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**Implementation of Machine Learning
Algorithms within Credit Risk
Modelling**

Master's thesis

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Declaration of Authorship

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

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Abstract

This Master's thesis deals with the custom machine learning implementation framework that was developed in Python and applied to the application scoring data of US home equity loans (HMEQ). The ML framework involves eight classification models, namely Logistic Regression, Decision Tree, Gaussian Naive Bayes, K-Nearest Neighbors, Random Forest, Gradient Boosting, Support Vector Machine, and Neural Network. It further consists of data exploration, data preprocessing using ADASYN oversampling and Optimal Binning with Weight-of-Evidence, a custom feature selection algorithm that utilizes both Bayesian Optimization and Forward Sequential Feature Selection, and a custom model selection algorithm employed based on Bayesian Optimization and weighted ranking of individual metric ranks. In this thesis, metrics such as F1 score, MCC, AUC, Kolmogorov-Smirnov Distance, Somers' D, etc., are evaluated. Instead of using standard classification threshold of 0.5, an optimal threshold is calculated using Youden index. The final model is Gradient Boosting trained on the features selected by Neural Network. This model is further evaluated using both model performance assessment and black-box model explainability inspection. The final model is deployed as a web application using Flask and HTML, which requires filling in the loan application form and outputs the loan approval result, probability of default, and LIME plot, i.e., local explainability of the black-box model around the single prediction.

Keywords: machine learning, credit risk, loans, probability of default, Python

Abstrakt

Tato diplomová práce se zabývá implementací vlastního rámce strojového učení (ML), který byl vyvinut v Pythonu a aplikován na aplikační scoringová data amerických hypotečních úvěrů (HMEQ). Tento ML rámec zahrnuje 8 klasifikačních modelů, jmenovitě logistickou regresi, rozhodovací strom, Gaussovský nainvní Bayes, k-nejbližších sousedů, náhodný les, gradientní boosting, model podpůrných vektorů a neuronovou síť. Dále je zde zahrnutá explorace dat, zpracování dat pomocí ADASYN a optimálního binningu s Weight-of-Evidence, vlastní algoritmus pro výběr prediktorů využívající Bayesovskou optimalizaci a Forwardovou sekvenční selekci prediktorů a vlastní algoritmus pro výběr finálního modelu na základě Bayesovské optimalizace a váženého rankingu dle jednotlivých metrik. V této práci jsou evaluovány metriky jako F1 skóre, MCC, AUC, Kolmogorov-Smirnovova vzdálenost, Somersův D atd. Namísto použití standardního klasifikačního prahu 0,5 se optimální prahová hodnota vypočítává pomocí Youdenova indexu. Finálním vybraným modelem je gradientní boosting trénovaný na prediktorech vybraných neuronovou sítí. Tento model je dále evaluován na základě hodnocení výkonnosti modelu a inspekce vysvětlitelnosti black-box modelu. Finální model je nasazen jako webová aplikace využívající Flask a HTML, do které se vyplní formulář žádosti o úvěr a vrátí výsledek o schválení úvěru, pravděpodobnost defaultu a LIME - lokální vysvětlitelnost black-box modelu okolo samotné predikce.

Klíčová slova: strojové učení, machine learning, kreditní riziko, úvěry, pravděpodobnost defaultu, Python

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Acronyms

ML	Machine Learning
HMEQ	Home Equity Data Set
PD	Probability of Default
LGD	Loss Given Default
EAD	Exposure At Default
ECL	Expected Credit Loss
LR	Logistic Regression
GNB	Gaussian Naive Bayes
DT	Decision Tree
KNN	K–Nearest Neighbors
RF	Random Forest
GB	Gradient Boosting
SVM	Support Vector Machine
NN	Neural Network
MLP	Multi-Layer Perceptron
SFS	Sequential Forward Selection
MSE	Mean Squared Error
CCP	Cost–Complexity Pruning
WoE	Weight–of–Evidence
SMOTE	Synthetic Minority Oversampling Technique
RFE	Recursive Feature Elimination
CDF	Cumulative Distribution Function
TP	True Positive
FP	False Positive

TPR	True Positive Rate
FPR	False Positive Rate
TN	True Negative
FN	False Negative
Prec.	Precision
Rec.	Recall
Acc.	Accuracy
MCC	Matthews Correlation Coefficient
ROC	Receiver Operating Characteristic
AUC	Area Under the Curve
KS	Kolmogorov–Smirnov Distance
SD	Somers' D
BS	Brier Score Loss
Thres.	Threshold
ReLU	Rectified Linear Unit
Tanh	Hyperbolic Tangent
ADASYN	Adaptive Synthetic Sampling
GP	Gaussian Process
EI	Expected Improvement
SHAP	SHapley Additive exPlanations
LIME	Local Interpretable Model–Agnostic Explanations
CPU	Central Processing Unit
HTML	Hypertext Markup Language

Chapter 1

Introduction

Machine learning is becoming increasingly important in the financial industry as it can bring competitive edge. Many financial institutions have already utilized the machine learning techniques for assessing creditworthiness of the clients and predicting their future behavior (PwC 2023). As the backbone of most financial institutions, credit risk modelling plays an integral role in ensuring the stability and profitability of these establishments as it primarily revolves around assessing the likelihood that a borrower will default on a debt by failing to make required payments.

Conventional methodologies for credit risk assessment have relied on statistical techniques and rule-based systems, which have been known to deliver sound results. However, with the exponential growth of data in recent years, financial institutions are confronted with the challenge and opportunity to extract valuable insights from this information deluge. In an era where data-driven decision making is becoming the norm rather than the exception, the application of machine learning in credit risk modelling is not just an interesting research area, but also a future practical necessity.

In this thesis, the main goal is to implement a custom machine learning framework developed in Python, which includes data exploration, data pre-processing, Bayesian hyperparameter optimization, feature selection, model selection, model recalibration, and model evaluation, and further to develop a custom web application, within which the trained model is deployed, into a production environment, using Flask and HTML with CSS and JavaScript elements. Such comprehensive machine learning framework is applied on an exemplary data set of US home equity loans (HMEQ) acquired from Credit

Risk Analytics (Baesens *et al.* 2016). Regardless of the potential discrepancy between such exemplary data set and the current state of the loan market, the objective of this thesis is rather to showcase a versatile machine learning implementation framework that can be effectively employed for diverse data sets, transcending industry boundaries and fulfilling varying analytical requirements. In this thesis, we employ eight different machine learning algorithms, namely Logistic Regression, Decision Tree, Gaussian Naive Bayes, K-Nearest Neighbors, Random Forest, Support Vector Machine, Gradient Boosting, and Neural Network. As evaluation metrics in order to assess model's performance, we use F1 score, Precision, Recall, Accuracy, Matthews Correlation Coefficient, Area Under the (ROC) Curve (henceforth AUC), Kolmogorov–Smirnov Distance, Somers' D, Brier Score Loss and Log Loss.

This thesis is divided into five chapters (2-5). Chapter 2 regards the theoretical background which introduces the credit risk modelling and machine learning concepts. Particularly, credit risk definition, regulation and credit scoring approaches are presented. Furthermore, machine learning terminology, machine learning algorithms and evaluation metrics are described. Moreover, more advanced machine learning techniques are introduced, such as ADASYN oversampling, Optimal Binning, Bayesian hyperparameter optimization or Forward Sequential Feature Selection.

Chapter 3 assesses literature review from both credit risk modelling and machine learning fields. Moreover, we propose five hypotheses either based on HMEQ-based studies (Aras 2021; Zurada *et al.* 2014), or based on researches related to machine learning application in different sectors (de Hond *et al.* 2023; Pintelas *et al.* 2020; Wu *et al.* 2018).

In Chapter 4, we present very extensive machine learning implementation framework, including a description of repository and environment structure of given implementation. Within the data exploration, we describe the analyzed data, inspect distributions of variables and also perform statistical association analysis in order to infer some relationships between the default and the predictors and between the predictors themselves. In the data preprocessing, we perform split of data into training set (for model building, hyperparameter tuning and feature selection), validation set (for model selection) and test set (for model evaluation). Further we perform ADASYN oversampling to balanced skewed default distribution and employ Optimal Binning which bins numerical predictors into interval bins and categorical predictors into categori-

cal group bins, optimally with respect to the default status. Such bins are then transformed using Weight-of-Evidence.

In the modelling part, we employ Bayesian Optimization for hyperparameter tuning and propose two custom algorithms. Feature selection algorithm which takes each model, tunes it with Bayesian Optimization and performs Forward Sequential Feature Selection, which returns a subset of optimal predictors per each model. Further, model selection algorithm which takes each model, tunes it with Bayesian Optimization on each subset of optimal predictors, and then evaluates it on the validation set using the proposed range of evaluation metrics. Instead of using standard classification threshold of 0.5, we compute an optimal threshold using Youden index. Additionally, each model is then ranked accordingly to each evaluation metric and afterwards, a rank score is calculated for each model as a weighted average of individual ranks, where the weights are explicitly defined by the author. The model with the highest rank score is then selected as the final model.

Within the model recalibration part, the final model retrained on the joined training set and validation set, as well as the optimal threshold is recalculated in order to enhance model's performance. In the evaluation section, the model is evaluated on the test set. Particularly, we assess model's performance by constructing confusion matrix or ROC curve, as well as by computing evaluation metrics mentioned above and comparing them with the results of the non-recalibrated model in order to assess impact of recalibration. Further, model explainability is inspected using feature importances and SHAP summary plot for global explainability of the model.

In the final part of machine learning implementation, we deploy the final model into a production environment as a web application using Flask and HTML with CSS and JavaScript elements. Prior the deployment, the final model and the optimal threshold are recalibrated on the joined training set, validation set and test set in order to enhance model's ability to generalize. The web application is temporarily deployed on PythonAnywhere cloud platform and it requires to fill in a loan application form. Once the form is submitted, the application processes the inputs and returns a result whether the loan would be approved or not according to the final model, as well as the probability of default. Further, this application also depicts LIME, i.e., local explainability of the model around given prediction, which shows how each predictor contributes to the prediction.

In the final Chapter 5, we summarize the results of this thesis. In particular, we assess the hypotheses proposed in Chapter 3, discuss the results of the machine learning implementation in this thesis with the results of Aras (Aras 2021) and Zurada (*Zurada et al.* 2014), present the key findings of machine learning implementation, outline the author's contribution in this thesis and lastly, propose various future research directions.

Chapter 2

Theoretical Background

This chapter provides an in-depth theoretical exploration of both credit risk and pertinent topics within the field of machine learning. The former describes basic credit risk definition, its key components, underlying regulation as well as the credit scoring approaches. The latter includes clarification of machine learning terminology for enhanced understanding in later chapters, an introduction to various machine learning algorithms used in empirical analysis of this thesis, and a definition of the metrics used to evaluate machine learning algorithms.

This chapter also delves into more sophisticated machine learning topics including the ADASYN oversampling methodology for handling imbalanced data sets, Bayesian Optimization for tuning the models' hyperparameters, Optimal Binning as a method for preprocessing data, and Forward Sequential Feature Selection as a technique for selecting the most optimal features.

2.1 Credit Risk

According to Gregory (Gregory 2012), credit risk can be defined as the risk that the client may be unable to unwilling to make a payment or fulfil loan contractual obligations, which is often known generically as default. However, default can have various forms and definition. The most common definition of default is based on days past due (DPD), particularly, the default event occurs when client is more than 90 days overdue on his loan (Brezigar-Masten *et al.* 2021).

Bessis (Bessis 2015) also defines default event which can result from the following events:

- Temporary or indefinite delay in payments;
- Restructuring of debt obligations due to the deterioration of the borrower's creditworthiness;
- Bankruptcy.

The main objective in credit risk modelling is to estimate (expected) credit loss, which has three components and is defined as follows:

$$ECL = PD \times EAD \times LGD \quad (2.1)$$

where PD is the probability of default indicating likelihood of the client will not meet scheduled loan payments, EAD is the exposure at default is the amount size that is due to be repaid at the time of default, and LGD is loss given default indicating the loss in case of default occurrence (Doumpos *et al.* 2019).

2.1.1 Regulation

Basel II/III

Basel Committee on Banking Supervision (BCBS) introduced Capital Accord Basel II and Basel III in 2004 and 2010, respectively (Shakdwipee & Mehta 2017), with a goal to set higher risk management and internal control standards for banks (Witzany 2017). Regarding credit risk modelling, the former Accord introduced two approaches how to model credit risk:

- **Standardized Approach** - The simplest approach which imposes risk weights of assets based on the external credit ratings from credit rating agencies (CRA's) (Konno & Itoh 2016).
- **Internal Ratings Based (IRB) Approach** - More sophisticated approach which allows to use internal rating systems to assess the parameters such as PD, LGD and EAD (Baesens *et al.* 2016). Such approach is further divided into two sub-approaches:
 - **Foundation IRB approach** - Only PD is internally estimated by a bank, while LGD and EAD are determined by the Basel Accord or provided by the local regulator (Baesens *et al.* 2016).

- **Advanced IRB approach** - All the parameters, i.e., PD, LGD and EAD are estimated internally by a bank itself and also subject to regulatory satisfaction (Joseph 2013).

IFRS 9

International Accounting Standard Board (IASB) in cooperation with the Financial Accounting Standard Board (FASB) published International Financial Reporting Standard (IFRS) 9 in 2014 in order to replace IAS (International Accounting Standard) 39 (Temim 2016), which incorporates the forward-looking information, i.e., impact of macroeconomic projections on expected credit losses (Porretta *et al.* 2020). IFRS 9 also outlines three-stages approach considering changes in credit quality since initial recognition of the financial asset (Beerbaum 2015), also known as SICR (Significant Increase In Credit Risk). According to Bellini (Bellini 2019), the stages are defined as follows:

- **Stage 1** - The financial instrument is considered to be in Stage 1 if it has not had a SICR since initial recognition or if it has low credit risk at the reporting date.
- **Stage 2** - The financial instrument is considered to be in Stage 2 if it has experienced a SICR since initial recognition, but it does not have objective evidence of impairment at the reporting date.
- **Stage 3** - The financial instrument is considered to be in Stage 3 if it has objective evidence of impairment at reporting date.

In case of Stage 1, 12-month ECL is calculated, while in case of Stage 2 and Stage 3, lifetime ECL is calculated (Gornjak 2017). While the aim of IFRS 9 regards the financial reporting which should follow a general purpose to provide information to those outside the firm to support decision usefulness, whereas Basel II/III seeks to decrease the frequency and cost of bank failures and to protect the financial system as whole by limiting the frequency and cost of systemic crises (Beerbaum 2015).

For more information about the differences between IFRS 9 and Basel II/III, please, refer to the study of Beerbaum and Ahmad (Beerbaum 2015).

2.1.2 Credit Scoring

Credit scoring is an assessment of the credit quality of the client which uses techniques for finding the criteria that best discriminate between defaulters and non-defaulters (Bessis 2015). From such perspective, we distinguish two basic types of credit scoring:

Application Scoring

As the name indicates, the application scoring is used to assess the credit-worthiness of the client at the moment of loan application which supports the decision whether a bank should approve or reject the loan application (Baesens *et al.* 2016). The most common variables which are used in application scoring and can be acquired from the loan application are for instance: age, gender, marital status, income, employment status and others (Baesens *et al.* 2016).

Behavioral Scoring

Behavioral scoring takes into account the observed client's recent or past behavior and starts once the loan has been approved (Van Gestel & Baesens 2009). In contrast to application scoring, which is static and takes into account only information from the loan application, behavioral scoring accumulates the information retrieved from the monitoring of the repayments and financial behavior of the client (Van Gestel & Baesens 2009).

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).
- **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.
- **Supervised Learning** - Process reflecting the ability of an algorithm to generalize knowledge from the data having with target or label cases, so that the algorithm can be used to predict new (unlabelled) cases (Berry *et al.* 2020). In other words, the learning process is supervised by the target variable, hence the 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** - The data is split into k folds (subsets) and the model is trained k times, each time on $k-1$ folds and evaluated on the remaining fold, in order to obtain reliable estimates of the model generalization error (Tatsat *et al.* 2020), or so called cross-validation score.
- **Overfitting** - Situation, when the model has small error during the training, but also a high test error (Forsyth 2019). The model is too complex and just purely memorizes the data on which is trained on, but cannot generalize well on unseen data.
- **Black-box model** - Models which are very accurate but also are very complex hard to interpret (Pintelas *et al.* 2020).
- **White-box model** - Models which are comprehensible and transparent but usually are less accurate (Pintelas *et al.* 2020).

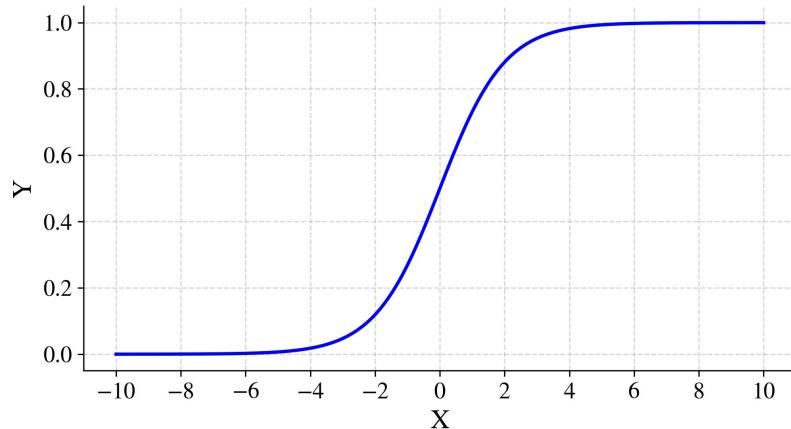
2.3 Algorithms

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, logistic regression is not a regression algorithm, but rather a classification algorithm as 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 a probability score prediction, it uses a logistic (sigmoid) function, which maps any real value into a probability and takes a S-shaped curve (Zaidi 2022), 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:

$$\ln \left(\frac{P}{1 - P} \right) = \beta_0 + \sum_{i=1}^n \beta_i X_i \quad (2.2)$$

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:

$$P = \Pr(Y = 1 | X) \quad (2.3)$$

Therefore, the term within the natural logarithm is 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.

$$\frac{P}{1 - P} = \frac{\Pr(Y = 1 | X_1, X_2, \dots, X_n)}{\Pr(Y = 0 | X_1, X_2, \dots, X_n)} \quad (2.4)$$

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

$$P = \frac{1}{1 + e^{-(\beta_0 + \sum_{i=1}^n \beta_i X_i)}} \quad (2.5)$$

Regarding the loss function minimized when estimating the model's parameters, the logistic regression uses the cross-entropy loss function, also known as log loss. This loss function is also used as an evaluation metric for the model's performance, which is further described in Subsection 2.4.6. Let us denote the loss function as $L(y, p)$, where y is the actual target values and p is the predicted probability scores. To this loss function, we can also additionally employ a regularization term C in order to prevent overfitting (Pramoditha 2021) by penalizing the coefficients' magnitudes. We distinguish 3 types of regularization (penalty) types:

- **L1** - Lasso regularization, which takes the absolute value of the coefficients' magnitudes.

$$L(y, p)_{L1} = L(y, p) + C \sum_{j=1}^k |w_j| \quad (2.6)$$

- **L2** - Ridge regularization, which squares the coefficients' magnitudes.

$$L(y, p)_{L2} = L(y, p) + C \sum_{j=1}^k w_j^2 \quad (2.7)$$

- **Elastic Net** - Combination of L1 and L2 regularizations, where α indicates the weight of L1 penalty.

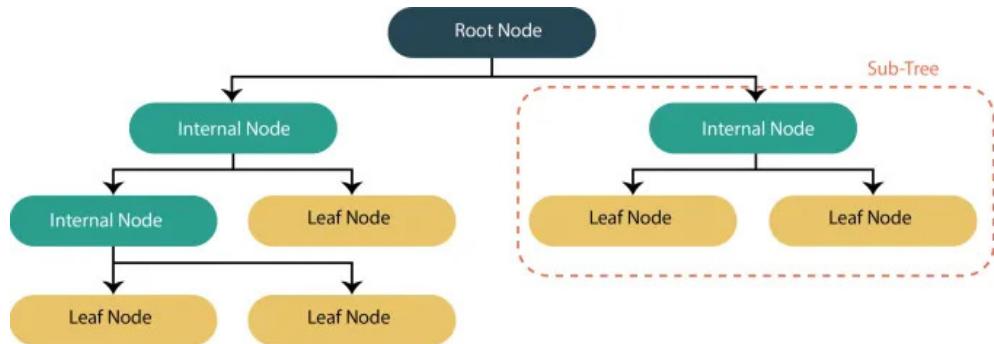
$$L(y, p)_{ElasticNet} = L(y, p) + C \sum_{j=1}^k [\alpha |w_j| + (1 - \alpha)w_j^2] \quad (2.8)$$

2.3.2 Decision Tree

Decision Tree 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 process 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:

$$E = - \sum_{i=1}^n p_i \log_2 (p_i) \quad (2.9)$$

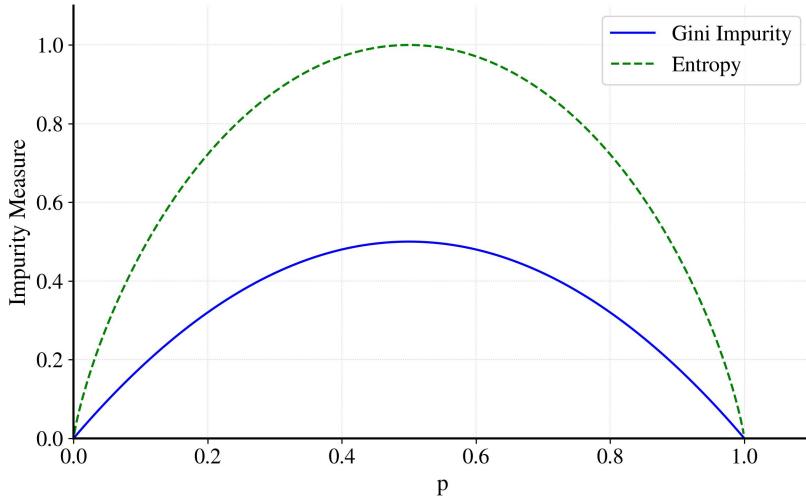
where p_i is the probability of the occurrence of the event i , or in other words, it is a fraction of the observations belonging to the class i within given node. In

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:

$$G = 1 - \sum_{i=1}^n p_i^2 \quad (2.10)$$

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, Decision Tree 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 Bayes theorem which is defined as:

$$\Pr(C = c | E) = \frac{\Pr(C = c) \times \Pr(E | C = c)}{\Pr(E)} \quad (2.11)$$

where $\Pr(C = c | E)$ 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 , i.e., the probability we would assign to the class c before seeing any evidence E , $\Pr(E | C = c)$ is the probability of seeing the evidence E conditional on the given class c , and $\Pr(E)$ 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:

$$\Pr(Y | X) = \frac{\Pr(Y) \times \Pr(X | Y)}{\Pr(X)} \quad (2.12)$$

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 2015). Therefore, instead of computing the probability of all features together, conditional on the class event, for each feature X we compute the conditional joint probability of X given the class event. Hence:

$$\Pr(X | Y) = \prod_{i=1}^n \Pr(X_i | Y) \quad (2.13)$$

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 posterior probability of the class event Y conditional on the subset of features

X can be expressed as:

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

During the training process, the Naive Bayes algorithm computes $\Pr(Y)$ and $\Pr(X | Y)$ 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 $\Pr(X | Y)$ for both default and non-default class. Specifically, based on the new instance's features X , we determine the computed $\Pr(Y)$ and $\Pr(X | Y)$ for both classes and afterwards, as a predicted class, we choose such class with the highest posterior probability. In general, the prediction while maximizing posterior probability is given as:

$$\Pr(Y | X) = \operatorname{argmax}_{y \in Y} \Pr(X | Y = y) \times \Pr(Y = y) \quad (2.15)$$

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.

$$\Pr(Y | X) = \max(\Pr(Y = 1 | X), \Pr(Y = 0 | X)) \quad (2.16)$$

where:

$$\Pr(Y = 0 | X) = \Pr(Y = 0) \times \prod_{i=1}^n \Pr(X_i | Y = 0) \quad (2.17)$$

respectively:

$$\Pr(Y = 1 | X) = \Pr(Y = 1) \times \prod_{i=1}^n \Pr(X_i | Y = 1) \quad (2.18)$$

This algorithm works well only if the features are categorical. However, most of the data sets 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:

$$\Pr(X = x | Y = 1) = \frac{1}{\sqrt{2\pi\sigma_{X|Y=1}^2}} \exp\left(-\frac{(x - \mu_{X|Y=1})^2}{2\sigma_{X|Y=1}^2}\right) \quad (2.19)$$

where $\mu_{X|Y=1}$ and $\sigma_{X|Y=1}$ is the mean and variance of X , respectively, given the class event $Y = 1$. Afterwards, $\Pr(X = x | Y = 1)$ derived from the Gaussian distribution can be substituted into Equation 2.18.

