PRAGUE UNIVERSITY OF ECONOMICS AND BUSINESS

FACULTY OF FINANCE AND ACCOUNTING

Department of Banking and Insurance

Application of Machine Learning Algorithms within Credit Risk Modelling

Master's thesis

Author: Bc. Petr Nguyen

Study program: Banking and Insurance & Data Engineering

Supervisor: prof. PhDr. Petr Teplý, Ph.D.

Year of defense: 2023

Declaration of Authorship

I, as an author, hereby declare that I wrote and compiled the Master's thesis *"Application of Machine Learning Algorithms within Credit Risk Modelling"* independently, using only the resources and literature listed in bibliography.

25th May 2023, Prague

Petr Nguyen

Abstract

The abstract should concisely summarize the contents of a thesis. Since potential readers should be able to make their decision on the personal relevance based on the abstract, the abstract should clearly tell the reader what information he can expect to find in the thesis. The most essential issue is the problem statement and the actual contribution of described work. The authors should always keep in mind that the abstract is the most frequently read part of a thesis. It should contain at least 70 and at most 120 words (200 when you are writing a thesis). Do not cite anyone in the abstract.

Keywords: machine learning, data science, credit risk, probability of default, loans, mortgages

Abstrakt

Nutnou součástí práce je anotace, která shrnuje význam práce a výsledky v ní dosažené. Anotace práce by neměla být delší než 200 slov a píše se v jazyce práce (tj. česky, slovensky či anglicky) a v překladu (tj. u anglicky psané práce česky či slovensky, u česky či slovensky psané práce anglicky). Anotace práce by neměla být delší než 200 slov a píše se v jazyce práce (tj. česky, slovensky či anglicky) a v překladu (tj. u anglicky psané práce česky či slovensky, u česky či slovensky psané práce anglicky). V abstraktu by se nemělo citovat.

Klíčová slova: machine learning, data science, kreditní riziko, pravděpodobnost defaultu, úvery, hypotéky

Acknowledgments

I, as an author, would like to express my deepest gratitudes and thanks to my supervisor prof. PhDr. Petr Teplý, Ph.D. for his help and significant advices throughout my thesis. Last but not least, I would like to also thank to my family for an enormous support during my studies.

Contents

List of Tables

List of Figures

Acronyms

ML Machine Learning

PD Probability of Default

AUC Area Under the Curve

LR Logistic Regression

RF Random Forest

GB Gradient Boosting

MLP Multi-Layer Perceptron

DT Decision Tree

KNN K–Nearest Neighbors

ADASYN Adaptive Synthetic Sampling

WoE Weight–of–Evidence

Chapter 1

Introduction

TBD

This document serves two purposes. First, it is a template and example for a master's thesis. Second, the text in all sections contains some useful information on structuring and writing your thesis.

The introduction should consist of three parts (as paragraphs, not to be structured into multiple headings): The first part deals with the background of the work and describes the field of research. It should also elaborate on the general problem statement and the relevance. The second part should describe the focus of the thesis, typically the paragraph starts with a phrase like "The objective of this thesis is ...." The last part should describe the structure of the thesis, for instance in the following manner. The thesis is structured as follows: Chapter 2 cites some formal requirements of the faculty and the frequently asked questions about the template, Chapter 3 gives some hints on basic formatting features and covers also acronyms, figures, boxes and tables. Chapter 4 gives a recommendation on the usage of hyphens in English language in LaTeX and explains how to use the itemize and quote environments and shows a few enumerate-based environments. Chapter 5 presents a checklist of common mistakes to avoid. **??** contains numerous hints. Chapter 6 summarizes our findings.

Chapter 2

Theoretical Background

2.1 Credit Risk

TBD

2.1.1 Regulation

TBD

Basel III

TBD

IFRS 9

TBD

2.1.2 Credit Scoring

TBD

Application Scoring

TBD

Behavioral Scoring

TBD

2.2 Machine Learning Terminology

In order to avoid confusion and ensure clear understanding in this thesis, it is necessary to provide precise definitions for machine learning terminology that may be easily confused with statistical terminology due to their similar meanings but different naming conventions.

- **Target variable** - Dependent variable, output variable or response variable, which we want to predict or classify (Y). In this case we want to predict a defaut status (Yes or No).
- **Feature** - Predictor, attribute, independent variable or explanatory variable (X), which we want to use to predict the target variable Y. In tabular data, one feature is represented by one column.
- **instance** - Observation, example, record, data point, case or a row in tabular data.
- **Training** - Fitting process, learning process or estimation of the model's parameters using the training data.
- **Weights** - Coefficient or parameters learnt during the training process.
- **Supervised Learning** - Process reflecting the abilty of an algorithm to generelize knowledge from the data having with target or label cases, so that the algorithm can be used to predict new (unlabelled) cases (Alloghani *et al.* 2020). In other words, the learning process is supervised by the target variable, hence the output model can be used to predict the target variable for new data, either using classification (when having categorical target variable) or regression (when having continuous target variable).
- **Cross–validation** - When being limited by the small dataset size, the data is split the data into k folds (subsets) and the model is trained k times, each time on $k-1$ folds and validated on the remaining fold, in order to btain reliable estimates of the model generalization error (Tatsat *et al.* 2020).

- **Overfitting** - Situation, when the model has small error during the training, but also a high tet error (Forsyth 2019). The model is too complex just purely memorizes the data on which is trained on, but cannot generalize and predict well on unseen data.

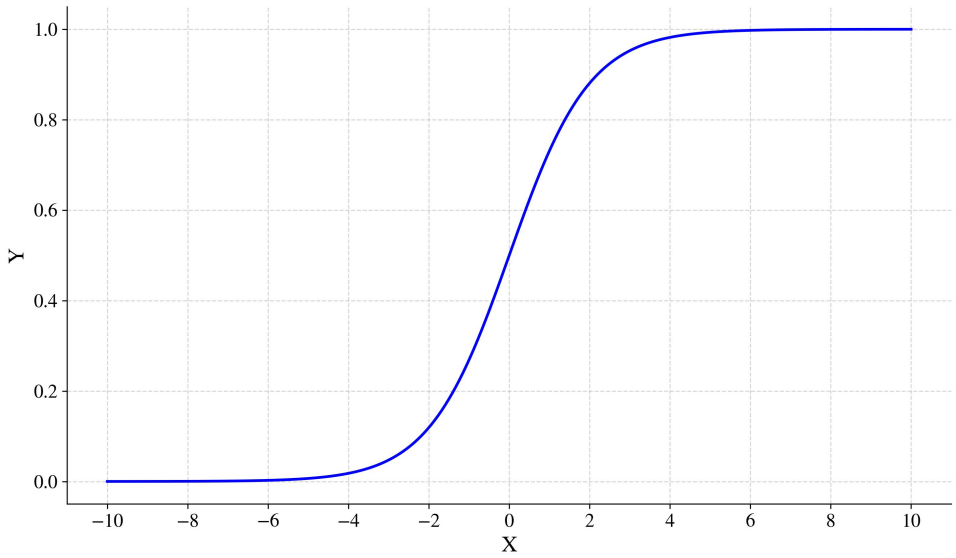
2.3 Algorithms

In this section, several algorithms, which are used in the machine learning implementation, are described. Since the goal is to predict whether or not given client will default, henceforth only (binary) classification algorithms as a part of the supervised learning are described. In other words, regression models and unsupervised learning algorithms are out of the scope of this thesis.

2.3.1 Logistic Regression

Despite the algorithm's name, it is actually not a regression but rather a classification model. In contrast, a linear regression's target variable is continuous whereas regarding a logistic regression, the target variable is categorical (or rather dichotomous in case of binary classification) (Wendler & Gröttrup 2021). For the probability estimation it is using a logistic, or so-called sigmoid function, which maps any real value within the range of 0 to 1 and takes a S-shaped curve as can be seen in Figure 2.1.

Figure 2.1: Logistic function



Source: Author's simulation in Python

The linear form of the logistic regression with n features can be written as:

$$\ln\left(\frac{P}{1-P}\right) = \beta_0 + \sum_{i=1}^{n} \beta_i X_i \tag{2.1}$$

where P is the probability of the occurred event, conditional on the set of given features. Let us denote $Y = 1$ as an observed target instance where the event occurred (e.g., default), then:

$$P = \Pr(Y = 1 \mid X) \tag{2.2}$$

Therefore, the term within the natural logarithm are the odds or more particularly, the ratio of the probability of the event with respect to the probability of non-event, both conditional on the same set of given features.

$$\begin{aligned} \frac{P}{1-P} &= \frac{\Pr(Y = 1 \mid X_1, X_2, \ldots, X_n)}{1 - \Pr(Y = 1 \mid X_1, X_2, \ldots, X_n)} \\ &= \frac{\Pr(Y = 1 \mid X_1, X_2, \ldots, X_n)}{\Pr(Y = 0 \mid X_1, X_2, \ldots, X_n)} \end{aligned} \tag{2.3}$$

Referring to the previous equations, solving for P, henceforth we get a final equation for computing the probability of occurred event with usage of logistic regression:

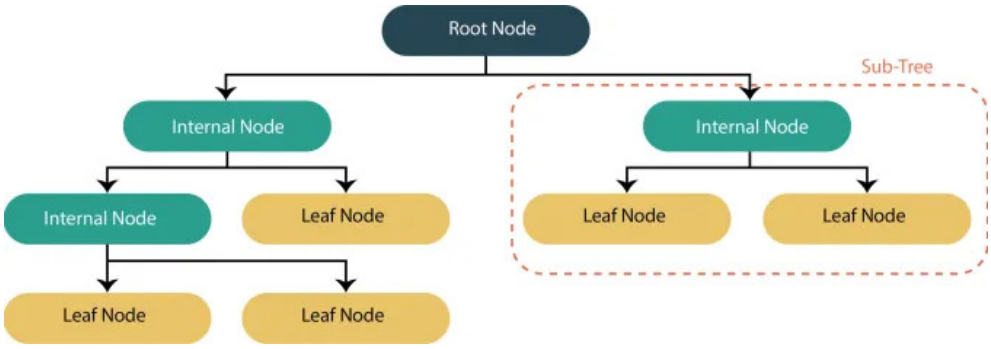
$$P = \frac{1}{1 + e^{-\left(\beta_0 + \sum_{i=1}^{n} \beta_i X_i\right)}} \tag{2.4}$$

2.3.2 Decision Tree

Decision tree (DT) is a rule–based algorithm which aims to partition the data into smaller and more homogeneous subsets. Such tree contains nodes, which are also visualized in Figure 2.2, namely:

- Root node - the topmost node of the tree where the splitting begins.
- Internal node - the non–terminal nodes as a result of the split and can be further split into another subsets.
- Leaf node - the terminal nodes as a results of the split and cannot be further split into another subsets.

Figure 2.2: Decision Tree's Nodes



Source: (Gauhar 2020)

The splitting process is based on the homogeneity or so called purity of the node with respect to the target variable (Provost & Fawcett 2013). In other words, we want to have the node as pure as possible which means that the node should contain as high proportion of one class as possible. In this case, the node should either contain high proportion of defaulters or non–defaulters, respectively. Such splitting processs starts from the root node and continues until the leaf nodes are pure enough or until the stopping criteria are met. The stopping criteria can be either a maximum depth of the tree, minimum number of observations within the node or minimum number of observations within the

leaf node. One way to measure impurity is using Entropy which ranges from 0 to 1 and is defined as:

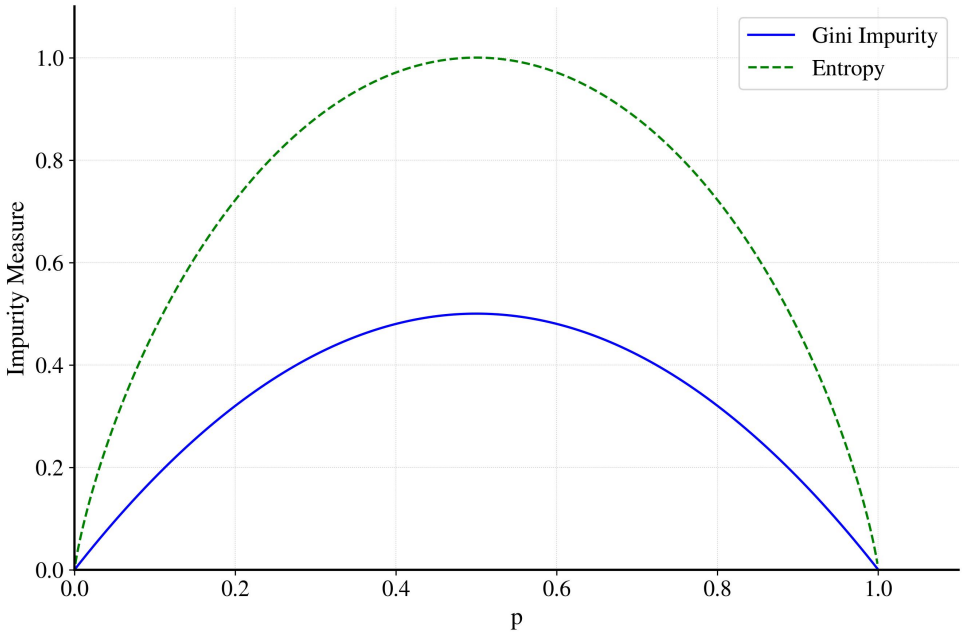
$$E = -\sum_{i=1}^{n} p_i \log_2 (p_i) \tag{2.5}$$

where p_i is the probability of the occurrence of the event i, or in other words, it is a fraction of the observations belonging to the class i within given node. In credit risk modelling terms, it is a proportion of defaulters within given node and $1 - p_i$ is a proportion of non–defaulters within given sample. The lower Entropy value, the purer the node is, i.e., the more homogeneous the subset is, where the frequency of one class is dominant to other class. Therefore, the goal is to minimize the Entropy value since we want to have the purest nodes as possible, i.e., the nodes where is either a high proportion of defaulters or non–defaulters. However, the Entropy is not the only way to measure the impurity of the node. Another way is using Gini Impurity which ranges from 0 to 0.5 and is defined as:

$$G = 1 - \sum_{i=1}^{n} p_i^2 \tag{2.6}$$

Both impurity measures are depicted in Figure 2.3 which we want to both of them minimize. Thus, we choose such feature and such rule which result in the lowest impurity measure. Such process is repeated until the stopping criteria are met or until the leaf nodes are pure enough.

Figure 2.3: Gini Impurity vs. Entropy



Source: Author's simulation in Python

After the training, the DT predicts the target variable based on the rules which are stored in the tree. The prediction process starts from the root node and continues until the leaf node is reached. Within the leaf node, the prediction can be either the most frequent class within the node or the probability of the occurrence of the event, i.e., the proportion of defaulters within given node.

2.3.3 Naive Bayes

Naive Bayes is a classification and probabilistic machine learning algorithm which is based on the Bayes theorem:

$$\Pr(C = c \mid E) = \frac{\Pr(C = c) \times \Pr(E \mid C = c)}{\Pr(E)} \tag{2.7}$$

where:

- $\Pr(C = c \mid E)$ is the posterior probability which is the probability that the target variable C takes on the class of interest c after taking the evidence E.
- $\Pr(C = c)$ is the prior probability of the class c is the probability we would assign to the class c before seeing any evidence E.
- $\Pr(E \mid C = c)$ is the probability of seeing the evidence E conditional on the given class c.
- $\Pr(E)$ is the probability of the evidence E.

With regards to the binary classification, we can substitute Y as a target variable instead C, and set of features X which will refer to the set of evidence E., henceforth the probability of Y using the Naive Bayes algorithm can be mathematically expressed as:

$$\Pr(Y \mid X) = \frac{\Pr(Y) \times \Pr(X \mid Y)}{\Pr(X)} \tag{2.8}$$

One of the assumptions of this algorithm is the conditional probabilistic independence among the features. Since all the X features' values combinations do not have to appear at all, we assume their independence (Cichosz 2014).

Therefore, instead of computing the probability of all features together, conditional on the class event, for each feature X we the conditional joint probability of X given the class event. Hence:

$$\Pr(X \mid Y) = \prod_{i=1}^{n} \Pr(X_i \mid Y) \tag{2.9}$$

Furthermore, the second adjustment is applied to the denominator of the Bayes theorem, i.e., $\Pr(X)$ - since such probability is constant over all the values of the class event, we can omit it from the equation. Therefore, the probability of the class event Y can be expressed as:

$$\Pr(Y \mid X) = \prod_{i=1}^{n} \Pr(X_i \mid Y) \times \Pr(Y) \tag{2.10}$$

During the training process, the Naive Bayes algorithm computes $\Pr(Y)$ and $\Pr(X \mid Y)$ for each class event Y and each feature X. In terms of default status, it calculates the proportion of defaulters $\Pr(Y = 1)$ and non–defaulters $\Pr(Y = 0)$ within given training sample as well as the proportion of defaulters and non–defaulters within given feature X.

When it comes to the predictions or classification of new instances, we use the trained Naive Bayes model, i.e., the computed probabilities $\Pr(Y)$ and $\Pr(X \mid Y)$ for both default and non–default class. Specifically, based on the new instance's features X, we determine the computed $\Pr(Y)$ and $\Pr(X \mid Y)$ for both classes and aftewards, as a predicted class, we choose such class with the highest posterior probability. In general, the prediction while maximizing posterior probability is given as:

$$\Pr(Y \mid X) = \text{argmax}_{y \in Y} \Pr(X \mid Y = y) \times \Pr(Y = y) \tag{2.11}$$

Specifically, in terms of binary classification for prediction of given class, whether it is default or non–default, we can compute the probability of the default event (1) and non–default event (0) and choose the class with the higher probability.

$$\Pr(Y \mid X) = \max\left(\Pr(Y = 1 \mid X), \Pr(Y = 0 \mid X)\right) \tag{2.12}$$

where:

$$\Pr(Y = 0 \mid X) = \Pr(Y = 0) \times \prod_{i=1}^{n} \Pr(X_i \mid Y = 0) \tag{2.13}$$

respectively:

$$\Pr(Y = 1 \mid X) = \Pr(Y = 1) \times \prod_{i=1}^{n} \Pr(X_i \mid Y = 1) \tag{2.14}$$

This algorithm works well if the features are categorical. However, most of the datasets contain continuous features as well. Therefore, we introduce **Gaussian Naive Bayes** algorithm which is suitable for continuous features. Such algorithm assumes that the features follow Normal (Gaussian) distribution, given the class label (Jahromi & Taheri 2017). Assuming the class event $Y = 1$, we can derive probability density function of particular value x of the continuous feature X as:

$$\Pr(X = x \mid Y = 1) = \frac{1}{\sqrt{2\pi\sigma^2_{X|Y=1}}} \exp\left(-\frac{\left(x - \mu_{X|Y=1}\right)^2}{2\sigma^2_{X|Y=1}}\right) \tag{2.15}$$

where $\mu_{X|Y=1}$ and $\sigma_{X|Y=1}$ is the mean and variance of X, respectively, given the the class event $Y = 1$.

2.3.4 K-Nearest Neighbors

The goal of K-nearest Neighbors algorithm (also known as KNN) is to find k instances that are most similar to particular instances y in the n-dimensional space, where n is the number of features. The principle of this algorithm consists in the similarity between the instances as it assumes that the similar instances are close to each other. Based on the predetermined k neighbors, it will predict the class based on the k nearest instances.

There are several ways how to measure the distance. The most used one is the Euclidean distance. Geometrically, it is a straight line between the two points and within two-dimensional space, it can be derived from the Pythagorean theorem, where the hypotenuse is the straight line measuring the distance. In the n-dimensional space, we take the sum the squared differences between the data points x and y, underneath the square root in order to compute the total Euclidean distance.

$$d_{Euclidean}(x, y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2} \tag{2.16}$$

Other distance measure is the Manhattan distance measure, which is known as a city block distance, referring to the real-life problems, more particularly in order to reach particular destination, we have to take the path in between the blocks. Mathematically, it is similar to the Euclidean distance, but instead of squared differences, it sums the absolute differences between the data points.

$$d_{Manhattan}(x, y) = \sqrt{\sum_{i=1}^{n} |x_i - y_i|} \tag{2.17}$$

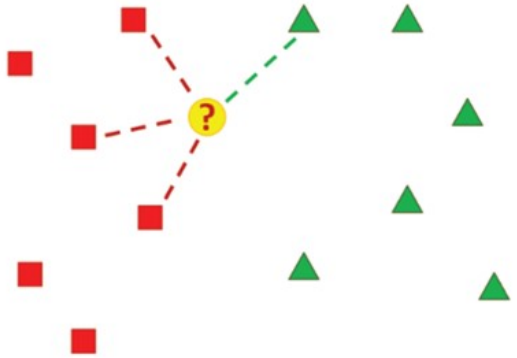
The last measure is the Minkowski distance which is the generalized form Euclidean or Manhattan distance respectively. It depends on p which represents the order of the norm. Hence, the Euclidean distance has the second order of the norm, whereas Manhattan distance has the first order of the norm.

$$d_{Minkowski}(x, y) = \sqrt[p]{\sum_{i=1}^{n} |x_i - y_i|^p} \tag{2.18}$$

Within the training process, KNN memorizes training instances and afterwards when it encounters a new instance, it tries to search for such training instance(s) which most strongly resembles the new instance (Witten *et al.* 2011). Therefore, After the training process, when it comes to the prediction, the KNN compares the new instance to the training instances, calculates the distances between the the new input and the training instances, and predicts the class based on on the majority voting within the k nearest neighbors, or predicts the probability scores as the fraction of positive instances within the k nearest neighbors.

On the following Figure 2.4, let us consider 2–dimensional space and that k is equal to 4, hence we are looking at four nearest neighbors for such new instance. Further, let us consider two classes - red squares and green triangles. By looking at the four nearest neighbors, we can observe that three out of the nearest neighbors are the red triangles. Therefore, when applying majority voting, KNN would predict such instance as a red triangle, or would predict a probability score of 0.75 for the red triangle.

Figure 2.4: K-Nearest Neighbors with $k = 4$



Source: (Mucherino *et al.* 2009)

2.3.5 Random Forest

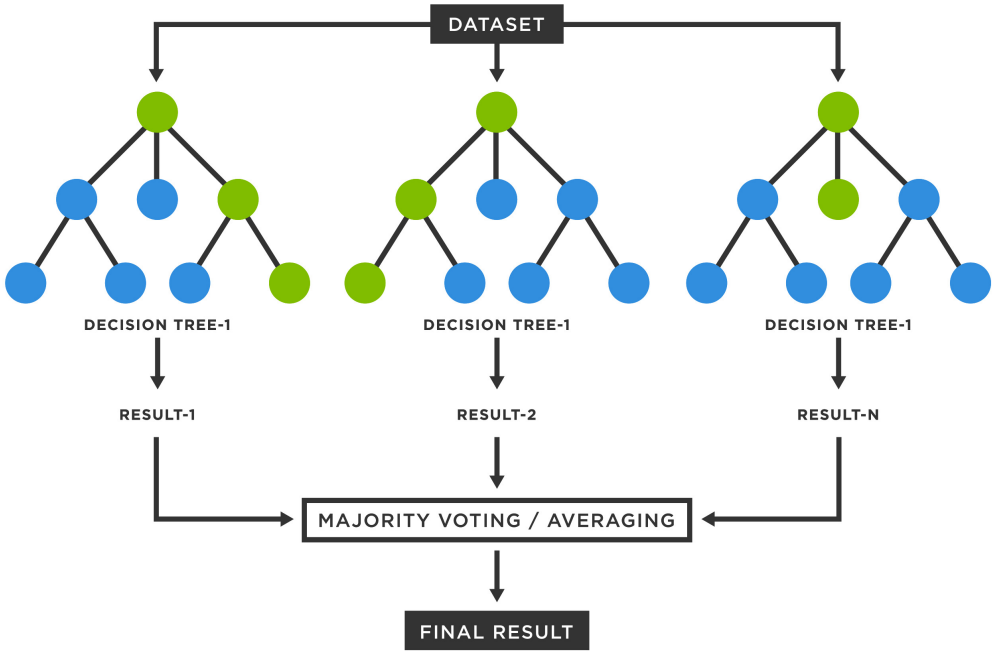
Random forest is an ensemble algorithm which is a collection of decision trees where each tree is independently trained on on a bootstrap sample of the training data (Han *et al.* 2011), i.e., on a on a set which is randomly sampled from the training data with replacement which has the same size as the training data. In such way, each bootstrap sample is unique and can contain duplicates of the original data or does not have to contain all the original data. Another aspect of randomness in such algorithm, particularly in the variability within trees, is the number of features considered for the split at each node. Instead of considering all the features of the length M, it randomly selects a subset of features of the length m (where $m < M$) and chooses the best split from the subset. The training process of individual decision tree is the same as described in Subsection 2.3.2.

Within classifying new instances, the random forest algorithm predicts the class based on the majority voting of the individual decision trees or predicts a probability as an average of the probabilities of the individual decision trees (Malley *et al.* 2011), thus:

$$\Pr\left(Y = 1 \mid X\right) = \frac{1}{B} \sum_{b=1}^{B} \Pr\left(Y = 1 \mid X, T_b\right) \tag{2.19}$$

where B is the number of trees and T_b is the b-th tree. Such algoritm is depicted on the Figure 2.5 for the visual representation.

Figure 2.5: Random Forest Diagram



Source: (TIBCO-Software 2023)

2.3.6 Gradient Boosting

In contrast to Random Forest whose trees are trained independently, i.e., in a parallel way, Gradient Boosting trains trees are trained in a sequential way, where each tree is trained on the residuals of the previous tree (Ayyadevara 2018), as a sequential building series of dependent weak learners, i.e., decision trees, in order to create a strong learner.

According to Dias (Dias *et al.* 2018), before adding any weak learners, first we need to initialize a model $F_0(x)$ which is a constant value computed by minimizing the sum of the loss function L over all training samples, i.e., we look for such γ constant which minimizes the loss function L, hence:

$$F_0(x) = \arg\min_{\gamma} \sum_{i=1}^{n} L\left(y_i, \gamma\right) \tag{2.20}$$

Then, for $m \in M$, where M is the total number of iterations or the number of tree estimators:

1. Compute pseudo–reisduals for each training sample pair (x_i, y_i) as the negative gradient of the loss function L with respect to the the prediction $F_{m-1}(x)$ of the previous model $F_{m-1}(x)$, hence:

$$r_{i,m} = -\left[\frac{\partial L\left(y_i, F\left(x_i\right)\right)}{\partial F\left(x_i\right)}\right]_{F(x)=F_{m-1}(x)} \tag{2.21}$$

2. Train a weak learner $h_m(x)$ on the with the training data as features and the pseudo–residuals as the target values $(x_i, r_{i,m})$, and then compute the learning rate γ_m which minimizes the loss function L when adding the weak learner $h_m(x)$ to the previous model $F_{m-1}(x)$, hence:

$$\gamma_m = \arg\min_{\gamma} \sum_{i=1}^{n} L\left(y_i, F_{m-1}\left(x_i\right) + \gamma h\left(x_i\right)\right) \tag{2.22}$$

3. Update the model $F_m(x)$ by adding the weak learner $h_m(x)$ with the learning rate γ_m, hence:

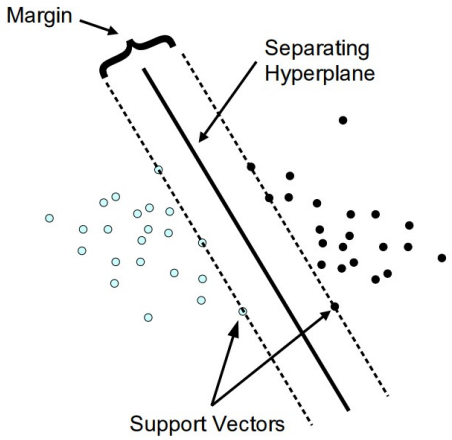
$$F_m(x) = F_{m-1}(x) + \gamma_m h(x) \tag{2.23}$$

Afterwards, such algorithm outputs the final model $F_M(x)$ as a combination of the initial model and the M weak learners.

2.3.7 Support Vector Machine

Support Vector Machine (henceforth SVM) is machine learning algorithm which can handle both linear and non–linear classification problems and tries to transform original training data into a higher dimension, where the class points are linearly separable by a (linear) decision boundary, also known as hyperplane (Han *et al.* 2011). In particular, SVM tries to maximize the margin which is the distance between the separating hyperplane and the support vectors, i.e., the training data points which are equally closest and parallel to such hyperplane (Tatsat *et al.* 2020), as shown in Figure 2.6.

Figure 2.6: Support Vector Machine 2D Hyperplane



Source: (Meyer 2015)

The hyperplane can be expressed as follows, where X are the features data, W is the vector of the weights and b is the intercept:

$$W \cdot X + b = 0 \tag{2.24}$$

Thus, the data points which lie above the hyperplane are classified as 1 and otherwise (Hsu & Lin 2002). Moreover, the distance between the hyperplane and any training data point is expressed as $\frac{1}{\|W\|}$, where $\|W\|$ is Euclidean the norm of the weight vector W. In order to maximize the margin, we maximize following term as we want to maximize both sides of below and above the hyperplane, therefore:

$$\min \frac{2}{\|W\|} \tag{2.25}$$

When the data are not linearly separable, SVM transforms the original data points into a higher dimensional space using non–linear mapping functions, also known as kernels (Han *et al.* 2011). In general, kernel function for the training tuples (X_i, X_j) can be expressed as:

$$K(X_i, X_j) = \phi(X_i) \cdot \phi(X_j) \tag{2.26}$$

where ϕ mapping function for high–dimensional transformation of the feature space. According to Patle, (Patle & Chouhan 2013) the most common kernel functions. where γ and r and d represent the kernel parameters, are:

- d–degree polynomial kernel:

$$K\left(X_i, X_j\right) = \left(1 + X_i \cdot X_k\right)^d \tag{2.27}$$

- Gaussian radial basis kernel:

$$K(X_i, X_j) = \exp\left(-\gamma \|X_i - X_j\|^2\right) \tag{2.28}$$

- Sigmoid kernel:

$$K(X_i, X_j) = \tanh(\gamma X_i \cdot X_j + r) \tag{2.29}$$

In some cases, the data cannot be linearly separable in higher dimensional space, i.e., we need to account for some potential errors, thus we introduce regularization factor C for penalizing the errors ξ, therefore, in order to maximize the margin as well as to allow for errors, we minizes the following term:

$$\min \frac{1}{2}\|W\| + C\sum_{i=1}^{N} \xi \tag{2.30}$$

Hence, by minimizing $\frac{1}{2}\|W\|$ we minimize the weights (i.e, maximize the margin), by minimizing ξ we reduce the number of training error, and by tuning C we balance between these two properties (Hsu & Lin 2002).

Note, that SVM do not predicted probability scores by default, but rather predicted classes based on the location whether the given data points are above or below the hyperplane. In order to obtain SVM's probabilities. as stated by Lin (Lin *et al.* 2007), the Platt scaling (Platt *et al.* 1999) can be applied as a surrogate model to estimate probability outputs. Particularly, it fits a logistic regression model with true labels as target variable and predictions produced by SVM as features to predict the probability scores. Hence:

$$\Pr\left(Y|f(x)\right) = \frac{1}{1 + \exp\left(A \cdot f(x) + B\right)} \tag{2.31}$$

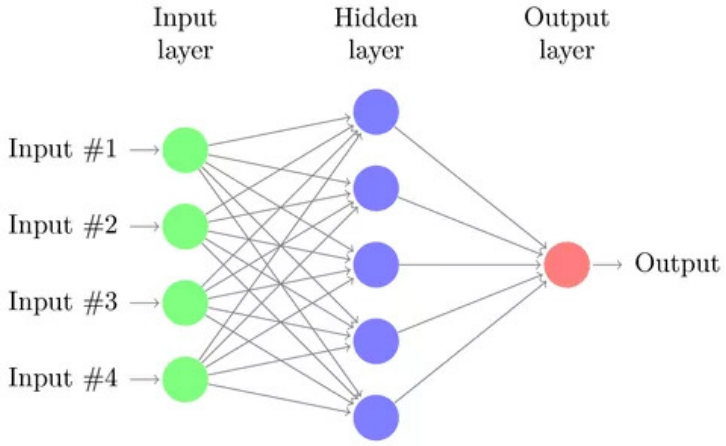
where, A and B are the coefficients of the logistic regression model.

2.3.8 Neural Network

Neural Network is a black–box machine learning algorithm which can handle very complex and non–linear relationship between. It contains several layers where each unit have a certain number of units. In general, we distinguish 3 type of layers as also visualized in Figure 2.7

- **Input layer** - The initial layer wghich contains n units, where n is the number of features within the dataset.
- **Output layer** - The final final layer which contains m units, where m is the number of classes within the target variable. Since we assume only binary classification algorithms, therefore the output layer contains only one unit.
- **Hiden layer** - The intermediate layer which is always between the two layers - either between the input and output layer or even between other hidden layers.

Figure 2.7: Neural Network Architecture



Source: (Dilmegani 2017)

The most common type of hidden layer is the fully connected layer where each unit is connected to each unit of the previous layer and to each unit in the next layer. Thus, each unit receives the inputs from the previous layer, performs the computation and feed the output to the next layer - such process is called *feed–forward*, thus feed–forward neural networks (Charu 2018). Within the receiving the inputs, let us assume an integration function g which performs a linear combination of the inputs x and the weights w, and adds a bias term b. Therefore, the ouput value z of the single unit in hidden layer is calculated as:

$$z = g\left(X, w\right) = b + \sum_{m=1}^{M} w_m x_m \tag{2.32}$$

where M indicates the number of units in the previous layer. Before the output value z is passed to the next layer, it is transformed by an activation function f

which is usually a non–linear function. The most common activation functions are:

- **ReLU** - Rectified Linear Unit (henceforth ReLU) is half–linear function which is rectified from the negative values to zero. The ReLU function is defined as:

$$f(z) = \max(0, z) \tag{2.33}$$

- **Tanh** - Hyperbolic tangent (henceforth Tanh) is another widely used non–linear activation function which reminds of the sigmoid function. The Tanh function is limited to the range between -1 and 1, and is defined as:

$$f(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \tag{2.34}$$

- **Sigmoid** - The logistic function was already described in Subsection 2.3.1. Such function is usually used in the last hidden layer before the output layer as it maps the output to the range between 0 and 1, i.e., the predicted probability for binary classification. In terms of z, the sigmoid function is defined as:

$$f(z) = \frac{1}{1 + e^{-z}} \tag{2.35}$$

The training of neural network is an iterative process, where within each iteration (also called as epoch), the neural network is fed with the input, pass through the (hidden) layers to the output. The output is then compared with the actual value and the error is calculated. Here comes another property of neural network which is the back–propagation, which updates all the weights and biases starting from the last layer by a small amount until the error is minimized as much as possible (Ayyadevara 2018). The error is then back-propagated through the network and the weights are updated. The process is repeated until the error is minimized.

2.4 Evaluation Metrics

This section focuses on particular measures through which it is possible to determine a predictive power of model in terms of its performance. The are

many ways, how to evaluate the model's performance, therefore, only the most common ones and the most relevant are further described. Note, since default prediction regards classification tasks, therefore regression's evaluation metrics are omitted. If not stated otherwise, the higher metric measure, the better the model's performance is.

2.4.1 Confusion Matrix and Derived Metrics

Confusion matrix is a table which summarizes the classification model's performance with respect to the actual classes and predicted classes. It is a square $n \times n$ matrix, where n determines number of classes within the target variable. Let us denote the confusion matrix as $C(f)$ for classification algorithm f. Its elements can be denoted as $c_{i,j}$ where i and j refer to the row and column indices, respectively, or more particularly, i refers to the actual class and j to the class predicted by the classifier f. Each element of the confusion matrix refers to the number of instances corresponding to actual class i and predicted class j (Japkowicz & Shah 2011). For instance, the element $c_2, 1$ would refer to the number of instances which have the actual class 2 but have been classified as class 1. Mathematically, the confusion matrix can be written as following:

$$C = c_{i,j} = \sum_{l=1}^{m} [(y_l = i) \wedge (f(x_l) = j)] \tag{2.36}$$

Or either in matrix form as:

$$C_{i \times j} = \begin{bmatrix} c_{1,1} & c_{1,2} & \cdots & c_{1,j} \\ c_{2,1} & c_{2,2} & \cdots & c_{2,j} \\ \vdots & \vdots & \ddots & \vdots \\ c_{i,1} & c_{i,2} & \cdots & c_{i,j} \end{bmatrix} \tag{2.37}$$

From the given matrix, the diagonal elements represent the numbers of correctly classified instances, whereas the non-diagonal elements represent the numbers of misclassified instances. Further, let us consider a binary classification - hence, the confusion matrix will have a form of 2×2.

$$C_{2 \times 2} = \begin{bmatrix} c_{1,1} & c_{1,2} \\ c_{2,1} & c_{2,2} \end{bmatrix} \tag{2.38}$$

We can this rewrite confusion matrix, assuming 2 target variable classes *Positive* and *Negative*, as:

$$C_{2\times 2} = \begin{bmatrix} TP & FN \\ FP & TN \end{bmatrix} \tag{2.39}$$

where:

- TP is the True Positive which refers to the number of instances which corresponds to the actual (*True*) class *Positive* and indeed have been correctly classified as class *Positive*.
- FP is the False Positive which refers to the number of instances which corresponds to the actual (*True*) class *Negative*, but have been incorrectly classified as class *Positive*. In the statistics and hypothesis–testing terms, it can be also called as Type 1 Error.
- FN is the False Negative which refers to the number of instances which corresponds to the actual class *Negative*, but have been incorrectly classified as class *Positive*. In the statistics and hypothesis–testing terms, it can be also called as Type 2 Error.
- TN is the True Negative which refers to the number of instances which corresponds to the actual class *Negative* and indeed have been correctly classified as class *Negative*.

Accuracy

Such metric ranges from 0 to 1 and it describes in relatives terms how many instances the model has correctly predicted. Thus, the goal is to minimize the number of False Positives and False Negatives, or in credit risk modelling terms, number of defaulters which the model has classified as non–defaulters and number of non–defaulters which the model has classified as defaulters. However, accuracy is inappropriate metric for evaluation when having imbalanced class, i.e., where the distribution of the target variable is skewed. In such case, the model can achieve a relatively high accuracy even though it is not able to predict the minority class correctly (Brownlee 2021), thus it would lead to the misleading results. This is the case of the credit risk modelling, when the loan portfolio oftenly have a lot of non–defaults and few defaults. Therefore, it is

deemed appropriate to consider other metrics when having imbalanced class.

$$Accuracy = \frac{TP + FN}{TP + TN + FP + FN} \tag{2.40}$$

Recall

Such metric is also known as True Positive Rate (TPR) or Sensitivity, which also ranges from 0 to 1, and it describes in relative terms how many actual *Positive* instances the model has correctly predicted out of all the actual *Positive* instances. Thus, the goal is to minimize the number of False Negatives, i.e., number of defaulters which the model has classified as non–defaulters. A lower value of recall could therefore indicates that either the model is not able to predict correctly the $True$ classes resulting in low number of True Positives and/or high number of False Negatives. Recall metris is useful when having imbalanced class and should be used instead of accuracy metric as it measures the model's ability to correctly identify instances of the minority class (i.e., defaults). Mathematically based on the confusion matrix elements, it can be computed as:

$$Recall = \frac{TP}{TP + FN} \tag{2.41}$$

Precision

This metric describes in relative terms how many predicted *Positive* instances are actually *Positive* out of all the predicted *Positive* instances. Thus, the goal is to minimize the number of False Positives, i.e., number of non–defaulters which the model has classified as defaulters. A lower value of precision could therefore indicates that either the model is not able to predict correctly the $True$ classes (low number of True Positives) or its prediction of $True$ classes is noisy (high number of False Positives). Precision is another metric which should be used instead of accuracy when having imbalanced class as it tt measures the model's ability to correctly identify instances of the minority class while minimizing false positives (i.e., non–default instances which the model has classified as default). Similarly, Precision also ranges from 0 to 1 and can be derived from the confusion matrix as follows:

$$Precision = \frac{TP}{TP + FP} \tag{2.42}$$

F1 Score

F1 score incorporates both Recall and Precision into a single value and takes on values between 0 and 1 as well. Is it defined as a weighted harmonic mean of these two metrics (Brabec *et al.* 2020) (where both Recall and Precision have uniform weights), and the goal is to minimize False Positives and False Negatives at the same time as within accuracy. Nevertheless, F1 score is deemed as more appropriate metric when dealing with imbalanced class as it provides more balanced evaluation of model's performance in imbalanced datasets compared to accuracy.

$$F1 = \frac{2 \times Precision \times Recall}{Precision + Recall} = \frac{2 \times TP}{2 \times TP + FP + FN} \tag{2.43}$$

Matthews Correlation Coefficient

The drawback of Recall, Precision and F1 score is they are asymmetric measures, i.e., they do not take into account the True Negatives. Therefore, such metrics' values will differ if we swap the positive and negative classes (Chicco & Jurman 2020), e.g., 1 would indicate non–default and vice versa. In order to overcome such drawback, Matthews Correlation Coefficient can be used as it is symmetric and it takes into account all the four elements of the confusion matrix as well as it captures imbalanced class issue. Methodologically, Matthews Correlation Coefficient is defined as a discretization of Pearson correlation for the case of binary variables (Boughorbel *et al.* 2017). Pearson correlation coefficient is defined as:

$$r(x, y) = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}} \tag{2.44}$$

Thus, assuming that x is the vector of True labels and y is the vector of predictions, the Matthews Correlation Coefficient can be defined as:

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}} \tag{2.45}$$

Matthews correlation coefficient ranges from -1 to 1, where 1 indicates perfect model's predictions, -1 indicates that model misclassifies all the instances and 0 indicates that model's predictions are not better than random guessing.

