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Stacking Algorithm and Ensemble Modelling

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Abstract

Stacking and Ensemble models currently belong to the most powerful machine learning tools. In depth, this paper introduces and discusses the most important concepts of Stacking and Ensembling. In order to assess their predictive performance in the context of credit risk assessment, a empirical evaluation study is realized on behalf of the German Credit Dataset. Results show that Ensembling models, including a Random Forest and a Gradient Boosting model, outperform standard machine learning models on a broad set of evaluation metrics. Different versions of Stacked Generalization models were able to establish better predictions than their level 0 generalizers. Thereby, more sophisticated Stacking algorithms could establish even better results. The restriction of the subset of input predictions for the Stacked Generalization models was ineffective with regards to performance issues. The results strongly reinforce the value of Stacking and Ensembling strategies for prediction in credit risk assessment problems.

1 Motivation

"[W]hen our imperfect judgements are aggregated in the right way, our collective intelligence is often excellent." (Surowiecki, 2005, Foreword p.XIV)

In accordance with the title of his book, Surowiecki refers to what he calls the wisdom of crowds-phenomenon (Surowiecki, 2005). This social phenomenon describes that - under certain fulfilled criteria - the aggregates of individual judgements are superior to each individual judgement alone. While this effect can be found in the social world, it also applies to the world of statistics and machine learning. In the field of Stacking and Ensemble modelling, research has shown different ways in which the aggregation of predictive models can deliver a more powerful model. Such Stacking and Ensemble models

currently belong to the most powerful machine learning tools as can be seen by their success in data science competitions (e.g. on the data science competition website Kaggle). In the context of credit risk assessment, where banks need to estimate credit worthiness of potential customers, accurate predictions are particularly valuable. In comparison to alternative predictive models, Stacking and Ensemble methods have shown to be highly effective in this area (Yu et al., 2008; Zhu et al., 2017). The field of existing methods is however large. In depth, this paper will therefore introduce and apply the most important concepts, namely Bagging and the related Random Forest model (Breiman, 1996, 2001), the concept of boosting and the related Gradient Boosting model Freund and Schapire (1996); Friedman (2002) as well as the idea of Stacked Generalization (Wolpert, 1992).

The paper's structure is as follows: In the coming section, the different concepts of Stacking and Ensembling shall be introduced and their strengths and shortfalls will be discussed. In the following, the value of applying these models in the context of credit risk classification is discussed briefly. Subsequently, an empirical evaluation study that aims at applying the introduced Stacking and Ensemble models in such financial context is prepared. For that, firstly the credit risk data is presented, secondly the model building process is outlined and thirdly the metrics for model evaluation are introduced. In the next section, results of the empirical evaluation study are presented in detail. Finally, conclusions about comparative advantages and shortfalls of the models in the context of credit risk classification are drawn and needs of further research are identified.

2 Stacking and Ensembling Modelling

Ensemble learning generally refers to the combination of multiple hypotheses in order to obtain a more powerful hypothesis. In the context of machine learning, the term hypothesis refers to the output of an algorithm, which aims to learn a target function $f(\mathbf{x})$ by using a set the features \mathbf{x} . Each algorithm that is used in the combination process of an ensemble learner is called a *base learner*.

Different ways to combine the hypotheses of base learners exist. Generally, ensemble learning is most effective when diverse base learners are combined. Hereby, diversity refers to error diversity, implying that the different base learners have different strengths in capturing structure in the data. Brown et al. (2005) show that the combination methods of

ensemble learning strategies enhance such diversity. Furthermore, practical applications of ensembling techniques show, that Stacking and Ensemble models enhance diversity amongst their base learners by requiring different algorithms, different hyperparameter settings, different feature subsets and different training sets for their base learners (Güneş, 2017).

In the following, different techniques to combine the hypotheses of base learners will be introduced and their specific strengths and shortfalls are identified.

2.1 Bagging and the Random Forest model

The idea of Bagging was originally proposed by Breiman (1996). The term abbreviates bootstrap aggregating which refers to a manipulation of the training data: Each base learner m is fitted on a uniformly drawn random sample D_m^{train} from the training data D^{train} . Notably, D_m^{train} may contain duplicates of certain observational units, since sampling is done with replacement. The hypotheses of the base learners is then aggregated by averaging in case of a regression problem or majority voting in case of a classification problem.

In so far, bagging is a meta-algorithm that can be used with every type of base learner algorithm. However, especially unstable base learners that are sensitive to data manipulation should be combined (Breiman, 1996, p.124). Breiman therefore recommends to use Neural Networks, Decision Trees or subset selection in Linear Regression. By building the base learners on different subsets of the data, the bagging procedure enhances diversity amongst them and can lead to "substantial gains in accuracy" (Breiman, 1996, p.123).

