vcv = vcv[-3:,-3:]
print('Annualized Risk Premia')
print(12 * premia)

premia_stderr = np.diag(premia_vcv)
premia_stderr = Series(premia_stderr,index=['VWMe', 'SMB', 'HML'])
print('T-stats')
print(premia / premia_stderr)
```

29.4 Outputting LATEX

Automatically outputting results to LATEX or another format can eliminate export errors and avoid tedious work. This example show how two of the tables in the previous Fama-MacBeth example can be exported to a complete LATEX document, and how, if desired, the document can be compiled to a PDF. The first code block contains the imports needed and defines a flag which determines whether the output LATEX should be compiled.

```
# imports
import numpy as np
import subprocess

# Flag to compile output tables
compile_latex = True
```

The next code block loads the npz file created using the output from the Fama-MacBeth example. The second part shows a generic method to restore all variables. The loaded data is in a dictionary, and so iterating over the keys and using `globals()` (a dictionary) in the main program.

```
# Load variables
f = np.load('fama-macBeth-results.npz')
data = f.items()
# Manually load parameters and std errors
arp = f['arp']
arpSE = f['arpSE']
beta = f['beta']
betaSE = f['betaSE']
J = f['J']
Jpval = f['Jpval']

# Generic restore of all data in a npz file
for key in f.keys():
    globals()[key] = f[key]
f.close()
```

The document is stored in a list. The first few lines contain the required header for a LATEX document, including some packages used to improve table display and to select a custom font. All strings are raw `r''` so that \ does not have to be escaped (i.e. `r'\'` rather than `'\\'` in normal strings).

```
# List to hold table
latex = []
# Initializd LaTeX document
latex.append(r'\documentclass[a4paper]{article}')
```

```python
latex.append(r'\usepackage{amsmath}')
latex.append(r'\usepackage{booktabs}')
latex.append(r'\usepackage[adobe-utopia]{mathdesign}')
latex.append(r'\usepackage[T1]{fontenc}')
latex.append(r'\begin{document}')
```

Table 1 will be stored in its own list, and then `extend` will be used to add it to the main list. Building this table is simple string manipulation and use of `format`.

```python
# Table 1
table1 = []
table1.append(r'\begin{center}')
table1.append(r'\begin{tabular}{lrrr} \toprule')
# Header
colNames = [r'VWM$^e$','SMB','HML']
header = ''
for cName in colNames:
    header += ' & ' + cName

header += r'\\ \cmidrule{2-4}'
table1.append(header)
# Main row
row = ''
for a,se in zip(arp,arpSE):
    row += rf' & $\underset{{({se:0.3f})}}{{{a:0.3f}}}$'
table1.append(row)
# Blank row
row = r'\\'
table1.append(row)
# J-stat row
row = rf'J-stat: $\underset{{({float(Jpval):0.3f})}}{{{float(J):0.1f}}}$ \\'
table1.append(row)
table1.append(r'\bottomrule \end{tabular}')
table1.append(r'\end{center}')
# Extend latex with table 1
latex.extend(table1)
latex.append(r'\newpage')
```

Table 2 is a bit more complex, and uses loops to iterate over the rows of the arrays containing the βs and their standard errors.

```python
# Format information for table 2
sizes = ['S','2','3','4','B']
values = ['L','2','3','4','H']
# Table 2 has the same header as table 1, copy with a slice
table2 = table1[:3]
m = 0
for i in range(len(sizes)):
    for j in range(len(values)):
        row = f'Size: {sizes[i]}, Value: {values[j]} '
        b = beta[:,m]
        s = betaSE[m,1:]
        for k in range(len(b)):
            row += r' & $\underset{{({s[k]:0.3f})}}{{{b[k]: .3f}}}$'
        row += r'\\ '
        table2.append(row)
        m += 1
    if i<(len(sizes)-1):
        table2.append(r'\cmidrule{2-4}')

table2.append(r'\bottomrule \end{tabular}')
```

```
table2.append(r'\end{center}')
# Extend with table 2
latex.extend(table2)
```

The penultimate block finished the document, and uses `write` to write the lines to the LATEX file. `write` does not automatically insert the newline character, and so `\n` is added to each line.

```
# Finish document
latex.append(r'\end{document}')
# Write to table
with open('latex.tex','w') as fid:
    for line in latex:
        fid.write(line + '\n')
```

Finally, if the flag is set, `subprocess` is used to compile the LATEX. This assumes that `pdflatex` is on the system path.