2.4.2 ROC Curve and AUC

ROC Curve

In order to derive Area Under the Curve (henceforth AUC), first we need to define Receiver Operating Characteristics (henceforth ROC) curve. ROC curve is two-dimensional visualization of the model performance and shows trade–off beteen True Positive Rate (TPR) and False Positive Rate (FPR) based on varying the given threshold (Han *et al.* 2011). The former metric was already described in Section 2.4.1, the latter refers to the ratio of the number of $Negative$ instances which are classified as $Positive$ to the total number of the actual $Negative$ instances, hence:

$$FPR = \frac{FP}{TN + FP} \tag{2.46}$$

In order to construct ROC curve, we need to sort the instances by the predicted probability scores and based on the given probability score, we set a threshold - what will be above the threshold will be classified as $True$ instance and what is below the threshold will be classified as $False$ instance. Thus, each probability score threshold produces a differnt confusion matrix and hence, different TPR and FPR values (Fawcett 2006). Thus, if the probability is 1, the threshold will be 1 as well and hence:

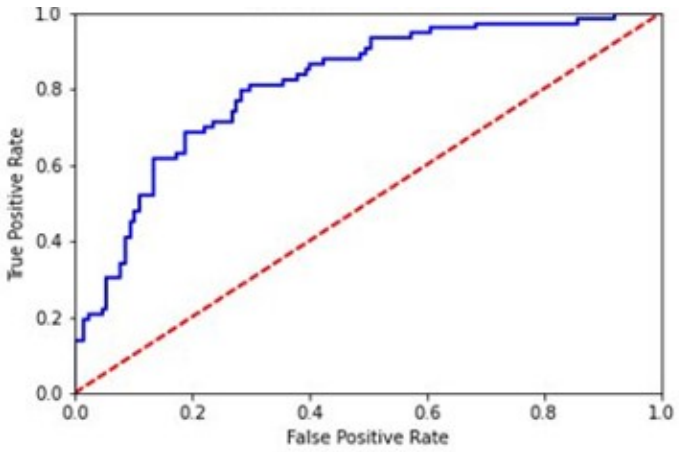
- TPR will be 0 because there is no probability which is higher than 1 and hence, everything will be classified as $Negative$ which will result into TP of 0, and subsequently into $Negative$ of 0 as well.
- FPR will be 0, too - since everything will be classified as $Negative$, therefore FP will be 0 which implies FPR to be 0, too.

On the other hand, if the probability is 0, the threshold will be 0 as well and hence:

- TPR will be 1 because there is no probability which is lower than 0 and hence, everything will be classified as $Positive$ which will result into FN of 0, and subsequently into TPR of 1.
- FPR will be 1, too - since everything will be classified as $Positive$, therefore TN will be 0 which implies FPR to be 1.

Thus, based on each threshold, the TPR and FPR will be to coordinates for single point within the graph and based on such points, we can construct the ROC curve, which can be depicted in Figure 2.8. Note that the diagonal line represents a random model which randomly guesses the *Positive* class half the time in such way, that FPR and TPR are the same, i.e., 0.5 (Fawcett 2006). Logically, a decent model should perform better than the random model, thus it the ROC curve should be above the diagonal line. Intuitively, the best possible theoretical model would have TPR of 1 and FPR of 0, meaning that all the $True$ actual classes should be predicted as $True$ and all the $False$ actual classes should not be classified as $True$ Within the ROC curve, the given curve reaches the left top corner which corresponds to the coordinates of TPR and FPR.

Figure 2.8: ROC Curve



Source: Author's results in Python.

AUC

AUC is basically the representation of ROC curve as a single number as it aggregates the performance on all possible thresholds ranging from 0 to 1. AUC can be interpreted as the probability that the randomly chosen actual $True$ instance is ranked higher than the randomly chosen actual $False$ instance (Janitza *et al.* 2013). As the AUC is an area present underneath the ROC curve, mathematically, it can be computed with the definite integral where x is the given threshold:

$$AUC = \int_0^1 TPR\left(FPR^{-1}(x)\right) dx \tag{2.47}$$

Since ROC curve is a probability curve, thus it is considering distribution

curve of TP and distribution curve of TN, separated by particular threshold - hence, TP would have probability scores above the given thresholds, whereas TN would have probability scores below the threshold. If these curves do not overlap, meaning the model can perfectly distinguish between the *Positive* and *Negative* values, therefore the AUC would be 1 and the ROC curve would reach the left top corner. However, this idealistic situation does not occur in the practice at all, but rather the two distributions are overlapping since the misclassification of the classes takes the place. The bigger overlap, the lower AUC is. If the distributions are completely overlapping, it implies the AUC of 0.5, meaning that the model cannot distinguish between the *Positive* and *Negative* classes, which is the worst scenario. On the other hand, if the distributions are totally opposite (meaning that the TP instances would have probability scores below the given threshold, whereas the TN instances would have probability scores above the given threshold), the AUC would be 0 since the model is predicting the *Positive* actual classes instead of *Negative* and vice versa (Narkhede 2018).

2.4.3 Kolmogorov-Smirnov Distance

The Kolmogorov-Smirnov (KS) Distance is non–parametric metric for assessing discriminant power of a model as it measures distance between the cumulative distribution functions (henceforth CDF) between two classes, and is quantified as a maximum vertical absolute difference between such two CDF's (Adeodato & Melo 2016). In credit risk modelling terms, we can express KS as follows:

$$\text{Kolmogorov Smirnov} = \max_{0 \leq t \leq 1} |F_D(t) - F_{ND}(t)| \tag{2.48}$$

where F_D and F_{ND} are the cumulative distribution functions of default and non-default cases, respectively, and t is the probability score threshold which ranges between 0 and 1. F_D and F_{ND} are defined as follows:

$$F_D(t) = \frac{1}{M_D} \sum_{i=1}^{M_D} I[f(x_i) \leq t] \tag{2.49}$$

$$F_{ND}(t) = \frac{1}{M_{ND}} \sum_{i=1}^{M_D} I[f(x_i) \leq t] \tag{2.50}$$

where M_D and M_{ND} refer to the number of default and non-default cases, respectively, and I is the indicator function which is equal to 1 if the condition

is true and 0 otherwise (Doumpos *et al.* 2019).

2.4.4 Somer's D

The Somers' D is a metric which is part of the Kendall family of ranking measures. Particularly, assuming X-Y pairs, a Kendall's τ_a is defined as:

$$\tau\left(X, Y\right) = \mathrm{E}\left[\mathrm{sign}(X_i - X_j)\mathrm{sign}(Y_i - Y_j)\right] \tag{2.51}$$

Equivalently, Kendall's τ_a can be defined as the difference between the probability that the two X-Y pairs are *concordant* and the probability that they are *discordant*. X-Y pair is concordant if the larger of the X values is paired with with larger of the Y values, i.e, $X_i < X_j$ and $Y_i < Y_j$. In contrast, X-Y pair is discordant if the larger of X values is associated with smaller of Y values or vice versa, i.e, $X_i < X_j$ and $Y_i > Y_j$, or $X_i > X_j$ and $Y_i < Y_j$ (Newson 2002). Therefore, Somers' D can be defined as the difference between the two conditional probabilities of concordance and discordance, given that the two X values are unequal (Newson 2014) as follows:

$$D\left(Y \mid X\right) = \frac{\tau\left(X, Y\right)}{\tau\left(X, X\right)} \tag{2.52}$$

In case of a binary classification, X values would represent *True* labels and Y values would represent predicted probability scores as rank vectors. Such metric ranges from -1 to +1 (likewise as Matthews correlation coefficient +1). Thus, the higher value of Somers' D, the model's better ability to distinguish between borrowers who are likely to default and those who are not.

2.4.5 Brier Score Loss

Methodologically, Brier Score Loss is calculated in the same way as Mean Squared Error (MSE). However, Brier Score Loss is applied to the predicted probabilities (i.e., assumes that the target variable is dichotomous) (Comotto 2022), whereas MSE is rather used in regression tasks where is no assumption regarding the continuous target variable. Henceforth, Brier Score Loss is defined as a mean squared error between the $True$ labels (y) and the predicted

probabilities ($\hat{y}$) as follows:

$$\text{Brier Score Loss} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \tag{2.53}$$

Brier Score Loss ranges from 0 to 1, where the the ideal scenario would be Brier Score Loss of 0 - in such case, the model would be perfect predictive power.

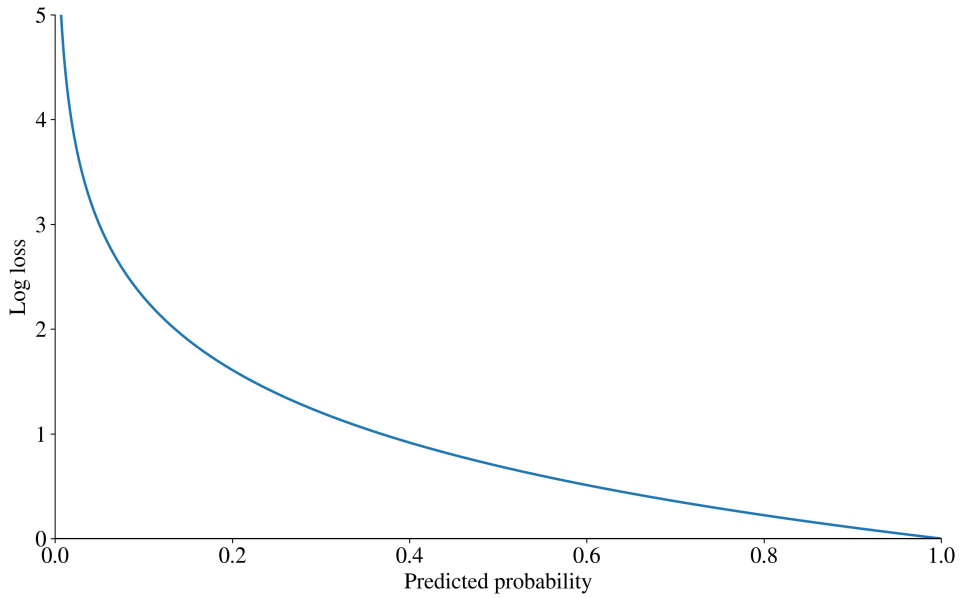
2.4.6 Log Loss

Log loss, also know as logistic loss or cross–entropy loss, is a loss function metric which takes *True* labels and predicted probabilities as an input and the minimize the difference between these two in a logarithmic function's form. Particularly, it indicates how close the predicted probabilities are to the corresponding $True$ labels. The more predicted probabilities diverges from the actual value, the more the log loss function penalizes the model's performance (Dembla 2020).

$$\text{Log Loss} = -\frac{1}{N}\sum_{i=1}^{N} y_i \ln(p_i) + (1 - y_i)\ln(1 - p_i) \tag{2.54}$$

Logically, the lower Log loss value, the better performance of the model is. As depicted in Figure 2.9, we can observe the closer the predicted probability is closer to 1 with respect to the actual target class being equal to 1, the more is the log loss function closer to 0 which is desired in terms of model's performance.

Figure 2.9: Log Loss Function when $Y = 1$



Source: Author's simulation in Python

2.5 ADASYN Oversampling

Since this thesis pertains to the dataset of defaulted loans, which target variable distribution is heavily skewed, i.e., the class is strongly imbalanced as the frequency distribution of the majority class is significantly higher than the frequency distribution of the minority class. In case of defaulted loans, the majority class would be non–default status and the minority class would be default status. This can cause serious degradation in model's performance as most of the models assume well–balanced class distributions, hence such models would be biased towards the majority class and would not be able to predict the minority class accurately (Prati *et al.* 2009).

To overcome this issue, one would use random undersampling or random oversampling to deal with the class imbalanced issue. The former randomly eliminates majority class instances whereas the latter randomly duplicates minority class instances. However, both have particular drawbacks, as the random under-sampling may lead to a a significant loss of information, and random oversampling is lead to the high degree of repetation of minority instances. Both then could lead to model's overfitting and detoriation in model's performance (He & Ma 2013). This might be a significant issue when the target

variable distribution is heavily imbalanced - assume that we have a dataset of 1,000 instances where 990 instances belongs to majority class and 10 instances to minority class. If we perform random undersampling in order to balance the target variable distribution, we would have to remove 980 instances and end up with undersampled dataset of 20 instances, which is not acceptable for model training. On the other hand, if we perform random oversampling, we would end up with 1,980 instances, where 980 instances would be the same as in the original dataset, which would lead to the model's overfitting.

Therefore, the Adaptive Synthetic Sampling (henceforth ADASYN) technique is used for oversampling the minority class. ADASYN generates synthetic instances of the minority class based on the nearest neighbors of the minority class instances. Such approach is more effective than Synthetic Minority Oversampling Technique (henceforth SMOTE) which also uses nearest neighbors to generate synthetic instances of minority class, as it generates more synthetic instances which are hard–to–learn by K-Nearest Neighbors given the density distributtions, whereby SMOTE generates synthetic instances uniformly for each minority instance. (He *et al.* 2008).

In other words, ADASYN generates more synthetic instances in regions where the density of the majority class within K nearest neighbors of minority instance is higher and fewer synthetic instances in regions where the density is lower, thereby ADASYN focuses on generating more hard–to–learn minority instances. Thereby, it makes easier for the machine learning model to learn the decision boundary between the minority and majority classes and boost the model's performance by focusing on hard–to–learn instances (He *et al.* 2008).

Before oversampling algorithm's execution, first we need to calculate the number of instances of minority class to be synthetically generated in order to balance the target variable distribution. The number of instances to be generated G is calculated as follows:

$$G = (m_l - m_s) \times \beta \tag{2.55}$$

where m_l is the number of majority class instances, m_s is the number of minority class instances and β indicates the desired ratio between the numbers of majority and minority class instances after oversampling.

Then for each minority class instance x_i, using K-nearest Neighbors with

Euclidean distance calculate the ratio r_i as:

$$r_i = \frac{\delta_i}{K} \tag{2.56}$$

where δ_i is the number of majority class instances within the K nearest neighbors of x_i. In such case, higher r_i indicates dominance of the majority class in given specific neighborhood of x_i (Nian 2018). Subsequently, all the r_i ratios are normalized as:

$$\hat{r}_i = \frac{ri}{\sum_{i=1}^{m_s} r_i} \tag{2.57}$$

In such way that sum of all the normalized $\hat{r}_i$ ratios is equal to 1. Hence, we can denote $\hat{r}_i$ as the density distribution.

$$\sum_{i=1}^{m_s} \hat{r}_i = 1 \tag{2.58}$$

Finally, the oversampling process is initialized. For each minority class instance x_i, calculate the number of instances to be synthetically generated based on the respective density distribution $\hat{r}_i$ and the total number of instances to be synthetically generated G. Thus, for the minority classes with higher density, it generates more synthetic instances, since those instances are hard–to–classify by the K-Nearest Neighbors.

$$G_i = G \times \hat{r}_i \tag{2.59}$$

Further, for each minority class instance x, generate G_i synthetic instances s_i as follows:

$$s_i = x_i + (x_{zi} - x_i) \times \lambda \tag{2.60}$$

where x_{zi} represents the radnomly chosen minority class instance within the K nearest neares neighbors for x_i, and $\lambda \in [0, 1]$ is a random number.

2.6 Optimal Binning

In the context of data preprocessing, it is crucial to consider the most appropriate feature transformation method that optimizes the performance of machine learning models. Although common approaches such as dummy encod-

ing, standardization, logarithmic transformation, and normalization are widely used, they may not always be suitable for a given dataset due to the presence of certain characteristics. For instance, dummy encoding (also known as one–hot encoding) may not be suitable for categorical features with a large number of categories as it could lead to the curse of dimensionality, therefore, it may result in the decrease of model's performance (Bera *et al.* 2021). Standardization may not be appropriate for features with a large number of outliers as it may result in a loss of information. Similarly, logarithmic transformation may not be appropriate for features with a large number of zeros, and normalization may not be suitable for features with a significant number of outliers.

Therefore, alternative approaches such as discretization or binning are increasingly being used. Binning is a categorization process to transform a continuous variable into a small set of groups or bins (Zeng 2014). This approach enables the identification of outliers within bins and reduce their impact, and additionally, it can capture missing values without requiring the removal or imputation of such values. As a result, binning is a more flexible and versatile feature transformation method that can effectively handle different types of datasets and is particularly useful in cases where other methods may not be appropriate.

In this thesis, we employ the `BinningProcess` from the `optbinning` module in Python for an optimal binning of both numeric and categorical features with respect to the target variable, developed by Guillermo Navas–Palencia (Navas-Palencia 2020). This approach involves grouping the values of a continuous variable into discrete intervals, or "bins", based on their relationship with the target variable. Similarly, for categorical features, the approach involves grouping the categories based on their relationship with the target variable. In general, the optimal binning is solved by iteratively merging an initial granular discretization until imposed constraints are satisfied. Particularly, the optimal binning process consists of two phases - pre–binning process (for generating initial granular discretization) and subsequent optimization (for satisfying imposed constraints). The former phase usually uses decision tree to generate initial split points to create pre–bins which are further merged while maximizing Information Value (also known as Jeffreys' divergence) while accounting for the constraints. (Navas-Palencia 2020) Such constraints are:

- Creation of separate bins for missing values: Since missing values can

have a significant impact on the target variable, hence is important to create a separate bin for them.

- Minimum bin size constraint - at least 5 % of the total number of instances: Such constraint ensures a bin's representativness.
- Each bin should have at least one instance of each target class: Application of such constraint allows to compute divergence measure.

Thus, the optimal binning process, the goal is the maximize discriminatory power among bins, i.e., divergence measure. For more information about optimal binning, please refer to (Navas-Palencia 2020).

After the binning process, the bins as categorical values needed to be encoded into numeric values. The most common approach in credit risk modelling is Weight–of–Evidence (henceforth WoE) encoding. The WoE is a commonly used measure of the strength of association between a binary target variable and an independent variable. According to Witzany (Witzany 2017), the WoE of categorical value c can be expressed as the change between the overal log odds ratio and the log odds ratio given the value c, hence:

$$WoE\left(c\right) = \ln\left(\Pr\left(c \mid Y = 0\right)\right) - \ln\left(\Pr\left(c \mid Y = 1\right)\right) \tag{2.61}$$

Assuming feature X and its respective bin b_i, thus $b_i \in X$, we can express WoE in terms of b as follows:

$$WoE_{X,b} = \ln\left(\frac{\Pr\left(X = b \mid Y = 0\right)}{\Pr\left(X = b \mid Y = 1\right)}\right) \tag{2.62}$$

According to Navas–Palencia (Navas-Palencia 2020), the WoE for bin i can be also computed as:

$$WoE_i = \ln\left(\frac{r_i^{ND}/r_T^{ND}}{r_i^D/r_T^D}\right) \tag{2.63}$$

where r_i^{ND} is the number of non–default instances in given bin i, r_i^D is the number of default instances in the given bin i, r_T^{ND} is the total number of non–default instances in whole sample and r_T^D is the total number of default instances in whole sample. Thus, positive WoE value is indicates larger distribution of non–defaults, i.e. higher likelihood of non–default, while negative WoE value indicates larger distribution of defaults, i.e., higher likelihood of default.

2.7 Hyperparameter Bayesian Optimization

Most of the machine learning models are configured by a set of hyperparameters which are not learned during the training process but need to be set beforehand. Such hyperparameters' values must be carefully chosen and considerably impact model's performance (Bischl *et al.* 2023). It is needed to point that the difference between parameter and hyperparameter - while paramater value is learnt during the training process from the data, on the other hand, hyperparameter value is set before the training process and cannot be learnt from the data (Owen 2022). In case of logistic regression, the parameters are estimated coefficients and intercept, while the hyperparameters are for instance regularization parameter, optimization solver etc.

Thus, it is recommended to select optimal hyperparameter values instead of relying on default hyperparameters. Nonetheless, selecting optimal hyperparameter values can be very challenging, especially when there are many hyperparameters to tune. Fortunately, in machine learning practice already exist several methods how to choose the best hyperparameters' values. The most common ones are Grid Search and Random Search. The former approach tries all the possible combinations of hyperparameters' values from predetermined hyperparameter space, which can be very computationally expensive, when the number of hyperparameters is large (Marinov & Karapetyan 2019), when the space of hyperparameter's values is too wide or when the dataset is too large. Regarding the latter approach, instead of trying al the possible combinations from the grid, it randomly selects samples of hyperparameters combinations. Although such approach can be less computationally expensive, it does not guarantee to find the global optimum. Another issue pertaining to both approach is that they do not consider any information from previous iterations and rather check all possible hyperparameter combinations or randomly select hyperparameter combinations, respectively.

The compromise for such drawbacks is hyperparameter tuning with Bayesian Optimization, which is able to find the best hyperparameters' values in less time and with less computational resources than Grid Search and also, it leads to better model's performance than Random Search despite the longer optimization time (Drahokoupil 2022). Bayesian Optimization is a hyperparameter tuning method which uses infromation from previous iterations in order to make more informed decsion about which hyperparameters' values to try next.

The main property of hyperparameter tuning is the objective function which we want to optimize (i.e., maximize or minimize in case of a score and loss, respectively), which input is the hyperparameters' values and the output is the score or loss. However, the objective function is not known beforehand and is very computionally expensive to evaluate.

Therefore, Bayesian Optimization uses a surrogate function which is the approximation and probability representation of the objective function. The most common surrogate function is the Gaussian Process (henceforth GP) which is able to produce accurate approximations as well as the uncertainty around the approximations (Wang 2020). According to Owen (Owen 2022), GP is utilized as the prior for the objective function along the posterior, which we want to update while. In other words, the prior captures the initial belief about the objective function, while the posterior is the updated distribution combining the prior belief and the observed evaluations of the objective function, i.e., it reflects the current belief about the objective function, hence the relation between the hyperparameters' values and the score or loss. GP is the generalization of the normal distribution and describes the distribution over functions (not the distribution of a random variable), hence the objective function f follows a normal distribution with noise as:

$$y = f(x) + \epsilon \tag{2.64}$$

Let us nedote, set $f_{1:n} = \{f(x_1), f(x_2), \ldots, f(x_n)\}$ as a set of n observations of the objective function, where $m(x_{1:n})$ is the mean function and K is the covariance kernel. Hence, such set follows normal distribution as well:

$$f_{1:n} \sim N(m(x_{i:n}), K) \tag{2.65}$$

Henceforht, the distribution of prediction generated by GP also follows normal distribution as:

$$p(y \mid x, D) \mid N\left(y \mid \mu^*, \sigma^{*2}\right) \tag{2.66}$$

where μ^* and σ^{*2} can by analytically derived from the K kernel, and D represents observed data regarding the previously evaluated iterions of hyperparameters' values.

Furthermore, Bayesian Optimization also employs acquisition function which accounts for which set of hyperparameters should be used in the next iteration

(Owen 2022). Particularly, the next hyperparameters' set is chosen based on the location where the acquisition function is maximized. The most common acquisition function is the Expected Improvement (henceforth EI), which is according to Owen (Owen 2022) defined as follows assuming that $\sigma(x) \neq 0$:

$$EI(x) = \left(\mu(x) - f\left(x^{+}\right)\right) \times \Phi(Z) + \sigma(x) \times \phi(Z) \tag{2.67}$$

where $\sigma(x)$ is the uncertainty, $\mu(x)$ is the expected performance which are both captured by surrogate model. $f(x^{+})$ indicates the current best value of the objective function, $\Phi(Z)$ and $\phi(Z)$ are the cumulative distribution function and probability density function of the standard normal distribution, respectively. Moreover, EI allows to balance between exploration and exploitation, where the former refers to the searching for the uknown regions where the objective function may have higher values, i.e, the hyperparameters' values which have not been evaluated yet, while the latter refers to the searching near the best observed values of the objective function, i.e.,near by the hyperparameters' values which have been evaluated already. Referring to Owen (Owen 2022), higher expected performance $\mu(x)$ compared to the current best value $f(x^{+})$ will favor the exploitation process, whereby a very high uncertainty $\sigma(x)$ will support exploration process.

2.8 Forward Sequential Feature Selection

Instead of using all the features in dataset, we use only the subset of the most relevant ones, which can further reduce the dimensionality of dataset, boost model performance, save computational resources and reduce overfitting. Such process is called feature selection and can be defined as the process of detecting the most relevant features and discarding the noisy redundant ones. (Bolón-Canedo *et al.* 2015).

With respect to the target variable, we distinguish 2 most common types of feature selection approaches: (1) filter methods and (2) warapper methods. Using the former approach, the feature selection is independent on a machine learning model itself, but rather is performed using univariate statistical tests, such as correlation measures, Chi–square test, Fisher score and others (Kaushik 2016), and chooses those ones with the highest or lowest values. This approach is used when we prefer lower computational cost and faster feature selection

process, but since it does no take into account the model itself, it does not have to able to select the features which would be optimal for particular model. Regarding the latter approach, the feature selection is based on a specific machine learning model and follows a greedy search approach by evaluating all the possible combinations of features against the evaluation metric criteria (Verma 2020). Although, such approach is very computationally expensive, it is able to select the optimal features for a particular model.

The most common wrapper method for feature selection is Recursive Feature Elimination (henceforth RFE). Such method takes a machine learning model as an base estimator, fit the model on whole set of features, computes and ranks their coefficients or feature importances, eliminates the least important features and repeats the process until the desired number of features is reached (Brownlee 2020) or until the stop criteria is met. However, the drawback of RFE is that it always requires feature importances or coefficients to compute, which is not suitable for models which do not produce any coefficients nor feature importances, such as KNN or Naive Bayes. Therefore, this approach is not implemented in this thesis.

Instead, the feature selection is performed with Sequential Feature Selection (henceforth SFS). Such method is iteratively adding (or removes) features the set sequentially. Hence, there are two approaches, Forward SFS and Backward SFS. The former approach keeps adding features to the set until the desired number of features is reached, while the latter approach starts with the whole set of features and removes them until the desired number of features is reached. In this thesis, Forward SFS is used since it was way more computationally efficient than Backward SFS within author's analysis. Forward SFS starts with an empty set of features and afterwards, variant features are sequentially added until the desired number of features is reached or until the addition of extra features does not reduce the criterion (Verma 2021). According to Scikit-learn's documentation (scikit-learn 2023a), at each stage, SFS chooses the best feature to add based on the cross–validation score.

Chapter 3

Literature Review

In this thesis, we examine the studies pertaining to machine learning applications in credit scoring, as well as studies addressing the wide range of machine learning implementations outside the credit scoring domain. The intent is to highlight certain machine learning techniques from non-credit scoring contexts that may be applicable to credit scoring and inspect whether they have positive or negative impact which will be further assessed within hypotheses testing. In the context of the studies related to machine learning in credit scoring, we inspect not only the studies focusing on the data set analyzed in this thesis, but we aksi also about the studies encompassing analyses of variety of distinct data sets. This inclusive approach is emplopyed to foster a more comprehensive and holistic understanding of the subject and to enable the identification of potentially valuable insights and methodologies that can be applied across different data sets within the credit scoring field.

It is a known fact that the distribution of the default status is imbalanced in the credit scoring domain, since the non–default cases are overpresented compared to the default cases. Several studies have already address such issue. For instance, Owusu and others (Owusu *et al.* 2023) employed ADASYN oversampling on the peer-to-peer loans data from American Lending Club, which exhibited an improvement in the model's performance in comparison to other benchmark studies. Another way to address such imbalance issue is changing the classication cut–off point. By default, the cut–off point is set to 0.5, which means that the predicted probability of default is greater than 0.5. Kazemi and others (Kazemi *et al.* 2023) demonstrated that utilization the customized cut–off points leads to a more accurate classification compared to the default

threshold value of 0.5, based on German and Australian credit data sets available to the public in the UCI machine learning data repository.

Whether to choose transparent, white–box model such as logistic regression or a complex, black–box model such as ensemble models or nerual network depends on various factors, such as type of the data set, sample size, data preprocessing techniques, hyperparameter tuning, or even a software used to implement the model. While Teplý and Polena (Teplý & Polena 2020) suggest that Logistic Regression is the best performing model on peer-to-peer loans data from Lending Club, Aniceto and others (Aniceto *et al.* 2020) demonstrate that the ensemble models, namely Random Forest and AdaBoost, outperformed the Logistic Regression on a large Brazilian bank's loan data set.

In this thesis, a dataset of US home equity loans (HMEQ) is analyzed, which is further described in Subsection 4.2.1. Regarding the studies pertaining to the HMEQ data set, the study of Aras (Aras 2021) and the study of Zurada (Zurada *et al.* 2014) are deemed to best the most relevant to this thesis.

With respect to the former study, the author performed imputation of missing values with mode and mean, respectively and for an evalutation, and used test size of size 596 instances. Author also performed an oversampling on the training set using Random Oversampling in order to balanced the default status distribution. Regarding the fitted models which are also used in this thesis, the author used KNN, Random Forest (RF), SVM, Decision Tree (DT), Gaussian Naive Bayes (GNB) and Logistic Regression (LR). Such models were also tuned using Grid Search method with 10–fold cross validation.

Within the evalutation, author assessed Accuracy (Acc.), Recall (Rec.), Precision (Prec.), F1 and Matthews Correlation Coefficient (MCC) metrics. The particular results are summarized in Table 3.1. Since the default distribution is imbalanced on the test set, the most relevant metrics are F1 and MCC. As can be seen, only three models exceeded the 0.8 and 0.75 threshold for F1 and MCC, respectively, namely KNN, RF and SVM. Whereas Gaussian Naive Bayes and Logistic Regression performed poorly as they did not even exceeded 0.5 threshold for F1 and MCC, respectively. However, it is not appropriate to compare the computed the metrics with the results of this thesis, since the test set size is different, did not performed feature selection and probably used a default classification threshold of 0.5.

Table 3.1: Evaluation Results (Aras 2021)

Model	Acc.	Rec.	Prec.	F1	MCC
KNN	0.953	0.789	0.980	0.874	0.853
RF	0.930	0.789	0.858	0.822	0.779
SVM	0.926	0.756	0.869	0.809	0.766
DT	0.898	0.683	0.792	0.734	0.674
GNB	0.795	0.480	0.504	0.492	0.364
LR	0.705	0.691	0.381	0.491	0.334

Source: (Aras 2021)

If we rank the models by each computed metric descendingly,we can explicitly derive a rank score as an average of the ranks. Based on the rank scores, we can then rank the models, as shown in Table 3.2. As can be seen, KNN dominantly outperformed all the models across all the metrics, while the black–box models such as Random Forest and SVM performed also performed well but not as well as KNN. On the other hand, Gaussian Naive Bayes and Logistic Regression performance exhibited very unsatisfactory performance. Therefore, according to Aras, it is expected that KNN and the black–box models (Random Forest and/or SVM) would perform well on the HMEQ data set.

Table 3.2: Evaluation Results - Ranked (Aras 2021)

Model	Acc.	Rec.	Prec.	F1	MCC	Score	Rank
KNN	1	1	1	1	1	1	1
RF	2	1	3	2	2	2	2
SVM	3	2	2	3	3	2.6	3
DT	4	4	4	4	4	4	4
GNB	5	5	5	5	5	5	5
LR	6	3	6	6	6	5.4	6

Source: Ranking of (Aras 2021)

The latter study pertains to the reasearch conducted by Zurada and others (Zurada *et al.* 2014). Likewise Aras, they also analyzed various classification models, but only relevant ones to this thesis are further discussed. Namely, the authors trained Neural Network (NN), Decision Tree (DT), Support Vector Machine (SVM), K–Nearest Neighbors (KNN) and Logistic Regression (LR), using Weka software. Authors did not mention which imputation technique

did they use, nor the data split ratio (i.e., the test size used for an evulation), but likwise Aras, they conducted a hyperparameter tuning using Grid Search with 10–fold cross validation.

The evalulation results are depicted in Table 3.3, namely the computed metrics such as Accuracy (Acc.), Recall (Rec.) and AUC. As can be seen, KNN model, which was the best one in case of Zurada's study, yielded a very deteriorated performance, while Logistic regression still performed badly. On the other hand the Neural Network was the best performing model as a black–box model. Surprisingly, also Decision Tree showcased relatively high performance in contrast to Zurada's study, where Decision Tree's performace was quite weak.

Table 3.3: Evaluation Results (Zurada *et al.* 2014)

Model	Acc.	Rec.	AUC
NN	0.869	0.590	0.863
DT	0.889	0.548	0.844
SVM	0.848	0.346	0.810
KNN	0.791	0.334	0.826
LR	0.836	0.304	0.794

Source: (Zurada *et al.* 2014)

The same interpretation can be derived from ranking the results in the same way as in Zurada's study, as shown in Table 3.4. Hence, it is expected that Neural Network would perform well on the HMEQ data set, while Logistic Regression's performance would be unsatisfactory.

Table 3.4: Evaluation Results - Ranked (Zurada *et al.* 2014)

Model	Acc.	Rec.	AUC	Score	Rank
NN	2	1	1	1.33	1
DT	1	2	2	1.67	2
SVM	3	3	4	3.33	3
KNN	5	4	3	4.00	4
LR	4	5	5	4.67	5

Source: Ranking of (Zurada *et al.* 2014)

Although, both Zurada and Aras ranked the Logistic Regression as the worst performing model and SVM was ranked according to them as the third best

model, they did not agree on the ranking of Decision Tree and KNN models. Such a disagreement can be attributed to the fact they both used different data preprocessing techniques, as well as different hyperparameters' spaces for fine tuning the models and probably also different softwares, random seed, and data split. We also need to account for a relatively small sample size of the HMEQ data set, which can lead to a high variance in the results. Therefore, several steps and procedures are applied in this thesis in order to ensure the reliable and robust results and estimates, which are further described in Section 4.4.

3.1 Hypotheses

In this section, we formulate the hypotheses, which are partially derived from the literature review disscused above and are further tested, i.e., rejected or not rejected, in Chapter 5 based on the empirical analysis regarding the machine learning implementation in Chapter 4.

Hypothesis #1: *The recalibration of the model enhaces model performance on HMEQ data set.*

The study of de Hond and others (de Hond *et al.* 2023) focuses on the model re-training (recalibration) in order to improve the model performance, based on the health record data from Leiden University Medical Center and Amsterdam University Medical Center fore prediction of readmissions or deaths after ICU discharge. Such effect is being achieved by either re-training the model on the and newest additional data, hence by increasing the sample size within the model training, we expect the model's predictive power to be enhanced. Such approach is further discussed in Subsection 4.4.4 and assessed in Subsection 4.5.1.

Hypothesis #2: *Either Neural Network or KNN model outperforms all the models on HMEQ data set.*

Based on the studies of Aras (Aras 2021) and Zurada and others (Zurada *et al.* 2014), the highest ranked models in terms of performance were KNN and Neural Network, respectively. Those two models outperformed the traditional Logistic Regression, and incase of Aras, KNN also outperformed Decision Tree, Gaussian Naive Bayes, SVM and even Random Forest. Therefore, we expect

that at least one of those two models will outperform all the other models on the HMEQ data set.

Hypothesis #3: *Black–box models perform better than the white–box models on HMEQ data set.*

(Loyola-Gonzalez 2019)

Hypothesis #4: *The longer execution time of a model, the better performance on HMEQ data set.*

Although, the research paper's objective of Wu and others (Wu *et al.* 2018) does not directly regard the relationship between the training (execution) time and the model performance, but rather the accuracy of indoor localization techniques in two different environments. Howeover, such study also inspects the evaluation of Bayes Net, SVM and Random Forest models, including their execution time. As shown in Table 3.5, we can observe that there is a trade-off between model performance and the execution time, as the SVM has the highest accuracy and moderate execution time, while the Bayes Net has the lowest accuracy, but also the shortest execution time. Therefore, we expect a positive association between the execution time and the model performance.

Table 3.5: Accuracy vs. Execution Time (Wu *et al.* 2018)

Model	Acc.	Time (seconds)
Bayes Net	0.8521 / 0.8474	0.56 / 1.15
SVM	0.9328 / 0.9590	1.79 / 3.21
RF	0.9070 / 0.9574	4.92 / 8.84

Source: Ranking of (Wu *et al.* 2018)

Hypothesis #5: *The main default drivers are the debt and/or delinquency features on HMEQ data set.*

In the study of Zurada and others (Zurada *et al.* 2014), the authors also inspect the significance of features in order to reduce the dimensionality. In particular, the authors employed both using correlation analysis with the target as well as ranking according to information gain. In case of HMEQ data set, the most significant features are debt–to–income ratio, number of derogatory public records and number of delinquent credit lines. Thus, these features are expected to be the most important indicators when predicting a default.

Chapter 4

Empirical Analysis - Machine Learning Implementation

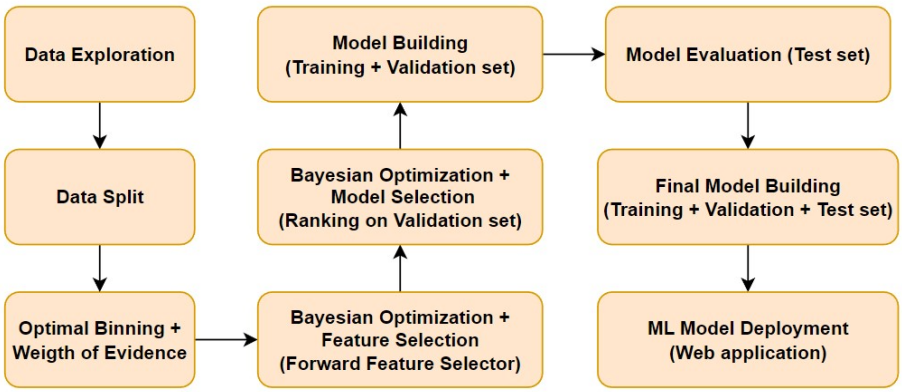
This chapter focuses on the main part of this thesis, particularly on the practical example of machine learning implementation. The machine learning framework deployed in this thesis is shown in Figure 4.1.

- **Data Exploration** - this part of the framework is focused on the exploration of the data in order to infer some insights about the data quality, distribution of the variables, statistical testing or association analysis.
- **Data Split** - this part of the framework is focused on the splitting of the data which are used separaterly in diferrent tasks such as model training, model selection and model evaluation.
- **Optimal Binning and WoE Encoding** - this part of the framework is focused on the optimal binning and the WoE encoding of the features as the main part of the feature preprocessing.
- **Feature Selection** - this part of the framework is focused on the feature selection in order to reduce the dimensionality of the data and to improve the performance of the machine learning models - each input model estimator is tuned with Bayesian Optimization.
- **Model Selection** - this part of the framework is focused on the model selection in order to find the best model based on the ranking - each input model is tuned with Bayesian Optimization on the subsets of selected features.
- **Model Building (Evaluation)** - this part of the framework is focused

on the recalibration of the final model by re-training it on the joined training and validation sets, which will be further evaluated.

- **Model Evaluation** - this part of the framework is focused on the evaluation of the final model on the unseen data from test set.
- **Model Building (Deployment)** - this part of the framework is focused on the final recalibration of the final model by re-training it on the joined training, validation and test sets, which will be further deployed into a production.
- **Model Deployment** - this part of the framework is focused on the deployment of the final model into a production as a web application.

Figure 4.1: Machine Learning Framework



Source: Author's results

4.1 Repository and Environment Structure

The whole machine learning implmenetation as the scope of this thesis is done mainly using Python Programming Language and further with collaboration of Git and HTML. The whole repository can be found in the separate appendix or is available on the GitHub repository `https://github.com/petr-ngn/FFU_VSE_Masters_Thesis_ML_Credit_Risk_Modelling`. The repository structure is shown in Figure 4.2.

