A comparison between three kinds of models

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ABSTRACT

After receiving the task to solve, our goal was to build multiple solutions to solve it and compare them. First of all, we compare two different types of really important and famous frameworks for Neural Network: Keras[1] and Pytorch[2]. Then we compare the approach based on Neural Network against a completely different approach in Machine Learning, known as SVM. Finally, we validate, by cross-validation, and test all the models on two different machines to see the performances.

1. INTRODUCTION

Our first aim is to show our journey from being without any previous knowledge of the frameworks to being able to write two fully working Multi-Layer Perceptrons networks (MLP) with two different shapes. We use two different structures to better understand how they work and how to extend them. The development has been really tough because of the differences between the two frameworks.
We were curious about how to deal with Support Vector Machines (SVM) and so, we choose it too; since we are dealing with a regression task we use a different kind of SVM called Support Vector Regression (SVR) implemented by scikit-learn[3]. The choice of these three models has been done to test all parts of course and to solve in the best way possible the given task. Talking about the task, we have 20 features and 2 target values, each of these are real numbers (they comes from sensors); no other assumption of the data has been done. We have found interesting patterns in the target values, about this it will be discussed later in this report. In order to test our models, we used Hold-out technique to split, initially, the data and then to validate the model; particularly, we used k-fold cross-validation and grid search. The developed code has been done by Python 3.7. The code is completely automatized; from the main script the user can interact with the models by choosing either if he wants to cross-validate or test one particular instance of a single model, or all of those. All the code is available on Github [4] and in the directory where this file is.

2. METHOD

First of all, we choose some main functionality that we were sure to be common to all the model or at least common to the Neural Network models, they are data import, data visualization, loss function (Mean Euclidian Distance), validation schema and test schema. Once we choose how to organize the shared part, we start to implement it.

- For data import and other small tasks of numeric values manipulation, we use *numpy* library [5].
- For both plotting learning curves and results of predictions in a 2D plot, we use *matplotlib* [6].
- Since the results on the blind set will be evaluated using the Mean Euclidian Error, we use it too as a *loss* in order to have more similar results. We implemented it by ourself using the tensor interface of the frameworks. For SVM, we just use this function to evaluate the results in the different parts of the process using numpy lists instead of tensors.
- For the Grid Search, there is online some automatic tool but we decided to implement it on our own. We did it with just 3/4 nested *for* loops, with no parallelization. In the phase of grid-search we also plot every learning curve, of course, we produced a huge amount of images, in this report we show just the most relevant.
- As activation function for the MLP we used and tested both Sigmoid and Rectified Linear Unit (ReLU)
- We choose to use Stochastic Gradient Descend as learning algorithm because during the course we understood very well how it works; moreover, it provides suitable smoothness properties for optimizing problems.
- About the preprocessing, we haven't done any kind of it in the beginning, not even plotting the targets in a 2D plot. We did it in the end; more detail will be discussed in section 3.
- We choose Mini batch learning; the batch size is chosen in the validation phase.
- As weights initialization technique we use the Glorot initialization (also known as Xavier). It initializes each weight with a small Gaussian value with mean = 0.0 and variance based on the fan-in and fan-out of the unit.
- According to the hold-out technique, at the beginning of the project, we split the dataset into two parts, the first one consists of randomly chosen 1.595 samples (90.09% of the entire dataset); the second one of 170 examples (9.91% of the entire dataset). The latter is used to test all the three models at the end of the validation process to choose the best one and give a true estimation of its generalization error.
- As validation schema, we use k-Fold cross-validation implemented by scikit-learn to not have any bias from the choose of the validation set. We always shuffle the sample before the division in folds. We use k = 10 because for each fold we have 90% of the dataset for training and 10% for validation. As a score for a model, we use the average over all the losses of the folds.

We started using Keras with TensorFlow backend [7] considering 3 hidden-layers network and a quite small amount of units per layer. We also experimented a "pyramid" shape, where at each level there are fewer units than the previous one.

For the Pytorch model, we decided to implement a two hidden layers network and a quite high amount of units per layer without any particular shape. In both Neural Network models, all the connection between a level and its next one are dense.
As we said in the Introduction chapter, together with the MLP we wanted to experiment a different approach to Machine Learning, and so we started to look for a good SVM framework to use. We found out that the best one is *libsvm* [8]. Instead of using it, we use the scikit-learn implementation based on *libsvm*. It provides a better integration in Python and the other utilities of scikit.
Since we are dealing with a regression task we use SVR, a special kind of SVM. They share the same principles, but it SVR differs on use an epsilon insensitive loss and two slack variables for each data point.

3. EXPERIMENTS

Once we choose the main structure of the models and the main techniques to use, we started to develop the models and tune the hyperparameters.

Let's talk shorty of how we plot the learning curves of our Neural Network models. Every point that we plot is defined in this way: (number of epoch, metrics at the end of that epoch), we use metric in the sense of loss or accuracy. For "at the end of that epoch" we mean the value of metric after a number of updates = (number of samples/batch size). Since we run ten-fold cross-validation we could plot ten learning curve. In order to not have such a confusing plot, we just consider four or five random fold, and we plot them both on validation set and training set. In this type of plots it isn't really important to understand which fold goes well or not, but just the variance between their behaviour, so it is ok to see them in black and white. In the Section 3.3 we talk about the SVM plot.