```
# Compile if needed
if compile_latex:
    exit_status = subprocess.call(r'pdflatex latex.tex', shell=True)
else:
    print("\n".join(latex))
```

Chapter 30

Quick Reference

30.1 Built-ins

import

`import` is used to import modules for use in a program.

from

`from` is used to import selected functions from a module in a program.

def

`def` is used to denote the beginning of a function.

return

`return` is used return a value from a function.

range

`range` is an iterator commonly used in `for` loops.

tuple

A `tuple` is an immutable collection of other types, and is initialized using parentheses, e.g. `(a,)` for a single element tuple or `(a,b)` for a 2-element tuple.

list

A `list` is a mutable collection of other types, and is initialized using square brackets, e.g. `[a]` or `[a,b]`.

dict

`dict` initialized a dictionary, which is a list of named values where the names are unique.

set, frozenset

`set` initializes a set which is a unique, mutable collection. `frozenset` is an immutable counterpart.

`for`

`for` being a for loop, and should have the structure `for` *var* `in` *iterable* : .

`while`

`while` begins a while loop, and should have the structure `while` *logical* :

`break`

`break` terminates a loop prematurely.

`continue`

`continue` continues a loop without processing any code below the continue statement.

`try`

`try` begin a block which can handle code which may not succeed. It must be followed by an `except` statement.

`except`

`except` catches errors generated in a `try` statement.

`if`

`if` begins an `if` . . . `elif` . . . `else`, and should have the structure `if` *logical* :

`elif`

`elif` stands for else if, and can be used after an `if` statement to refine the expression. It should have the structure `elif` *logical* :

`else`

`else` finalizes an `if` block and executes if no previous path was taken.

`print`

`print` outputs information to the console.

`file`

`file` opens a file for low-level file reading and writing.

30.1.1 `file` Methods

File methods operate on a file object, which is initialized using `file`. For example, `f = file('text.txt','r')` opens the file text.txt for reading, and `close` is used as `f.close()`.

close

`close` closes an open file handle, and flushes any unwritten data to disk.

flush

`flush` flushes any unwritten data to disk without closing the file.

read

`read` reads data from an open file.

readline

`readline` reads a single line from an open file.

readlines

`readlines` reads one or more lines from an open file.

write

`write` writes a single line to a file without appending the new line character.

writelines

`writelines` writes the contents of an iterable (e.g. a list) to a file without appending the new line character to each line.

30.1.2 String (`str`) Methods

String methods operate on strings. For example, `strip` can be used on a string `x = 'abc '` as `x.strip()`, or can be directly used as `' abc '.strip()`.

split

`split` splits a string at every occurrence of another string, left to right.

rsplit

`rsplit` splits a string at every occurrence of another string, right to left.

join

`join` combines an iterable of strings using a given string to combine.

strip

`strip` removes leading and trailing whitespace from a string.

`lstrip`

`lstrip` removes leading whitespace from a string.

`rstrip`

`rstrip` removes trailing whitespace from a string.

`find`

`find` returns the index of the first occurrence of a substring. -1 is returned if not found.

`rfind`

`rfind` returns the index of the first occurrence of a substring, scanning from the right. -1 is returned if not found.

`index`

`index` behaves like `find`, but raises an error when not found.

`count`

`count` counts the number of occurrences of a substring.

`upper`

`upper` converts a string to upper case.

`lower`

`lower` coverts a string to lower case.

`ljust`

`ljust` right pads a string with whitespace or a specified character up to a given width.

`rjust`

`rjust` left pads a string with whitespace or a specified character up to a given width.

`center`

`center` left and right pads a string with whitespace or a specified character up to a given width.

`replace`

`replace` returns a copy of a string with all occurrences of a substring replaced with an alternative substring.

`format`

`format` formats and inserts formattable objects (e.g. numbers) into a string.

30.1.3 Operating System (`os`)

os.system

`system` executes (external) system commands.

os.getcwd

`getcwd` returns the current working directory.

os.chdir

`chdir` changes the current working directory.

os.mkdir

`mkdir` creates a new directory, but requires all higher level directories to exist.

os.makedirs

`makedirs` creates a directory at any level, and creates higher level directories if needed.

os.rmdir

`rmdir` removes an empty directory.

os.listdir

`listdir` returns the contents of a directory. See `glob.glob` for a more useful form.

os.path.isfile

`path.isfile` determines whether a string corresponds to a file.

os.path.isdir

`path.isdir` determines whether a string corresponds to a directory.

30.1.4 Shell Utilities (`shutil`)

shutil.copy

copy copies a files using either a file name to use for the copy or a directory to use as a destination, in which case the current file name is used.