2.3.4 K-Nearest Neighbors

The goal of K-nearest Neighbors algorithm (henceforth 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.

$$d_{Euclidean}(x, y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2} \quad (2.20)$$

Other distance measure is the Manhattan distance measure, also known as a city block distance. In contrast to the Euclidean distance, but instead of squared differences, it sums the absolute differences between the data points.

$$d_{Manhattan}(x, y) = \sqrt{\sum_{i=1}^n |x_i - y_i|} \quad (2.21)$$

The last measure is the Minkowski distance which is the generalized form

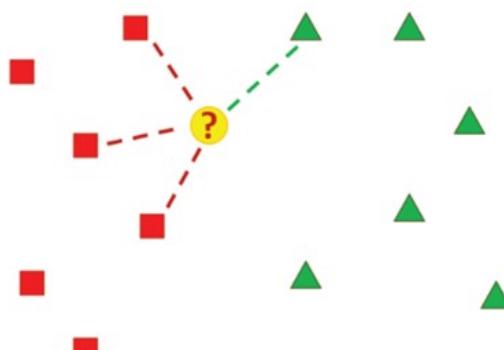
Euclidean or Manhattan distance respectively. It depends on p which represents the order of the norm. Hence, the Euclidean distance has the second order of the norm, whereas Manhattan distance has the first order of the norm.

$$d_{Minkowski}(x, y) = \sqrt[p]{\sum_{i=1}^n |x_i - y_i|^p} \quad (2.22)$$

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.* 2016). 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 score as the fraction of positive instances within the k nearest neighbors.

In 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 four 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 a bootstrap sample of the training data (Han *et al.* 2011), i.e., on a set which is randomly sampled from the training data with replacement and 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:

$$\Pr(Y = 1 | X) = \frac{1}{B} \sum_{b=1}^B \Pr(Y = 1 | X, T_b) \quad (2.23)$$

where B is the number of trees and T_b is the b -th tree.

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:

$$F_0(x) = \arg \min_{\gamma} \sum_{i=1}^n L(y_i, \gamma) \quad (2.24)$$

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

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

$$r_{i,m} = - \left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)} \right]_{F(x)=F_{m-1}(x)} \quad (2.25)$$

2. Train a weak learner $h_m(x)$ 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:

$$\gamma_m = \arg \min_{\gamma} \sum_{i=1}^n L(y_i, F_{m-1}(x_i) + \gamma h(x_i)) \quad (2.26)$$

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

$$F_m(x) = F_{m-1}(x) + \gamma_m h(x) \quad (2.27)$$

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) 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 2.5.

Figure 2.5: Support Vector Machine 2D Hyperplane



Source: (Meyer 2009)

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:

$$W \cdot X + b = 0 \quad (2.28)$$

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:

$$\min \frac{2}{\|W\|} \quad (2.29)$$

When the data are not linearly separable, SVM transforms the original data points into a higher dimensional space using non-linear mapping function, also

known as kernel (Han *et al.* 2011). In general, kernel function for the training tuples (X_i, X_j) can be expressed as:

$$K(X_i, X_j) = \phi(X_i) \cdot \phi(X_j) \quad (2.30)$$

where ϕ is mapping function for high-dimensional projection 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:**

$$K(X_i, X_j) = (1 + X_i \cdot X_k)^d \quad (2.31)$$

- **Gaussian radial basis kernel:**

$$K(X_i, X_j) = \exp(-\gamma \|X_i - X_j\|^2) \quad (2.32)$$

- **Sigmoid kernel:**

$$K(X_i, X_j) = \tanh(\gamma X_i \cdot X_j + r) \quad (2.33)$$

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 minimize the following term:

$$\min \frac{1}{2} \|W\|^2 + C \sum_{i=1}^N \xi \quad (2.34)$$

Hence, by minimizing $\frac{1}{2} \|W\|^2$ 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 does not predict probability scores by default, but rather predict 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 probabilities. Particularly, it fits logistic regression with true labels Y as target variable and predictions produced by SVM ($f(x)$) as features. Therefore the predicted probability score can be expressed as:

$$\Pr(Y|f(x)) = \frac{1}{1 + \exp(A \cdot f(x) + B)} \quad (2.35)$$

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 layer has a certain number of units (neurons). In general, we distinguish 3 type of layers as also visualized in Figure 2.6:

- **Input layer** - The initial layer which contains n units, where n is the number of features within the data set.
- **Output layer** - The 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.
- **Hidden 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 2.6: Neural Network Architecture



Source: (Dilmegani 2022)

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*, hence 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 output value z of the single unit in hidden layer is calculated as:

$$z = g(X, w) = b + \sum_{m=1}^M w_m x_m \quad (2.36)$$

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 non-linear 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:

$$f(z) = \max(0, z) \quad (2.37)$$

- **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:

$$f(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \quad (2.38)$$

- **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:

$$f(z) = \frac{1}{1 + e^{-z}} \quad (2.39)$$

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. There 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 2014). 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:

$$C = c_{i,j} = \sum_{l=1}^m [(y_l = i) \wedge (f(x_l) = j)] \quad (2.40)$$

Or either in matrix form as:

$$C_{i \times j} = \begin{bmatrix} c_{1,1} & c_{1,2} & \cdots & c_{1,j} \\ c_{2,1} & c_{2,2} & \cdots & c_{2,j} \\ \vdots & \vdots & \ddots & \vdots \\ c_{i,1} & c_{i,2} & \cdots & c_{i,j} \end{bmatrix} \quad (2.41)$$

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 classifica-

tion - hence, the confusion matrix will have a form of 2×2 :

$$C_{2 \times 2} = \begin{bmatrix} c_{1,1} & c_{1,2} \\ c_{2,1} & c_{2,2} \end{bmatrix} \quad (2.42)$$

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

$$C_{2 \times 2} = \begin{bmatrix} TP & FN \\ FP & TN \end{bmatrix} \quad (2.43)$$

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*.

From such confusion matrix, we can derive several metrics which are further described on the following pages.

Accuracy

Such metric ranges from 0 to 1 and it describes in relative 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 often have a lot of non-defaults and few defaults. Therefore, it is deemed appropriate to consider other metrics when having imbalanced class.

$$\text{Accuracy} = \frac{TP + FN}{TP + TN + FP + FN} \quad (2.44)$$

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 indicate 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 metric 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:

$$\text{Recall} = \frac{TP}{TP + FN} \quad (2.45)$$

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 indicate 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 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:

$$\text{Precision} = \frac{TP}{TP + FP} \quad (2.46)$$

F1 Score

F1 score incorporates both Recall and Precision into a single value and takes on values between 0 and 1 as well. It is 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 data sets compared to Accuracy.

$$F1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} = \frac{2 \times TP}{2 \times TP + FP + FN} \quad (2.47)$$

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., class 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:

$$r(x, y) = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (2.48)$$

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:

$$MCC = \frac{TP \times TN - FP \times FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}} \quad (2.49)$$

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 between 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:

$$FPR = \frac{FP}{TN + FP} \quad (2.50)$$

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 different 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 TPR 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 2.7. 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).

Figure 2.7: ROC Curve



Source: Author's results in Python.

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 .

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 (Janitz 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:

$$AUC = \int_0^1 TPR(FPR^{-1}(x)) dx \quad (2.51)$$

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:

$$\text{Kolmogorov Smirnov} = \max_{0 \leq t \leq 1} |F_D(t) - F_{ND}(t)| \quad (2.52)$$

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:

$$F_D(t) = \frac{1}{M_D} \sum_{i=1}^{M_D} I[f(x_i) \leq t] \quad (2.53)$$

$$F_{ND}(t) = \frac{1}{M_{ND}} \sum_{i=1}^{M_{ND}} I[f(x_i) \leq t] \quad (2.54)$$

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:

$$\tau(X, Y) = E[\text{sign}(X_i - X_j)\text{sign}(Y_i - Y_j)] \quad (2.55)$$

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 the 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:

$$D(Y | X) = \frac{\tau(X, Y)}{\tau(X, X)} \quad (2.56)$$

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 (henceforth 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 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:

$$\text{Brier Score Loss} = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2 \quad (2.57)$$

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

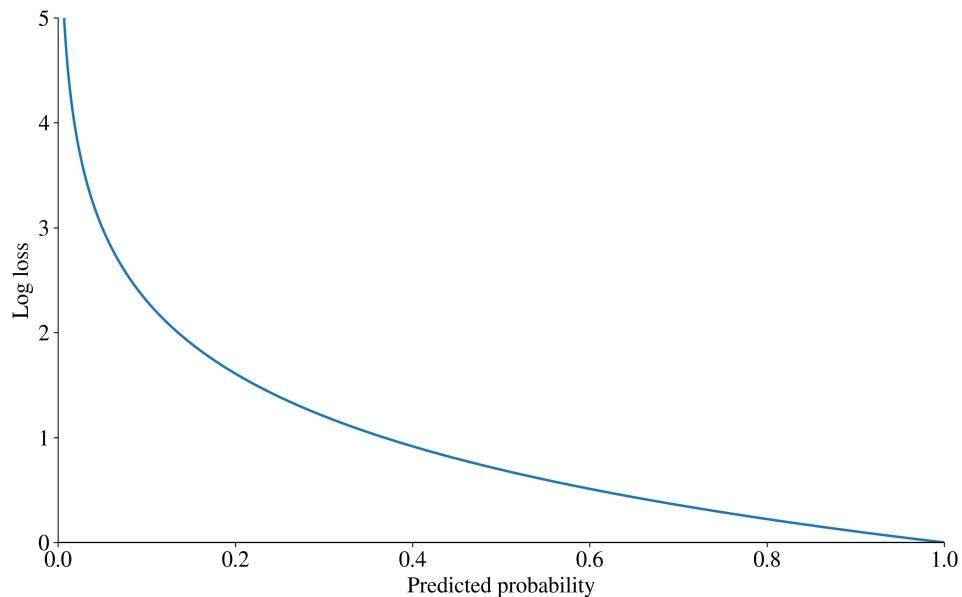
2.4.6 Log Loss

Log loss, also known as logistic loss or cross-entropy loss, is a loss function metric which takes *True* labels and predicted probabilities as an input and then minimizes 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 diverge from the actual value, the more the log loss function penalizes the model's performance (Dembla 2020).

$$\text{Log Loss} = -\frac{1}{N} \sum_{i=1}^N y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i) \quad (2.58)$$

Logically, the lower Log loss value, the better performance of the model is. As depicted in Figure 2.8, 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 2.8: Log Loss Function for $Y = 1$



Source: Author's simulation in Python

2.5 ADASYN Oversampling

Since this thesis pertains to the data set of defaulted loans, which target variable distribution is heavily skewed, it is needed to emphasize the imbalanced class issue, 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 significant loss of information, and random oversampling is lead to the high degree of repetition of minority instances. Both then could lead to model's overfitting and deterioration 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 data set 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 data set 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 data set, which would lead to the model's overfitting.

Therefore, the Adaptive Synthetic Sampling (henceforth ADASYN) technique is used for oversampling the minority class in this thesis. 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, however, ADASYN generates more synthetic instances which are hard-to-learn by K-Nearest Neighbors given the density distributions, whereby SMOTE gener-

ates synthetic instances uniformly for each minority class 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:

$$G = (m_l - m_s) \times \beta \quad (2.59)$$

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:

$$r_i = \frac{\delta_i}{K} \quad (2.60)$$

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:

$$\hat{r}_i = \frac{r_i}{\sum_{i=1}^{m_s} r_i} \quad (2.61)$$

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.

$$\sum_{i=1}^{m_s} \hat{r}_i = 1 \quad (2.62)$$

Finally, the oversampling process is initialized. For each minority class in-

stance 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.

$$G_i = G \times \hat{r}_i \quad (2.63)$$

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

$$s_i = x_i + (x_{zi} - x_i) \times \lambda \quad (2.64)$$

where x_{zi} represents the randomly chosen minority class instance within the K nearest 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 encoding, standardization, logarithmic transformation, and normalization are widely used, they may not always be suitable for a given data set 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.

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.

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. As Navas-Palencia states (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 should be observed within given bin. Such constraint ensures a bin's representativeness.
- **Each bin should have at least one instance of each target class:** Application of such constraint allows to compute divergence measure.

Thus, using the optimal binning process, the goal is to 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 need 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 overall log odds ratio and the log odds ratio given the value c , hence:

$$WoE(c) = \ln(\Pr(c | Y = 0)) - \ln(\Pr(c | Y = 1)) \quad (2.65)$$

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

$$WoE_{X,b} = \ln\left(\frac{\Pr(X = b | Y = 0)}{\Pr(X = b | Y = 1)}\right) \quad (2.66)$$

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

$$WoE_i = \ln\left(\frac{r_i^{ND}/r_T^{ND}}{r_i^D/r_T^D}\right) \quad (2.67)$$

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 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 Bayesian Hyperparameter 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 parameter 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 data set is too large. Regarding the latter approach, instead of trying all 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 information from previous iterations in order to make more informed decision 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 computationally 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. 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:

$$y = f(x) + \epsilon \quad (2.68)$$

Let us denote $f_{1:n} = \{f(x_1), f(x_2), \dots, f(x_n)\}$ 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:

$$f_{1:n} \sim N(m(x_{1:n}), K) \quad (2.69)$$

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

$$p(y | x, D) \mid N(y | \mu^*, \sigma^{*2}) \quad (2.70)$$

where μ^* and σ^{*2} can be analytically derived from the K kernel, and D represents observed data regarding the previously evaluated iterations 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 $\sigma(x) \neq 0$:

$$EI(x) = (\mu(x) - f(x^+)) \times \Phi(Z) + \sigma(x) \times \phi(Z) \quad (2.71)$$

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 unknown 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 data set, we use only the subset of the most relevant ones, which can further reduce the dimensionality of data set, 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 2023), 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 2022). 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. In particular, 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 2023g), at each stage, SFS chooses the best feature to add based on the cross-validation score.

2.9 Theoretical Summary

In this chapter, we have introduced the theoretical background of the thesis. In particular, in Section 2.1, we have described the traditional credit risk parameters, i.e., PD, LGD, and EAD, as well as the credit risk regulation regarding Basel II/III and IFRS 9, and also scoring methods, namely application and behavioral scoring. Pertaining to the machine learning part, its terminology has been introduced in order to avoid any misunderstanding in the following chapters Section 2.2.

Furthermore, as classification algorithms, following 8 algorithms have been described in Section 2.3 and are also employed in empirical analysis of this thesis: Logistic Regression, Decision Tree, Gaussian Naive Bayes, KNN, Random Forest, Gradient Boosting, SVM and Neural Network.

For assessment of model's performance, we have defined following metrics in Section 2.4, which are used in empirical analysis of this thesis: Accuracy, Precision, Recall, F1 score, Matthews Correlation Coefficient, AUC, Kolmogorov–Smirnov Distance, Somers' D, Brier Score Loss and Log Loss.

Moreover, another advanced machine learning techniques have been presented, particularly, ADASYN oversampling for dealing with imbalanced, i.e., skewed distribution of the target variable (Section 2.5), Optimal Binning for data preprocessing using discretization with respect to the target variable (Section 2.6), Bayesian Optimization for hyperparameter tuning of models (Section 2.7), and lastly, Forward Sequential Feature Selection for selecting subsets of optimal features (Section 2.8). All these techniques are employed in empirical analysis of this thesis as well.

Chapter 3

Literature Review

Within the literature review, our objective is to explore the application and implementation of machine learning in credit scoring. We will examine relevant studies in two areas: machine learning applications specifically related to credit scoring and machine learning implementations in various other domains. The aim is to identify machine learning techniques from non-credit scoring contexts that could potentially be useful in credit scoring. We will evaluate the impact of these techniques through hypothesis testing.

Regarding studies related to machine learning in credit scoring, we will analyze not only the researches focused on the HMEQ data set used in this thesis, but also studies that involve different data sets. This comprehensive approach is intended to develop a broader understanding and facilitate the discovery of valuable insights and methodologies that can be applied across various data sets in 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 (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 classification cut-off point. By default, the cut-off point is set to 0.5, which means that if the predicted probability score exceeds the threshold, it will be classified as default and vice versa. Kazemi (Kazemi *et al.* 2022) demonstrated that utilization of the customized cut-off points leads to a more accurate classifi-

cation 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 neural 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 Teply and Polena (Teply & Polena 2020) suggest that Logistic Regression is the best performing model on peer-to-peer loans data from Lending Club, Aniceto (Aniceto *et al.* 2020) demonstrates 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 data set 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 be 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, author used test size of size 596 instances. Author also performed an oversampling on the training set using Random Oversampling in order to balance the default status distribution. Regarding the fitted models which are also used in this thesis, 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 exceed 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 not the same, and the data preprocessing and modelling is different as well.

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, one would expect that KNN and Random Forest 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 research conducted by Zurada (Zurada *et al.* 2014). Likewise Aras, author also analyzed various classification models, but only relevant ones to this thesis are further discussed. Namely, Zurada 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 likewise Aras, they conducted a hyperparameter tuning using Grid Search with 10-fold cross validation.

The evaluation 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, 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 performance 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 insights can be derived from ranking the results in the same way as in Zurada's study, as shown in Table 3.4. Hence, one would expect 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, different hyperparameters' spaces for fine tuning 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 to ensure the reliable and robust results and estimates, which are further described in Section 4.3 and Section 4.4.

3.1 Hypotheses

In this section, we formulate the hypotheses, which are partially derived from the literature review discussed above and are further tested in Section 5.1, i.e., rejected or not rejected, based on the empirical analysis regarding the machine learning implementation in Chapter 4.

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

The study of de Hond (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 for a prediction of readmissions or deaths after ICU discharge. Such effect is being achieved by re-training the model on the 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 (Zurada *et al.* 2014), the highest ranked models in terms of performance were KNN and Neural Network, respectively. These two models outperformed the traditional Logistic Regression, and in case 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.*

Following the Section 2.2, there is a trade-off between the model performance and the interpretability, where the black-box models are more complex and less interpretable, but also more accurate, while the white-box models are less complex and more interpretable, but also less accurate (Pintelas *et al.* 2020). With respect to the algorithms described in Section 2.3, we deem Logistic Regression as a white-box model, since it is interpretable thanks to the estimated coefficients which can indicate the strength and direction impact of each feature on the target variable adjusting for all other features (Park 2013). Another white-box model is a Gaussian Naive Bayes as it is based on the Bayes theorem and Gaussian distribution, thus only prior probabilities and conditional means and variances need to be computed per each feature according to Equation 2.18 and Equation 2.19. Decision Tree can be considered as a white-box model, assuming that the decision tree is small (Goethals *et al.* 2022), i.e., if the tree is not too deep and wide, which enhance the comprehensible interpretation of the model.

One would say that KNN is a white-box model, since it just looks for k closest neighbours around given data point. However, the interpretation of the model might not be straightforward if the k is large and/or when having higher number of features which increases the dimensionality, as the model might be too complex. According to Loyola-Gonzalez (Loyola-Gonzalez 2019), KNN is considered as a black-box model since it is highly dependent on the distance function which might bias the classification results and change in a distance function can lead to different outcomes. Therefore, we consider KNN as a black-box model. Regarding the rest of the models, they are deemed as black-box models due to the following reasonings:

- **SVM** - Very complex mathematical operations involved in such algorithm make it difficult to interpret the model (Loyola-Gonzalez 2019).
- **NN** - The more layers and units within each layer does the neural network have, the less transparent and comprehensible the model is (Bathaei 2018).
- **RF, GBM** - Such ensemble models consist out of multiple decision trees,

which are combined together to form a more complex model. Therefore, the interpretation of such models is not straightforward.

Therefore, we expect that the black–box models will outperform the white–box models on the HMEQ data set in overall.

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

Although, the research paper’s objective of Wu (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. However, 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 relationship 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: (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 (Zurada *et al.* 2014), the author also inspected the significance of features in order to reduce the dimensionality. In particular, the authors employed both correlation analysis with the target variable as well as ranking according to information gain. In this case, the most significant features are debt–to–income ratio and number of delinquent credit lines. Therefore, these features are expected to be the most important indicators when predicting a default.

Chapter 4

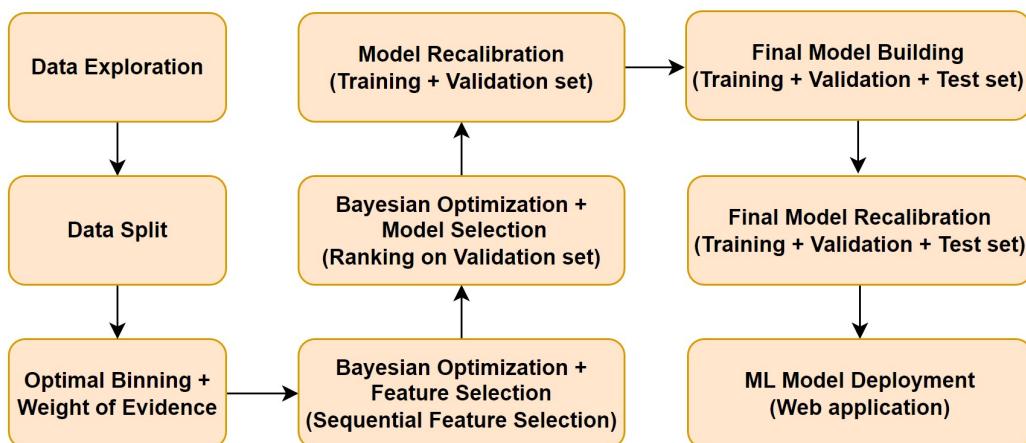
Empirical Analysis - Machine Learning Implementation

This chapter focuses on the main part of this thesis, particularly on employing the custom machine learning implementation framework. The machine learning framework deployed in this thesis is shown in Figure 4.1 as is described from the high-level-point view as follows:

- **Data Exploration** - Exploration of the data in order to infer some insights about the data quality, distribution of the variables, statistical testing and association analysis.
- **Data Split** - Splitting of the data which are used separately in different tasks such as model training, hyperparameter tuning, feature selection, model selection and model evaluation.
- **Optimal Binning and WoE Encoding** - Optimal binning and the WoE encoding of the features as the main part of the feature preprocessing.
- **Feature Selection** - Feature selection with Forward Sequential Feature Selection in order to reduce the dimensionality of the data and to improve the performance of the machine learning models - each input model is tuned with Bayesian Optimization.
- **Model Selection** - Model selection based on weighted ranking where the weights are defined explicitly by the thesis' author, in order to find the best model. Each input model is tuned with Bayesian Optimization on each subset of selected features.

- **Model Recalibration (Evaluation)** - Recalibration (Re-training) of the final model by re-training it on the joined training and validation sets, which will be further evaluated.
- **Model Evaluation** - Evaluation of the final model on the unseen data from test set in order to assess model's predictive power as well as model's explainability.
- **Model Recalibration (Deployment)** - 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** - Deployment of the final model into a production as a web application.

Figure 4.1: Machine Learning Framework



Source: Author's Framework

4.1 Repository and Environment Structure

The whole machine learning implementation as the scope of this thesis is developed 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-ognn/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 sub-directories of the trained and fitted objects for features preprocessing, feature selection and model selection, including the final objects used in evaluation or 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 ML modelling, feature selection, model selection and model evaluation;
- `Scikit-optimize` - for more advanced hyperparameter tuning;
- `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, as shown in Figure 4.3:

Figure 4.3: Environment Setup Command

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

Source: Author's command at Anaconda

An user should aware of his current path directory in the terminal. In order to install the file `requirements.yml`, one needs 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 in Figure 4.4 shows the former approach:

Figure 4.4: Environment Setup Command with Directory Change

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

Source: Author's command at Anaconda

To preserve the reproducibility of this solution and consistency 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 every time when replicating the solution. Some `Scikit-learn` or `Scikit-optimize` objects have optional argument `n_jobs` which utilizes the number of central processing units (CPU) cores used during the parallelizing computation. Such argument is 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 which can be used in the pre-processing 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 (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 Table 4.1, 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 contains following categories - Administration (**Office**), Sales, Manager (**Mgr**), Professional Executive (**ProfExe**), Self-employed (**Self**), and Other.