The Random Forest model uses the bagging principle and supplements it with the random subspace approach (Ho, 1998; Breiman, 2001). This approach builds each base learner on a random sample with replacement of all available features, which implies a decorrelation of the base learners' hypotheses. For Random Forests, the Decision Trees is the preferred base learner algorithm (cp. Breiman, 2001).

A big strength of the Random Forest is the reduction in prediction variance compared to single Decision Trees, which stems from the diversification. Clearly, the computational costs of a Random Forest can be much higher than those of a single Tree, since computational time increases linearly to the number of consulted Trees. Due to the independent building of the individual base learners, Random Forest model building can be accelerated by parallelization on different cores of the computer. Breiman further notes that Random Forests give "useful internal estimates of error, strength, correlation and variable importance" (Breiman, 2001, p.10). Hence, even though decision rules of Random Forests are less transparent than those of single Decision Trees due to the sampling, relative variable importances can be calculated as a by-product by randomly permuting

features and examining their influence on the prediction. As a single weakness, growing a large random forest can be computationally expensive. Breiman proves that the generalization error of the ensemble converges almost surely to a limit with increasing number of Trees (Breiman, 2001, p.30). In practice, the number of Trees is however restricted by the amount of available computational resources.

2.2 Boosting and the Gradient Boosting model

Beneath Bagging, another powerful ensembling technique is Boosting. It builds on the idea that the aggregation of weak base learners may lead to a strong learner. In their Adaboost algorithm, Freund and Shapire (1996) start with an ensemble of one weak learner and iteratively add one more weak learner that aims to correct for the (pseudo) residuals of the current ensemble. Thereby, the calculation of these residuals is based on an iterative reweighting of the data. The weights of each datapoint x_i for model m depend on the prediction accuracy of the current ensemble hypothesis for that datapoint $h_{\{1,2,\ldots,m-1\}}^{ensemble}(x_i)$.

With Boosting, it is possible to decrease the training error to zero (Freund and Schapire, 1996, p.11ff.). Furthermore, as long as base learners are better than random guessing, the Boosting technique is also able to reduce the generalization error independent of the base learning algorithm.

A development of the Boosting idea is the (Stochastic) Gradient Boosting model, which is currently the most commonly used Boosting model (Friedman, 2001, 2002). In contrast to the data weighting scheme in the Adaboost algorithm, Gradient Boosting minimizes the gradient of a loss function of the error by applying gradient descent. Typically, small Decision Trees are used as base learners of the Gradient Boosting model due to their propensity towards high prediction bias. Additionally, Gradient Boosting integrates the bagging idea. Friedman shows, that this integration could substantially improve accuracy and execution speed of the model (Friedman, 2002).

The possibility to be executed fast is a reason for the heavy use of Gradient Boosting models for machine learning problems. Furthermore, they allow to gain insights into the dependence of target and features by enabling partial dependence plots (Friedman, 2001, p.1219ff.). However, due to its nature, Gradient Boosting models are highly prone to overfit the training data and therefore must be accompanied with regularization methods (Friedman, 2002, p.1203). Therefore most of the parameters of the Gradient Boosting model deal with this problem of overfitting.

2.3 Stacked Generalization model

Stacked Generalization models has been introduced by Wolpert (1992) and defines a way to combine multiple predictive algorithms by using a second-level algorithm. In contrast to Bagging or Boosting, Stacked Generalization is typically applied to a space of different base learner algorithms. The idea is, that different kinds of models that are applied to the learning problem are able to capture only part of the problem. Combining models with diverging strengths in the right way then leads to improved predictive accuracy. Stacked Generalization is therefore also referred to as a second-stage model.

The Stacking algorithm involves partitioning of training dataset $D^{train} = (\mathbf{x}^{train}, y^{train})$ into $J = \{1, 2, ..., J\}$ disjoint parts $D_1^{train}, D_2^{train}, ..., D_J^{train}$. For each of these subsets D_j^{train} , called level 0 learning set, a base learner $m \in \{1, 2, ...M\}$, also referred to as level 0 generalizer, is built on behalf of the training dataset D_{-j}^{train} that does not include subset j. (Wolpert, 1992, cp.). In each iteration, the model built on D_{-j}^{train} is used to predict the target feature in subset D_j^{train} . The predictions of the J subsets are then combined again in order to obtain a prediction of the target over the whole training dataset D^{train} . Besides that, each level 0 generalizer is used to predict on the test dataset D^{test} . Due to the level 0 generalizers being built J times on different disjoint subsets of the training data, Stacked Generalization can be seen as a sophisticated form of cross-validation. The next step is building a meta learner, referred to as level 1 generalizer, that produces a prediction by using the training dataset predictions of the M level 0 generalizers as inputs.