Figure 4.2: Repository Structure

```
|--- data
|  |--- interim_dat.csv
|  |--- preprocessed_data.csv
|  |--- raw_data.csv
|
|--- flask_app
|  |--- inputs
|  |  |--- inputs_flask_app_dict.pkl
|  |
|  |--- templates
|  |  |--- index.html
|  |  |--- results.html
|  |
|  |--- static
|  |
|  |--- app.py
|
|--- models
|  |--- feature_preprocessing
|  |--- feature_selection
|  |--- model_selection
|  |--- objects_FINAL
|
|--- plots
|--- Masters_Thesis.ipynb
|--- README.md
|--- requirements.yml
```

Source: Author's results at GitHub

- `data` - directory containing the raw data, partially preprocessed data (`interim`) and the final preprocessed data.
- `flask_app` - directory containing the Flask application which is used for the deployment of the model. Particularly, it contains the `app.py` file which is the main back-end file of the application, the `templates` and `static` subdirectories which contain the front-end HTML files for

the application, and the `inputs` subdirectory which contains the input dictionary for the application (such as the trained model, threshold, final features etc.).

- `models` - directory containing the the subdirectories of the trained and fitted objects for features preprocessing, feature selection and model selection, including the final objects used in deployment.
- `plots` - directory containing the plots generated within the main Python notebook.
- `Masters_Thesis.ipynb` - main Python notebook containing the main part of the machine learning Implementation, such as exploratory analysis, data preprocessing, training and evaluation of the models.
- `README.md` - README file containing the description of the repository.
- `requirements.yml` - file containing the list of the required packages and their specific versions used in this project.

This particular solution is developed in Python version 3.10.9 and these are the main packages and modules used in this project:

- `NumPy`, `Pandas` - for data manipulation and analysis.
- `Matplotlib`, `Seaborn` - for data visualization.
- `Scipy` - for statistical analysis.
- `OptBinning` - for optimal binning of features with respect to the target.
- `ImbLearn` - for handling imbalanced data using oversampling.
- Scikit-learn - for feature selection, model selection and model evaluation.
- Scikit-optimize - for more advanced hyperparameter optimization.
- Flask - for deployment of the model as web application.

To replicate this solution, one may download this repository as a zip file or either can clone this repository using Git to the local repository. Before running any files or scripts, it is important to set the environment for such project using the file `requirements.yml`. This can be done by running the following command in the Anaconda terminal which will create the new environment with the name `FFU_VSE_Masters_Thesis` and install all the required packages:

```
>> conda env create -n FFU_VSE_Masters_Thesis -f requirements.yml
```

Be aware of your current path directory in your terminal. In order to install the file `requirements.yml`, you need to define a path to the directory, where such file is located. To achieve this, the user has to either change the path in the terminal using `cd` command, insert the path directory before the `requirements.yml` in terminal, or to copy the file `requirements.yml` to the current path directory. The following code shows the former approach:

```
>> cd C:\Users\ngnpe\FFU_VSE_Masters_Thesis_ML_Credit_Risk_Modelling
>> conda env create -n FFU_VSE_Masters_Thesis -f requirements.yml
```

To preserve the reproducibility of this solution and conistency of the results, the random seed is instantiated to `42`, so for instance data split, model optimization or training would be deterministic and not totally random everytime when replicating the solution.

Some `Scikit-learn` or `Scikit-optimize` objects have optional argument `n_jobs` which utilizes the number of CPU cores used during the parallelizing computation. Such argument was set to `-1`, hence all the processors are used in order to speed up the training or optimization process.

4.2 Data Exploration

This section is focused on exploration of the analyzed loan data set, particularly on data set description, distribution analysis and association analysis, in order to infer potential valuable insights and hypotheses which can be used in the preprocessing or modelling part.

4.2.1 Data Set Description

The analyzed data set pertains to the HMEQ data set which contains loan application information and default status of 5,960 US home equity loans. Such data set was acquired from Credit Risk Analytics website[1] (Baesens *et al.* 2016). Since this data set regards the loan application scoring data, using macroeconomic or other external data is omitted due to the data set characteristics as well as modelling with behavioral scoring. Thus our goal is to predict whether the loan applicant will or would default based on provided information from the loan application.

As can be seen in **??**, the data set contains 13 columns, 12 features and 1 target variable `BAD` indicating whether the loan was in default (`1`) or not (`0`). Amongst the 12 features, there are 10 numeric features and 2 categorical features, namely `REASON` which contains 2 categories - Debt consolidation (`DebtCon`) and Home improvement (`HomeImp`), and `JOB` which fontains following categories - Administration (`Office`), Sales, Manager (`Mgr`), Professional Executive (`ProfExe`), Self-employed (`Self`), and Other.

[1] `http://www.creditriskanalytics.net/datasets-private2.html`

Table 4.1: Data Set Columns

Variable	Description	Data type
BAD	Default status	Boolean
LOAN	Requested loan amount	numeric
MORTDUE	Loan amount due on existing mortgage	numeric
VALUE	Value of current underlying collateral property	numeric
REASON	Reason of loan application	categorical
JOB	Job occupancy category	categorical
YOJ	Years of employment at present job	numeric
DEROG	Number of derogatory public reports	numeric
DELINQ	Number of delinquent credit lines	numeric
CLAGE	Age of the oldest credit line in months	numeric
NINQ	Number of recent credit inquiries	numeric
CLNO	Number of credit lines	numeric
DEBTINC	Debt-to-income ratio	numeric

Source: (Baesens *et al.* 2016)

After the initial data inspection, data does not contain any duplicates but does contain missing values, which are summarized in Table 4.2. Most of the missing values contains the feature `DEBTINC` with 1,267 missing observations, whereas columns indicating default status (`BAD`) or requested loan amount (`LOAN`) do not contain any missing values, which is expected as the bank should have the available information about their loans whether they have defaulted or not, and since this data set pertains to the application scoring, when applying for a loan, an applicant should always fill out the requested loan amount.

Table 4.2: Missing Values Summary

Columns	# NA's	% NA's
BAD	0	0.00 %
LOAN	0	0.00 %
MORTDUE	518	8.69 %
VALUE	112	1.88 %
REASON	252	4.23 %
JOB	279	4.68 %
YOJ	515	8.64 %
DEROG	708	11.88 %
DELINQ	580	9.73 %
CLAGE	308	5.17 %
NINQ	510	8.56 %
CLNO	222	3.72 %
DEBTINC	1267	21.26 %

Source: Author's results in Python

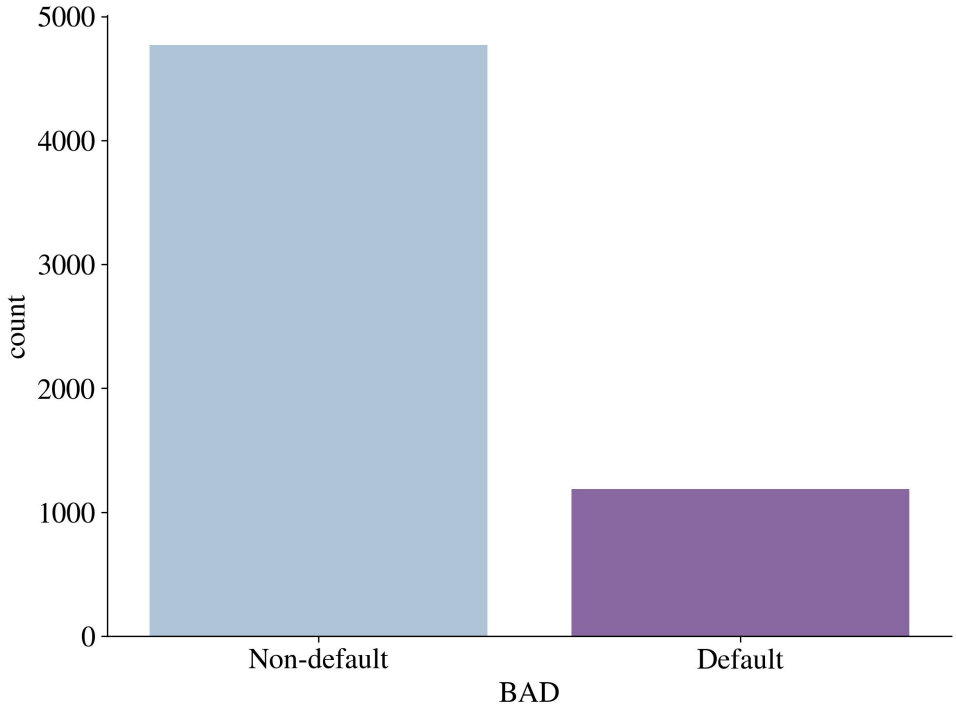
4.2.2 Distribution Analysis

In this subsection, we inspect the distribution of our variables, including the target variable and the features. Such distribution inspection may help us to identify potential outliers, missing values, and other potential issues with the data set.

Default Distribution

Regarding the the target variable distribution, from the Figure 4.3 we can observe that the default status distribution is heavily imbalanced, as most of the loans have not defaulted yet. Particularly, 80.05% of the observations have been labelled as non-default (4,771 observations) and 19.95% observations labelled as default (1,189 observations). This may cause problems in the modelling part, as the model may be biased towards the majority class, i.e., the non-default class. Such imbalanced class issue will be further treated in Subsection 4.3.1.

Figure 4.3: Default status distribution



Source: Author's results in Python

Numeric Features' Distribution

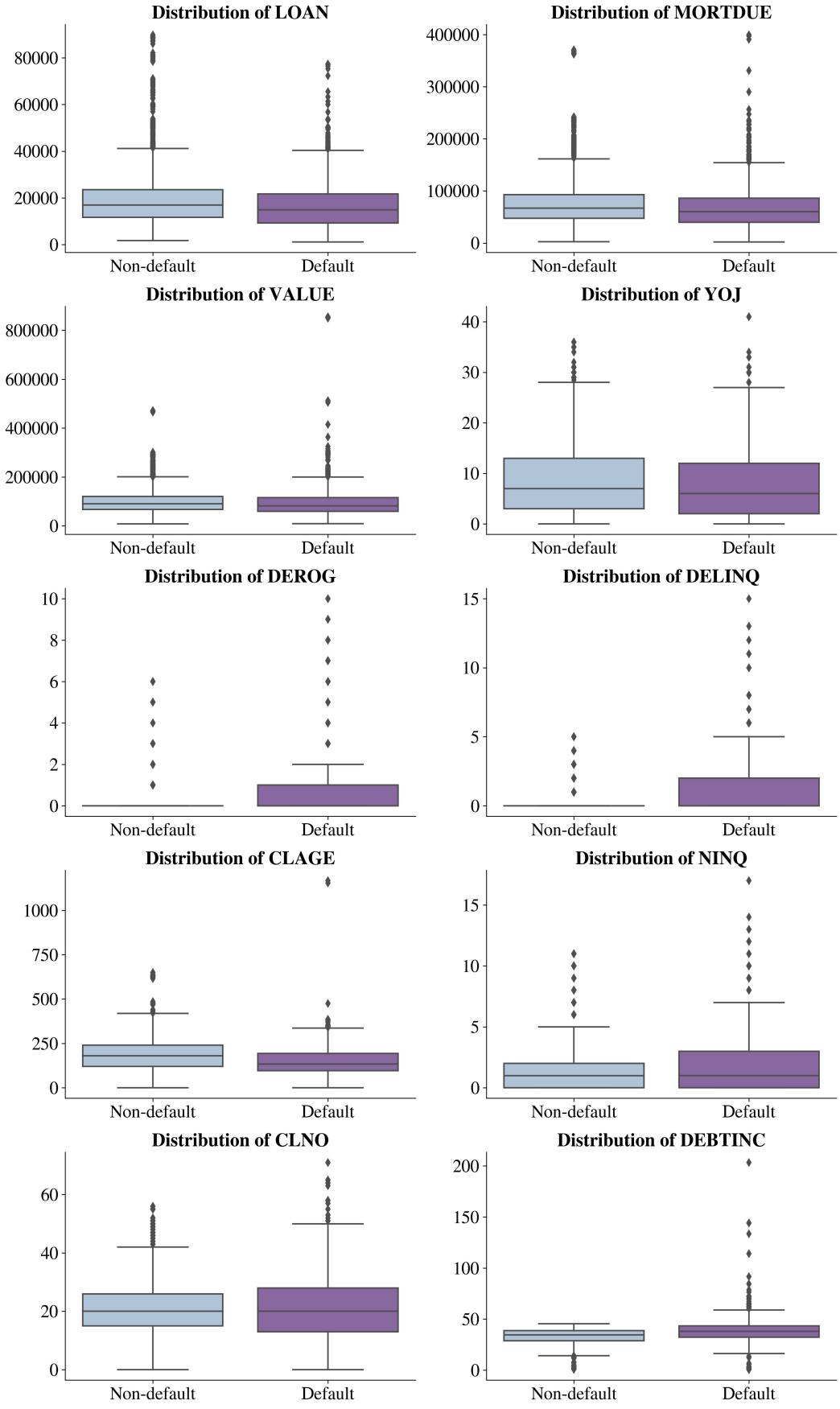
Regarding the numeric features, it can be observed that most of them exhibit a positive skewness and contain outliers, as illustrated in Figure 4.4, which depicts the conditional distribution of the numeric features with respect to the default status via boxplots.

All the outliers appear to be valid, indicating that they have not arisen due to data entry errors. This can be attributed to the non-negative nature of all the numeric features, which makes it impossible to have negative values for features such as the number of years at present job or the number of delinquent credit lines, among others. Additionally, the maximum values of the given features are not unrealistically high, further corroborating the validity of the outliers. However, it is necessary to treat these outliers as they can bias a model's weights or coefficients, particularly in the case of logistic regression or neural networks. Outliers can also jeopardize distance calculations in the case of KNN, or in general, affect the position and orientation of the decision boundary. Such factors can lead to overfitting and inaccurate and biased predictions. A detailed explanation of the outlier treatment is provided in Subsection 4.3.2.

Concerning the target variable, it can be observed that there are some dif-

ferences in the distribution shapes of DEROG and DELINQ, which exhibit less skewness and lower dispersion for non-default cases as compared to default cases. Since both features indicate negative information about delinquency, it is expected that a higher value for these features would increase the likelihood of loan default. Referring to the feature DEBTINC, it does not exhibit any extreme values for non-default cases, but some extreme values are present for default cases. From this, it can be inferred that if the debt-to-income ratio is too high, indicating that the applicant's income is not sufficient to cover their debt, the loan is more likely to end in default. The association between the default status and the numeric features is further investigated in Section 4.2.3.

Figure 4.4: Conditional distribution of numeric features



Source: Author's results in Python

Due to the fact that the boxplots do not capture the missing values occurred in given features, it is also important to inspect the numbers and proportions of missing values in each feature, conditional on the default status. As can be seen in Table 4.3, n_0 refers to the number of missing values in given feature for non-default cases, n_1 refers to the number of missing values in given feature for default cases. N_0 and N_1 refer to the total number non–default cases and default cases respectively, therefore n_0/N_0 refers to the proportion of missing values in given feature for non-default cases, and n_1/N_1 refers to the proportion of missing values in given feature for default cases.

Pertaining to the feature `DEBTINC`, we can observe a significant difference in the number of missing values between the default and non-default cases. Out of all defaulted loans, 66.11 % had missing debt–to–income ratio, whereas only 10.08 % out of all non-defaulted loans had missing debt–to–income ratio. Therefore, there could be a strong association between the missing debt–to–income ratio and the default.

Similarly, the table depicts a significant difference with respect to `VALUE` as 0.15 % had missing collateral property value out of all non–defaulted loan, and 8.92 % defaulted loans had missing collateral property value. It can be inferred that loan applicants who withhold information on their collateral property value or debt-to-income ratio are more likely to default on their loans. This may be due to negative information that they are trying to conceal, such as an excessively high debt or low income, or a low collateral property value. Such associations are further investigated in Section 4.2.3.

Table 4.3: Numeric features NA's table

Feature	n_0	n_1	n_0/N_0	n_1/N_1
LOAN	0	0	0 %	0 %
MORTDUE	412	106	8.64 %	8.92 %
VALUE	7	105	0.15 %	8.83 %
YOJ	450	65	9.43 %	5.47 %
DEROG	621	87	13.02 %	7.32 %
DELINQ	508	72	10.65 %	6.06 %
CLAGE	230	78	4.82 %	6.56 %
NINQ	435	75	9.12 %	6.31 %
CLNO	169	53	3.54 %	4.46 %
DEBTINC	481	786	10.08 %	66.11 %

Source: Author's results in Python

Categorical Features' Distribution

Regarding the distribution of categorical features, the data set includes 2 nominal features, namely `REASON` and `JOB`. The conditional distribution of categorical features on the default status is visualized using barplots in Figure 4.5. The plot indicates that most loan applicants applied for debt consolidation, while most job occupancies were labeled as `Other`.

With respect to the default status, there appears to be no significant difference between the default and non-default cases in terms of the relative distribution of the `REASON` feature. However, a slight difference is observed between the default and non-default cases in terms of the relative distribution of the `JOB` feature. Specifically, the categories `Office`, `ProfExe`, and `N/A` exhibit a relatively higher proportion of non-default cases than default cases. Hence, a moderate association between the `JOB` feature and the default status is possible, as further investigated in Section 4.2.3.

Figure 4.5: Conditional distribution of categorical features

Source: Author's results in Python

4.2.3 Association Analysis

In this subsection, we aim to examine potential relationships between the variables by analyzing their associations. Firstly, we investigate the association between the default status and the features. Subsequently, we explore the association among the features themselves.

Association between default status and numeric features

To measure the association between the target variable and the numeric features, we use the Point-Biserial correlation coefficient, which is the Pearson's product moment correlation coefficient between a continuous variable and a dichotomous variable (Kornbrot 2014). This coefficient ranges from -1 to +1

and can be used to assess the strength and direction of the relationship between a continuous variable and a binary variable. The formula for computing this coefficient is as follows:

$$r_{pb,X} = \frac{\mu\left(X|Y=1\right) - \mu\left(X|Y=0\right)}{\sigma_X} \sqrt{\frac{N\left(Y=1\right) \times N\left(Y=0\right)}{N\left(N-1\right)}} \tag{4.1}$$

Here, $\mu\left(X|Y=1\right)$ and $\mu\left(X|Y=0\right)$ represent the means of the given numeric feature X conditional on the default status and non-default status, respectively, while σ_X denotes the standard deviation of X. The values of $N\left(Y=1\right)$ and $N\left(Y=0\right)$ indicate the number of observations with default status and non-default status, respectively, and N represents the total number of observations within the feature X.

The following Table 4.4 displays the computed Point-Biserial coefficient for each numeric feature with respect to the default status, along with its statistical significance. The results show that features such as `DEROG`, `DELINQ`, and `DEBTINC` are moderately and positively associated with the default status at the 1% statistical significance level. These findings support the observations made in Section 4.2.2 regarding the positive associations of these features with the default status. It can be inferred that these features may serve as important predictors in the model.

Table 4.4: Point–Biserial Correlation table

Feature	**Coefficient**	**Significance**
LOAN	-0.075	***
MORTDUE	-0.048	***
VALUE	-0.030	**
YOJ	-0.060	***
DEROG	0.276	***
DELINQ	0.354	***
CLAGE	-0.170	***
NINQ	0.175	***
CLNO	-0.004	
DEBTINC	0.200	***

*: $p < 0.10$, **: $p < 0.05$, ***: $p < 0.01$

Source: Author's results in Python

Association between default status and categorical features

In order to measure the strength of the relationship between the dichotomous default status and categorical variables, we employ Cramer's V, which ranges from 0 to 1 and is defined as:

$$CV_X = \sqrt{\frac{\chi^2}{N\,(k-1)}} \tag{4.2}$$

As noted in Section 4.2.2, the association between the default status and `REASON` is weak, as evidenced by the Cramer's V value being close to zero. Conversely, the association between the default status and `JOB` is slightly stronger, as the categories `Office`, `ProfExe`, and `N/A` exhibit a higher proportion of non-default cases than default cases. Both `REASON`'s and `JOB`'s associations with default status are statistically significant at the 1% significance level.

While statistical significance is important, it does not necessarily indicate that a feature is a strong predictor of the target variable. Ultimately, the usefulness of a feature in predicting the target variable is determined by the performance metrics of the model.

Table 4.5: Cramer's V Association table

Feature	**Coefficient**	**Significance**
REASON	0.038	***
JOB	0.120	***

*: $p < 0.10$, **: $p < 0.05$, ***: $p < 0.01$

Source: Author's results in Python

Association between default status and missing values

Given that the loan data set contains missing values, it is necessary to examine whether the missingness is associated with the default status. One possible approach is to encode the feature with missing values as a binary variable, where 1 indicates the presence of a missing value and 0 otherwise.

To quantify the strength of association between the two binary variables, the Phi coefficient is used, which is defined as:

$$\phi_X = \sqrt{\frac{\chi^2}{n}} \tag{4.3}$$

In line with the finding regarding the `DEBTINC` and `VALUE` in Section 4.2.2, there is a strong and statistically significant association between the missing debt-to-income ratio and default status, and a moderate and statistically significant association between the missing collateral property value and default status, as shown in Table 4.6. Therefore, we can anticipate that these features will be crucial indicators in default prediction. Further details on feature selection are presented in Subsection 4.4.2.

Table 4.6: Phi Correlation Coefficient table

Feature	**Coefficient**	**Significance**
LOAN	0.000	
MORTDUE	0.003	
VALUE	0.254	***
REASON	0.004	
JOB	0.064	***
YOJ	0.056	***
DEROG	0.070	***
DELINQ	0.061	***
CLAGE	0.030	**
NINQ	0.039	***
CLNO	0.018	
DEBTINC	0.547	***

*: $p < 0.10$, **: $p < 0.05$, ***: $p < 0.01$

Source: Author's results in Python

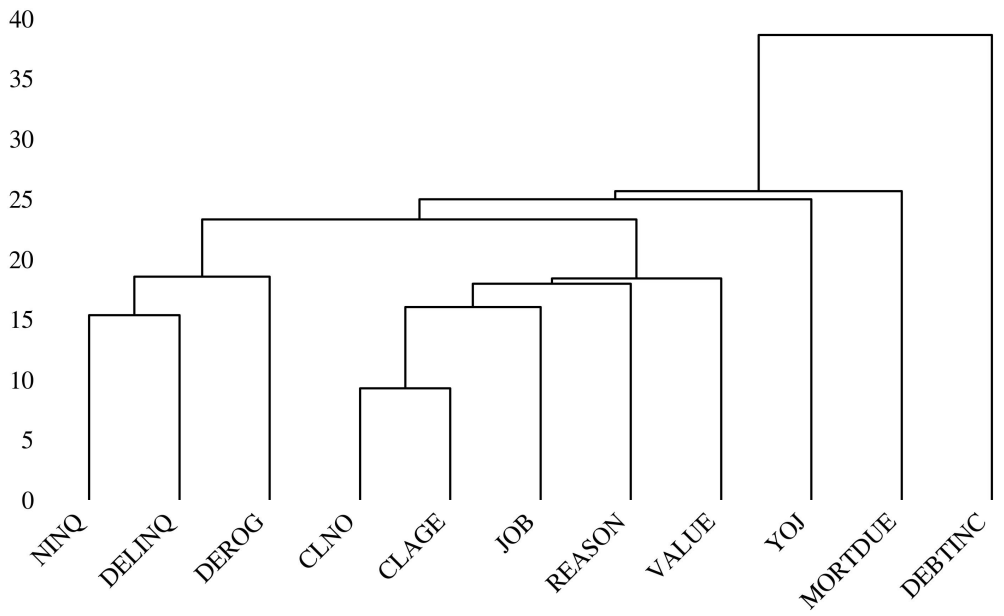
Missing Values Association

Additionally, it is imperative to investigate the relationship between missing values and default status, as well as the interrelationship between the missing values themselves. A common approach to identifying patterns of missing data in a data set is through the use of a dendrogram, which clusters variables hierarchically based on the occurrence of missing values. This method groups variables into clusters based on the similarity of their missing value patterns, such that variables with comparable patterns of missingness are clustered to-

gether. Conversely, variables with dissimilar patterns of missingness are placed in separate clusters. The dendrogram is constructed by merging the two closest clusters iteratively until all variables are in the same cluster. The distance between the clusters at each step of the merging process is shown on the y-axis of the dendrogram, and the order in which the variables are merged is displayed on the x-axis.

In Figure 4.6, the hierarchical clustering of the data set's variables is illustrated, excluding the default status and requested loan amount feature `LOAN`, as these variables do not contain any missing values. As depicted in the dendrogram, the `CLNO` and `CLAGE` features have the most similar patterns of missing values occurrences. Therefore, it can be inferred that a significant number of loan applicants tend to omit information regarding their number of credit lines (`CLNO`) and the age of their most recent credit line (`CLAGE`) when submitting their loan applications.

Figure 4.6: Nullity dendrogram



Source: Author's results in Python

Multicolinearity Analysis

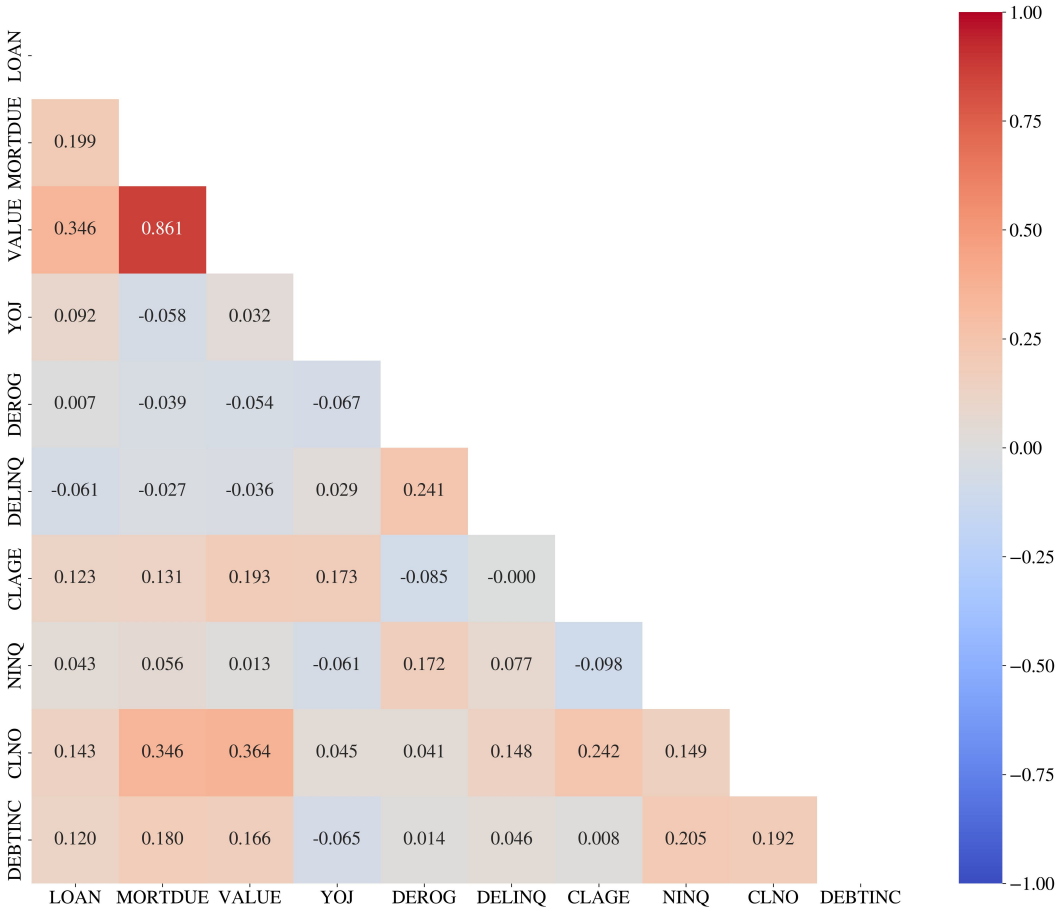
To quantify the association between the numerical features, Pearson correlation coefficient is often used. However, it is highly sensitive to outliers and makes assumptions regarding the normal distribution and linear relationship between variables. Consequently, Spearman correlation coefficient is utilized

as an alternative, as it is a non-parametric measure that does not make any assumptions regarding the distribution of variables or the linearity of their relationship. The Spearman correlation coefficient is defined as follows:

$$\rho_{spearman} = 1 - \frac{6 \sum_{i=1}^{n} d_i^2}{n\left(n^2 - 1\right)} \tag{4.4}$$

In the Figure 4.7, we can observe a very strong correlation between the `MORTDUE` and `VALUE` features. Such multicolinearity can cause problem in predictions na model's overfitting. Therefore, a feature selection is recommended - such selection is further described in Subsection 4.4.2.

Figure 4.7: Spearman Correlation Matrix



Source: Author's results in Python

4.3 Data Preprocessing

In this section, the process of preprocessing data is described as the crucial step in the machine learning modelling. Particularly, the the process of dividing data for various tasks, oversampling due to the imbalanced class issue, discretization of features and Weight–of–Eveidence transformation are further discussed and described.

4.3.1 Data Split and ADASYN Oversampling

To ensure appropriate model training and unbiased evaluation, it is necessary to split data into separate sets for various purposes. Specifically, the data set is split into three sets: (1) training set for training the model, perform feature selection or hyperparameter tuning, (2) validation for hyperparameter tuning, and (3) test set for assess the model performance on the unseen data (Subasi 2020). In this thesis, the data is plit into training, validation and test sets in ratio of 70:15:15, which ensures sufficient amount of data for training, hence the model would be able to generalize well, while keeping the validation and test sets large enough to provide reliable evaluation of the model's performance.

The data is split using stratified split to preserve the default status distribution, which is highly imbalanced. Stratification ensures that the distribution of defaults and non-defaults remains the same across all sets, thereby avoiding overfitting and data leakage. Using stratification, each set had 80 % non-defaults and 20 % defaults. This method enables accurate prediction since the model is trained and evaluated on the same population (Igareta 2021). However, stratification alone may not be sufficient for dealing with imbalanced classes. Therefore, ADASYN oversampling is performed as described in Section 2.5. Note that ADASYN oversampling is performed on the training set only after the split to avoid data leakage and biased evaluation.

In Python, the data are divided and oversampled using a custom function `data_split()`. This function first employs the `train_test_split()` function from the `scikit-learn` module to split the data into training, validation, and test sets with a stratification technique. Next, the `ADASYN()` class from the `imblearn` module is used to oversample the training set. This is achieved by generating synthetic instances of the minority class based on the five nearest neighbors and Euclidean distance.

However, the `ADASYN()` class from `imblearn` is not designed to handle missing values or categorical features encoded as character. To overcome this limitation, the following approach is taken:

1. Separate the categorical and numeric features;
2. Impute the missing values with arbitrary values:
   - Categorical features: string `'N/A'`;
   - Numeric features: number `99999999999999` - such value is chosen since it is highly unlikely to be present in the data set.
3. Convert the categorical features into dummy variables;
4. Join the numeric features with the dummy variables;
5. Perform the oversampling on the joined data set;
6. Convert the dummy variables back into categorical features;
7. Retrieve back the missing values:
   - Categorical features: replace string `'N/A'` with `np.nan`;
   - Numeric features: for each feature X if its value exceeds the original maximum value, then replace it with `np.nan`;

The following Table 4.7 shows the default distribution of the individual sets before and after oversampling. The training set after ADASYN oversampling was balanced, while the default distribution remained the same across the validation and test sets before and after oversampling, which is desirable due to stratification.

Table 4.7: Sample sizes of split sets

Set	**# instances**	**% defaults**	**% non–defaults**
Training	4,171	19.95 %	80.05 %
Training (oversampled)	6,437	48.13 %	51.87 %
Validation	895	20.00 %	80.00 %
Test	894	20.00 %	80.00 %

Source: Author's results in Python

Since ADASYN increases the sample size by generating, i.e., adding new instances into the sample, it may have an impact on the distribution of the

features. After the inspection in Python, it have no significant impact on the numeric features as the distributions before and after ADASYN oversampling do not differ that much. However, pertaining to the categorical features, a significant impact of ADASYN oversampling can be observed as can be seen in Table 4.8 and Figure 4.8, respectively, which depict the distribution of categorical features on the subsample of default cases within the training set, particularly distribution before and after the oversampling. As such, n_B and n_A refer to the number of default cases within given category before and after oversampling, respectively, N_B and N_A represents the total number of default cases before and after oversampling, respectively.

Within the `REASON` feature, we can observe a significant increase the proportion of defaulted clients who applied for a loan due to the debt consolidation (`DebtCon`) among all the defaulters after an oversampling - particularly, the ratio has increased by 12.20 percentage points. On the other hand, the proportion of defaulted clients who applied for a loan due to the home improvement (`HomeImp`) has decreased by 9.69 percentage points, indicating lower distribution of such clients in the oversampled set. Regarding the `JOB` feature, we can observe a substantial increase in the proportion in the of defaulted managers (`Mgr`) among all the defaulters after oversampling by 38.75 percentage points. On the other hand, the proportion of defaulted clients who are labelled as `Others` has decreased by 17.15 percentage points.

Table 4.8: ADASYN Impact on Categorical Features' Distribution

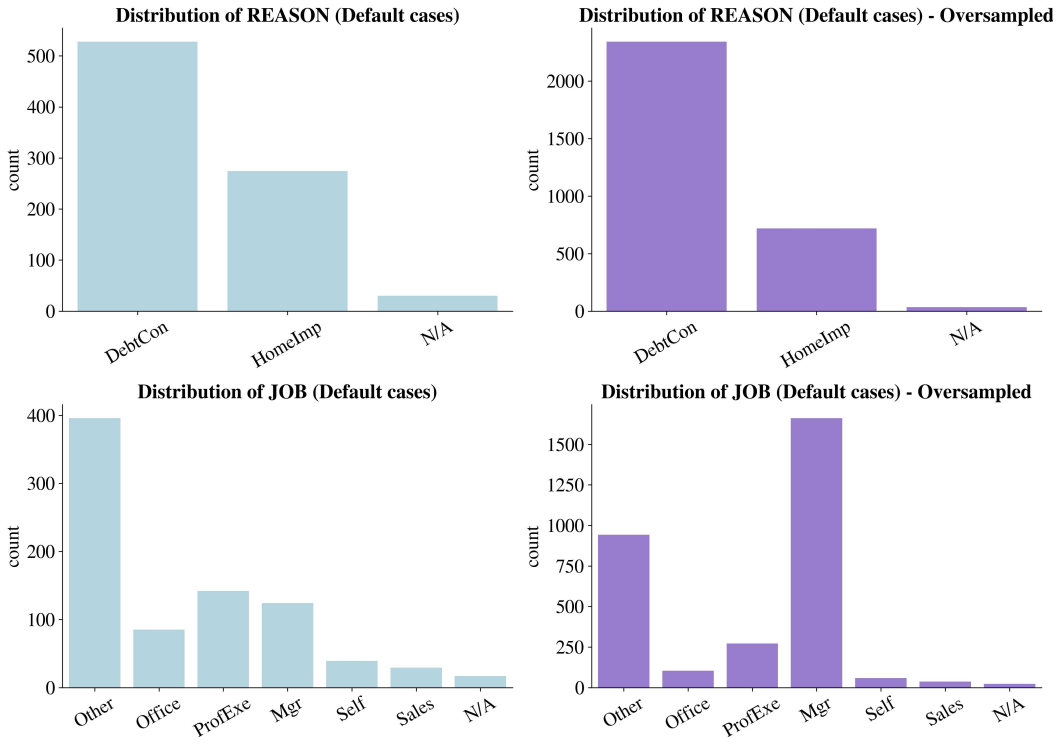
Featuew	Category	n_B	n_A	n_B/N_B	n_A/N_A	Diff.
REASON	DebtCon	528	2,344	63.46 %	75.66 %	12.20 p.p.
REASON	HomeImp	274	720	32.93 %	23.24 %	-9.69 p.p.
REASON	N/A	30	34	3.61 %	1.10 %	-2.51 p.p.
JOB	Mgr	124	1,662	14.9 %	53.65 %	38.75 p.p.
JOB	Other	396	943	47.6 %	30.44 %	-17.16 p.p.
JOB	ProfExe	142	272	17.07 %	8.78 %	-8.29 p.p.
JOB	Office	85	104	10.22 %	3.36 %	-6.86 p.p.
JOB	Self	39	58	4.69 %	1.87 %	-2.82 p.p.
JOB	Sales	29	36	3.49 %	1.16 %	-2.33 p.p.
JOB	N/A	17	23	2.04 %	0.74 %	-1.30 p.p.

Source: Author's results in Python

Such findings regarding the significant increases in the proportion of default

cases regarding the `DebtCon` and `Mgr` categories are given to the nature of ADASYN oversampling. As explained before, ADASYN generates more synthetic default class instances in the neighborhood of such default instances, which are hard–to–learn for ADASYN. In other words, ADASYN creates more default instances for such default instances where the density of the non–default class is relatively high in given default instance's neighborhood. Therefore, default instances which either are managers or applied for a loan due to the debt consolidation are difficult–to–learn for ADASYN, thus ADASYN replicates more instances with such characteristics, hence this results in a higher proportion of default cases in the oversampled set for such category.

Figure 4.8: ADASYN Impact of Categorical Features' Distribution



Source: Author's results in Python

4.3.2 Optimal Binning and Weight–of–Evidence

As already described in autorefsec:optbinningtheory, the optimal binning is employed as a data preprocessing step in this thesis. Particularly, we employ `BinningProcess` class from the `optbinning` module in Python - such class optimally discretizes the continuous features into interval bins and optimally groups categorical features' categories into sub-group categories with respect to the target variable while maximizing Information Value, and afterwards such bins are encoded using WoE (Navas-Palencia 2020). Besides discretizing and grouping, it also creates special bins for capturing missing values.

In this thesis, this data preprocessing step is wrapped into a custom function `woe_binning()` in Python. First, the `BinningProcess` class is fitted on the training set only in order to avoid data leakage, while it learns the split points for binning, event rates, WoE coefficients etc, and afterwards, such fitted `BinningProcess` class is used to transform training, validation and test set.

The following Figure 4.9 depicts the distribution of WoE bins for each feature. It can be observed that binning captures either linear, non-linear, monotonic, or non-monotonic relationships between the default status and the numeric features in terms of WoE. Regarding the `DELINQ` feature, a monotonic relationship can be observed, where the higher number of delinquent credit lines, the lower the WoE coefficient, indicating a larger distribution of defaults with respect to non-defaults in the given bin. Thus, the higher the number of delinquent credit lines, the higher the likelihood of defaulting in terms of WoE.

