XAI - Final Project

Professor: Carlos Andres Peña
Assistant: Shabnam Ataee

June 2021

Data Set

Data Set

- Description. The goal of this project is to verify the impact of pesticides and soil care products on the health and quality of vineyard soils in Switzerland.
- Data Set. The following vineyard soil samples are available:
  - *104 soil samples in 2015*
  - *73 soil samples in 2016*
- For each soil sample, there exists
  - *2683 features as input variables*
    - Available in CSV files *'ProtistAmpliconSequenceVariants_ASV_2015.csv' & 'ProtistAmpliconSequenceVariants_ASV_2016.csv'*
  - *'Cu_mg_kg' as target (output variable)*
    - Available as a column in CSV files *'Env_2015.csv' & 'Env_2016.csv'*
  - The first column in all CSV files is considered as *index*.

- Note. *The provided data is confidential.*

Data Set (Cont.)

- Train Set. We consider data set in 2015 as train set.
- Test Set. We consider data set in 2016 as test set.

- The values of target variable *'Cu_mg_kg'* are float numbers. This is a *regression problem by default*. In this project, we ask you to convert it into a *classification problem with 4 different classes* in such a way that the values of *'Cu_mg_kg'* in the train set are *equally distributed* between these four classes.

Problem

Overall Problem

Question 1. What are *the most relevant features* (Feature Selection) in this classification problem?

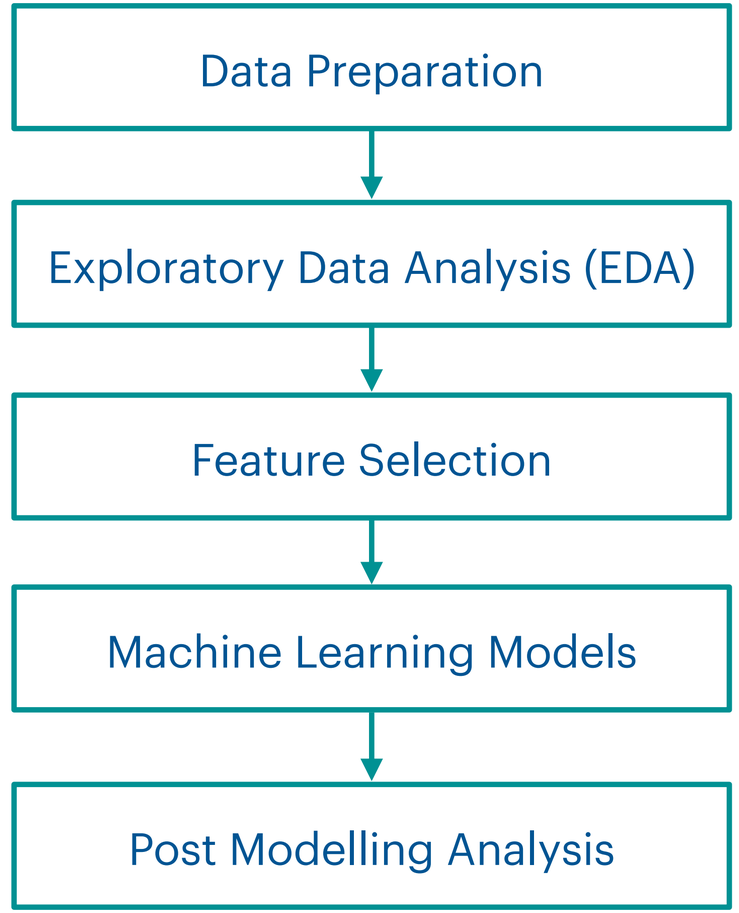
Question 2. How could we predict *class of 'Cu_mg_kg'* in *vineyard soil samples* in 2016 using *interpretability-oriented machine learning (ML)* models?

- Note. This problem is a *classification problem*.