shutil.copyfile

`copyfile` copies a file using a file name.

shutil.copy2

`copy2` is identical to copy only that (some) file meta-data is also copied.

shutil.copytree

copytree copies an entire directory tree to a destination that must not exist.

shutil.move

move moves a directory tree to a destination which must not exist.

shutil.make_archive

make_archive creates zip, gztar and bztar archives.

shutil.rmtree

rmtree recursively removes a directory tree.

30.1.5 Regular Expressions (`re`)

re.findall

findall returns all occurrences of a regular expression in a string as a list.

re.split

split splits a string on occurrences of a regular expression.

re.sub

sub substitutes a string of each occurrence of a regular expression.

re.finditer

finditer works similarly to findall, only returning an iterable object rather than a list.

re.compile

compile compiles a regular expression for repeated use.

30.1.6 Dates and Times (`datetime`)

datetime.datetime

datetime initializes a date-time object.

datetime.date

date initializes a date object.

datetime.time

time initializes a time object.

datetime.timedelta

`timedelta` represents the difference between two `datetime`s.

datetime.datetime.replace

`replace` replaces fields in a date-time object. `replace` is a method of a date-time, date or time object.

datetime.datetime.combine

`combine` combines a date object and a time object and returns a date-time object. `combine` is a method of a date-time, date or time object.

30.1.7 Other

These function all are contained in other modules, as listed to the left of the dot.

glob.glob

`glob.glob` returns a directory listing allowing for wildcards.

subprocess.call

`subprocess.call` can be used to run external commands.

textwrap.wrap

`textwrap.wrap` wraps a long block of text at a fixed width.

30.2 NumPy (`numpy`)

The functions listed in this section are all provided by NumPy. When a function is listed using only the function name, this function appears in the NumPy module, and so can be accessed as `numpy`.*function*, assuming that NumPy was imported using `import` `numpy`. When a function name contains a dot, for example `linalg.eig`, then the function `eig` is in the `linalg` module of `numpy`, and so the function is accessed as `numpy.linalg.eig`.

30.2.1 Core NumPy Types

dtype

`dtype` is used for constructing data types for use in arrays.

array

`array` is the primary method for constructing arrays from iterables (e.g., a list). Variables created using `array` have type `numpy.ndarray`.

30.2.2 `ndarray`

`ndarray` is the core array data type provided by NumPy. Attributes are accessed directly from an array, e.g. `x.dtype`, and methods are calls to functions which operate on an array, e.g. `x.sum()`.

Attributes

T

T returns the transpose of an array.

dtype

dtype returns the data type of an array.

flat

flat returns a 1-dimensional iterator for an array.

imag

imag returns the imaginary portion of an array.

real

real returns the real portion of an array.

size

size returns the total number of elements of an array.

ndim

ndim returns the number of dimensions of an array.

shape

shape returns the shape of an array as a tuple with ndim elements. shape can also be used to set the shape using a tuple, e.g. x.shape=(10,5) as long as the number of elements does not change.

Methods

all

all returns True if all elements evaluate to True (i.e. not False, None or 0). axis can be used to compute along a particular axis.

any

any returns True if any element evaluates to True. axis can be used to compute along a particular axis.

argmax

argmax returns the index of the maximum of an array. axis can be used to compute along a particular axis.

argmin

argmin returns the index of the minimum of an array. axis can be used to compute along a particular axis.

argsort

`argsort` returns the indices needed to sort an array. `axis` can be used to compute along a particular axis.

astype

`astype` allows an array to be viewed as another type (e.g., `recarray`) and copies the underlying.

conj, conjugate

`conj` and `conjugate` both return the complex-conjugate element-by-element.

copy

`copy` returns a copy of an array.

cumprod

`cumprod` returns the cumulative product of an array. `axis` can be used to compute along a particular axis.

cumsum

`cumsum` return the cumulative sum of an array. `axis` can be used to compute along a particular axis.

dot

`dot` computes the dot-product (standard matrix multiplication) or an array with another array.

flatten

`flatten` returns a copy of an array flattened into a 1-dimensional array.

max

`max` returns the maximum value of an array. `axis` can be used to compute along a particular axis.

mean

`mean` returns the average of an array. `axis` can be used to compute along a particular axis.

min

`min` returns the minimum of an array. `axis` can be used to compute along a particular axis.

nonzero

`nonzero` returns the indices of the non-zero elements of an array.

prod

`prod` computes the produce of all elements of an array. `axis` can be used to compute along a particular axis.

ravel

ravel returns a flattened view of an array without copying data.

repeat

repeat returns an array repeated, element-by-element.

reshape

reshape returns returns an array with a different shape. The number of elements must not change.