A non-linear relationship can be observed with respect to the `YOJ` feature, where the WoE coefficient is positive for applicants who have recently started working at their new job (i.e., number of years at the present job is less than 1) and for applicants who have been working at their current job for a relatively long time (i.e., number of years at the present job is higher than 19). Thus, applicants who have been working for a longer time have stable income and are more creditworthy and less likely to default. Regarding applicants who have recently started working at their new job, it is possible that they are less likely to default since the `YOJ` feature does not capture the applicant's total number of years of work experience, but only the number of years at the present job. Thus, in the given data set, applicants who have recently started working at their new job have a relatively higher total number of years of work experience, making them more creditworthy and less likely to default. On the other hand,

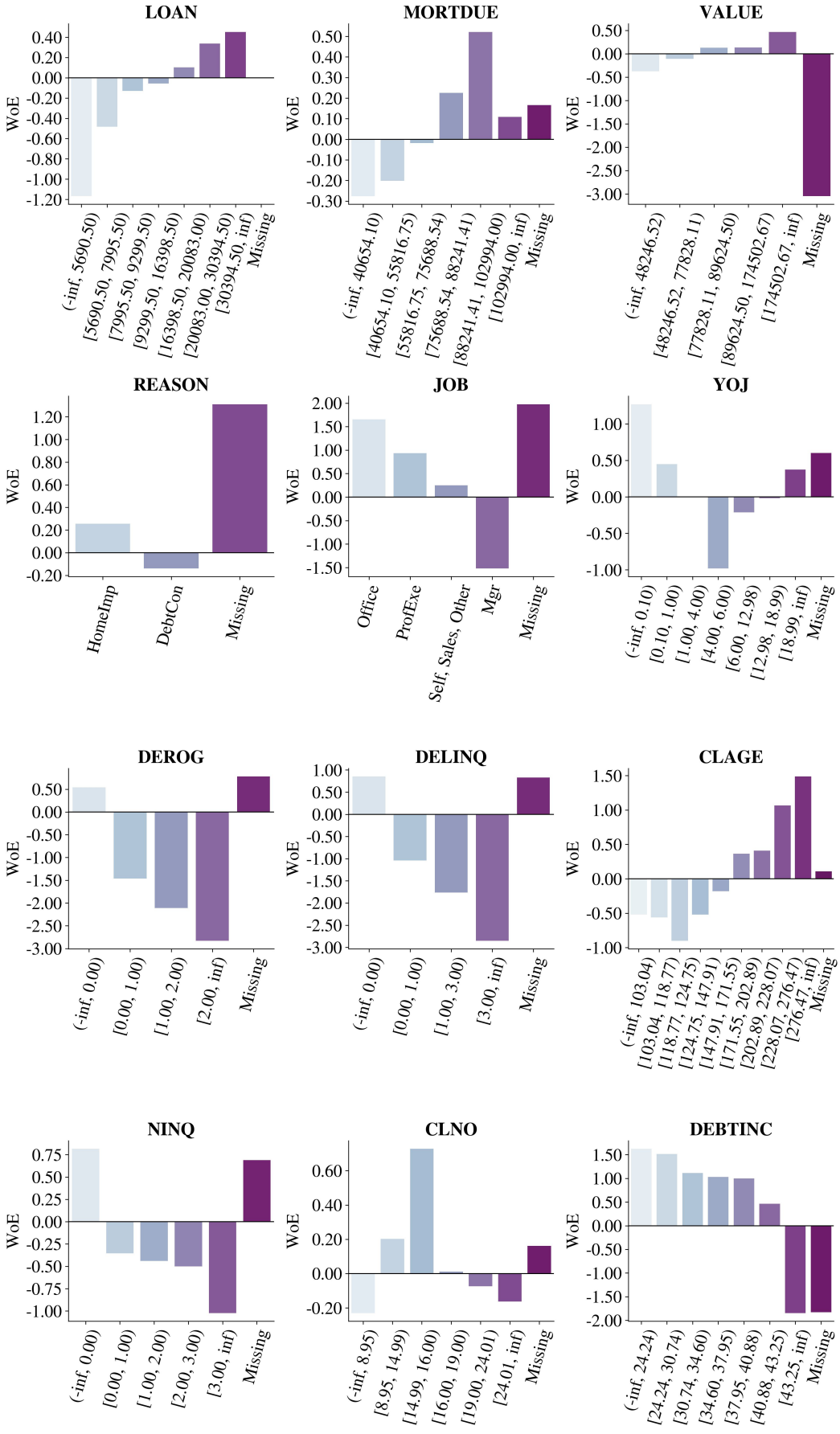
for applicants who have been working at their present job between 1 and 19 years, the WoE coefficient is negative. This relationship seems to be complex and can be influenced by other factors not present in the data set, such as the applicant's age, total number of years of work experience, education, etc.

As already mentioned numeric and categorical features contain a separate bin capturing missing values, which can be a useful indicator when training a model. This is evident in the `DEBTINC` feature, where the bin capturing missing values has the most negative WoE coefficient, indicating that there is a larger distribution of defaulters compared to non-defaulters. This finding was already raised in Section 4.2.3 in terms of the strong and statistically significant association between the default status and the missing values in `DEBTINC`.

Within the `JOB` feature, specifically regarding the `Mgr` category, we can observe the direct impact of ADASYN oversampling as already described by Table 4.8. Since ADASYN generated more default class instances for original default instances who are managers, this results in higher default rate within such job category, thus to the larger distribution of defaulters compared to non–defaulters, which is quantified in the negative WoE value.

QUESTION FOR SUPERVISOR: should I also decsribe the WoE distribution for other features as well or is this sufficient?

Figure 4.9: WoE Bins Distribution



Source: Author's results in Python

4.4 Modelling

Once the data are finally preprocessed, the next step regards the modelling part which includes hyperparameter tuning, feature selection, model selection and model building.

In Python, 8 different machine learning models from `Scikit-learn` module are used for the default status prediction, which were already described in Section 2.3, namely:

- **Logistic Regression** - `LogisticRegression()`
- **Decision Tree** - `DecisionTreeClassifier()`
- **Gaussian Naive Bayes** - `GaussianNB()`
- **K-Nearest Neighbors** - `KNeighborsClassifier()`
- **Random Forest** - `RandomForestClassifier()`
- **Gradient Boosting** - `GradientBoostingClassifier()`
- **Support Vector Machine** - `SVC()`
- **Multi–Layer Percepton** (*Neural Network*) - `MLPClassifier()`

4.4.1 Hyperparameter Bayesian Optimization

In this thesis, hyperparameter tuning of models is performed using Bayesian Optimization as described in Section 2.7. In Python, a custom function, `bayesian_optimization()`, is implemented to perform hyperparameter tuning using Bayesian Optimization. This function utilizes `BayesSearchCV` class from the `Scikit-optimize` module, with a 10-fold stratified cross-validation scheme and 50 iterations, while maximizing the F1 score. As a surrogate function, Gaussian Process is used (scikit-learn 2023h). The use of `BayesSearchCV` with stratified cross-validation in the hyperparameter tuning process provides a robust and reliable approach to selecting the optimal hyperparameters for the model, while the incorporation of Bayesian Optimization enables the efficient exploration of the hyperparameter space. By maximizing the F1 score, the hyperparameters selected through this process will result in a model with improved performance. Note, that the hyperparameter tuning is performed solely on training set in order to preserve the independence of the validation and test set, and avoid the information/data leakage as well.

For each model, the Bayesian Optimization algorithm performs 50 iterations while searching for the best hyperparameters values that maximize the F1 score. Within each iteration, a 10-fold stratified cross-validation is conducted to evaluate the model's cross–validation F1 score. Moreover, for each model, we specify the hyperparameter space, i.e., particular hyperparameters to be tuned and their possible ranges which the hyperparameter can take. The ranges are specified using `Integer` class to define interval of integers, `Real` to define interval of float numbers, and `Categorical` to define a list of possible (categorical) values. Note that not all the available hyperparameters are tuned, but only the most relevants due to the time complexity of the Bayesian Optimization algorithm. The definition of hyperparameter space for each model is described further in the following subsubsections.

Logistic Regression

The first hyperparameter **`Intercept`** allows to specify whether the intercept should be estimated or not. The next hyperparameter is the **`C penalty factor`** as a regularization term to prevent overfitting by adding such term to the objective loss function (Pramoditha 2021). Particularly, in case of Logistic Regression, C penalty factor is the regularization term which penalizes the coefficients' magnitudes. The is related to the **`Penalty`** hyperparameter, which allows to specify the norm used in the penalization. The most common penalty is $L1$ (also known as Lasso) penalty which which takes the absolute value of the coefficients' magnitudes. The logistic regression's loss function is the cross–entropy (also known as Log Loss) which is further described in Subsection 2.4.6. Then, the loss function with $L1$ penalty is defined as follows:

$$L(y,p)_{L1} = L(y,p) + C\sum_{j=1}^{k} \mid w_j \mid \tag{4.5}$$

Another penalty is $L2$ (also known as Ridge) penalty, which is more strict in penalization than $L1$ as it squares the coefficients' magnitudes. The loss function with $L2$ penalty is defined as follows:

$$L(y,p)_{L2} = L(y,p) + C\sum_{j=1}^{k} w_j^2 \tag{4.6}$$

The third penalty norm is the *ElasticNet* which combines both $L1$ and $L2$. The loss function with *ElasticNet* penalty is defined as follows:

$$L(y,p)_{ElasticNet} = L(y,p) + C\sum_{j=1}^{k}\left[\alpha \mid w_j \mid +(1-\alpha)w_j^2\right] \tag{4.7}$$

where α indicates the weight of $L1$ penalty in the *ElasticNet* penalty and refers to the *L1 ratio* hyperparameter. Moreover, the **`Class weight`** hyperparameter is a hyperparameter which allows to assign higher importance to the minority class instances during the training process.

Furthermore, **`Solver`** hyperparameter is used to specify which optimization algorithm should be used to estimate the coefficients' values. According to Hale (Hale 2019), Scikit-learn provides five solvers for Logistic Regression, namely *lbfgs* (Limited-memory Broyden-Fletcher-Goldfarb-Shanno) which approximates the second derivative matrix updates with gradient evaluations, *liblinear* (Library for Large Linear Classification) which uses coordinate descent algorithm, *newton-cg*, *sag* (Stochastic Average Gradient descent) as a variation of gradient descent and incremental aggregated gradient approaches using random sample of previous gradient values, and *saga* as an extension of *sag* which allows $L1$ regularization. For more information, please refer to the Scikit-learn documentation regarding Logistic Regression (scikit-optimize 2023). The last hyperparameter of Logistic Regression to tune in this thesis is the **`Intercept scaling`** which allows to scale the intercept.

Table 4.9: Logistic Regression - Hyperparameter Space

Hyperparameter	**Space**
Intercept	True, False
C factor	$<1 \times 10^{-6}$, 5>
Penalty	L1, L2, Elastic Net, None
Solver	lbfgs, liblinear, newton-cg, sag, saga
Class weight	None, balanced
L1 ratio	<0, 1>
Intercept scaling	True, False

Source: Author's results in Python

Decision Tree

The first hyperparameter of Decision Tree is the **`Criterion`** which allows to specify the function to measure the quality of a split - either Gini or Entropy impurity function. Another important hyperparameter is the **`Max depth`** which allows to specify the maximum depth of the tree. The last hyperparameter is the **`Max features`** which allows to specify the number of features to consider when looking for the best split (scikit-learn 2023g). Note, that **`Max features`** has a variable range of values depending on the number of features which is dependent on the number of features selected during feature selection (where the feature are iteratively selected and the model is trained and evaluated on each iteration).

Table 4.10: Decision Tree - Hyperparameter Space

Hyperparameter	**Space**
Criterion	Gini, Entropy
Max depth	<1, 10>
Max features	<1, `len(X.columns)`>

Source: Author's results in Python

Gaussian Naive Bayes

In case of Gaussian Naive Bayes, the only hyperparameter to tune is the **`Variance smoothing`** which allows to specify the portion of the largest variance of all features to be added to variances for calculation stability (scikit-learn 2023d), in order to smooth out the variances of each feature in case when the variance is zero.

Table 4.11: Gaussian Naive Bayes - Hyperparameter Space

Hyperparameter	**Space**
Variance smoothing	$<1 \times 10^{-9}, 1 \times 10^{-6}>$

Source: Author's results in Python

K–Nearest Neighbors

In KNN, it is crucial to specify the number of neighbors to consider during the classification process, which is depicted in the **`# neighbors`** hyperparam-

eter. Further, it is needed to select optimal distance measure, i.e., Euclidean, Manhattan or Minkowski as described in Subsection 2.3.4 - such selection refers to the **`Metric`** hyperparameter. Pertaining to the Minowski distance, we tune also the **`Norm order`** hyperparameter which allows to specify the power parameter within the distance calculation. Last but not least, KNN also allows to tune the **`Weights`** hyperparameter which allows to specify the weight function used in prediction - either uniform or distance. With the former function, all the points within each neighborhood are weighted uniformly and with the latter approach, the points are weighted inversely with respect to their distance. (scikit-learn 2023e).

Table 4.12: K–Nearest Neighbors - Hyperparameter Space

Hyperparameter	**Space**
# neighbors	<5, 20>
Metric	Euclidean, Manhattan, Minkowski
Norm order	<1, 5>
Weights	Uniform, Distance

Source: Author's results in Python

Random Forest

In in the Random Forest, we tune the number of base trees which are trained in parallel way in the ensemble, i.e., the **`# estimators`** hyperparameter. Similarly to Decision Tree, Random Forest allows to select the optimal split measure, i.e., Gini, Entropy or additionaly even Log Loss, which is depicted in the **`Criterion`** hyperparameter. Likewise Decision Tree, Random Forest also allows to specify the maximum depth of the tree as well as the the number of features to consider when looking for the best split, i.e., the **`Max depth`** hyperparameter and **`Max features`**, respectively. The **`Bootstrap`** hyperparameter allows to specify whether bootstrap samples are used when training the tree estimators. Similarly to Logistic Regression, Random Forest also has the **`Class weight`** hyperparameter which allows to specify the weight of each class in the classification process - *balanced* function takes the target variable to adjust the weights which are inversely proportional to class frequencies, whereas *subsample balanced* does almost the same, but the weights are computed based on the bootstrap samples. Last but not least, Random Forest also allows to tune the **`CCP alpha`** hyperparameter which allows to specify the complexity parameter

used for Minimal Cost-Complexity Pruning (CCP), in order to reduce the size of the tree estimators and avoid overfitting by remocing subtrees from the tree estimators which do not improve the performance (scikit-learn 2023c).

Table 4.13: Random Forest - Hyperparameter Space

Hyperparameter	**Space**
# estimators	<100, 1000>
Criterion	Gini, Entropy, Log Loss
Max depth	<1, 10>
Max features	<1, `len(X.columns)`>
Bootstrap	True, False
Class weight	None, balanced, subsample balanced
CCP alpha	$<1 \times 10^{-12}$, 0.5>

Source: Author's results in Python

Gradient Boosting

Likewise Random Forest, Gradient Boosting also allows to tune the number of base trees which are trained in sequential way in the ensemble, i.e., the **`# estimators`** hyperparameter, as well as the maximum depth of the tree and the number of features to consider when looking for the best split, i.e., the **`Max depth`** hyperparameter and **`Max features`**, respectively. Is it also need to tune the **`Learning rate`** hyperparameter which shrinks the contribution of each tree in order prevent overfitting. We can also select the optimal loss function of Gradient Boosting (**`Loss`** hyperparameter), either Log Log Loss or Exponential loss function - in the latter case, the model is equivalent to AdaBoost algorithm (scikit-learn 2023b). Moreover, the **`Criterion`** hyperparameter allows to specify measurement method of the split quality, i.e., MSE or Friedman MSE which improves the MSE with Friedman scores (scikit-learn 2023b).

Table 4.14: Gradient Boosting - Hyperparameter Space

Hyperparameter	Space
# estimators	<100, 1000>
Max depth	<1, 10>
Max features	<1, `len(X.columns)`>
Learning rate	<0.0001, 0.2>
Loss	Log Loss, Exponential
Criterion	MSE, Friedman MSE

Source: Author's results in Python

Support Vector Machine

Likewise Logistic Regression, SVM also allows to tune the **`C`** hyperparameter for the regularization, as well as the **`Kernel`** hyperparameter which specifies the kernel type to be used in the algorithm in order to map the data into higher dimensional space in order to find the optimal hyperplane which separates the classes. If the kernel is d-degree polynomial, we can also tune the **`Degree`** hyperparameter which specifies the degree of the polynomial kernel function. SVM also has the **`Class weight`** hyperparameter which assigns the weights to the input data based on the class frequencies in order to balance the classes.

Table 4.15: Support Vector Machine - Hyperparameter Space

Hyperparameter	Space
C factor	$<1 \times 10^{-6}$, 5>
Kernel	Linear, Poly, RBF, Sigmoid
Degree	<1, 10>
Class weight	balanced, None

Source: Author's results in Python

Multi–Layer Percepton

TBD

In the MLP, we tune the activation function applied in the hidden layers, namely Logistic, ReLU, Tanh which were already described in Subsection 2.3.8, and further Identity which is just a linear activation function, hence $f(z) = z$.

Regarding the optimization algorithm which refers to **`Solver`** hyperparameter, we can choose between *lbgfs*, *sgd* (Stochastic Gradient Descent) and *adam* (Adaptive Moment Estimation). The **`Learning rate`** can be either constant (i.e, 0.001), inversely scaled, i.e., gradually and inversely decreased with and inverse scaling exponent t (where t refers to the time step, by default $t = 0.5$), or adaptive, i.e., the learning rate is kept constant as long as the training loss keeps decreasing, otherwise it is divided by 5 (scikit-learn 2023f).

Table 4.16: Multi Layer Percepton - Hyperparameter Space

Hyperparameter	**Space**
Hidden layer size	<5, 500>
Activation function	Identity, Logistic, Tanh, ReLU
Solver	Adam, sgd, lbfgs
Learning rate	Constant, Adaptive, Invscaling

Source: Author's results in Python

4.4.2 Sequential Feature Selection

As the feature selection approach, Forward Sequential Feature Selection is employed in order to choose the optimal set of features as described in Section 2.8. Within machine learning implemenation, instead of fitting Forward SFS only with one model, Forward SFS is fitted for each input model in order to obtain the best subsets of features for each model, assuming the importance of each features varies across the models. Instead of using input models with default hyperparameters, each model is tuned with Bayesian Optimization in order to obtain the optimal hyperparameters for each model, which would further improve the performance of each model within SFS and therefore, it would lead to the more optimal selection of features. The custom feature selection algorithm is stated in Algorithm 1, thus, when having n input models, it returns n subsets of optimal features, one per each model:

Algorithm 1 Feature Selection Algorithm

1: **for** *model* $\in$ *models* **do**
2: *optimized_model* $\leftarrow$ BayesianOptimization(*model*)
3: *best_features* $\leftarrow$ ForwardSFS(*optimized_model*)
4: **end for**

Particularly, each input model is first tuned on the training set with Bayesian Optimization with 50 iterations and 10–fold stratified cross validation (in order to preserve the target variable distribution across the folds) while maximizing the F1 score - within author's machine learning implemenation, his custom function `bayesian_optimization()` is used. Once the model is tuned, the Forward SFS is fitted with such tuned model on the same training set with 10–fold stratified cross validation while maximizing the F1 score. Instead of selecting the fixed number of features, Scikit-learn's `SequentialFeatureSelector` class allows to set a stop criterion (`tol` parameter) which stops adding features if the objective score function is not increasing at least by `tol` between two consecutive feature additions (scikit-learn 2023a). Such paramaeter is set to the value which is close to zero, therefore the feature selection stops when the objective score function is not increasing anymore.

Such feature selection algorithm is wrapped into author's custom function `SFS_feature_selection()`. This function iteratively prints the process of the feature selection as can be seen in Figure 4.10, including the current step (Bayesian Optimization or Feature Selection), the execution time in minutes,

and the selected features per each model. Since we have 8 input models, we get 8 optimal subsets of features.

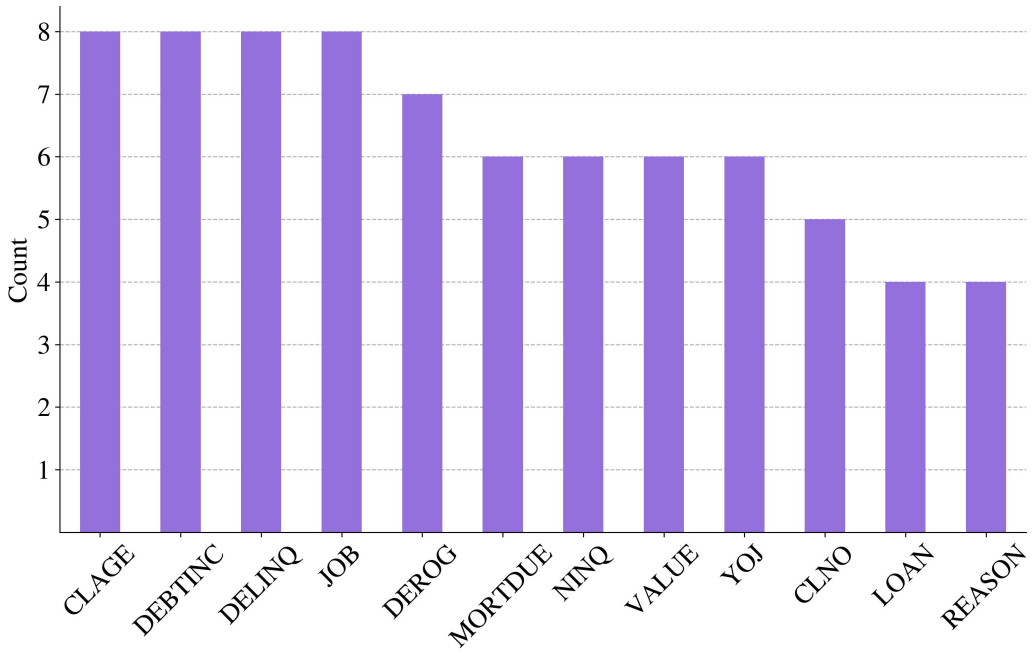
Figure 4.10: Feature Selection Print Statement

```
--------------------------------------------------------------------------------
---------------------------------------- 2/8 -----------------------------------
--------------------------------------------------------------------------------
------------------------------ FEATURE SELECTION WITH DT -------------------------
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------

1/4 ... Starting Bayesian Optimization on the whole set of features
2/4 ... Bayesian Optimization finished
3/4 ... Starting Forward Sequential Feature Selection
4/4 ... Forward Sequential Feature Selection with finished

Execution time: 0.8622 minutes

9 features selected: VALUE, JOB, YOJ, DEROG, DELINQ, CLAGE, NINQ, CLNO, DEBTINC

--------------------------------------------------------------------------------
--------------------------------------------------------------------------------


--------------------------------------------------------------------------------
---------------------------------------- 3/8 -----------------------------------
--------------------------------------------------------------------------------
------------------------------ FEATURE SELECTION WITH GNB -------------------------
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------

1/4 ... Starting Bayesian Optimization on the whole set of features
2/4 ... Bayesian Optimization finished
3/4 ... Starting Forward Sequential Feature Selection
4/4 ... Forward Sequential Feature Selection with finished

Execution time: 0.4152 minutes

6 features selected: MORTDUE, JOB, DELINQ, CLAGE, NINQ, DEBTINC

--------------------------------------------------------------------------------
--------------------------------------------------------------------------------
```

Source: Author's results in Python

The following Figure 4.11 depicts the reccurrence of the selected features. As can be seen, features such as `CLAGE`, `DEBTINC`, `DELINQ` and `JOB` were selected by each model. On the other hand, features such as `LOAN` and `REASON` were selected only four times. Therefore, it can be expected that such features which were selected every time will have significant impact in predictions.

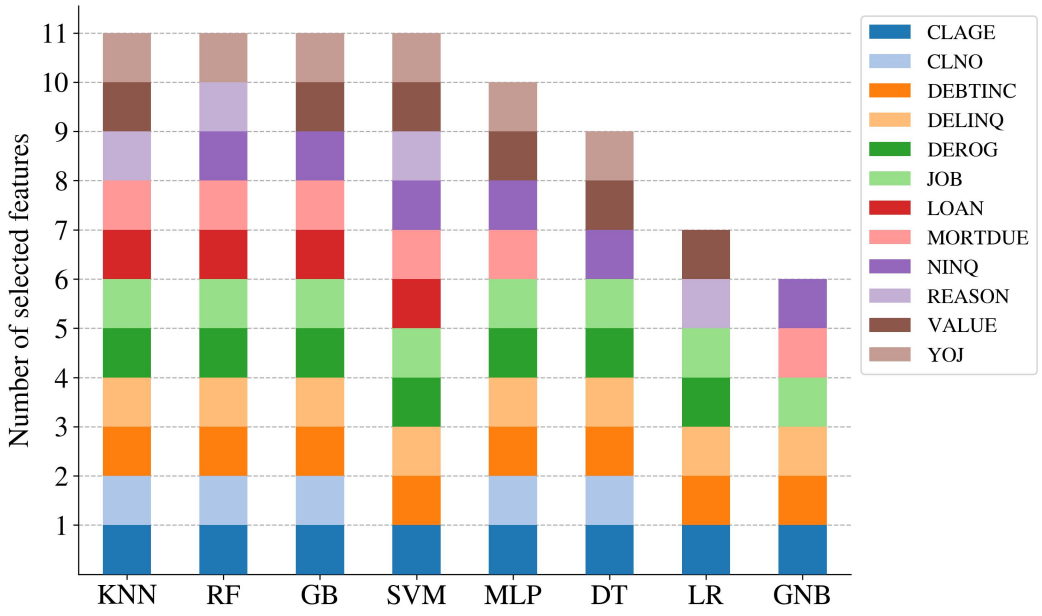
Figure 4.11: Reccurrence of Selected Features



Source: Author's results in Python

According to Figure 4.12, models such as K–Nearest Neighbors, Random Forest, Gradient Boosting and Support Vector Machine chose almost all the features as onlt one feature feature was eliminated. On the other hand, Gaussian Naive Bayes chose only 6. It seems to be that most of the features are important as each model has selected a higher amount of features. It is evident the more comples and/or black–box models require more features in contrast to transparant models such as Logistic Regression or Gaussian Naive Bayes.

Figure 4.12: Distribution of Selected Features per Model



Source: Author's results in Python

4.4.3 Model Selection

In combination with the pre–selected subsets of features, the next step regards the selection of the final model which will be further used within an evaluation and the deployment. The algorithm process is described in Algorithm 2 below:

Algorithm 2 Model Selection Algorithm

```
for model ∈ models do
    for features ∈ features_subsets do
        optimized_model ← BayesianOptimization(model, features)
        for metric ∈ evaluation_metrics do
            performance ← Evaluation(optimized_model, metric)
        end for
    end for
end for
```

Therefore, each input model is tuned on each subset of features selected within feature selection on the training set and subsequently, the optimized model is evaluated on the validation set. Thus, when having n input models and m subsets of selected features, we get $n \times m$ tuned models. $m \leq n$ because we exclude duplicated subset of selected features which can occur when more than one model choose the same subset(s) of features. Since there are 8 input

models and 8 unique subsets of selected features, the total number of tuned models is 64.

Metrics Space

When evaluating classification models using class-based metrics such as F1 score, Precision, Recall, Accuracy, Matthews Correlation Coefficient, a default classification threshold of 0.5 is often used. This threshold separates predicted classes based on whether the predicted probability score is higher or lower than 0.5. However, in real-world use cases, the 0.5 classification threshold may not be appropriate and according to (Esposito *et al.* 2021), such threshold is not appropriate when having imbalanced ata. Therefore, it is recommended to calculate an optimal threshold rather than relying on the default one. For such case, the Youden index is employed which is derived from ROC curve and enables the selection of an optimal classification threshold value. The Younden index searches for the threshold that maximizes the sum of True Positive Rate and True Negative Rate, decreased by 1 (Fluss *et al.* 2005), thus:

$$J = TPR + TNR - 1 \tag{4.8}$$

Mathematically, the optimal threshold using Youden index is derived as follows:

$$T_{opt} = \text{argmax}_{t\in[0,1]}\,(J) \tag{4.9}$$

In Python, the `roc_curve` function from `Scikit-learn` returns False Positive Rate instead of the True Negative Rate. Nevertheless, we can derive the True Negative Rate from False Positive Rate as follows:

$$TNR = 1 - FPR \tag{4.10}$$

Therefore:

$$T_{opt} = \text{argmax}_{t\in[0,1]}\,(TPR + (1 - FPR) - 1) \tag{4.11}$$

Note, that the optimal threshold is calculated based on the training set and henceforth is applied within the evaluation on validation set.

In order to ensure a more comprehensive and unbiased evaluation of a model's performance, it is recommended to consider multiple metrics rather than relying on a single metric alone. This approach provides a more generalized overview

of the model's performance across different aspects and helps to prevent any bias towards a single metric. To accomplish this, models can be ranked based on their performance on each individual metric, where a higher score or a lower loss indicates a better model, resulting in a higher rank for that metric. Subsequently, for each metric, the ranking of the models is determined, and the final ranking is calculated as a weighted average of these individual rankings. The weights have been set expertly and are summarized in Table 4.17.

Specifically, the highest weight (1.5) is assigned to the F1 score, which provides a balanced measure of a model's performance with respect to both False Positives and False Negatives. This metric is commonly used in classification tasks, particularly in imbalanced data sets, such as the validation set in our case, which has not been oversampled. In addition to the F1 score, higher weight is assigned to the Recall score as well (1.2), which is a metric that penalizes False Negatives. False Negatives occur when the model predicts a negative result (i.e., no default) for an instance that is actually positive (i.e., default). In the context of loan applications, one may prefer to reject a loan applicant who would not have defaulted (False Positive) rather than approving the application of a client who would have defaulted (False Negative). Therefore, it is appropriate to give higher weight to Recall in order to reduce the likelihood of False Negatives. Henceforth, the weights are assigned to different metrics based on their relevance to the models' ranking, with the highest weight given to F1 score and additional weight given to Recall to ensure that False Negatives are minimized.

Table 4.17: Model Ranking Weights table

Metric	Weight
F1 score	1.5
Recall	1.2
Precision	1
Accuracy	1
AUC	1
Somers' D	1
Kolmogorov Smirnov	1
Matthews Correlation Coefficient	1
Brier Score Loss	1

Source: Author's results in Python

Particularly, for each model a rank score is calculated in order to determine the final rank. The lower rank score indicates better model performance. For particular model M, the rank score as weighted sum of the individual ranks as follows:

$$RankScore_M = \frac{\sum_{i=1}^{k} r_i \times w_i}{\sum_{i=1}^{k} w_i} \tag{4.12}$$

where k is the number of metrics used to evaluated the model M, r_i is the rank order of i–th metric for given model M and w_i is the weight assigned to the i–th metric. Such metric lies in interval $< 1, k >$, where 1 would indicate a perfect model performance across the all metrics.

QUESTION: Should we also add this metric for better interpretability or is the metric defined above sufficient?

For better interpretability, we can normalize the rank scores which would range from 0 to 1 where 1 would indicate a perfect performance of the model.

$$NormRankScore_M = 1 - \frac{RankScore_M - k}{k - 1} \tag{4.13}$$

Model Selection Results

The custom function `model_selection()` iteratively prints the process of the model tuning and evaluation on each subset of features, in order to keep the track of such process as it is depicted in Figure 4.13. Particularly, it prints which model on which features is being tuned and evaluated, exeuction time, optimal threshold, F1 score on the validation set and the best hyperparameters.

Figure 4.13: Model Selection Print Statement

```
--------------------------------------------------------------------------------
------------------------------------ 56/64 -------------------------------------
--------------------------------------------------------------------------------
--------------------------- BAYESIAN OPTIMIZATION OF SVM ------------------------
-------------------------- WITH FEATURES SELECTED BY MLP -------------------------
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------

1/2 ... Starting Bayesian Optimization on the subset of features (10 features):
        MORTDUE, VALUE, JOB, YOJ, DEROG, DELINQ, CLAGE, NINQ, CLNO, DEBTINC
2/2... Bayesian Optimization finished

Execution time: 22.0695 minutes

F1 Score on Validation set: 0.7102272727272726

Optimal classification threshold: 0.6477

Tuned hyperparameters of SVM:

    C: 4.999999999999999
    break_ties: False
    cache_size: 200
    class_weight: balanced
    coef0: 0.0
    decision_function_shape: ovr
    degree: 1
    gamma: scale
    kernel: rbf
    max_iter: -1
    probability: True
    random_state: 42
    shrinking: False
    tol: 1.102507160381566e-09
    verbose: False

--------------------------------------------------------------------------------
--------------------------------------------------------------------------------
```

Source: Author's results in Python

The final output of the function `model_selection()` is table which summarizes the model's computed metrics as depicted in Table 4.18. As can be seen, the best models in terms of ranking are the Gradient Boosting models which in general have the highest score metrics and the lowest loss metrics. On the other hand, the worst-performing models are Gaussian Naive Bayes models.

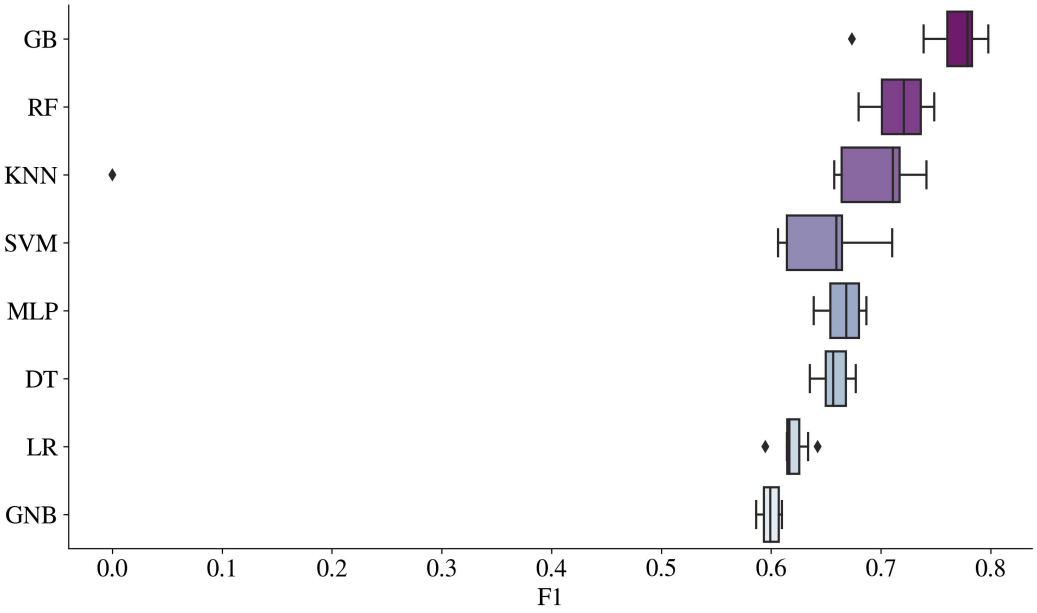
Table 4.18: Model Selection Results

Tuned model	**FS model**	# Features	Time	Thres	F1	Prec	Rec	Acc	AUC	SD	KS	MCC	JC	BS	Log Loss	Score	Rank
GB	MLP	10	738.19	0.4955	0.7809	0.7853	0.7765	0.9128	0.9515	0.9030	0.7751	0.7265	0.6406	0.0666	0.2487	3.48	1
GB	KNN	11	767.90	0.5072	0.7978	0.7912	0.8045	0.9184	0.9587	0.9175	0.7989	0.7467	0.6636	0.0687	0.4135	3.82	2
GB	SVM	11	904.84	0.5053	0.7896	0.8155	0.7654	0.9184	0.9555	0.9109	0.7961	0.7397	0.6524	0.0718	0.3486	4.17	3
GB	GB	11	686.26	0.4132	0.7799	0.7778	0.7821	0.9117	0.9543	0.9086	0.7989	0.7247	0.6393	0.0703	0.3372	4.29	4
GB	RF	11	802.55	0.4973	0.7775	0.7841	0.7710	0.9117	0.9541	0.9081	0.7961	0.7225	0.6359	0.0669	0.2803	4.37	5
RF	KNN	11	356.24	0.4725	0.7486	0.7326	0.7654	0.8972	0.9226	0.8452	0.7109	0.6843	0.5983	0.0923	0.3232	8.66	6
GB	DT	9	719.92	0.4729	0.7675	0.7697	0.7654	0.9073	0.9407	0.8814	0.7556	0.7096	0.6227	0.0808	0.4693	8.87	7
RF	GB	11	310.63	0.4517	0.7385	0.7135	0.7654	0.8916	0.9200	0.8400	0.7123	0.6709	0.5855	0.0886	0.3135	9.47	8
RF	MLP	10	397.42	0.4761	0.7357	0.7181	0.7542	0.8916	0.9179	0.8358	0.7081	0.6679	0.5819	0.0879	0.3084	10.39	9
GB	LR	7	1008.69	0.4362	0.7388	0.7000	0.7821	0.8894	0.9219	0.8438	0.7081	0.6706	0.5858	0.0886	0.3925	10.79	10
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
DT	MLP	10	54.19	0.5000	0.6427	0.6374	0.6480	0.8559	0.8133	0.6266	0.5810	0.5524	0.4735	0.1254	2.0008	50.38	55
GNB	GB	11	23.04	0.1829	0.5970	0.4893	0.7654	0.7933	0.8531	0.7063	0.5810	0.4880	0.4255	0.1310	0.6461	50.50	56
GNB	KNN	11	22.98	0.3588	0.6093	0.5219	0.7318	0.8123	0.8479	0.6957	0.5698	0.5024	0.4381	0.1367	0.6686	50.81	57
GNB	DT	9	23.11	0.2241	0.6063	0.5095	0.7486	0.8056	0.8467	0.6935	0.5768	0.4991	0.4351	0.1316	0.6370	50.85	58
GNB	MLP	10	23.11	0.2194	0.6013	0.5000	0.7542	0.8000	0.8493	0.6986	0.5768	0.4930	0.4299	0.1319	0.6360	50.99	59
DT	GNB	6	53.14	0.5000	0.6354	0.6284	0.6425	0.8525	0.8187	0.6375	0.5838	0.5430	0.4656	0.1251	2.1679	51.74	60
GNB	GNB	6	23.05	0.4787	0.5950	0.5039	0.7263	0.8022	0.8356	0.6711	0.5559	0.4835	0.4235	0.1470	0.5280	54.53	61
LR	GNB	6	95.14	0.4561	0.5948	0.5121	0.7095	0.8067	0.8379	0.6758	0.5531	0.4831	0.4233	0.1319	0.4180	54.97	62
GNB	SVM	11	22.91	0.1991	0.5885	0.4872	0.7430	0.7922	0.8425	0.6850	0.5712	0.4756	0.4169	0.1345	0.6721	55.15	63
GNB	RF	11	23.25	0.3413	0.5864	0.4943	0.7207	0.7966	0.8288	0.6577	0.5545	0.4720	0.4148	0.1486	0.7040	57.85	64

Source: Author's results in Python

In order to gain a more detailed understanding of the model selection results, the distribution of computed metrics is plotted. In Figure 4.14, the F1 score distribution is visualized for each input model. An outlier can be observed in KNN where the F1 score is 0.

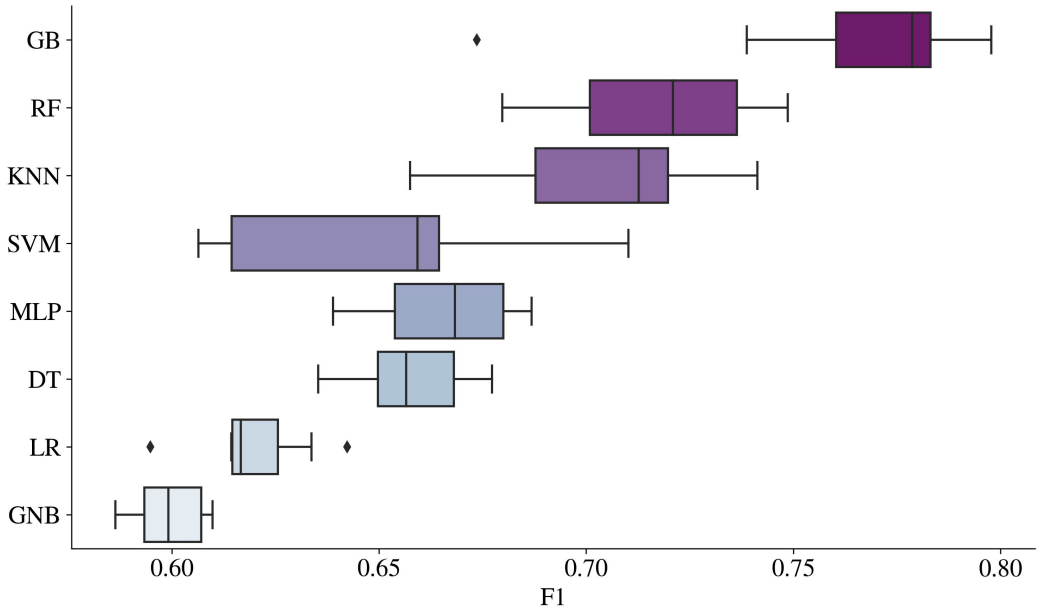
Figure 4.14: F1 Score Distribution



Source: Author's results in Python

Such outlier is removed in Figure 4.15 to gain a more general insight into the F1 score distribution. It can be observed that Gradient Boosting models have the highest F1 scores of around 80 %. Another tree ensemble model, Random Forest, is performing well as the second best. However, more transparent models such as Logistic Regression and Naive Bayes are performing poorly, having F1 scores around 60 %. Surprisingly, black box models such as Support Vector Machine and Neural Network are outperformed by the less complex KNN model. Nonetheless, given the relatively small sample size, KNN performs better than Neural Network and non-linear SVM on small data sets.