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 are observed within 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

Variable	# 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

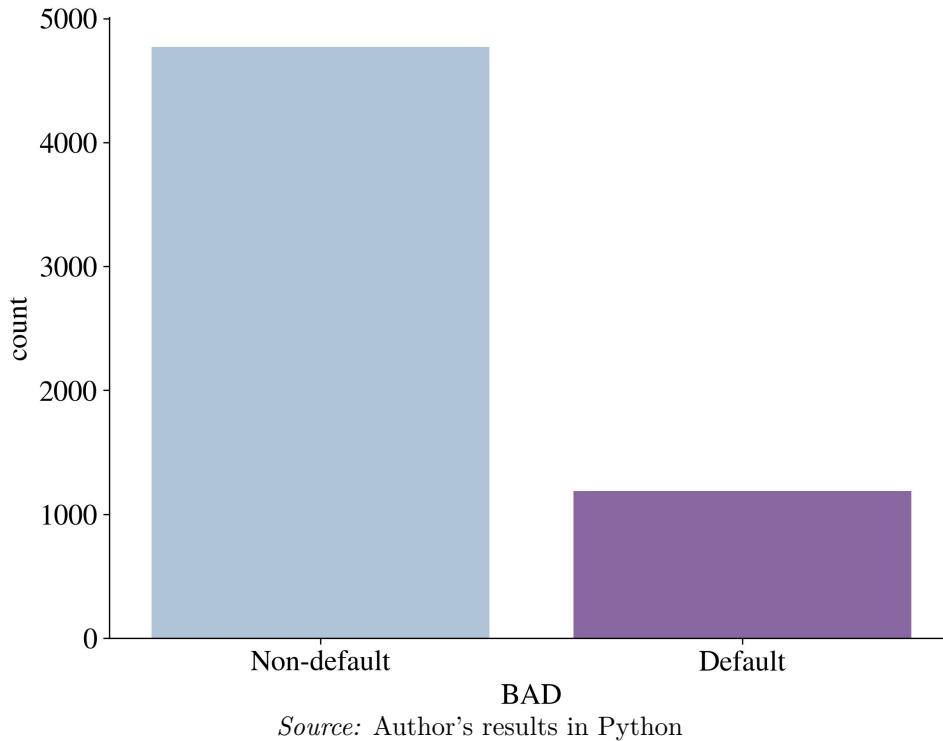
4.2.2 Distribution Analysis

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 outliers, and other potential issues with the data set.

Default Distribution

Regarding the the target variable distribution, from the Figure 4.5 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 4.5: Default Distribution



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 4.6, which depicts the conditional distribution of the numeric features with respect to the default status via boxplots.

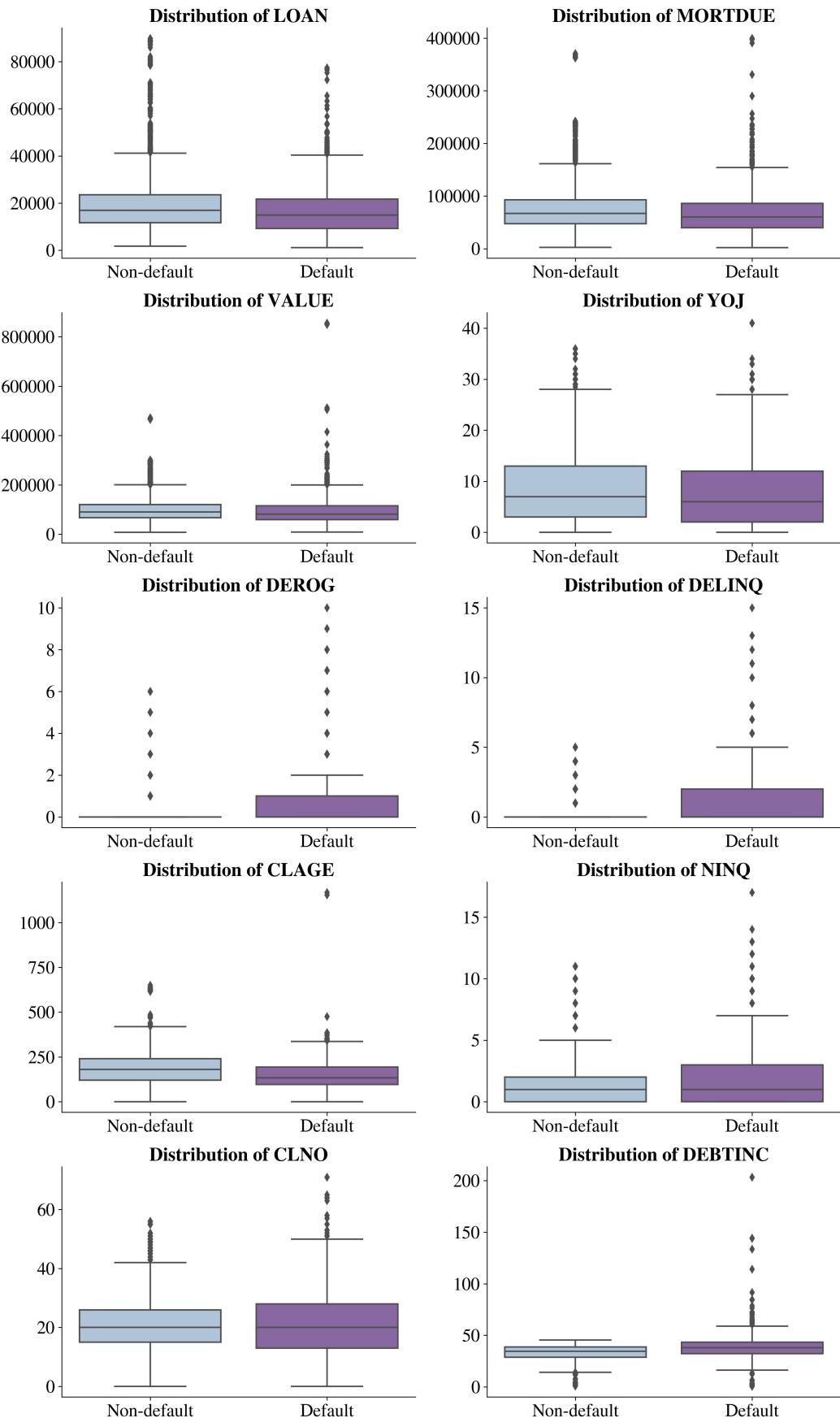
All the outliers appear to be valid, indicating that they have not arisen due to data entry errors. This can be attributed to the non-negative nature of all the numeric features, which makes it impossible to have negative values for features such as the number of years at present job or the number of 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.

Since the features are positively skewed a lot, they do not follow Guassian (normal) distribution. Additionally, Shapiro–Wilk test is conducted in order to assessed whether the features' distributions are significantly different from a normal distribution. According to such test, all the numeric features' distributions do not follow normal distribution on 1% statistical significance level. For a reference, see Table A.1 in Appendix A.

Figure 4.6: 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 Summary

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 %

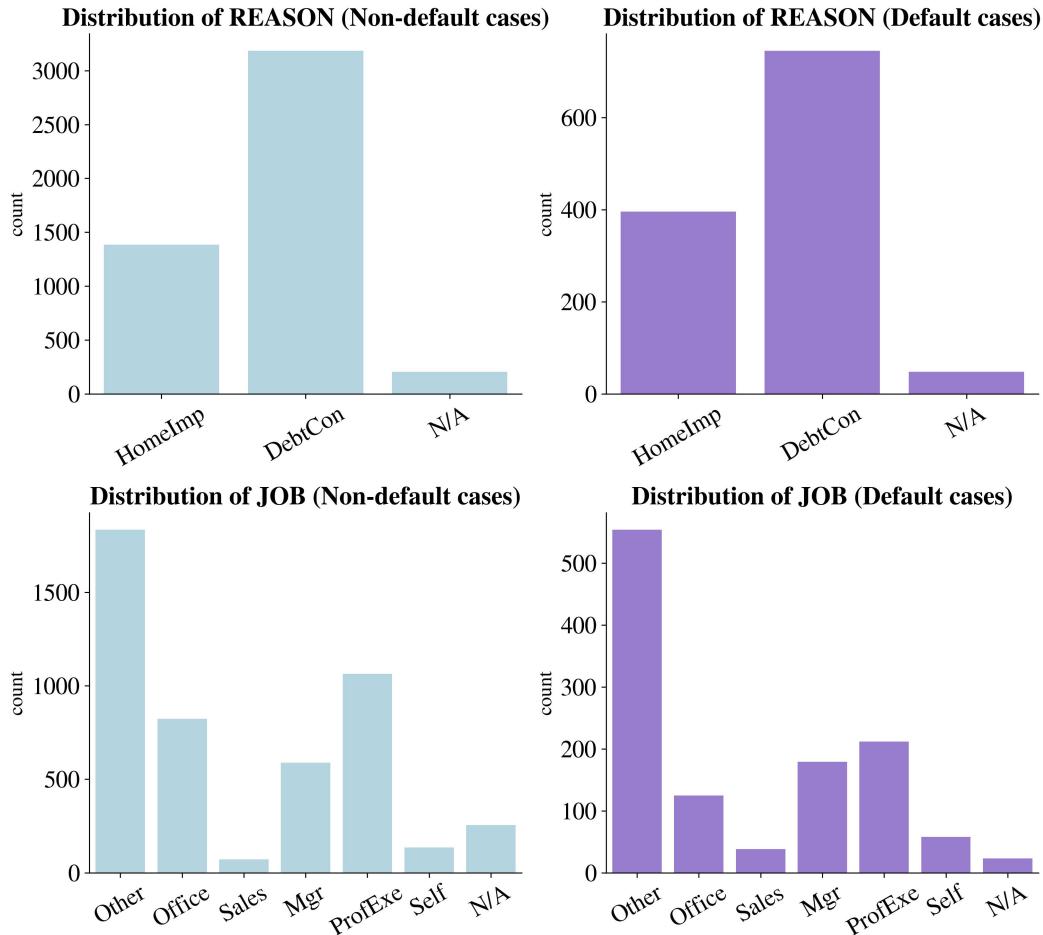
Source: Author's results in Python

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 4.7. 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 strong 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 4.7: 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 2015). 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:

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

Here, $\mu(X|Y=1)$ and $\mu(X|Y=0)$ 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 $N(Y=1)$ and $N(Y=0)$ 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 - Numeric Features vs. Default

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:

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

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 - Categorical Features vs. Default

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:

$$\phi_X = \sqrt{\frac{\chi^2}{n}} \quad (4.3)$$

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 - NA's vs. Default

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

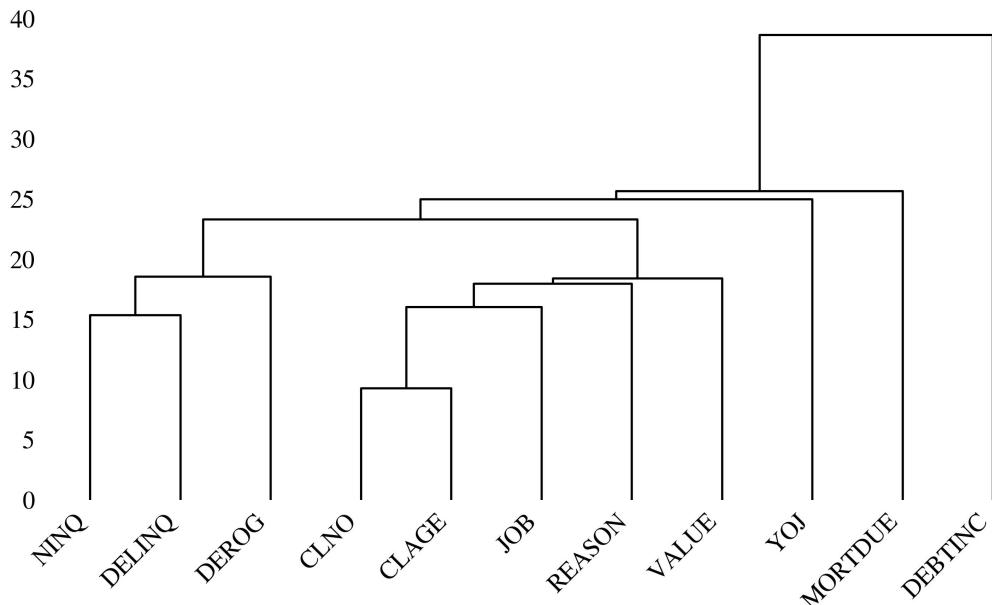
Missing Values Association

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 4.8, 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 4.8: Nullity Dendrogram



Source: Author's results in Python

Note that the target variable is imbalanced, therefore, the dendrogram depicted in Figure 4.8 is not representative for the default cases. Therefore, we can also inspect the dendrogram for the default cases only, as shown in Figure 4.9. As can be seen, the hierarchy has changed compared the hierarchy in Figure 4.8. It can be observed that a significant number of loan applicants tend to omit information regarding their number of credit lines (**CLNO**) and

the number of delinquent credit lines (**DELINQ**) when submitting their loan applications. Especially regarding the second feature, this might indicate a common delinquency problem among the applicants and thus, higher probability of default.

Figure 4.9: Nullity Dendrogram (default cases)



Source: Author's results in Python

Multicollinearity 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:

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

In the Figure 4.10, we can observe a very strong correlation between the **MORTDUE** and **VALUE** features. Such multicollinearity 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 4.10: Spearman Correlation Matrix



Source: Author's results in Python

Regarding the association between categorical features, namely REASON and JOB, the Cramer's V coefficient is used. The Cramer's V coefficient results in a value of 0.149 while being statistically significant 1% statistical significance level, thus we observe a weak association between the two features.

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, ADASYN oversampling due to the imbalanced class issue, discretization of features and Weight-of-Evidence 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 split into training, validation and test sets with 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 `999999999999999` - 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 its 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 default distribution in training set after ADASYN oversampling is balanced, while the default distribution remains the same across the validation and test sets, which is desirable due to stratification.

Table 4.7: Data Split Summary

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 has no significant impact on the numeric features as the distributions before and after ADASYN oversampling do not differ that much, as can be seen Figure A.1 in Appendix A. 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 4.11, respectively, which depict the distribution of categorical features on the sub-sample 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. 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.

Table 4.8: ADASYN Impact on Categorical Features' Distribution

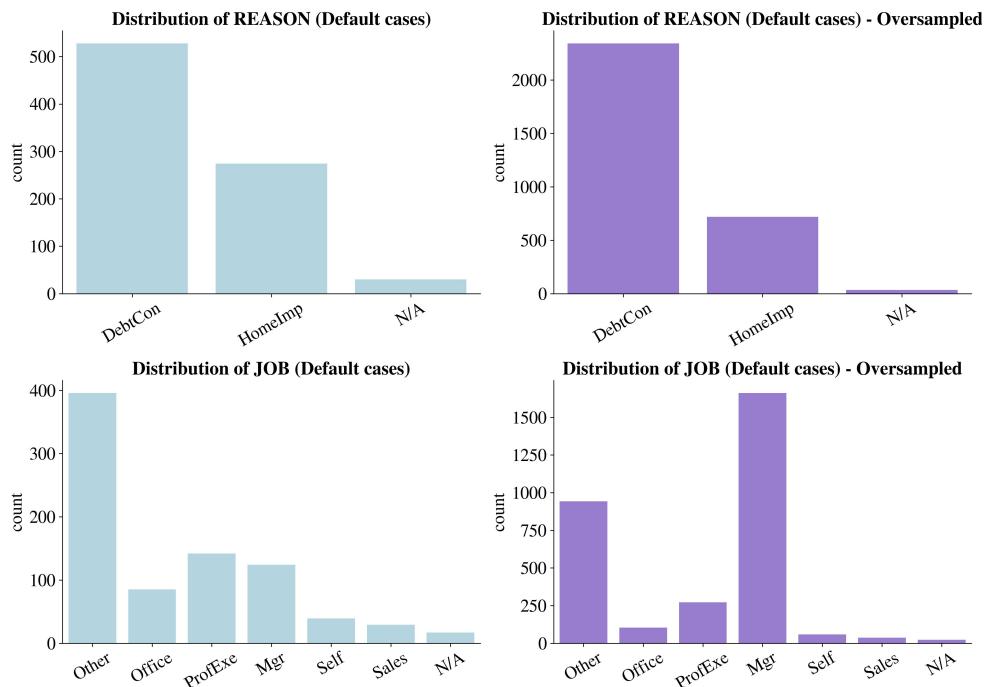
Features	Category	n_B	n_A	n_B/N_B	n_A/N_A	Diff.
REASON	DebtCon	528	2,344	63.46 %	75.66 %	12.20 p.p.
REASON	HomeImp	274	720	32.93 %	23.24 %	-9.69 p.p.
REASON	N/A	30	34	3.61 %	1.10 %	-2.51 p.p.
JOB	Mgr	124	1,662	14.9 %	53.65 %	38.75 p.p.
JOB	Other	396	943	47.6 %	30.44 %	-17.16 p.p.
JOB	ProfExe	142	272	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 already explained, 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 4.11: ADASYN Impact of Categorical Features' Distribution



Source: Author's results in Python

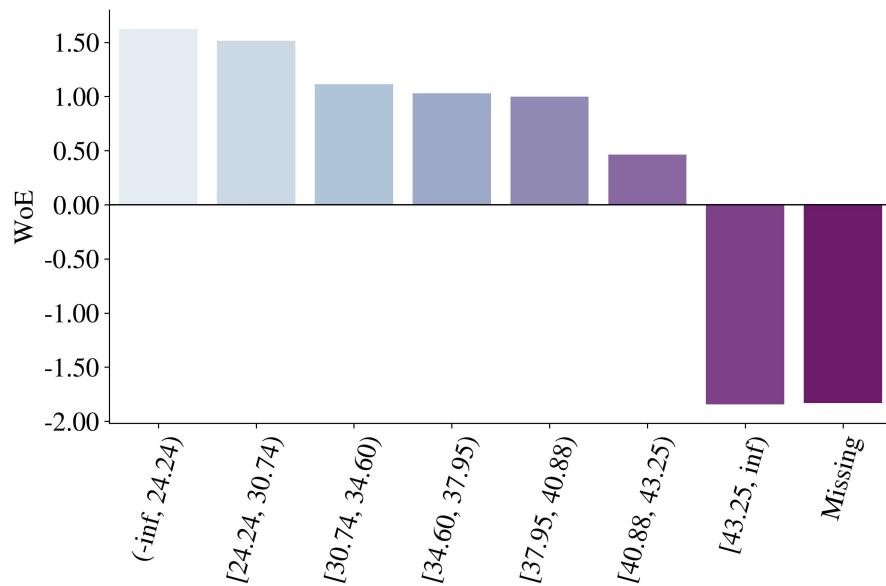
4.3.2 Optimal Binning and Weight-of-Evidence

As already described in Section 2.6, 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 then is used to transform training, validation and test set.

The following Figure 4.12 depicts the WoE bins distribution for the `DEBTINC` feature. It is evident that the bin capturing the missing values has the most negative WoE coefficient, which indicates larger distribution of defaulters compared to non-defaulters in such bin. We can further observe a monotonic relationship between the WoE coefficients and the bins, as the debt-to-income ratio increases, the WoE coefficient decreases, thus higher likelihood of default. Therefore, we expect if the debt-to-income ratio is either missing or extremely high, it will have a significant impact on the likelihood of default.

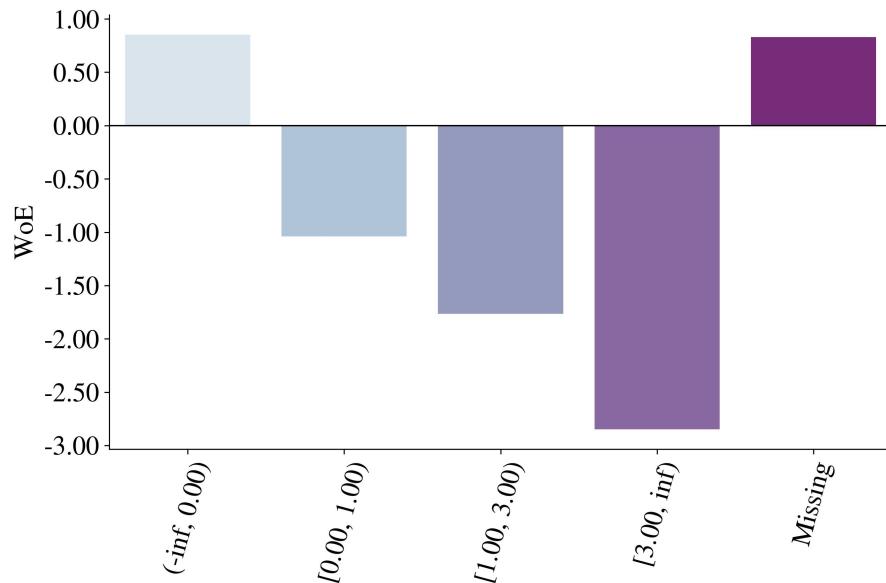
Figure 4.12: WoE Bins Distribution - Debt–To–Income Ratio



Source: Author's results in Python

Another monotonic relationship can be observed in case of DELINQ feature as can be seen in Figure 4.13. With increasing number of delinquent credit lines, the WoE coefficient decreases, indicating larger distribution of defaulters compared to non-defaulters. Therefore, we expect that the higher the number of delinquent credit lines will lead to the the higher the likelihood of default.

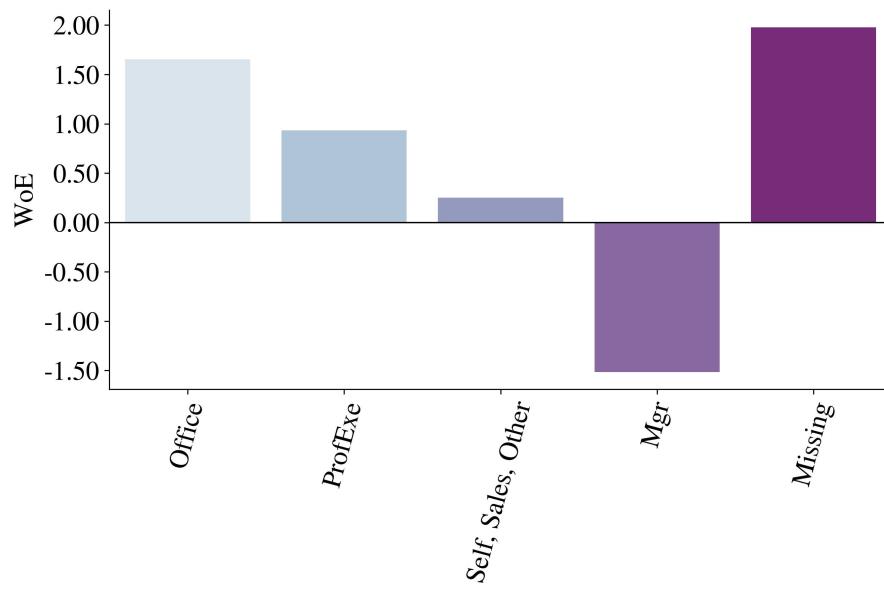
Figure 4.13: WoE Bins Distribution - Number of Delinquent Credit Lines



Source: Author's results in Python

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. Figure 4.14 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.

Figure 4.14: WoE Bins Distribution - Job Occupancy



Source: Author's results in Python

The WoE bins distributions of other features are depicted Figure A.2 in the Appendix Appendix A.

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 recalibration. In Python, eight different machine learning classification 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 Perceptron (Neural Network)** - `MLPClassifier()`
 - Henceforth, we terms such as Neural Network and Multi-Layer Perceptron are used interchangeably.