Wolpert shows that this stacking procedure is able to reduce the bias of the base learners and thus minimizes the generalization error rate. He even recommends to use a version of Stacked Generalization in any real-world problem (Wolpert, 1992, p.2).

Different meta learning algorithms can be used for the combination of base learners. An optimal meta algorithm finds the best way to use the strengths of the base learners. Overfitting problem is especially present in Stacked Generalization models. This is due to the base learners all predicting the same target (Güneş, 2017). As a consequence, cross-validation and regularization can be used. Further more, the chosen meta learning algorithm should not be sensible to collinearity. It is therefore especially recommended to use Regularized Regression, Gradient Boosting or hill climbing methods (Güneş et al., 2017).

3 Credit Risk Assessment

Techniques of Stacking and Ensemble modelling are applied to predictive problems of a broad range of topics. This paper will especially focus on the application of Ensemble Learning in credit risk classification problems. Credit risk assessment and especially its modelling is an important part in the field of financial risk management since for most small- and medium-sized banks, interests on loans are still the primary financial source (Jacobson et al., 2006, p.2). The banking supervision accord Basel II, that was published in 2004 and applies to member states of the European Union since 2007, restricted the buffer capital on banks and therefore makes it especially important for them to estimate the riskiness of loan applicants (Basel Committee on Banking Supervision, 2004). For that, banks need to be able to distinguish between risky and non-risky applicants. Two opposing factors determine the banks' business rules regarding loans: On the one hand, more loans are better for the bank. On the other hand, a bank can not afford to make to many bad decisions, since this would eventually lead to a collapse of the bank. A good strategy on granting loans will therefore be a compromise. Minimizing the fraction of bad decisions thus increases banks' revenue.

Applying Ensemble Learning techniques to credit risk modelling has already proven to be highly valuable. Zhu et al. (2017) investigate credit risk assessment for small-and medium-sized Chinese enterprises. For that, they carry out an experiment in which they compare the predictive performance of individual machine learning methods and Ensembling methods of different complexity. They find especially the more complex ensembling methods to be of outstanding discriminative accuracy (Zhu et al., 2017, p.46f.). Yu et al. (2008) successfully apply an Ensemble learner comprising six levels of stacked Neural Networks in order to evaluate credit risk at the measurement level. Hereby, they further incorporate the Bagging approach. They conclude, that such technique "provides a promising solution to credit risk analysis" (Yu et al., 2008, p.1443).

4 Methodology

In order to evaluate and compare the introduced Stacking and Ensemble models, an empirical evaluation study is conducted. The quantlets for replication of the study can be found in the Appendix B or accessed in the corresponding github repository. In this section, the dataset used for the evaluation study is presented, the model building process is explained in detail and the metrics for evaluation are introduced.

4.1 Data description

The empirical evaluation study of this paper uses the German Credit Dataset from the UCI machine learning repository (Dheeru and Karra Taniskidou, 2017). This dataset classifies people as either being good or bad customers for a bank with respect to credit risk. It comprises a total number of 1000 observations and 20 features. Tables 2 and

3 in the Appendix present the summary statistics for the numerical and the categorical features in the original dataset, respectively. To ensure better model performance, the numerical data is standardized before model building. The dataset is partitioned into a training dataset, comprising 750 observations, and into a test dataset, comprising 250 observations.

4.2 Model building process

The model building process consists of feature selection, model training and tuning as well as prediction. For the purpose of this study, an extensive set of models went through this process: a Random Forest model and a Gradient Boosting model represent the Ensemble learners. Furthermore, both models are built a second time as level 0 generalizers for the Stacked Generalization models. Additionally, a Decision Tree, a Neural Network as well as a Logistic Regression model are built in order to provide a diverse set of level 0 generalizers for the Stacking. Four different such Stacked Generalization models are built by using different subsets of base learners' predictions and different combiner algorithms.

Before training the models, feature selection is a critical step. The aim of feature selection is dimension reduction. Building the models on an optimal subset of features may reduce their training time, reduce the variance and may make the model more easily interpretable (Guyon and Elisseeff, 2003). Since, the optimal subset of features depends on each model, a wrapper approach for feature selection is applied to each model specifically. Each model-specific wrapper approach starts with building an intercept model and sequentially adding the next best feature by using a sequential foreward selection approach. The wrapper approach stops when adding another feature cannot increase the AUC measure (see section 4.3) by at least 0.00001 units. All wrapper approaches are run on 3-fold cross-validation in order to avoid overfitting problems. Notably, a larger number of folds leads to instabilities due to the small sample size. Subsequently, the subset of features identified by the model-specific wrapper approaches is used for training of the corresponding models. Since the Random Forest and the Gradient Boosting models are built as Ensemble models as well as level 0 generalizers for the Stacked Generalization models, independent wrapper approaches are applied for both versions.

