

# Machine Learning – Project 1

Pierre Fouche, Matthias Leroy and Alexandre Poussard  
*MSc Data Science – EPFL, Switzerland*

**Abstract**—The aim of this paper is to make classification of particles over results' experiments. Thus, given a set of features that describe the decay signature of a collision event, we tried to predict if this event was a Higgs boson signal or some background information. We will expose the different machine learning algorithms we tried and the evaluations we made that finally led us to the ridge regression.

## I. FEATURES ANALYSIS AND DATA PREPARATION

The training set is composed of 250 000 samples of each 30 features representing 30 experimental measurements. During our dataset exploratory analysis, we noticed that the 23rd column is discrete and categorical with values in the set 0,1,2,3. We then decided to divide our training set into 3 subsets (because number 2 and 3 have the same -999). Then in the doc, they explained depending on those 4 categories, other features are defined or not which allows us to split the data based on these categories. We also notice that for 2 and 3, features are defined in the same way and so we can merge data set 2/3 and obtain 3 datasets. However, we still have non-defined values in the first column and we decide to split again for each Jet into 2 smaller datasets which contains defined OR nondefined values. We then have 6 datasets depending on jets and Mass and with only defined values. This allows us to have two benefits: smaller training dataset (for computation) and more precise one.

We then normalize/standardize the data and focus on polynomial basis and feature engineering.

For each subset, we have at the beginning, said  $N$  rows and  $D$  features. For the polynomial basis, which goal is to add other features for better training, we then have a subset with still  $N$  rows but  $D*d$  ( $d = \text{max degree}$ ). This degree is defined thanks to the cross-validation according to the model we use. See Section ?? . Instead of trying to find a different degree for each training dataset we could have chosen a common one big enough to satisfied each set. We would gain in test rapidity but risk to overfit the data. Then, we decide to add more features by modifying and combining existing ones depending on our training set. In fact, features engineering increase considerably our classification precision, but in return our training model asked for more memory and take longer to process. Thus, we try different method in order to find the best trade-off that we could make for each training set. First of all we compute

the cross term matrix of our  $D$  original features (the one to one product for each column) and get  $C = (D*(D-1))/2$  new features. Then, we decide to add the square, square root and cubic root of these combinations. Thus, if we apply each of these new features of one of our training set, it will be finally composed of  $N$  samples and  $D*d+C*4$  features. However, we did not add all these features to all of our training set. In fact, we evaluate the importance of each one of them with our cross validation test and populate our set according to the losses we get.

## II. MODELS AND METHODS

In order to make our predictions, we tested 6 different machine learning methods, that we tried to improve according to the results, and the validation evaluations we got. Thus, we started to think about the better way to evaluate our models, and we finally decided to implement a 5-fold cross-validation (it seems to us a reasonable choice since we got validation sets of 50 000 samples which is equivalent to a 20% – 80% split of test and training data).

First of all, we tried a linear regression using a gradient descent. Our first questioning was to find a correct learning rate  $\gamma$  in order to converge to the best parameters  $w^*$  for the minimum cost function that we could possibly find with this optimization algorithm. After testing different values for  $\gamma$  it was finally possible to make our first prediction. It was very encouraging but we want to test other algorithm before started to optimize one. Thus, we implemented a stochastic gradient descent. We had to use a standard mini-batch-size-1. We did the same work, and try to optimize the step-size. However, whatever its value was, we did not succeed to find a smaller loss that we got with the batch gradient descent. The only benefit of this methods was the computational cost, in fact the convergence's speed was a little bit faster. However, at this step of the challenge, we were more concerned about efficiency and precision of the results rather than complexity as long as our computer succeeded to get a result. Moreover, we could have tried mini-batch SGD and found a trade-off between speed and loss. However, we could most probably not have a better loss than with gradient descent and we did not want to persevere knowing that we could find optimum  $w^*$  parameters with least squares regression using normal equations. Actually, the solution is obtained explicitly by solving these normal equations and thus, optimize what we tried to do with gradient descents models. We get indeed better predictions

using Least Square and we get a categorization accuracy of (—) on Kaggle. From this result, we tried to improve it with extended features vectors. Thus, we added a polynomial basis in order to increase the representational power of the linear model. That's why we ran our cross-validation in order to determine the degree  $M$  that minimize our validation error for each of our 6 training sets. And we finally got our best prediction score. However, we noticed that the error for the training sets and the validation sets occasionally disagreed a little for the best degrees. Thus, it could be resulting of an overfitting problem. Therefore, in order to reduce our variance we tried to regularize our linear model by using ridge regression using normal equations. In fact, most of the work was to determine the hyperparameters, since for this model we have to find a  $\lambda$  parameter that best regularize our model by penalize complex ones for every polynomial basis we wanted to test. Therefore, after running our 5-fold cross-validation we find a set of 6 *degree*,  $\lambda$  couples for each dataset, that minimize the losses. Finally, we got a better prevision than with the Least Square model, we obtained (—) on Kaggle. Surprisingly, the *lambdas* that gave us the best results were very small, thus, Least Square model was not overfitting that much. Finally, we implemented the logistic regression. We had good hope for this model because it is supposed to be optimized for classification problems. However, the *Newton's method* that we tried did not satisfy us. Indeed, we had hard time to compute our parameters  $\gamma$  (for the gradient descent) and the degrees of our polynomial basis. In fact, the *Hessian* of the loss function was very costly, and we did not succeed to estimate a good estimation (it seems that our computers had not enough memory for the work we asked). And finally, our results was worst than for the ridge regression. Then, we implement a regularized logistic regression...

