Plume Labs data challenge : predict pollution in an Asian megacity

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***Abstract*— This report our participation and solution proposed for the "Plume Labs data challenge". It was part of the "Advanced machine learning" course of the Ecole Polytechnique led by M. Le Pennec and Mrs. D'alche-Buc.**

I. INTRODUCTION

Plume Labs is a french start-up aiming at providing people insights about the pollution in the atmosphere. In particular, they use pollutants measures gathered from international meteorological agencies to compute a score, the plume labs "air quality index" in different cities in the world. This score takes into accounts multiple pollutants and toxic gas such as fine particles, ozone or nitrogen dioxide.

II. TASK OVERWIEW

Presently, the start-up is able to gather large amounts of data and process them in order to compute the quality index in real time. They now want to use this expertise to make predictions of the amount of pollutants in the future. More precisely, they want us to predict the concentrations of 4 different pollutants during the next 24 hours.

In order to achieve that, they gave us measurements from different meteorological stations in an Asian megacity. The set of measurements aggregates the measures of 18 stations. There are 2 categories of stations :

- The first category is composed of 17 stations having measured pollutants levels during the previous 24 hours.
- The second category is composed of the station on which we want to make the prediction. For this station we have no pollutant data but we are given the meteorological features (humidity, dew point, cloud cover, temperature, etc.) of the previous 24 hours as well as weather forecasts for the next 24h.

Thus, we have to implement the classical machine learning pipeline, summarized by the following graph :

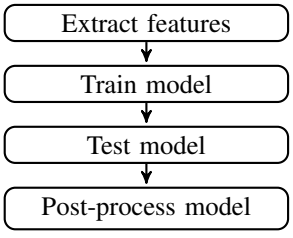


Fig. 1: The process to be implemented

A. Extract features

The data we are given is already "clean", there are no missing or strange values. Moreover, the number of features provided is large: we have approximately 1k different measurements in the data set. Thus, we focused this part of the process on feature selection and also on how to re-arrange the features to train different models.

B. Train model

Here is the most tricky part of the challenge. We are facing a multi-regression problem : we want to predict the levels of 4 different pollutants for the next 24 hours. In other words, we have to be able to perform, for each example in the train or in the test sets, 96 regressions. Moreover, as far as it is a time-related prediction problem, we have to be able to include in our models the time information.

C. Test model

To test our models we used classical cross-validation on sub-samples of the initial data. The quality of the prediction was assessed using the Mean Squared Error (MSE).

D. Post-process model

Keeping in mind the "shape" and characteristics of the data on which we want to predict was fundamental in this challenge. After predicting, we used logical considerations to post-process the predictions in order to increase our accuracy.

Finally, after finding a good predictive model on our local set, we made submissions on the Ecole Normal Superieure data challenge platform (https://challengedata.ens.fr) on which the challenge was hosted.

III. ANALYSIS OF THE DATASET

At the beginning of the project, we tried to understand better the given dataset performing different analysis on the data.

A. Description of the data

The data is organized in a very specific manner. When we import the dataset we get the following matrix :

$$
\begin{array}{cc}
 & \begin{array}{ccc} hour_{-24} & \dots & hour_{-1} \end{array} \\
\begin{array}{c} measures - day_1 - hour_1 \\ \vdots \\ measures - day_N - hour_{24} \end{array} & \begin{pmatrix} mes_(1,1) & \dots & mes_(1,P) \\ \vdots & & \vdots \\ mes_(N,1) & \dots & mes_(N,P) \end{pmatrix}
\end{array}
$$

Fig. 2: This teh representation of a feature-block. Each measure is made on 24h, thus for each pollutants and for each stations we have that kind of blocks composed of 24 columns : one column per hour. The total dataset is just a vertical concatenation of that kind of blocs

We also noticed that, and this is really important, from a line to the following, the measures are made with a 1-hour time interval. Because of that, we observed "propagating" values in the data set, and we took advantage of this information latter in the post-processing. (see the specific part of the report)

B. Features available

The given data is heterogeneous : even though it's clear that we have to categories of stations (described before) among the pollutants-describing stations, there are differences. Some of them are measuring just one type or two of pollutant while other measure all pollutants... For that reason, we do not have the same quantity of information for all the pollutants.