resize

resize changes the size shape of an array in-place. If the new size is larger then new entries are 0 filled. If the new size is smaller, then the elements selected are ordered according by their order in ravel.

round

round returns an array with each element rounded to a provided number of decimals.

sort

sort sorts an array (in-place). axis can be used to compute along a particular axis.

squeeze

squeeze returns an array with any singleton dimensions removed.

std

std returns the standard deviation of an array. axis can be used to compute along a particular axis.

sum

sum returns the sum of an array. axis can be used to compute along a particular axis.

tolist

tolist returns a list of an array. If the array has more than 1 dimension, the list will be nested.

trace

trace returns the sum of the diagonal elements.

transpose

transpose returns a view of the array transposed. x.transpose() is the same as x.T.

var

var returns the variance of an array. axis can be used to compute along a particular axis.

view

`view` returns a view of an array without copying data.

Methods and Attributes as functions

Many of the `ndarray` methods can be called as functions and behave identically, aside from taking the array as the first input. For example, `sum(x, 1)` is identical to `x.sum(1)`, and `x.dot(y)` is identical to `dot(x,y)`. The following list of functions are identical to their method: `all`, `any`, argmax, argmin, argsort, `conj`, `cumprod`, `cumsum`, diagonal, `dot`, `imag`, `real`, mean, std, `var`, `prod`, `ravel`, repeat, `squeeze`, `reshape`, std, `var`, trace, `ndim`, and `squeeze`.

Functions with different behavior

round

`around` is the function name for `round`. `around` is preferred as a function name since `round` is also the name of a built-in function which does not operate on arrays.

resize

Using `resize` as a function returns the resized array. Using `resize` as a method performs the resizing in-place.

sort

Using `sort` as a function returns the sorted array. Using `sort` as a method performs the sorting in-place.

size

Using `size` as a function can take an additional argument `axis` specifying the axis to use. When used without an argument `size(x)` is identical to `x.size`.

shape

Using `shape` as a function only returns the shape of an array. The attribute use of `shape` also allows the shape to be directly set, e.g. `x.shape`=3,3.

max

`amax` is the function name for the method `max`. `amax` is preferred as a function name since `max` is also the name of a built-in function which does not operate on arrays.

min

`amin` is the function name for the method `min`. `amin` is preferred as a function name since `min` is also the name of a built-in function which does not operate on arrays.

30.2.3 Array Construction and Manipulation

linspace

`linspace` creates an n-element linearly spaced vector between a lower and upper bound.

logspace

`logspace` creates a logarithmically spaced (base-10) vector between a lower and upper (log-10) bound.

arange

`arange` creates an equally spaced vector between a lower and upper bound using a fixed step size.

ones

`ones` creates an array of 1s.

zeros

`zeros` creates an array of 0s.

empty

`empty` creates an array without initializing the values.

eye

`eye` creates an identity array.

identity

`identify` creates an identity array.

meshgrid

`meshgrid` creates 2-dimensional arrays from 2 1-dimensional arrays which contain all combinations of the original arrays.

tile

`tile` block repeats an array.

broadcast_arrays

`broadcast_arrays` produces the broadcasted version of 2 broadcastable arrays.

vstack

`vstack` vertically stacks 2 or more size compatible arrays.

hstack

`hstack` horizontally stacks 2 or more size compatible arrays.

vsplit

`vsplit` splits an array into 2 or more arrays vertically.

hsplit

`hsplit` splits an array into 2 or more arrays horizontally.

split

`split` splits an array into 2 or more arrays along an arbitrary axis.

concatenate

`concetenate` combines 2 or more arrays along an arbitrary axis.

delete

`delete` deletes elements from an array. `axis` can be used to delete along a particular axis.

flipud

`flipud` flips an array top-to-bottom.

fliplr

`fliplrud` flips an array left-to-right.

diag

`diag` returns the diagonal from a 2-dimensional array, or returns a diagonal 2-dimensional array when used with a 1-dimensional input.

triu

`triu` returns the upper triangular array from an array.

tril

`tril` returns the lower triangular array from an array.

30.2.4 Array Functions

kron

`kron` returns the Kronecker product of 2 arrays.

trace

`trace` returns the sum of the diagonal elements of an array.

diff

`diff` returns the 1st difference of an array. An optional second input allows for higher order differencing. `axis` can be used to compute the difference along a particular axis.

30.2.5 Input/Output

`loadtxt`

`loadtxt` loads a rectangular array from a text file. No missing values are allowed. Automatically decompresses gzipped or bzipped text files.

`genfromtxt`

`genfromtxt` loads text from a data file and can accept missing values.

`load`

`load` loads a npy or npz file.

`save`

`save` saves a single array a NumPy data file (npy).

`savez`