3.1 KERAS Multi-Layer Perceptrons

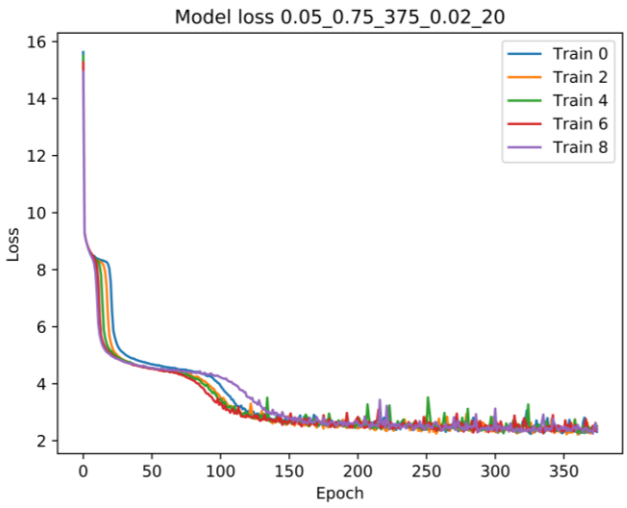


Figure 1 Learning curve of an unstable model. eta = 0.05, alpha = 0.75, epochs = 375, lambda 0.02, batch size = 64

Implementing the basic structure in Keras was quite easy and quick; in our opinion, this framework works with a high level of abstraction. It provides every aspect of a Neural Network, but as a drawback, it doesn't let the programmer has the control of some aspect of what it is going on under the hood. Thanks to the online documentation of the framework we started to develop our idea, 3 hidden-layer NN with this structure: the first one (the nearest to the input layer) of 26 unit, the second of 24 and the final hidden layer of 22 units. So we built it following this rule, with $c = 2$:

$$Unit\_at\_level_i = Unit\_at\_level_{i-1} - c$$

Then we started the grid-search with a value of *eta* (learning rate) too high. For this reason, our first models were unstable as we can see in **Figure 1**.

Then we restarted the grid-search with a low value of *eta* around 0.001, in order to let the model go slow and stable to the solution. As *alpha* (momentum parameter) around 0.8 as *lambda* (penalization term for norm 2 regularization) 0.02 and batch size 64.

In this initial phase of grid-search it there was some other problem, for example, we selected a set of *lambda* too high and the model was unable to learn, and so it went in underfitting. As we can see in **Figure 2**.

At this phase, we used the sigmoid activation function, and after some steps over the grid search, we found some good parameters in terms of smoothness of the learning curve and loss on the validation set (around 1.5). We found a weird behaviour in more or less all plots; there were "stairs shapes" that is some plateaux and some parts where loss function had steep descend. Moreover, the needed epochs were very high (around 450). As we can see in **Figure 3.**

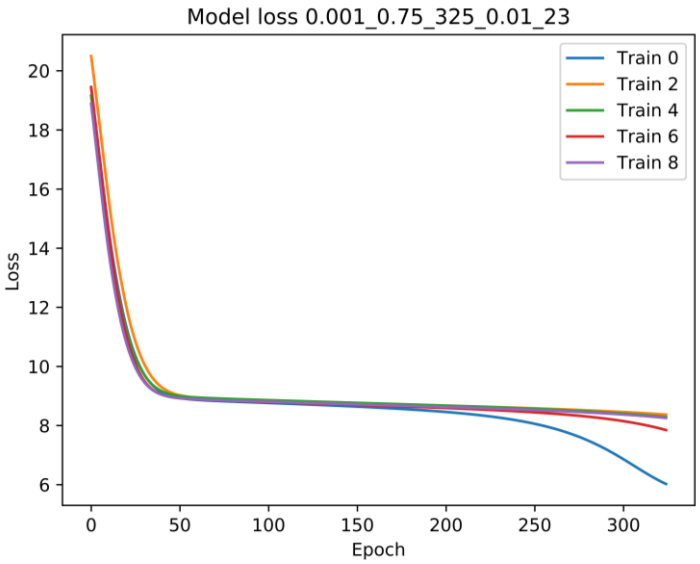


Figure 2 Learning curve of undefitted model.
eta = 0.001, alpha = 0.75, epochs = 325,
lambda 0.01, batch size = 23

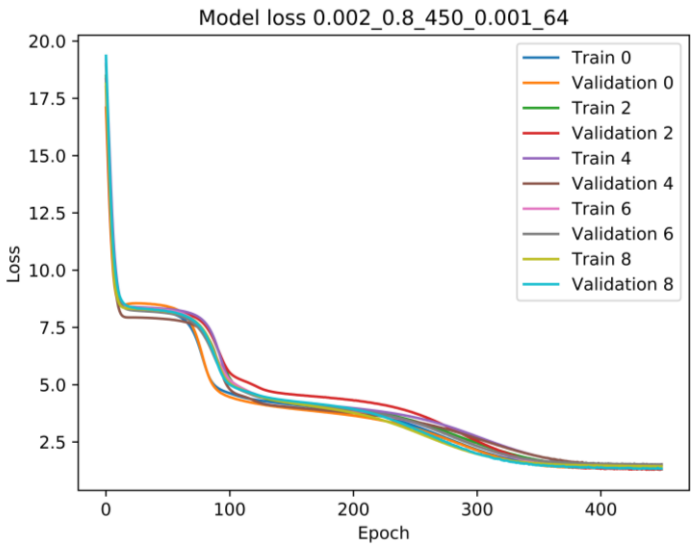


Figure 3 Learning curve of the first model with sigmoid activation function.
eta = 0.002, alpha = 0.8, epochs = 450,
lambda 0.001, batch size = 64