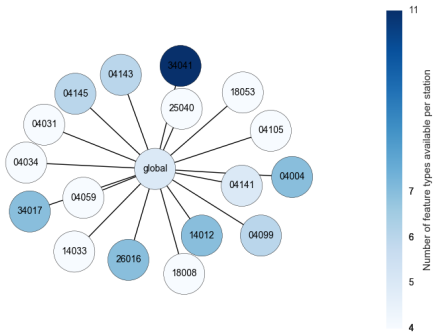


Fig. 3: Here are listed the stations contributing to the final prediction we are going to make on a station named "global" above. Global contains some meteorological data, the other measure the pollutants levels. From that graph, it appears clearly that the richness of information from a station to another is not the same.

An other way to understand this is to look at the total number of features per station or the total number of features per type of features :

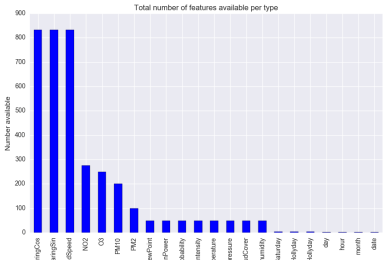


Fig. 4: Every stations except "global" have wind measures but... only few stations have PM2 measures,for instance.

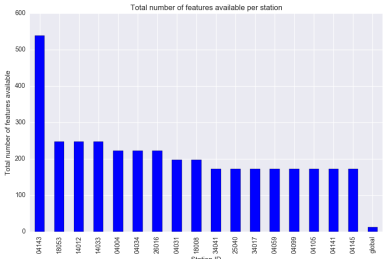


Fig. 5: One station has a lot more information than the other : it's the station on which we are asked to make the prediction. This is logical because this specific station measures a lot of meteorological features, in general on 24h or 48h time windows

C. Correlation between features

Because of the specific distribution of columns in the dataset, we wanted to check the correlation between the input features (columns of the training dataset) and the correlation between the features we want to predict (observed values used for training). In fact, some

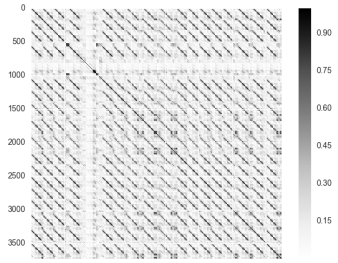


Fig. 6: Here, each pixel value, p_{ij} is the correlation between the column i and the column j. The main phenomenon observable here is the presence of multiple small diagonal lines of high-correlation. They are due to the wind measures. The wind measure at an hour h in a station s_x is always highly correlated to the wind measured at the same hour in a station s_y and this is true $\forall x, y$.

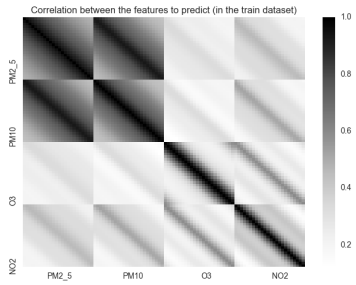


Fig. 7: Here is the same matrix than before but, here, calculated on the 96 columns we want to predict in the training set. First, we can observe that we have 16 squared sub-blocks : they correspond to the columns of different pollutants. In each sub-block, the values observed measure the correlation of a pollutant at hour h_x with itself at hour h_{x+t} : all pollutants are highly correlated to themselves on close hours (black diagonals) but the correlation diminishes when time increases. This is quite understandable. Secondly, the fine particles (PM_{10},PM_2) are less volatile than gases (NO_2, O_3) : their levels of self-correlation are higher. Finally, PM_2 and PM_{10} are obviously highly correlated but this is less true for gases.

From this information, 2 resolutions were adopted :

- We have to test multi-models, that is to say models based on the observations of just one pollutant predicting the same pollutant or models trained on all observations but predicting, again, on pollutant only.
- We have to feature engineer the wind features. They are highly correlated and this characteristic can perturb our models (and increases the training time for no additional value).

D. Behavior of the pollutants concentration

Finally, we also checked the pollutants concentrations' behavior. From the train set it is easy to track the pollutants in each station hour by hour : each line correspond to an hour of measure. Thus, we arbitrarily took the "hour -1" of each station for each pollutants.