`savez` saves an array or set of arrays to a NumPy data file (npz).

`savez_compressed`

`savez_compressed` saves an array or set of arrays to a NumPy data file (npz) using compression.

`savetxt`

`savetxt` saves a single array to a text file.

30.2.6 nan Functions

`nansum`

`nansum` returns the sum of an array, ignoring NaN values. `axis` can be used to compute along a particular axis.

`nanmax`

`nanmax` returns the maximum of an array, ignoring NaN values. `axis` can be used to compute along a particular axis.

`nanargmax`

`nanargmax` returns the index of the maximum of an array, ignoring NaN values. `axis` can be used to compute along a particular axis.

`nanmin`

`nanmin` returns the minimum of an array, ignoring NaN values. `axis` can be used to compute along a particular axis.

`nanargmin`

`nanargmin` returns the index of the minimum of an array, ignoring NaN values. `axis` can be used to compute along a particular axis.

30.2.7 Set Functions

`unique`

`unique` returns the set of unique elements of an array.

`in1d`

`in1d` returns a Boolean array indicating which elements of one array are in another.

`intersect1d`

`intersect1d` returns the set of elements of one array which are in another.

`union1d`

`union1d` returns the set of elements which are in either of 2 arrays, or both.

`setdiff1d`

`setdiff1d` returns the set of elements on one array which are not in another.

`setxor1d`

`setxor1d` returns the set of elements which are in either or 2 arrays, but not both.

30.2.8 Logical and Indexing Functions

`logical_and`

`logical_and` compute the value of applying `and` to the elements of two broadcastable arrays.

`logical_or`

`logical_or` compute the value of applying `or` to the elements of two broadcastable arrays.

`logical_xor`

`logical_xor` compute the value of applying `xor` to the elements of two broadcastable arrays.

`logical_not`

`logical_not` compute the value of applying `not` to the elements of an array.

`allclose`

`allclose` returns `True` if all elements of two arrays differ by less than some tolerance.

array_equal

array_equal returns True if two arrays have the same shape and elements.

array_equiv

array_equiv returns True if two arrays are equivalent int eh sense that one array can be broadcast to become the other.

find

find returns the indices of an array where a logical statement is true. The indices returned correspond to the flattened array.

argwhere

argwhere returns the indices from an array where a logical condition is True.

extract

extract returns the elements from an array where a logical condition is True.

isnan

isnan returns a Boolean array indicating whether the elements of the input are nan .

isinf

isinf returns a Boolean array indicating whether the elements of the input are inf .

isfinite

isfinite returns a Boolean array indicating whether the elements of the input are not inf and not nan.

isposinf

isposinf returns a Boolean array indicating whether the elements of the input are inf.

isneginf

isneginf returns a Boolean array indicating whether the elements of the input are -inf

isreal

isreal returns a Boolean array indicating whether the elements of the input are either real or have 0j complex component.

iscomplex

iscomplex returns a Boolean array indicating whether the elements of the input are either have non-zero complex component.

`is_string_like`

`is_string_like` returns `True` if the input is a string or similar to a string.

`isscalar`

`isscalar` returns `True` if the input is not an array.

`is_numlike`

`is_numlike` returns `True` if the input is numeric.

`isvector`

`isvector` returns `True` if the input has at most 1 dimension which is not unity.

30.2.9 Numerics

`nan`

`nan` represents Not a Number.

`inf`

`inf` represents infinity.

`finfo`

`finfo` can be used along with a data type to return machine specific information about numerical limits and precision.

30.2.10 Mathematics

`log`

`log` returns the natural logarithm of the elements of an array.

`log10`

`log10` returns the bast-10 logarithm of the elements of an array.

`sqrt`

`sqrt` returns the square root of the elements of an array.

`exp`

`exp` returns the exponential of the elements of an array.

`absolute`

`absolute` returns the absolute value of the elements of an array.

sign

sign returns the sign of the elements of an array.

30.2.11 Rounding

floor

floor rounds to next smallest integer.

ceil

ceil round to next largest integer

30.2.12 Views

asarray

asarray converts its input to an ndarray if it is not, and avoids copies if its input is already an ndarray.

30.2.13 `rec`

rec.array

rec.array construct record arrays.

30.2.14 `linalg`

linalg.matrix_power

matrix_power raises a square array to an integer power.

linalg.cholesky

cholesky computes the Cholesky factor of a positive definite array.

linalg.qr

qr computes the QR factorization of an array.

linalg.svd

svd computes the singular value decomposition of an array.

linalg.eig

eig computes the eigenvalues and eigenvectors of an array.

linalg.eigh

eigh computes the eigenvalues and eigenvectors of a Hermitian (symmetric) array.

`linalg.cond`

`cond` computes the conditioning number of an array.

`linalg.det`

`det` computes the determinant of an array.

`linalg.slogdet`

`slogdet` computes the log determinant and the sign of the determinant of an array.