Pipeline

Pipeline

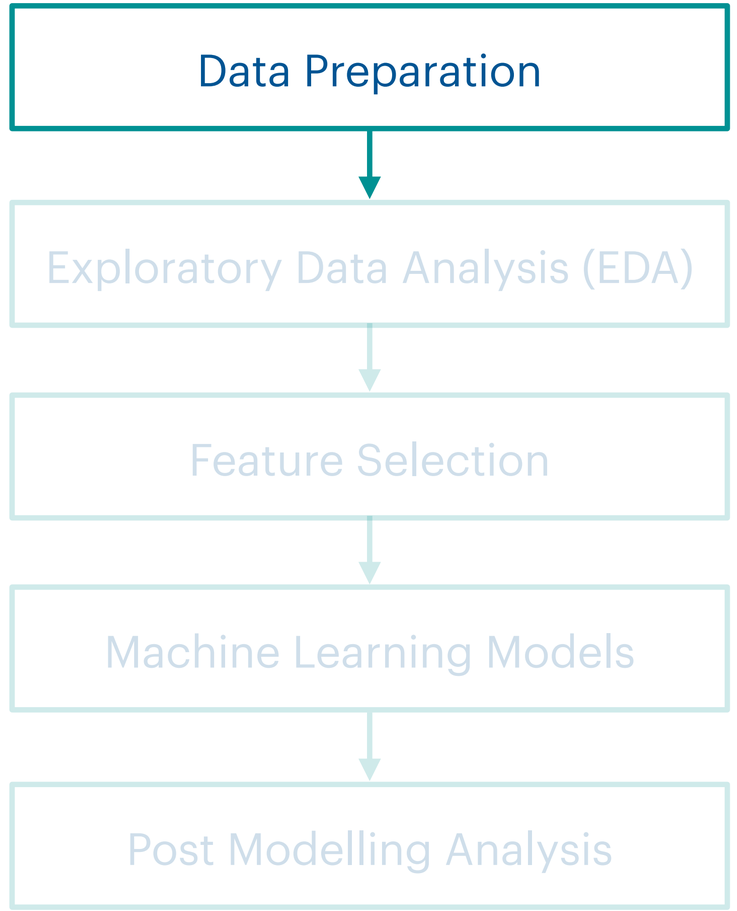
- Follow the proposed pipeline to solve this classification problem.



Data Preparation

Data Preparation

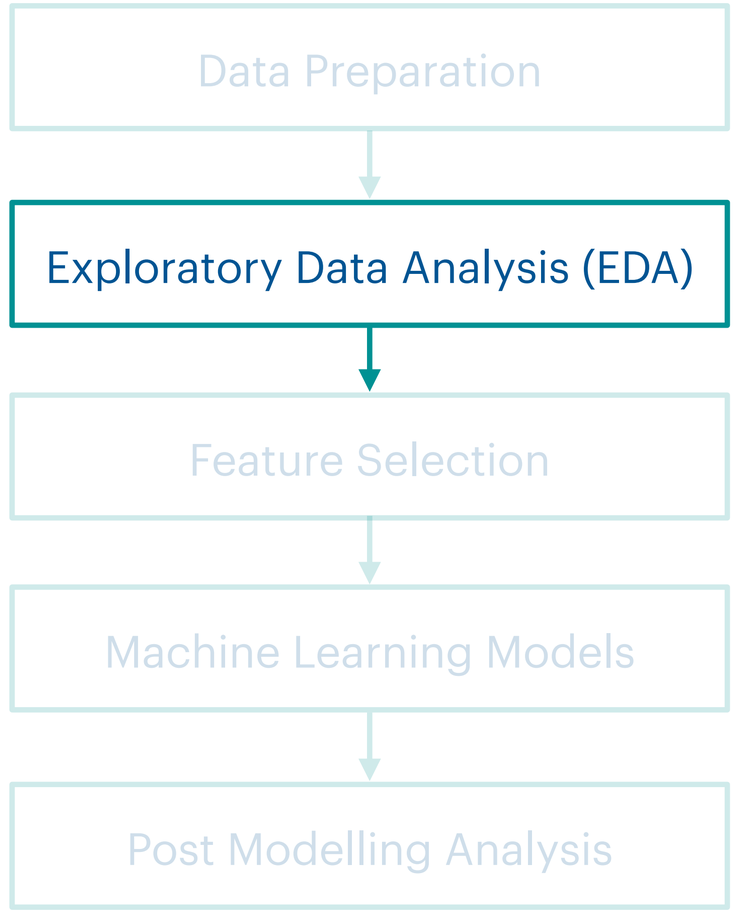
- Data Preparation is composed of *formatting* and also *cleaning* data from *missing values* and *outliers*. Prepare data for the next steps.
- The values of *'Cu_mg_kg'* are float numbers. Convert this regression problem into a *classification problem with 4 different classes* in such a way that the values of *'Cu_mg_kg'* in the train set are *equally distributed* between these four classes.



