# WhizzML Tutorials

The BigML Team

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MACHINE LEARNING MADE BEAUTIFULLY SIMPLE

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## About this Document

This document contains a collection of WhizzML tutorials, organized by complexity. These are intended to help the user write his/her own WhizzML Scripts and Libraries.

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### Introduction

As you have read in the WhizzML Primer document,<sup>1</sup> WhizzML is a powerful tool for automating Machine Learning (ML) workflows and implementing higher-level ML algorithms.

This document contains tutorials for writing these WhizzML workflows and algorithms. The tutorials are organized into three categories: Part I, Part II and Part III.

In the beginner tutorials, we go over each piece of the code in detail, explaining WhizzML language concepts and its standard library. As the tutorials get more advanced, we leave these details behind to focus on higher level concepts.

<sup>&</sup>lt;sup>1</sup>https://bigml.com/whizzml

# Part I

# Beginner

We'll start with a few basic tutorials that demonstrate just a few of the most basic features of WhizzML. It might be handy to have the WhizzML Reference nearby as you go through these examples.

### Model or Ensemble?

In this tutorial, we'll do a simple test to determine whether a single tree or an ensemble is a better fit for a given dataset. We'll go over every line of the code here, but you can also grab it from our WhizzML examples repository<sup>1</sup> on Github.

The idea here is simple: We can use WhizzML to build both single trees and ensembles of trees as predictors. BigML can also conduct evaluations of predictors on datasets. So our script will:

- Split our datasets into two parts, training and testing
- Train a single tree on the training data
- Train an ensemble of trees on the training data
- Evaluate both on the testing data
- Compare the evaluations to decide which is better

#### 1.1 Creating the Training and Testing Sets

The first thing we need to do is split our datasets into two parts. Taken together, these two functions do exactly that.

As you can see, the sample-dataset function takes three parameters, ds-id, which is the identifier for the input dataset, rate which is the amount of the data that we want to keep, and oob, a Boolean value that says whether to use the sample specified, or its complement. That is, if rate is 0.75 and oob is false, we'll get 75% of the data in our sample. If oob is true, we'll get the other 25%.

This is important to our split as we want our training and testing data to be mutually exclusive (so we can't "cheat" by training on testing points before the test). In fact, you can see this at work in split-dataset. Here we return a list of two datasets created by sample-dataset, where the only

<sup>&</sup>lt;sup>1</sup>https://github.com/whizzml/examples/tree/master/model-or-ensemble

parameter we've varied is oob. This will give us a two mutually exclusive datasets, one of which we'll use to train, and the other to test.

#### **1.2** Creating Predictors

The next thing we need to do is create our single tree and our ensemble. Given a dataset identifier, ds-id, creating a model from it with default configuration parameters is as simple as calling the built-in procedure create-model:

```
(create-model ds-id)
```

For the ensemble, we have the corresponding **create-ensemble** primitive, although in this case we will want to also provide a configuration parameter: the number of models in the forest, **size**:

(create-ensemble ds-id {"number\_of\_models" size})

In both cases, the **create** procedure will first check that the dataset that is used has reached its **finished** state (i.e., has status code 5), waiting if necessary for it, and then request the creation of the corresponding model or ensemble. The result of the call will be the identifier of the new resource.

#### **1.3 Evaluating Predictors**

The last major step is to evaluate the models on the testing data. To that end, we can use the WhizzML built-in 'create-evaluation', that takes as inputs the identifier of the resource to evaluate (a model or an ensemble in our case) and the identifier of the test dataset to use for the evaluation. Thus, our code performing evaluations will be very straightforward:

```
(create-evaluation model-id test-dataset-id)
(create-evaluation ensemble-id test-dataset-id)
```

These calls will return the corresponding evaluation identifiers. We will want to, first, wait until they are finished, and, once they are completed, fetch them and extract from the full resource map the quantity that we are going to use to assess the quality of our model or ensemble, namely, the average F-measure. These two steps are encapsulated in the helper function quality-measure, that we define as follows:

```
(define (quality-measure ev-id)
 (let (ev (fetch (wait ev-id)))
   (ev ["result" "model" "average_f_measure"])))
```

As you can see, we first call wait with the evaluation's identifier to make sure the evaluation is finished before fetching it. wait will eventually return that identifier again if everything is fine, and then we use that identifier again as the argument of fetch, that recovers the full map of the evaluation. All that is left is to access the nested field "average f measure" within that map:

As you can see, we use the evaluation map itself, ev, as a function to perform the lookup, passing to it the path to the desired key as a list, ["result" "model" "average\_f\_measure"].

#### 1.4 The Whole Workflow

Finally, we're ready to put it all together.

```
;; Function encapsulating the full workflow
(define (model-or-ensemble src-id)
 (let (ds-id (create-dataset src-id)
                                        ;; full dataset
        ids (split-dataset ds-id 0.8)
                                        ;; split it 80/20
        train-id (ids 0)
                                        ;; the 80% for training
                                        ;; and 20% for evaluations
        test-id (ids 1)
       m-id (create-model train-id)
        e-id (create-ensemble train-id {"number_of_models" 15})
       m-f (quality-measure (create-evaluation m-id test-id))
        e-f (quality-measure (create-evaluation e-id test-id)))
   (log-info "model f " m-f " / ensemble f " e-f)
   (if (> m-f e-f) m-id e-id)))
```

The final function looks basically like our itemized list at the top of this tutorial. We first create a dataset using the input source identifier. We then split this dataset using the function split-dataset above that gives us a list of two sub-datasets. We can use the returned list as a procedure to pull out the first and second elements of this list into train-id and test-id, respectively. We then make our single tree and our ensemble and evaluate them both, pulling the value for the F-measure out of the evaluation.

Depending on which value for the F-measure is better, we return the identifier of the better thing, and we're done!

#### **1.5** Extension to Regression

In the above code, we use a quality metric, the average value of F1, that is only available when our problem is a classification. For regressions (that is, models where our objective field is numeric), that metric is not available and our script will raise an error.

We can easily fix the problem and extend our script so that it supports regression problems by picking a convenient quality metric for them. A good choice is **r\_squared**, which can be found nested following the path ["result" "model" "r\_squared"] in the evaluation map.

Instead of **f-measure** we will use a new function, **quality-measure** that will first try to find the average F measure and, in case it is not found, will fallback to **r\_squared**:

```
;; Function to extract a quality measure from the evaluation results
(define (quality-measure ev-id)
  (let (ev (fetch (wait ev-id)))
      (or (ev ["result" "model" "average_f_measure"] false)
            (ev ["result" "model" "r_squared"] false)
            (raise "The models couldn't be evaluated"))))
```

The implementation of this function also shows a simple example of error signaling using raise.

#### 1.6 Summing Up

We have seen an example of how we can use WhizzML to do simple model selection with some basic code and no external libraries. We have written our first simple functions to abstract away implementation details, such as **quality-measure**, seen how to create and fetch BigML resources and access its properties, and simple error handling.

### **Dataset Transform**

We'll start with a script that will remove a field from a dataset if it has "too much" missing data. As those of you who have dealt with production data know, sometimes there are fields which are missing a lot of data. So much so, that we want to ignore the field altogether.

BigML will automatically detect bad fields like this and ignore them automatically if we create a predictive model. But what if **we** want to specify the required "completeness" of the data field? How can we eliminate fields that have, say, 95% non-missing data?

#### We can use WhizzML!

Let's Do it! Use the WhizzML reference guide<sup>1</sup> if you need it along the way.

To reiterate our goal, we want to write a function that:

- 1. Given a dataset and a specified threshold (e.g. 0.95)
- 2. Returns a new dataset with only the fields that are more than 95% populated.

We can define the base function here.

#### 2.1 Filtered-Dataset

Hey, slow down! Ok. Let's take it step-by-step.

We define a new function called filtered-dataset that takes two arguments: Our starting dataset dataset-id, and a threshold (e.g., 0.95)

(define (filtered-dataset dataset-id threshold) ...)

What do we want this function to do? We want it to return a new dataset, hence:

(create-and-wait-dataset ...)

But we don't just want any old dataset, we want one based off our old dataset:

<sup>&</sup>lt;sup>1</sup>https://bigml.com/whizzml

"origin\_dataset" dataset-id

And we also want to exclude some fields from our old dataset!

"excluded\_fields" (...)

