

Data Science

Deadline – January 13th 2023 @ (23:59)

I. GENERAL DESCRIPTION

A. Project Goal

The goal of the data science project is to help students **to understand the impact of the different choices** made along the data science process (*KDD process*). In order to achieve this goal, students are asked to address two distinct domains and two different tasks: **classification** and **forecasting**.

B. Delivery

Students only have to deliver **a report** describing the results obtained over the exploration of both datasets and tasks. The report should contain a technical description of the procedures performed over the data, the corresponding results, the decisions taken and possible justifications for those results.

You can imagine, you are writing a report to be read by your supervisor, not your client, and so the description shall be technical and not from the domain point of view.

The report may be written in Portuguese or English, but has to follow the **template**, providing all the charts required and without exceeding the number of characters allowed per section. Exceeding text will not be considered.

The report file shall be named **report_X.pdf** (replacing X by the team number) and has to be submitted through **Fénix** before the deadline stated on the first page

Excellence

Excelling projects have three major characteristics.

First, they show an acute understanding of the data characteristics and their impact on the discovery, formulating hypothesis to explain differences in performance.

Second, robust assessments go beyond simple performance indicators, studying different and adequate parameters, and deriving trends from the experiments.

Third, poor results are not acceptable, and there is always something that we can learn from the data.

Plagiarism

Plagiarism is an act of fraud. We will apply state-of-the-art software to detect plagiarism. Students involved in projects with evidence of plagiarism will be reported to the IST pedagogical council in accordance with IST regulations.

II. WORK TO DEVELOP

The project consists of performing only **the first iteration of the KDD-process**, when training a set of models over two distinct datasets, not considering any additional iteration. In particular, data profiling, data preparation, modeling and evaluation steps have to be performed for each task.

There are two tasks to perform over the datasets: **classification** and **forecasting**.

In both situations, the goal is not only to describe the best models learned, but to understand the impact of the available options on the produced models performance.

Students may choose the mining tool to apply, between **python** (using *scikit-learn*), **R** and any other language. Other business intelligence platform may be used but discouraged, since they are not prepared to deliver the charts required.

A. Classification

The datasets for the classification task in this project were collected from the Kaggle platform, and are available for **download** in **Fénix section Project**.

- **Health domain - Diabetes 130 US hospitals for years 1999-2008**
 - classification **file** = diabetic_data.csv **target** = readmitted
 - description available on <https://www.kaggle.com/datasets/brandao/diabetes>
- **Climate domain - Predict Droughts using Weather & Soil Data**
 - classification **file** = drought.csv **target** = drought
 - description available on <https://www.kaggle.com/datasets/cdminix/us-drought-meteorological-data>
 - the data to be used was sampled from the original data, reducing the number of records, combining all data and binary labeling the records

Data Profiling

For the first task, data should be characterized along the four perspectives: dimensionality, distribution, sparsity and granularity.

When in the presence of symbolic variables, and since `sklearn` is not able to deal with them correctly, students have to choose a **new encoding for those variables**, before proceeding with the correlation analysis.

Remember that data profiling is used as a mean to best understand the data and mostly for identifying the required transformations to apply to the original data, in the following step. These transformations aim to improve the performance of classification techniques, to be applied during the modeling phase.

In particular, students should perform a statistical analysis of the datasets in advance and summarize relevant implications in the report, such as the underlying distributions and hypothesize feature dependency.

Data Preparation

At this stage, data shall be transformed solving the problems identified in the previous task.

For this purpose, students are asked to apply preparation techniques in a predefined order (shown in Figure 1), in a manner to minimize the operations performed.

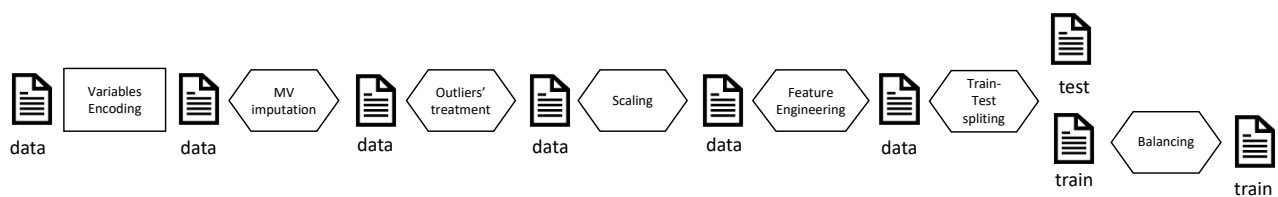


Figure 1 Data preparation methodology for the classification task

Variables encoding is the first step to apply, and it is only required in the presence of symbolic variables, and shall directly result from the *granularity* analysis performed in the data profiling step. Among the techniques available you encounter *transforming into numeric* and *dummification*. Different choices have usually to be made for each variable. Only a choice per variable shall be applied, without applying more than one alternative.