Exploratory Data Analysis (EDA)

Exploratory Data Analysis (EDA)

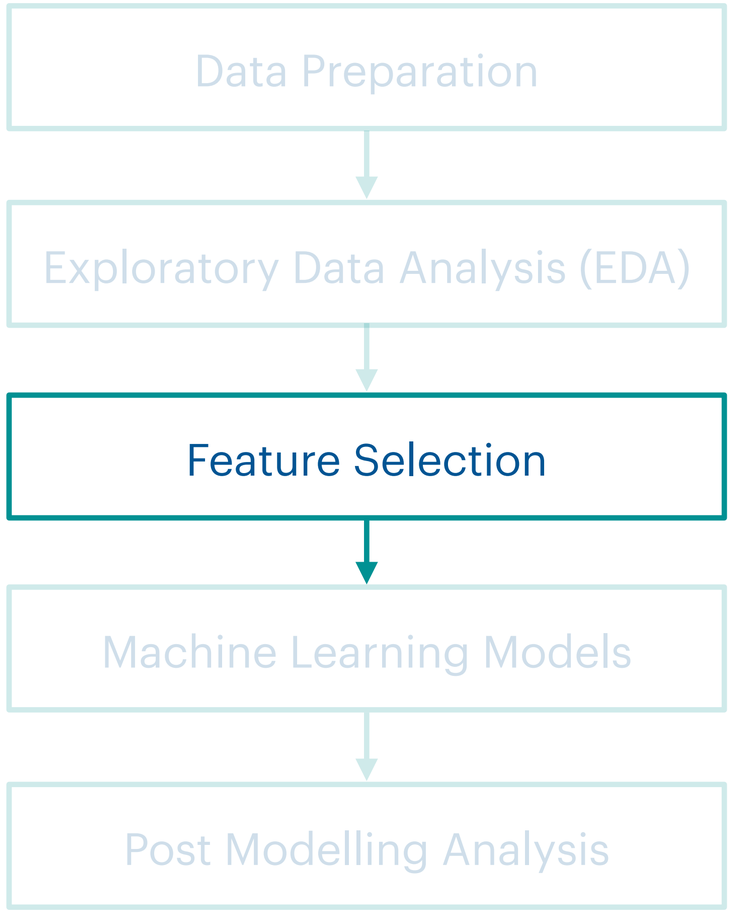
- Do some kind of Exploratory Data Analysis (EDA) to become more familiar with the given data sets.



Feature Selection

Feature Selection

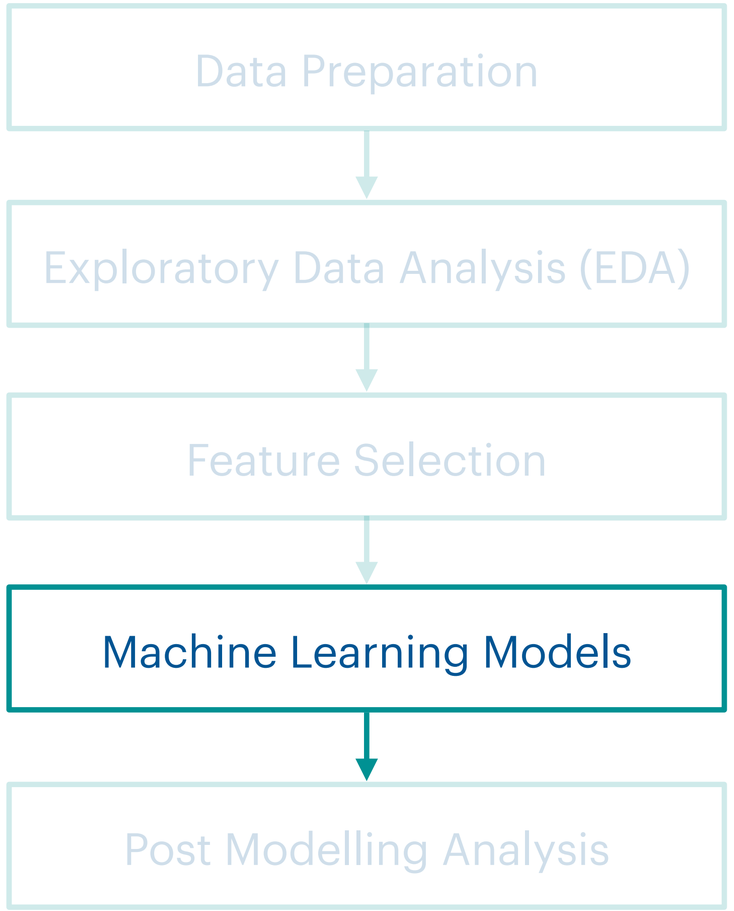
- Use a Feature Selection technique to select a subset of features
  - *Size(selected_features) should be between 100 and 200. (i.e., one order of magnitude reduction)*