Ah, but which fields do we want to exclude? We can let a new function called excluded-fields figure that out for us.

But for now, all we need to know is that this new function (excluded-fields) takes two arguments: our old dataset and our specified threshold.

The line above becomes: (indentation removed for clarity)

```
"excluded_fields" (excluded-fields dataset-id threshold)
```

As we progress, keep in mind that we want this new function (excluded-fields) to return a list of field names (e.g. ["field\_1" "field\_2" "field\_3"])

Great! We defined our base function. Now we have to tell our new function, excluded-fields how to give us the list that we want.

#### 2.2 Excluded-Fields

Wow what? You can use that code for reference, but don't be intimidated. We'll go over each piece.

First we define the function, declaring its two arguments: our original dataset, and the threshold we want to use.

(define (excluded-fields dataset-id threshold) ... )

Before we write any more code, let's talk about the meat of this function. We want to look at all the columns (fields) of this dataset, and find the ones that are missing too much data. We'll keep the names of these "bad" fields so that we can exclude them from our new dataset.

To do this, we can use the function filter. It takes two arguments: a list and a predicate. filter will return a new list composed of the elements in the original list that satisfy the predicate. In our case, the predicate is that the field has to have at least 95% of the data.

The first argument given to filter is our predicate. The predicate should be a function that either evaluates to true or false based on each element of the list we pass to it. If the predicate returns true, then that element of the list is kept. Otherwise, it is thrown out.

We can define this predicate function using lambda.

lambda is like any other function definition. We have to tell it the name of the thing we are passing into it

(field-name)

and also tell it what we are going to do with that thing.

```
(> threshold <percent-of-data-that-the-field-has>)
```

In our case, we are checking to see if the threshold is *greater than* the amount of data present. We will keep the field-name(s) that *do not* have enough data. (Because remember, these are the fields that will be excluded from our new dataset!)

Cool! But two things are still missing from our filter.

```
1. all-field-names
```

2. <percent of data that the field has>

How do we get these?

The first isn't too difficult because BigML datasets have this information readily available. We just have to fetch it from BigML first.

(fetch dataset-id)

and then specify which value we want to get.

```
((fetch dataset-id) "input_fields")
```

Nice.

To figure out what percent of the rows are populated for a specific field, we get to... Define a new function!

But before we do that, let's talk about some things we skipped over in our excluded-fields function. Here it is again, for convenience.

#### What is let?

let is the preferred method for declaring local variables in WhizzML.

- We set the value of data to the result of (fetch dataset-id).
- We set the value of all-field-names to the result of (get data "input\_fields").
- We set the value of total-rows to the result of (get data "rows"). (We didn't talk about this yet. It's one of the values we need to pass to the present-percent function)

let is useful for a couple of reasons in this function. First, we use data twice. So we can avoid the repetition of writing (fetch dataset-id) twice. Second, naming these variables at the top of the function makes the rest much easier to read!

So to wrap up this excluded-fields function, let's talk through what it does again. First, it declares local variables that we'll need. Then, it takes the list of all-field-names and filters it based on a function that checks its "present percent" of data points. We keep the names of the fields that *do not* meet our criteria. Cool!

Now, we'll go over that present-percent function

#### 2.3 Present-Percent

```
(define (present-percent data field-name total-rows)
  (let (fields (data "fields"))
      (- 1 (/ (missing-count field-name fields) total-rows))))
```

Ah. Not so bad.

To calculate the percentage of data points that are present in a given field, we need a few things. First of all, the big collection of data from our dataset (data). Second, the name of the field we are inspecting (field-name). Last, the total number of rows in our dataset (total-rows).

We'll set another local variable using let and call it fields. This is another object containing data about each of the fields. We'll be using it below.

```
(let (fields (data "fields")) ...)
```

Then, we divide the missing-count from the field by the total-rows. This gives us a "missing percent"

```
(/ (missing-count field-name fields) total-rows))
```

We subtract the "missing percent" from one and that gives us the "present percent"!

```
(- 1 (/ (missing-count field-name fields) total-rows))
```

But missing-count is another function! Yes it is!

#### 2.4 Missing-Count

```
(define (missing-count field-name fields)
  (fields [field-name "summary" "missing_count"]))
```

missing-count takes two arguments. First, the name of the field we are inspecting (field-name) and second, the fields object we mentioned earlier. It holds a bunch of information about each of the dataset fields.

To get the count of missing rows of data from the field, we do this:

```
(fields [field-name "summary" "missing_count"])
```

It lets us access an inner value (i.e. 10) from a data object structured like so:

And... That's it! We have now written all the pieces to make our filtered-dataset function work! All together, the code should look like this:

```
(define (missing-count field-name fields)
  (fields [field_name "summary" "missing_count"]))
```

And we can run it just like this:

(filtered-dataset "dataset/83hs0sj3819sdkd92k" 0.75)

And get a result like this:

"dataset/..." - a new dataset without those empty fields.

# Part II

# Intermediate

Now that we've mastered the basics, let's take a look at some more involved workflows. Here, we'll be dealing with multiple resource types and using many of the standard library functions to accomplish our task.

### **Covariate Shift**

If this is your first time writing WhizzML, we suggest you start with one of the examples in Part I, since we won't explain *all* the details in this walkthrough.

In this post, we'll write a WhizzML script that automates a process to investigate Covariate Shift. To get an understanding of what we're trying to do, read this article first.<sup>1</sup>

Again, use the WhizzML reference guide<sup>2</sup> if you need help along the way.

Our goal is to write a function that:

- Given two datasets (one that represents the data used to train a predictive model, one that represents production data)
- Returns an indication of whether the distribution of data has changed.

As we read in the article, the indicator of change in our data distribution is called the phi coefficient. Our WhizzML script will return us this number, so lets name our base function phi-coefficient.

#### 3.1 Phi-Coefficient

#### What are we doing here?

To start, the function takes three arguments. The first two are ids for our training and production datasets, respectively. We call them training-dataset and production-dataset. The third argument, seed, is used to make our sampling deterministic. We'll talk about this later.

There's quite a bit going on in this function, but it's all broken into manageable pieces. First, we use let to set local variables. These local variables are the result of a few different functions which we will have to define.

The local variables are comb-data, ids, model and eval. After these are set, we can compute the phi coefficient with the function avg-phi.

<sup>&</sup>lt;sup>1</sup>http://blog.BigML.com/2014/01/03/simple-machine-learning-to-detect-covariate-shift/

<sup>&</sup>lt;sup>2</sup>https://bigml.com/whizzml

#### 3.1.1 Comb-Data

comb-data is the result of (combined-data training-dataset production-dataset)

Here we're combining the two datasets into one big dataset. But before they are combined, we have to do a transformation on each dataset (add the "Origin" field). We'll talk about that transformation when we define combined-data.

The result of our comb-data dataset looks something like this:

$field_1$	field_2		"Origin"
123	124		"Training"
123	124		"Production"
123	124		"Production"
123	124	• • •	"Training"

#### 3.1.2 Ids

Next, we have a variable called ids. This is a list of dataset-ids that is the result of

(split-dataset comb-data 0.8 seed)

What our split-dataset function does is takes the comb-data (one big dataset) and randomly splits it into two datasets. We split it so that we can train a predictive model with the larger portion of the split, and then evaluate its performance on the smaller part.

The split-dataset function returns something like this

["dataset/83bf92b0b38gbgb" "dataset/83hf93gf012bg84b20"].

#### 3.1.3 Model

model is a BigML predictive model resource. We are creating this model from the first element of our ids list: "dataset" (head ids). The model is built to predict whether the value for the "Origin" field is "Training" or "Production". Thus, the "objective\_field" is "Origin". "objective\_field" "Origin".

#### 3.1.4 Eval

eval is a BigML evaluation resource. To create an evaluation, we need two arguments: a predictive model and a dataset we want to test the model against. Our model is stored in model and our dataset is the second element in the ids list, that is, the element in position 1: (ids 1)

#### 3.1.5 Avg-Phi

We're done with the local variables, but what does the whole **phi-coefficient** function return - what's our end product?

```
(avg-phi eval)
```

That line gives us the average phi score for the evaluation we just created. A bunch of information is stored inside the eval data object that will be retrieved from BigML. But of course, we have to tell the function avg-phi how to get what we want! We'll save that for later.

• • •

So we have built our base function and understand its components. Now we have to go back and build the functions we haven't defined yet, specifically comb-data, split-dataset, model-evaluation and avg-phi. We'll start with comb-data.