After many other experiments, we decided to use ReLU activation function since we had 3 layers; in fact, it has been demonstrated that ReLU ensures better training of deeper networks [9]. This modification changed completely the learning curves. Indeed, with it, we obtained the same results with fewer epochs (just 70!) than sigmoid, and there weren't any more weird plateaux and "stairs", as we can see in figure **Figure 4**.

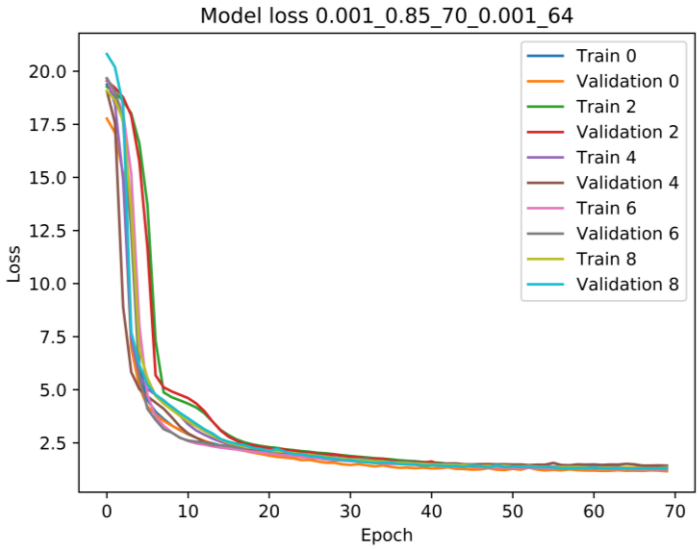


Figure 4 Learning curve of the first model with ReLU activation function

Then we also found out that the same results were reachable with fewer units, so we increased the *c* of the formula to 3, in order to have our levels with 25-22-19 units. Since we changed the activation function and a bit the number of units, we started again the grid search for the hyperparameters. We found what in our opinion was the best hyperparameters: eta = 0.001, alpha = 0.84, lambda = 0.0006, batch size = 64, number of epochs = 170. The average result on the training set, validation set, and the result on our internal test set is in Section 3.5. We can see the final plot of the learning curve of this model in **APPENDIX A1**.

3.2 PYTORCH Multi-Layer Perceptrons

The first thing to say about this framework is that it has a lower level of abstraction; for example, we need to implement the *forward* [10] function of the net and so how the net computes its output. Nevertheless, it provides high-level functionality like *autograd* [10] for the execution of the backpropagation. In this framework, we decided to build a different MLP, with one layer less and more units per layer than the Keras model, so two hidden layers of 35/45 units per layer. For us, it has been really useful this book [11]. The main issue compared to the previous framework is the implementation of the loss function. In Pytorch, we implemented this Mean Euclidian Error explicitly using tensors to work faster on GPU using "the cuda semantics" [12], in order to make the tensors operation be done efficiently by our Nvidia© GPU and not simply in CPU. We will show later, how our different Nvidia© GPUs works for the same task. Another issue found during the implementation of this model was the construction of the mini-batch algorithm. In fact, we did it all on our own moving indexes according to the batch size. With the knowledge acquired in the previous model, the hyperparameters tuning was faster than before. For the same reason explained in the previous model, we always use ReLU activation function. In the first part, we thought that the learning curves were smooth. During the construction of the plots we found out another small problem, if we zoom in the epochs, the learning curves were a bit shaky as we can see in

Figure 5. This discovery was useful not only to understand the behaviour of the learning curves at the ending part of the training phase but also to visualize better how the different curves of training and validation were distant from each other. So, we changed our plotting technique accordingly as we can see in **Figure 5**.

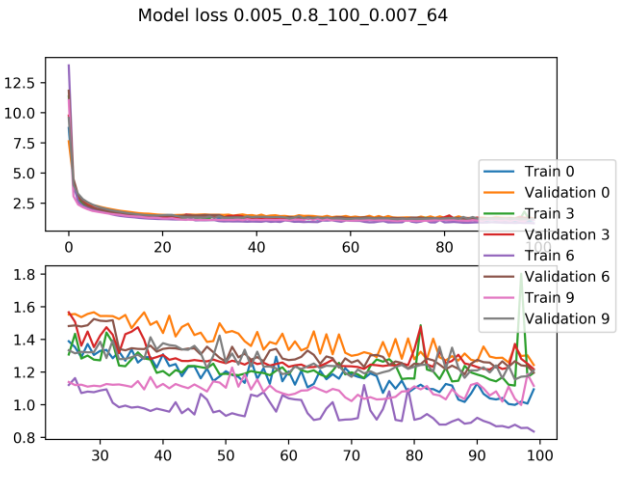


Figure 5
Top: Learning curve of epochs[0,100]
Bottom: Learning curve of epochs [25,100]
eta = 0.005, alpha = 0.8, epochs = 100, lambda = 0.007, batch size = 64