The training process for each model generally consists of establishing a broad-grid tuning of all relevant hyperparameters on the training dataset in order to find the (locally) optimal parameter choices. In order to avoid overfitting on the training dataset, each combination of hyperparameters is tested by a 3-fold cross-validation process. For the Random Forest and the Gradient Boosting model, their tuned versions can directly be used for prediction on the test dataset. For the Stacked Generalization models, the training dataset is partitioned into five disjoint subsets. Each of the five level 0 gener-

alizers is then build in five iterations as described in section 2.3. Again, each iteration involves a parameter tuning on 3-fold cross-validation. All level 0 generalizers are then used to predict the observations in the test dataset. Stacking model 1 is then built by averaging over the probabilistic predictions of all five level 0 generalizers. Stacking model 2 is constructed by averaging over the probabilistic predictions of the three best predictions of level 0 generalizers in terms of AUC measure. For that, the correlations of the level 0 generalizers on the training data must be investigated in order to avoid multicollinearity problems. Stacking model 3 is built by using again all level 0 predictions and a Gradient Boosting model as combining algorithm. Finally, Stacking model 4 is constructed by combining all level 0 predictions by using a Logistic Regression combiner. The parameters of the combining algorithms are again tuned under 3-fold cross-validation.

4.3 Evaluation metrics

In credit risk modelling, the misclassification costs are often type-specific. This means that a false negative prediction may have different costs for the bank than a false positive prediction. When misclassification costs are known, a cost-sensitive model building strategy should be consulted. Since in the context of this paper misclassification costs are however unknown, equal misclassification costs for false negative and false positive predictions are assumed. Furthermore, the broad field of cost-sensitive learning may serve as a topic for other studies. The following metrics are used to evaluate the models.

AUC: In the model building process, tuning of model parameters for each model m is evaluated on the Area Under Curve (AUC) metric. Tuning on the AUC is especially recommended when facing probabilistic predictions, since the metric generalizes over all possible cut-off thresholds that could be used to transform probabilistic into binary predictions. The AUC is a ranking indicator that measures the area under the receiver operating characteristic curve (ROC curve) (Hanley and McNeil, 1982). For a probabilistic prediction, like in the context of this study, a visualization of the ROC curve can be obtained by plotting the sensitivity against 1- specificity for all cut-off thresholds between zero and one. The AUC value can therefore take values between zero and one as well. A random model would obtain an AUC value of 0.5, which can thus function as a benchmark value in model evaluation on AUC. In a statistical sense, the AUC estimates the probability that a randomly chosen correct prediction is correctly ranked higher than a randomly chosen false prediction. For model m, the AUC can be calculated as

$$AUC^{m} = \frac{1}{P \times N} \sum_{j=1}^{P} \sum_{k=1}^{N} (\hat{y}_{j}^{m} - \hat{y}_{k}^{m})$$
 (1)

, whereby P and N denote the positive (in our case good) and negative (bad) instances amongst the outcome values in the credit data. Further, \hat{y}_j^m and \hat{y}_k^m are the predictions of model m for the positive instance y_j and the prediction for the negative instance y_k , respectively.

Accuracy: Another important metric in evaluation of classification models is the Accuracy metric, which can be interpreted as the percentage of correctly classified points. In contrast to the AUC, probabilistic predictions must be transformed into binary predictions for the Accuracy metric, which implies selecting a cut-off threshold. For the purpose of this study, a natural cut-off threshold of 0.5 is chosen.

$$Accuracy^{m} = \frac{TP^{m} + TN^{m}}{FP^{m} + FN^{m} + TP^{m} + TN^{m}}$$
(2)

, whereby TP^m is the number of true positive predictions for model m and TN^m , FP^m and FN^m are the corresponding number of true negatives, the number of false positives and the number of false negatives for model m, respectively.

Logarithmic Loss: The Logarithmic Loss is a metric for evaluating class predictions that penalizes for a high confidence about incorrect classifications. For the case of a binary outcome, the Logarithmic Loss is given by

$$LogLoss^{m} = -\frac{1}{N} \sum_{i=1}^{N} (y_{i} \times \log(p_{i}^{m}) + (1 - y_{i}) \times \log(1 - p_{i}^{m}))$$
 (3)

, whereby p_i^m is model m's prediction for observation y_i .