For the rest of the preparation steps to consider, students have to apply at least two alternatives, to evaluate the impact of each one and to choose the most promising, according the procedure illustrated in Figure 2.

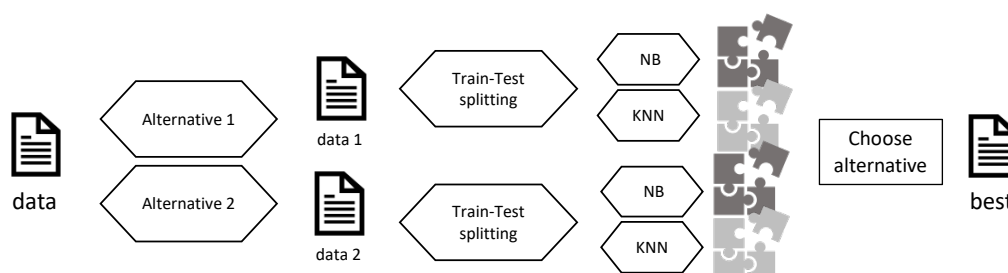


Figure 2 Decision process for each preparation step in the classification task

The proposal here is to process each alternative transformation and then assess the impact of the resulting datasets on training classification models through KNN and Naïve Bayes, by measuring their performance.

In this manner, for each preparation step, students have to apply at least two different preparation techniques concerning a single preparation step, in order to obtain different prepared datasets. With each one of these datasets, train both a KNN and a Naïve Bayes model. Compare the results obtained from the different datasets and identify the dataset that led to the best results, and proceed with the chosen one to the next preparation step.

We suggest the use of both Naïve Bayes and KNN to train these models, due to their simplicity and the reduced number of parameters to tune. Besides that, the different nature of both approaches limit the chances of choosing a technique best suited for a particular approach.

After training the different models, we chose the preparation technique that presents the best improvement when compared with the previous dataset. In this manner, after the training we may face 4 possibilities:

- none of the alternative preparation techniques applied improve the results: so, we should **keep the previous dataset** and proceed for the next step;
- one of the alternatives lead to the training of better models using both approaches: so, we **chose the dataset** resulting from this transformation to proceed for the next step;
- the alternative supporting the improvement is different for each learning technique: so, it is necessary to evaluate in which of the models the improvement was higher, and choose the technique responsible for that increase;
- the improvements are residual: so, it is our choice to continue with the previous dataset, or to follow with the technique that theoretically should present higher improvements.

Remember that you should only consider applying the technique if the data requires it. For example, if a dataset has no missing values, there is no need to perform missing values imputation. **Although, that fact has to be mentioned in the report, and the decisions of not applying some preparation ask have to be justified.**

Some additional remarks:

- It is not possible to train models over missing values with `sklearn`; in this manner, the original dataset has to be replaced by one of the prepared ones to proceed to the next step.
- Balancing has to be applied only to the training dataset, and consequently data partition has to be done previously.
- When in the presence of temporal data, data partition shall use older data to train and newer to test, in order to not use future data to classify past data. In any other case, partition shall be random.
- Feature selection and generation may be applied before or after balancing. In either case, its study may be done as for the other preparation techniques, using only KNN and Naïve Bayes, to assess their results.

Modeling

During the modeling step, students are asked to train a set of classification models to learn the concepts identified by the target variable for both datasets. In particular, students have to apply several machine learning methods and corresponding training algorithms, namely: **Naïve Bayes**, **kNN**, **Decision Trees**, **Multi-Layer Perceptrons**, **Random Forests** and **Gradient Boosting**.

Again, the goal is to study the impact of the different options available. This time the different parameterizations for each training algorithm.

The use of automatic optimizations offered on *autoML* frameworks are strongly discouraged, since they find the best parameters but do not give any intermediate results allowing for performing the impact analysis required.

The training data shall be the same for all the training methods, corresponding to the result of the preparation step – the dataset that led to the best performance of KNN and Naïve Bayes.