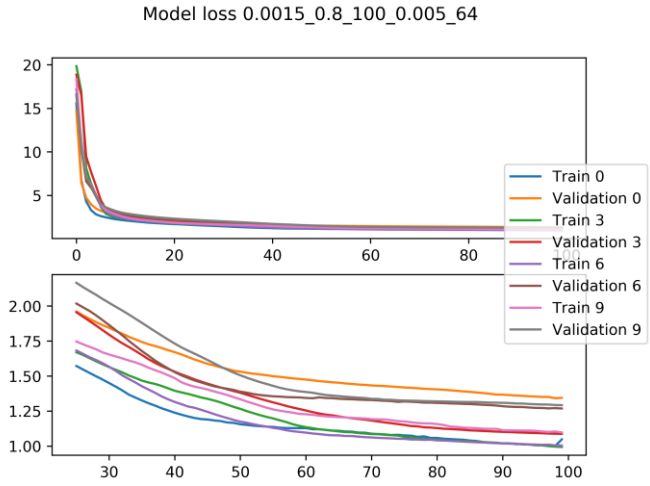


Figure 6
Top: Learning curve of epochs[0,100]
Bottom: Learning curve of epochs [25,100]
eta = 0.0015, alpha = 0.8, epochs = 100, lambda = 0.005, batch size = 64

Found this issue, we restarted again a new phase of hyperparameters tuning, with fewer values than before. After that, the graphs were a lot smoother in the ending part of the learning phase. As we can see in **Figure 6.** Our best hyperparameters are: eta = 0.0015, alpha = 0.9, lambda = 0.002, batch size = 64, number of epochs = 135. The average result on the training set, validation set, and the result on our internal test set is in Section 3.5. We can see the final plot of the learning curve of this model in **APPENDIX A2.**

3.3 SCIKI-LEARN Support Vector Regression

One of the biggest issue found in this model was the concept of learning in a totally different approach. As seen in the course, an important choice regards the kernel to use. We started with Radial basis function (RBF). Our model needs three parameters, each of one of these controls the complexity of the system. The first is *gamma* that defines how far the influence of a single training example reaches, with low values meaning "far" and high values mining "close". The second parameter that we use is *C*, the third is *epsilon*. We started the grid search over the space to find the best value that minimizes the loss. As we said before, the task given is of regression, so we use SVR. This model is different from the first one because of it use an *epsilon* (third parameter) to construct the epsilon-insensitive tube. Once we found what we wanted to tune, we found that if we use only the SVR, we cannot solve the task because it is a multiple regression task. Of course, it is possible to solve the same task considering one regressor per target. In the beginning, we try to do by our own, but in order

to be sure that all the executions run efficiently, we decided to use a support library *MultiOutputRegressor*[13] provided by scikit-learn. Another import issue was the plotting of the learning curve; here the concept of learning is completely different because there aren't epochs; instead, we work only with the training sample. As we studied, the learning curve of SVR can be plotted by (number of examples, loss).

Since we were totally new with this type of model we started in a wide range of exponential, values = [0.01, 0.01, 0.1,1, 10]. Because of the dataset is noise and we haven't enough confidence we didn't try values bigger than 10 since with high *C* less training errors are allowed. For *gamma* we started with a small value in order to let the Gaussian function has a large variance. We also checked a range of values near 0.1 for epsilon. In the **APPENDIX A3,** we can see some of the Learning Curves generate by the grid search. The best hyperparameters are *C* = 8, *gamma* = 0.05 and *epsilon* = 0.2. The average result on the training set, validation set, and the result on our internal test set is in Section 3.5. We can see the plot of the learning curve of the best SVM model in **Figure 6**.

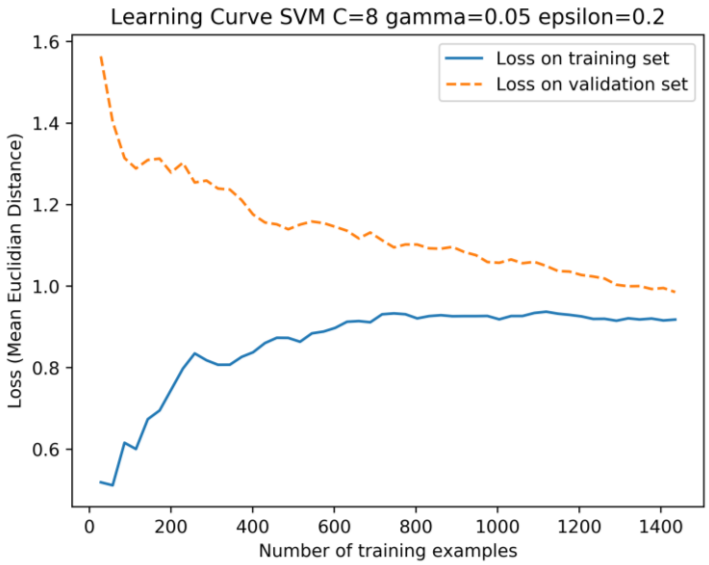


Figure 6 Learning curve of the final SVR model

3.4 Comparison Nvidia© GTX 850M - Nvidia© GTX 1650M

Our laptops are:

- **PC1**: Asus N56J, Intel® Core ™ i7 – 4710HQ, NVIDIA® GeForce® GTX 850M, 16 GB RAM, Windows 10.
- **PC2**: Dell Inspiron 7590, Intel® Core™ i7 – 9750H, NVIDIA® GeForce® GTX 1650M, 16 GB RAM , Windows 10.

In **Figure 7** there is a simple bar chart that visualizes the time in seconds needed by our laptops to execute this set of steps: 1) train and evaluate the models in 10 folds 2) train again the models on the whole dataset 3) predict the result for the blind set. 4) plotting the results.

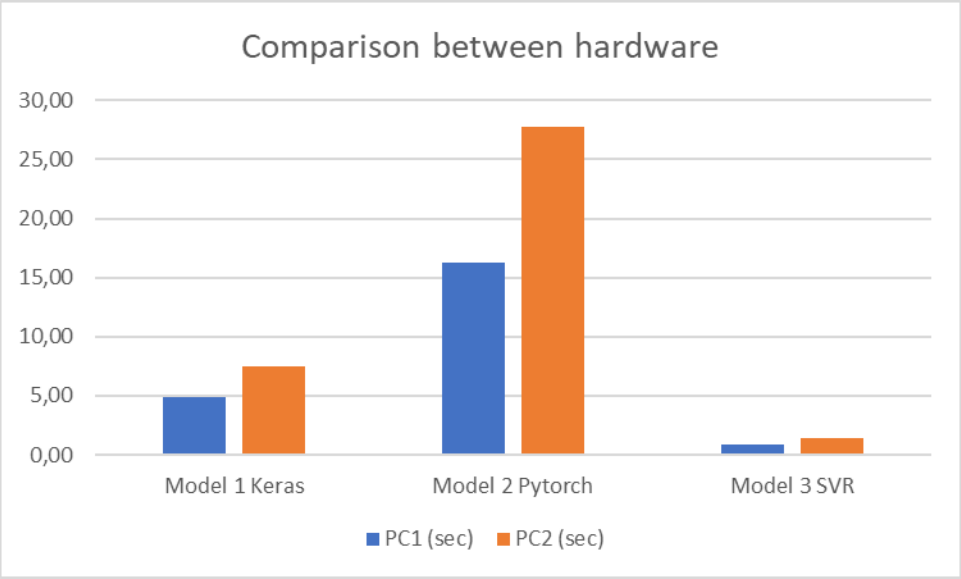


Figure 7 Comparison of time needed by the models

As we can see Pytorch got the worst performances than the other, also because our implementation has some problem in allocating tensors from *numpy* n-dimensional array.

3.5 MONK'S RESULTS

To solve monk dataset we use a simple Keras MLP with one hidden layer of 4 units. All tests use batch size = 25.

Task	Eta	Momentum	Lambda	MSE (TR/TS)	Accuracy (TR/TS) (%)[i]
MONK 1	0.25	0.85	0	0.0016/0.0024	100%/100%
MONK 2	0.2	0.75	0	0.0007/0.0105	100%/100%
MONK3	0.2	0.75	0	0.0395/0.496	95%/93%
MONK3 (reg.)	0.4	0.75	0.0001	0.0128/0.0270	99%/95%

Table 1. Average prediction results obtained for the MONK's tasks.