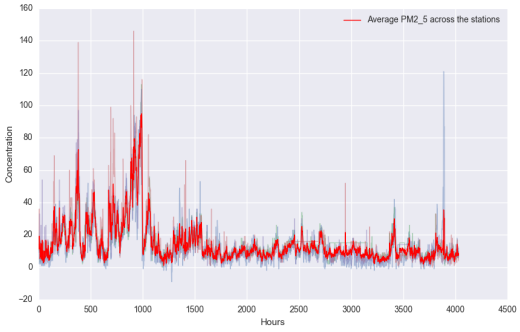


Fig. 8: In the PM2 levels we can see a relative stability from an hour to another. There few deviance in the measures between the stations is quite low.

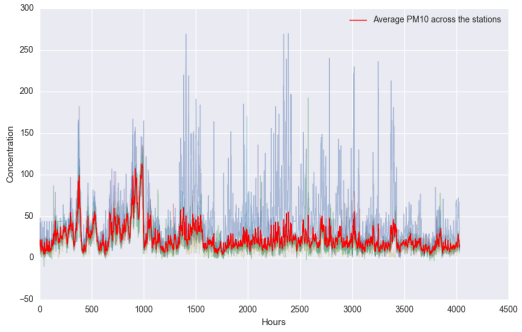


Fig. 9: As you can see, the levels observed for PM10 are close to PM2's ones. We also notice the presence of an outlier station (blue curve) for which the measured values are often very far from the mean value.

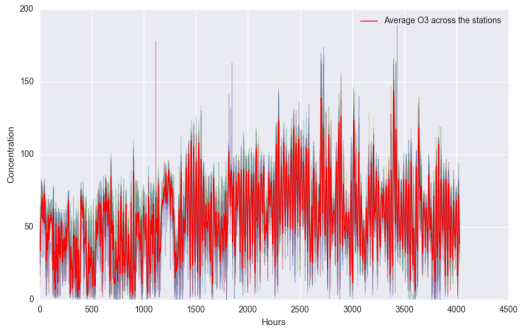


Fig. 10: Clearly, we can verify the volatility of O_3 that we intuited from the second correlation matrix. From an hour to another we see huge variations. Nevertheless, the measured values, for each stations are close to the "mean" value.

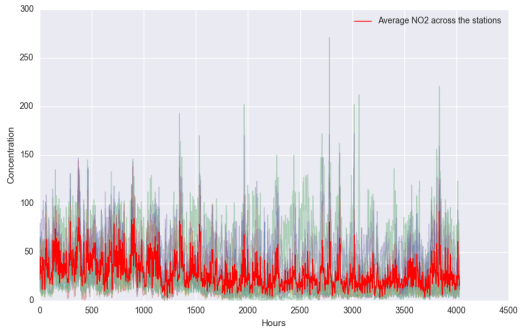


Fig. 11: Finally, here are the observed values for NO2. We find again a high volatility and, also, an important deviation between stations...

IV. FIRST APPROACH

A. Ridge and Lasso

After analyzing the dataset and having a better understanding of the task at hand, we started experimenting with the regression task. Our first approach was to use a linear model,

more specifically a **ridge regression** which is consists in minimizing linear least squares function with an L2 penalty. The L2 penalty controls the complexity of the model through regularizing the weights to keep them small, thus controlling over-fitting.

The intuition behind using the ridge regression was mainly driven by the fact that our problem is quite high dimensional. In fact, we have 3729 features in our data-set. We chose Ridge over Lasso for a very simple reason: Some of our features are highly correlated (such as hourly measurements of PM2-5 and PM-10). If we use L1 penalty, if two features are correlated in order to ensure sparsity of the solution, only one of the two features will be picked. In contrast, if we use L2 penalty, the two correlated features will be both included in the model and their corresponding coefficients will be shrinked. In the case of both regressors, the penalization hyper-parameter C was selected using cross-validation. The obtained hyper-parameter was C=0.1 in both cases.

	MSE
Ridge Regression	0.83 (+/- 0.02)
Lasso Regression	0.84 (+/- 0.01)

TABLE I: Mean cross validation score using MSE on the training dataset

B. Random Forests and Feature Importance

Our second approach to the model was to use ensemble methods. Since we have some noisy data in our training set, we came to the conclusion that we need a more robust model. We therefore opted for ensemble methods.

We have therefore opted for a Random Forest Regressor. We therefore build the following model: For each hourly target value of a specific pollutant, we build a random forest regressor which takes as an input the entire train dataset. We hence obtain 24 models for each pollutant amounting to 96 models in total.