#### 3.2 Comb-Data

Again, this function combines two datasets. We tell BigML what datasets we want to combine using the origin\_datasets parameter and passing it a list of dataset ids.

But what are train-data and prod-data?

Those are helper functions that add the "Origin" field we talked about.

- train-data adds the "Origin" field with the value "Training" in each row
- prod-data adds the "Origin" field with the value "Production" in each row

They are defined here:

```
(define (train-data dataset-id)
  (with-origin-field dataset-id "Training"))
(define (prod-data dataset-id)
  (with-origin-field dataset-id "Production"))
```

Since we are doing pretty similar things in both functions, (adding an "Origin" field) we can separate that logic into its own function. Here it is:

In that function we are...

- Creating a new dataset from an existing one "origin\_dataset" dataset-id
- Adding a new field "new\_fields" [...]
- Giving the new field a column name and label "name" "Origin" "label" "Origin"
- Setting the row's value "field" value.

The value will either be the string "Production" or "Training". This string is passed in as an argument where prod-data and train-data are defined.

Nice. Now let's go over split-dataset.

#### 3.3 Split-Dataset

• What are we splitting? dataset-id. The input dataset.

- How are we splitting it 80%/20%? 90%/10%? We can do whatever we want. This is determined by rate.
- How are we going to shuffle our data before we split it? The seed determines this.

As you can see, we are sampling the same dataset twice. One sample will be used to build a predictive model, the other will be used to evaluate the predictive model.

sample-dataset is another function. Here it is below:

#### 3.4 Sample-Dataset

This function is what actually interacts with BigML. We create a new dataset, passing in the **rate**, the original dataset (dataset-id), whether it is out\_of\_bag or not (we'll go over this) and the seed used to determine how the original dataset was shuffled.

Here's a little diagram that will help explain how the seed and out\_of\_bag (oob) work.

	(seed = "123")		(seed	= "hi12")	
	(rate = 0.5)		(rate	= 0.5)	
-Original Dataset-	- New dataset -		- Anothe	er dataset	-
Id   field_1	Id   field_1		Id	field_1	
1 "hello"	1 "hello"	х	1	"hello"	х
2 "hi"	2 "hi"	х	2	"hi"	oob
3 "ok"	3 "ok"	oob	3	"ok"	х
4 "yeah"	4 "yeah"	oob	4	"yeah"	oob

So if out\_of\_bag is set to true, we grab the rows labeled "oob". Otherwise, we grab the ones marked "x" The seed just changes which rows we label "oob" and "x". The seed also enables this whole process to be deterministic. So if you run the phi-coefficient function with the same seed (and the same datasets), you'll get the same results!

Cool. That wraps up our sample-dataset and split-dataset functions. Next up, model-evaluation.

#### 3.5 Model-Evaluation

```
(define (model-evaluation model-id dataset-id)
  (create-and-wait-evaluation {"model" model-id "dataset" dataset-id}))
```

We apologize if you were hoping for something more exciting. This function is just a wrapper for the method included with /whizzml, create-and-wait-evaluation. As you can see, we are simply creating an evaluation with a model and a dataset.

Our last function is...

#### 3.6 Avg-Phi

```
(define (avg-phi ev-id)
  ((fetch ev-id) ["result" "model" "average_phi"]))
```

Pretty simple too!

We take the evaluation ev-id and fetch its data from BigML (fetch ev-id). Then we access the average\_phi attribute nested under "model" and "result".

The data object looks like this:

(fetch ev-id) ;; -> { "result" { "model" { "average\_phi" 0.834 }}}

• • •

And there we have it. A WhizzML script that helps predict covariate shift.

#### 3.6.1 All Together:

```
(define (with-origin-field dataset-id value)
 (create-and-wait-dataset {"origin_dataset" dataset-id
                            "new_fields" [{"field" value
                                           "name" "Origin"
                                           "label" "Origin"}]))
(define (train-data dataset-id)
 (with-origin-field dataset-id "Training"))
(define (prod-data dataset-id)
 (with-origin-field dataset-id "Production"))
(define (combined-data training-dataset production-dataset)
 (create-and-wait-dataset {"origin_datasets" [(train-data training-dataset)
                                               (prod-data production-dataset)]}))
(define (sample-dataset dataset-id rate oob seed)
 (create-and-wait-dataset {"sample_rate" rate
                            "origin_dataset" dataset-id
                            "out_of_bag" oob
                            "seed" seed}))
(define (split-dataset dataset-id rate seed)
 (list (sample-dataset dataset-id rate false seed)
        (sample-dataset dataset-id rate true seed)))
(define (model-evaluation model-id dataset-id)
 (create-and-wait-evaluation {"model" model-id "dataset" dataset-id}))
(define (avg-phi ev-id)
 ((fetch ev-id) ["result" "model" "average_phi"]))
(define (phi-measure training-dataset production-dataset seed)
 (let (comb-data (combined-data training-dataset production-dataset)
        ids (split-dataset comb-data 0.8 seed)
       model (create-and-wait-model {"dataset" (ids 0)
                                      "objective_field" "Origin"})
        ev-id (model-evaluation model (ids 1)))
      (avg-phi ev-id)))
```

We can run our function like this:

```
(phi-measure "datast/ei9202i390203" "dataset/s93999303f09" "test-run-1") -> 0.82
(phi-measure "datast/ei9202i390203" "dataset/s93999303f09" "test-run-2") -> -0.4
```

But. . .

As we read in the article, it is best to do this process several times and look at the average of the results. How could we add some more code to to do this programmatically?

Here's one implementation.

#### 3.7 Multi-Phis

Again, we are giving this function our training-dataset and production-dataset. But we are also passing in n, which is the number of phi-coefficients we want to calculate.

As you can see, we are defining a loop.

Within this loop, we set some variables.

- seeds, we give the default (starting) value of (range 0 n)
  - If we pass in 4 for the value of n then the initial value of seeds = [0 1 2 3]
- out is our output. We will add the result of a phi-coefficient run each time through the loop.
  - Initially, out = []

We also define the end-scenario.

- If seeds is empty, then we return a map with the values list and average. (we'll explain these in a bit)
- If seeds is not empty, we go back to the loop, but define values for seeds and out.
- seeds = (tail seeds). This grabs everything but the first element of seeds
  - So the first time through, it might be [0 1 2 3], then it will be [1 2 3], then [2 3]...
- out = (append out (phi-coefficient ...)) We take the result of our phi-coefficient function and add it to the out list.
  - First time through, it's [], then [-0.0838], then [-0.0838, 0.1240] ...

The seed we will use for each of these phi-coefficient runs will be "test-0", "test-1", "test-2" etc. Thats what (str "test-" (head seeds)) is doing - joining the string "test-" with the first element of the seeds list.

The last thing we should discuss is the end-case return value:

```
{"list" out
    "average" (/ (reduce + 0 out) (count out))}
```

The value of "list" (out) is just the list of phi-coefficient values from each run. The "average" is... Yep. The average of all the runs. reduce adds up the elements. count counts the number of elements. / divides the first by the second.

You got it! The average of many phi-coefficients between two datasets, to help predict covariate shift.

Example run<sup>3</sup>:

```
(multi-phis 3 "dataset/56c3af3f7e0a8d6cca01292e" "dataset/574ef59546522f61f2000444")
;; -> { :list [0.03824, -0.10747, -0.08768], :average -0.05230 }
```

#### Cool

Take a second and think about what you can accomplish now in a few clicks with this WhizzML Script.

- 1. Make a bunch of predictive models
- 2. Evaluate their performances
- 3. Get the knowledge of whether your data characteristics have changed

Sweet!

And even more powerful... The knowledge to automate your own processes!

 $<sup>^{3}</sup>$ Since we used the same dataset for the Training and Production data, it guesses the wrong value for the "Origin" nearly every time! That's why the phi-coefficient values are all close to -1.

### Best-K

BigML has an implementation of G-means clustering built into the cluster API.<sup>1</sup> G-means clustering is an enhancement to K-means clustering that seeks to find the optimal value of K under the assumption that the neighborhood of points around the centroid of a cluster should have a Gaussian distribution in a certain sense.<sup>2</sup> In our API, G-means clustering is invoked by omitting the number K of centroids for K-means clustering, *e.g*:

Assuming a priori that clusters in a dataset conform to the assumptions of the G-means algorithm may be inappropriate. In addition, the G-means method for determining K incrementally fissions clusters and adjusts the resulting clusters appropriately, so that in many cases not every value of K is considered. This proclivity of the algorithm to split a cluster into two clusters is determined by the critical\_value parameter, but frequently there aren't principled ways to select its value.