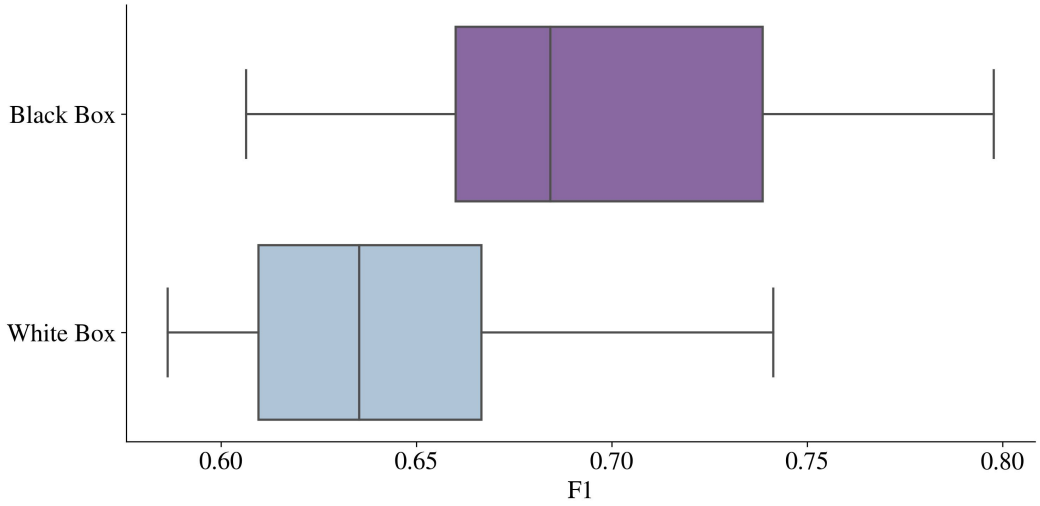
Figure 4.15: F1 Score Distribution - without outlier



Source: Author's results in Python

As depicted in Figure 4.16, the distribution of F1 score (without the outlier) across the model type. Although, both score distributions overlap, it is evident, that black–box models outperform white–box model in terms of F1 score in overall as expected.

Figure 4.16: F1 Score Distribution (Black–box/White–box dimension) - without outlier

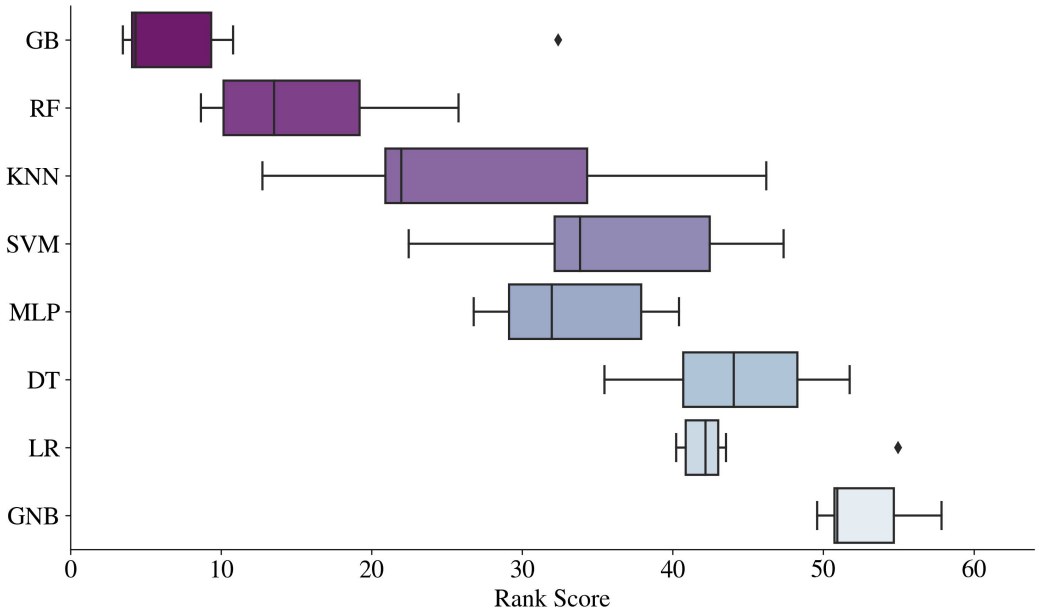


Source: Author's results in Python

We can also consider not only F1 score but also other metrics, which is

quantified in the rank score calculated according to Equation 4.12. As shown in Figure 4.17, we can observe that the order of models ranked by the rank score is identical as the order of the models ranked by F1 score in Figure 4.14. Hence, across all the metrics, the Gradient Boosting perform the best in overall while Gaussian Naive Bayes do not perform well at all.

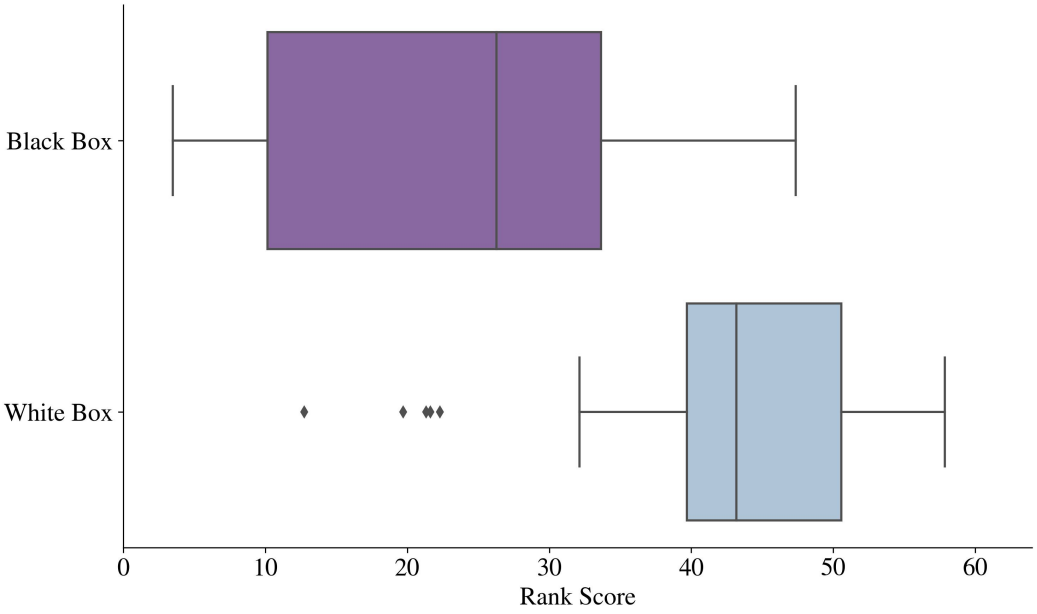
Figure 4.17: Rank Score Distribution



Source: Author's results in Python

As expected, also, the black–box models are ranked higher than the white–box models according to the rank score as shown in Figure 4.18. This is evident also from Table 4.18 where the black–box models, namely Gradient Boosting and Random Forest, dominated amongst the first 10 ranked models.

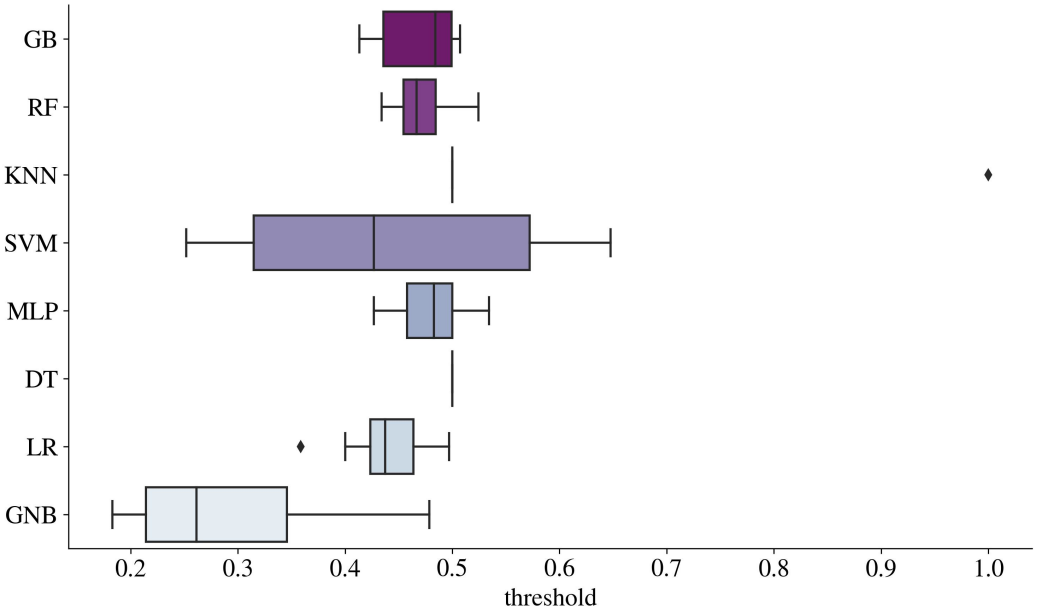
Figure 4.18: Rank Score Distribution (Black–box/White–box dimension)



Source: Author's results in Python

The optimal threshold distribution for each base model is presented in Figure 4.19. We can observe an outlier in KNN having a threshold value of 1, which explains the F1 score outlier found previously in Figure 4.14.

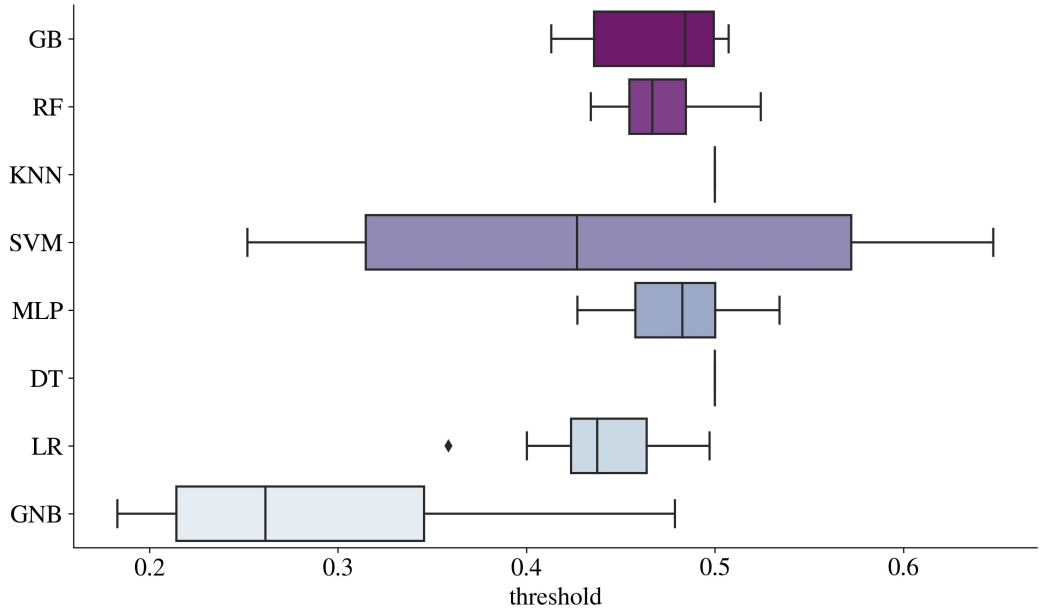
Figure 4.19: Threshold Distribution



Source: Author's results in Python

In order to obtain a better insight into the distribution of optimal thresholds, the outlier in KNN is excluded, resulting in the threshold distribution depicted in Figure 4.20. The optimal threshold values are mostly distributed below 0.5, indicating that the models are generally more conservative. The most conservative model is Gaussian Naive Bayes, which has a median threshold value around 0.25.

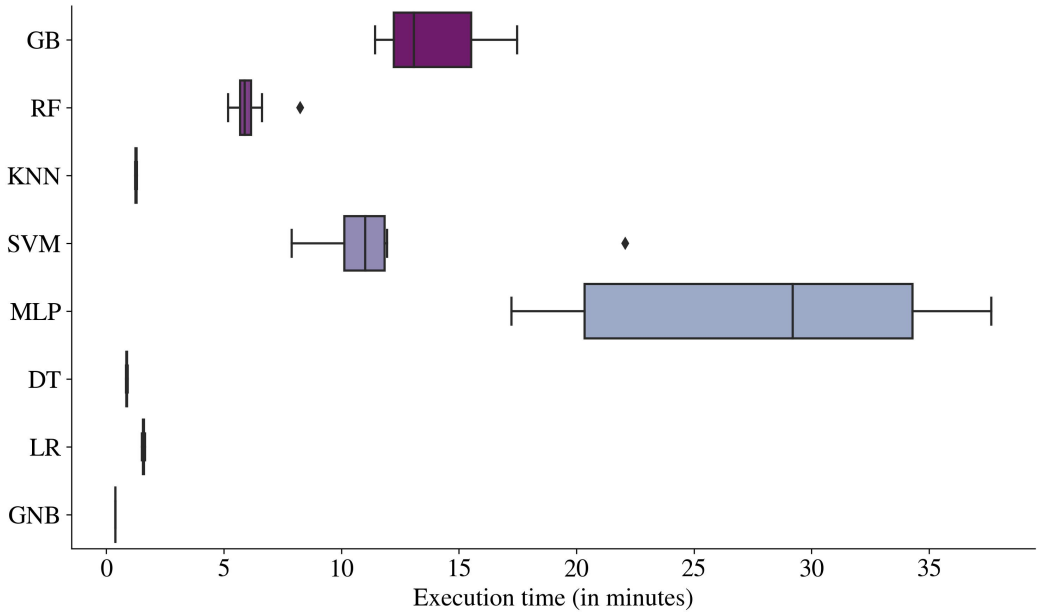
Figure 4.20: Threshold Distribution - without outlier



Source: Author's results in Python

Upon examining the execution time of each model, it can be observed that the transparent and non-complex models such as Logistic Regression, Gaussian Naive Bayes, or even Decision Tree, which take around only 1 minute to optimize themselves, also perform poorly, as already inspected in Figure 4.15. Conversely, the most time-consuming models are undoubtedly the Neural Network models, which take around 30 minutes to optimize themselves. Other time-consuming models include Gradient Boosting and Support Vector Machine, which take around 13 and 11 minutes to optimize themselves, respectively. This finding suggests that longer execution time does not necessarily lead to better performance, as the Neural Network models are significantly outperformed by several other models.

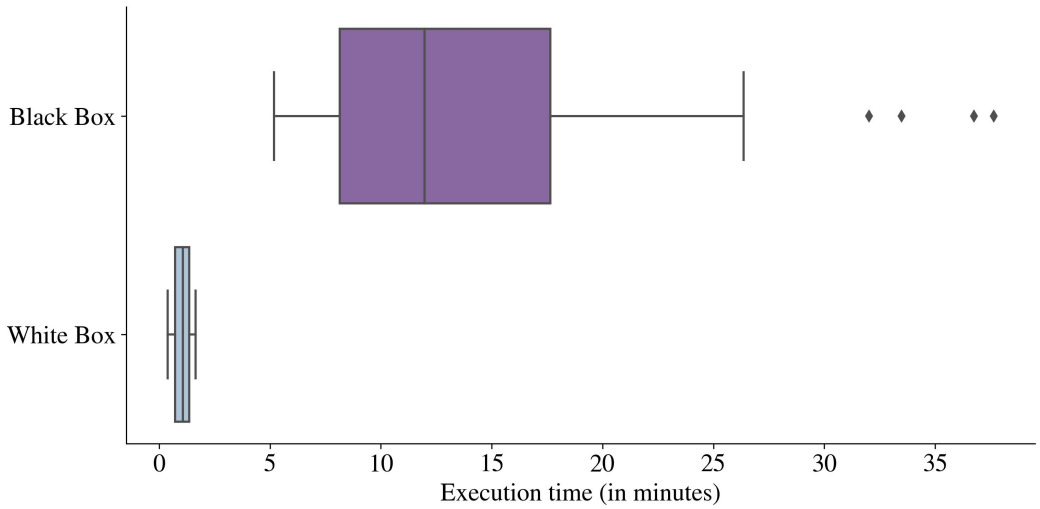
Figure 4.21: Execution Time Distribution



Source: Author's results in Python

We can inspect the execution from another perspective as shown in Figure 4.22. It can be observed that black–box models take a significant amount of time ot opimize than the white–box models which is given due to the complexity of the black–box models.

Figure 4.22: Execution Time Distribution (Black–box/White–box dimension)

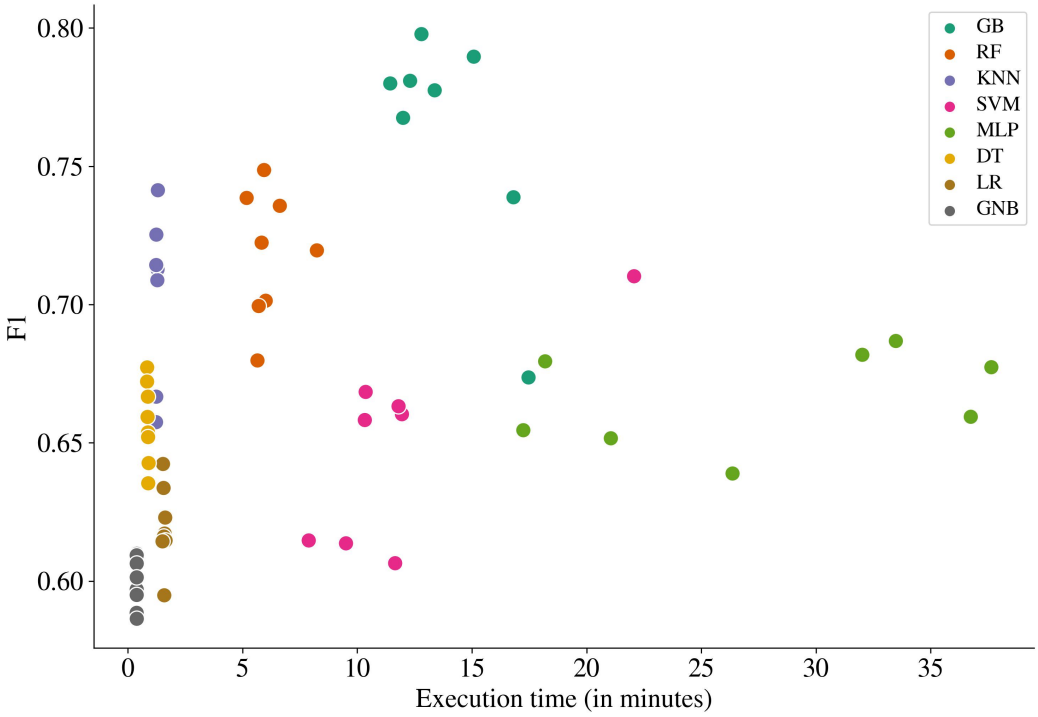


Source: Author's results in Python

The execution time and the F1 score are inspected together using a scat-

terplot, as shown in Figure 4.23. A cluster of non-complex and transparent models, such as Logistic Regression, Gaussian Naive Bayes, Decision Tree, and KNN, can be observed around the vertical line near 0 execution time. These models are quick to optimize, but their F1 scores are generally low, except for KNN. Further, their variance in execution time is quite low, regardless of the feature subset they are optimized on. On the other hand, the Neural Network models always perform poorly, regardless of the length of the execution time. Furthermore, the variance of the F1 scores is quite low for these models, indicating that the execution time does not have a significant impact on the F1 score in the case of Neural Networks.

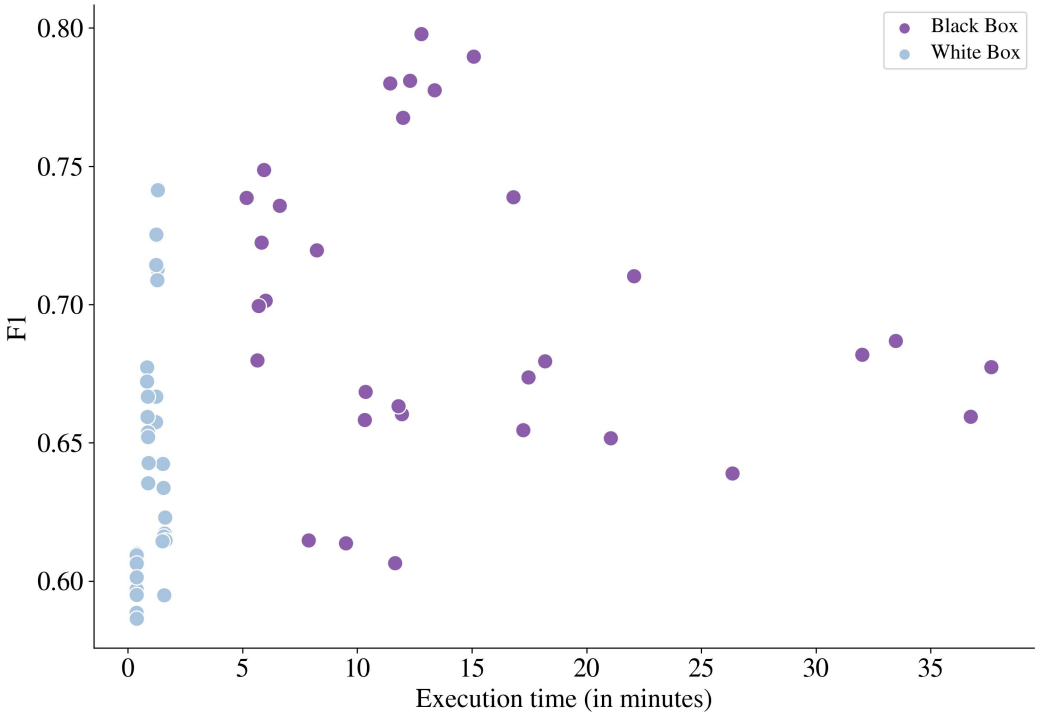
Figure 4.23: Execution Time vs. F1 Scatterplot - without outlier



Source: Author's results in Python

Such separation of of the black–box and white–box models is more evident from Figure 4.24 where the white–box models points are light blue-colored and the black–box models are purple-colored. While the execution time of white–box models seems to be constant regardless the score, the points of black–box models are more dispersed across the execution time–F1 dimension.

Figure 4.24: Execution Time vs. F1 Scatterplot (Black–box/White–box dimension) - without outlier



Source: Author's results in Python

To summarize this subsection, the best and final model is the Gradient Boosting Classifier which was optimized on the subset of features selected by Multi-Layer Percepton - both the model information and its final hyperparameters' values are described in Table 4.19. Such model is then used in the next modelling steps, including the recalibration, evaluation and deployment.

Table 4.19: Final Model Information

Final Model	Gradient Boosting
FS Model	Multi–Layer Percepton
Final Features	MORTDUE, VALUE, JOB, YOJ, DEROG, DELINQ, CLAGE, NINQ, CLNO, DEBTINC
Threshold	0.4955
F1	0.7809
# estimators	1,000
Criterion	Friedman MSE
Max depth	10
Max features	1
Loss	Log loss
Learning rate	0.0150

Source: Author's results in Python

4.4.4 Model Recalibration

In order to ensure that the final model performs well on unseen data, it is common practice to employ the recalibration approach, which involves retraining the model on both the training and validation sets. By doing so, the sample size used for training is increased. As such, the retraining (or so called recalibration) model lead (or are expected to lead) to markedly improved model performance (de Hond *et al.* 2023). The recalibrated model is then used to evaluate the performance of the final model on the test set, which is the ultimate measure of a model's performance.

In addition to recalibrating the final model, it is crucial to recalibrate the threshold value for assigning class labels based on predicted probabilities. The optimal threshold value can be determined using the training and validation sets. Such threshold is recalibrated based on the training and validation set. In this thesis, the optimal threshold value is found to be **0.45109**, which is then used for evaluating the final model's performance on the test set. By recalibrating the threshold value, the model's performance is further improved, resulting in more accurate predictions. After the recalibration process, we can observe that the model is more conservative as its optimal classification threshold has decreased. The impact on the model's performance is further assessed in Subsection 4.5.1.

Moreover, the recalibration process helps to mitigate overfitting issues, which occur when the model is only trained on the training set. By incorporating the validation set into the training process, the recalibrated model can better generalize to new data and improve its overall performance on the test set. The inclusion of the validation set during the recalibration process does not cause any data leakage issues since this set was already used during model selection to evaluate each model's performance. Therefore, using the validation data for recalibration is a sound practice that helps to ensure the reliability and accuracy of the final model.

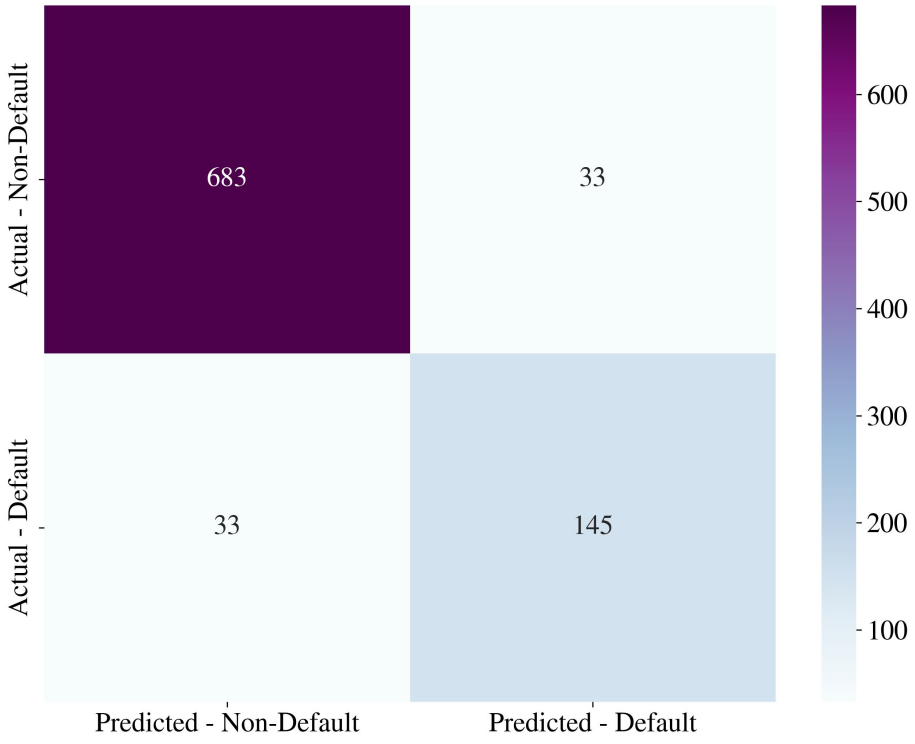
4.5 Model Evaluation

After recalibrating the model and threshold, the final step in evaluating the model's performance is to test it on previously unseen data, specifically the test set. This evaluation is critical to determine whether the model can generalize well to new data beyond the training, feature selection, and model selection phases. During the evaluation, the recalibrated classification threshold of 0.45109, determined in the model recalibration process, is also used.

4.5.1 Model Performance Assessment

In Figure 4.25, the confusion matrix for the final model, based on the test set and using the recalibrated threshold, is presented. The matrix shows that the model is generalizing well, having correctly predicted 145 defaults and misclassified only 33 defaults and further, correctly predicted 683 non–defaults and misclassified only 33 non–defaults. Such a result indicates that the model is a good fit for the data and can provide useful predictions for the problem at hand.

Figure 4.25: Confusion Matrix



Source: Author's results in Python

In order to obtain a better understanding of the model's performance on previously unseen data, we computed several metrics that were used during the model selection process. These metrics are presented in Table 4.20. The results indicate that the model performs well on the unseen data, with most of the scores metrics around 80 % to 90 %. Furthermore, the loss metrics are relatively low, indicating that the model can effectively distinguish between defaults and non-defaults. Overall, these results suggest that the model is performing well and is suitable for predicting defaults. The results suggest that the model has a good balance between correctly identifying defaults and non-defaults, as well as minimizing false positives and false negatives. This further confirms the model's ability to accurately predict defaults.

Table 4.20: Metrics Evaluation

Metric	Value
F1	0.8146
Precision	0.8146
Recall	0.8146
Accuracy	0.9262
AUC	0.9564
Somers' D	0.9128
KS	0.7915
MCC	0.7685
Brier Score Loss	0.0594
Log Loss	0.2163

Source: Author's results in Python

The following Table 4.21 shows the impact of recalibration on the model's performance metrics. M_{NR} denotes the final model which was not recalibrated at all (i.e., was trained only on the training set), whereas M_R denotes the recalibrated model (i.e., trained on the joined training and validation set). Respectively, M_{NR} uses its threshold computed bas on the training set (0.4955), and M_R uses its threshold computed on the joined training and validation set(0.45109). As can be seen, the recalibration indeed has a positive impact on the metrics evaluation as all the metric scores have increased, while the metric loss functions decreased. We can observe the most significant decrease in the Log Loss function, which decreased by 8.09 %, while the objective function F1 score has increased by 3.30 % thanks to to increase in both Precision and

Recall. Therefore, the recalibration process is deemed desired and appropriate in terms of model's performance.

Table 4.21: Recalibration Impact on Metrics Evaluation

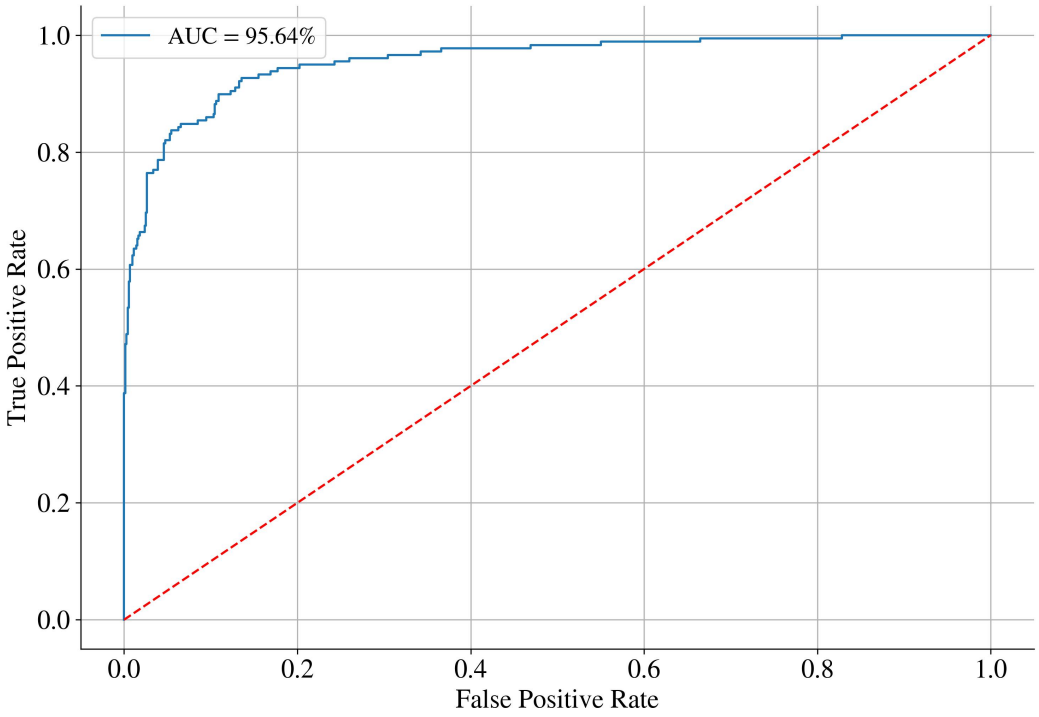
Metric	M_{NR}	M_R	**Diff.**
F1	0.7886	0.8146	3.30 %
Precision	0.8023	0.8146	1.53 %
Recall	0.7753	0.8146	5.07 %
Accuracy	0.9172	0.9262	0.98 %
AUC	0.9518	0.9564	0.48 %
Somers' D	0.9037	0.9128	1.01 %
KS	0.7845	0.7915	0.89 %
MCC	0.7373	0.7685	4.23 %
Brier Score Loss	0.0632	0.0594	-6.11 %
Log Loss	0.2353	0.2163	-8.09 %

Source: Author's results in Python

To further evaluate the performance of the (recalibrated) model, we can visualize the ROC curve, as presented in Figure 4.26. The curve illustrates the trade-off between the true positive rate and the false positive rate at various classification thresholds. An ideal ROC curve should have an area under the curve (AUC) value of 100 %, indicating a perfect classifier, while a random classifier would have an AUC of 50 %.

From the curve, we observe that the AUC value of the model is 95.55 %, indicating a high degree of accuracy in distinguishing between defaults and non-defaults. The curve covers most of the area under the diagonal line, indicating that the model is performing well in differentiating the two classes. Therefore, the results suggest that the model is performing well and is capable of accurately identifying potential defaulters.

Figure 4.26: ROC Curve



Source: Author's results in Python

4.5.2 Model Explainability

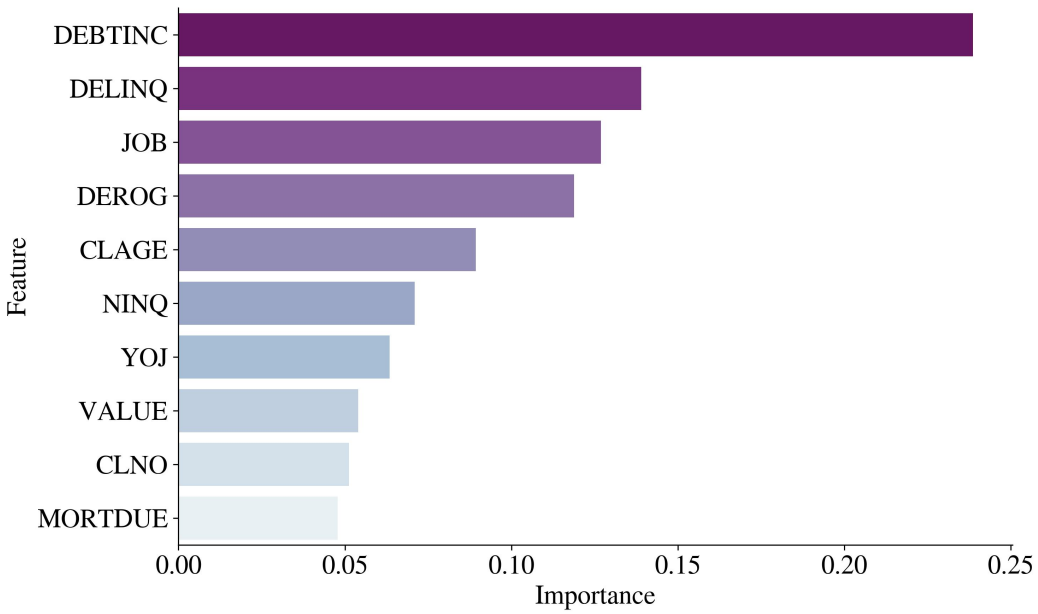
To gain insights into the impact of the features used in the final model, we can inspect the feature imporances of the final model, which is a part of family of tree ensemble algorithms. As the names indicates, it is the score value representing the importance of the features, i.e., the higher score, the more important the feature is. Basically, it is the measure of how much a feature contributes to the overall performance of the model. Overall, the feature importance plot provides valuable insights into the factors that are most important in predicting loan defaults. It can be used to identify which features are contributing the most to the model's accuracy and to guide future feature selection efforts. According to Bonaccorso (Bonaccorso 2020), feature importance is the measure proportional to the impurity reduction that a particular feature allows us to achieve, and is defined as:

$$\mathrm{FI}\left(\bar{x}^{(i)}\right) = \frac{1}{N}\sum_{k=1}^{N}\sum_{j=1}^{L}\frac{n(j)}{M}\delta I_j^i \tag{4.14}$$

where $\text{FI}\left(\bar{x}^{(i)}\right)$ referes to the feature importance of the feature i, $n(j)$ is the number of samples reaching the node j, δI_j^i represents the impurity reduction at node j after the splitting using the feature j, M is total number of samples in the data set used to built the model, and N refers to the number of tree estimators used within an ensemble model.

The following Figure 4.27 depicts the feature importances of all the selected features on which the model was trained. The two most important features used in the final model are `DEBTINC` and `DELINQ`, which are crucial delinquency indicators in determining whether a borrower would be able to repay their loan. These two features have a significant impact on the model's ability to accurately predict loan defaults, with high feature importance scores. This is also in line with the findings from the exploratory analysis, WoE distribution or feature selection.

Figure 4.27: Feature Importance



Source: Author's results in Python

Thus, understanding the impact of individual features on model performance can be useful in identifying areas for improvement, as well as in identifying the most significant factors that drive loan defaults. By focusing on these important features, lenders and policymakers can better understand and address the underlying factors that contribute to default risk, ultimately leading to better lending decisions and improved outcomes for borrowers and lenders alike.

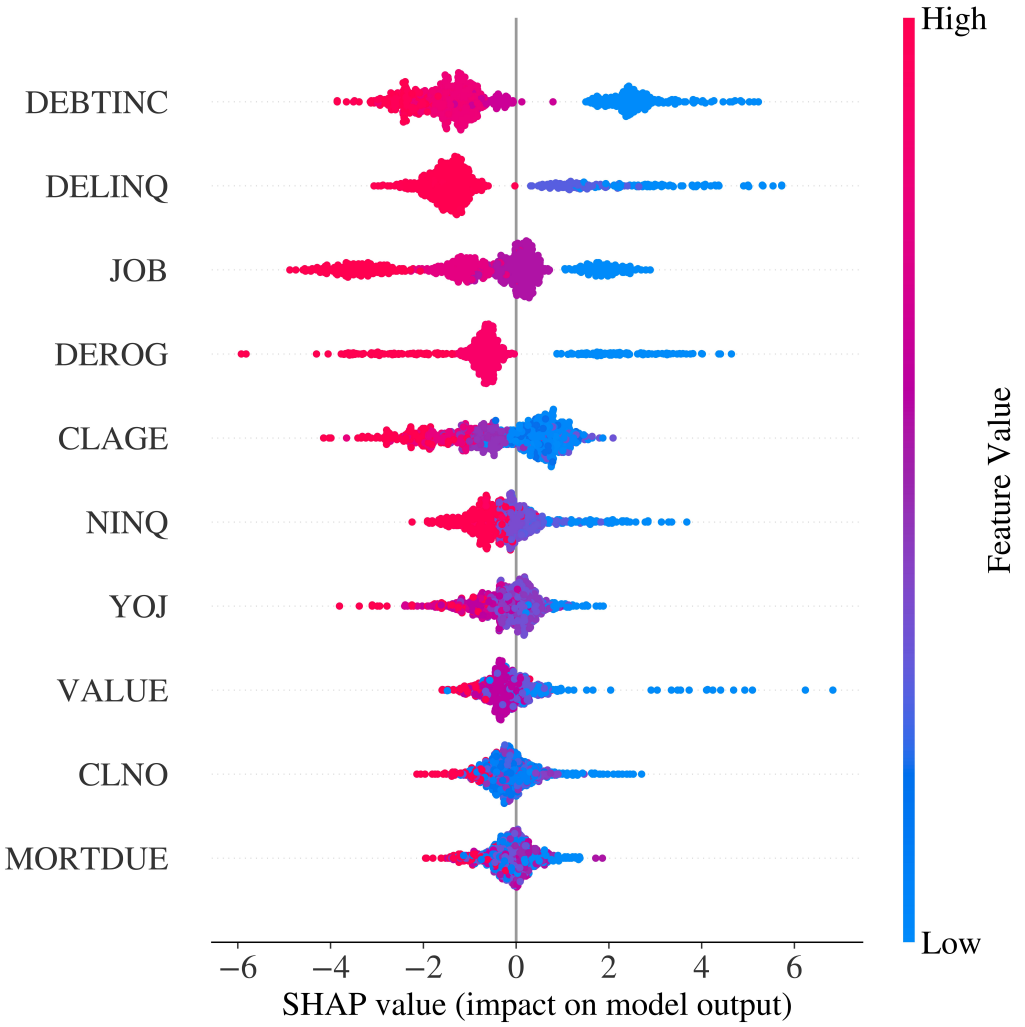
ADD BRIEF THEORY ABOUT THE SHAP VALUES

To gain further insights into the impact of the features on the final model's predictions, the SHapley Additive exPlanations (henceforth SHAP) summary plot is displayed in Figure 4.28. The SHAP summary plot provides a clear visualization of the contribution each feature makes to a prediction and is used for a black box model explainability. Each dot in the plot represents a feature and its corresponding SHAP value. The color of the dot represents the feature's value, with red indicating high values and blue indicating low values. The position of the dot on the x-axis represents the impact of the feature on the prediction, with features on the right-hand side contributing more positively to the prediction, and features on the left-hand side contributing more negatively.

Since our data points are encoded in WoE values, the higher (the more positive) value, the larger distribution of non-defaulters compared to defaulters, and vice versa, the lower (the more negative) value, the larger distribution of defaulters compared to non-defaulters. For the most important features, we can observe that the blue values (negative WoE values) and red values (positive WoE values) are quite separable. Negative WoE values are positively contributing to the predictions, and the positive WoE values are negatively contributing to the predictions. This means that the more negative the WoE value, the more likely the borrower is to default, and vice versa.