Brier Score: The models will further be assessed on the Brier Score, which is identical to the Mean Squared Error metric in statistics. For model m, the Brier score is defined as

Brier^m =
$$\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i^m)^2$$
 (4)

, whereby \hat{y}_i^m denotes the predicted probability of model m for observation y_i .

5 Results

In the following, the results of the empirical application of Stacking and Ensemble models on a credit risk classification problem will be presented. Table 1 shows the evaluations of all models on the test dataset with respect to the metrics AUC, Accuracy, Logarithmic Loss and Brier Score.

	AUC	Accuracy	LogLoss	Brier
Ensemble model: Random Forest	0.78	0.73	0.52	0.18
Ensemble model: Gradient Boosting	0.78	0.72	0.52	0.18
Level 0 generalizer: Decision Tree	0.69	0.65	0.60	0.21
Level 0 generalizer: Logit Regression	0.71	0.74	0.57	0.19
Level 0 generalizer: Neural Network	0.76	0.74	0.53	0.18
Level 0 generalizer: Random Forest	0.73	0.69	0.56	0.19
Level 0 generalizer: Gradient Boosting	0.80	0.74	0.52	0.17
Stacking model 1: Average, all predictions	0.77	0.64	0.24	0.18
Stacking model 2 Average, best predictions	0.77	0.63	0.25	0.18
Stacking model 3: GB, all predictions	0.78	0.61	0.29	0.17
Stacking model 4: LR, all predictions	0.81	0.64	0.30	0.16

Table 1: Model performances on the test dataset. Values rounded on two digits after comma. Abbreviations GB and LR denote Gradient Boosting and Logistic Regression that are used as combiner algorithms.

Since all models were tuned on the AUC metric, the comparison on behalf of this metric is most informative. The two Ensemble models, namely the Random Forest and the Gradient Boosting model, score highly on the AUC metric with a value of 0.78. In terms of AUC, they even outperform most level 0 generalizers, especially the Decision Tree and the Logistic Regression. It can be concluded that they rank a randomly chosen correct prediction comparatively comparatively higher than a randomly chosen false prediction in comparison with the level 0 generalizers. Notably, the Gradient Boosting level 0 generalizer and the Random Forest level 0 generalizer perform a bit different when compared to their counterparts. This may origin from the decreased size of training dataset due to the partitioning that was applied for building the level 0 generalizers.

The four Stacking models were built on top of the level 0 generalizers. Figure 1 shows the correlations of the predictions of the level 0 generalizers on the training data. It can be seen that the predictions of the level 0 generalizers are (mostly) correlated positively, which seems intuitive since they all predict the target in the similar context. However, correlations are not perfect (all < |0.9|). This reveals diversity of predictions, which already indicates that combining them may increase predictive performance.

Indeed, Table 1 reveals that the four Stacking models clearly outperform their level 0 generalizers in terms of AUC. Stacking models 1, 2 and 3 that are based on averaging predictions as well as a Gradient Boosting combiner have similar high AUC performance than the Random Forest and the Gradient Boosting model. Stacking model 4 that is based on combining level 0 predictions by Logistic Regression even shows a better AUC performance than the Random Forest and the Gradient Boosting model. For visual comparison, Figure 2 shows the ROC curves related to the AUC values for all models.

With regards to the Accuracy, the Logistic Regression and the Neural Network per-

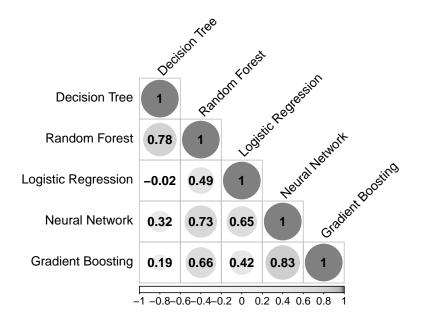


Figure 1: Correlation plot of training dataset predictions of level 0 generalizers.