Fortunately, using WhizzML we can implement an alternative to G-means for determining K based on the Pham-Dimov-Nguyen algorithm.<sup>3</sup> Pham, Dimov, and Nguyen define a measure of concentration f(K) on a K-means clustering and use that as evaluation function to determine the best K. This tutorial presents an example implementation of the PDN-based algorithm that finds the best number K of centroids for K-means clustering in an arbitrary range of  $K_{\min}$  to  $K_{\max}$ .

The full code for this tutorial is available in our whizzml examples repository<sup>4</sup> on Github.

#### 4.1 Code Overview

We first present a brief overview of the WhizzML functions in this package that implement the Pham-Dinov-Nguyen approach to estimating the best number of centroids K for a K-means clustering. We then review a few brief example functions using the top-level functions in the package.

<sup>&</sup>lt;sup>1</sup>https://bigml.com/developers/clusters

<sup>&</sup>lt;sup>2</sup>https://blog.bigml.com/2015/02/24/divining-the-k-in-k-means-clustering/

<sup>&</sup>lt;sup>3</sup>http://www.ee.columbia.edu/~dpwe/papers/PhamDN05-kmeans.pdf

<sup>&</sup>lt;sup>4</sup>https://github.com/whizzml/examples/tree/master/best-k

```
ids (create* "cluster" clist))
(map fetch (wait* ids))))
```

Inputs:

- dataset: (string) Dataset identifier of the dataset to be clustered
- args: (map) Arguments for the cluster operation
- k-min: (number) Minimum value of K
- k-max: (number) Maximum value of K

Output: (list) Cluster metadata for created clusters

We begin with a function generate-clusters to create a collection of K-means clusterings for an arbitrary range k-min  $\leq K \leq$  k-max of centroids. The input map args for the WhizzML cluster function is expanded to fargs with the input dataset, the number K of centroids, and the name for each cluster instance. After setting up the list of arguments for generating each cluster in the collection, the routine uses the common idiom create\*, wait\* to generate the returned set of candidate BigML Cluster objects in parallel.<sup>5</sup>

```
(define (extract-eval-data cluster)
  (let (id (cluster "resource")
        k (cluster "k")
        n (count (cluster "input_fields"))
        within_ss (cluster ["clusters" "within_ss"])
        total_ss (cluster ["clusters" "total_ss"]))
        {"id" id "k" k "n" n "within_ss" within_ss "total_ss" total_ss}))
```

Inputs:

• cluster: (string) Cluster identifier of the cluster

**Output:** (map) Cluster metadata used to compute the evaluation function f(K)

To simplify the implementation of the PDN algorithm, we next define a helper function to extract certain metadata items from the full metadata for a cluster. The metadata returned by extract-eval-data are just the items needed to compute the PDN evaluation function f(K). These include the number K of centroids in the K-means clustering, the number of covariates n considered in the K-means computation, the total sum-squared distance between the items in the cluster and the cluster centroid for all clusters  $S_k$  (within\_ss), and finally  $S_1$  available in the metadata for every cluster (total\_ss).

We could have included this helper function in the generate-clusters function. We chose here to define it separately for illustrative purposes. Users may find other application-specific alternatives.

```
(define (alpha-func n)
 (let (alpha_2 (- 1 (/ 3 (* 4 n)))
        w (/ 5 6))
      (lambda (k)
        (if (<= k 2)
            alpha_2
            (+ (* (pow w (- k 2)) alpha_2) (- 1 (pow w (- k 2)))))))
```

Inputs:

• n: (number) Number of covariates

**Output:** (function) Weighting function  $\alpha(K)$ 

 $<sup>^{5}</sup>$ The reader might have observed this routine illustrates how WhizzML is not a pure functional language. The primary intent of WhizzML is to orchestrate BigML operations through side effects such as, in this case, creating BigML clusters from a BigML dataset.

As discussed in more detail below, the Pham-Dimov-Nguyen algorithm is based on an evaluation function f(K) that includes a weighting  $\alpha(K)$  function parameterized on the number of covariates n. The weighting function in the Pham-Dimov-Nguyen paper is in recursive form. This factory function returns the closed-form equivalent:

$$\alpha(K) = \begin{cases} 1 - 3/4n & k = 2\\ (5/6)^{k-2}\alpha(2) + \left[1 - (5/6)^{k-2}\right] & k > 2 \end{cases}$$

In the same manner as we do next with evaluation-func, we can implement  $\alpha(K)$  as the partial application of a function  $\alpha(K, n)$  for n. We realize this partial function application as a factory function apply-func. This factory function defines a closure that in turn includes n and returns an anonymous function lambda(k) as  $\alpha(K)$ .

Inputs:

• n: (number) Number of covariates

**Output:** (function) Weighting function  $\alpha(K)$ 

The Pham-Dimov-Nguyen approach to finding the best K has at its core an evaluation function f(K). The version in the Pham-Dimov-Nguyen paper is a function of a single argument K that internally includes  $S_K$  and  $S_{K-1}$  (the within\_ss field of the cluster metadata map returned by extract-eval-data). The form returned by this factory function has the  $S_K$  and  $S_{K-1}$  values as arguments.

$$f(K, S_K, S_{K-1}) = \begin{cases} 1 & k = 1 \text{ or } S_{K-1} = 0 \text{ or } S_{K-1} \text{ undefined} \\ S_K / [\alpha(K)S_{K-1}] & \text{otherwise} \end{cases}$$

Following the conventions of functional programming languages we can implement  $f(K, S_K, S_{K-1})$  as the partial application of a function  $f(K, S_K, S_{K-1}, n)$  for n.

This factory function evaluation-func defines a closure that in turn includes n and returns an anonymous function lambda(k sk skm) as  $f(K, S_K, S_{K-1})$ . Note also that the weighting function  $\alpha(K)$  in the PDN evaluation f(K) could have been a subfunction inside this evaluation-func. As discussed previously, for illustrative purposes we instead have implemented it as the returned result of a separate factory function alpha-func.

```
(define (evaluate-clusters clusters)
 (let (cmdata (map extract-eval-data clusters)
    n ((cmdata 0) "n")
    fe (evaluation-func n))
 (loop (in cmdata
        out []
        ckz {})
    (if (= [] in)
        out
        (let (ck (head in)
            ckr (tail in)
            k (ck "k")
            within_ss (ck "within_ss")
        within_ssz (if (<= k 2) (ck "total_ss") (ckz "within_ss"))</pre>
```

cko (assoc ck "fk" (fe k within\_ss within\_ssz)))
(recur ckr (append out cko) ck)))))

Inputs:

• clusters: (list) Cluster metadata maps ordered by K

**Output:** (list) Sequence of maps that have the field fk with the value  $f(K, S_K, S_{K-1})$  added

Having defined a number of component functions, we pull them together in evaluate-clusters. This function applies the Pham-Dimov-Nguyen evaluation function f(K) to a list that ranges over K of the K-means clusters for a dataset. The result is a list over K of items that include the value of f(K).

In more detail, evaluate-clusters applies the evaluation function  $f(K, S_K, S_{K-1})$  returned by evaluation-func as fe to the cluster metadata returned by extract-eval-data as cmdata. The body of the function is a loop that iterates over the in list of metadata maps returned by extract-eval-data and sequentially builds the out list of metadata maps. Each map in the out list is the source map in the list list augmented with the value  $f(K, S_K, S_{K-1})$  as fk of the evaluation function fe applied to the data values Kand  $S_K$  (within\_ss) from the input map. In addition, the input cluster metadata map ck to an iteration of the loop is passed back into the next iteration as the source ckz for the value of  $S_{K-1}$ .

```
(define (clean-clusters evaluations cluster-id logf)
 (for (x evaluations)
    (let (id (x "id")
        _ (if logf (log-info "Testing for deletion " id " " cluster-id)))
    (if (!= id cluster-id)
        (prog (delete id)
                (if logf (log-info "Deleted " id))))))))
    cluster-id)
```

Inputs:

- evaluations: (list) Sequence of maps of evaulation results for the clusters
- cluster-id: (string) Cluster to save (not delete)
- logf: (boolean) Flag to enable logging

Output: (string) Returns the cluster-id supplied as an input.