Using this approach, we manage to improve the performance of our model. To better evaluate this performance, we use on top of the mean squared error the "R2" or "R-squared" score which stands for coefficient of determination. R2 measures how well are the target data replicated by the model. The R2 score is computed as follows:

$$R = 1 - SS_{res}/SS_{tot} \tag{1}$$

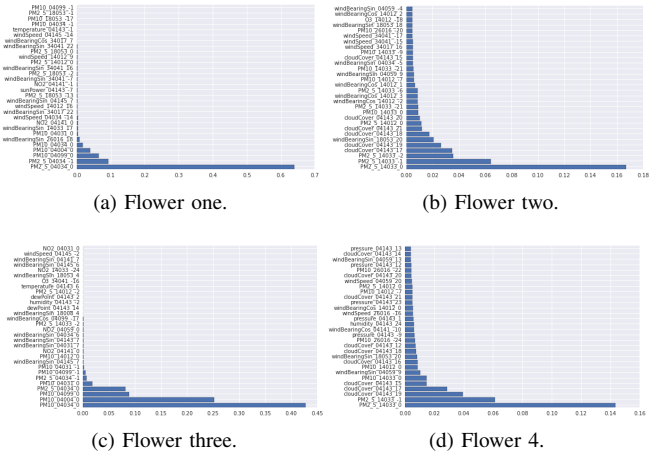
$$SS_{tot} = \sum (y_i - \overline{y}) \tag{2}$$

$$SS_{res} = \sum (predy_i - y_i)) \tag{3}$$

Where $\overline{y}$ is the mean of the target values and $predy_i$ are the values predicted.

C. Post-processing with predicted values propagation

If you read carefully the section "Analysis of the dataset" you know that the given dataset is vertically **and** horizontally ordered by hours. Thus, we observe in the dataset "propagation" of constant values. In other words : the values on the inverted diagonals of the matrix of prediction are constant because they concern the same hours of prediction !



(a) Flower one. (b) Flower two.

(c) Flower three. (d) Flower 4.

Fig. 12: My flowers.

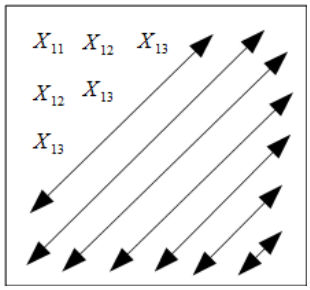


Fig. 13: For each pollutants measures, you observe this pattern of propagating values on inverted diagonals. This is caused by the order of the set of examples.

The data on which we want to predict is organized exactly in the same way. This is a real strong information because we know, now, that the predicted matrix must show a propagating pattern. Now, if you combine this information with the fact (detailed before) that predicting the first hour of each pollutant levels (that is to say predicting the first column of each pollutant) is a lot more easy than predicting the next hours then you obtain the following method :

- Step 1: Predict the first column of each pollutant as precisely as possible, for example using random forests with a large number of estimators
- Step2: Predict the other columns with a constantly decreasing number of estimators to gain time. The quality of the prediction of the other columns is, then, a lot diminished, but we do not care because of step 3
- Step3: Post-processing of the prediction : propagate the values from the firsts columns in the way displayed on fig.12. Note : when we propagate we simply erase the predictions made before with newer values from the firsts columns.

Apart from increasing our scores a lot, this post-processing allowed us to decrease tremendously the computational cost

of the training and, thus, dedicate that extra time to train more complex and more precise models for predicting the first columns.

D. Conclusions of the first approach

- On this dataset, random forests are the best learner we found.
- Training one model per column is clearly a better way to address the problem.
- The quality of our prediction depends of the pollutant and the predicted hour: while PM_2 and PM_{10} levels can be predicted with high confidence, volatile gases like NO_2 and O_3 are more difficult to fit.
- This 96 regression problem can be re-interpreted as a 4 regression problem: the order of the data set allows us to propagate predicted values in a way such that we no longer need to train all the forests.

V. IMPROVED MODELS

From the previous section we understand now that all the challenge resides in making the prediction of the first columns of each pollutants as precise as possible (and the propagate the values to recover the prediction matrix), especially NO_2 and O_3's ones.

VI. CONCLUSIONS

A good understanding of the task and the data's characteristics was fundamental the perform well on that challenge.

Now that we have finished this project we deserve listening to a nice funk tune. That's what I'm gonna do. Thank you Erwan, stay fresh bro.