Overall, the SHAP summary plot provides a valuable tool for interpreting and understanding the complex decision-making process of the final model. The plot enables us to examine the impact of individual features on the model's output and helps us to identify which features are most influential in the model's decision-making process. By understanding the relative importance of each feature, we can gain deeper insights into the creditworthiness assessment process and make more informed decisions in the lending industry.

Figure 4.28: SHAP Summary Plot



Source: Author's results in Python

4.6 Machine Learning Deployment

This section describes the process of taking a trained machine learning model and making it available for use in the real world. It involves taking the model from a development environment and integrating it into a production environment where it can be used to make predictions or decisions based on new data. In this thesis, the machine learning model is deployed as web application using Flask and HTML.

4.6.1 Final Model Recalibration

Before deploying the model in a production setting, a meticulous process is undertaken to ensure optimal performance. This involves conducting a final recalibration of the model using the entire data set, comprising the training, validation, and test sets. The purpose of this recalibration is to fine-tune the model parameters, thereby maximizing its ability to generalize and yield accurate predictions.

The test set, which has been employed previously during the model evaluation phase, is incorporated into the recalibration process without any risk of data leakage. By including the test set, the sample size for training is expanded, thereby increasing the model's capacity to generalize effectively.

Upon completion of the recalibration, the final classification threshold for deployment is determined to be **0.3358**. This value is derived from a comprehensive analysis of the training, validation, and test sets, which ensures that the model's generalization capabilities are further enhanced for optimal performance in real-world applications.

4.6.2 Flask and HTML Web Application

In this case, the machine learning model was deployed into a web application using Flask and HTML. The application is temporarily deployed on the Cloud server on the **PythonAnywhere** platform and is accessible here: `http://ml-credit-risk-app-petrngn.pythonanywhere.com/`. However, the application will be shut down after the thesis defense and will not be available online anymore due to the budget reasons. Nevertheless, the code for the application

is available in the GitHub repository, and the application can be run locally using any Python compiler.

Furthermore, prior to deployment, we need to prepare several Python inputs for the web application, including:

- **Model** - the final model recalibrated on the training, validation and test set.
- **Threshold** - the final classification threshold recalibrated on the training, validation and test set.
- **Features** - the final features used in the final model.
- **Data Frame** - the input tabular object used in the web application to store the loan applicant's inputs.
- **Optimal Binning Transformator** - fitted `BinningProcess` object for binning and WoE-encoding of the loan applicant's inputs.
- **WoE Bins** - a set of bins and WoE values used for mapping the WoE values to missing values.
- **LIME explainer** - fitted `LimeTabularExplainer` object for local explainability of model's prediction.

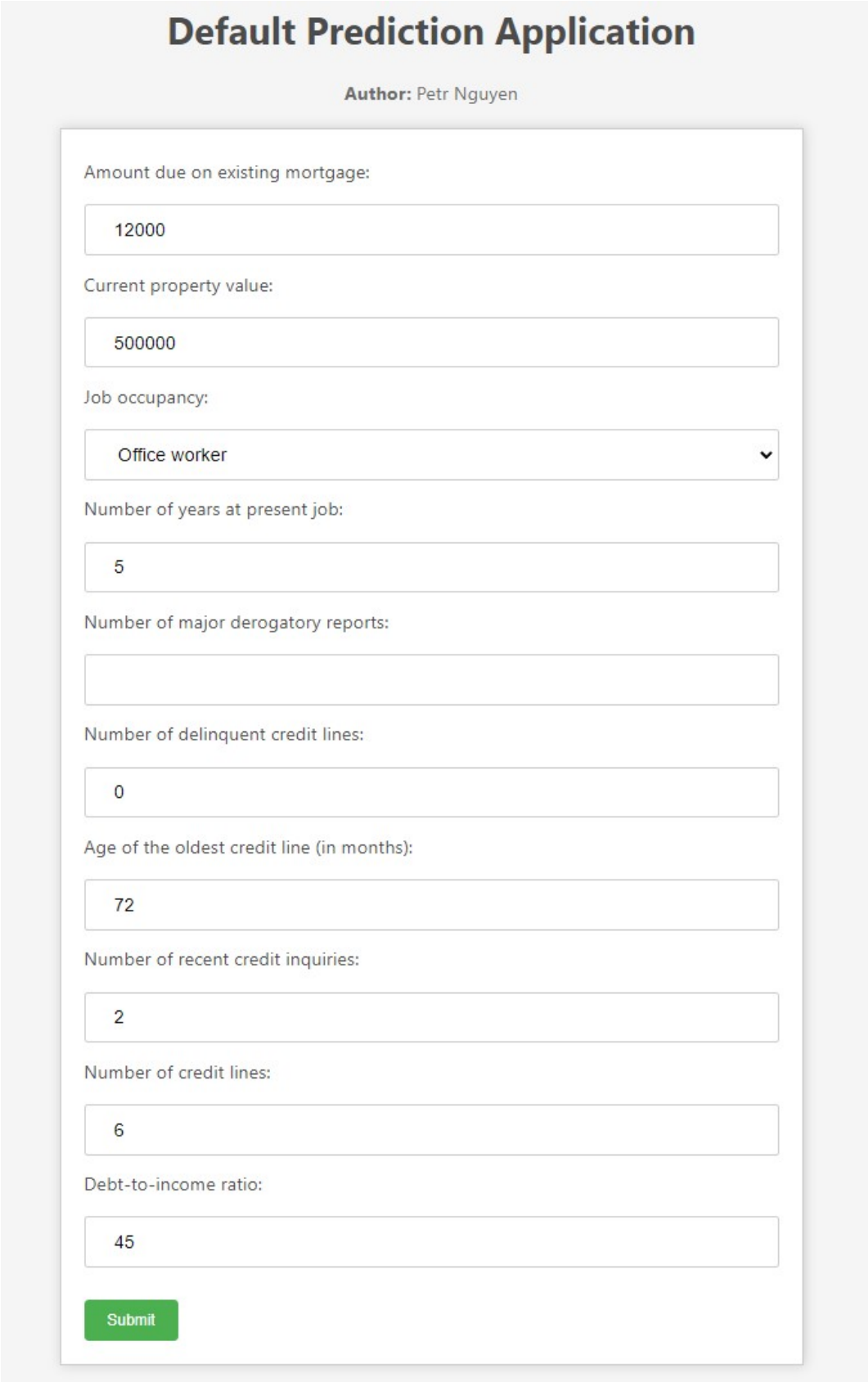
Such inputs required for the machine learning application are exported in the `.pkl` format using the `dill` module. This format allows for efficient and easy-to-use serialization and deserialization of the inputs. The pickled file is then loaded directly into the Flask application.

For the back-end of the web application, Flask is used to deploy the machine learning model. The Flask application is written in the `app.py` file, which is stored in the `flask_app` directory. The front-end of the web application is coded in HTML, with CSS and JavaScript elements used to enhance the user interface.

The web application first renders a HTML page, as shown in Figure 4.29. This page contains a loan application form, in which the user or the loan applicant fills in the respective field values that correspond to the features on which the machine learning model was trained. The form is designed to capture the necessary information required for the model to make a prediction about the loan applicant's application. Note that not all fields in the loan application form need to be filled out. This is because the missing values in certain features

may indicate a higher risk of default. Conversely, one may choose to impose a restriction on the form, requiring all fields to be filled out. However, this could result in a lower number of received applications from delinquent clients, as they may not have all the necessary information to complete the form.

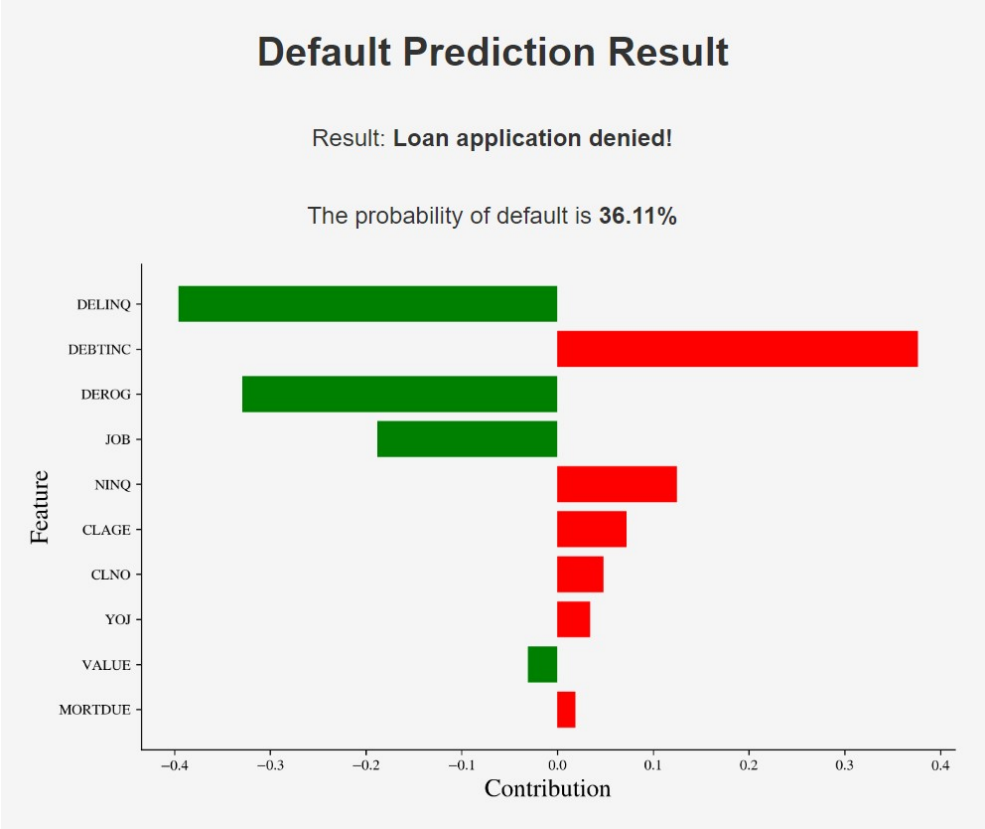
Figure 4.29: Flask Web Application Form



Source: Author's results in Python

Once, the loan application form is submitted, the web application uses the pickled input to transform the data from the loan application form and use it in the recalibrated model in order to get the result, whether the given loan applicant would repay his loan based on predetermined threshold. The result is then displayed in the web application, as shown in Figure 4.30. Particularly, the web application returns whether the loan application would be denied or approved based on the model's output and also the probability score of default.

Figure 4.30: Flask Web Application - Prediction Result



Source: Author's results in Python

Besides the prediction results, it also displays the Local Interpretable Model-Agnostic Explanations (henceforth LIME) of the black–box model with respect to the inputs submitted within the form. LIME focuses on the local explainability of the black box model around the black–box prediction as it generates a new data set consisting of perturbed samples around the given prediction and then trains a surrogate linear model on the new data set. Such local interpretable, surrogate model should be a good approximation of the black box model in the vicinity of the given prediction, i.e., the local interpretable model

is then used to explain the prediction of the black box model (Ribeiro *et al.* 2016).

The LIME explanation of input instances x is given as follows:

$$\xi(x) = \arg\min_{g \in G} L(f, g, \pi_x) + \Omega(g) \tag{4.15}$$

where f is the original black–box model, g is the surrogate model, L is the loss functions measuring how far is the explanation $\xi(x)$ far from the prediction produced by black–box model f, and $\Omega(g)$ is the complexity of the surrogate model g.

The explanation is given in terms of the feature importance, which is represented by the magnitude of the feature's coefficient in the local interpretable model. The higher the magnitude of the coefficient, the more important the feature is in the prediction of the black box model. Therefore, as it is shown in Figure 4.30, the red bars indicate positive contribution to the probability of default whereas green bars indicate negative contribution to the probability of default. In other words, The features with red bars indicate that the client would not probably repay his loan and vice versa. The contributions' magnitudes are in line with the findings from feature imporance or SHAP values which is focused on the global explainability of the black–box model (not local explainability), that features such as debt–to–income ratio (`DEBTINC`) or number of deliquent credit lines (`DELINQ`) have the largest impact of the probability default. Particularly, a high value of debt–to–income ratio causes higher probability default, whereas no delinquent credit lines leads to the lower probability default.

Chapter 5

Hypotheses' Testing

Result #1: *The recalibration of the model does enhaces model performance on HMEQ data set.*

We fail to reject the **Hypothesis #1** because all we observe improvements in the metrics within evaluation on test set when the final model was re-trained on the joined training and validation set instead solely On the training set. Particularly, all the score metrics and loss metrics have increased and decreased, respectively, as can be seen in Table 4.21.

Result #2: *Neural Network and KNN model do not outperform all the models on HMEQ data set.*

We reject the **Hypothesis #2** as the final model, which is the best performing, is the Gradient Boosting model as described in Table 4.19. KNN was also outperformed by the Random Forest and in case of Neural Network, it was outperformed by SVM as well as can be seen in Figure 4.17. If we aggregate the model selection results, we can observe that the best KNN model had the 11th highest rank, while Neural Network (MLP) exhibited unsatisfactory performance with the 22nd highest rank as can be seen in Table 5.1.

Table 5.1: Aggregated Ranks of Models

Model	Rank
GB	1
RF	6
KNN	11
SVM	19
MLP	22
DT	33
LR	40
GNB	55

Source: Author's results in Python

Result #3: *Black–box models does perform better than the white–box models on HMEQ data set.*

We fail to reject the **Hypothesis #3** as the black–box models truly outperformed the white–box models as can be seen in Figure 4.18 which depicts the distribution of ranks for both black–box and white–box models. Most of the white–box models were ranked in the bottom half within the model selection, whereas the 10 best performing models consisted out of black–box models only, namely Gradient Boosting and Random Forest. Even though some black–box models' performances were weak and other white–box models exhibited relatively high ranks, we can still conclude that the black–box models outperformed the white–box models on average as the median of the black–box models' ranks is lower than the white–box models' median.

Result #4: *The longer execution time of a model does not indicate better performance on HMEQ data set.*

We reject the **Hypothesis #4** as according to Figure 4.21, even though the Neural Network (MLP) model had the longest execution time on average, it underperformed several models such as Gradient Boosting, Random Forest, KNN and SVM which took significantly less time to execute. The same can be observed from Figure 4.23, where Neural Network performed poorly regardless the length of the execution time.

Hypothesis #5: *debt and delinquency features are the main default drivers on HMEQ data set.*

We fail to reject the **Hypothesis #5** according to Figure 4.27 which depicts the feature importance of the final model (Gradient Boosting). As can be seen, the most important features are debt–to–income ratio `DEBTINC` and number of delinquent credit lines `DELINQ`. Based on the SHAP values depicted in Figure 4.28, we can observe that the negative values of textttDEBTINC and `DELINQ` positively contribute to the model's predictions of the target variable, whereas the positive values negatively contribute to the model's predictions. In other words, the higher value of such features, the higher probability of default and vice versa. Since the features' values are encoded as WoE, the negative WoE values indicates larger distribution of defaulters compared to non–defaulters in given bins. Based on the WoE bins distribution in Figure 4.9, we can observe negative WoE values for bins where the debt–to–income ratio is extremely high or is missing. Regarding to the number of delinquent credit lines, we can observe a negative WoE value for bin corresponding to the relatively high number of delinquent credit lines. Therefore, if the loan applicant has either high or missing debt–to–income ratio and/or relatively high number of delinquent credit lines, he would be likely to default.

Chapter 6

Conclusion

TBD

The conclusion should briefly summarize the problem statement and the general content of the work and the emphasize on the main contribution of the work.

When writing the conclusion keep in mind that some readers may not have gone through the whole thesis, but have jumped directly to the conclusion after having read the abstract in order the decide on the personal relevance of the thesis. Therefore, the conclusion should be self contained, which means that a reader should be able to understand the essence of the conclusion without having to read the whole thesis.

The conclusion typically ends with an outlook that describes possible extensions of the presented approaches and of planned future work.

Bibliography

Adeodato, P. J. & S. B. Melo (2016): "On the equivalence between kolmogorov-smirnov and roc curve metrics for binary classification." *arXiv preprint arXiv:1606.00496* .

Alloghani, M., D. Al-Jumeily, J. Mustafina, A. Hussain, & A. Aljaaf (2020): "Supervised and unsupervised learning for data science." *Supervised and Unsupervised Learning for Data Science* .

Aniceto, M. C., F. Barboza, & H. Kimura (2020): "Machine learning predictivity applied to consumer creditworthiness." *Future Business Journal* **6(1)**: pp. 1–14.

Aras, S. (2021): "Bagging and boosting classifiers for credit risk evaluation." *REFLECTIONS OF ECONOMIC DEVELOPMENT* p. 121.

Ayyadevara, V. K. (2018): "Pro machine learning algorithms." *Apress: Berkeley, CA, USA* .

Baesens, B., D. Roesch, & H. Scheule (2016): *Credit risk analytics: Measurement techniques, applications, and examples in SAS*. John Wiley & Sons.

Bera, D., R. Pratap, & B. D. Verma (2021): "Dimensionality reduction for categorical data." *IEEE Transactions on Knowledge and Data Engineering* .

Bischl, B., M. Binder, M. Lang, T. Pielok, J. Richter, S. Coors, J. Thomas, T. Ullmann, M. Becker, A.-L. Boulesteix *et al.* (2023): "Hyperparameter optimization: Foundations, algorithms, best practices, and open challenges." *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery* **13(2)**: p. e1484.

Bolón-Canedo, V., N. Sánchez-Maroño, & A. Alonso-Betanzos (2015): *Feature selection for high-dimensional data*. Springer.

Bonaccorso, G. (2020): *Mastering Machine Learning Algorithms: Expert techniques for implementing popular machine learning algorithms, fine-tuning your models, and understanding how they work*. Packt Publishing Ltd.

Boughorbel, S., F. Jarray, & M. El-Anbari (2017): "Optimal classifier for imbalanced data using matthews correlation coefficient metric." *PloS one* **12(6)**: p. e0177678.

Brabec, J., T. Komárek, V. Franc, & L. Machlica (2020): "On model evaluation under non-constant class imbalance." In "Computational Science–ICCS 2020: 20th International Conference, Amsterdam, The Netherlands, June 3–5, 2020, Proceedings, Part IV 20," pp. 74–87. Springer.

Brownlee, J. (2020): "Recursive feature elimination (rfe) for feature selection in python." Retrieved April 28, 2023.

Brownlee, J. (2021): "Failure of classification accuracy for imbalanced class distributions." *MachineLearningMastery.com* .

Charu, C. A. (2018): "Neural networks and deep learning: a textbook."

Chicco, D. & G. Jurman (2020): "The advantages of the matthews correlation coefficient (mcc) over f1 score and accuracy in binary classification evaluation." *BMC genomics* **21**: pp. 1–13.

Cichosz, P. (2014): *Data mining algorithms: explained using R*. John Wiley & Sons.

Comotto, F. (2022): "Evaluation metrics: Leave your comfort zone and try mcc and brier score." Medium. Retrieved April 30, 2023.

Dembla, G. (2020): "Intuition behind log-loss score." Medium. Retrieved April 30, 2023.

Dias, P., S. Experian, B. Melissa Forti, M. Witarsa, & S. Experian (2018): "A comparison of gradient boosting with logistic regression in practical cases." In "URL: https://www. sas. com/content/dam/SAS/support/en/sasglobal-forum-proceedings/2018/1857-2018. pdf," .

Dilmegani, C. (2017): "Dark side of neural networks explained [2023]." AI-Multiple. Retrieved April 30, 2023.

Doumpos, M., C. Lemonakis, D. Niklis, & C. Zopounidis (2019): "Analytical techniques in the assessment of credit risk." *EURO Advanced Tutorials on Operational Research. Cham: Springer International Publishing.[Google Scholar]* .

Drahokoupil, J. (2022): "Application of the xgboost algorithm and bayesian optimization for the bitcoin price prediction during the covid-19 period." *FFA Working Papers* **4**: p. Article 2022.006.

Esposito, C., G. A. Landrum, N. Schneider, N. Stiefl, & S. Riniker (2021): "Ghost: adjusting the decision threshold to handle imbalanced data in machine learning." *Journal of Chemical Information and Modeling* **61(6)**: pp. 2623–2640.

Fawcett, T. (2006): "An introduction to roc analysis." *Pattern recognition letters* **27(8)**: pp. 861–874.

Fluss, R., D. Faraggi, & B. Reiser (2005): "Estimation of the youden index and its associated cutoff point." *Biometrical Journal: Journal of Mathematical Methods in Biosciences* **47(4)**: pp. 458–472.

Forsyth, D. (2019): *Applied machine learning*. Springer.

Gauhar, N. (2020): "Decision tree: A classification algorithm." `https://learnwithgauhar.com/decision-tree-a-classification-algorithm/`. Accessed on April 30, 2023.

Hale, J. (2019): "Don't sweat the solver stuff." *Medium* Retrieved May 1, 2023.

Han, J., M. Kamber, & J. Pei (2011): *Data Mining: Concepts and Techniques*. Morgan Kaufmann, 3rd edition.

He, H., Y. Bai, E. A. Garcia, & S. Li (2008): "Adasyn: Adaptive synthetic sampling approach for imbalanced learning." In "2008 IEEE International Joint Conference on Neural Networks (IEEE World Congress on Computational Intelligence)," pp. 1322–1328.

He, H. & Y. Ma (2013): *Imbalanced Learning: Foundations, Algorithms, and Applications*. Wiley-IEEE Press.

de Hond, A. A., I. M. Kant, M. Fornasa, G. Cinà, P. W. Elbers, P. J. Thoral, M. S. Arbous, & E. W. Steyerberg (2023): "Predicting readmission or death after discharge from the icu: External validation and retraining of a machine learning model." *Critical Care Medicine* **51(2)**: pp. 291–300.

Hsu, C.-W. & C.-J. Lin (2002): "A comparison of methods for multiclass support vector machines." *IEEE transactions on Neural Networks* **13(2)**: pp. 415–425.

Igareta, A. (2021): "Stratified sampling: You may have been splitting your dataset all wrong."

Jahromi, A. H. & M. Taheri (2017): "A non-parametric mixture of gaussian naive bayes classifiers based on local independent features." In "2017 Artificial intelligence and signal processing conference (AISP)," pp. 209–212. IEEE.

Janitza, S., C. Strobl, & A.-L. Boulesteix (2013): "An auc-based permutation variable importance measure for random forests." *BMC bioinformatics* **14(1)**: pp. 1–11.

Japkowicz, N. & M. Shah (2011): *Evaluating learning algorithms: a classification perspective*. Cambridge University Press.

Kaushik, S. (2016): "Introduction to feature selection methods with an example (or how to select the right variables?)." Accessed: April 30, 2023.

Kazemi, H. R., K. Khalili-Damghani, & S. Sadi-Nezhad (2023): "Estimation of optimum thresholds for binary classification using genetic algorithm: An application to solve a credit scoring problem." *Expert Systems* **40(3)**: p. e13203.

Kornbrot, D. (2014): "Point biserial correlation." *Wiley StatsRef: Statistics Reference Online* .

Lin, H.-T., C.-J. Lin, & R. C. Weng (2007): "A note on plattâ€™s probabilistic outputs for support vector machines." *Machine learning* **68**: pp. 267–276.

Loyola-Gonzalez, O. (2019): "Black-box vs. white-box: Understanding their advantages and weaknesses from a practical point of view." *IEEE access* **7**: pp. 154096–154113.

Malley, J., J. Kruppa, A. Dasgupta, K. Malley, & A. Ziegler (2011): "Probability machines consistent probability estimation using nonparametric learning machines." *Methods of information in medicine* **51**: pp. 74–81.

Marinov, D. & D. Karapetyan (2019): "Hyperparameter optimisation with early termination of poor performers." In "2019 11th Computer Science and Electronic Engineering (CEEC)," pp. 160–163. IEEE.

Meyer, D. (2015): "Support vector machines." *The Interface to libsvm in package e1071* **28**: p. 20.

Mucherino, A., P. Papajorgji, & P. M. Pardalos (2009): *Data mining in agriculture*, volume 34. Springer Science & Business Media.

Narkhede, S. (2018): "Understanding auc - roc curve." Medium. Retrieved April 28, 2023.

Navas-Palencia, G. (2020): "Optimal binning: mathematical programming formulation." *arXiv preprint arXiv:2001.08025* .

Newson, R. (2002): "Parameters behind â€śnonparametricâ€ť statistics: Kendall's tau, somersâ€™ d and median differences." *The Stata Journal* **2(1)**: pp. 45–64.

Newson, R. B. (2014): "Interpretation of somers' d under four simple models."

Nian, R. (2018): "An introduction to ADASYN (with code!)." Medium. Retrieved on May 2, 2023 from `https://medium.com/@ruinian/an-introduction-to-adasyn-with-code-1383a5ece7aa`.

Owen, L. (2022): *Hyperparameter Tuning with Python*. Packt Publishing, 1st edition. Original work published 2022.

Owusu, E., R. Quainoo, S. Mensah, & J. K. Appati (2023): "A deep learning approach for loan default prediction using imbalanced dataset." *International Journal of Intelligent Information Technologies (IJIIT)* **19(1)**: pp. 1–16.

Patle, A. & D. S. Chouhan (2013): "Svm kernel functions for classification." In "2013 International Conference on Advances in Technology and Engineering (ICATE)," pp. 1–9. IEEE.

Platt, J. *et al.* (1999): "Probabilistic outputs for support vector machines and comparisons to regularized likelihood methods." *Advances in large margin classifiers* **10(3)**: pp. 61–74.

Pramoditha, R. (2021): "How to mitigate overfitting with regularization." Medium. Retrieved May 1, 2023.

Prati, R. C., G. E. Batista, & M. C. Monard (2009): "Data mining with imbalanced class distributions: concepts and methods." In "IICAI," pp. 359–376.

Provost, F. & T. Fawcett (2013): *Data Science for Business: What you need to know about data mining and data-analytic thinking.* " O'Reilly Media, Inc.".

Ribeiro, M. T., S. Singh, & C. Guestrin (2016): """ why should i trust you?" explaining the predictions of any classifier." In "Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining," pp. 1135–1144.

scikit-learn (2023a): "Sequentialfeatureselector." `https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.SequentialFeatureSelector.html#sklearn.feature_selection.SequentialFeatureSelector`. Retrieved April 28, 2023.

scikit-learn (2023b): "sklearn.ensemble.gradientboostingclassifier." `https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.GradientBoostingClassifier.html#sklearn.ensemble.GradientBoostingClassifier`. Retrieved April 28, 2023.

scikit-learn (2023c): "sklearn.ensemble.randomforestclassifier." `https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html#sklearn.linear_model.LogisticRegression`. Retrieved April 28, 2023.

scikit-learn (2023d): "sklearn.naive_bayes.gaussiannb." `https://scikit-learn.org/stable/modules/generated/sklearn.naive_`

bayes.GaussianNB.html#sklearn.naive_bayes.GaussianNB. Retrieved April 28, 2023.

SCIKIT-LEARN (2023e): "sklearn.neighbors.kneighborsclassifier." https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KNeighborsClassifier.html#sklearn.neighbors.KNeighborsClassifier. Retrieved April 28, 2023.

SCIKIT-LEARN (2023f): "sklearn.neural_network.mlpclassifier." https://scikit-learn.org/stable/modules/generated/sklearn.neural_network.MLPClassifier.html#sklearn.neural_network.MLPClassifier. Retrieved April 28, 2023.

SCIKIT-LEARN (2023g): "sklearn.tree.decisiontreeclassifier." https://scikit-learn.org/stable/modules/generated/sklearn.tree.DecisionTreeClassifier.html#sklearn.tree.DecisionTreeClassifier. Retrieved April 28, 2023.

SCIKIT-LEARN (2023h): "skopt.bayessearchcv." https://scikit-optimize.github.io/stable/modules/generated/skopt.BayesSearchCV.html#. Retrieved April 28, 2023.

SCIKIT-OPTIMIZE (2023): "sklearn.linear_model.logisticregression." https://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html#sklearn.ensemble.RandomForestClassifier. Retrieved April 28, 2023.

SUBASI, A. (2020): *Practical machine learning for data analysis using python*. Academic Press.

TATSAT, H., S. PURI, & B. LOOKABAUGH (2020): *Machine Learning and Data Science Blueprints for Finance*. O'Reilly Media.

TEPLÝ, P. & M. POLENA (2020): "Best classification algorithms in peer-to-peer lending." *The North American Journal of Economics and Finance* **51**: p. 100904.

TIBCO-SOFTWARE (2023): "What is a random forest?" https://www.tibco.com/reference-center/what-is-a-random-forest. Retrieved April 30, 2023.

Verma, V. (2020): "A comprehensive guide to feature selection using wrapper methods in python." https://www.analyticsvidhya.com/blog/2020/10/a-comprehensive-guide-to-feature-selection-using-wrapper-methods-in-python/. Retrieved April 30, 2023.

Verma, Y. (2021): "A complete guide to sequential feature selection." https://analyticsindiamag.com/a-complete-guide-to-sequential-feature-selection/. Retrieved April 28, 2023.

Wang, W. (2020): "Bayesian optimization concept explained in layman terms." Medium. Accessed: April 29, 2023.

Wendler, T. & S. Gröttrup (2021): *Data Mining with SPSS Modeler: Theory, Exercises and Solutions*. Cham: Springer.

Witten, I. H., E. Frank, M. Hall, & C. Pal (2011): *Data Mining: Practical Machine Learning Tools and Techniques*. Morgan Kaufmann, 4th edition.

Witzany, J. (2017): *Credit risk management*. Springer.

Wu, Z., L. Jiang, Z. Jiang, B. Chen, K. Liu, Q. Xuan, & Y. Xiang (2018): "Accurate indoor localization based on csi and visibility graph." *Sensors* **18(8)**: p. 2549.

Zeng, G. (2014): "A necessary condition for a good binning algorithm in credit scoring." *Applied Mathematical Sciences* **8(65)**: pp. 3229–3242.

Zurada, J., N. Kunene, & J. Guan (2014): "The classification performance of multiple methods and datasets: Cases from the loan credit scoring domain." *Journal of International Technology and Information Management* **23(1)**: p. 5.

Appendix A

Additional Figures and Tables

Appendix B

Source Codes

B.1 Python Notebook Code

```
import warnings

warnings.filterwarnings("ignore")

import os
import numpy as np
import pandas as pd
import matplotlib
```

```
import matplotlib.pyplot as plt
from matplotlib import ticker
import seaborn as sns
import time
import math
import missingno
from itertools import combinations

from scipy.stats import chi2_contingency, ks_2samp, pointbiserialr, somersd
from imblearn.over_sampling import ADASYN

from optbinning import BinningProcess

from sklearn.model_selection import train_test_split, StratifiedKFold
from sklearn.feature_selection import SequentialFeatureSelector
from sklearn.metrics import (
        accuracy_score,
        recall_score,
        precision_score,
        f1_score,
        matthews_corrcoef,
        brier_score_loss,
        confusion_matrix,
        roc_curve,
        roc_auc_score,
```

```
        log_loss,
)


from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier
from sklearn.naive_bayes import GaussianNB
from sklearn.ensemble import RandomForestClassifier, GradientBoostingClassifier
from sklearn.neighbors import KNeighborsClassifier
from sklearn.svm import SVC
from sklearn.neural_network import MLPClassifier

from skopt import BayesSearchCV
from skopt.space import Real, Categorical, Integer
import shap

import lime
import dill

data = pd.read_csv("./data/raw_data.csv")
```