4.4.1 Bayesian Hyperparameter 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-optimize 2023a). 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 relevant 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. C is the regularization strength, and it is used to specify the regularization penalty, i.e., the hyperparameter `Penalty`. If the penalty is set to *ElasticNet*, we can also tune $L1$ ratio, which refers to the α parameter in Equation 2.8. 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 2023b). 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 2023a). 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	$<1, \text{len}(\text{X.columns})>$

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 vari-

ance of all features to be added to variances for calculation stability (scikit-learn 2023b), 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` hyperparameter. 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 2023d).

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 the Random Forest, we tune the number of base trees which are trained in parallel way in the ensemble, i.e., the `# estimators` hyperparameter. Sim-

ilarly 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 removing subtrees from the tree estimators which do not improve the performance (scikit-learn 2023f).

Table 4.13: Random Forest - Hyperparameter Space

Hyperparameter	Space
# estimators	$<100, 1000>$
Criterion	Gini, Entropy, Log Loss
Max depth	$<1, 10>$
Max features	$<1, \text{len}(\mathbf{X.columns})>$
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 2023c). 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 2023c).

Table 4.14: Gradient Boosting - Hyperparameter Space

Hyperparameter	Space
# estimators	$<100, 1000>$
Max depth	$<1, 10>$
Max features	$<1, \text{len}(X.\text{columns})>$
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 Perceptron

Regarding the MLP, we use one hidden layer where we tune the number of units as represented by the **Hidden layer size** hyperparameter. We also tune the **Activation function** applied in the hidden layer, 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 *lbfgs*, *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 2023e).

Table 4.16: Multi Layer Perception - 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 (henceforth SFS) is employed in order to choose the optimal set of features as described in Section 2.8. Within machine learning implementation, instead of fitting Forward SFS only with one model, Forward SFS is fitted for each input model in order to obtain the best subset 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:    $optimized\_model \leftarrow \text{BAYESIANOPTIMIZATION}(model)$ 
3:    $best\_features \leftarrow \text{FORWARDSFS}(optimized\_model)$ 
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 2023g). 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 4.15, 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 4.15: 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
-----
```

Source: Author's results in Python

The following Figure 4.16 depicts the recurrence 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.

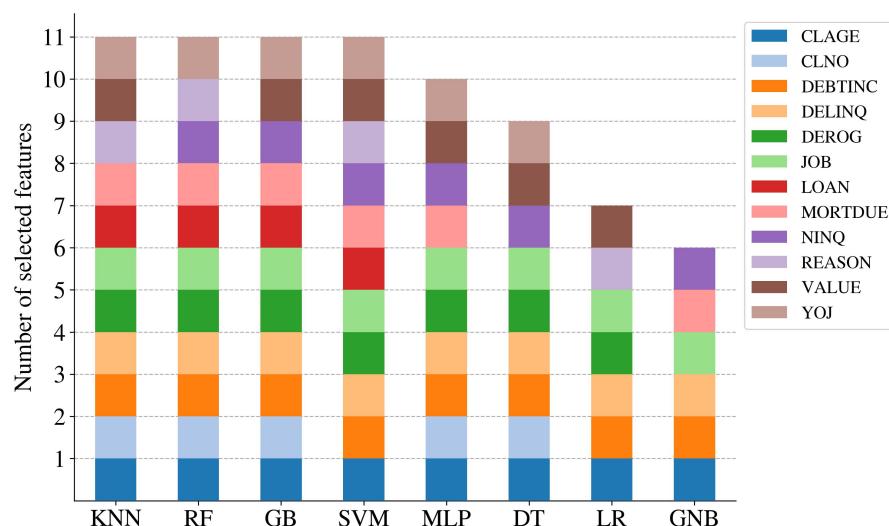
Figure 4.16: Recurrence of Selected Features



Source: Author's results in Python

According to Figure 4.17, models such as KNN, Random Forest, Gradient Boosting and SVM chose almost all the features as only one 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 complex black-box models require more features in contrast to transparent models such as Logistic Regression or Gaussian Naive Bayes.

Figure 4.17: 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

```

1: for model  $\in$  models do
2:   for features  $\in$  features_subsets do
3:     optimized_model  $\leftarrow$  BAYESIANOPTIMIZATION(model, features)
4:     for metric  $\in$  evaluation_metrics do
5:       performance  $\leftarrow$  EVALUATION(optimized_model, metric)
6:     end for
7:   end for
8: 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 standard 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 data.

Therefore, it is recommended to calculate an optimal threshold rather than relying on the standard 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 Youden 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:

$$J = TPR + TNR - 1 \quad (4.5)$$

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

$$T_{opt} = \operatorname{argmax}_{t \in [0,1]} (J) \quad (4.6)$$

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:

$$TNR = 1 - FPR \quad (4.7)$$

Therefore:

$$T_{opt} = \operatorname{argmax}_{t \in [0,1]} (TPR + (1 - FPR) - 1) \quad (4.8)$$

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

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 can be calculated as weighted average of the individual ranks as follows:

$$RankScore_M = \frac{\sum_{i=1}^k r_i \times w_i}{\sum_{i=1}^k w_i} \quad (4.9)$$

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. Based on the rank scores, we assign the final ranks where rank of 1 indicates the best performing model whereas rank k determines the worst performing model.

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 4.18. Particularly, it prints which model on which features is being tuned and evaluated, execution time, optimal threshold, F1 score on the validation set and the best hyperparameters.

Figure 4.18: Model Selection Print Statement

```
-----  
----- 7/64 -----  
----- BAYESIAN OPTIMIZATION OF LR -----  
----- WITH FEATURES SELECTED BY SVM -----  
-----  
  
1/2 ... Starting Bayesian Optimization on the subset of features (11 features):  
      LOAN, MORTDUE, VALUE, REASON, JOB, YOJ, DEROG, DELINQ, CLAGE, NINQ, DEBTINC  
2/2... Bayesian Optimization finished  
  
Execution time: 1.493 minutes  
  
F1 Score on Validation set: 0.6160919540229886  
  
Optimal classification threshold: 0.4003  
  
Tuned hyperparameters of LR:  
  
      C: 0.2768320429063577  
      class_weight: balanced  
      dual: False  
      fit_intercept: True  
      intercept_scaling: 25.603205585229382  
      l1_ratio: 0.5230523280543836  
      max_iter: 100  
      multi_class: auto  
      n_jobs: -1  
      penalty: elasticnet  
      random_state: 42  
      solver: saga  
      tol: 0.0001  
      verbose: 0  
      warm_start: False  
-----  
-----
```

Source: Author's results in Python

The final output of the function `model_selection()` is a 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, followed by another ensemble mode, Random Forest. On the other hand, the worst-performing models are Gaussian Naive Bayes models. In the first ten worst performing models, we can observe also that Decision Tree and Logistic Regression, as white-box models, perform poorly.

Table 4.18: Model Selection Results

Tuned model	FS model	# Features	Exec. Time	Thresh.	F1	Prec.	Rec.	Acc.	AUC	SD	KS	MCC	BS	Log Loss	Score	Rank
GB	MLP	10	12.21	0.4955	0.7809	0.7853	0.7765	0.9128	0.9515	0.9030	0.7751	0.7265	0.0666	0.2487	3.30	1
GB	RF	11	13.30	0.4973	0.7775	0.7841	0.7709	0.9117	0.9541	0.9081	0.7961	0.7225	0.0669	0.2803	3.97	2
GB	KNN	11	12.80	0.5072	0.7978	0.7912	0.8045	0.9184	0.9587	0.9175	0.7989	0.7467	0.0687	0.4135	4.08	3
GB	SVM	11	15.00	0.5053	0.7896	0.8155	0.7654	0.9184	0.9555	0.9109	0.7961	0.7397	0.0718	0.3486	4.32	4
GB	GB	11	11.38	0.4132	0.7799	0.7778	0.7821	0.9117	0.9543	0.9086	0.7989	0.7247	0.0703	0.3372	4.39	5
RF	KNN	11	5.80	0.4725	0.7486	0.7326	0.7654	0.8972	0.9226	0.8452	0.7109	0.6843	0.0923	0.3232	8.48	6
GB	DT	9	12.03	0.4729	0.7675	0.7697	0.7654	0.9073	0.9407	0.8814	0.7556	0.7096	0.0808	0.4693	8.80	7
RF	GB	11	5.07	0.4517	0.7385	0.7135	0.7654	0.8916	0.9200	0.8400	0.7123	0.6709	0.0886	0.3135	9.22	8
RF	MLP	10	6.54	0.4761	0.7357	0.7181	0.7542	0.8916	0.9179	0.8358	0.7081	0.6679	0.0879	0.3084	10.20	9
GB	LR	7	16.79	0.4362	0.7388	0.7000	0.7821	0.8894	0.9219	0.8438	0.7081	0.6706	0.0886	0.3925	11.03	10
...
GNB	DT	9	0.36	0.2241	0.6063	0.5095	0.7486	0.8056	0.8467	0.6935	0.5768	0.4991	0.1316	0.6370	49.56	55
GNB	MLP	10	0.36	0.2194	0.6013	0.5000	0.7542	0.8000	0.8493	0.6986	0.5768	0.4930	0.1319	0.6360	49.68	56
GNB	KNN	11	0.35	0.3588	0.6093	0.5219	0.7318	0.8123	0.8479	0.6957	0.5698	0.5024	0.1367	0.6686	50.58	57
DT	MLP	10	0.83	0.5000	0.6427	0.6374	0.6480	0.8559	0.8133	0.6266	0.5810	0.5524	0.1254	2.0008	52.10	58
SVM	GNB	6	6.38	0.1821	0.5788	0.4718	0.7486	0.7821	0.8393	0.6786	0.5768	0.4633	0.1355	0.4354	53.11	59
DT	GNB	6	0.82	0.5000	0.6354	0.6284	0.6425	0.8525	0.8187	0.6375	0.5838	0.5430	0.1251	2.1679	53.31	60
GNB	SVM	11	0.36	0.1991	0.5885	0.4872	0.7430	0.7922	0.8425	0.6850	0.5712	0.4756	0.1345	0.6721	53.65	61
GNB	GNB	6	0.36	0.4787	0.5950	0.5039	0.7263	0.8022	0.8356	0.6711	0.5559	0.4835	0.1470	0.5280	53.79	62
LR	GNB	6	1.53	0.4561	0.5948	0.5121	0.7095	0.8067	0.8379	0.6758	0.5531	0.4831	0.1319	0.4180	54.02	63
GNB	RF	11	0.36	0.3413	0.5864	0.4943	0.7207	0.7966	0.8288	0.6577	0.5545	0.4720	0.1486	0.7040	57.08	64

Source: Author's results in Python

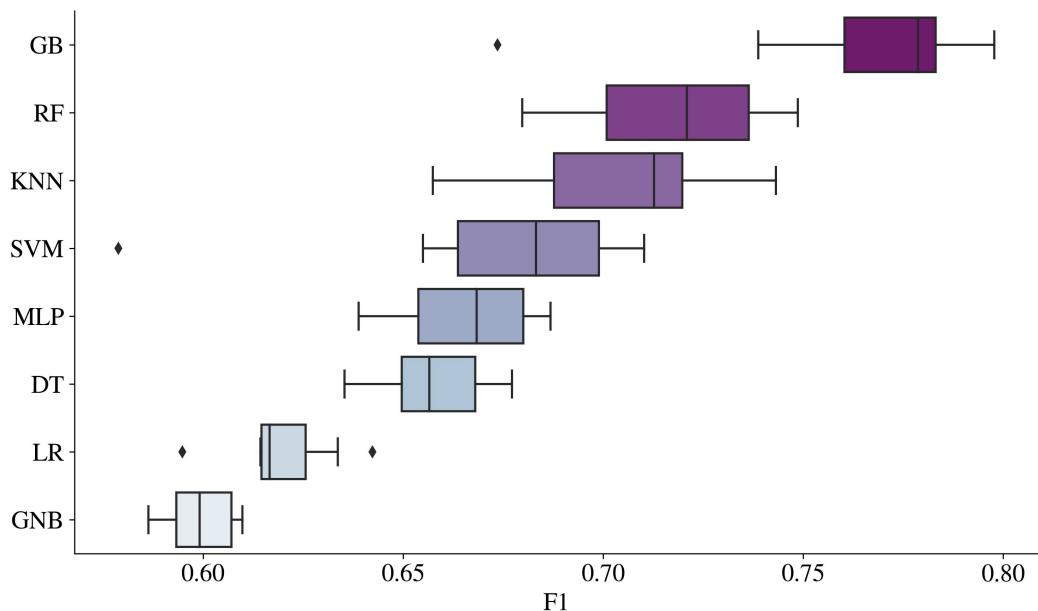
In order to gain a more detailed understanding of the model selection results, the distribution of computed metrics is plotted. In Figure 4.19, the F1 score distribution is visualized for each input model. An outlier can be observed in KNN where the F1 score is 0.

Figure 4.19: F1 Score Distribution



Source: Author's results in Python

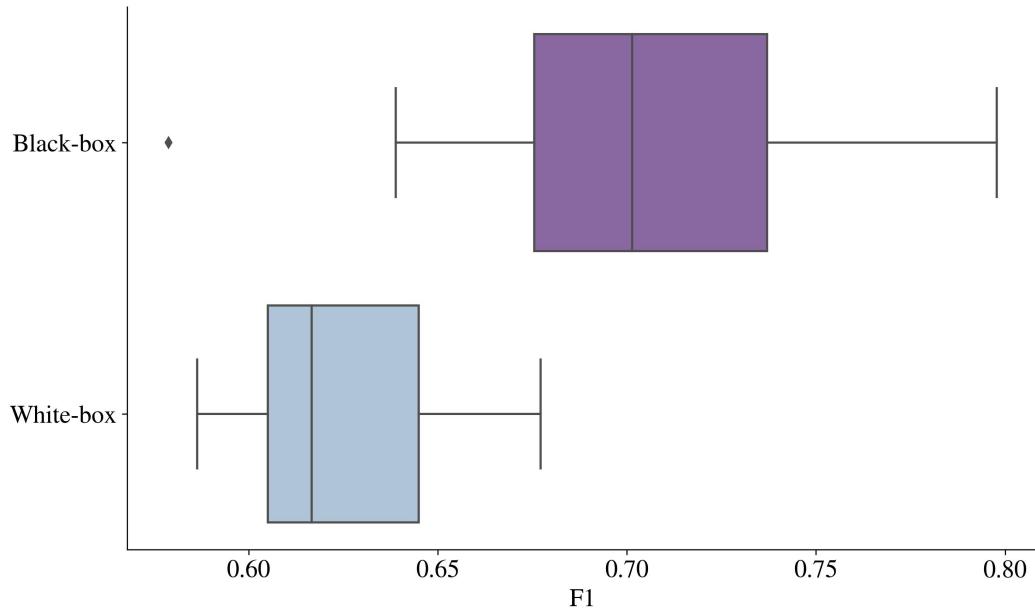
Such outlier is removed in Figure 4.20 to gain a more general insight into the F1 score distribution. It can be observed that Gradient Boosting models have the highest F1 scores of around 80 %. Another tree ensemble model, Random Forest, is performing well as the second best. However, more transparent models such as Logistic Regression and Naive Bayes are performing poorly, having F1 scores around 60 %.

Figure 4.20: F1 Score Distribution - *without outlier*

Source: Author's results in Python

As depicted in Figure 4.21, it visualizes 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.

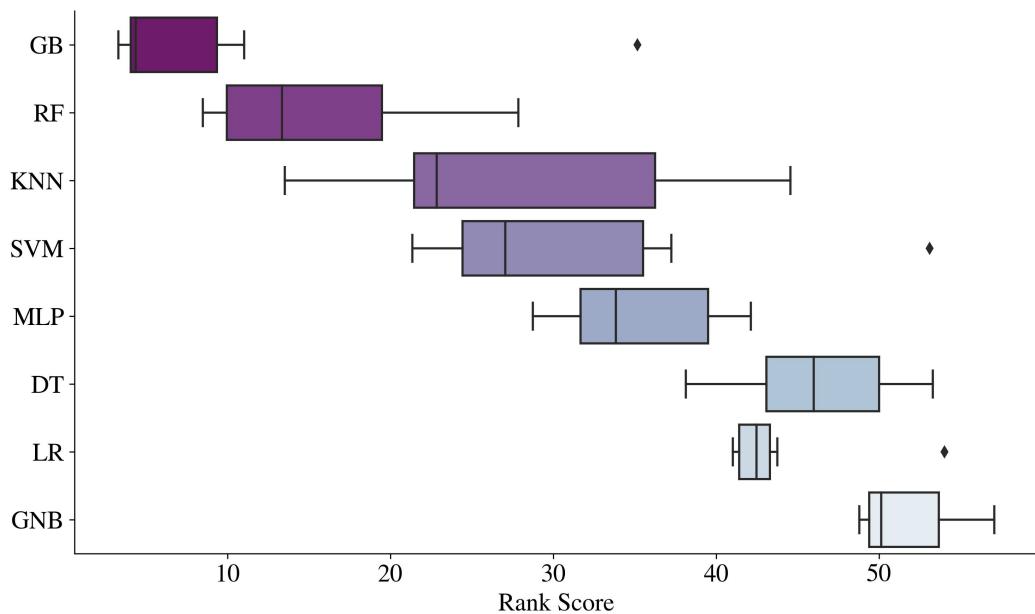
Figure 4.21: F1 Score Distribution (Black-box/White-box dimension) - *without outlier*



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 4.9. As shown in Figure 4.22, 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 4.19. Hence, across all the metrics, the Gradient Boosting perform the best in overall while Gaussian Naive Bayes does not perform well at all.

Figure 4.22: 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 4.23. 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 4.23: 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 4.24. We can observe an outlier in KNN having a threshold value of 1, which explains the F1 score outlier found previously in Figure 4.19.

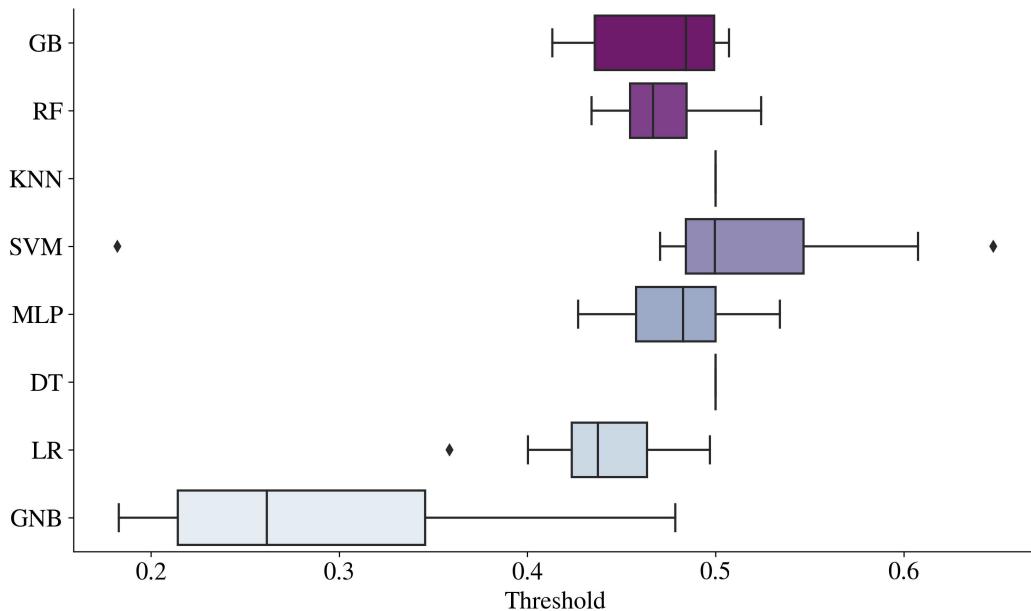
Figure 4.24: Threshold Distribution



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 4.25. 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 4.25: 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 4.20. 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.

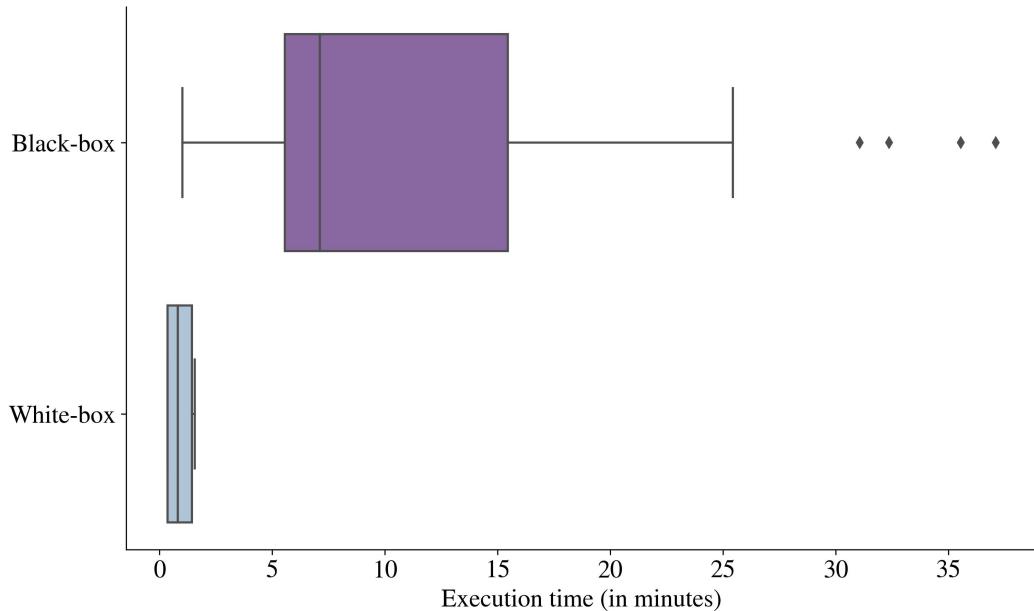
Figure 4.26: Execution Time Distribution



Source: Author's results in Python

We can inspect the execution time from another perspective as shown in Figure 4.27. It can be observed that black-box models take a significant amount of time to optimize than the white-box models which is given due to the complexity of the black-box models. Further we can notice that some of the black-box models took only few minutes to optimized themselves. This corresponds to KNN models and it can be attributed to the small sample size as of data set as well as lower data set dimensionality (i.e., low number of features) and further given the lower number of k neighbors (which is constrained to 10 at most as depicted in Table 4.12).

Figure 4.27: Execution Time Distribution (Black-box/White-box dimension)



Source: Author's results in Python

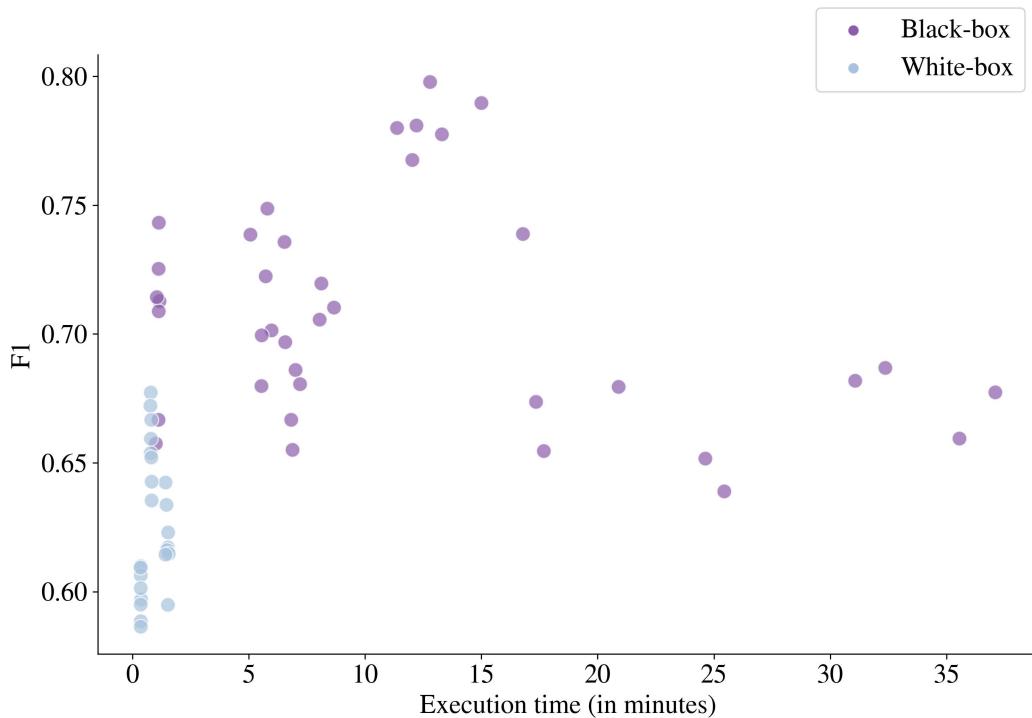
The execution time and the F1 score are inspected together using a scatterplot, as shown in Figure 4.28. A cluster of non-complex and transparent models, such as Logistic Regression, Gaussian Naive Bayes, and Decision Tree, can be observed around the vertical line near 0 execution time. These models are quick to optimize, but their F1 scores are generally low. 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 4.28: Execution Time vs. F1 Scatterplot - *without outlier*

Source: Author's results in Python

Such separation of the black-box and white-box models is more evident from Figure 4.29 where the white-box models points are light blue-colored and the black-box models are purple-colored. While the score of white-box models seems to be constant regardless the execution time length, the points of black-box models are more dispersed across the execution time–F1 score dimension.