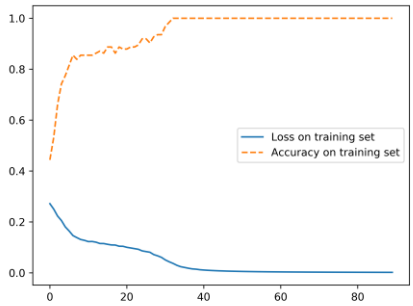
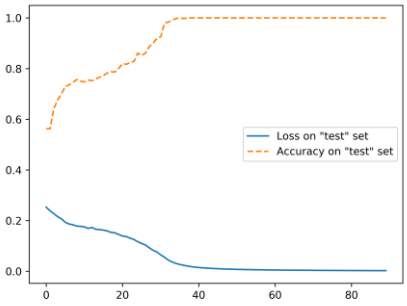
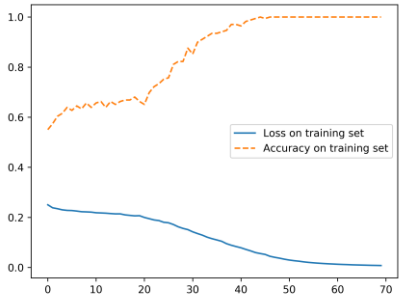
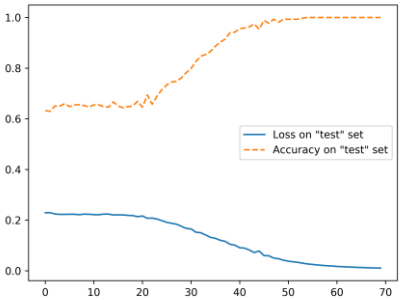
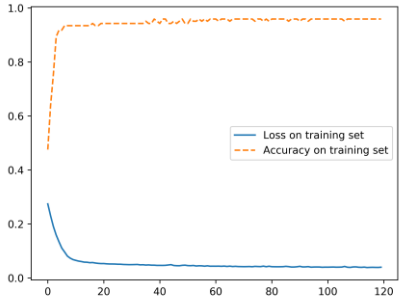
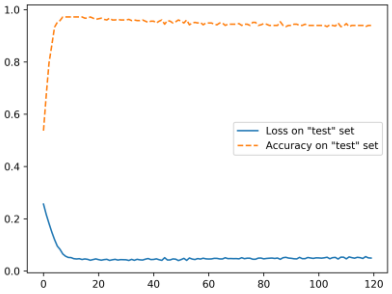
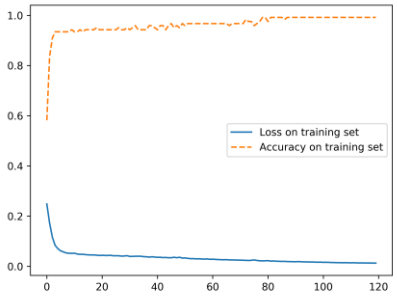
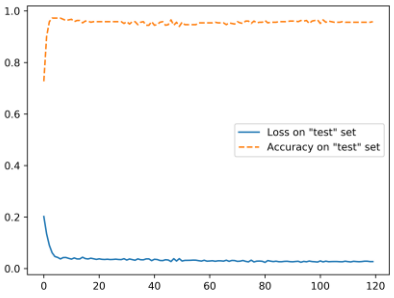
	Plot of loss and accuracy Training Set	Plot of loss and accuracy Test Set
MONK 1		
MONK 2		
MONK 3		
MONK 3 (reg)		

Table 2. Plots of the MSE and accuracy for the 3 MONK's benchmarks.

3.5 CUP RESULTS

In the end, of the process of model selection, we wrote a script that tests all the final models on our internal test set. Results on training and validation are the average over the 10 folds. The results are in **Table 3**:

	Training Set	Validation Test	Test Set
Model 1 Keras	1.1552	1.2756	1.2353
Model 2 Pytorch	1.0385	1.1882	1.2081
Model 3 SVR	0.9096	1.0457	1.0632

Table 3 Final results

Given these results, we choose Model 3 SVR.

4. CONCLUSIONS

In the **APPENDIX B** we can see the plots in a cartesian plane of the results of our models just to "visual compare" the different shapes.
After this project, we can say that with its level of abstraction Keras permit to develop faster the code than Pytorch. Nevertheless, if you know what you are doing (in terms of theory background), Pytorch is more accurate than Keras because of the lower level of abstraction since it permits a strong control over the code. In the end, we can say that SVM are very powerful tools and in particular *libsvm* (and other libraries based on it, like scikit-learn) implements efficiently all the functionalities; also, it provides a quite easy programming interface.

NICKNAME: BOFMON
BLIND TEST RESULTS: BOFMON_ML-CUP19-TS.csv

W*e agree to the disclosure and publication of my name, and of the results with preliminary and final ranking*.

REFERENCES

[1] https://keras.io/

[2] https://pytorch.org/

[3] https://scikit-learn.org/stable/

[4] https://github.com/aboffa/MachineLearningProject

[5] https://numpy.org/

[6] https://matplotlib.org/

[7] https://www.tensorflow.org/api_docs/python/tf/keras/backend

[8] https://www.csie.ntu.edu.tw/~cjlin/libsvm/

[9] Xavier Glorot, Antoine Bordes and Yoshua Bengio (2011). Deep sparse rectifier neural networks. AISTATS. Rectifier and softplus activation functions. The second one is a smooth version of the first.

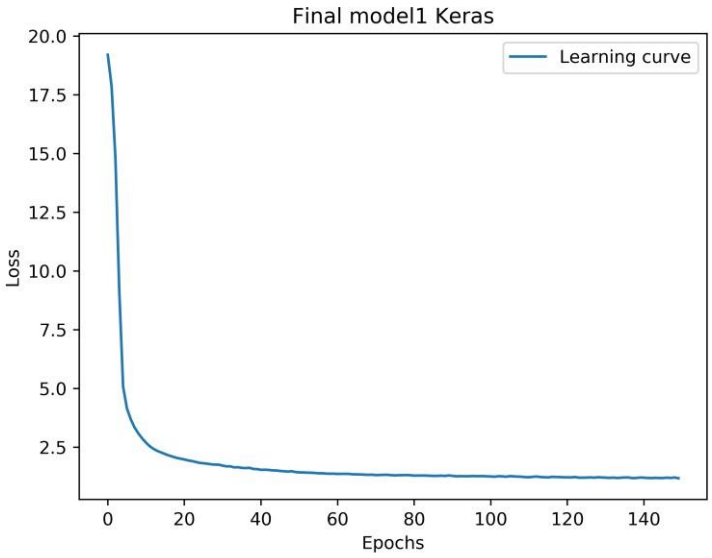
[10] https://pytorch.org/docs/stable/index.html