### III. IMPROVING PREDICTION

After, we found our best prediction, we asked ourself how we could continue to improve it. in fact, at the begining of the challenge we tried the model we implemented directly on the dataset we get. Without thinking about analyse, preprocessing and features engineering. It ended up with a very high bias over our estimation. In fact, it was not bother us to much when we start because the training and validation errors were very close when we ran the cross validation but, the error itself was not small enough for our prediction goal.

Scientific papers usually begin with the description of the problem, justifying why the problem is interesting. Most importantly, it argues that the problem is still unsolved, or that the current solutions are unsatisfactory. This leads to the main gist of the paper, which is "the idea". The authors then show evidence, using derivations or experiments, that the idea works. Since science does not occur in a vacuum, a proper comparison to the current state of the art is often part

of the results. Following these ideas, papers usually have the following structure:

#### Abstract

Short description of the whole paper, to help the reader decide whether to read it.

#### Introduction

Describe your problem and state your contributions.

#### Models and Methods

Describe your idea and how it was implemented to solve the problem. Survey the related work, giving credit where credit is due.

#### Results

Show evidence to support your claims made in the introduction.

#### Discussion

Discuss the strengths and weaknesses of your approach, based on the results. Point out the implications of your novel idea on the application concerned.

#### Summary

Summarize your contributions in light of the new results.

## IV. TIPS FOR GOOD WRITING

The ideas for good writing have come from [?], [?], [?].

### A. Getting Help

One should try to get a draft read by as many friendly people as possible. And remember to treat your test readers with respect. If they are unable to understand something in your paper, then it is highly likely that your reviewers will not understand it either. Therefore, do not be defensive about the criticisms you get, but use it as an opportunity to improve the paper. Before your submit your friends to the pain of reading your draft, please *use a spell checker*.

### B. Abstract

The abstract should really be written last, along with the title of the paper. The four points that should be covered [?]:

- 1) State the problem.
- 2) Say why it is an interesting problem.
- 3) Say what your solution achieves.
- 4) Say what follows from your solution.

### C. Figures and Tables

Use examples and illustrations to clarify ideas and results. For example, by comparing Figure 1 and Figure 2, we can see the two different situations where Fourier and wavelet basis perform well.

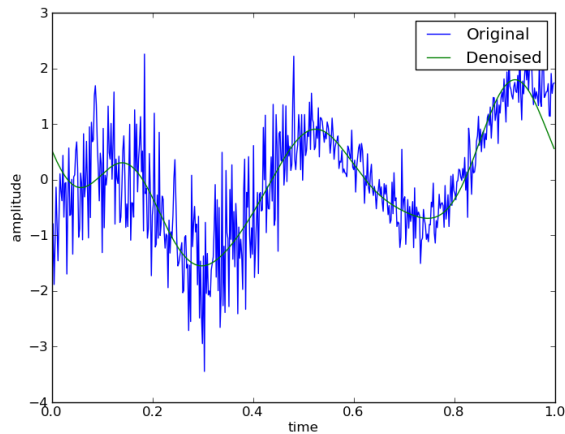


Figure 1. Signal compression and denoising using the Fourier basis.

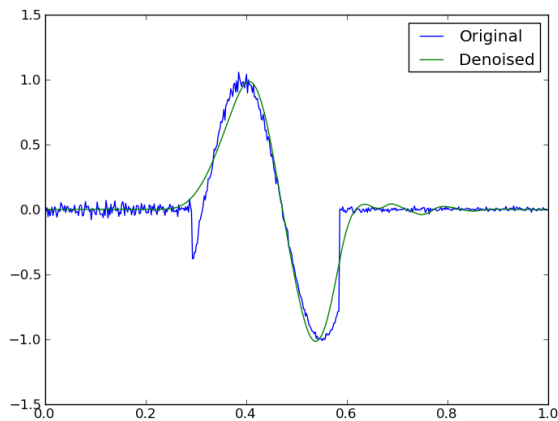


Figure 2. Signal compression and denoising using the Daubechies wavelet basis.

#### D. Models and Methods

The models and methods section should describe what was done to answer the research question, describe how it was done, justify the experimental design, and explain how the results were analyzed.