Before we define the final, top-level functions we define two more helper functions. The first is this straightforward helper function clean-clusters that deletes the BigML cluster objects created as intermediate computation results, except for the cluster specified by cluster-id.

Inputs:

- dataset: (string) Identifier of dataset to be processed with the cluster operation.
- cluster-arg: (map) Arguments for cluster function
- k: (number) Number of centroids for cluster operation

**Output:** (string) Returns the cluster-id of the created cluster.

The second helper function best-cluster is also required by some of our top-level functions. It performs a single K-means clustering with the specified number K of centroids. The input map args for the

WhizzML cluster function is expanded to ckargs with the identifier of the input dataset, the number K of centroids k, and the name for the cluster instance.

Inputs:

- dataset: (string) identifier of dataset to be processed with the cluster operation.
- args: (map) Arguments for cluster function
- k-min: (number) Minimum value of K
- k-max: (number) Maximum value of K
- clean: (boolean) Flag to delete all but the optimal cluster
- logf: (boolean) Flag to enable logging

Output: (list) Pham-Dimov-Nguyen evaluations of the clusters.

This function combines the generate-clusters and evaluate-clusters functions to create a list of K-means clusters with a range of centroids and a list of metadata maps that include the Pham-Dimov-Nguyen evaluation function f(K) values for those clusters.

The args argument is a map that one can use to optionally specify all of the parameters for the K-means cluster function except the dataset, the number of centroids k, and the cluster name parameters. (See the the BigML developer documentation<sup>6</sup> for details.) The dataset, args, and k-min and k-max, are passed directly to the generate-clusters function. The list of cluster metadata for the clusters it creates is passed directly to the evaluate-clusters function.

This function can be used as top-level function to just return the list of Pham-Dimov-Nguyen evaluation functions f(K) result over the specified number of centroids k-min to k-max (inclusive). When called as top-level function, the clean parameter can be specified as true to automatically delete the BigML cluster objects created after the PDN evaluations are computed. Setting the boolean parameter logf to true causes generation of log data.

Inputs:

- dataset: (string) identifier of dataset to be processed with the cluster operation.
- cluster-arg: (map) Arguments for cluster function
- k-min: (number) Minimum value of K

<sup>&</sup>lt;sup>6</sup>https://bigml.com/developers/clusters#cl\_cluster\_arguments

- k-max: (number) Maximum value of K
- clean: (boolean) Flag to delete all but the optimal cluster
- logf: (boolean) Flag to enable logging
- **Output:** (string) Cluster identifier of best K-means cluster as determined by Pham-Dimov-Nguyen evaluation function.

This top-level function uses the Pham-Dimov-Nguyen algorithm to create the best K-means clustering and returns the identifier of the BigML cluster object for the number of centroids K that results in the smallest (best) value of the PDN evaluation function f(K).

The clusters-args and best-args parameters are maps that one can use to optionally specify all of the parameters for the cluster function except the dataset, the number of centroids k, and the cluster name parameters (See the the BigML developer documentation<sup>7</sup> for details). args is used in the search phase to find the best K. best-args allows one to specify different args for the final stage of clustering with the best K. In particular, one might do clustering on a subset of the dataset during the search phase to save time and other resources, then do the best clustering on the full dataset. If best-args matches args, the result for the best K generated with args during the search phase is returned by best-k-means. If best-args differs from args, the dataset is re-clustered with the best K and the identifier of that cluster is returned by best-k-means.

This function is called by **best-batchcentroid** to do the actual clustering. It can also be called directly if one only needs the best WhizzML cluster object and not the full WhizzML batchcentroid and annotated dataset.

Inputs:

- dataset: (string) Identifier of dataset to be processed with the cluster operation.
- cluster-arg: (map) Arguments for cluster function
- k-min: (number) Minimum value of K
- k-max: (number) Maximum value of K
- clean: (boolean) Flag to delete all but the optimal cluster
- logf: (boolean) Flag to enable logging

Output: (string) Identifier of created batchcentroid

This final top-level routine first uses the **best-k-means** function to generate a best K-means clustering determined by the Pham-Dimov-Nguyen evaluation function f(K). It then creates a BigML batchcentroid object and BigML dataset annotated with clusters numbers in the best K-means clustering of the supplied dataset.

#### 4.2 Examples

We conclude with a few brief examples of how to use the top-level functions and some additional application suggestions.

<sup>&</sup>lt;sup>7</sup>https://bigml.com/developers/clusters#cl\_cluster\_arguments

Using the Top-Level Functions The main top-level function can be called to generate the best BigML batchcentroid and an annotated BigML dataset for an input dataset with the identifier ds-id as:

```
(define batchcentroid-id (best-batchcentroid ds-id {} 1 10 {} false false))
```

If only the best K-means BigML cluster object is required, perhaps for evaluating different ranges of k-min to k-max, one can use the top-level function:

(define cluster-id (best-k-means ds-id {} 1 10 {} false false))

Finally, if one only seeks the list of Pham-Dimov-Nguyen evaluation function f(K) results for the K-means clusterings for k-min to k-max, one can use the top-level function:

(define evaluations (evaluate-k-means ds-id {} 1 10 false false))

Specifying clean as true causes these top-level functions to delete the intermediate BigML datasets created during the computation. Other information generated during execution of function can be logged by specifying logf as true.

Using args and best-args The input args can be used to specify a custom map of arguments for the BigML cluster function that generates the collection of clusters for k-min to k-max in the evaluation phase. Similarly, the input best-args in the best-k-means and best-batchcentroid functions can be used to specify a custom map of arguments for the K-means cluster operation with the best number K of centroids.

As an example, suppose we have a dataset that has two fields depvar1 and depvar2 that we consider to be dependent variables predicted from the remaining fields of the dataset. We'd like to discover the best number of clusters when only the remaining fields are considered by the K-means algorithm. In addition, we believe we can get a reasonable estimate for the best K if we only use 20% of the dataset in the evaluation phase. We can limit the K-means cluster computations according to these constraints by specifying

```
(define ds-id "dataset/...")
(define cfargs {"excluded_fields" ["depvar1" "depvar2"]})
(define cargs (assoc cfargs "seed" "test seed" "out_of_bag" false "sample_rate" 0.2))
(define evaluations (evaluate-k-means ds-id cargs 1 10 false false))
(define cluster-id (best-k-means ds-id cargs 1 10 cfargs false false))
(define batchcentroid-id (best-batchcentroid ds-id cargs 1 10 cfargs false false))
```

Segmented Searches for the Best K In some cases we might have a first guess for the best K. When we run the evaluations over an initial range k-min to k-max we find that the values of f(K) over that range do not exhibit a clear and unambiguous minimum. Rather than re-run the evaluations over the initial range k-min to k-max, we can simply rerun it over additional subranges.

For instance, we can run:

```
(define evaluations (evaluate-k-means ds-id cargs 1 10 false false))
(define evaluations (evaluate-k-means ds-id cargs 10 20 false false))
(define evaluations (evaluate-k-means ds-id cargs 20 30 false false))
```

to cover the total range k-min = 1 to k-min = 30.

There is one detail to note here. The initial value  $f(K_{\min})$  for  $K_{\min} > 1$  is an approximation. By overlapping the ranges as shown in the example, the initial value for any  $K_{\min} > 1$  can be discarded. In this case, f(K) over the full range  $1 \le K \le 30$  can be assembled by composing f(K) for  $1 \le K \le 10$ from the first run,  $11 \le K \le 20$  from the second run, and  $21 \le K \le 30$  from the third run.

# Part III

# Advanced

The purpose of the Advanced tutorials is to demonstrate porting high-level Machine Learning algorithms to the WhizzML language. Writing the scripts in this section requires a thorough understanding of Machine Learning concepts. To this end, lower level WhizzML concepts will not be explained in detail here. For more basic instruction regarding the WhizzML language, refer to the Part I or Part II tutorials, or the WhizzML Language Reference guide.

### **Gradient Boosting**

Gradient tree boosting has become one of the more popular algorithms in the machine learning world, thanks in part to a number of open-source software packages as well as some high profile public successes.