Machine Learning Models

Interpretability-Oriented Machine Learning Models

- Use *one baseline* and *two different interpretability-oriented machine learning models* to solve this regression problem.
  - *Baseline*
  - *Model A*
  - *Model B*
- At least in one of the proposed models, use *grid search* to tune hyper-parameters.



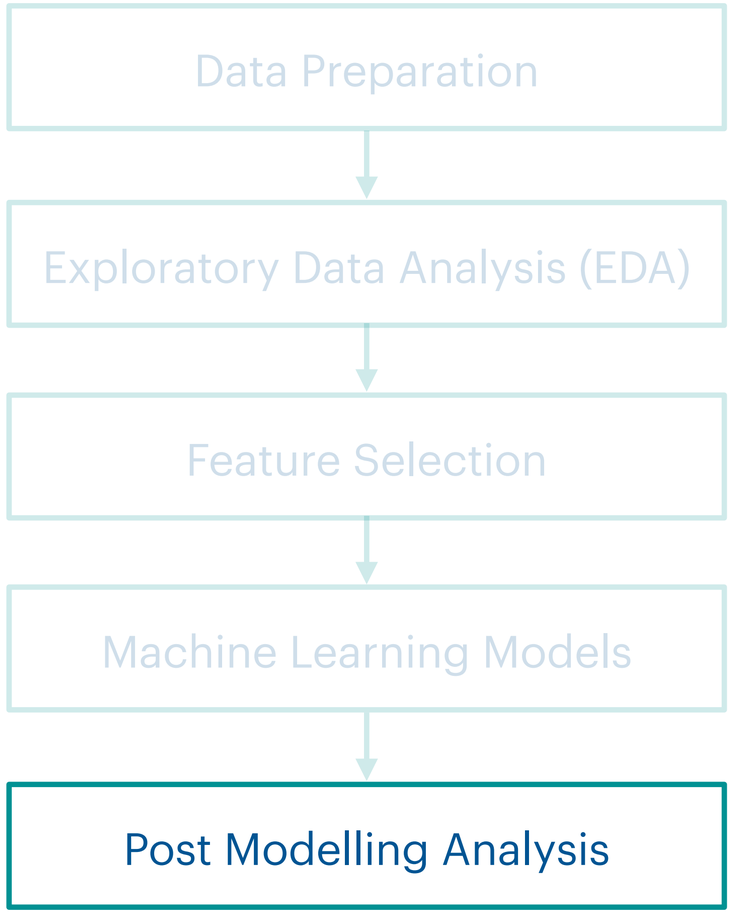
Evaluation Metrics

- For each model, calculate the following evaluation metrics on the test set:
  - Accuracy
  - Recall
  - Precision
  - F1-Score

Post Modelling Analysis

Post Modelling Analysis

- In Post Modelling Analysis,
  - Compare the different models in terms of *performance* and *interpretability*.
  - Analyse the *trade-off* between performance and interpretability.
  - Select one model that you consider as the best one and analyse it carefully.



Optional Section with Bonus

Optional Section
with Bonus

- Consider this problem as a regression problem and repeat the last two phases of the pipeline *(Machine Learning Models & Post-Modelling Analysis)* to solve this regression Problem.
- *Mean-Absolute-Error (MAE)* is a metric to evaluate the performance of regression models. It is the mean of the absolute values of each prediction error on all instances of the test set.
  - For each model, calculate *MAE* on test set.

* Bonus: Up to 0.5 additional points in your worst note (Labs average, Test 1, or Project)