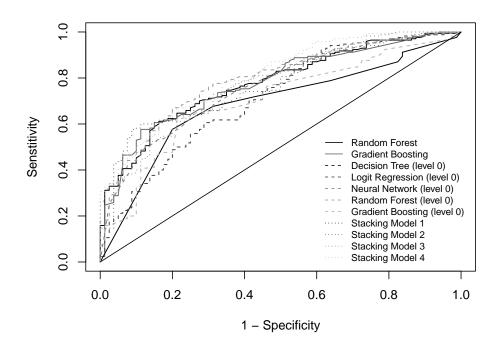


Figure 2: Receiver Operating Characteristic (ROC) curves for all models.

form about equally well as the two Ensemble models. The Decision Tree is however outperformed by the Random Forest and the Gradient Boosting model. Interestingly, all four Stacking models show relatively bad values on the Accuracy metric. Regarding the relation of Accuracy and AUC, it can be concluded that the Stacking and Ensemble models do not necessarily perform better on the cut-off threshold of 0.5, which is implied by the Accuracy metric. However, generalizing over all possible cut-off threshold they clearly outperform most level 0 generalizers as can be seen by the corresponding AUC values and the corresponding ROC curves in Figure 2. Furthermore, this indicates that the standard cut-off threshold for probabilistic predictions of 0.5 may not be optimal for those models.

The Logarithmic Loss metric gives even more information on the particular strengths and weaknesses of the models. Contrasting the level 0 generalizers with the Random Forest and the Gradient Boosting model, the latter show a slightly smaller Logarithmic Loss. The four Stacking models however, reveal a much better performance on behalf of the Logarithmic Loss metric. It can be concluded, that the Ensemble models and even more the Stacking models do not place as high confidences on their incorrect predictions.

Regarding the Brier Score, differences are not that present. In tendency, the Stacking and Ensemble Models perform slightly better on that metric than the level 0 generalizers. One time more, this shows that in binary classification a good model is not only defined by its errors but rather by which observations it is able to classify correctly.

With regards to all calculated metrics, Stacking models are be able to capture the structure in the data most effective. Already a simple averaging approach, as applied for Stacking models 1 and 2, leads to increased performance when compared to the level 0 models. Interestingly, reducing the set of level 0 generalizers, like for Stacking model 2, does not add more value. Nevertheless, it shall be noted that such restriction of input predictions could still decrease computational costs. Applying a more sophisticated level 1 combiner, like Gradient Boosting or Logistic Regression, furthermore improves prediction. In particular, the Logistic Regression combiner is able to increase AUC performance.

6 Conclusion

This paper aimed to discuss and evaluate Stacking and Ensemble models in a financial application of credit risk assessment. Focus was set on introducing the concepts of Bagging, Boosting and Stacked Generalization as well as the corresponding Random Forest and Gradient Boosting models. In depth, it was explained how Bagging and Boosting aim at increasing performance by decreasing generalization variance of base learners and by decreasing generalization bias of base learners, respectively. Moreover, the Stacked Generalization model was outlined, that seeks for the optimal way to combine the specific

strengths of level 0 generalizers in order to increase predictive performance even more.

A broad set of different Stacking and Ensemble models as well as standard machine learning models was applied and evaluated to a classification problem of credit risk assessment. Thereby, the Random Forest model and Gradient Boosting model outperformed standard machine learning models on behalf of the calculated metrics. Furthermore, all four Stacked Generalization approaches were able to establish a better performance on AUC, Logarithmic Loss and Brier Score than their level 0 generalizers. With regards to Accuracy metric, they performed worse, suggesting that the metric-implied cut-off threshold of 0.5 being suboptimal. Even a simple combiner algorithm like averaging could increase performance of the Stacking model, while the Logistic Regression combiner performed best. Restricting the subset of input predictions seems to be ineffective with regards to performance issues. To conclude, Stacking and Ensemble models could show their comparative strengths in this study. The results strongly confirm their value for prediction issues in credit risk assessment.

While this study focused on predicting binary outcomes, further research could evaluate the performance of Stacking and Ensemble models for regression problems in a similar context. A shortfall of Stacking and Ensemble models is their need of much computational resources caused by their complexity. In the context of *scalability*, current research tests ideas that restrict computational costs, e.g. by adaptive parallelization (Li et al., 2014) or by improving intra-model algorithms like stochastic gradient descent (Bottou, 2012). A further problem of such models is the absence of proven statistical properties like unbiasedness, consistency or asymptotic theory for construction of confidence intervals. In order to use machine learning models for research purposes, such properties are however necessary. Only recently, the field of *machine learning in economics* emerged, where the development of such properties is aimed at (see Athey (2017), Wager and Athey (in press)). Developments in this field of research will also enable better application of machine learning models to financial research problems.

A Appendix - Summary Tables

	Mean	Std. Dev.	Median	Minimum	Maximum
Duration	20.90	12.06	18.00	4.00	72.00
Amount	3271.26	2822.74	2319.50	250.00	18424.00
Installment Rate	2.97	1.12	3.00	1.00	4.00
Residence Duration	2.85	1.10	3.00	1.00	4.00
Age	35.55	11.38	33.00	19.00	75.00
Number of Credits	1.41	0.58	1.00	1.00	4.00
Number of Liable People	1.16	0.36	1.00	1.00	2.00

Table 2: Summary statistics for numerical features in the German Credit Dataset.