Evaluation

Evaluation of the obtained models should be done as usual, through confidence measures and evaluation charts. A thorough comparison of the adequacy of the models should be presented taking into consideration the adequacy of their behavior against the properties of each dataset and their observed performance.

For this purpose the analysis of each classification technique should be done at three different levels:

- the analysis of the impact of the different parameters on models performance;
- the description of the best model found for each classification technique, and its performance;
- the study of overfitting when learning the best model.

Critical Analysis

After identifying the best models learnt with the different ML methods, a critical analysis shall be presented. In particular, students shall compare the best models for each method,

concerning their content and performance. This analysis may incorporate an individual explanation for each model found, but also a cross analysis of the different results.

B. Forecasting

The datasets for the forecasting task only consider univariate time series, were collected from the same domains as the data used for classification, and again can be downloaded in **Fénix section Project**.

- **Health domain - Diabetes**
 - classification **file** = diabetes.csv **target** = glucose
 - description available on <https://archive.ics.uci.edu/ml/datasets/diabetes>
- **Climate domain - Predict Droughts using Weather & Soil Data**
 - classification **file** = drought_score.csv **target** = score
 - description available on <https://www.kaggle.com/datasets/cdminix/us-drought-meteorological-data>

Note that in both cases, the data to be used was sampled from the original data and is ready to use, not requiring additional selection.

Data Profiling

In the forecasting context, profiling gives particular attention to the granularity analysis of the target variable, but also to the distribution and its stationarity.

Data Preparation

Like for classification, data preparation shall follow a pre-defined sequence of operations, in order to reduce the number of datasets to analyze.

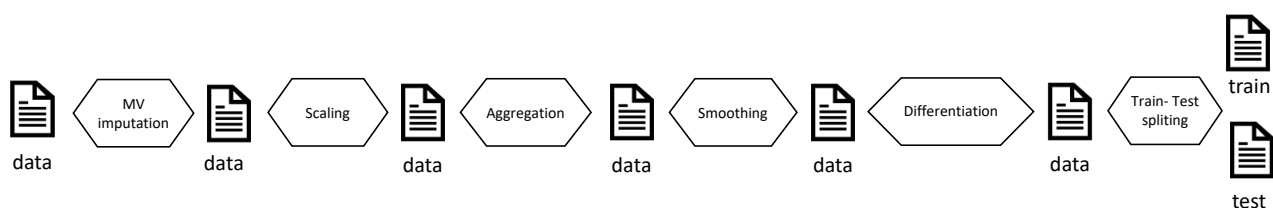


Figure 3 Data preparation methodology for the forecasting task

Now, after missing value imputation, a scaling transformation shall be applied, followed by the study of the best aggregation and smoothing operations. The last transformation to apply shall be the differentiation.

Aggregation shall consider two levels of aggregation and differentiation shall be tested as the first and second derivatives.

Regarding data partition, remember that time series are temporal data, and so test data shall always be posterior to any train data.

The decision over which operation leads to better results shall be based on the persistence model.

Modeling

The forecasting task has to explore the application of **Simple Average**, **Persistence model**, **Rolling Mean**, **ARIMA** and **LSTMs**, for training a single model for each domain.

As for classification, different parametrizations shall be applied over the same dataset. Again the use of *autoML* tools is discouraged for the same reasons.

Evaluation

Like before, evaluation of the obtained models should be done as usual, through confidence measures and evaluation charts, now in the forecasting context. A thorough comparison of the adequacy of the models shall be presented taking into consideration the adequacy of their behavior against the properties of each dataset and their observed performances.

For this purpose the analysis of each forecasting technique shall be done at two different levels:

- the analysis of the impact of the different parameters on models performance;
- the description of the best model found for each forecasting technique;

Critical Analysis

As before, the critical analysis shall compare the different best models obtained, explaining the different achievements with the different techniques.

III. EVALUATION CRITERIA

The project will be evaluated as a *whole*. Nevertheless, we provide below a decomposition of the total project score for the purpose of guidance and prioritization:

CLASSIFICATION	55%	FORECASTING	45%
Data profiling	5%	Data profiling	5%
Data preparation	10%	Data preparation	10%
Modeling and Evaluation		Modeling and Evaluation	
Naïve Bayes	2%	Simple Average	2%
KNN	3%	Persistence model	2%
Decision Trees	5%	Rolling mean	3%
Multi-layer perceptron	5%	ARIMA	3%
Random Forests	5%	LSTMs	5%
Gradient Boosting	5%		
Critical analysis	15%	Critical analysis	15%

Good Work !!!