B.1.1 Data Exploration

```
data.info()
```

```
no_duplicates = data.duplicated(subset = [col for col in data.columns if col != 'BAD']).sum()
print(f"Duplicates check: {no_duplicates} duplicated rows.")


def categorical_numeric_vars(df: pd.DataFrame, target:str = "BAD") -> tuple[list, list]:

    cat_vars = [col for col in df.columns if df[col].dtypes == "O" and col != target]
    num_vars = [col for col in df.columns if col not in cat_vars + [target]]

    print(f"Categorical features: {', '.join(cat_vars)}")
    print(f"Numeric features: {', '.join(num_vars)}")

    return (cat_vars, num_vars)

cat_vars, num_vars = categorical_numeric_vars(data)


def default_distribution_plot(df, target="BAD", export=True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"

    # Replacing the Booleans with non-default/default strings for visualization
    df_plot = df[[target]].copy().replace({0: "Non-default", 1: "Default"})
```

```
# Figure's initialization
fig, ax = plt.subplots(figsize=(8, 6))

# Default distribution
sns.countplot(data=df_plot, x=target, palette="BuPu",
              order=list(df_plot[target].unique())[::-1], ax=ax)

# Increase the fontsize for xlabel and ylabel
ax.set_ylabel(ax.yaxis.label.get_text(), fontsize=17)
ax.set_xlabel(ax.xaxis.label.get_text(), fontsize=17)

# Increase the fontsize for xticks and yticks
plt.xticks(fontsize=17)
plt.yticks(fontsize=17)

# Removing upper and right axes spines
ax.spines["top"].set_visible(False)
ax.spines["right"].set_visible(False)

plt.tight_layout()

# Exporting plot
if export:
    os.makedirs("./plots/", exist_ok=True)
```

```
        plt.savefig(f"./plots/Default_Distribution.jpg", dpi=300)

    plt.show()

default_distribution_plot(data)


def numeric_distribution_plot(df: pd.DataFrame, num_vars: list,
                              plot_type: str, target: str = "BAD",
                              export: bool = True):

    def custom_int_formatter(x, pos):
        return f"{x:.0f}"

    #Possible plot types
    plot_types = {"boxplot": sns.boxplot,
                  "violinplot": sns.violinplot,
                  "histogram": sns.histplot}

    #Plot type parameter check
    if plot_type not in plot_types.keys():
                plot_types = ','.join([key for key in plot_types.keys()])
        raise ValueError(f"Invalid plot type. Please, select one of these available plot types: {plot_types}")
```

```
matplotlib.rcParams["mathtext.fontset"] = "stix"
matplotlib.rcParams["font.family"] = "STIXGeneral"

#Plot either boxplots or violinplots
if plot_type in ["boxplot", "violinplot"]:

    #replace 0/1's with (Non)-default texts for visualization's sake.
    df_plot = df.copy()
    df_plot[target] = df_plot[target].replace({0: "Non-default", 1: "Default"})

    #Figure's and axes' initialization
    fig, axs = plt.subplots(nrows = 5, ncols = 2, figsize = (12, 20))

    for ax, var in zip(axs.ravel(), num_vars):

        #Boxplot/violinplot
        plot_types[plot_type](data = df_plot, x = target, y = var, ax = ax,
                              palette = "BuPu", order = ["Non-default", "Default"])

        ax.set_title(f"Distribution of {var}", size = 19, fontweight = "bold")
        ax.tick_params(axis = "both", which = "major", labelsize = 18)
        ax.set(xlabel = None)
        ax.set(ylabel = None)
        ax.spines["top"].set_visible(False)
        ax.spines["right"].set_visible(False)
```

```
            ax.yaxis.set_major_formatter(matplotlib.ticker.FuncFormatter(custom_int_formatter))

        plt.tight_layout()

        #Exporting the plots
        if export:
            os.makedirs("./plots/", exist_ok = True)
            plt.savefig(f"./plots/Numeric_Features_Distribution_{plot_type.capitalize()}s.jpg", dpi = 300)
        plt.show()


    #Plot histograms
    elif plot_type == "histogram":
        def integer_formatter(x, pos):
            return f"{int(x)}"

        #Figure's and axes' initialization
        fig, axs = plt.subplots(nrows = len(num_vars), ncols = 2, figsize = (12, 25))

        #Column index
        col_ind = 0
        # Axis index
        # (if the value is even, the plot will be located on the left side, otherwise on the right side)
        axis_count = 0
```

```
for ax in axs.ravel():

    #Accessing the feature name.
    var = num_vars[col_ind]
    #Subsetting the data based on the feature.
    var_series = df[var]

    # Calculating the bin size for given feature ensuring that both conditional plots
    # (left and right) will have the same number of bins.
    # Using rule of thumb (Scott, 1979)
    # https://stackoverflow.com/questions/33458566/how-to-choose-bins-in-matplotlib-histogram

    R = var_series.max() - var_series.min() #Range of the feature's values
    n = len(var_series) #Number of feature's values
    sigma = var_series.std() #Standard deviation of the feature's values

    #Number of bins
    no_bins = int(R*(n**(1/3))/(3.49*sigma))

    # The left side (even axis_count) depicts the features' distribution
    # conditional on the non-default cases.
    if axis_count % 2 == 0:
        #Subsetting the data for non-default cases only.
        df_subset= df.query(f"{target} == 0")
        #Number of missing values within given feature
```

```
no_missings = df_subset[var].isna().sum()
# Percentage of missing values within subset of given feature
# (i.e., percentage of missing values of given feature within the non-default cases)
pct_missings = no_missings/df_subset.shape[0] * 100

# Histogram with kernel density function
# binrange to ensure that both left and right plot will have the same data range.
plot_types[plot_type](data = df_subset, x = var, ax = ax, bins = no_bins,
                      binrange = ((var_series.min(), var_series.max())),
                      kde = True, color = "lightblue")

ax.set_title(f"Distribution of {var} (Non-default cases)", size = 17, fontweight = "bold")
ax.tick_params(axis = "both", which = "major", labelsize = 15, rotation = 30)
ax.set(xlabel = None)
ax.set_ylabel(ax.get_ylabel(), fontsize=15)
ax.xaxis.set_major_formatter(ticker.FuncFormatter(integer_formatter))
ax.spines["top"].set_visible(False)
ax.spines["right"].set_visible(False)

#Inserting a text box with an information about the missing values.
ax.text(0.7, 0.9, f"Number of NA's: {no_missings} ({pct_missings:.1f}%)",
        horizontalalignment = "center", verticalalignment = "center",
        fontsize = 14,
        transform = ax.transAxes, bbox = dict(facecolor = "pink", alpha = 0.3))
```

```
# The right side (odd axis_count) depicts the features' distribution
# conditional on the default cases.
else:
    #Subsetting the data for default cases only.
    df_subset = df.query(f"{target} == 1")
    #Number of missing values within given feature
    no_missings = df_subset[var].isna().sum()
    # Percentage of missing values within subset of given feature
    # (i.e., percentage of missing values of given feature within the default cases)
    pct_missings = no_missings/df_subset.shape[0] * 100

    # Histogram with kernel density function
    # binrange to ensure that both left and right plot will have the same data range.
    sns.histplot(data = df_subset, x = var, ax = ax, bins = no_bins,
                 binrange = ((var_series.min(), var_series.max())),
                 kde = True, color = "mediumpurple")

    ax.set_title(f"Distribution of {var} (Default cases)", size = 17, fontweight = "bold")
    ax.tick_params(axis = "both", which = "major", labelsize = 15, rotation = 30)
    ax.set(xlabel = None)
    ax.set_ylabel(ax.get_ylabel(), fontsize=15)
    ax.xaxis.set_major_formatter(ticker.FuncFormatter(integer_formatter))
    ax.spines["top"].set_visible(False)
    ax.spines["right"].set_visible(False)
```

```
                #Inserting a text box with an information about the missing values.
                ax.text(0.7, 0.9, f"Number of NA's: {no_missings} ({pct_missings:.1f}%)",
                        horizontalalignment = "center", verticalalignment = "center",
                        fontsize = 14,
                        transform = ax.transAxes, bbox = dict(facecolor = "pink", alpha = 0.3))

                #Proceeding with the next feature
                col_ind += 1

            #Switching to the left/right side of the figure
            axis_count +=1

        plt.tight_layout()

        #Exporting the plots
        if export:
            os.makedirs("./plots/", exist_ok = True)
            plt.savefig(f"./plots/Numeric_Features_Distribution_{plot_type.capitalize()}s.jpg", dpi = 300)

        plt.show()


numeric_distribution_plot(data, num_vars, plot_type = "boxplot")
numeric_distribution_plot(data, num_vars, plot_type = "violinplot")
numeric_distribution_plot(data, num_vars, plot_type = "histogram")
```

```python
def normality_test(data: pd.DataFrame, num_vars: list) -> pd.DataFrame:

    from scipy.stats import shapiro

    output_df = pd.DataFrame(columns = ["Feature", "Shapiro-Wilk", "Significance", "Result"])

    for i, col in enumerate(num_vars):
        temp_df = data.copy()
        temp_df = temp_df[temp_df[col].notna()].copy()

        output_df.loc[i, "Feature"] = col

        shapiro_stat, shapiro_p = shapiro(temp_df[col])
        shapiro_significance_stars = "***" if shapiro_p < 0.01 else "**" if shapiro_p < 0.05 \
                                        else "*" if shapiro_p < 0.1 else ""
        shapiro_significance_result = "Normally distributed" if shapiro_p > 0.05 \
                                      else "Not normally distributed"

        output_df.loc[i, "Shapiro-Wilk"] = round(shapiro_stat,4)
        output_df.loc[i, "Significance"] = shapiro_significance_stars
        output_df.loc[i, "Result"] = shapiro_significance_result

    return output_df
```

```
normality_test(data, num_vars)


def num_na_table(df: pd.DataFrame, num_vars: list, target: str = "BAD") -> pd.DataFrame:
    output_df = pd.DataFrame(index = num_vars,
                        columns = ["# of NA's (Y=0)", "# of NA's (Y=1)",  "% of NA's (Y=0)", "% of NA's (Y=1)"])
    for num in num_vars:
        output_df.loc[num, "# of NA's (Y=0)"] = df.query(f"{target} == 0")[num].isna().sum()
        output_df.loc[num, "# of NA's (Y=1)"] = df.query(f"{target} == 1")[num].isna().sum()

        pct_nd = df.query(f"{target} == 0")[num].isna().sum()/df.query(f"{target} == 0").shape[0] * 100
        pct_d = df.query(f"{target} == 1")[num].isna().sum()/df.query(f"{target} == 1").shape[0] * 100
        output_df.loc[num, "% of NA's (Y=0)"] = pct_nd
        output_df.loc[num, "% of NA's (Y=1)"] = pct_d

    return output_df

num_na_table(data, num_vars)


def categorical_distribution_plot(df: pd.DataFrame, cat_vars: list,
                                  target: str = "BAD", export: bool = True):
```

```
#Figure's and axes' initialization
fig, axs = plt.subplots(nrows = len(cat_vars),ncols = 2, figsize = (11, 10))

#Column index
col_ind = 0
# Axis index
# (if the value is even, the plot will be located on the left side, otherwise on the right side)
axis_count = 0

matplotlib.rcParams["mathtext.fontset"] = "stix"
matplotlib.rcParams["font.family"] = "STIXGeneral"

for ax in axs.ravel():

    #Accessing the feature name
    var = cat_vars[col_ind]
    # Subsetting the data based on the feature with subsequent replacing missing values
    # with N/A's strings (for visualization's sake).
    var_target_df = df[[var, target]].copy().fillna("N/A")

    #If the feature has some missing values, put the N/A category at the end of the plot.
    if var_target_df.query(f"{var} == 'N/A'").shape[0] != 0:
        categories = [cat for cat in var_target_df[var].unique() if cat != "N/A"] + ["N/A"]
    else:
        categories = var_target_df[var].unique()
```

```
# The left side (even axis_count) depicts the features' distribution
# conditional on the non-default cases.
if axis_count % 2 == 0:

    sns.countplot(data = var_target_df.query(f"{target} == 0"), x = var,
                  ax = ax, order = categories, color = "lightblue")

    ax.set_title(f"Distribution of {var} (Non-default cases)", size = 19, fontweight = "bold")
    ax.tick_params(axis = "both", which = "major", labelsize = 18)
    ax.tick_params(axis = "x", rotation = 30, which = "major", labelsize = 18)
    ax.set(xlabel = None)
    ax.set_ylabel(ax.get_ylabel(), fontsize=15)
    ax.spines["top"].set_visible(False)
    ax.spines["right"].set_visible(False)


# The right side (odd axis_count) depicts the features' distribution
# conditional on the default cases.
else:

    sns.countplot(data = var_target_df.query(f"{target} == 1"), x = var,
                  ax = ax, order = categories, color = "mediumpurple")

    ax.set_title(f"Distribution of {var} (Default cases)", size = 19, fontweight = "bold")
```

```
            ax.tick_params(axis = "both", which = "major", labelsize = 18)
            ax.tick_params(axis = "x", rotation = 30, which = "major", labelsize = 18)
            ax.set_ylabel(ax.get_ylabel(), fontsize=15)
            ax.set(xlabel = None)
            ax.spines["top"].set_visible(False)
            ax.spines["right"].set_visible(False)

            #Proceeding with the next feature
            col_ind += 1

        #Switching to the left/right side of the figure
        axis_count += 1

    plt.tight_layout()

    #Exporting the plots
    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/Categorical_Features_Distribution.jpg", dpi = 300)

    plt.show()


categorical_distribution_plot(data, cat_vars)
```

```
def cat_na_table(df: pd.DataFrame, cat_var: str, target: str = "BAD") -> pd.DataFrame:
    temp_df = df.copy()
    temp_df[cat_var] = temp_df[cat_var].fillna("N/A")
    output_df = pd.DataFrame(index = list(temp_df[cat_var].unique()),
                             columns = ["# (Y=0)", "# (Y=1)",  "% (Y=0)", "% (Y=1)"])

    for cat in output_df.index:
        output_df.loc[cat, "# (Y=1)"] = temp_df.query(f"{target} == 1 and {cat_var} == '{cat}'").shape[0]
        output_df.loc[cat, "# (Y=0)"] = temp_df.query(f"{target} == 0 and {cat_var} == '{cat}'").shape[0]
        pct_d = round(output_df.loc[cat, "# (Y=1)"]/temp_df.query(f"{target} == 1").shape[0], 4)* 100
        pct_nd = round(output_df.loc[cat, "# (Y=0)"]/temp_df.query(f"{target} == 0").shape[0] , 4)* 100
        output_df.loc[cat, "% (Y=1)"] = pct_d
        output_df.loc[cat, "% (Y=0)"] = pct_nd

    return output_df

cat_na_table(data, "JOB")
cat_na_table(data, "REASON")

def point_biserial_corr_table(data: pd.DataFrame, num_features, target = 'BAD') -> pd.DataFrame:

    output_df = pd.DataFrame(columns = ['Feature', 'Point-Biserial Correlation', 'Significance'])
    for i, col in enumerate(num_features):
```

```
        temp_df = data[data[col].notna()].copy()
        coef, p_value = pointbiserialr(temp_df[target], temp_df[col])
        output_df.loc[i, 'Feature'] = col
        output_df.loc[i, 'Point-Biserial Correlation'] = round(coef, 3)

        significance_stars = '***' if p_value <= 0.01 else '**' if p_value <= 0.05 else \
                             '*' if p_value <= 0.1 else ' '
        output_df.loc[i, 'Significance'] = significance_stars

    return output_df


point_biserial_corr_table(data, num_vars)


def cramer_v_table(data: pd.DataFrame, cat_features, target = 'BAD') -> pd.DataFrame:

    output_df = pd.DataFrame(columns = ['Variable #1', 'Variable #2', "Cramer's V", 'Significance'])

    pairs = list(combinations(cat_features + [target], 2))

    pairs = [sorted(pair) for pair in pairs]

    pairs = sorted(pairs)
```

```
    for i, pair in enumerate(pairs):
        temp_df = data.copy()
        temp_df = temp_df[temp_df[pair[0]].notna()]
        temp_df = temp_df[temp_df[pair[1]].notna()]

        cross_tab = pd.crosstab(temp_df[pair[0]], temp_df[pair[1]])
        chi2, p_value, *_ = chi2_contingency(cross_tab, correction = False)

        N = cross_tab.sum().sum()
        k = min(cross_tab.shape)
        cr_v = np.sqrt((chi2/N) / (k-1))

        significance_stars = '***' if p_value <= 0.01 else '**' if p_value <= 0.05 else \
                             '*' if p_value <= 0.1 else ' '

        output_df.loc[i, 'Variable #1'] = pair[0]
        output_df.loc[i, 'Variable #2'] = pair[1]
        output_df.loc[i, "Cramer's V"] = round(cr_v, 3)

        significance_stars = '***' if p_value <= 0.01 else '**' if p_value <= 0.05 else \
                             '*' if p_value <= 0.1 else ' '
        output_df.loc[i, 'Significance'] = significance_stars

    return output_df
```

```
cramer_v_table(data, cat_vars)


def phi_correlation(var1, var2) -> float:

    cross_tab = pd.crosstab(var1, var2)

    chi2, p_value, *_ = chi2_contingency(cross_tab)
    n = cross_tab.sum().sum()

    phi = np.sqrt(chi2/n)

    return phi


def na_phi_corr_table(data: pd.DataFrame, target = 'BAD') -> pd.DataFrame:

    output_df = pd.DataFrame(columns = ['Feature', 'Phi Correlation', 'Significance'])

    for i, col in enumerate(data.drop(target, axis = 1).columns):
        na_indicator = [1 if pd.isnull(i) else 0 for i in data[col]]
        cross_tab = pd.crosstab(data[target], na_indicator)
        chi2, p_value, *_ = chi2_contingency(cross_tab)
        n = cross_tab.sum().sum()
```

```
        phi = np.sqrt(chi2/n)
        significance_stars =  '***' if p_value <= 0.01 else '**' if p_value <= 0.05 else \
                              '*' if p_value <= 0.1 else ' '

        output_df.loc[i, 'Feature'] = col
        output_df.loc[i, 'Phi Correlation'] = round(phi, 3)
        output_df.loc[i, 'Significance'] = significance_stars

    return output_df

na_phi_corr_table(data)


def spearman_corr_matrix_plot(df: pd.DataFrame, num_var: list, export: bool = True):

    #Figure's initialization
    plt.figure(figsize = (16,13))
    matplotlib.rcParams['mathtext.fontset'] = 'stix'
    matplotlib.rcParams['font.family'] = 'STIXGeneral'
    #Corelation matrix heatmap
    heatmap = sns.heatmap(df[num_var].corr(method = "spearman"), vmin = -1, vmax = 1,
                          mask = np.triu(np.ones_like(df[num_var].corr())),
                          annot = True, cmap  = "coolwarm",  fmt = ".3f",
                          xticklabels = num_var, yticklabels = num_var,
```

```
                        annot_kws={"size": 19})

    plt.xticks(fontsize = 19)
    plt.yticks(fontsize = 19)

    cbar = heatmap.collections[0].colorbar
    cbar.ax.tick_params(labelsize=19)

    plt.tight_layout()

    #Exporting the plots
    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/Spearman_Correlation_Matrix_Numeric_Features.jpg", dpi = 300)

    plt.show()


spearman_corr_matrix_plot(data, num_vars)


def na_dendrogram(df:pd.DataFrame, export:bool = True, plot_suffix:str = ""):

    matplotlib.rcParams['mathtext.fontset'] = 'stix'
    matplotlib.rcParams['font.family'] = 'STIXGeneral'
```

```
    #True/False values indicating whether a column has some NA's.
    na_columns_indicators = df.describe(include = "all").T["count"] < df.shape[0]
    #Filtering the column names having NA's.
    na_columns = df.columns[na_columns_indicators]
    #Subsetting the data based on the NA's columns.
    final_df_dendogram = df[na_columns]

    #Plotting the dendrogram
    missingno.dendrogram(final_df_dendogram, orientation = "top", figsize = (10, 6), fontsize = 11)
    #plt.title("Dendrogram of variables having NA's", size = 13, fontweight = "bold")
    plt.yticks(fontsize=17)
    plt.xticks(rotation=45, fontsize=17)

    plt.tight_layout()

    #Exporting the plot
    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/NA_Dendrogram{plot_suffix}.jpg", dpi = 300)

    plt.show()

na_dendrogram(data)
na_dendrogram(data[data['BAD'] == 1], plot_suffix = "_defaults")
```

B.1.2 Data Preprocessing

```
def data_split(
        df: pd.DataFrame,
        test_size: float,
        validation_size: float,
        seed: int,
        num_vars,
        cat_vars,
        oversampling: str = "None",
        target: str = "BAD",
) -> tuple[pd.DataFrame, pd.Series, pd.DataFrame, pd.Series, pd.DataFrame, pd.Series]:

        # Separating the target variable (Y) and the features (X)
        Y = df[target]
        X = df.drop(target, axis=1)

        # Stratified split into training set, validation set and test set
        X_temp, X_test, y_temp, y_test = train_test_split(
                X, Y, stratify=Y, test_size=test_size, random_state=seed
        )
        X_train, X_valid, y_train, y_valid = train_test_split(
                X_temp, y_temp, stratify=y_temp, test_size=validation_size, random_state=seed
        )
```

```
# ADASYN Oversampling
if oversampling == "ADASYN":

        # ADASYN initialization
        adasyn = ADASYN(random_state=seed, n_jobs=-1)

        # Temporary imputing of missing values
        # (separately for categorical and numeric features)
        # ADASYN cannot work with NA's, thus we replace them with arbitrary values.
        X_train_imputed = pd.concat(
                (
                        X_train[cat_vars].copy().fillna("NAN"),
                        X_train[num_vars].copy().fillna(99999999999999),
                ),
                axis=1,
        )[X_train.columns].copy()

        # Dummy encoding of categorical features
        # ADASYN cannot work with categorical features, thus we need to encode them.
        for cat in cat_vars:
                X_cat_dummies = pd.get_dummies(X_train_imputed[[cat]])
                X_train_imputed = X_train_imputed.drop(cat, axis=1)
                X_train_imputed = pd.concat((X_train_imputed, X_cat_dummies), axis=1)

        # Oversampling on the training set.
```

```
X_train_final, y_train_final = adasyn.fit_resample(
        X_train_imputed, pd.DataFrame(y_train)
)

# Converting dummies back into the original categorical features.
for cat in cat_vars:
        X_train_final[cat] = (
                X_train_final.loc[
                        :, [col for col in X_train_final.columns if cat in col]
                ]
                .idxmax(axis=1)
                .str.replace(f"{cat}_", "")
        )
        X_train_final = X_train_final.drop(
                [col for col in X_train_final.columns if f"{cat}_" in col], axis=1
        )

# Replacing the NA's strings back to NA's with respect to the categorical features.
X_train_final = X_train_final.replace({"NAN": np.nan})

# Replacing back the missing values (99999999999999) with NA's in such case
# whether the value is exceeding the maximum value of given numeric feature before imputing.
for num in num_vars:
        max_value = X_train[num].max()
        X_train_final[num] = X_train_final[num].apply(
```

```
                                    lambda x: np.nan if x > max_value else x
                                )

                y_train_final = y_train_final[target]

                X_train_final = X_train_final.reindex(columns=X_train.columns)

                return X_train_final, y_train_final, X_valid, y_valid, X_test, y_test

        # No oversampling
        else:

                return X_train, y_train, X_valid, y_valid, X_test, y_test


seed = 42
test_size = 0.15
validation_size = test_size/(1 - test_size)

(
    X_train,
    y_train,
    X_valid,
    y_valid,
    X_test,
```

```
    y_test,
) = data_split(data, test_size, validation_size, seed, num_vars, cat_vars, oversampling="ADASYN")

(
    X_train_orig,
    y_train_orig,
    X_valid_orig,
    y_valid_orig,
    X_test_orig,
    y_test_orig,
) = data_split(data, test_size, validation_size, seed, num_vars, cat_vars)


def print_data_info(**kwargs):

    for name, _set in kwargs.items():

        no_dashes = 50
        no_dashes_name_left = int((no_dashes - len(name) - 1)/2)*"-"
        no_dashes_name_right  = f"{(no_dashes - len(name) - len(no_dashes_name_left) - 2)*'-'}"

        data_info = f"{_set['features'].shape[0]} instances, {_set['features'].shape[1]} features"
        no_dashes_data_info_left = int((no_dashes - len(data_info) - 1)/2)*"-"
        no_dashes_data_info_right = f'{(no_dashes - len(data_info) - len(no_dashes_data_info_left) - 2)*"-"}'
        pct_d = np.sum(_set['target']) / _set['target'].shape[0]*100:
```

```
        pct_nd = np.sum(_set['target'] == 0)/ _set['target'].shape[0]*100
        target_info = f"Default: {pct_d:.2f}%  | Non-default: {pct_nd:.2f}%"
        no_dashes_target_info_left = int((no_dashes - len(target_info) - 1)/2)*"-"
        length_dashes_target_info_right = (no_dashes - len(target_info) - len(no_dashes_target_info_left) - 2)
        no_dashes_target_info_right = f'{length_dashes_target_info_right*"-"}'


        print(no_dashes*"-")
        print(f"{no_dashes_name_left} {name} {no_dashes_name_right}")
        print(f"{no_dashes_data_info_left} {data_info} {no_dashes_data_info_right}")
        print(f"{no_dashes_target_info_left} {target_info} {no_dashes_target_info_right}")
        print(no_dashes*"-", "\n")

print_data_info(Training = {'features': X_train, 'target': y_train},
                Validation = {'features': X_valid, 'target': y_valid},
                Test = {'features': X_test, 'target': y_test})
```

```
def woe_binning(
        x_train_set: pd.DataFrame,
        y_train_labels: pd.Series,
        cat_vars: list,
        export: bool = True,
        **kwargs,
) -> tuple[dict, pd.DataFrame]:
```

```
binning_path = "./models/feature_preprocessing"
final_objects_path = "./models/objects_FINAL"

# Initializing the binning process object.
bn = BinningProcess(
        variable_names=list(x_train_set.columns),
        categorical_variables=cat_vars
)

# Fitting the binning on training set.
bn.fit(x_train_set, y_train_labels)

# DataFrame including binned categories' information.
bins_woe = pd.DataFrame()

for i in x_train_set.columns:

        var = bn.get_binned_variable(i).binning_table.build()
        var = var[(~var["Bin"].isin(["Special", "Totals"]))]
        var["Variable"] = i

        bins_woe = pd.concat((bins_woe, var))

bins_woe = bins_woe.loc[:, ~bins_woe.columns.isin(["JS"])]
```

```
if export:
        for save_path in [binning_path, final_objects_path]:
                os.makedirs(save_path, exist_ok=True)
                bn.save(f"{save_path}/binning_woe_object.h5")
                bins_woe.to_csv(f"{save_path}/woe_bins.csv",
                   index = False)

# Transforming both training set and test set
# based on the fitted training binning.
def woe_bin_transform(bn_fit, x_set):
        x_set_binned = bn_fit.transform(x_set, metric="woe")
        x_set_binned.index = x_set.index

        return x_set_binned

X_binned_sets = {"X_train_binned": woe_bin_transform(bn, x_train_set)}
x_set_copy = X_binned_sets["X_train_binned"].copy()

for col in x_set_copy.columns:
        na_woe = (bins_woe
                .query('Variable == @col and Bin == "Missing"')["WoE"]
                .values[0]
                )
        x_set_copy.loc[x_train_set[col].isna(), col] = na_woe
```

```
    X_binned_sets["X_train_binned"] = x_set_copy

    for name, x_set in kwargs.items():
        X_binned_sets[f"{name}_binned"] = woe_bin_transform(bn, x_set)
        x_set_copy = X_binned_sets[f"{name}_binned"].copy()
        for col in x_set_copy.columns:
            na_woe = (bins_woe
                      .query('Variable == @col and Bin == "Missing"')
                      ["WoE"]
                      .values[0])
            x_set_copy.loc[x_set[col].isna(), col] = na_woe
        X_binned_sets[f"{name}_binned"] = x_set_copy

    return (X_binned_sets, bins_woe, bn)


X_binned_sets, woe_bins, binning_transformator = woe_binning(X_train, y_train, cat_vars,
                                                             X_valid = X_valid, X_test = X_test)
X_train_binned, X_valid_binned, X_test_binned = (xset for i, xset in X_binned_sets.items())

X_binned_sets_orig, woe_bins_orig, binning_transformator_orig = woe_binning(X_train_orig, y_train_orig,
                                                                            export = False, cat_vars,
                                                                            X_valid = X_valid_orig,
                                                                            X_test = X_test_orig)
X_train_binned_orig, X_valid_binned_orig, X_test_binned_orig = (xset for i, xset in X_binned_sets_orig.items())
```

```
def prep_data_export(features: tuple, labels: tuple,
                     ind_sets: tuple = ("Training", "Validation", "Test"),
                     csv_name:str = '') -> pd.DataFrame:

    df_list = []

    #Join each pair of features and labels data, assign to it a set indicator,
        # append to the list and then,
        #  transform that list into a data frame (and export it).
    for feat, lab, ind in zip(features, labels, ind_sets):

        temp = pd.concat((lab, feat), axis = 1)
        temp["set"] = ind
        df_list.append(temp)

    dfs = [df for df in df_list]

    final_df = pd.concat(dfs, axis = 0).sort_index()

    if len(csv_name) != 0:
        os.makedirs("./data/", exist_ok = True)
        final_df.to_csv(f"./data/{csv_name}.csv", index = False)
```

```
    return final_df


interim = prep_data_export((X_train_binned, X_valid_binned, X_test_binned),
                           (y_train, y_valid, y_test),
                           ("Training", "Validation", "Test"),
                           csv_name = "interim_data")


def categorical_distribution_plot_OS(df_orig: pd.DataFrame, df_os, cat_vars: list,
                                     target: str = "BAD", class_val = 1, export: bool = False):

    #Figure's and axes' initialization
    fig, axs = plt.subplots(nrows = len(cat_vars),ncols = 2, figsize = (14, 10))

    #Column index
    col_ind = 0
    #Axis index (if the value is even, the plot will be located on the left side, otherwise on the right side)
    axis_count = 0

    matplotlib.rcParams['mathtext.fontset'] = 'stix'
    matplotlib.rcParams['font.family'] = 'STIXGeneral'

    class_title_name = 'Default' if class_val == 1 else 'Non-Default'
```

```
for ax in axs.ravel():

    #Accessing the feature name
    var = cat_vars[col_ind]
    # Subsetting the data based on the feature with subsequent replacing missing values#
    # with N/A's strings (for visualization's sake).
    var_target_df_orig = df_orig[[var, target]].copy().fillna("N/A")
    var_target_df_os = df_os[[var, target]].copy().fillna("N/A")

    #If the feature has some missing values, put the N/A category at the end of the plot.
    if var_target_df_orig.query(f"{var} == 'N/A'").shape[0] != 0:
        categories_orig = [cat for cat in var_target_df_orig[var].unique() if cat != "N/A"] + ["N/A"]
    else:
        categories_orig = var_target_df_orig[var].unique()

    #If the feature has some missing values, put the N/A category at the end of the plot.
    if var_target_df_os.query(f"{var} == 'N/A'").shape[0] != 0:
        categories_os = [cat for cat in var_target_df_os[var].unique() if cat != "N/A"] + ["N/A"]
    else:
        categories_os = var_target_df_os[var].unique()

    # The left side (even axis_count) depicts the features' distribution
    # conditional on the non-default cases.
    if axis_count % 2 == 0:
```

```
        sns.countplot(data = var_target_df_orig.query(f"{target} == {class_val}"), x = var,
                      ax = ax, order = categories_orig, color = "lightblue")

        ax.set_title(f"Distribution of {var} ({class_title_name} cases)", size = 19, fontweight = "bold")
        ax.tick_params(axis = "both", which = "major", labelsize = 18)
        ax.tick_params(axis = "x", rotation = 30, which = "major", labelsize = 18)
        ax.set(xlabel = None)
        ax.set_ylabel(ax.get_ylabel(), fontsize=18)
        ax.spines["top"].set_visible(False)
        ax.spines["right"].set_visible(False)


    #The right side (odd axis_count) depicts the features' distribution conditional on the default cases.
    else:

        sns.countplot(data = var_target_df_os.query(f"{target} == {class_val}"), x = var,
                      ax = ax, order = categories_os, color = "mediumpurple")

        ax.set_title(f"Distribution of {var} ({class_title_name} cases) - Oversampled",
                     size = 19, fontweight = "bold")
        ax.tick_params(axis = "both", which = "major", labelsize = 18)
        ax.tick_params(axis = "x", rotation = 30, which = "major", labelsize = 18)
        ax.set_ylabel(ax.get_ylabel(), fontsize=18)
        ax.set(xlabel = None)
        ax.spines["top"].set_visible(False)
```

```
            ax.spines["right"].set_visible(False)

            #Proceeding with the next feature
            col_ind += 1

        #Switching to the left/right side of the figure
        axis_count += 1

    plt.tight_layout()

    #Exporting the plots
    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/Categorical_Features_Distribution_OS_{class_title_name}.jpg", dpi = 300)

    plt.show()


categorical_distribution_plot_OS(pd.concat((X_train_orig, y_train_orig), axis = 1),
                                 pd.concat((X_train, y_train), axis = 1),
                                   cat_vars, class_val = 1, export = True)

df_temp = pd.DataFrame(columns = ['Feature', 'Category', '# (Y=1)', '# (Y=1) - Oversampled',
                                  '% (Y=1)','% (Y=1) - Oversampled'])
i = 0
```

```
orig_temp_df = pd.concat((X_train_orig, y_train_orig), axis = 1).copy()
temp_df = pd.concat((X_train, y_train), axis = 1).copy()
for cat_var in cat_vars:
    orig_temp_df[cat_var] = orig_temp_df[cat_var].fillna("N/A")
    temp_df[cat_var] = temp_df[cat_var].fillna("N/A")

    for category in orig_temp_df[cat_var].unique():
        df_temp.loc[i, 'Feature'] = cat_var
        df_temp.loc[i, 'Category'] = category

        count_d = orig_temp_df.query(f"{cat_var} == '{category}' and BAD == 1").shape[0]
        count_d_os = temp_df.query(f"{cat_var} == '{category}' and BAD == 1").shape[0]
        df_temp.loc[i, '# (Y=1)'] = count_d
        df_temp.loc[i, '# (Y=1) - Oversampled'] = count_d_os

        pct_d = df_temp.loc[i, '# (Y=1)'] /  orig_temp_df.query("BAD == 1").shape[0]
        pct_d_os = df_temp.loc[i, '# (Y=1) - Oversampled'] /  temp_df.query("BAD == 1").shape[0]
        df_temp.loc[i, '% (Y=1)'] = round(pct_d * 100, 2)
        df_temp.loc[i, '% (Y=1) - Oversampled'] = round(pct_d_os * 100, 2)
        i += 1

df_temp['rel diff'] = df_temp['% (Y=1) - Oversampled'] - df_temp['% (Y=1)']
df_temp.reindex(df_temp['rel diff'].abs().sort_values(ascending=False).index)
```

```
def numeric_distribution_plot_OS(df_orig: pd.DataFrame, df_os: pd.DataFrame, num_vars: list,
                                 plot_type: str, target: str = "BAD", class_val = 1,
                                 export: bool = True):

    #Possible plot types
    plot_types = {"boxplot": sns.boxplot,
                  "violinplot": sns.violinplot
                  }

    #Figure's and axes' initialization
    fig, axs = plt.subplots(nrows = len(num_vars),ncols = 2, figsize = (11, 45))

    #Column index
    col_ind = 0
    #Axis index (if the value is even, the plot will be located on the left side, otherwise on the right side)
    axis_count = 0

    matplotlib.rcParams['mathtext.fontset'] = 'stix'
    matplotlib.rcParams['font.family'] = 'STIXGeneral'

    class_title_name = 'Default' if class_val == 1 else 'Non-Default'

    for ax in axs.ravel():
```

```
#Accessing the feature name
var = num_vars[col_ind]

# The left side (even axis_count) depicts the features' distribution
# conditional on the non-default cases.
if axis_count % 2 == 0:

    plot_types[plot_type](data = df_orig.loc[df_orig[target] == class_val], y = var, ax = ax,
                          color = "lightblue")

    ax.set_title(f"Distribution of {var} ({class_title_name} cases)", size = 17)
    ax.tick_params(axis = "both", which = "major", labelsize = 15)
    ax.tick_params(axis = "x", rotation = 30, which = "major", labelsize = 15)
    ax.set(xlabel = None)
    ax.set_ylabel(ax.get_ylabel(), fontsize=15)
    ax.spines["top"].set_visible(False)
    ax.spines["right"].set_visible(False)

#The right side (odd axis_count) depicts the features' distribution conditional on the default cases.
else:

    plot_types[plot_type](data = df_os.loc[df_os[target] == class_val], y = var, ax = ax,
                          color = "mediumpurple")

    ax.set_title(f"Distribution of {var} ({class_title_name} cases) - Oversampled", size = 17)
```

```
            ax.tick_params(axis = "both", which = "major", labelsize = 15)
            ax.tick_params(axis = "x", rotation = 30, which = "major", labelsize = 15)
            ax.set_ylabel(ax.get_ylabel(), fontsize=15)
            ax.set(xlabel = None)
            ax.spines["top"].set_visible(False)
            ax.spines["right"].set_visible(False)

            #Proceeding with the next feature
            col_ind += 1

        #Switching to the left/right side of the figure
        axis_count += 1

    plt.tight_layout()

    #Exporting the plots
    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/Numeric_Features_Distribution_{plot_type.capitalize()}s.jpg", dpi = 300)

    plt.show()


numeric_distribution_plot_OS(pd.concat((X_train_orig, y_train_orig), axis = 1),
                             pd.concat((X_train, y_train), axis = 1), num_vars,
```

```
                                plot_type = "violinplot", export = False)

def woe_bins_plot(bins_woe: pd.DataFrame, export: bool = True):

    matplotlib.rcParams['mathtext.fontset'] = 'stix'
    matplotlib.rcParams['font.family'] = 'STIXGeneral'


    fig, axs = plt.subplots(nrows = 4, ncols = 3, figsize = (13, 22))

    for i, ax in zip(bins_woe["Variable"].unique(), axs.ravel()):

        temp = bins_woe.loc[bins_woe["Variable"] == i]
        sns.barplot(x = temp.index, y = "WoE", data = temp, ax = ax, palette = "BuPu")
        ax.axhline(y = 0, color = "black", linewidth = 1)


        cat = False

        for j in temp["Bin"]:
            if isinstance(j, np.ndarray):
                cat = True
                break
        if cat == False:
            labels = list(temp["Bin"])
```

```
        elif cat == True:
            temp_bins = [k if type(k) == str else str(list(k)) for k in temp["Bin"]]
            labels = [k..replace("[", "").replace("]", "").replace("'","") for k in temp_bins]

        ax.set_title(i, size = 20, fontweight = "bold")
        ax.set_xticklabels(labels, rotation = 75, size = 19)
        ax.set_yticklabels(['%.2f' % y for y in ax.get_yticks()], size = 19)
        ax.set_xlabel(ax.get_xlabel(), fontsize=19)
        ax.set_ylabel(ax.get_ylabel(), fontsize=19)

        ax.spines["top"].set_visible(False)
        ax.spines["right"].set_visible(False)


    fig.tight_layout()


    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/WoE_Distribution.jpg", dpi = 300)

    plt.show()
```

```
woe_bins_plot(woe_bins)
```