Feature	Category	Count	Fraction
Customer Classification	good	700	70%
(Outcome Feature)	bad	300	30%
Account Status	x < 0 DM	274	27.4%
	$0~\mathrm{DM} < x < 200~\mathrm{DM}$	269	26.9%
	x >= 200 DM	63	6.3%
	no account	394	39.4%
Credit History	no credits taken/all paid back duly	40	4%
	all credits at this bank paid back duly	49	4.9%
	existing credits paid back duly till now	530	53%
	delay in paying off in the past	88	8.8%
	critical account	293	29.3%
Purpose	car (new)	234	23.4%
	car(used	103	10.3%
	furniture/equipment	12	1.2%
	radio/television	181	18.1%
	domestic appliances	280	28%
	repairs	12	1.2%
	education	22	2.2%
	vacation	50	5%
	retraining	9	0.9%
	business	97	9.7%
Savings	x < 100 DM	603	60.3%
	100 <= x < 500 DM	103	10.3%
	$500 \le x \le 1000 \text{ DM}$	63	6.3%
	x > = 1000 DM	48	4.8%
	unknown/no savings	183	18.3%

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Feature	Category	Count	Fraction
Employment Duration	unemployed	62	6.2%
	x < 1 year	172	17.2%
	$1 \le x \le 4 \text{ years}$	339	33.9%
	$4 \le x < 7 \text{ years}$	174	17.4%
	x >= 7 years	253	25.3%
Status and Sex	male: divorced/separated	50	5%
	female: divorced/separated/married	310	31%
	male: single	548	54.8%
	male: married/widowed	92	9.2%
Other Debtors	none	907	90.7%
	co-applicant	41	4.1%
	guarantor	52	5.2%
Property	real estate	282	28.2%
	savings agreement/life insurance	232	23.2%
	car or other	332	33.2%
	unknown/no property	154	15.4%
Other Installment Plans	bank	139	13.9%
	stores	47	4.7%
	none	814	81.4%
Housing	rent	179	17.9%
	own	713	71.3%
	for free	108	10.8%
Job	unemployed/ unskilled - non-resident	22	2.2%
	unskilled - resident	200	20%
	skilled employee / official	630	63%
	management/self-employed/officer	148	14.8%
Telephone	none	596	59.6%
	yes	404	40.4%
Foreign Worker	yes	963	96.3%
-	no	37	3.7%

 Table 3: Summary statistics for categorical features in the German Credit Dataset.