`linalg.solve`

`solve` solves a just-identified set of linear equations.

`linalg.lstsq`

`lstsq` finds the least squares solutions of an over-identified set of equations.

`linalg.inv`

`inv` computes the inverse of a square array.

30.2.15 `random`

`random.rand`

`rand` returns standard uniform pseudo-random numbers. Uses n inputs to produce an n-dimensional array.

`random.randn`

`randn` returns standard normal pseudo-random numbers. Uses n inputs to produce an n-dimensional array.

`random.randint`

`randing` returns uniform integers on a specified range, exclusive of end point. Uses an n-element tuple to produce an n-dimensional array.

`random.random_integers`

`random_integers` returns uniform integers on a specified range, inclusive of end point. Uses an n-element tuple to produce an n-dimensional array.

`random.random_sample`

`random_sample` returns standard Uniform pseudo-random numbers. Uses an n-element tuple to produce an n-dimensional array.

`random.random`

`random` returns standard Uniform pseudo-random numbers. Uses an n-element tuple to produce an n-dimensional array.

random.standard_normal

`standard_normal` returns standard normal pseudo-random numbers. Uses an *n*-element tuple to produce an *n*-dimensional array.

random.sample

`sample` returns standard Uniform pseudo-random numbers. Uses an *n*-element tuple to produce an *n*-dimensional array.

random.shuffle

`shuffle` shuffles the elements of an array in-place.

random.permutation

`permutation` returns a random permutation of an array.

random.RandomState

`RandomState` is a container for the core random generator. `RandomState` is used to initialize and control additional random number generators.

random.seed

`seed` seeds the core random number generator.

random.get_state

`get_state` gets the state of the core random number generator.

random.set_state

`set_state` sets the state of the core random number generator.

Random Number Generators

Random number generators are available for distribution in the following list: `beta`, `binomial`, `chisquare`, `exponential`, `f`, `gamma`, `geometric`, `laplace`, `logistic`, `lognormal`, `multinomial`, `multivariate_normal`, `negative_binomial`, `normal`, `poisson`, `uniform`.

30.3 SciPy

30.3.1 Statistics (`stats`)

30.3.1.1 Continuous Random Variables

Normal (`norm`), Beta (`beta`), Cauchy (`cauchy`), χ^2 (`chi2`), Exponential (`expon`), Exponential Power (`exponpow`), F (`f`), Gamma (`gamma`), Laplace/Double Exponential (`laplace`), Log-Normal (`lognorm`), Student's *t* (`t`)

stats.*dist*.rvs

rvs generates pseudo-random variables.

stats.*dist*.pdf

pdf returns the value of the PDF at a point in the support.

stats.*dist*.logpdf

logpdf returns the log of the PDF value at a point in the support.

stats.*dist*.cdf

cdf returns the value of the CDF at a point in the support.

stats.*dist*.ppf

ppf returns the value of the random variable from a point in (0,1). PPF is the same as the inverse CDF.

stats.*dist*.fit

fit estimates parameters by MLE.

stats.*dist*.median

median returns the median of random variables which follow the distribution.

stats.*dist*.mean

mean returns the mean of random variables which follow the distribution.

stats.*dist*.moment

moment returns non-central moments of random variables which follow the distribution.

stats.*dist*.var

var returns the variance of random variables which follow the distribution.

stats.*dist*.std

std returns the standard deviation of random variables which follow the distribution.

30.3.1.2   Statistical Functions

stats.mode

mode returns the empirical mode of an array.

stats.moment

moment computes non-central moments of an array.

stats.skew

skew computes the skewness of an array.

stats.kurtosis

kurtosis computes the *excess* kurtosis of an array.

stats.pearsonr

pearsonr computes the correlation of an array.

stats.spearmanr

spearmanr computes the rank correlation of an array.

stats.kendalltau

kendalltau computed Kendall's τ, which is similar to a correlation, from an array.

stats.normaltest

normaltest computes a Jarque-Bera like test for normality.

stats.kstest

kstest computes a Kolmogorov-Smirnov test for a specific distribution.

stats.ks_2samp

ks_2samp computes a Kolmogorov-Smirnov test from directly from two samples.

stats.shapiro

shapire computes the Shapiro-Wilks test of normality.

30.3.2 Optimization (`optimize`)

30.3.2.1 Unconstrained Function Minimization

optimize.fmin_bfgs

fmin_bfgs minimizes functions using the BFGS algorithm.

optimize.fmin_cg

fmin_cg minimizes functions using a Conjugate Gradient algorithm.

optimize.fmin_ncg

fmin_ncg minimizes functions using a Newton-Conjugate Gradient algorithm.

30.3.2.2 Derivative Free Unconstrained Function Minimization

`optimize.fmin`

`fmin` minimizes a function using a simplex algorithm.

`optimize.fmin_powell`

`fmin_powell` minimizes a function using Powell's algorithm.

30.3.2.3 Constrained Function Minimization

`optimize.fmin_slsqp`

`fmin_slsqp` minimizes a function subject to inequality, equality and bounds constraints.

`optimize.fmin_tnc`

`fmin_tnc` minimizes a function subject to bounds constraints.

`optimize.fmin_l_bfgs_s`

`fmin_l_bfgs_s` minimizes a function subject to bounds constraints.

`optimize.fmin_colyba`