The algorithm is, as bagged classifiers and random forests, an ensemble of weak learners, combined to make a strong one. The primary difference with boosting is that each successive weak model is, in a sense, trained on the mistakes of the previously learned models. With gradient boosting, a gradient is calculated with respect to the current model collection, and each model represents a gradient "step" in that direction.

Because the gradient steps are expressed as trees, one way to code this algorithm is using WhizzML to specify and string together the various steps in the algorithm, and allow BigML's computing infrastructure to handle the heavy lifting of calculation over all points in the dataset and the individual modeling steps.

The full code for this tutorial is available in our whizzml examples repository<sup>1</sup> on Github.

Advanced Tutorial Alert! This tutorial is pretty advanced. It assumes a significant level of comfort with WhizzML and with a bit of high-ish level mathematics. If you feel like you're in over your head, you can always head back to the Part I or the Part II sections to get your feet on firmer ground before you continue here.

It might also be helpful to have some of the other WhizzML reference material<sup>2</sup> on hand to help you as you follow along.

#### 5.1 Algorithm Overview

As mentioned above, gradient tree boosting is an iterative algorithm that learns an ensemble of decision trees. Each tree is trained on the mistakes of all previous trees, and so each tree represents a step towards more correct predictions.

Gradient tree boosting is a gradient descent algorithm in the most general sense of that term, in which an objective function is minimized via gradient descent. Normally, however, the gradient steps to be taken are computed analytically from a parameterized model by differentiating the objective with respect to these parameters. In gradient tree boosting, we have only the predictions of the model on the training data as our expression of the current model parameters. Thus, we compute the gradient at each of the training data points and use decision trees to craft an approximate representation.

More specifically, suppose our current predictions for the training data are represented as an  $n \times k$  matrix of probabilities, where n is the number of points and k is the number of classes. These probabilities are expressions of the model parameters. Without going into the actual objective function used, it turns out that a reasonable approximation for the gradient at the training data points is simply  $\hat{y} - p_i$ , where  $\hat{y}$  is 1 if the true class is class  $i \in 1...k$  and 0 otherwise.

<sup>&</sup>lt;sup>1</sup>https://github.com/whizzml/examples/tree/master/gradient-boosting

<sup>&</sup>lt;sup>2</sup>https://bigml.com/whizzml

We then train a model (rather, k models, one for each class) to approximate this difference at each of the training points, then uses the model to predict the value on the training data. Why is this necessary, as we know the value of the objective at these points already (that's how we trained the model!)? First, as it's important that we don't overfit the training data, we'll learn a "shallow" tree so the predictions will be different from the true values, and should be a good proxy for the predictions we'd see on new data.

With the predictions for this gradient "step" in hand, we can sum them onto our current running sum of gradient steps, then use the *softmax transform* to turn these sums into probabilities. We use the softmax function here for more than just convenience; the objective function that we glossed over two paragraphs ago has this softmax operation as an important part of it, so not using it here would be mathematically invalid.

With these probabilities in hand, we can recompute the gradient at the training points and iterate the algorithm. The algorithm stops generally if you reach some predetermined number of iterations or cease to make improvement for a while (we'll do the later here).

You're left finally with an  $m \times k$  matrix of models, where m is the number of gradient steps you took and k is the number of classes. To predict probabilities for a new point, predict a score for that point with each model, sum these scores "down the columns" so you're left with k sums, one for each class, then apply the softmax transform to get your per-class probabilities.

Yes, this is a lot of information. And we're ignoring quite a bit; we're not going to mess with learning rates, shrinkage, or regularization. But you could if you wanted! Check out these slides<sup>3</sup> for more information if you want to dig deeper.

All right, enough exposition. Let's write some code.

#### 5.2 Helper Functions

Before we get into the guts of the algorithm, we're going to introduce a few helper functions.

```
;; A constant added to the generated field names to let us know that
;; we generated them
(define boost-id "__bmlboost")
;; The names of the fields contain ground truth - if there are k
;; classes, this is k columns, one for each class. If the true class
;; for a given point is the nth class, the value in column in for that
;; point is 1, else it is zero.
(define (truth-names nclasses)
  (map (lambda (i) (str boost-id "_truth_" i)) (range nclasses)))
;; For each of the "names" classes below, we are generating field
;; names, one for each class, at each iteration of the algorithm.
;; This generates a unique field name given a prefix `name` and an
;; iteration number.
(define (field-names nclasses iteration name)
  (map (lambda (i) (str boost-id "_" name "_" i "_iter_" iteration))
       (range nclasses)))
;; The names for the fields containing the total scores (the running
;; sum of all gradient steps) at iteration `iteration`
(define (sum-names nclasses iteration)
  (field-names nclasses iteration "sum"))
;; The names for the fields containing the scores at iteration `iteration`
```

<sup>&</sup>lt;sup>3</sup>https://homes.cs.washington.edu/~tqchen/pdf/BoostedTree.pdf

```
(define (pred-names nclasses iteration)
  (field-names nclasses iteration "prediction"))
;; Field names for the softmax probabilities at iteration `iteration`
  (define (softmax-names nclasses iteration)
    (field-names nclasses iteration "softmax"))
;; The field name for the gradients (the objective for each class) at
;; each iteration
  (define (grad-names nclasses iteration)
    (field-names nclasses iteration)
    (field-names nclasses iteration)
```

As we make our way through the algorithm, we're going to create a lot of new columns in our dataset. We'll create new columns for the gradients at each step, the running sums at each step, and the predictions of the gradient trees at each step. These functions will return unique names for each type of column; one for each class at any given iteration of the algorithm

```
;; Helper methods to add fields to the given dataset using flatline
;; expressions
(define (make-fields names exprs)
  (let (make-field (lambda (i) {"name" (names i) "field" (exprs i)}))
    (map make-field (range (min (count exprs) (count names))))))
(define (add-fields dataset new-fields input-ids)
  (let (req {"origin_dataset" dataset "new_fields" new-fields})
    (if (empty? input-ids)
        (create-and-wait-dataset req)
        (create-and-wait-dataset (assoc req "input_fields" input-ids)))))
```

Here's how we'll actually create all of those new columns. The top function make-fields takes a list of column names and list of flatline expressions. It then creates a list of maps with the names and expressions in each one. The bottom function takes this list, puts into a BigML resource request and creates a copy of the argument dataset with the new columns appended. If input-ids is specified, it retains only those fields from the original dataset.

Wait, you haven't heard of flatline? That's BigML's DSL for dataset transformation. As you'll see, using WhizzML to compose flatline expressions that transform your data allows you to do a ton of interesting things. You can get more familiar with flatline by perusing the user's guide here.<sup>4</sup>

<sup>&</sup>lt;sup>4</sup>https://github.com/bigmlcom/flatline/blob/master/user-manual.md

(count (obj ["summary" "categories"]))))

Finally, a few miscellaneous helpers: get-num-classes does what it says on the box, gets the number of classes in the objective field. get-inputs gets the original input fields for the dataset, a handy thing to know when you're adding a whole bunch of columns at each iteration, get-objectives gets the field ids of the objective fields (one for each class) with the gradient columns at a given iteration.

#### 5.3 Computing the Gradients Given Probabilities

Recall that the first thing we have to do is compute the gradient at each of the training data points. We're going to use flatline to subtract the currently predicted probability for each class from the true objective value, then put that value in a new set of columns (again, one for each class).

This requires us to have a predicted probability for each point. During the first iteration, we're just going to assume all classes have equal probability.

We first get the names of the columns where we're going to put the gradient values in next-names. Then we get the currently predicted probabilities for each class. If it's an iteration other than the first, we compose a flatline expression that pulls out the value from the appropriate column, given by softmax-names.

We can then write a little internal function, fexp, which subtracts the two columns values. Of course, we have to (map fexp (range nclasses)) so that we get an expression for each class, then use new-fields and add-fields to add them to the dataset.

#### 5.4 Learning the Gradient Models

Now that we have our collection of gradient columns, we're going to learn a tree to represent each one.

Here we get the input and objectives for each model (remember, get-inputs returns the original input fields for the data, minus the fields we've generated ourselves). The input fields will always be the same, but we will learn one model per objective field (that is, one per class).

We do this with the inline function create, which takes the template req for the model request and adds an objective field. We then (map create oids) to create one model for each objective in oids and wait for them to complete.