Figure 4.29: 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 **MLP** - 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 Perceptron
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 re-training the model on both the training and validation sets. By doing so, the sample size used for training is increased. As such, the re-training (or so called recalibration) model leads (or is 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.

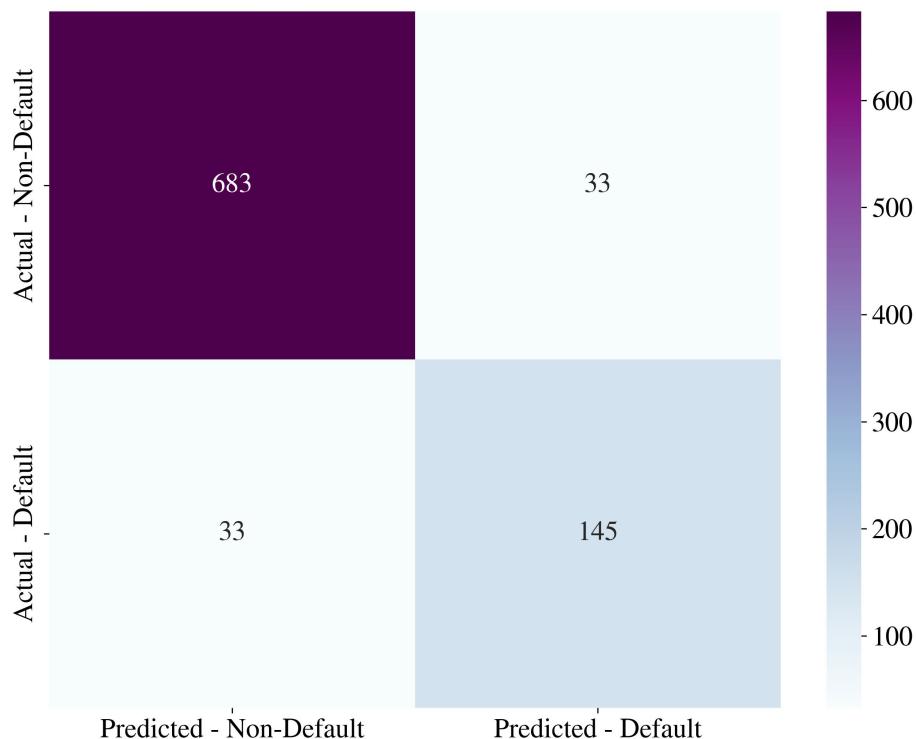
4.5 Model Evaluation

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 4.30, 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 4.30: 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. Particularly, out of all test instances, the model predicts correctly 92.62 %. Model also predicts 81.46 % instances out of all the actual default instances. Also, out of all predicted default instances, model predict 81.46 % instances correctly to be actually default instances. 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., 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 an 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 4.31. 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 4.31: ROC Curve



Source: Author's results in Python

4.5.2 Model Explainability

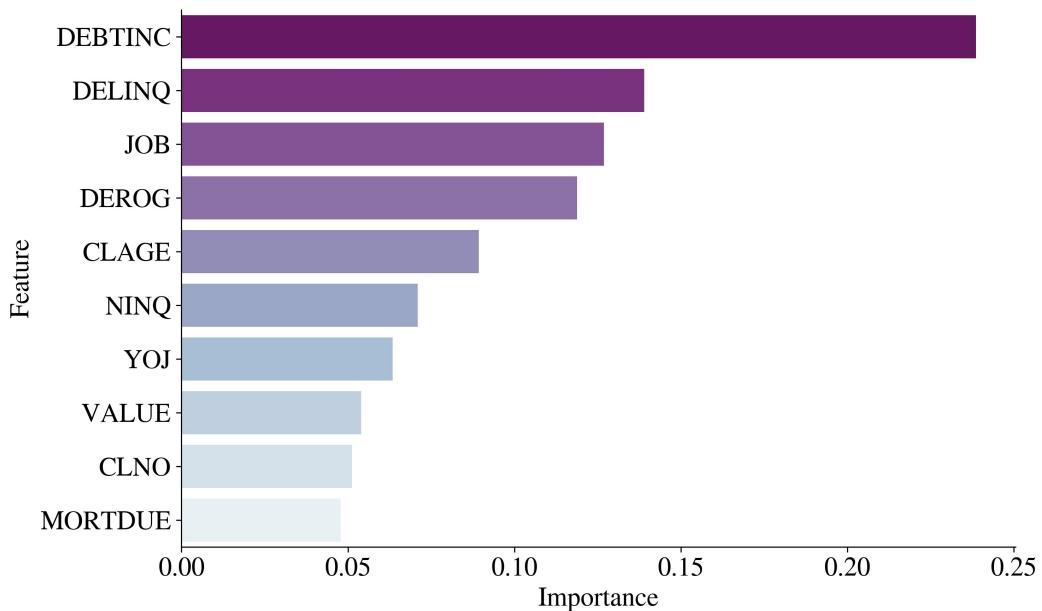
To gain insights into the impact of the features used in the final model, we can inspect the feature importances of the final model, which is a part of family of tree ensemble algorithms. As the name indicates, it is the score value representing the importance of the features, i.e., the higher score, 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:

$$\text{FI}(\bar{x}^{(i)}) = \frac{1}{N} \sum_{k=1}^N \sum_{j=1}^L \frac{n(j)}{M} \delta I_j^i \quad (4.10)$$

where $\text{FI}(\bar{x}^{(i)})$ refers 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 4.32 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 debt and 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 4.32: Feature Importance



Source: Author's results in Python

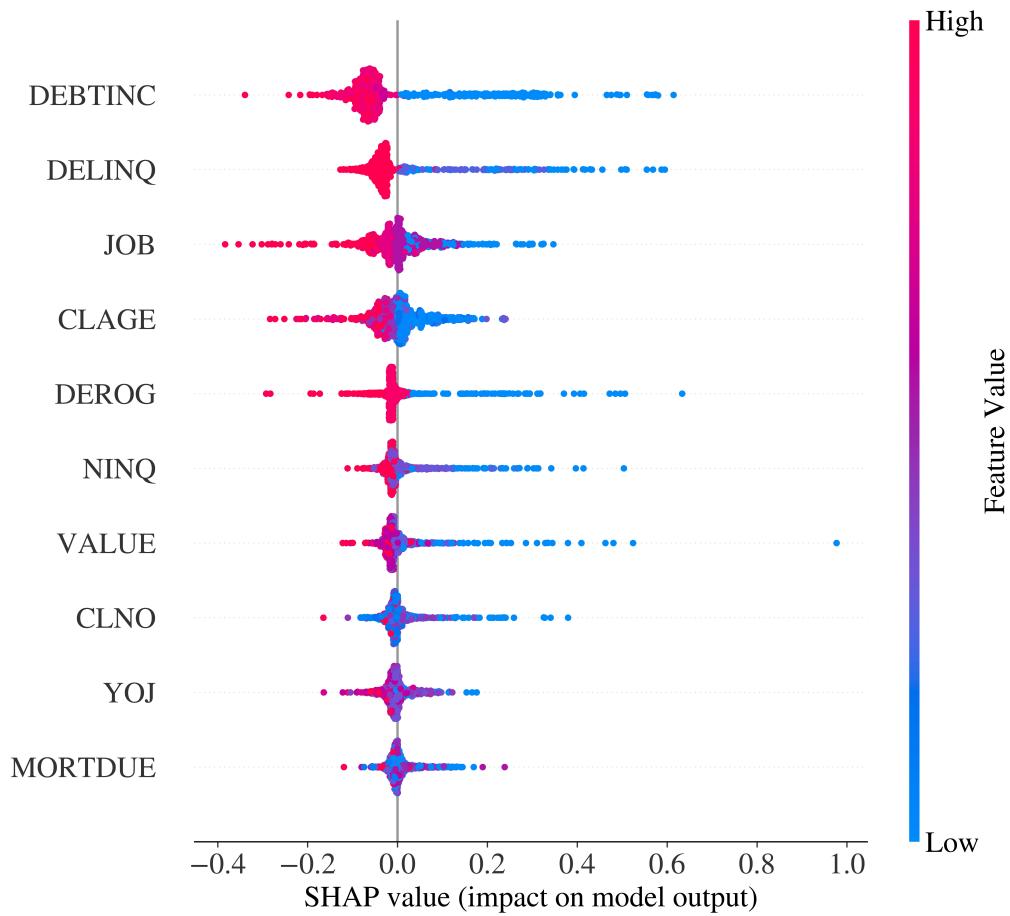
Thus, understanding the impact of individual features on model performance can be useful in identifying areas for improvement, as well as in identifying the most significant factors that drive loan defaults. By focusing on these important features, lenders and policymakers can better understand and address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

To gain further insights into the impact of the features on the final model's predictions, the SHapley Additive exPlanations (henceforth SHAP) values can be calculated. Particularly, the SHAP value is defined as the mean marginal contribution of each feature value across all possible values in the feature space, while considering feature importance (Bhattacharya 2022). The following Figure 4.33 depicts SHAP summary plot which provides a clear visualization of the contribution each feature makes to a prediction and global explainability of the model predictions. 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 4.33: 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 is 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** - 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 4.34. 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 4.34: Flask Web Application Form

Default Prediction Application

Author: Petr Nguyen

Amount due on existing mortgage:

Current property value:

Job occupancy:

Number of years at present job:

Number of major derogatory reports:

Number of delinquent credit lines:

Age of the oldest credit line (in months):

Number of recent credit inquiries:

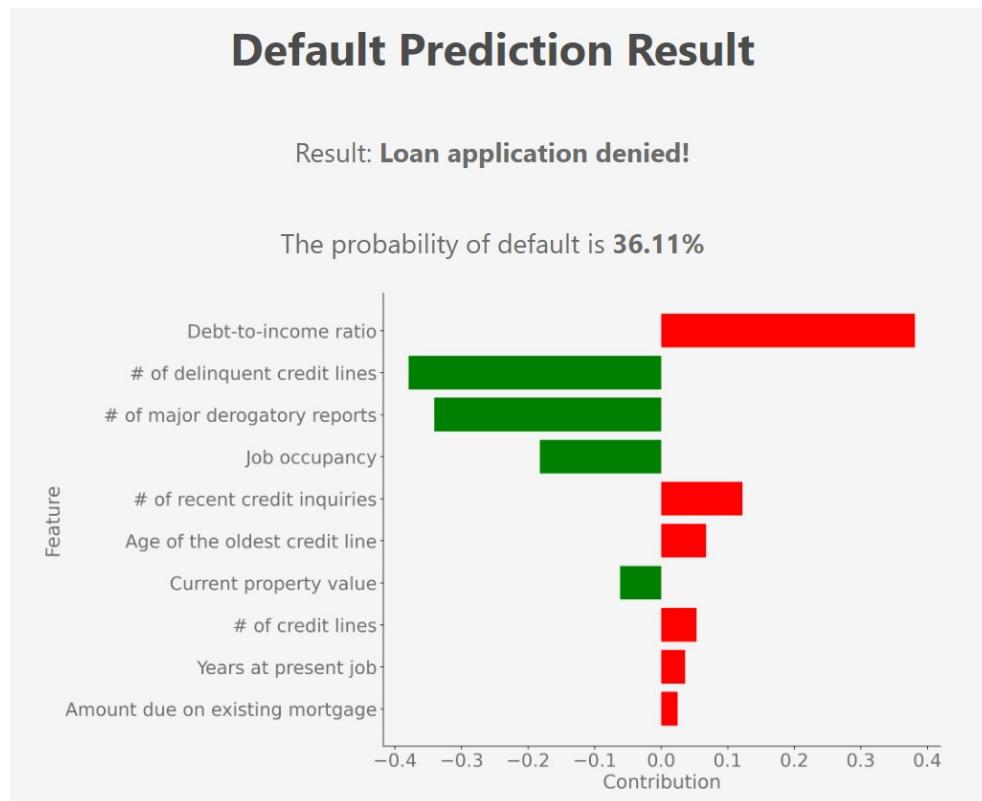
Number of credit lines:

Debt-to-income ratio:

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 4.35. 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 4.35: 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:

$$\xi(x) = \arg \min_{g \in G} L(f, g, \pi_x) + \Omega(g) \quad (4.11)$$

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 4.35, 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 importance 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 delinquent 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

Summary of Results

In this chapter, we evaluate the hypotheses presented in Section 5.1, as outlined in Section 3.1. These evaluations are based on the results obtained from the implementation of machine learning techniques described in Chapter 4. Furthermore, we compare our results with those of previous studies on HMEQ-based studies (Aras 2021; Zurada *et al.* 2014) in Section 5.2. Additionally, we provide a summary of the key findings derived from the machine learning implementation from Chapter 4 in Section 5.3. Moreover, we delve into the author's contributions to the field of credit risk modelling and machine learning in Section 5.4. Lastly, we address the key recommendations to improve this thesis and its machine learning implementation or for future research in Section 5.5.

5.1 Hypotheses' Testing

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

We fail to reject the **Hypothesis #1** because we observe improvements across all 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. In particular, all the score metrics and loss metrics have increased and decreased, respectively, as can be seen in Table 4.21. Hereby, we can confirm that the recalibration of the model truly boost the model predictive power on HMEQ data set.

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 4.22. If we aggregate the model selection results by looking the highest rank per each model, we can observe that the best KNN model had the 12th highest rank, while Neural Network (MLP) exhibited unsatisfactory performance with the 26th highest rank as can be seen in Table 5.1. Therefore, our results are not in line with the outcomes of respective studies (Aras 2021; Zurada *et al.* 2014) which reported that Neural Network and KNN model outperformed all the models on HMEQ data set, respectively.

Table 5.1: Max–Aggregated Ranks of Models

Model	Rank
GB	1
RF	6
KNN	12
SVM	17
MLP	26
DT	35
LR	39
GNB	52

Source: Author's results in Python

Result #3: *Black–box models DO 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 4.23, 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 that 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 4.26, 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 4.28, where Neural Network performed poorly regardless the length of the execution time.

Result #5: *Debt and delinquency features ARE the main default drivers on HMEQ data set.*

We fail to reject the **Hypothesis #5** according to Figure 4.32 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 4.33, we can observe that the negative values of DEBTINC 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 4.12 and Figure 4.13, respectively, we can observe negative WoE values for bins where the debt–to–income ratio is extremely high or is missing and 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.

5.2 Comparison with other HMEQ Studies

Within the literature review in Chapter 3, we discussed the studies of Aras (Aras 2021) and Zurada (Zurada *et al.* 2014) which analyzed the HMEQ data set, i.e., the same data set as in this thesis. In this section, we contrast their results with those of this thesis. Particularly, we compare the models' rankings from Table 3.2 and Table 3.4, respectively, with the thesis' author's rankings derived from Table 5.1, which is summarized in the following Table 5.2. Upon examination, it is apparent that none of the studies considered the Gradient Boosting model, which happens to be the best-performing model in this thesis.

With respect to the study of Aras (Aras 2021), when excluding our Gradient Boosting model, we can agree that Random Forest and KNN are the top-performing models. However, there is a discrepancy in the order of their performance. Aras found that KNN outperformed Random Forest, whereas in this thesis, Random Forest outperformed KNN. Furthermore, it is worth noting that the worst-performing models, namely Decision Tree, Logistic Regression, and Gaussian Naive Bayes, align with both this thesis and Aras' study. Specifically, Aras identified Logistic Regression as the worst-performing model, while in this thesis, Gaussian Naive Bayes exhibited the poorest performance.

Regarding the Zurada's study (Zurada *et al.* 2014), we again concur that Logistic Regression is one of the worst performing models. However, there are significant disparities in the rankings of other models compared to the results obtained in this thesis. It is evident from the findings that MLP was identified as the best performing model in Zurada's study, whereas in this thesis, MLP was ranked as the 5th best performing model, placing it in the second half of the ranked models. In contrast, while KNN was ranked as the 3rd best performing model in this thesis, it received the position of the 2nd worst performing model according to Zurada. Conversely, Zurada ranked Decision Tree as the best second performing model, while in this thesis, it was positioned as the 6th best performing model. However, both Zurada's and Aras' studies, consistent with this thesis, ranked the SVM model in the middle range, aligning with our findings.

Table 5.2: Ranking Results Comparison based on HMEQ Data Set

Model	This Thesis	(Aras 2021)	(Zurada <i>et al.</i> 2014)
GB	1	-	-
RF	2	2	-
KNN	3	1	4
SVM	4	3	3
MLP	5	-	1
DT	6	4	2
LR	7	6	5
GNB	8	5	-

Source: Author's results in Python, Rankings of (Aras 2021), (Zurada *et al.* 2014)

It is important to note that the author of the thesis, Aras, and Zurada employed distinct data preprocessing techniques and different data splits, leading to variations in the training, tuning, and evaluation samples, resulting in disparate outcomes. While Zurada and Aras utilized Grid Search with cross-validation for hyperparameter tuning, the author of the thesis employed Bayesian Optimization with stratified cross-validation. Besides, each author used different hyperparameters' spaces.

Additionally, each author utilized different evaluation metrics. Aras utilized Accuracy, Recall, Precision, F1, and Matthews Correlation Coefficient, while Zurada employed Accuracy, Recall, and AUC. In contrast, the author of the thesis employed a broader range of metrics, including Accuracy, Recall, Precision, F1, Matthews Correlation Coefficient, AUC, Kolmogorov-Smirnov Distance, Somers' D, Brier Score Loss, and Log Loss. Moreover, it is worth mentioning that the authors may have used different software tools. The thesis' author utilized Python, while Zurada employed Weka, and the software used by Aras is unknown. These various factors contribute to the discrepancies in the obtained results among the studies and the thesis. Therefore, it is advisable to refrain from making direct comparisons due to the incomparability of the results.

5.3 Key Findings

The key findings of this thesis are summarized in the following list. We exclude such findings which are derived from the hypotheses' testing in Section 5.1, namely that the most important features for predicting default are the number of delinquent credit lines `DELINQ` and the debt-to-income ratio `DEBTINC`, and that the Gradient Boosting model outperforms all other models in terms of the majority of evaluation metrics etc.

- ADASYN oversampling generates more default-case instances which are managers according to `JOB` feature as described in depicted in Table 4.8 and Figure 4.11. This is attributed to ADASYN nature as it generates more synthetic instances for such default-case instances which are hard-to-learn, therefore default clients who are managers are hard-to-learn according to ADASYN and its underlying KNN algorithm as described in Subsection 4.3.1. By generating more synthetic learn for instances which are hard-to-learn, ADASYN oversampling is expected to improve the model's performance.
- We can also observe the impact of missing values within default prediction, particularly in case of debt-to-income ratio `DEBTINC`. As can be seen in Figure 4.12, the WoE corresponding the bin capturing missing values has a negative value of (approx. -2), which indicates a larger distribution of defaulters compared to non-defaulters. Referring to the WoE values, the SHAP summary plot (Figure 4.33) depicts the global model explainability and the contribution of each feature to the predictions. As can be seen in case of `DEBTINC`, the blue values (i.e., negative WoE values) contributes positively to the default, hence when the debt-to-income ratio is missing, the model is more likely to predict default for such instance.
- Another finding regards the features `DEBTINC` and `DELINQ`. The higher debt-to-income ratio and/or the higher number of delinquent credit lines, the higher the probability of default. This is evident from the WoE values in Figure 4.12 and Figure 4.13, respectively, and the SHAP summary plot in Figure 4.33.
- Most of the models are conservative as most of their optimal thresholds obtained using Youden index are below the standard classification threshold of 0.5 as depicted in Figure 4.25.

- Ensemble models, such as Gradient Boosting and Random Forest, perform better than SVM or Neural Network (MLP), while the transparent models such as Decision Tree, Logistic Regression, and Gaussian Naive Bayes perform the worst. This is depicted in Figure 4.22.
- Black–box models which are complex tend to select more features than transparent white box–models within feature selection (Figure 4.16).

5.4 Contributions

The primary contribution of the thesis author involves the implementation of a customized machine learning framework on a credit risk dataset consisting of performing and non-performing US home equity loans, as described in Figure 4.1 from high–level point of view. This framework encompasses several key steps.

Firstly, the author conducts data exploration (Section 4.2), including distribution and association analysis. To address the imbalanced distribution of defaults, an advanced approach utilizing ADASYN oversampling is employed (Subsection 4.3.1). Additionally, a preprocessing step utilizing Optimal Binning is implemented to discretize feature values into bins optimized with respect to the default status, while also capturing the impact of extreme and missing values by converting them into Weight-of-Evidence values (Subsection 4.3.2).

The author then utilizes custom wrapped algorithms for both feature selection and model selection. These algorithms incorporate Bayesian Optimization for hyperparameter tuning based on the chosen classification models (Subsection 4.4.1). Within the feature selection algorithm, each model is tuned and used within Forward Sequential Feature Selection to determine the subset of optimal features (Subsection 4.4.2). Within the model selection algorithm, each model is tuned and trained on subsets of selected features, determining an optimal threshold for classification using the Youden index, and subsequently evaluated on a validation set using a variety of metrics (Subsection 4.4.3). The models are ranked based on these metrics, considering explicit weights defined by the author. The best performing model is selected for final evaluation on the test set and for deployment.

To enhance the model’s performance and generalization ability, the author performs recalibration of the model and threshold prior to evaluation, by join-

ing the training and validation sets into one set used for model recalibration (Subsection 4.4.4). The evaluation process encompasses various approaches, including the assessment of the model’s performance using a confusion matrix, evaluation metric scores and losses, and ROC curve analysis (Subsection 4.5.1). The impact of recalibration on the evaluation is also examined. Additionally, the author assesses the explainability of the black-box model by analyzing feature importances and SHAP values (Subsection 4.5.2).

Another significant contribution involves deploying the model as a web application using Flask and HTML (Section 4.6). The deployed application is recalibrated alongside its threshold on the joined training, validation and test sets to enhance model’s ability to generalize. Such application is temporarily hosted and deployed on PythonAnywhere cloud platform and made publicly accessible. Users are required to complete a loan application form, with the fields corresponding to the features on which the model was trained. After submission, the application provides a result and default prediction, accompanied by explainability insights using LIME, which highlights the contribution of each feature to the prediction (Subsection 4.6.2).

5.5 Recommendations

Despite the complexity of the custom machine learning solution applied in this thesis, and the hundreds of hours invested by the author, it still has its limitations and drawbacks. We aim to address these issues in this section and provide suggestions for future studies.

1. **Use more relevant and actual data** - Given the nature of the data set analyzed in this thesis, it might not be the most relevant for the current market situation. Thus, using an up-to-date data would either lead to a more realistic generalization (Kumar *et al.* 2021) or an improvement in model’s performance (Karatas *et al.* 2020).
2. **Use bigger data** - Since the real bank data sets often contain hundreds of thousands or even millions of instances, and the number of features can be in hundreds or even higher, it would be beneficial to use bigger data sets to train the models on. Therefore, having bigger sample size for the training, we can enhance model’s performance (Ng *et al.* 2020), as the model would be able to learn more complex patterns in the data.