`fmin_colyba` minimizes a function subject to inequality and equality constraints.

30.3.2.4 Scalar Function Minimization

`optimize.fmin_bound`

`fmin_bound` minimizes a function in a bounded region.

`optimize.golden`

`golden` uses a golden section search to minimize a scalar function.

`optimize.brent`

`brent` uses Brent's method to minimize a scalar function.

30.3.2.5 Nonlinear Least Squares

`optimize.lstsq`

`lstsq` performs non-linear least squares minimization of a function which returns a 1-dimensional array of errors.

30.3.3 Input/Output (`io`)

`io.loadmat`

`loadmat` loads a MATLAB data file.

`io.savemat`

`savemat` saves an array or set of arrays to a MATLAB data file.

30.4 Matplotlib

30.4.1 2D plotting

`plot`

`plot` plots a 2-dimensional line or set of lines.

`pie`

`pie` produces a pie chart.

`hist`

`hist` computes and plots a histogram.

`scatter`

`scatter` produces a scatter plot.

`bar`

`bar` produces a vertical bar chart.

`barh`

`barh` produces a horizontal bar chart.

`contour`

`contour` produces a 2-dimensional contour representation of 3-dimensional data.

30.4.2 3D plotting

`plot`

`plot` using the optional keyword argument `zs` produces 3-dimensional plots.

`plot_wireframe`

`plot_wireframe` plots a 3-dimensional wire-frame surface.

`plot_surface`

`plot_surface` plots a 3-dimensional solid surface.

30.4.3 Utility Commands

`figure`

`figure` opens a new figure or changes the current figure to an existing figure.

`add_axes`

`add_axes` adds a single axes to a figure.

`add_subplot`

`add_subplot` adds a subplot to a figure.

`show`

`show` updates a figure and pauses the running of a non-interactive program until the figure is closed.

`draw`

`draw` updates a figure.

`close`

`close` closes figures. `close('all')` closes all figures.

`legend`

`legend` adds a legend to a plot or chart using the information in `label` keyword arguments.

`title`

`title` adds a title to a plot or chart.

`savefig`

`savefig` exports figures to common file formats including PDF, EPS, PNG and SVG.

30.4.4 Input/Output

`csv2rec`

`csv2rec` reads data in a CSV file and returns a NumPy record array. Columns are automatically types based on the first few rows of the input array, and importing dates is supported.

30.5 pandas

The format `DataFrame.`*method* is used to indicate that method is called directly on a DataFrame (e.g. `x.`*method*`()`).

30.5.1   Data Structures

Series

Series constructs the 1-dimensional array-like (or column-like) structure underlying a DataFrame.

TimeSeries

TimeSeries is a sub-class of Series where the index is a set of datetimes.

DataFrame

DataFrame constructs the primary 2-dimensional array-like (or table-like) structure in pandas.

30.5.2   Series/DataFrame Methods

drop

drop drops rows or columns using a list of labels.

dropna

dropna drops rows containing null-values.

drop_duplicates

drop_duplicates drops rows that contain duplicate values.

values

values returns the NumPy array underlying the DataFrame.

index

values returns an Index object containing the index labels.

fillna

fillna allows null-values to be filled with another value.

T, transpose

T transposes a DataFrame and is used as a property (i.e. df.T). transpose is identical except that it is used as a method (i.e. df.transpose())

sort

sort sorts a DataFrame using either index or column labels or values in one or more columns.

sort_index

sort_index is identical to sort except for the keyword argument names.

pivot

`pivot` reshapes a DataFrame

stack

`stack` creates a single Series representation of a DataFrame.

unstack

`unstack` converts a single Series representation to a Series.

concat

`concat` concatenates two DataFrames into a single DataFrame. `concat` is a function which operated on DataFrames and is not a method.

append

`append` concatenates a DataFrame to the existing DataFrame.

reindex

`reindex` changes the index and/or column labels.

reindex_like

`reindex_like` reindexes a DataFrame using the index of another DataFrame.

reindex_axis

`reindex_axis` reindexes one axis of a DataFrame.

merge

`merge` performs a SQL-like join of two DataFrames using index values to construct the union.

join

`join` performs a SQL-like join of two DataFrames using values in columns to construct the union.

update

`update` updates the values of cells in one DataFrame using index labels.

groupby

`groupby` produces a DataFrameGroupBy object that can be used to compute grouped statistics or plots.

apply

`apply` applies a function column- or row-wise to a DataFrame.

applymap

`applymap` applies a function element-by-element to a DataFrame.

pivot_table

`pivot_table` produces an Excel-like grouping of a DataFrame using one or more columns to group.

count

`count` returns the number of non-null values for each variable in a DataFrame.

describe

`describe` produces summary statistics about the variables in a DataFrame.

value_counts

`value_counts` performs histogramming on a DataFrame.

30.5.3 Graphics

DataFrame.plot

`plot` produces a plot of data in a DataFrame. A keyword argument `kind` can be used to produce line plots (default), bar (`'bar'`), horizontal bar (`'barh'`) or kernel density plots (`'kde'` or `'density'`).

DataFrame.hist

`hist` produces a histogram plot.