[11] Eli Stevens, Luca Antiga (2020). Deep Learning with Pytorch. Essential Excerpts. Manning Author Picks. https://pytorch.org/assets/deep-learning/Deep-Learning-with-PyTorch.pdf

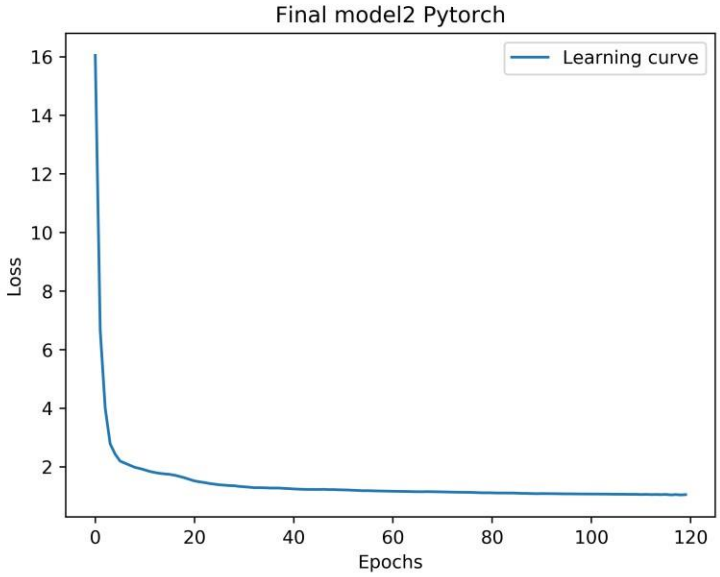
[12] https://pytorch.org/docs/stable/notes/cuda.html

[13] https://scikit-learn.org/stable/modules/generated/sklearn.multioutput.MultiOutputRegressor.html

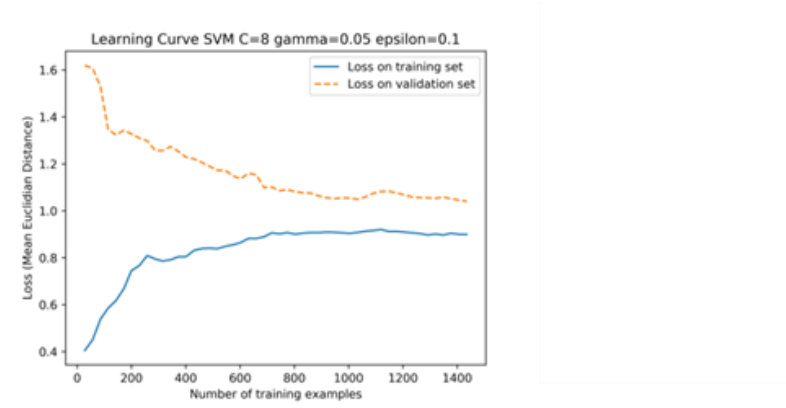
APPENDIX A (LEARNING CURVES)