The model refers to the underlying mathematical model or structure which you use to describe your problem, or that your solution is based on. The methods on the other hand, are the algorithms used to solve the problem. In some cases, the suggested method directly solves the problem, without having it stated in terms of an underlying model. Generally though it is a better practice to have the model figured out and stated clearly, rather than presenting a method without specifying the model. In this case, the method can be more easily evaluated in the task of fitting the given data to the underlying model.

The methods part of this section, is not a step-by-step,

directive, protocol as you might see in your lab manual, but detailed enough such that an interested reader can reproduce your work [?], [?].

The methods section of a research paper provides the information by which a study's validity is judged. Therefore, it requires a clear and precise description of how an experiment was done, and the rationale for why specific experimental procedures were chosen. It is usually helpful to structure the methods section by [?]:

- 1) Layout the model you used to describe the problem or the solution.
- 2) Describing the algorithms used in the study, briefly including details such as hyperparameter values (e.g. thresholds), and preprocessing steps (e.g. normalizing the data to have mean value of zero).
- 3) Explaining how the materials were prepared, for example the images used and their resolution.
- 4) Describing the research protocol, for example which examples were used for estimating the parameters (training) and which were used for computing performance.
- 5) Explaining how measurements were made and what calculations were performed. Do not reproduce the full source code in the paper, but explain the key steps.

#### E. Results

Organize the results section based on the sequence of table and figures you include. Prepare the tables and figures as soon as all the data are analyzed and arrange them in the sequence that best presents your findings in a logical way. A good strategy is to note, on a draft of each table or figure, the one or two key results you want to address in the text portion of the results. The information from the figures is summarized in Table I.

When reporting computational or measurement results, always report the mean (average value) along with a measure of variability (standard deviation(s) or standard error of the mean).

#### V. TIPS FOR GOOD SOFTWARE

There is a lot of literature (for example [?] and [?]) on how to write software. It is not the intention of this section to replace software engineering courses. However, in the interests of reproducible research [?], there are a few guidelines to make your reader happy:

- Have a README file that (at least) describes what your software does, and which commands to run to obtain results. Also mention anything special that needs to be set up, such as toolboxes<sup>1</sup>.
- A list of authors and contributors can be included in a file called AUTHORS, acknowledging any help that you

<sup>1</sup>For those who are particularly interested, other common structures can be found at <http://en.wikipedia.org/wiki/README> and <http://www.gnu.org/software/womb/gnits/>.

| Basis              | Support         | Suitable signals       | Unsuitable signals     |
|--------------------|-----------------|------------------------|------------------------|
| Fourier<br>wavelet | global<br>local | sine like<br>localized | localized<br>sine like |

Table I  
CHARACTERISTICS OF FOURIER AND WAVELET BASIS.

may have obtained. For small projects, this information is often also included in the README.

- Use meaningful filenames, and not `temp1.py`, `temp2.py`.
- Document your code. Each file should at least have a short description about its reason for existence. Non obvious steps in the code should be commented. Functions arguments and return values should be described.
- Describe how the results presented in your paper can be reproduced.

#### A. *LaTeX* Primer

*LaTeX* is one of the most commonly used document preparation systems for scientific journals and conferences. It is based on the idea that authors should be able to focus on the content of what they are writing without being distracted by its visual presentation. The source of this file can be used as a starting point for how to use the different commands in *LaTeX*. We are using an IEEE style for this course.

1) *Installation*: There are various different packages available for processing *LaTeX* documents. On OSX use *MacTeX* (<http://www.tug.org/mactex/>). On Windows, use for example *MikTeX* (<http://miktex.org/>).

2) *Compiling LaTeX*: Your directory should contain at least 4 files, in addition to image files. Images should be in `.png`, `.jpg` or `.pdf` format.

- `IEEEtran.cls`
- `IEEEtran.bst`
- `groupXX-submission.tex`
- `groupXX-literature.bib`

Note that you should replace `groupXX` with your chosen group name. Then, from the command line, type:

```
$ pdflatex groupXX-submission
$ bibtex groupXX-literature
$ pdflatex groupXX-submission
$ pdflatex groupXX-submission
```

This should give you a PDF document `groupXX-submission.pdf`.

3) *Equations*: There are three types of equations available: inline equations, for example  $y = mx + c$ , which appear in the text, unnumbered equations

$$y = mx + c,$$

which are presented on a line on its own, and numbered equations

$$y = mx + c \tag{1}$$

which you can refer to at a later point (Equation (1)).

4) *Tables and Figures*: Tables and figures are “floating” objects, which means that the text can flow around it. Note that `figure*` and `table*` cause the corresponding figure or table to span both columns.

## VI. SUMMARY

The aim of a scientific paper is to convey the idea or discovery of the researcher to the minds of the readers. The associated software package provides the relevant details, which are often only briefly explained in the paper, such that the research can be reproduced. To write good papers, identify your key idea, make your contributions explicit, and use examples and illustrations to describe the problems and solutions.

## ACKNOWLEDGEMENTS

The author thanks Christian Sigg for his careful reading and helpful suggestions.