DataFrame.boxplot

`boxplot` produces a boxplot of the data in a DataFrame.

DataFrame.scatter_plot

`scatter_plot` produces a scatter plot of two series.

DataFrame.scatter_matrix

`scatter_matrix` produces a matrix of bivariate scatter plots with histograms or kernel density estimates along the diagonal.

DataFrame.lag_plot

`lag_plot` produces a scatter plot of a time series against its lag.

30.5.4 Input/Output

read_excel

`read_excel` reads both Excel 97/2003 and 2007/10/13 files and requires both the filename and the sheet name.

read_csv

`read_csv` reads csv and other delimited files.

read_stata

`read_stata` reads STATA data files.

read_table

`read_table` reads general delimited files.

read_hdf

`read_hdf` reads data from HDF5 files (usually created using `DataFrame.to_hdf`)

read_html

`read_html` reads html tables.

read_json

`read_html` reads data from JavaScript Object Notation.

DataFrame.to_excel

`to_excel` writes data to an Excel file.

DataFrame.to_csv

`to_csv` writes data to a CSV file.

DataFrame.to_string

`to_string` writes data to a string variable or buffer (file or StringIO).

DataFrame.to_latex

`to_latex` writes data to a LaTeX file.

DataFrame.to_stata

`to_stata` writes data to a STATA data file.

DataFrame.to_hdf

`to_hdf` writes data to a HDF5 data file.

DataFrame.to_html

`to_hdf` writes data to a HTML data table.

`DataFrame.to_json`

`to_hdf` writes data to a JSON string.

30.6 IPython

?*partial*, ?module.*partial*

`?`*partial* list any known objects – variables, functions or modules – which match the wild card expression *partial* where *partial* can be any string.

function?, magic?

?*function*, ?*magic*, ?*module*, *function*?, *magic*? and *module*? all pretty print the docstring for a function, magic word or module.

function??, magic??

??*function*, ??*magic*, ??*module*, *function*??, *magic*?? and *module*?? all pretty print the entire function, magic word or module, including both the docstring and the code inside the function.

!command

!*command* is used to run a system command as if executed in the terminal. For example, `!`copy file`.py backup.py` will copy file.by to backup.py. An output can be used to capture the command window text printed by the command to a local variable. For example, `dirListing = !dir *.py` will capture the contents to running a directory listing for all py files. This can then be parsed or used for error checking.

%bookmark

`%bookmark` allows bookmarks to be created to directories. Manage IPython's bookmark system. For example, the current directory can be bookmarked using `%bookmark currentDir`, and can be returned to using `%cd currentDir` (assuming the current directory doesn't contain a directory named currentDir).

%cd

`%cd` changes the current working directory. In Windows, \, \\ or / can be used as directory separators. In Linux, / should be used to separate directories. `%cd` support tab completion, so that only a few letters are needed before hitting the tab key to complete the directory name.

%clear, %cls

`%clear` and `%cls` both clear the terminal window (but do not remove any variables, functions or modules).

%edit

`%edit` opens the editor for py files, and is usually used `%edit` *filename*`.py`.

%hist

`%hist` lists command history. `%hist -g` *searchterm* can be used to search for a specific term or wildcard expression.

%lsmagic

`%lsmagic` lists all defined magic functions.

%magic

`%magic` prints detailed information about all magic functions.

%pdb

`%pdb` controls the use of the Python debugger.

%pdef

`%pdef` prints only the definition header (the line beginning with `def`) for functions.

%precision

`%precision` sets the display precision. For example `%precision 3` will show 3 decimal places.

%prun

`%prun` runs a statement in the profiler, and returns timing and function call information. Use `%run -p` *file-name.py* to profile a standalone file.

%psearch

`%psearch` searches for variables, functions and loaded modules using wildcards.

%pwd

`%pwd` shows the current working directory.

%pycat, %more, %less

`%pycat`, `%more` and `%less` all show the contents of a file in the IPython window.

%pylab

`%pylab` initializes pylab if not initialized from the command line.

%quickref

`%quickref` shows a reference sheet for magic commands.

%reset

`%reset` resets the session by removing all variables, functions and imports defined by the user.

%reset_selective

`%reset_selective` *re* resets all names which match the regular expression *re*.

%run

`%run` *filename.py* executes a file containing Python code in the IPython environment.

%time

`%time` *code* provides the time needed to run the code once. `%timeit` is often more useful.

%timeit

`%timeit` *code* times a segment of code, and is useful for finding bottlenecks and improving algorithms. If *code* is very fast, multiple runs are used to improve timing accuracy.

```
>>> %timeit x=randn(100,100);dot(x.T,x)
1000 loops, best of 3: 758 us per loop
```

%who

`%who` lists all variables in memory.

%who_ls

`%who_ls` returns a sorted list containing the names of all variables in memory.

%whos

`%whos` provides a detailed list of all variables in memory.

%xdel

`%xdel` *variable* deletes the variable from memory.

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