#### 5.5 Scoring Instances with the Models

The next step is to use our learned models to predict gradient values for the training data.

```
;; Predict the value of the gradient for all points in the dataset
;; Need to predict one at a time so we can preserve all fields
(define (batch-predict dataset iteration mod-ids)
 (let (pnames (pred-names (count mod-ids) iteration))
   (loop (last-ds dataset mids mod-ids names pnames)
      (if (empty? mids)
       last-ds
        (let (req {"all_fields" true
                   "output_dataset" true
                   "model" (head mids)
                   "dataset" last-ds
                   "prediction_name" (head names)}
              bp (create-and-wait-batchprediction req)
              new-ds ((fetch bp) "output_dataset_resource")
              _ (wait-forever new-ds))
              (recur new-ds (tail mids) (tail names)))))))
```

This code works by first getting names for the columns where we'll put the predictions (pnames). We then loop over these names and the corresponding model identifiers, creating a batchprediction for each one. We'll do these serially, as we want to preserve predictions from previous models when we make a new one, so the dataset created by the first batchprediction will provide the input fields for the second, and so on for each model.

Note that we have to create-and-wait-batchprediction and later wait separately for the created dataset; the readiness of the batch prediction does not imply readiness for the output dataset resource.

#### 5.6 Summing the Model Scores Into The Current Model

Now we have to sum our predicted scores into our running totals. We'll use flatline again.

This looks a lot like the function we used to compute the gradient and follows the same general pattern. First we pull out the names "source" and "destination" columns for the flatline operation (in this case, last-sums and this-preds, and this-sums respectively.

We then create a function fexp that will take a class index i, pick out the *i*th name from each of the aforementioned lists, and compose the flatline expression that adds the two columns. Of course, if we're on the first iteration of the algorithm ((empty? last-sums)) then the current sum is just the current prediction.

We can then (map fexp (range classes)) to do this for each class, resulting in a new running sum for each class. Finally, we use make-fields and add-fields to add the list of new columns to the dataset.

#### 5.7 Computing Probabilities From Scores

Essentially the last step in the algorithm is to turn the set of running sums into probabilities that can feed into the next iteration of the algorithm. For this we'll use the *softmax transform* to massage the values into a proper distribution. What is it? Suppose you've got k classes and a score for each class  $s_1, s_2, \ldots, s_k$ . We define the probability  $p_i$  for class i as:

$$p_i = \frac{e^{s_i}}{\sum_j e^{s_j}}$$

so that the probability vector is the vector of scores exponentiated, then normalized.

```
;; Create the softmax probabilities from the given scores
(define (create-softmax-probs dataset nclasses iteration)
   (let (this-sums (sum-names nclasses iteration)
        this-softmaxs (softmax-names nclasses iteration)
        fl-exp (lambda (name) (flatline "(exp (f {{name}}))"))
        exp-sum (str "(+ " (join " " (map fl-exp this-sums)) ")")
        fexp (lambda (name) (str "(/ " (fl-exp name) " " exp-sum ")"))
        new-fields (make-fields this-softmaxs (map fexp this-sums)))
        (add-fields dataset new-fields [])))
```

Again, we rely on flatline to do the heavy lifting. We get the source and destination columns as before in this-sums and this-softmaxs. We then compose a flatline expression equivalent to the above equation. Note that we do it by parts here for convenience, first defining an "exponentiator" in fl-exp, then the denominator in exp-sum, and finally the closure that will make the final expression for each column in fexp. One more invocation of new-fields and add-fields and we have our new probabilities.

#### 5.8 Putting It All Together

Having the new probabilities in place we can iterate the above steps:

Here we assume that we start with trained models, and execute an entire iteration using the functions defined above, so that we come all the way back to the point where we can train models again.

All that's left is to iterate that function until a stopping condition, along with a few set up and tear down steps.

```
(define (gradient-boost dataset)
 (let (objective (dataset-get-objective-id dataset)
        inputs (default-inputs dataset objective)
       nclasses (get-num-classes dataset objective)
        formatted (format dataset nclasses inputs objective))
    (loop (ds formatted
           iteration 1
           total-imp 0
           imp-1 0
           imp-2 0
           models [])
      (log-info "Iteration " iteration)
      (let (sets (bootstrap ds iteration)
            train (sets 0)
            test (sets 1)
            last-gradient (sum-gradient test nclasses (- iteration 1))
            _ (log-info "Gradient: " last-gradient)
            new-models (learn-trees train nclasses (- iteration 1))
            new-test (create-fields test iteration new-models)
            this-gradient (sum-gradient new-test nclasses iteration)
            _ (log-info "Gradient: " this-gradient)
            this-imp (- last-gradient this-gradient)
            pct (* (/ (+ this-imp imp-1 imp-2) (+ this-imp total-imp)) 100))
        (log-info "Improvement over last 3 iterations: " pct "%")
        ;; Stop arbitrarily at 1% improvement over last three iterations
        (if (> pct 1)
          (recur (create-fields ds iteration new-models)
                 (+ iteration 1)
                 (+ total-imp this-imp)
                 this-imp
                 imp-1
                 (append models new-models))
          models)))))
```

It seems like a lot, but the main bits are the stopping condition (we keep track of the last three total gradient magnitudes and stop if they represent less than 1% of the total improvement) and also the fact that we learn over a bootstrap sample of our original dataset. That is, at each iteration we learn over some of the dataset and check improvement over the other part. As such, we have to call create-fields on both the training and the test sets

#### 5.9 Conclusion

We've implemented a "vanilla" version of gradient tree boosting in WhizzML. Hopefully, we've proven along the way that it's possible to implement many complex machine learning algorithms in WhizzML, and thereby gain the power of BigML's infrastructure behind your implementation.

### Anomaly-Based Covariate Shift

Detecting Covariate Shift and Dataset Shift in new production data relative to previously trained predictive models is always a challenge. BigML has discussed a method for doing this<sup>1</sup> based on the Matthews Correlation Coefficient (Phi Coefficient) computed from the confusion matrix for a predictive model. A tutorial also describes a WhizzML package for implementing this method (see the "Covariate Shift" section). This tutorial describes an alternative method that can be easily implemented using WhizzML that can be useful for some types of data.

In the alternative method we describe here, we use the WhizzML anomaly detection functions. The method computes an average anomaly score of the production dataset relative to the model training dataset as a measure of the covariate shift between the training dataset and the production dataset. An anomaly detector is trained from the same dataset used to train the model. This anomaly detector is then used to derive a batch anomaly score for the production dataset. Finally, the average value of that batch anomaly score is computed as an indicator of covariate shift.

The full code for this tutorial is available in our whizzml examples repository<sup>2</sup> on Github.

#### 6.1 Code Overview

We first review the functions in the package to explain the anomaly-based approach to covariate-shift estimation.

Inputs:

- dst-id: (string) ID of the dataset to be sampled.
- rate: (float) A value between 0 and 1 that specifies the size of the bagged sample. For example, 0.8 means that 80% of original dataset is in the bagged sample.
- oob: (boolean) Selects whether we want the bagged (false) chunk of data or the out of bag (true) chunk. For example, if the rate is 0.75, and oob is false, we get 75% of the data. If oob is true, we get the other 25%.
- seed: (string) A string used to make the sampling deterministic (repeatable)

Output: (string) ID of the new dataset object.

<sup>&</sup>lt;sup>1</sup>https://blog.bigml.com/2014/01/03/simple-machine-learning-to-detect-covariate-shift/

<sup>&</sup>lt;sup>2</sup>https://github.com/whizzml/examples/tree/master/anomaly-shift

To build a practical anomaly-based covariate shift detector, we need to derive sample from the anomaly detector training dataset and the production dataset. This helper routine wraps the basic dataset creation function to isolate configuration of that function so that it can be easily modified to support other sampling options in other applications. This basic version simply creates a deterministic sample determined by **seed** parameter of a size determined jointly by **rate** and **oob** from the source dataset specified by **dst-id**.

Inputs:

- anomaly-id: (string) ID of the anomaly detector object.
- dst-id: (string) ID of the production dataset object.