3. **Use behavioral scoring data** - The data set used in this thesis is based on the application data only, however, the behavioral scoring data is often used in the real-world applications as well. Therefore, it would be also beneficial to use behavioral scoring data which would dynamically capture the client's information about his behavior and it would help the bank to make more informed decision about how to deal with the existing clients (Li & Zhong 2012).
4. **Use macroeconomic data** - Using macroeconomic data such as GDP, unemployment rate, inflation rate, interest rate etc. would allow to create macroeconomic forecasts, i.e., to take into account possible changes in the macroeconomic changes by incorporating forward-looking information (Jakubik *et al.* 2007). Thanks to that, one would be able to achieve more reliable estimates by dynamically capturing the current economic state.
5. **Use TensorFlow/Keras or PyTorch for NN development** - In this thesis, we used Neural Network (Multi-Layer Perceptron) from `Scikit-learn` module. However, in ML engineering or deep learning, the Neural Networks are mostly developed using TensorFlow/Keras or Keras modules which are more efficient and provide more flexibility (Gevorkyan *et al.* 2019).
6. **Django for ML deployment** - In this thesis, Flask framework was used for ML deployment as a web application. Although Flask is a great tool for ML deployment when it comes to the small projects or micro-framework solutions, it is not suitable for production environment. Therefore, we recommend to use Django framework for ML deployment, which is a full-stack Python-based web application framework and is more suitable for production environment and creating larger and more complex database-backed websites and applications (Khatri & Jonhs 2023).
7. **ML application in other credit risk modelling components** - Besides applying ML prediction models in credit risk for default prediction (i.e., PD), it would be also beneficial to apply ML models in other credit risk modelling components, such as LGD and EAD, or subsequently in ECL as well (Munkhdalai *et al.* 2019; Grzybowska & Karwanski 2020) or even for macroeconomic forecasting (Hall 2018).
8. **Hyperparameter Optimization with Optuna** - In this thesis, we used Bayesian Optimization from `Scikit-optimize` module for hyperpa-

rameter optimization. However, there is more efficient framwork, namely Optuna module, which is deemed as the next-generation hyperparameter optimization software which allows to construct the hyperparameter search space dynamically, efficient implementation of searching and pruning strategies and it also provides a versatile architecture which can be deployed in scalable distributed computing or light-weight experiments conducted through interactive interface (Akiba *et al.* 2019).

9. **H2O ML module** - H2O is an automated machine learning module which is more efficient than **Scikit-learn** and provides more flexibility in terms of faster scoring capabilities or producing high quality models suitable for deployment in enterprise envinronment (LeDell & Poirier 2020). According to H2O's documentation, it provides wrapper functions which perform a large number of modelling-related tasks that would typically require many lines of code and it can be also used for automating the machine learning workflow including automatic training and tuning of many models (H2O.ai 2023).

Chapter 6

Conclusion

The main contribution of this thesis is conducting a custom machine learning implementation framework on a credit risk data set of US home equity loans (HMEQ), including training, tuning and selecting from the eight classification algorithms with further deployment and development of a custom web application.

We have covered the theoretical background of credit risk, machine learning, particular machine learning algorithms and the evaluation of classification models, including more advanced machine learning techniques such as ADASYN oversampling, Optimal Binning, Bayesian Optimization or Forward Sequential Feature Selection, as all described in Chapter 2. In Chapter 3 we have proposed five hypotheses, including the literature review with the main focus on HMEQ-based studies of Aras (Aras 2021) and Zurada (*Zurada et al.* 2014).

The Chapter 4 pertains to the very extensive empirical analysis, i.e., machine learning implementation on HMEQ data set. This includes the high-level overview of the custom machine learning framework, repository and environment structure in Python (Section 4.1), data exploration, data preprocessing, hyperparameter tuning, feature selection, model selection, model recalibration, model evaluation and final machine learning deployment. Such implementation is employed with random seed of 42 in order to ensure reproducibility of the results.

Within data exploration (Section 4.2), we first delve into the description of the data set, particularly, what variables or how many instances does it contains (Subsection 4.2.1). Also, distribution analysis is performed (Subsection 4.2.2) as an inspection of the default distribution (Section 4.2.2) as well as the distri-

bution of the features conditional on the default and non-default classes (Section 4.2.2, Section 4.2.2). Further, an association analysis (Subsection 4.2.3) is conducted using Point–Biserial Coefficient (Section 4.2.3), Cramer’s V (Section 4.2.3), Phi Coefficient (Section 4.2.3), Spearman Correlation Coefficient (Section 4.2.3) or Nullity dendograms (Section 4.2.3), in order to infer some association between the default and the features or the feature themselves.

This chapter further describes an implementation of data preprocessing (Section 4.3), including the data split into training set (for hyperparameter tuning, feature selection and model training), validation set (for model selection), and test set (for model evaluation). Such data is split into ratio 70:15:15 with stratification in order to preserve the global distribution of the defaults across the samples. It also includes ADASYN oversampling in order to balance the default distribution, which is performed on the training set only in order to avoid data leakage (Section 4.3). The next step of data preprocessing involves Optimal Binning (Subsection 4.3.2), which is utilized using `optbinning` module in Python developed by Navas–Palencia (Navas-Palencia 2020). This module is employed in order to discretize the numeric features into interval bins and categorical features into subgroups of categories, both are optimally binned with respect to the default. Optimal binning also captures both linear and non-linear relationships and also extreme and missing values, hence no replacement or imputation of outliers of missing values is needed. Afterwards, these bins as categorical values are transformed using Weight–of–Evidence (WoE) with respect to the defaults. The optimal binning and WoE transformation are fitted on the training set only in order to avoid data leakage, based on which other sets are transformed.

Chapter 4 also includes modelling part (Section 4.4), which includes Bayesian Optimization, feature selection and model selection. In this thesis, we use eight classification models from `scikit-learn` module, namely Logistic Regression, Decision Tree, Gaussian Naive Bayes, K–Nearest Neighbors, Random Forest, Gradient Boosting, Support Vector Machine, and Neural Network (Multi–Layer Perceptron). Bayesian Optimization is used for hyperparameter tuning, particularly we use `scikit-optimize` module. We use Bayesian Optimization with 50 iterations, stratified 10–fold cross–validation, while maximizing F1 score. For each model, we further define hyperparameters’ space over which the model is tuned (Subsection 4.4.1). The feature selection is performed using custom algorithm developed by the author, which iterates over the models. Particu-

larly, for each model, it tunes it with Bayesian Optimization on training set, and such tuned model is used as an input estimator within Forward Sequential Feature Selection on training set, which returns subset of optimal features for given model. Since we have eight models, we obtain eight subset of features. Within the model selection Subsection 4.4.3, each model is tuned on each subset of selected features on training set, and then is evaluated on the validation set. On the validation set, we evaluate several evaluation metrics, such as F1 score, Precision, Recall, Accuracy, Matthews Correlation Coefficient, AUC, Kolmogorov–Smirnov Distance, Somers’ D, Brier Score Loss and Log Loss. Instead of using standard classification threshold of 0.5, we compute an optimal threshold using Youden index. Since we have eight models and eight subset of features, we obtain 64 models in total. Afterwards, all the models are ranked on each metric, based on which we calculate a rank score as a weighted average of the individual ranks, where the weights are set explicitly by the author. Based on the rank score, we determine the final rank. The model with the highest rank (i.e., rank of 1) is then selected as the final model for both evaluation and deployment. The final model is **Gradient Boosting** which was trained on the features selected by **Multi-Layer Perceptron**.

In the next part of Chapter 4, we delve into model recalibration and model evaluation. Pertaining to model recalibration (Subsection 4.4.4), the final model is retrained (recalibrated) on the joined training and validation set as (1) by increasing the training sample size we enhance the model’s performance and ability to generalize, and (2) we already used validation set within model selection, thus no data leakage occurs. Together with the model itself, we also recalculate the optimal threshold using Youden index. The recalibrated optimal threshold used for an evaluation is **0.45109**. The final model is further assessed in evaluation part on the test set (Section 4.5). First we inspect model’s performance (Subsection 4.5.1) using confusion matrix and the evaluation metrics defined previously and further we construct a ROC curve as an indicator, whether given model performs better than a random guess. We inspect the impact of the recalibration on the model’s performance as well. Further, we assess the model explainability (Subsection 4.5.2) by exploring its feature importances, i.e., how each feature contributes to the model’s performance, and by SHAP summary plot which depicts the global explainability of the model and how each future contributes to the predictions.

The final section of Chapter 4 regards the machine learning deployment of the

model into a production as a web application (Section 4.6). Such application is built using Flask framework for back-end and HTML with CSS and JavaScript elements for front-end. Prior the deployment, the final model and its optimal threshold are retrained on the whole data set (training, validation and test set) in order to enhance the model’s performance and ability to generalize, since we already used the test set within the evaluation part. The final optimal threshold used in the deployment is **0.3358**. The web application itself is temporarily deployed on PythonAnywhere cloud platform which is accessible via the following link: <http://ml-credit-risk-app-petrngn.pythonanywhere.com/>. Such application requires to fill in the loan application form where its fields correspond to the features on which the final model was trained (Figure 4.34). After a submission of the form, the application processes the inputs, bins them and transforms them into WoE values and afterwards, it predicts the result, whether the loan is rejected or approved based on the optimal threshold, and the probability of default. The result is then displayed on the web page (Figure 4.35). The application also displays LIME which depicts the local Explainability of the model around the given prediction, i.e., it shows the contribution of each feature to the prediction.

In the last Chapter 5, we summarize the results of this thesis. Particularly, we assess hypotheses’ testing (Section 5.1) which is depicted in the following table Table 6.1.

Table 6.1: Hypotheses’ Results

#	Hypothesis	Rejected
H1	<i>The recalibration of the model enhances model performance on HMEQ data set.</i>	NO
H2	<i>Either Neural Network or KNN model outperforms all the models on HMEQ data set.</i>	YES
H3	<i>Black-box models perform better than the white-box models on HMEQ data set.</i>	NO
H4	<i>The longer execution time of a model, the better performance on HMEQ data set.</i>	YES
H5	<i>The main default drivers are the debt and/or delinquency features on HMEQ data set.</i>	NO

Source: Author’s Results

This chapter also includes the discussion of the model rankings results with

the results of the studies of Aras (Aras 2021) and Zurada (Zurada *et al.* 2014) as discussed in Section 5.2. While the results of Aras' study are in line with the results of this thesis, i.e., Random Forest and K-Nearest Neighbors perform well whereas Decision Tree, Logistic Regression and Gaussian Naive Bayes perform poorly, the results of Zurada's study are not in line with the results of this thesis, as its best models are Multi-Layer Perceptron and Decision Tree, which are outperformed by Gradient Boosting, Random Forest, K-Nearest Neighbors and Support Vector Machine. Further, Zurada ranks K-Nearest Neighbors as one the worst performing models (after Logistic Regression), whereas K-Nearest Neighbors performs well in this thesis and outperforms Support Vector Machine, Multi-Layer Perceptron, Decision Tree, Logistic Regression and Gaussian Naive Bayes. Since either thesis' author, Zurada and Aras used different data preprocessing steps, hyperparameter tuning approach and spaces, evaluation metrics and software tools, we should refrain from making direct comparisons due to the incomparability of the results, given the factors mentioned above.

Regarding the key findings of this thesis, particularly of the machine learning implementation Section 5.3, besides the findings observed within hypotheses' testing and studies' comparisons, we further observe that ADASYN oversampling generates more default-case instances which are managers which is attributed to the nature of ADASYN oversampling, which generates more synthetic default-case samples for such default cases which are hard-to-learn by ADASYN, thus defaulted managers are hard-to-learn by ADASYN (Subsection 4.3.1). By generating more syntehetic instances which are hard-to-learn, it is expected that the model's performance will be enhanced. Another finding regards the impact of the missing value of debt-to-income ratio within default prediction, in particular, if the debt-to-income ratio is missing, it increases the probability of default (Figure 4.33), since bin capturing missing values has negative WoE coefficient (Figure A.2). Following this observation, also higher of debt-to-income ratio and/or number of delinquent credit lines increase the probability of default as can be seen in SHAP summary plot (Figure 4.33) and WoE distribution (Figure A.2). Further, most of the models are conservative since their optimal thresholds are lower than the standard classification threshold 0.5, i.e., they are more likely to reject the loan application than to approve it, as depicted in Figure 4.25. Moreover, ensemble models, such as Gradient Boosting and Random Forest, outperform Support Vector Machine

and Multi-Layer Perceptron, whereas the less complex, white-box models, such as Decision Tree, Logistic Regression and Gaussian Naive Bayes have very poor performance, as shown in Figure 4.22. Last but not least, Black-box models which are complex require more features than transparent white box-models to perform well within feature selection (Figure 4.16).

In the final part, we discuss the contribution of this thesis which is further elaborated in detail in Section 5.4, and the recommendations for future research Section 5.3, given the limitation of the analyzed data set which might not be representative for the current situation in the financial industry. We recommend to use more relevant actual data to capture current market situation; use bigger data to increase the training sample size; use macroeconomic data to dynamically capture the current economic state; use TensorFlow/Keras or PyTorch for development of Neural Network which is more versatile than Scikit-learn; use Django for machine learning deployment which is more suitable for full-stack projects than Flask; implement machine learning in other components of credit risk modelling, such as EAD, LGD, recovery rates or ECL itself; use Optuna module for hyperparameter tuning which is the state-of-the-art hyperparameter optimization framework; use H2O module for automated machine learning.

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Appendix A

Additional Figures and Tables

TBD

Table A.1: Normality Test - Shapiro–Wilk

Feature	Shapiro-Wilk	Significance	Result
LOAN	0.8519	***	Not normally distributed
MORTDUE	0.8802	***	Not normally distributed
VALUE	0.81	***	Not normally distributed
YOJ	0.9078	***	Not normally distributed
DEROG	0.336	***	Not normally distributed
DELINQ	0.4578	***	Not normally distributed
CLAGE	0.9346	***	Not normally distributed
NINQ	0.6909	***	Not normally distributed
CLNO	0.9665	***	Not normally distributed
DEBTINC	0.8272	***	Not normally distributed

Source: Author's results in Python

Figure A.1: ADASYN Impact of Numeric Features' Distribution

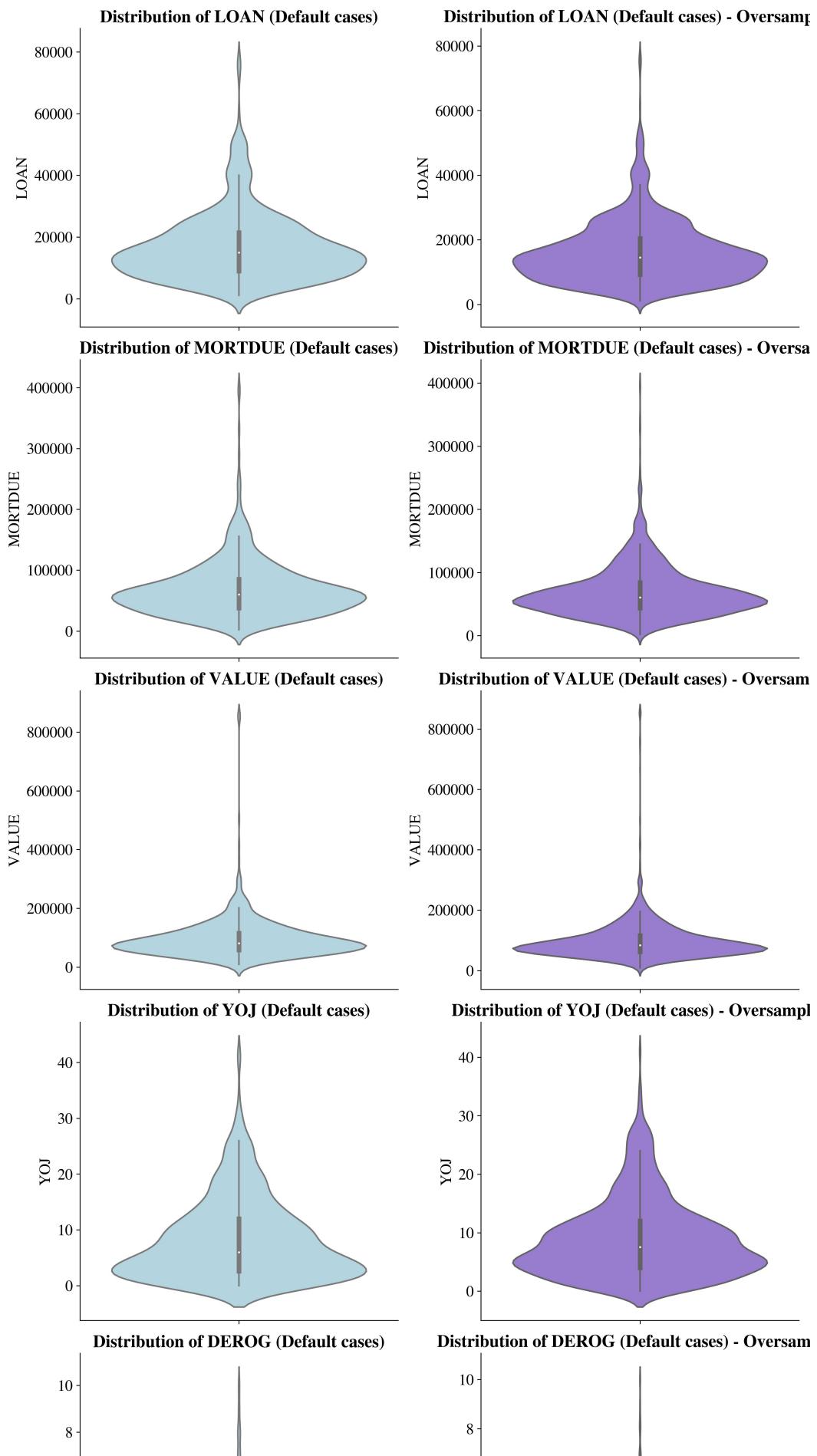
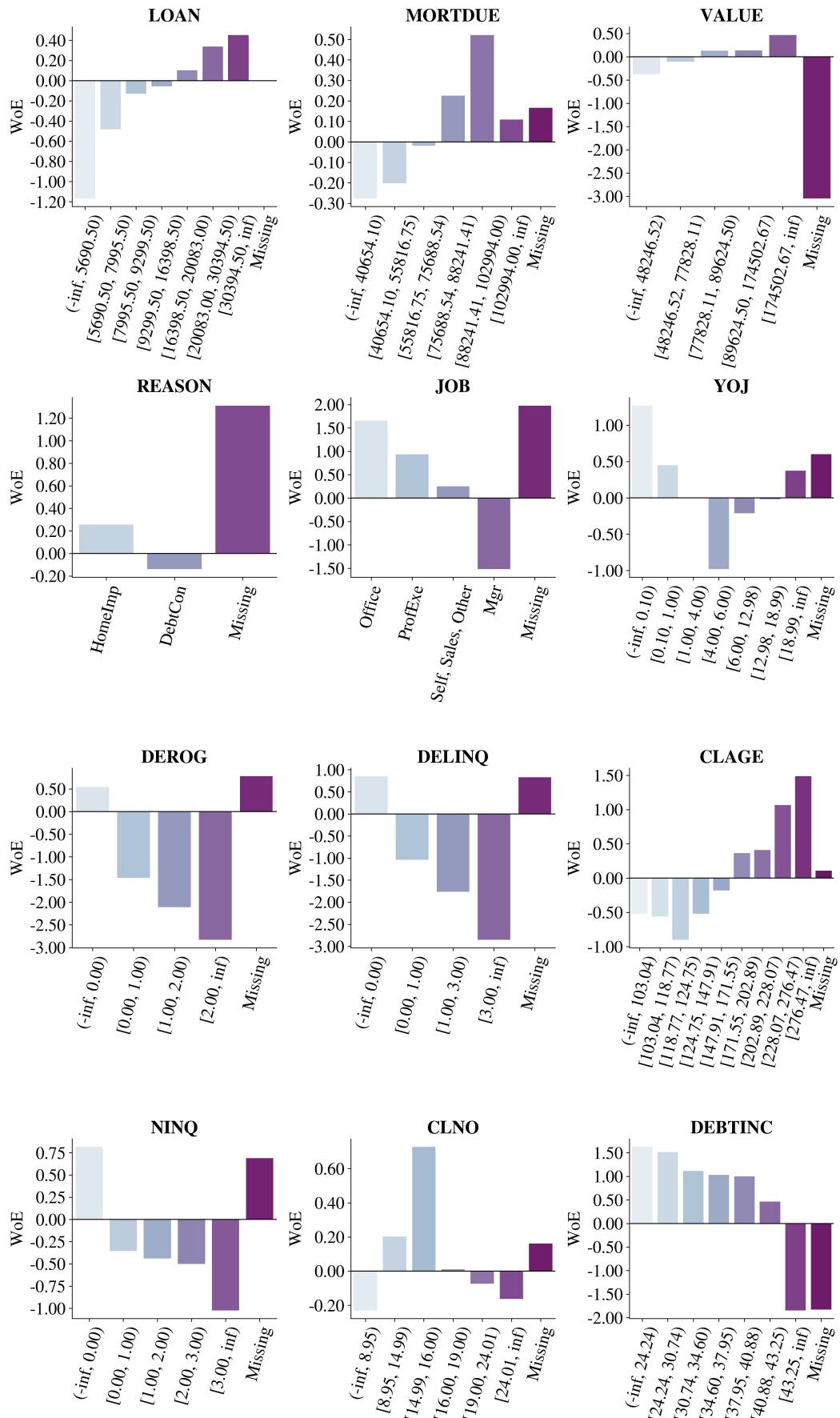