B.1.3 Modelling

```
models_dict = {
               "LR": LogisticRegression(random_state = seed, n_jobs = -1),
               "DT": DecisionTreeClassifier(random_state = seed),
               "GNB": GaussianNB(),
               "KNN": KNeighborsClassifier(n_jobs = -1),
               "RF": RandomForestClassifier(random_state = seed, n_jobs = -1),
               "GB": GradientBoostingClassifier(random_state = seed),
               "SVM": SVC(probability = True, random_state = seed),
               "MLP": MLP(random_state = seed)
              }


def bayesian_optimization(model, x_train: pd.DataFrame, y_train:
                          pd.Series, seed: int, objective_function: str = "f1"):

    estimator = model

    #Adjustment of max_features hyperparameter within the final model selection.
    max_features = len(x_train.columns)
```

```
#Defining a searching space of possible ranges of hyperparameters, given the model.

if type(model) == type(RandomForestClassifier()):

    search_space = {
                    "n_estimators": Integer(100, 1000),
                    "criterion": Categorical(["gini", "entropy", "log_loss"]),
                    "max_depth": Integer(1, 10),
                    "max_features": Integer(1, max_features),
                    "class_weight": Categorical(["balanced", "balanced_subsample", None]),
                    "bootstrap": Categorical([True, False]),
                    "ccp_alpha": Real(0.000000000001, 0.5, prior="log-uniform"),
                    }



elif type(model) == type(GradientBoostingClassifier()):

    search_space = {
                    "n_estimators": Integer(100, 1000),
                    "loss": Categorical(["log_loss", "exponential"]),
                    "max_depth": Integer(1, 10),
                    "learning_rate":Real(0.0001, 0.2, prior="log-uniform"),
                    "max_features": Integer(1, max_features),
                    "criterion": Categorical(["friedman_mse", "squared_error"]),
```

```
                    }


elif type(model) == type(LogisticRegression()):

    search_space = {
                    "fit_intercept": Categorical([True, False]),
                    "C": Real(0.000001, 5, prior = "log-uniform"),
                    "penalty": Categorical(["l1", "l2", "none", "elasticnet"]),
                    "solver": Categorical(["lbfgs", "liblinear", "newton-cg", "sag", "saga"]),
                    "class_weight": Categorical(["balanced", None])
                    }

    for solver in ["lbfgs", "liblinear", "newton-cg", "sag", "saga"]:
        if solver == "lbfgs" or solver == "newton-cg":
            search_space["penalty"] = Categorical(["l2", "none"])
        elif solver == "sag":
            search_space["penalty"] = Categorical(["l2", "elasticnet"])
            search_space["l1_ratio"] = Real(0, 1, prior = "uniform")
        elif solver == "liblinear":
            search_space["penalty"] = Categorical(["l1", "l2", "none", "elasticnet"])
            if search_space["penalty"] == "l2":
                search_space["dual"] = Categorical([True, False])
            if search_space["fit_intercept"]:
```

```
                search_space["intercept_scaling"] = Real(0.1, 100.0, prior="log-uniform")
        else:
            search_space["penalty"] = Categorical(["l1", "l2", "none", "elasticnet"])
            search_space["l1_ratio"] = Real(0, 1, prior = "uniform")
            search_space["solver"] = Categorical(["saga"])
```

```
elif type(model) == type(SVC()):
    search_space = {
                    "C": Real(0.000001, 5, prior = "log-uniform"),
                    "kernel": Categorical(["linear", "poly", "rbf", "sigmoid"]),
                    "degree": Integer(1, 10),
                    "class_weight": Categorical(["balanced", None])
                   }
```

```
elif type(model) == type(MLPClassifier()):
    search_space = {
                    "hidden_layer_sizes": Integer(5, 500),
                    "activation": Categorical(["logistic", "identity", "tanh", "relu"]),
                    "solver": Categorical(["lbfgs", "sgd", "adam"]),
                    "learning_rate": Categorical(["constant", "invscaling", "adaptive"]),
                   }
```

```
elif type(model) == type(DecisionTreeClassifier()):

    search_space = {
                    "criterion": Categorical(["gini", "entropy"]),
                    "max_depth": Integer(1, 10),
                    "max_features": Integer(1, max_features),
                    }


elif type(model) == type(GaussianNB()):

    search_space = {
                    "var_smoothing": Real(1e-9, 1e-6, prior = "log-uniform")
                   }


elif type(model) == type(KNeighborsClassifier()):

    search_space = {
                    'n_neighbors': Integer(5, 20),
```

```
                    'weights':  Categorical(['uniform', 'distance']),
                    'metric': Categorical(['minkowski', 'manhattan', 'euclidean']),
                    'p': Integer(1, 5)
                   }


#Initialization of the stratified 10-fold cross validation.
stratified_cv = StratifiedKFold(n_splits = 10, shuffle = True, random_state = seed)

# Initialization of the Bayesian Optimization.
# using the stratified 10-fold cross validation and given model,
# while maximizing the objective function F1 score.
bayescv = BayesSearchCV(estimator = estimator,
                        search_spaces = search_space,
                        scoring = objective_function, cv = stratified_cv,
                        n_jobs = -1, n_iter = 50,
                        random_state = seed)

#Fitting the Bayesian optimization algorithm on the training data.
bayescv.fit(x_train, y_train)

#Outputs the model with the best tuned hyperparameters with respect to F1 score.
return bayescv.best_estimator_
```

```
def SFS_feature_selection(x_train:pd.DataFrame, y_train:pd.Series,
                  models_dict:dict, seed:int, objective_function: str = "f1",
                  sfs_method: str = 'forward', export:bool = True) -> pd.DataFrame:

    #Printing output settings and functions
    dashes = 115 * "-"
    count = 1

    def print_FS(name: str, dashes: str,
                 count: int, models_dict: dict):

        print(dashes)
        order = f"{count}/{len(models_dict.keys())}"
        no_dashes_left = int((len(dashes) - len(order) - 1)/2)*"-"
        no_dashes_right  = f"{(len(dashes) - len(order) - len(no_dashes_left) - 2)*'-'}"
        print(f"{no_dashes_left} {order} {no_dashes_right}")
        print(dashes)

        text_ = f"FEATURE SELECTION WITH {name.upper()}"

        no_dashes_left_ = int((len(dashes) - len(text_) - 1)/2)*"-"
        no_dashes_right_  = f"{(len(dashes) - len(text_) - len(no_dashes_left_) - 2)*'-'}"
        print(f'{no_dashes_left_} {text_} {no_dashes_right_}')
        print(dashes)
        print(dashes, "\n")
```

```
def print_FS_exec_time(time, number_features: int,
                       selected_feats: list, dashes: str):

    print(f'    Execution time: {round(time, 4)} minutes', "\n")
    print(f'    {number_features} features selected: {", ".join(selected_feats)}', "\n")
    print(dashes)
    print(dashes, "\n")
    print()


#Definitions of paths for exported files
opt_models_path = "./models/feature_selection/opt_models"
feat_select_path = "./models/feature_selection/feat_select_objects"
df_feat_select_path = "./models/feature_selection"

# Empty list for storing all the models with their tuned hyperparameters,
# number of features selected, and names of selected features.
models_feats_list = []

# For each model, tune its hyperparameters using Bayesian Optimization.
# Then use the tuned model for feature selection using Forward Sequential Feature Selector,
# while maximizing an objective function F1 Score.
for model_name, model in models_dict.items():
```

```
print_FS(model_name, dashes, count, models_dict)

start = time.time()
print("    1/4 ... Starting Bayesian Optimization on the whole set of features")

#Tuning the hyperparameters of the model using Bayesian Optimization.
tuned_model = bayesian_optimization(model, x_train, y_train, seed, objective_function)

print("    2/4 ... Bayesian Optimization finished")

#Initialization of the stratified 10-fold cross validation.
stratified_cv = StratifiedKFold(n_splits = 10, shuffle = True, random_state = seed)

print(f"    3/4 ... Starting {sfs_method.capitalize()} Sequential Feature Selection")

# Initialization of the Forward Sequential Feature Selector 10-fold Cross Validation
# in order to select the optimal number of features
# based on the model with tuned hyperparameters and maximizing F1 score function.
# Instead of selected a fixed number of features, we use an auto selection which stops adding features
# when the objective function (F1) is not incremented by at least "tol"
# between two consecutive feature additions.

sfs = SequentialFeatureSelector(tuned_model, n_features_to_select = "auto",
                                direction = sfs_method, scoring = objective_function,
                                cv = stratified_cv, n_jobs = -1, tol = 0.0000000000000000001)
```

```
sfs.fit(x_train, y_train)

print(f"    4/4 ... {sfs_method.capitalize()} Sequential Feature Selection with finished", "\n")
end = time.time()

#Extracting the final selected features and number of the selected features.
selected_feats = x_train.columns[sfs.get_support()].tolist()
number_features = len(selected_feats)

print_FS_exec_time((end - start)/60, number_features, selected_feats, dashes)

#Exporting both fitted tuned model and feature selection object.
if export:
    for save_path, export_obj, save_name in zip([opt_models_path, feat_select_path],
                                                [tuned_model, sfs],
                                                ["FS_tuned", "SFS_with"]):

        os.makedirs(save_path, exist_ok = True)
        with open(f'{save_path}/{save_name}_{model_name}.h5', "wb") as save_obj:
            dill.dump(export_obj, save_obj)

#Appeding all the model's information from both Bayesian Optimization an Sequential Feature Selection.
models_feats_list.append([model_name, #name of the tuned base model
                          number_features, #number of selected features
                          selected_feats, #list of selected features' names
```

```
                                (end - start)/60 #execution time
                                ])

            count += 1

    # Storing all the models with their tuned hyperparameters,
    # number of features selected, and names of selected features.
    feat_sel_cols = ["model_name",
                     "n_features", "final_features", "execution_time"]

    feat_sel = pd.DataFrame(models_feats_list, columns = feat_sel_cols)

    # Exporting the data frame storing all the models' information
    # from both Bayesian Optimization an Sequential Feature Selection.
    if export:
        with open(f"{df_feat_select_path}/feat_selection_df_ORIGINAL.pkl", "wb") as feat_select_df_save:
            dill.dump(feat_sel, feat_select_df_save)

    return feat_sel


feat_selection_df = SFS_feature_selection(X_train_binned, y_train, models_dict, seed)


def selected_features_recurrence(df: pd.DataFrame, export: bool = True):
```

```
matplotlib.rcParams['mathtext.fontset'] = 'stix'
matplotlib.rcParams['font.family'] = 'STIXGeneral'

df_plot = (
            pd.get_dummies(df["final_features"]
                           .apply(pd.Series)
                           .stack()
                          )
            .sum(level = 0)
            .sum()
            .reset_index()
            .rename(columns = {"index": "Model", 0: "Count"})
            .sort_values("Count", ascending = False)
          )

fig, ax = plt.subplots(nrows = 1, ncols = 1, figsize = (11, 7))



df_plot.plot.bar(x = "Model", y = "Count", color = "mediumpurple",
                 legend = False, ax = ax, zorder = 2)

ax.grid(which = "major", axis = "y", linestyle = "--", zorder = 0)
```

```
    # set title and axis labels
    #plt.title("Recurrence of the selected features", size = 13, fontweight = "bold")
    #plt.xlabel("Features", size = 14)
    plt.xlabel(None)
    plt.ylabel("Count", size = 20)
    plt.yticks(range(1, df_plot['Count'].max() + 1), size = 20)
    plt.xticks(size = 20, rotation = 45)

    plt.legend().set_visible(False)

        #Removing upper and right axes spines
    axes = plt.gca()
    axes.spines["top"].set_visible(False)
    axes.spines["right"].set_visible(False)

    plt.tight_layout()

    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/Recurrence_Selected_Features.jpg", dpi = 300)

    plt.show()


selected_features_recurrence(feat_selection_df)
```

```
def selected_features_dist(df: pd.DataFrame, export: bool = True):

    matplotlib.rcParams['mathtext.fontset'] = 'stix'
    matplotlib.rcParams['font.family'] = 'STIXGeneral'

    df_plot = (
        pd.concat(
            (
                df[["model_name"]],
                pd.get_dummies(
                    df["final_features"]
                    .apply(pd.Series)
                    .stack()
                )
                .sum(level=0)
            ),
            axis=1
        )
        .copy()
    )

    df_plot["totals"] = df_plot.drop("model_name", axis=1).sum(axis=1)
    df_plot = (
        df_plot
```

```
    .sort_values(by="totals", ascending=False)
    .drop("totals", axis=1)
)

fig, ax = plt.subplots(nrows=1, ncols=1, figsize=(11, 7))

colors = plt.cm.tab20.colors

df_plot.plot(
    x="model_name",
    y=[col for col in df_plot.columns if col != "model_name"],
    kind="bar",
    stacked=True,
    figsize=(10, 6),
    ax=ax,
    color=colors,
    zorder=3
)

ax.grid(which="major", axis="y", linestyle="--", zorder=0)
#plt.title("Distribution of Selected Features", size=15, fontweight="bold")
plt.xlabel(None)
plt.ylabel("Number of selected features", size=19)
plt.xticks(size=19, rotation=0)
plt.yticks(range(1,
```

```
                    df_plot[[col for col in df_plot.columns if col != "model_name"]].sum(axis=1).max() + 1),
            size=19)
    plt.legend(bbox_to_anchor=(1, 1), fontsize=14)

    # Removing upper and right axes spines
    axes = plt.gca()
    axes.spines["top"].set_visible(False)
    axes.spines["right"].set_visible(False)

    plt.tight_layout()

    if export:
        os.makedirs("./plots/", exist_ok=True)
        plt.savefig(f"./plots/Selected_Features_Distribution.jpg", dpi=300)

    plt.show()


selected_features_dist(feat_selection_df)


def remove_duplicated_selected_feats(df:pd.DataFrame, export:bool = True) -> pd.DataFrame:

   df_feat_select_path = "./models/feature_selection"
```

```
#Filtering indices of duplicated selected features
feat_duplicated_ind = (
                        df["final_features"]
                       .apply( lambda x: ", ".join(x))
                       .duplicated(keep = False)
                       .values
                      )

if sum(feat_duplicated_ind) != 0:
    #Keeping the model which was the fastest to execute and drop the others
    duplicated_models = (
                         df[feat_duplicated_ind]
                         .sort_values("execution_time")
                         .reset_index(drop = True)
                        )

    drop_models = (
                   duplicated_models
                   .loc[1:,'model_name']
                   .values
                  )

    keep_model = duplicated_models.head(1)["model_name"].values[0]

    models_name_join = ', '.join(duplicated_models["model_name"].tolist())
```

```
        final_feat_selection_df = (
                                  df[~df["model_name"].isin(drop_models)]
                                  .reset_index(drop = True)
                                  )
        filter_row = (final_feat_selection_df["model_name"] == keep_model)
        final_feat_selection_df.loc[filter_row, "model_name"] = models_name_join

    else:
        final_feat_selection_df = df.copy()

    if export:
        with open(f"{df_feat_select_path}/feat_selection_df_FINAL.pkl", "wb") as feat_select_df_save:
            dill.dump(final_feat_selection_df, feat_select_df_save)

    return final_feat_selection_df


feat_selection_df_FINAL = remove_duplicated_selected_feats(feat_selection_df)


metrics_weights = {
                    "descending_rank": {
                                        "F1": 1.5,
                                        "Recall": 1.2,
```

```
                                    "Precision": 1,
                                    "Accuracy": 1,
                                    "AUC": 1,
                                    "Somers D": 1,
                                    "KS": 1,
                                    "MCC": 1
                                   },

                "ascending_rank": {
                                    "Brier Score Loss": 1,
                                    "Log Loss": 1
                                   }
                }


def calc_opt_threshold(model, x:pd.DataFrame, y:pd.Series) -> float:

    y_scores = model.predict_proba(x)[:, 1]

    fpr, tpr, thresholds = roc_curve(y, y_scores)

    youden_index = tpr + (1 - fpr) - 1
    threshold = thresholds[np.argmax(youden_index)]

    return threshold
```

```
def model_selection(x_train:pd.DataFrame, y_train:pd.Series,
                    x_val:pd.DataFrame, y_val:pd.Series,
                    models_dict:dict, feat_sel:pd.DataFrame,
                    seed:int, metrics_weights:dict,
                    target:str = "BAD", objective_function: str = "f1",
                    export:bool = True) -> pd.DataFrame:


    #Printing output settings functions
    dashes = 115 * "-"
    count = 1

    def print_model_selection(name: str, fs_name: str, feat_sel: pd.DataFrame,
                              models_dict: dict, dashes: str, count: int):

        print(dashes)

        order = f"{count}/{len(models_dict.keys())*feat_sel.shape[0]}"
        no_dashes_left = int((len(dashes) - len(order) - 1)/2)*"-"
        no_dashes_right  = f"{(len(dashes) - len(order) - len(no_dashes_left) - 2)*'-'}"

        print(f"{no_dashes_left} {order} {no_dashes_right}")
```

```
    print(dashes)

    text_ = f"BAYESIAN OPTIMIZATION OF {name.upper()}"
    text__ = f"WITH FEATURES SELECTED BY {fs_name.upper()}"

    no_dashes_left_ = int((len(dashes) - len(text_) - 1)/2)*"-"
    no_dashes_right_  = f"{(len(dashes) - len(text_) - len(no_dashes_left_) - 2)*'-'}"
    no_dashes_left__ = int((len(dashes) - len(text__) - 1)/2)*"-"
    no_dashes_right__  = f"{(len(dashes) - len(text__) - len(no_dashes_left__) - 2)*'-'}"

    print(f"{no_dashes_left_} {text_} {no_dashes_right_}")
    print(f"{no_dashes_left__} {text__} {no_dashes_right__}")
    print(dashes)
    print(dashes, "\n")


def exec_time_model_selection(name: str, opt_mod, time, evs_list: list,
                              threshold: float, dashes: str):

    print(f"    Execution time: {round(time, 4)} minutes", "\n")
    print(f"    {objective_function.capitalize()} Score on Validation set: {evs_list[0]}", "\n")
    print(f"    Optimal classification threshold: {round(threshold, 4)}", "\n")
    print(f"    Tuned hyperparameters of {name}:", "\n")
    for hyp, val in opt_mod.get_params().items():
```

```
            print(f"        {hyp}: {val}")
        print("")
        print(dashes, "\n")

#Path to save the model selection data frame.
model_selection_path = "./models/model_selection"

#Metrics space.
metrics = {
            "F1": f1_score,
            "Precision": precision_score,
            "Recall": recall_score,
            "Accuracy": accuracy_score,
            "AUC": roc_auc_score,
            "Somers D": somersd,
            "KS": ks_2samp,
            "MCC": matthews_corrcoef,
            "Brier Score Loss": brier_score_loss,
            "Log Loss": log_loss
            }

#Metrics categorization
probs_evs = ["AUC", "Brier Score Loss"]
class_evs = ["Precision", "Recall", "F1", "Accuracy", "MCC"]
```

```
#List for storing the results of the model selection.
tuned_list = []


#For each model, optimize it on the each subset of optimal features on training set
    # and then evaluate it on validation set with filtered features (using set of several metrics).
for model_name, model in models_dict.items():

    for _, row in feat_sel.iterrows():

        #Model name and feature selection method.
        fs_name = row["model_name"]

        #Final features
        final_features = row["final_features"]

        #Filtered training and validation sets based on the final features.
        X_train_filtered = x_train[final_features]
        X_val_filtered = x_val[final_features]

        print_model_selection(model_name, fs_name, feat_sel, models_dict, dashes, count)
        n_f = len(final_features)
        print(f"    1/2 ... Starting Bayesian Optimization on the subset of features ({n_f} features):")
        print(f'                {", ".join(final_features)}')
```

```
start = time.time()

#Bayesian Optimization
tuned_model = bayesian_optimization(model, X_train_filtered, y_train, seed, objective_function)

end = time.time()

#Optimal threshold calculation
threshold = calc_opt_threshold(tuned_model, X_train_filtered, y_train)

#Predicted probabilities and classes on validation set (using optimal threshold)
y_val_scores = tuned_model.predict_proba(X_val_filtered)[:, 1]
y_val_preds = pd.Series(y_val_scores).apply(lambda x: 1 if x > threshold else 0)

#List for storing calculated evaluation metrics.
evs_list = []

#Metrics calculation on validation set.
for metric_name, metric in metrics.items():
    if metric_name in probs_evs:
        evs_list.append(metric(y_val, y_val_scores))
    elif metric_name in class_evs:
        evs_list.append(metric(y_val, y_val_preds))
    elif metric_name == 'Log Loss':
        evs_list.append(metric(y_val, tuned_model.predict_proba(X_val_filtered)))
```

```
        elif metric_name == "Somers D":
            evs_list.append(metric(y_val, y_val_scores).statistic)
        elif metric_name == "KS":
            X_Y_concat = pd.concat((y_val, X_val_filtered), axis = 1)
            X_Y_concat["prob"] =  y_val_scores
            evs_list.append(metric(X_Y_concat.loc[X_Y_concat[target] == 1, "prob"],
                                   X_Y_concat.loc[X_Y_concat[target] == 0, "prob"]).statistic)

    #Storing the results of the model selection.
    tuned_list.append([model_name,
                       fs_name,
                       tuned_model,
                       len(final_features),
                       final_features,
                       (end - start)/60,
                       threshold] +
                       evs_list
                       )

#Exporting the final tuned model in .h5 format
    if export:
        os.makedirs(model_selection_path, exist_ok = True)
        os.makedirs(f"{model_selection_path}/models", exist_ok = True)

        with open(f"{model_selection_path}/models/{model_name}_with_{fs_name}.h5", "wb") as mod_save:
```

```
                dill.dump(tuned_model, mod_save)


        print("    2/2... Bayesian Optimization finished", "\n")

        exec_time_model_selection(model_name, tuned_model, (end - start)/60, evs_list, threshold, dashes)

        count += 1

#Model selection data frame.
model_sel_cols = ["tuned_model_name", "fs_model_name",
                  "sfs_object", "n_features",
                  "final_features", "execution_time",
                  "threshold"] + list(metrics.keys())

model_selection_df = pd.DataFrame(tuned_list, columns = model_sel_cols)

#Ranking the models based on the evaluation metrics and the provided weights.
for dict_name, metric_weight_dict in metrics_weights.items():

    #Ranking each metric.
    for metric in metric_weight_dict.keys():

            # Ranking the models whether the metric is ascending or descending
            # (score metrics are descending, loss metrics are ascending).
```

```
            order = True if dict_name == "ascending_rank" else False

            #Ranking
            model_selection_df[f"{metric}_rank"] = (
                                                    model_selection_df[[metric]]
                                                    .rank(ascending = order)
                                                    )

#Accessing individual ranking metrics columns.
ranked_cols = [rank for rank in model_selection_df.columns if "_rank" in rank]

unnested_metric_weights = {k: v for in_dict in metrics_weights.values() for k, v in in_dict.items()}


for i, row in model_selection_df[ranked_cols].iterrows():

    numerator = sum([row[col] * unnested_metric_weights[col.split("_")[0]] for col in ranked_cols])
    deniminator = sum(unnested_metric_weights.values())

    model_selection_df.loc[i, "avg_rank"] = numerator / deniminator


model_selection_df['final_rank'] = model_selection_df['avg_rank'].rank(ascending = True)

#Ordering the model selection data frame based on the final ranking.
```

```
    model_selection_df = (
                           model_selection_df
                          .drop(ranked_cols, axis = 1)
                          .sort_values("final_rank")
                          .reset_index(drop = True)
                          )

    #Exporting the model selection data frame.
    if export:
        with open(f"{model_selection_path}/model_selection_df.pkl", "wb") as model_select_df_save:
            dill.dump(model_selection_df, model_select_df_save)

    return model_selection_df



model_selection_df = model_selection(X_train_binned, y_train, X_valid_binned, y_valid,
                                     models_dict, feat_selection_df_FINAL, seed, metrics_weights)


(
    model_selection_df
    .loc[(model_selection_df
          .loc[:, ~model_selection_df
               .columns
```

```
                .isin(["final_features"])]
            .groupby("tuned_model_name")["final_rank"]
            .idxmin()),
        ~model_selection_df
        .columns
        .isin(["final_features"])]
    .sort_values("final_rank")
)


def plot_models_metrics(df: pd.DataFrame, metric: str, group_by: str = "tuned_model_name",
                        plot_name: str = "", export:bool = True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"

    plt.figure(figsize = (10, 6))  # Increase the figsize values to make the plot bigger
    sns.boxplot(data = df, x = metric, y = group_by, palette = "BuPu_r")

    axes = plt.gca()
    axes.spines["top"].set_visible(False)
    axes.spines["right"].set_visible(False)
    axes.set(ylabel = None)

    # Increase the fontsize for xticks and yticks
```

```
    plt.xticks(fontsize = 17)
    plt.yticks(fontsize = 17)

    # Increase the fontsize for x and y axis labels
    if metric == "execution_time":
        plt.xlabel(f"Execution time (in minutes)", fontsize = 17)
    else:
        plt.xlabel(metric, fontsize = 17)

    plt.tight_layout()

    if export:
        os.makedirs("./plots/", exist_ok=True)
        plot_name_save = metric.upper() if len(plot_name) == 0 else plot_name.upper()
        plt.savefig(f"./plots/{plot_name_save}_Distribution.jpg", dpi=300)

    plt.show()


plot_models_metrics(model_selection_df, "F1")
plot_models_metrics(model_selection_df[model_selection_df["F1"]>model_selection_df["F1"].min()],
                    "F1", plot_name = "F1_wo_outliers")

plot_models_metrics(model_selection_df, "threshold")
plot_models_metrics(model_selection_df[model_selection_df["threshold"] < model_selection_df["threshold"].max()],
```

```
                    "threshold", plot_name = "threshold_wo_outliers")

plot_models_metrics(model_selection_df, "execution_time")

for col in ["Precision", "Recall", "Accuracy", "AUC", "Somers D", "KS", "MCC", "Brier Score Loss", "Log Loss"]:
    plot_models_metrics(model_selection_df, col, export = "_".join([col]))


def scatter_metrics_plot(df: pd.DataFrame, metric_1: str, metric_2: str,
                         plot_name: str = "", export: bool = True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"

    plt.figure(figsize = (10, 7))
    plot_df = df.copy()
    sns.scatterplot(data = plot_df, x = metric_1, y = metric_2,
                    hue = "tuned_model_name", palette = "Set2", s = 100, alpha = 0.7)
    axes = plt.gca()
    axes.spines["top"].set_visible(False)
    axes.spines["right"].set_visible(False)

    # Increase the fontsize for xticks and yticks
    plt.xticks(fontsize=18)
    plt.yticks(fontsize=18)
```

```
if metric_1 == "execution_time":
    metric_xlabel = "Execution time (in minutes)"
else:
    metric_xlabel = metric_1

if metric_2 == "execution_time":
    metric_ylabel = "Execution time (in minutes)"
else:
    metric_ylabel = metric_2

# Increase the fontsize for x and y axis labels
plt.xlabel(metric_xlabel, fontsize = 18)
plt.ylabel(metric_ylabel, fontsize = 18)

plt.legend(bbox_to_anchor = (1.2, 1.1), fontsize = 18)  # Increase the fontsize for the legend
plt.tight_layout()

if export:
    os.makedirs("./plots/", exist_ok = True)
    plt.savefig(f"./plots/Scatterplot_{metric_1}_{metric_2}{plot_name}.jpg", dpi = 300)

plt.show()
```

```
scatter_metrics_plot(model_selection_df, "execution_time", "F1")
scatter_metrics_plot(model_selection_df[model_selection_df["F1"] > model_selection_df["F1"].min()],
                     "execution_time", "F1", plot_name = "_wo_outliers")


def print_final_model(df: pd.DataFrame, model_order: int = 0):

    final_model_path = "./models/model_selection/models"

    with open(os.path.join(final_model_path, f"{final_model_name}_with_{fs_model_name}.h5"), "rb") as mod_load:
        final_model = dill.load(mod_load)

    final_model_name = df.loc[model_order, "tuned_model_name"]
    fs_model_name = df.loc[model_order, "fs_model_name"]
    final_features = df.loc[model_order, "final_features"]
    final_threshold, final_hyperparameters = df.loc[model_order, "threshold"], final_model.get_params()

    #Final model

    print(f"Final model: {final_model_name.upper()}")
    print(f"Final model trained on features selected by: {fs_model_name.upper()}")
    print(f"Final subset of features: {', '.join(final_features)}")
    print(f"The final threshold: {final_threshold}")
    print("Final hyperparameters:")
```

```
    for hp_name, hp_value in final_hyperparameters.items():
        print(f"{(len('Final hyperparameters:') + 2) * ' '}{hp_name}: {hp_value}")


print_final_model(model_selection_df)


def data_filter_join(hyp_tuning_df: pd.DataFrame, x_train: pd.DataFrame,
                     x_valid: pd.DataFrame, x_test: pd.DataFrame,
                     y_train: pd.Series, y_valid: pd.Series,
                     model_order:int = 0) -> tuple[pd.Series, pd.DataFrame, pd.DataFrame]:

    #Final features
    final_features = [feat for feat in hyp_tuning_df.loc[model_order, "final_features"]]

    #Joined training and validation labels.
    y_train_valid = pd.concat((y_train, y_valid))

    #Filtered joined training and validation set based on final features.
    x_train_valid_filtered = pd.concat((x_train, x_valid))[final_features]

    #Filtered test set based on final features.
    x_test_filtered = x_test[final_features]

    return (y_train_valid, x_train_valid_filtered, x_test_filtered)
```

```
(
  y_train_valid,
  X_train_valid_binned_filtered,
  X_test_binned_filtered
) = data_filter_join(model_selection_df, X_train_binned, X_valid_binned, X_test_binned, y_train, y_valid)

preprocessed = prep_data_export((X_train_valid_binned_filtered, X_test_binned_filtered),
                                (y_train_valid, y_test),
                                ("Training_Validation", "Test"),
                                csv_name = "preprocessed_data")


def final_model_fit_eval(hyp_tuning_df: pd.DataFrame,
                         x_fit: pd.DataFrame, y_fit: pd.Series,
                         model_order: int = 0,
                         save_model: bool = True):

    final_model_path = "./models/model_selection/models"
    output_path = "./models/objects_FINAL"

    final_model_name = hyp_tuning_df.loc[model_order, "tuned_model_name"]
    fs_model_name = hyp_tuning_df.loc[model_order, "fs_model_name"]
```

```
    #Final model
    with open(os.path.join(final_model_path, f"{final_model_name}_with_{fs_model_name}.h5"), "rb") as mod_load:
        final_model = dill.load(mod_load)

    #Fitting the final model on the joined training and validation set
    final_model.fit(x_fit, y_fit)

    if save_model:
        with open(f"{output_path}/final_model_eval.h5", "wb") as mod_save:
            dill.dump(final_model, mod_save)

    return final_model


final_model_eval = final_model_fit_eval(model_selection_df, X_train_valid_binned_filtered, y_train_valid)

def get_final_features(model_selection_df: pd.DataFrame, model_order: int = 0) -> tuple[float, list]:

    final_features = model_selection_df.loc[model_order, "final_features"]

    return final_features


final_features = get_final_features(model_selection_df)
```

```
opt_threshold = calc_opt_threshold(final_model_eval, X_train_valid_binned_filtered, y_train_valid)
```

B.1.4 Evaluation

```
def conf_mat(model, X: pd.DataFrame, y: pd.Series, threshold: float) -> pd.DataFrame:

    y_scores = pd.Series(model.predict_proba(X)[:, 1])
    y_preds = y_scores.apply(lambda x: 1 if x > threshold else 0)

    confm = pd.DataFrame(
                         confusion_matrix(y, y_preds),
                         columns = ["Predicted - Non-Default", "Predicted - Default"],
                         index = ["Actual - Non-Default", "Actual - Default"]
                        )
    return confm


conf_matrix = conf_mat(final_model_eval, X_test_binned_filtered, y_test, opt_threshold)


def conf_mat_plot(conf_matrix: pd.DataFrame, export:bool = True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"
```

```
    plt.figure(figsize = (9, 7))
    #plt.title("Confusion matrix", size = 13, fontweight = "bold")


    ax = sns.heatmap(conf_matrix, annot=True, cmap = "BuPu", fmt = "g", annot_kws = {"size": 18})

    cbar = ax.collections[0].colorbar
    cbar.ax.tick_params(labelsize = 18)  # Set fontsize for color bar

    plt.xticks(size = 18)
    plt.yticks(size = 18)

    plt.tight_layout()


    if export:
        os.makedirs("./plots", exist_ok=True)
        plt.savefig(f"./plots/Confusion_Matrix.jpg", dpi=300)
    plt.show()


conf_mat_plot(conf_matrix)

def evaluation_metrics(model, X: pd.DataFrame, y: pd.Series,
```

```
                    threshold: float, target: str = "BAD") -> pd.DataFrame:

metrics = {
            "F1": f1_score,
            "Precision": precision_score,
            "Recall": recall_score,
            "Accuracy": accuracy_score,
            "AUC": roc_auc_score,
            "Somers D": somersd,
            "KS": ks_2samp,
            "MCC": matthews_corrcoef,
            "Brier Score Loss": brier_score_loss,
            "Log Loss": log_loss
            }


probs_evs = ["AUC","Brier Score Loss"]
class_evs = ["Precision", "Recall", "F1", "Accuracy", "MCC"]
evs_list = []

y_scores = model.predict_proba(X)[:, 1]
y_preds = pd.Series(y_scores).apply(lambda x: 1 if x > threshold else 0)

for metric_name, metric in metrics.items():
    if metric_name in probs_evs:
```

```
            evs_list.append([metric_name, metric(y, y_scores)])
        elif metric_name in class_evs:
            evs_list.append([metric_name, metric(y, y_preds)])
        elif metric_name == "Log Loss":
            evs_list.append([metric_name, metric(y, model.predict_proba(X))])
        elif metric_name == "Somers D":
            evs_list.append([metric_name, metric(y, y_scores).statistic])
        elif metric_name == "KS":
            X_Y_concat = pd.concat((y, X), axis = 1)
            X_Y_concat["prob"] =  y_scores
            evs_list.append([metric_name, metric(X_Y_concat.loc[X_Y_concat[target] == 1, "prob"],
                                                 X_Y_concat.loc[X_Y_concat[target] == 0, "prob"]).statistic])

    evaluation_df = pd.DataFrame(evs_list, columns = ["Metric", "Score"])

    return evaluation_df


evaluation_metrics(final_model_eval, X_test_binned_filtered, y_test, opt_threshold)


def ROC_curve_plot(model, X: pd.DataFrame, y: pd.Series, export:bool = True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"
```

```
y_pred = model.predict_proba(X)[:, 1]
fpr, tpr, _ = roc_curve(y, y_pred)
auc = roc_auc_score(y, y_pred)
plt.figure(figsize = (10, 7))
plt.plot(fpr,tpr,label = f"AUC = {auc*100:.2f}%")
plt.plot([0, 1], [0, 1], "r--")
plt.ylabel("True Positive Rate",  size = 18)
plt.xlabel("False Positive Rate",  size = 18)
plt.xticks(size = 18)
plt.yticks(size = 18)
plt.legend(prop={'size': 16})
#plt.title("ROC curve", size = 13, fontweight = "bold")
plt.grid()
axes = plt.gca()
axes.spines["top"].set_visible(False)
axes.spines["right"].set_visible(False)


plt.tight_layout()

if export:
    os.makedirs("./plots/", exist_ok = True)
    plt.savefig(f"./plots/ROC_curve_FINAL.jpg", dpi = 300)
plt.show()
```

```
ROC_curve_plot(final_model_eval, X_test_binned_filtered, y_test)


def feature_importance_plot(model, features: list, export:bool = True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"

    importances = model.feature_importances_

    plot_df = pd.DataFrame({"Feature": features, "Importance": importances})
    plot_df = plot_df.sort_values("Importance", ascending = False)

    plt.figure(figsize = (10, 6))
    sns.barplot(plot_df, x = "Importance", y = "Feature", palette = "BuPu_r")
    #plt.title("Feature Importances", fontsize = 15, fontweight = "bold")

    axes = plt.gca()
    axes.spines["top"].set_visible(False)
    axes.spines["right"].set_visible(False)

    axes.xaxis.label.set_size(18)
    axes.yaxis.label.set_size(18)
```

```
    plt.xticks(fontsize = 18)
    plt.yticks(fontsize = 18)

    plt.tight_layout()

    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/Feature_Importances.jpg", dpi = 300)

    plt.show()


feature_importance_plot(final_model_eval, final_features)


def GBC_SHAP_plot(model, X: pd.DataFrame, export: bool = True):

    matplotlib.rcParams["mathtext.fontset"] = "stix"
    matplotlib.rcParams["font.family"] = "STIXGeneral"


    explainer = shap.TreeExplainer(model, model_output = "probability", data = X)

    shap_values = explainer.shap_values(X)
```

```
    #Scaling the SHAP values in order to be between -1 and 1.
    #max_abs_shap = np.max(np.abs(shap_values))
    #scaled_shap_values = shap_values / max_abs_shap

    # Set plot size here
    plot_size = (16, 12)

    # Create a summary plot and specify the plot_size
# Set plot size
    plot_size = (8, 8)

    # Create a summary plot and specify the plot_size
    summary_plot = shap.summary_plot(shap_values,
                                     X.values,
                                     feature_names = X.columns,
                                     show = False,
                                     plot_size = plot_size,
                                     color_bar = True)

    # Increase fontsize of labels and ticks
    plt.gca().xaxis.label.set_size(18)
    plt.gca().yaxis.label.set_size(18)
    plt.xticks(fontsize = 18)
    plt.yticks(fontsize = 18)
```

```
    # Find the colorbar object and modify its fontsize
    colorbar = plt.gcf().get_axes()[-1]
    colorbar.tick_params(labelsize = 18)
    colorbar.set_ylabel("Feature Value", fontsize = 18)  # Increase fontsize of the "Feature Value" label

    plt.tight_layout()

    if export:
        os.makedirs("./plots/", exist_ok = True)
        plt.savefig(f"./plots/SHAP_summary_plot.jpg", dpi = 1200)

    plt.show()


GBC_SHAP_plot(final_model_eval, X_test_binned_filtered)


def final_model_fit_deploy(final_model, X: tuple, y: tuple, final_features: list,
                           target = "BAD", export: bool = True):

    df_list = []
    output_path = "./models/objects_FINAL"

    #Joining the features and labels from training, validation and test sets.
    for feat, lab in zip(X, y):
```

```
        temp = pd.concat((lab, feat), axis = 1)
        df_list.append(temp)
    dfs = [df for df in df_list]

    #Final model fit.
    final_df = pd.concat(dfs, axis = 0).sort_index()
    X_final = final_df[final_features]
    y_final = final_df[target]

    final_model.fit(X_final, y_final)

    #Exporting the final model.
    if export:
        with open(f"{output_path}/final_model_deploy.h5", "wb") as mod_save:
            dill.dump(final_model, mod_save)

    #Final classification threshold
    final_threshold = calc_opt_threshold(final_model, X_final, y_final)

    return (final_model, final_threshold)

(
  final_model_deployment, final_threshold_deployment
) = final_model_fit_deploy(final_model_eval,
                           (X_train_valid_binned_filtered, X_test_binned_filtered),
```

```
                                                    (y_train_valid, y_test),
                                                    final_features)

def flask_app_input_export(**kwargs):

    with open(r"flask_app\inputs\inputs_flask_app_dict.pkl", "wb") as f:
        dill.dump(kwargs, f)

    with open(r"models\objects_FINAL\inputs_flask_app_dict.pkl", "wb") as f:
        dill.dump(kwargs, f)


def lime_explanation(X: pd.DataFrame, export: bool = True):

    explainer = lime.lime_tabular.LimeTabularExplainer(
                                                        training_data = np.array(X),
                                                        feature_names = X.columns,
                                                        class_names = ["non-default", "default"],
                                                        mode = "classification"
                                                        )

    return explainer


lime_explainer = lime_explanation(pd.concat((X_train_valid_binned_filtered, X_test_binned_filtered)))
```

```
flask_app_input_export(woe_bins = woe_bins,
                       binning_transformator = binning_transformator,
                       final_model = final_model_deployment,
                       threshold = final_threshold_deployment,
                       final_features = final_features,
                       categorical_features = cat_vars,
                       input_df = pd.DataFrame(columns = X_train_binned.columns),
                       lime_explainer = lime_explainer)
```

B.2 Flask Web Application Code

```
import warnings

warnings.filterwarnings("ignore")
from flask import Flask, render_template, request
import pandas as pd
import numpy as np
import os
import lime
import dill
import matplotlib
```

```
import matplotlib.pyplot as plt


app = Flask(__name__)


current_dir = os.path.dirname(os.path.abspath(__file__))
input_file_path = os.path.join(current_dir, "inputs", "inputs_flask_app_dict.pkl")

with open(input_file_path, "rb") as f:
        inputs = dill.load(f)

with open(os.path.join(current_dir, "inputs", "explainer.pkl"), "rb") as f:
        lime_explainer = dill.load(f)


def lime_plot(input, model, lime_explainer):
        def custom_lime_plot(exp, pos_color: str = "red", neg_color: str = "green"):

                fig, ax = plt.subplots()
                vals = [i[1] for i in exp.as_list()][::-1]
                names = [
                        i[0].split(" <=")[0].split("< ")[-1].split(" >")[0] for i in exp.as_list()
                ][::-1]
                feat_dict = {
```

```
                "JOB": "Job occupancy",
                "REASON": "Reason of loan application",
                "LOAN": "Requested loan amount",
                "MORTDUE": "Amount due on existing mortgage",
                "VALUE": "Current property value",
                "YOJ": "Years at present job",
                "DEROG": "# of major derogatory reports",
                "DELINQ": "# of delinquent credit lines",
                "CLAGE": "Age of the oldest credit line",
                "NINQ": "# of recent credit inquiries",
                "CLNO": "# of credit lines",
                "DEBTINC": "Debt-to-income ratio",
            }
            names = [feat_dict[i] for i in names]
            colors = [pos_color if x > 0 else neg_color for x in vals]
            pos = np.arange(len(vals)) + 0.5

            ax.barh(pos, vals, align="center", color=colors)
            ax.set_yticks(pos)
            ax.set_yticklabels(names)

            return fig

plt.rcParams["font.family"] = "Segoe UI"
```

```
exp = lime_explainer.explain_instance(
        data_row=input, predict_fn=model.predict_proba
)

fig = custom_lime_plot(exp)
fig.set_size_inches(11, 9)

ax = plt.gca()
ax.spines["right"].set_visible(False)
ax.spines["top"].set_visible(False)
ax.set_ylabel("Feature", fontsize=21, color="#6c6c6c")
ax.set_xlabel("Contribution", fontsize=21, color="#6c6c6c")
ax.tick_params(axis="x", labelsize=20)
ax.tick_params(axis="y", labelsize=20)

plt.title("")
for xticklabel, yticklabel in zip(ax.get_xticklabels(), ax.get_yticklabels()):
        xticklabel.set_color("#6c6c6c")
        yticklabel.set_color("#6c6c6c")

fig.savefig(
        os.path.join(current_dir, "static", "lime_explanation.png"),
        format="png",
        bbox_inches="tight",
        dpi=300,
```

```
                transparent=True,
        )
        plt.close(fig)


@app.route("/")
def home():
        features = inputs["final_features"]
        categorical_features = inputs["categorical_features"]
        return render_template(
                "index.html", variables=features, categorical_features=categorical_features
        )


@app.route("/predict", methods=["POST"])
def predict():
        (
                woe_bins,
                woe_binning,
                model,
                threshold,
                final_features,
                categorical_features,
                input_df,
        ) = (input for _, input in inputs.items())
```

```
for feature in input_df.columns:
        if feature in final_features:
                if feature in categorical_features:
                        input_df.loc[0, feature] = (
                                str(request.form[feature]) if request.form[feature] else np.nan
                        )
                elif feature == "LOAN":
                        input_df.loc[0, feature] = (
                                int(request.form[feature]) if request.form[feature] else np.nan
                        )
                else:
                        input_df.loc[0, feature] = (
                                float(request.form[feature]) if request.form[feature] else np.nan
                        )
        else:
                input_df.loc[0, feature] = np.nan

input_df_woe = woe_binning.transform(input_df, metric="woe")

for feature in input_df_woe.columns:
        na_woe = woe_bins.query('Variable == @feature and Bin == "Missing"')[
                "WoE"
        ].values[0]
        input_df_woe.loc[input_df[feature].isna(), feature] = na_woe
```

```
        input_df_woe_FINAL = input_df_woe[final_features]
        pred_score = model.predict_proba(input_df_woe_FINAL)[:, 1]

        result = [
                "Loan application denied" if i > threshold else "Loan application approved"
                for i in pred_score
        ]

        lime_plot(input_df_woe_FINAL.iloc[0], model, lime_explainer)

        return render_template(
                "results.html",
                prediction=round(pred_score[0] * 100, 2),
                predicted_class=result[0],
        )


if __name__ == "__main__":
        app.run(debug=True)
```

B.3 HTML UI Codes

B.3.1 index.html

```
<!DOCTYPE html>
<html>
        <head>
                <style>
                        body {
                                font-family: Arial, sans-serif;
                                background-color: #f3f3f3;
                                color: #444;
                        }
                        form {
                                margin: 20px auto;
                                padding: 30px;
                                background-color: #ffffff;
                                border: 1px solid #e6e6e6;
                                box-shadow: 2px 2px 15px rgba(0, 0, 0, 0.1);
                                max-width: 700px;
                                border-radius: 5px;
                        }
                        h1 {
                                text-align: center;
                                color: #333;
```

```
        margin-bottom: 20px;
}

p {
        text-align: center;
        color: #666;
        margin-bottom: 30px;
}

label {
        display: block;
        margin-bottom: 5px;
        color: #555;
}

input[type="number"],
select {
        padding: 10px 20px;
        font-size: 16px;
        border: 1px solid #ccc;
        border-radius: 4px;
        width: 100%;
        box-sizing: border-box;
        margin: 10px 0;
        transition: border 0.3s;
```

```
}

input[type="submit"] {
        background-color: #4caf50;
        color: white;
        padding: 12px 30px;
        border: none;
        border-radius: 4px;
        cursor: pointer;
        margin-top: 30px;
        width: auto;
        transition: background-color 0.3s;
        display: block;
        margin-left: auto;
        margin-right: auto;
}

input[type="submit"]:hover {
        background-color: #45a049;
}

select:hover,
input[type="number"]:hover,
select:focus,
input[type="number"]:focus {
```

```
                        border-color: #4caf50;
                }
                .form-grid {
                        display: grid;
                        grid-template-columns: repeat(2, 1fr);
                        gap: 20px;
                }

                .form-grid > div {
                        grid-column: span 1;
                }
        </style>
</head>
<body>
        <h1>Default Prediction Application</h1>
        <p><b>Author:</b> Petr Nguyen</p>
        <form method="POST" action="/predict">
                <div class="form-grid">
                        {% for variable in variables %}
                        <div>
                                {% if variable == 'JOB' %}
                                <label for="JOB">Job occupancy:</label>
                                <select name="JOB">
                                        <option value=""></option>
                                        <option value="Mgr">Manager</option>
```

```
        <option value="Office">Office worker</option>
        <option value="ProfExe">Professional/Executive</option>
        <option value="Sales">Sales</option>
        <option value="Self">Self-employed</option>
        <option value="Other">Other</option>
</select>
<br />
{% elif variable == 'REASON' %}
<label for="REASON">Reason of loan application:</label>
<select name="REASON">
        <option value=""></option>
        <option value="DebtCon">Debt Consolidation</option>
        <option value="HomeImp">Home Improvement</option>
</select>
<br />
{% elif variable == 'LOAN' %}
<label for="LOAN">Requested loan amount:</label>
<input type="number" name="LOAN" min="0" required /><br />
{% elif variable == 'MORTDUE' %}
<label for="MORTDUE">Amount due on existing mortgage:</label>
<input type="number" name="MORTDUE" min="0" /><br />
{% elif variable =='VALUE' %}
<label for="VALUE">Current property value:</label>
<input type="number" name="VALUE" min="0" /><br />
{% elif variable == 'YOJ' %}
```

```
                    <label for="YOJ">Number of years at present job:</label>
                    <input type="number" name="YOJ" min="0" step="0.1" /><br />
                    {% elif variable == 'DEROG' %}
                    <label for="DEROG">Number of major derogatory reports:</label>
                    <input type="number" name="DEROG" min="0" /><br />
                    {% elif variable == 'DELINQ' %}
                    <label for="DELINQ">Number of delinquent credit lines:</label>
                    <input type="number" name="DELINQ" min="0" /><br />
                    {% elif variable == 'CLAGE' %}
                    <label for="CLAGE">Age of the oldest credit line (in months):</label>
                    <input type="number" name="CLAGE" min="0" /><br />
                    {% elif variable == 'NINQ' %}
                    <label for="NINQ">Number of recent credit inquiries:</label>
                    <input type="number" name="NINQ" min="0" /><br />
                    {% elif variable == 'CLNO' %}
                    <label for="CLNO">Number of credit lines:</label>
                    <input type="number" name="CLNO" min="0" /><br />
                    {% elif variable == 'DEBTINC' %}
                    <label for="DEBTINC">Debt-to-income ratio:</label>
                    <input type="number" name="DEBTINC" min="0" step="0.0000001" /><br />
                    {% endif %}
                </div>
                {% endfor %}
        </div>
        <input type="submit" value="Submit" />
```

```
                </form>
        </body>
</html>
```

B.3.2 results.html

```
<!DOCTYPE html>
<html>
        <head>
                <title>Default Prediction - Result</title>
                <style>
                        body {
                                font-family: "Segoe UI", Tahoma, Geneva, Verdana, sans-serif;
                                background-color: #f5f5f5;
                                color: #333;
                        }
                        h1 {
                                text-align: center;
                                color: #4c4c4c;
                                font-size: 2.5em;
                                margin-top: 50px;
                        }
                        p {
                                text-align: center;
```

```
                color: #6c6c6c;
                font-size: 1.5em;
                margin-top: 50px;
            }
            .box {
                background-color: #ccc;
                width: 200px;
                height: 200px;
                display: flex;
                justify-content: center;
                align-items: center;
                font-size: 24px;
                font-weight: bold;
                text-align: center;
                text-decoration: none;
                color: #333;
            }
            img {
                max-width: 100%;
            }
        </style>
</head>
<body>
        <h1>Default Prediction Result</h1>
        <p>Result: <b>{{predicted_class}}!</b></p>
```

```
            <p>The probability of default is <b>{{ prediction }}%</b></p>

            <img src="{{ url_for('static', filename='lime_explanation.png') }}"
                 alt="LIME Explanation" width="50%" style="display: block; margin: auto;" />
    </body>
</html>
```