**Output:** (string) ID of the created batchanomalyscore object.

We also will need to apply an anomaly detector derived from a training dataset to a production dataset. As with the sample-dataset, this helper routine wraps the WhizzML batch anomaly score computation function to isolate the configuration information so that it can be easily modified to use other evaluation options. This basic version simply applies the anomaly detector specified by anomaly-id to the dataset specified by dst-id and returns a BigML batchanomalyscore object. Because we specify all\_fields and output\_dataset as true in the WhizzML function to create the batchanomalyscore object, the returned metadata includes a reference to a dataset that includes the original production dataset with each item annotated with an additional member that contains the anomaly score for the item and additional metadata that includes the anomaly score results for the whole dataset.

```
(define (avg-anomaly evdst-id)
  (let (evdst (fetch evdst-id)
      score-field (evdst ["objective_field" "id"])
      sum (evdst ["fields" score-field "summary" "sum"])
      population (evdst ["fields" score-field "summary" "population"]))
      (/ sum population)))
```

Inputs:

• evdst-id: (string) ID of the batch anomaly score dataset object.

**Output:** (float) Average batch anomaly score from the results in the batch anomaly score dataset object.

Finally, we encapsulate the computation of the average anomaly score for the production dataset as a helper function that computes the average anomaly score from the annotated production dataset object returned by anomaly-evaluation. The metadata for this augmented production dataset object includes a ["objective\_field" "id"] member that contains the name of the score-field for the member with the object that has summary anomaly score results for the production dataset. The quotient of the members ["fields" score-field "summary" "sum"] and ["fields" score-field "summary" "population"] in that anomaly score member is returned as the average batch anomaly score for the production dataset object evdst-id.

```
score (avg-anomaly evdst-id))
(if clean
  (prog (delete evdst-id)
        (delete ev-id)
        (delete anomaly)
        (delete prodo-dst)
        (delete traino-dst)))
score))
```

Inputs:

- train-dst: (string) ID of the training dataset.
- train-exc: (list) Fields to exclude from the training dataset.
- prod-dst: (string) ID of the production dataset.
- prod-exc: (list) Fields to exclude from the production dataset.
- seed: (string) A string used to make the sampling deterministic (see the "sample-dataset" function).
- clean: (boolean) Delete intermediate datasets before exiting the function.

**Output:** (float) The average anomaly score between 0 and 1.

This top-level function combines the previous helper functions to compute the average anomaly score for a single production dataset relative to an anomaly detector built from the training dataset.

The function accepts a training dataset train-dst and a production dataset prod-dst along with a seed string to force deterministic sampling of both. 80% of the training dataset traino-dst is used to train an anomaly detector anomaly, ignoring the fields in the list train-exc. 20% of the production dataset prodo-dst is then evaluated with the anomaly detector to produce a BigML batchanomalyscore object ev-id. The batchanomalyscore ev-id metadata has the ID evdst-id for the anomated version of the production dataset. The metadata for this dataset includes the anomaly score information used by avg-anomaly to compute an average anomaly score for the sample of the production dataset.

Finally, if clean is specified as true the intermediate objects created by the function are deleted before the function returns the score.

```
(define (anomaly-loop train-dst
                      train-exc
                      prod-dst
                      prod-exc
                      seed
                      niter
                      clean
                      logf)
 (loop (iter 1
        scores-list [])
    (if logf
      (log-info "Iteration " iter))
    (let (score (anomaly-measure train-dst
                                  train-exc
                                  prod-dst
                                  prod-exc
                                  (str seed " " iter)
                                  clean)
          scores-list (append scores-list score))
      (if logf
        (log-info "Iteration " iter scores-list))
      (if (< iter niter)
        (recur (+ iter 1)
```

```
scores-list)
scores-list))))
```

#### Inputs:

- train-dst: (string) ID of the training dataset.
- train-exc: (list) Fields to exclude from the training dataset.
- prod-dst: (string) ID of the production dataset.
- prod-exc: (list) Fields to exclude from the production dataset.
- seed: (string) A string used to make the sampling deterministic (see the "sample-dataset" function).
- niter: (number) Number of iterations.
- clean: (boolean) Delete intermediate datasets before exiting the function.
- logf: (boolean) Enables logging.

Output: (list) A list of average anomaly scores between 0 and 1 for specified datasets over niter trials.

To facilitate logging and to illustrate the implementation of multiple train-evaluate iterations in way that can be easily augmented in specific applications, we implement iteration over the anomaly-measure as an explicit loop function.

The loop function inputs are an iteration count iter and a list of scores computed thus far scores-list. Each iteration of the loop generates a unique seed value for sampling the training and production datasets and computes the anomaly score with anomaly-measure. That score is appended to the scores-list. If niter iterations have not been completed, the iteration count is updated and the loop repeated.

```
(define (anomaly-measures train-dst
                           train-exc
                           prod-dst
                           prod-exc
                           seed
                           niter
                           clean
                           logf)
 (let (values (anomaly-loop train-dst
                              train-exc
                              prod-dst
                              prod-exc
                              seed
                              niter
                              clean
                              logf))
     values))
```

Inputs:

- train-dst: (string) ID of the training dataset.
- train-exc: (list) Fields to exclude from the training dataset.
- prod-dst: (string) ID of the production dataset.
- prod-exc: (list) Fields to exclude from the production dataset.
- seed: (string) A string used to make the sampling deterministic (see the "sample-dataset" function).
- niter: (number) Number of iterations.
- clean: (boolean) Delete intermediate datasets before exiting the function.

• logf: (boolean) Enables logging.

**Output:** (list) A list of average anomaly scores between 0 and 1 for the specified datasets over niter trials.

This top-level function computes a list of niter average anomaly scores for pairs of samples of the training dataset train-dst and the production dataset prod-dst. For illustration purposes we implement this function as a wrapper function around the anomaly-loop function that does the actual work and pass all of the input values including those mentioned and train-exc, prod-exc, seed, clean, and logf directly to that function. For other applications, alternative looping structures could be implemented.

```
(define (anomaly-estimate train-dst
                           train-exc
                           prod-dst
                           prod-exc
                           seed
                          niter
                           clean
                           logf)
 (let (values (anomaly-measures train-dst
                                  train-exc
                                  prod-dst
                                  prod-exc
                                  seed
                                  niter
                                  clean
                                  logf)
        sum (reduce + 0 values)
        cnt (count values))
    (/ sum cnt)))
```

#### Inputs:

- train-dst: (string) ID of the training dataset.
- train-exc: (list) Fields to exclude from the training dataset.
- prod-dst: (string) ID of the production dataset.
- prod-exc: (list) Fields to exclude from the production dataset.
- seed: (string) A string used to make the sampling deterministic (see the "sample-dataset" function).
- niter: (number) Number of iterations.
- clean: (boolean) Delete intermediate datasets before exiting the function.
- logf: (boolean) Enables logging.
- **Output:** (float) The average anomaly scores between 0 and 1 for the specified datasets for the niter trials.

Finally, in this top-level function we use anomaly-measures to compute a list of niter average anomaly scores for pairs of samples of the training dataset train-dst and the production dataset prod-dst. We then compute the average of the scores in that list and return that as a single measure of the covariate shift between the training dataset train-dst and the production dataset prod-dst.

#### 6.2 Examples

We end this tutorial description with a few examples of how to use the top-level functions.

If we only want an estimate of the data shift computed from a single pair of samples from the training dataset and the production dataset, we can use the top-level function:

```
(define cvshift-one (anomaly-measure "dataset/..."
[]
    "dataset/..."
[]
    "test-run-1"
    false))
```

In this example we don't exclude any of the fields from the training dataset and specify that we would like to preserve all of the intermediate objects created in the computation by specifying clean as false.

Suppose next that we are concerned our training or production datasets aren't uniform in some sense. Suppose also that the datasets include a dependent variable **idvar** that differs consistently between the two datasets potentially affecting the anomaly score. In this case, we can use the top-level function that generates a series of anomaly scores:

```
(define cvshift-set (anomaly-measures "dataset/..."
    ["idvar"]
    "dataset/..."
    ["idvar"]
    "test-run"
    20
    true
    true))
```

Here we specify we want a series of 20 train-evaluate iterations and that logging information should be generated by specifying logf as true. To manage storage on our BigML account we also define clean as true to delete all intermediate objects each iteration.

Finally, we can run a series of train-evaluate trials and then compute the average of the anomaly scores using the final top-level function as:

```
(define cvshift-avg (anomaly-estimate "dataset/..."
    ["idvar"]
    "dataset/..."
    ["idvar"]
    "test-run"
    20
    true
    true))
```

In this case we specify the same sequence of anomaly score computations and then take the average returned by the function as our estimate of covariate-shift between the training dataset train-dst and the production dataset prod-dst.