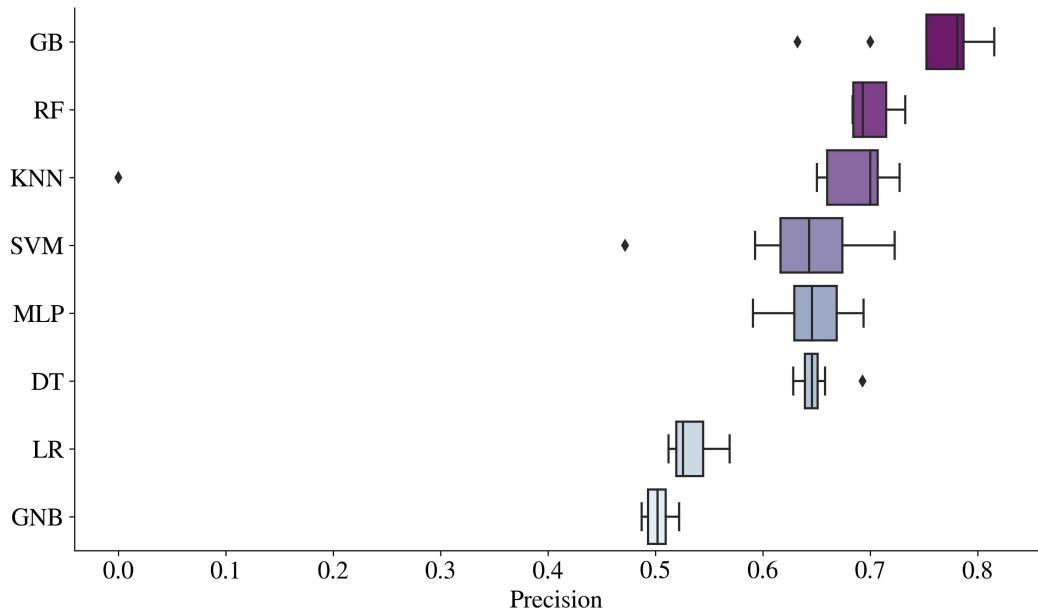
Figure A.2: WoE Bins Distribution



Source: Author's results in Python

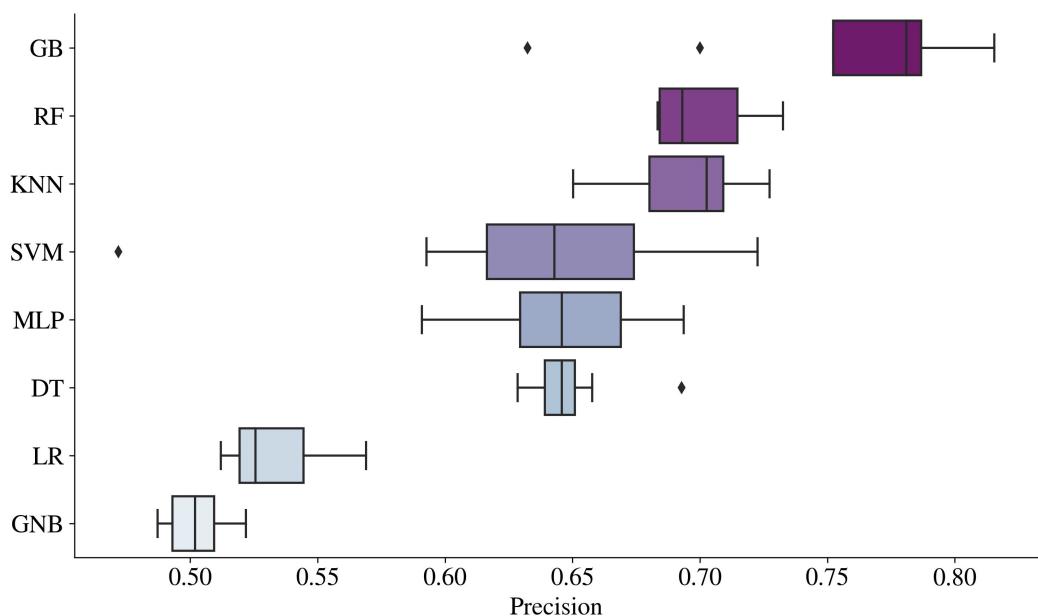
A.1 Model Selection Results

Figure A.3: Precision Distribution



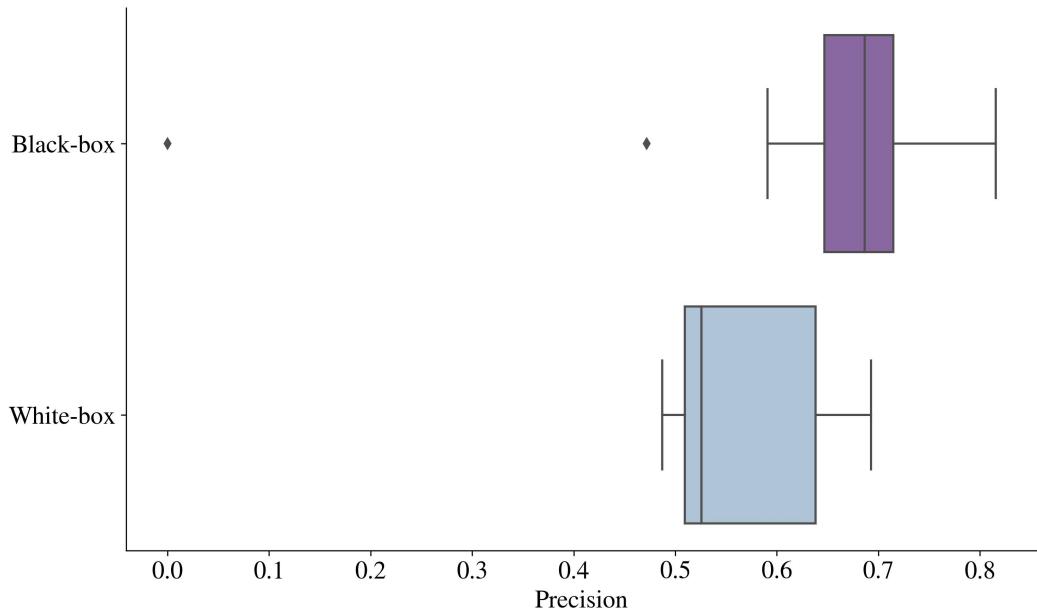
Source: Author's results in Python

Figure A.4: Precision Distribution - *without outlier*



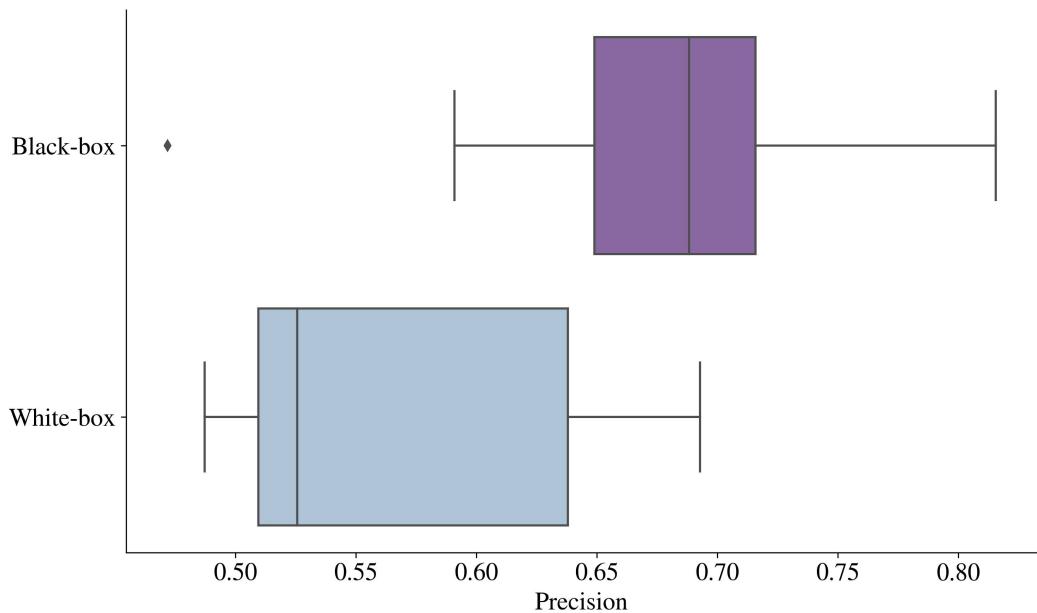
Source: Author's results in Python

Figure A.5: Precision Distribution (Black-box/White-box dimension)



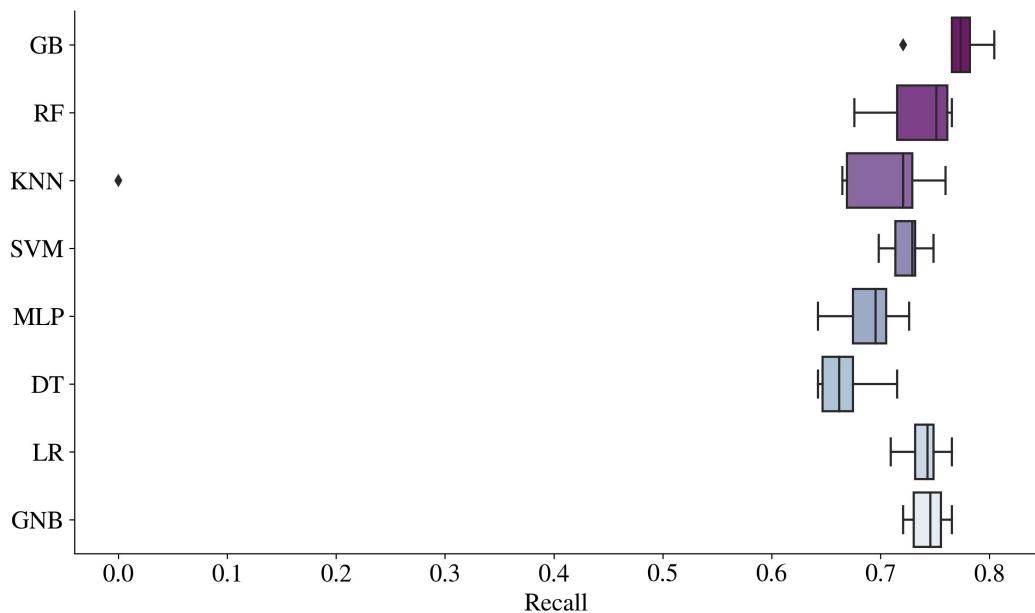
Source: Author's results in Python

Figure A.6: Precision Distribution (Black-box/White-box dimension) - *without outlier*

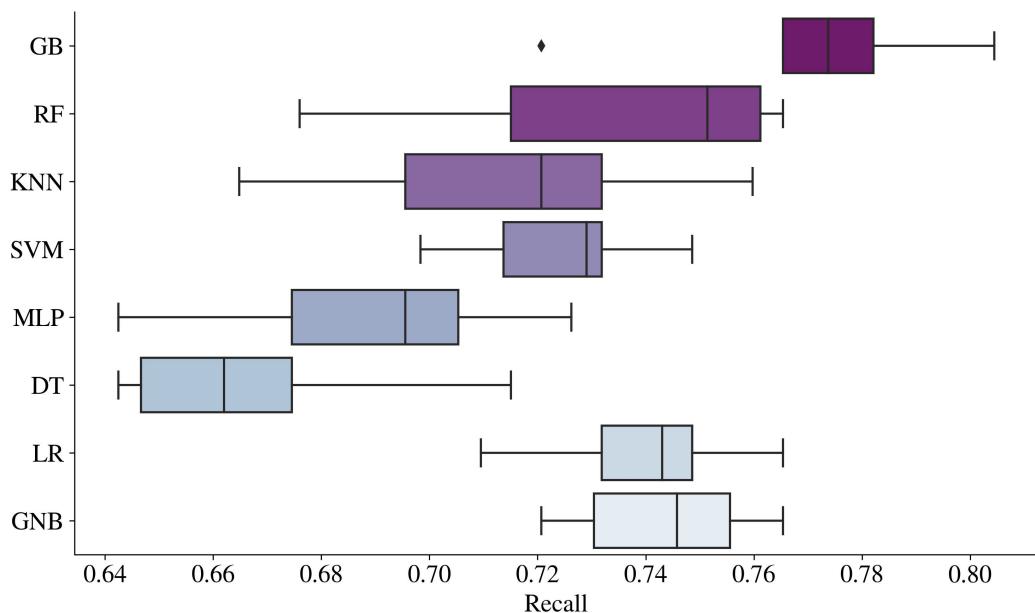


Source: Author's results in Python

Figure A.7: Recall Distribution

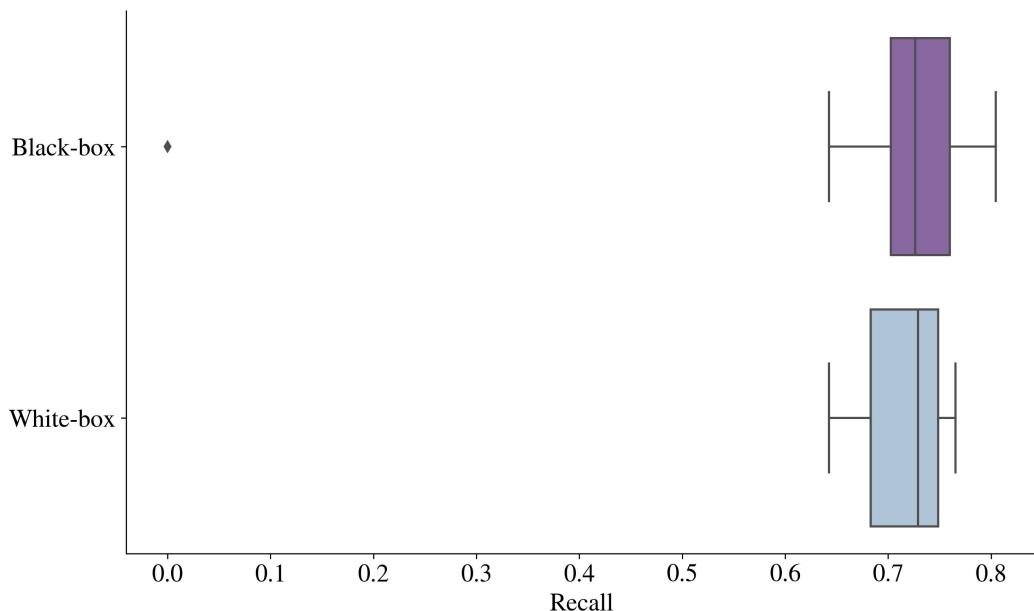


Source: Author's results in Python

Figure A.8: Recall Distribution - *without outlier*

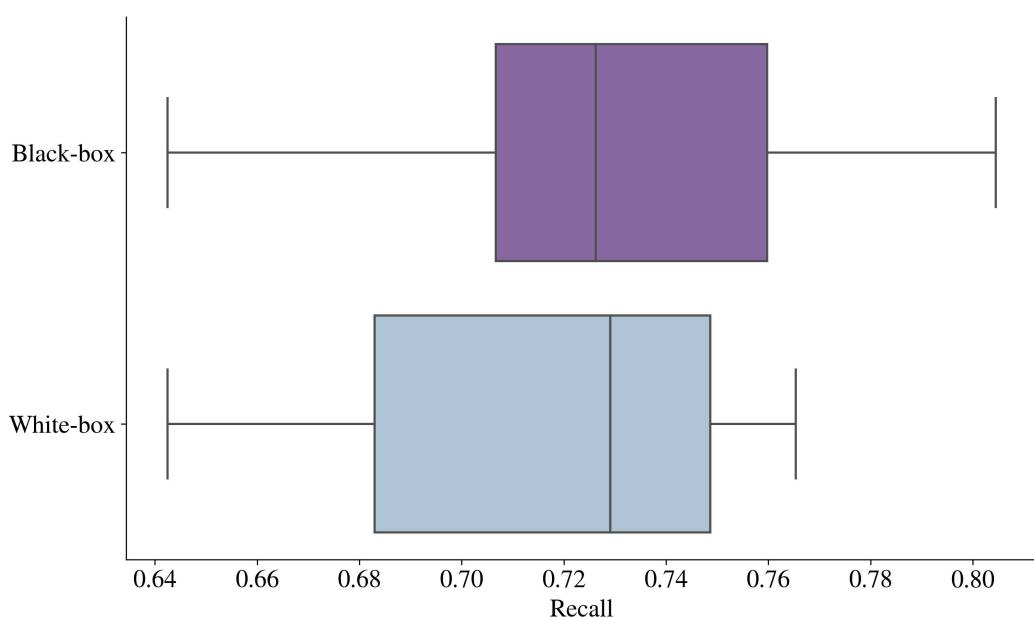
Source: Author's results in Python

Figure A.9: Recall Distribution (Black–box/White–box dimension)



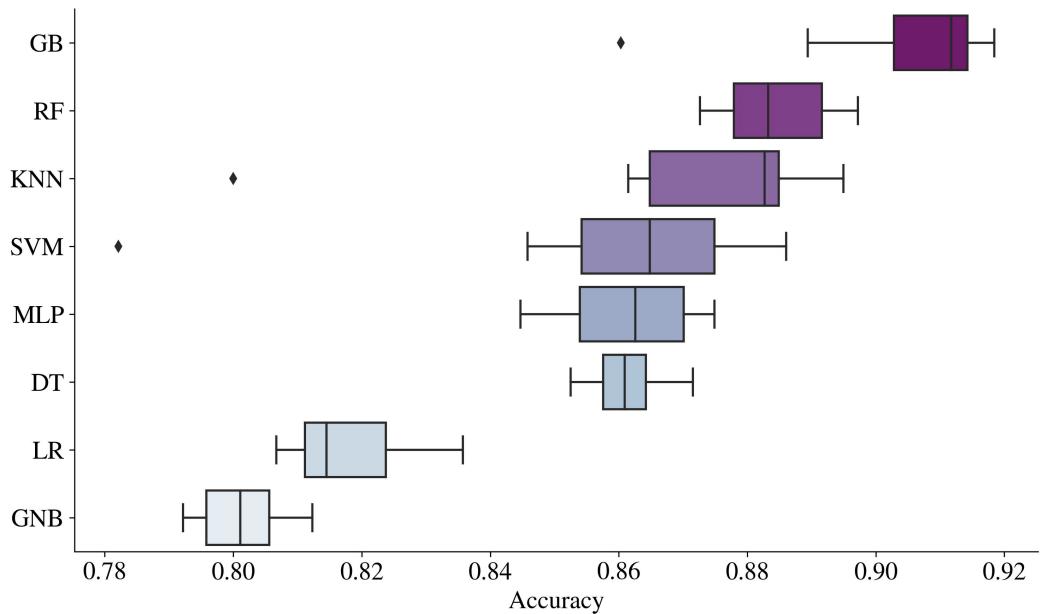
Source: Author's results in Python

Figure A.10: Recall Distribution (Black–box/White–box dimension)
- without outlier



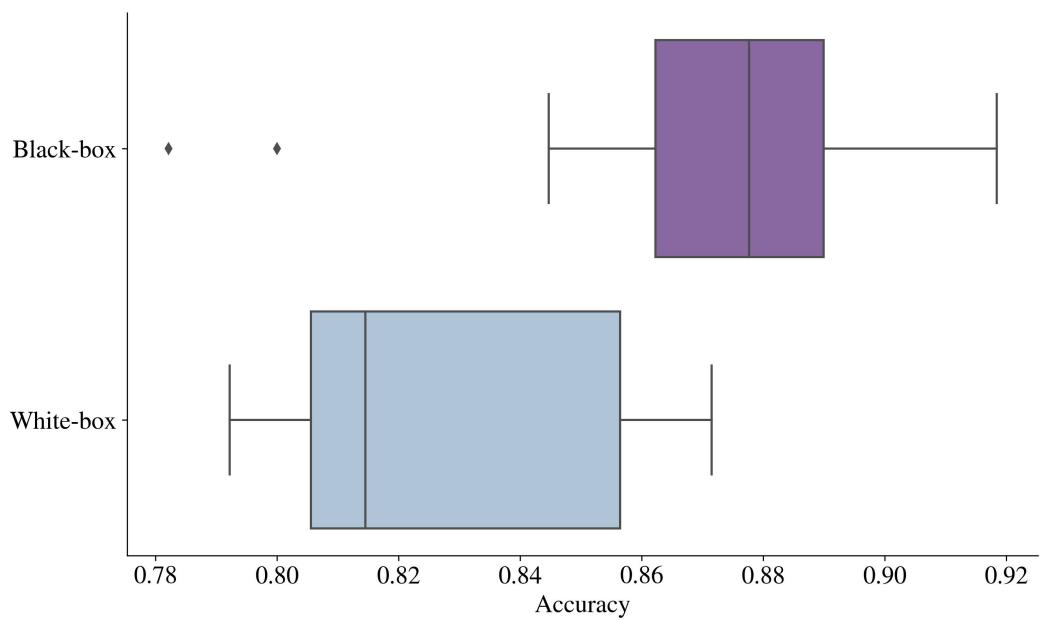
Source: Author's results in Python

Figure A.11: Accuracy Distribution



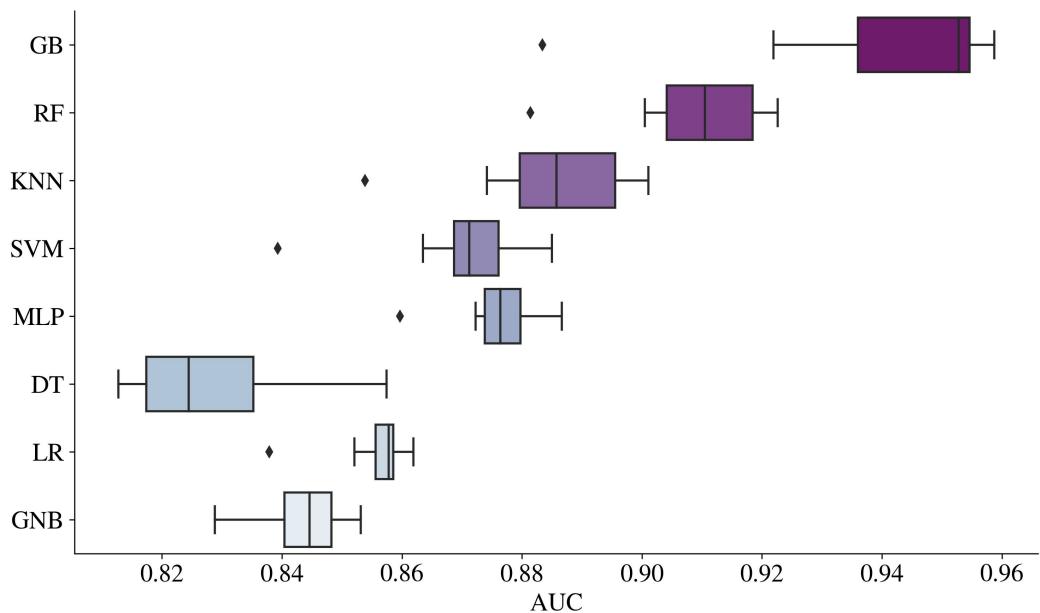
Source: Author's results in Python

Figure A.12: Accuracy Distribution (Black-box/White-box dimension)



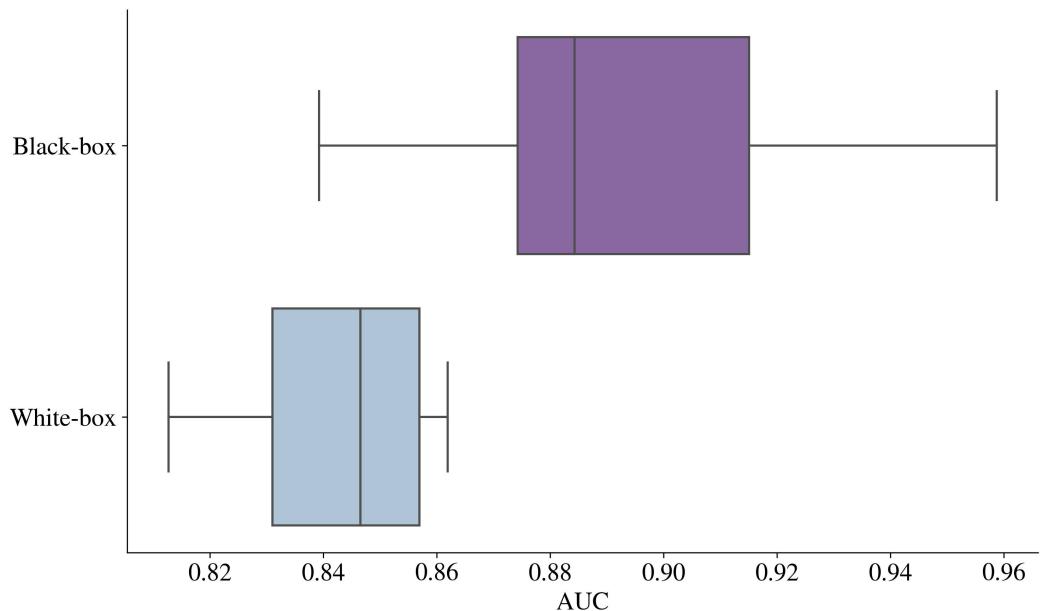
Source: Author's results in Python

Figure A.13: AUC Distribution



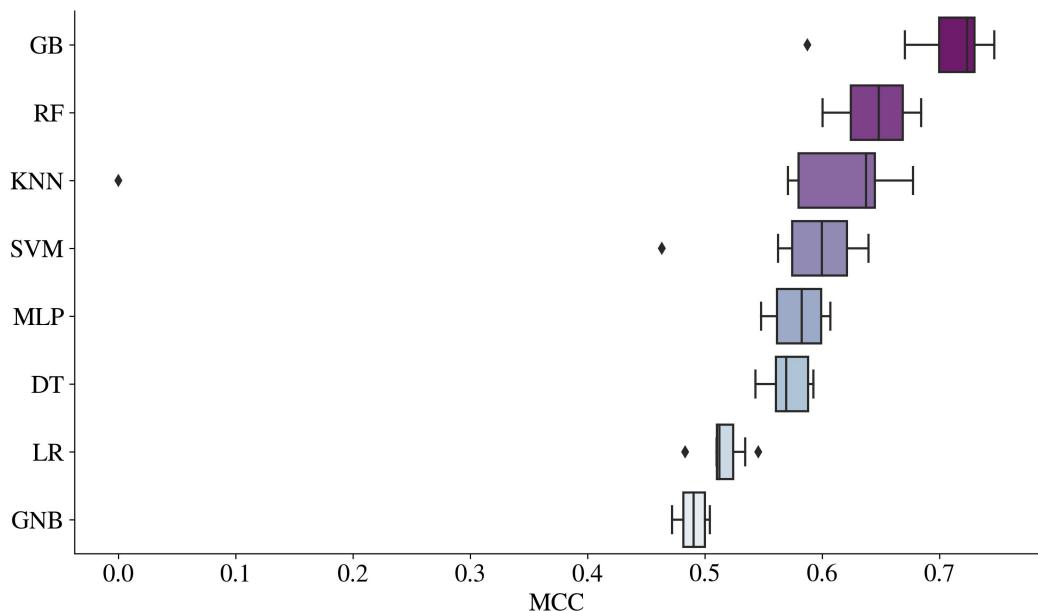
Source: Author's results in Python

Figure A.14: AUC Distribution (Black-box/White-box dimension)