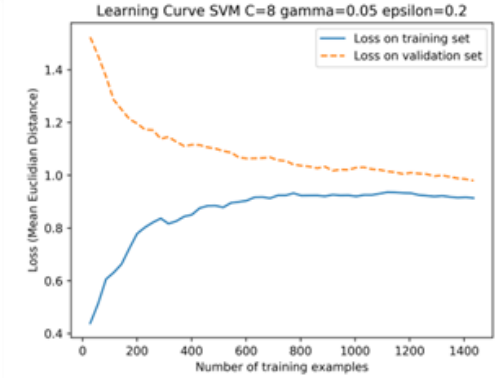


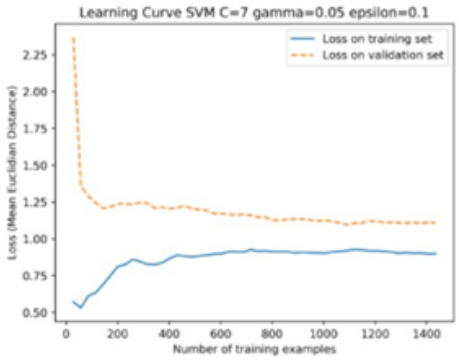
A1. LEARNING CURVES OF THE FINAL MODEL 1

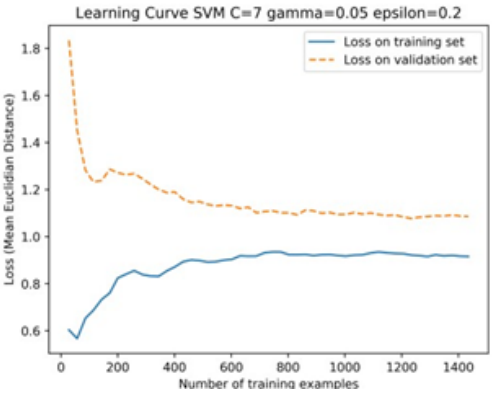


A2. LEARNING CURVES OF THE FINAL MODEL 2



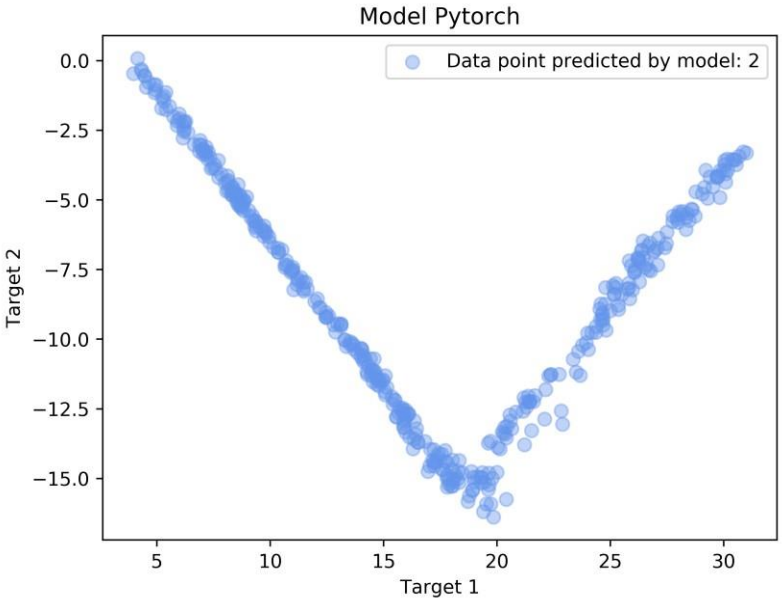




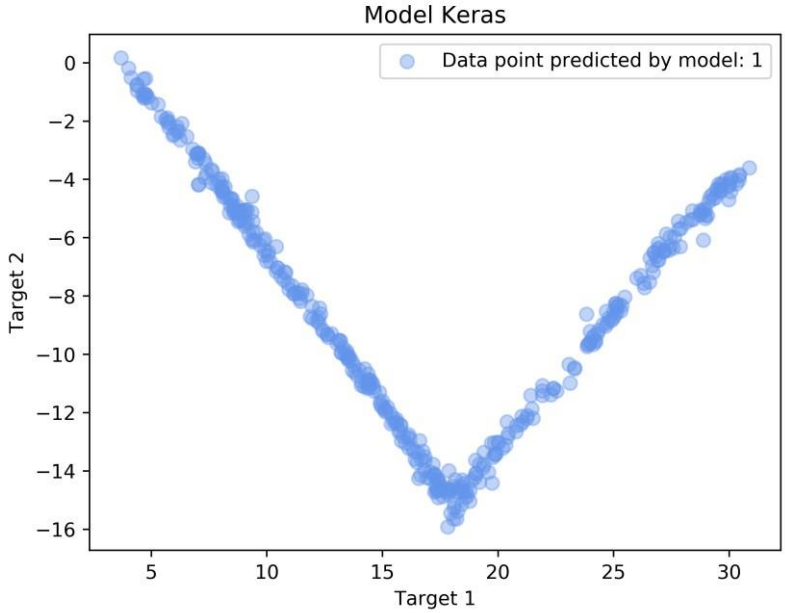


A3. LEARNING CURVES OF THE MODEL 3

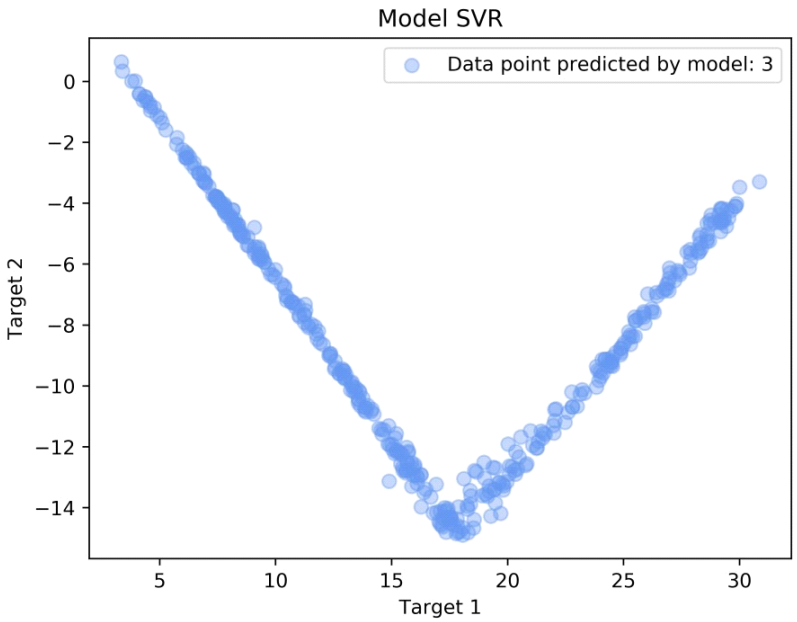
APPENDIX B (DATA VISUALIZATION)



B1. DATA VISUALIZATION OF THE FINAL MODEL 1



B2. DATA VISUALIZATION OF THE FINAL MODEL 2



B3. DATA VISUALIZATION OF THE FINAL MODEL 3