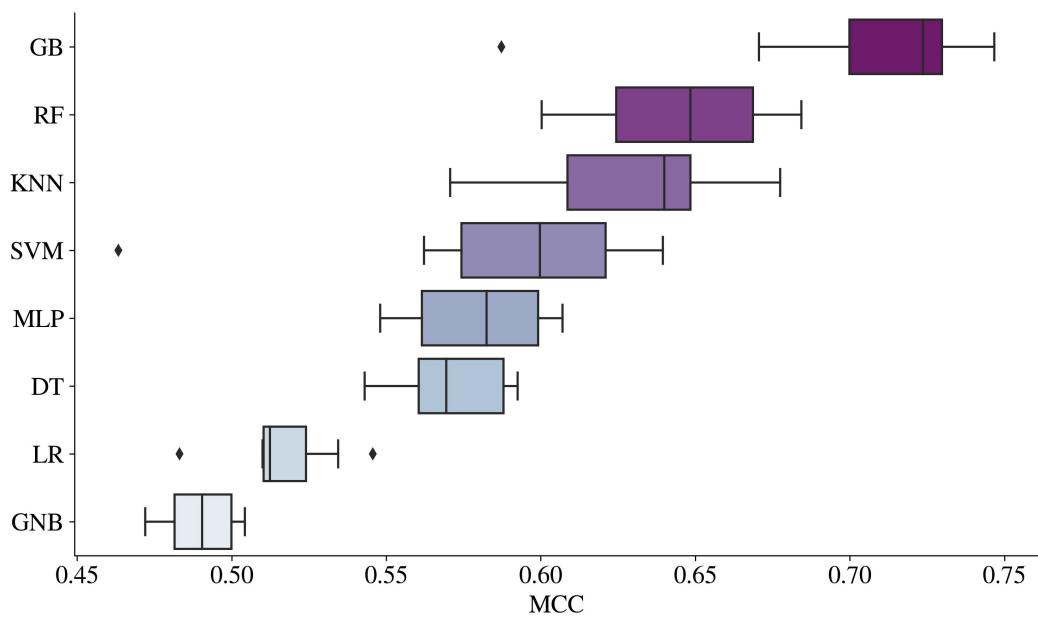


Source: Author's results in Python

Figure A.15: Matthews Correlation Coefficient Distribution

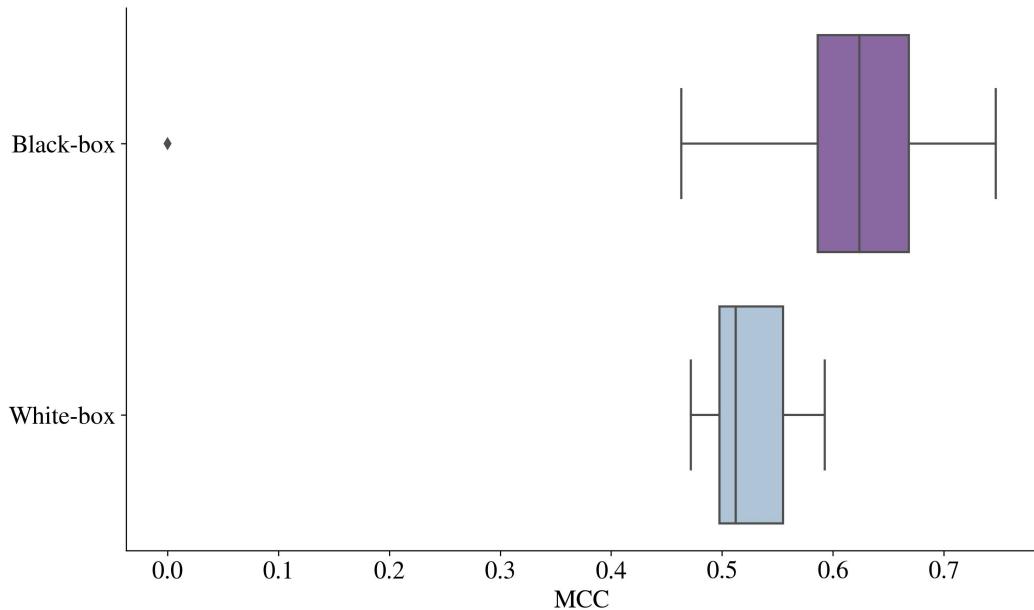


Source: Author's results in Python

Figure A.16: Matthews Correlation Coefficient Distribution - *without outlier*

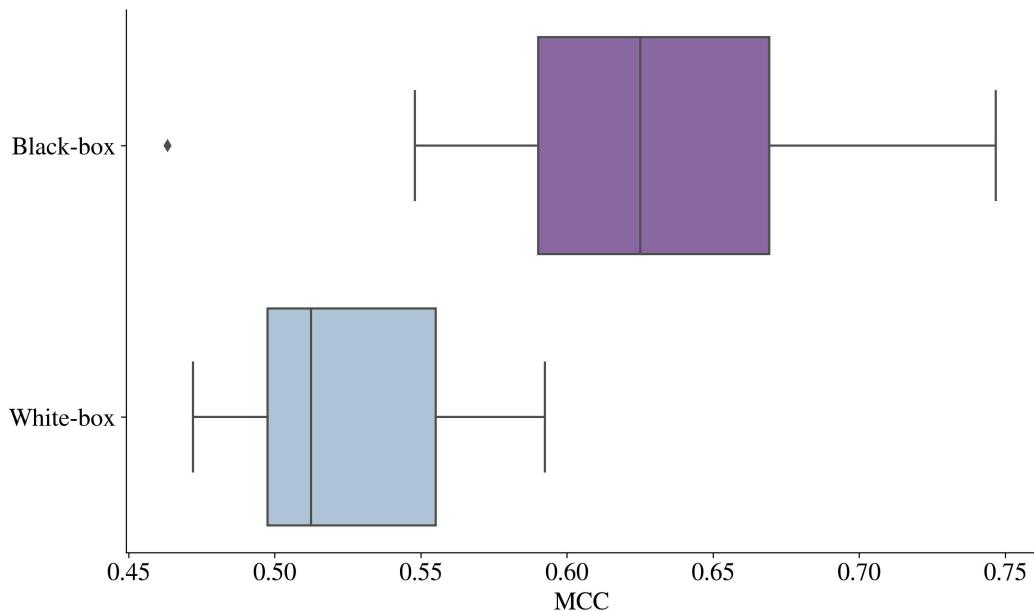
Source: Author's results in Python

Figure A.17: Matthews Correlation Coefficient Distribution (Black–box/White–box dimension)



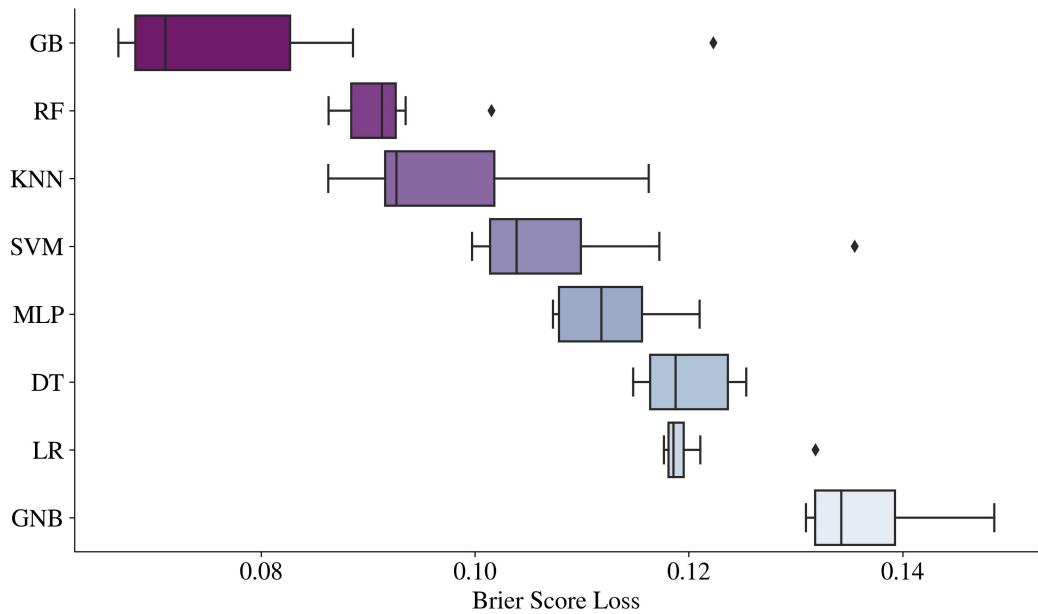
Source: Author's results in Python

Figure A.18: Matthews Correlation Coefficient Distribution (Black–box/White–box dimension) - *without outlier*



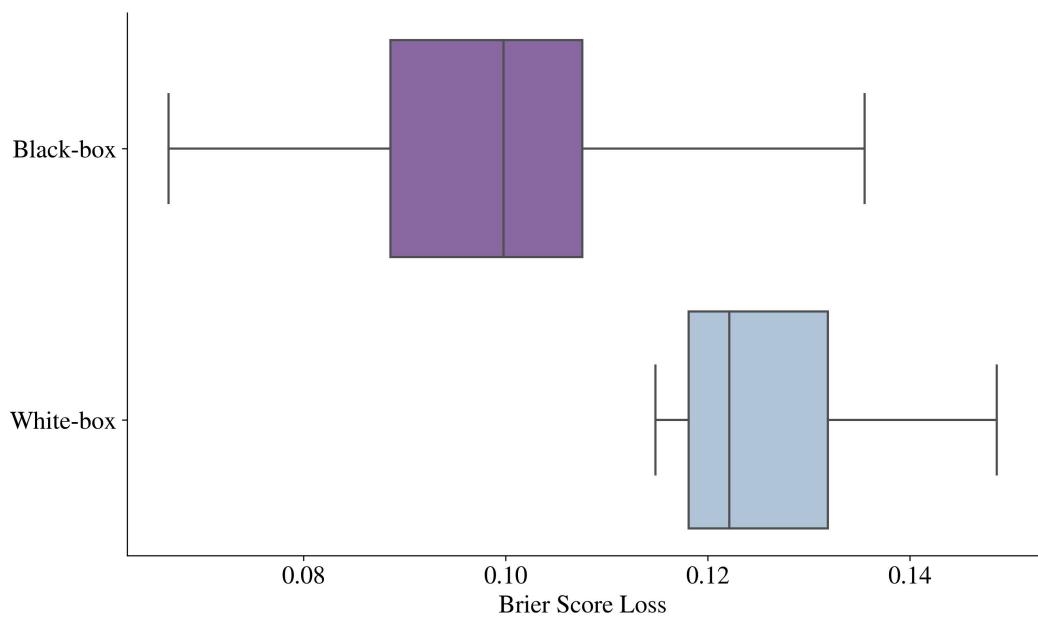
Source: Author's results in Python

Figure A.19: Brier Score Loss Distribution



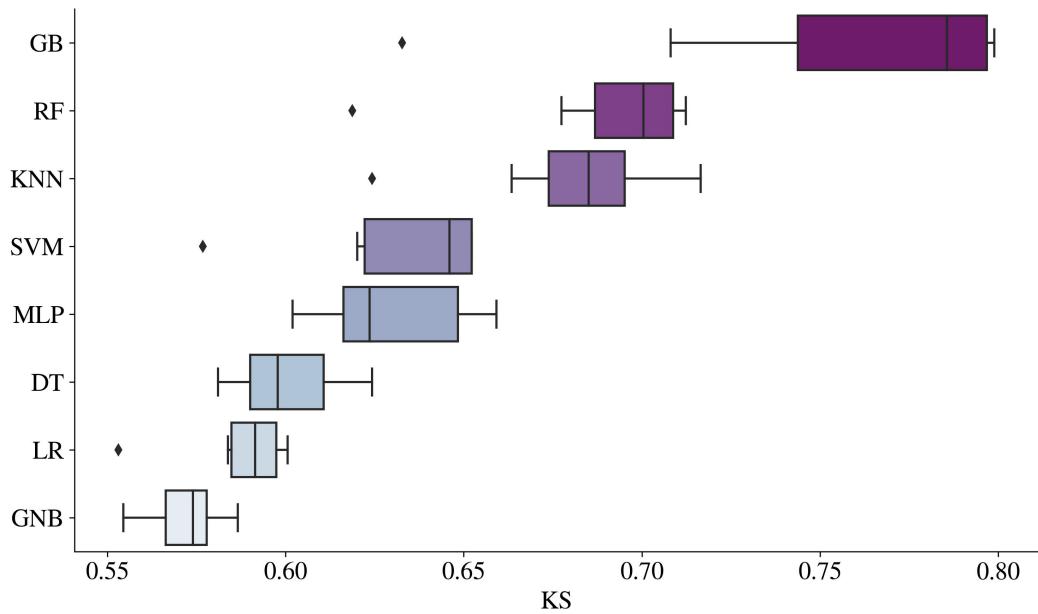
Source: Author's results in Python

Figure A.20: Brier Score Loss Distribution (Black-box/White-box dimension)



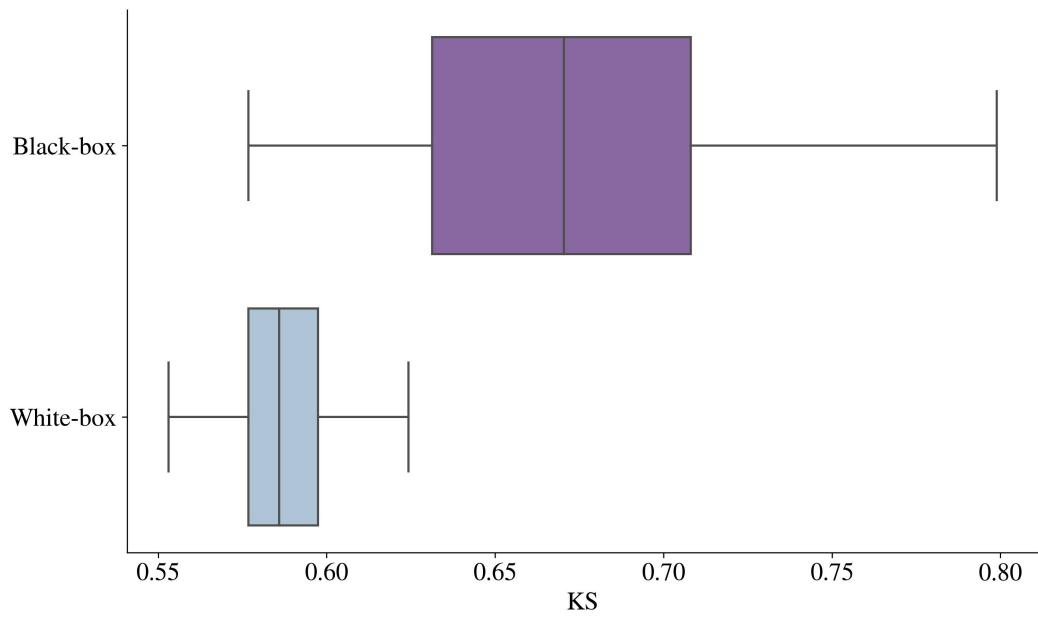
Source: Author's results in Python

Figure A.21: Kolmogorov–Smirnov Distance Distribution



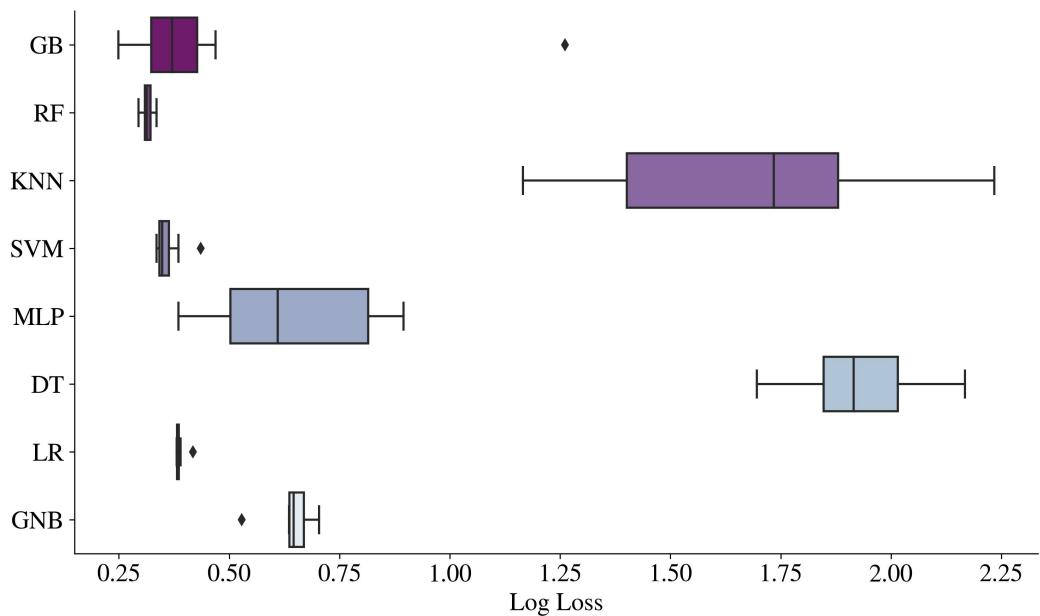
Source: Author's results in Python

Figure A.22: Kolmogorov–Smirnov Distance Distribution (Black–box/White–box dimension)



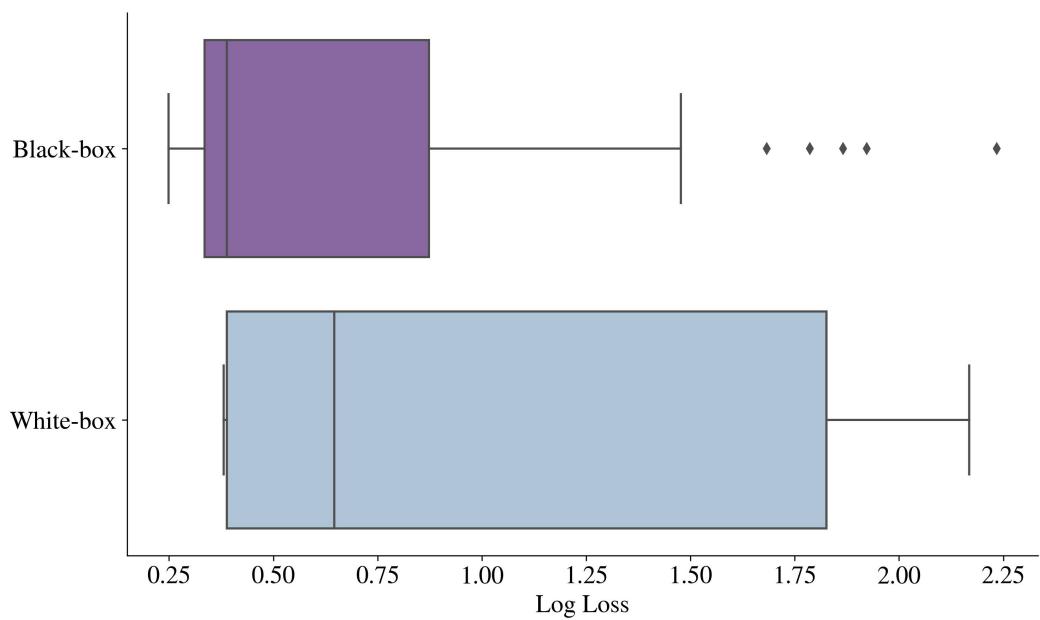
Source: Author's results in Python

Figure A.23: Log Loss Distribution



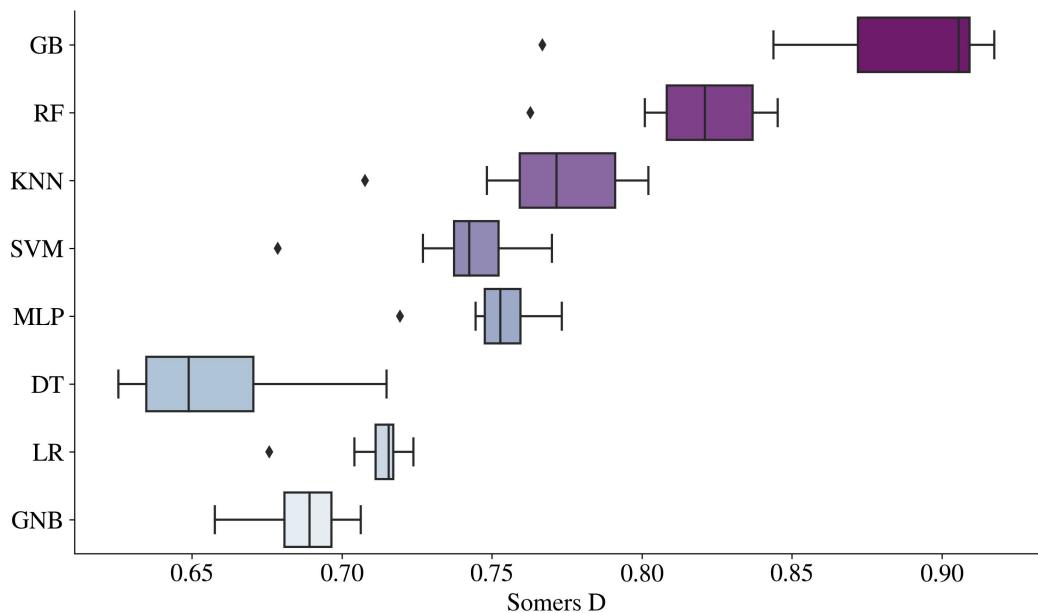
Source: Author's results in Python

Figure A.24: Log Loss Distribution (Black-box/White-box dimension)



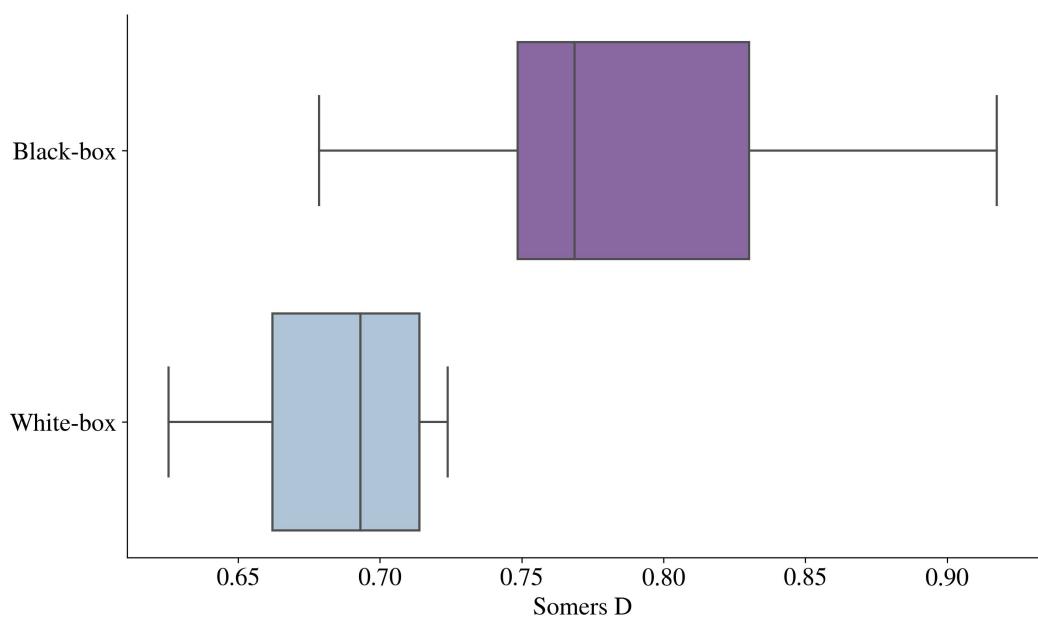
Source: Author's results in Python

Figure A.25: Somers' D Distribution



Source: Author's results in Python

Figure A.26: Somers' D Distribution (Black-box/White-box dimension)



Source: Author's results in Python