B Appendix - Code

1: Main file

```
# Numerical Introductory Course 2018
2
   # Topic: Stacking and Ensemble Modelling
   # Supervisor: Prof. Dr. Brenda L\'opez Cabrera
   # Student: Frederik Schreck
   8
10
   # Prepare environment
11
12
   # Install packages and set working directory to path of main.R file
13
   library("rstudioapi")
14
   setwd(dirname(rstudioapi::getActiveDocumentContext()$path))
15
16
   library("plyr")
17
  library("mlr")
18
   library("parallelMap")
19
   library("parallel")
20
   library("ggplot2")
21
   library("corrplot")
22
   library("glmnet")
23
   library("xtable")
24
   library("caret")
25
  library("caretEnsemble")
  library("gbm")
  library("ROCR")
28
29
   rm(list = ls(all = TRUE))
30
   graphics.off()
31
32
33
34
   # Loading dataset: German Credit Data
35
36
37
                     <- read.delim("dataset/german_credit_data.txt",</pre>
   creditdata
                                    header = FALSE, sep = " ")
39
40
   # Renaming of feature
41
   colnames(creditdata) <- c("account_status", "duration",</pre>
42
                             "credit_history", "purpose", "amount",
43
                             "savings", "employment_duration",
44
                             "installment_rate", "status_sex",
45
                            "other_debtors", "residence_duration",
46
                            "property", "age", "installment_plans",
47
48
                            "housing", "number_credits", "job",
49
                            "liable_people", "telephone",
                            "foreign_worker", "customer")
50
```

```
51
52
53
    # Feature Engineering
54
                            _____
55
56
    # Formatting and labelling
57
    creditdata $ duration
                                    <- as.numeric(creditdata$duration)</pre>
58
    creditdata $ amount
                                    <- as.numeric(creditdata$amount)</pre>
59
    creditdata$installment_rate <- as.numeric(creditdata$installment_rate)</pre>
    creditdata$residence_duration <- as.numeric(creditdata$residence_duration)</pre>
61
    creditdata$age
                                    <- as.numeric(creditdata$age)</pre>
62
    creditdata$number_credits
                                    <- as.numeric(creditdata$number_credits)</pre>
63
                                    <- as.numeric(creditdata$duration)</pre>
    creditdata$duration
64
    creditdata$liable_people
65
                                    <- as.numeric(creditdata$liable_people)</pre>
66
    creditdata$customer
                                    <- factor(creditdata$customer,</pre>
67
                                               levels = c(1, 2),
                                               labels = c("good", "bad"))
68
69
    # No problem of missing values
70
    apply(creditdata, 2, function(x) sum(is.na(x)))
71
72
73
    # Create summary tables for numeric and for categorical features
    numeric_vars <- lapply(Filter(is.numeric, creditdata),</pre>
74
                            function(x) rbind(mean = mean(x),
75
76
                                                sd = sd(x),
                                                median = median(x),
77
                                                minimum = min(x),
78
                                                maximum = max(x))
79
80
    print(xtable(t(data.frame(numeric_vars))),
81
         file="tables/summary_numeric.txt")
82
83
    cat_vars <- ldply(Filter(is.factor, creditdata),</pre>
84
                       function(x) t(rbind(names(table(x)),
85
86
                                             table(x),
87
                                             paste0(prop.table(table(x))*100,"%"))))
88
    colnames(cat_vars) <- c("feature", "category", "Count", "Fraction")</pre>
    print(xtable(data.frame(cat_vars)),
89
          file="tables/summary_categorical.txt")
90
91
    # Standardize numeric features for models performance
92
    creditdata$duration
                            <- scale(creditdata$duration)</pre>
    creditdata $ amount
                                   <- scale(creditdata$amount)</pre>
94
    creditdata$installment_rate <- scale(creditdata$installment_rate)</pre>
95
    creditdata$residence_duration <- scale(creditdata$residence_duration)</pre>
96
                                    <- scale(creditdata$age)</pre>
97
    creditdata$age
    creditdata$number_credits
                                    <- scale(creditdata$number_credits)</pre>
98
    creditdata$duration
                                    <- scale(creditdata$duration)</pre>
99
    creditdata$liable_people
                                   <- scale(creditdata$liable_people)</pre>
100
101
102
103
104
    # Data partitioning into training and testing data
105
106
107
    set.seed(2601)
```

```
idx <- sample(x = NROW(creditdata),</pre>
108
109
                   size = floor(0.75*NROW(creditdata)),
                   replace = FALSE)
110
    train <- creditdata[idx,]</pre>
111
    test <- creditdata[-idx,]</pre>
112
113
114
115
116
    # Feature Selection
117
                     ______
118
    'For each model, a wrapper approach is run on the training dataset
119
   in order to find the best subset of features. The optimal set of
120
    features is the then used in the subsequent model building part.
121
122
123
    The wrappers as well as the model tuning are evaluated on the AUC
124
    measure. Tuning of the hyperparameters in the wrapper is done by
    a grid-approach with 3-fold cross-validation process.
125
126
    For reproduction of the results, the output of the wrapper
127
    files can be accessed directly.'
128
129
130
    # Generate empty lists to store the models and their results in
             <- list() # Selected set of features used for each model
131
    model_lib <- list() # Model library</pre>
132
    yhat
              <- list() # Predictions on test dataset
133
134
135
    136
137
    source("gb_wrapper.R")
138
    # For replication purposes: gb_wrapper results
139
    train_wrapper <- mlr::createDummyFeatures(train, target = "customer")</pre>
140
               <- c("customer", "account_status.A11",
    vars$gb
141
                      "account_status.A14", "credit_history.A30",
142
                      "credit_history.A34", "purpose.A49", "savings.A63",
143
144
                      "savings.A65", "employment_duration.A75",
145
                      "other_debtors.A103", "property.A123",
                      "installment_plans.A143", "job.A174",
146
                      "telephone.A192")
147
148
149
    150
    source("rf_wrapper.R")
151
152
    # For replication purposes: rf_wrapper results
153
              <- c("customer", "account_status", "duration",
154
    vars$rf
                     "credit_history", "purpose", "savings",
155
                     "employment_duration", "other_debtors",
156
                     "residence_duration", "age", "installment_plans",
157
                     "housing", "job", "liable_people", "foreign_worker")
158
159
160
161
   'For the Stacked Generalization model, firstly the training data is
162
split into five disjoint sets. Secondly, the Random Forest model and
164 the Gradient Boosting model are rebuilt on that subset. For each
```

```
model, a new wrapper approach is applied to find the optimal subset
165
166
   of features.
167
   Additionally, a Decision Tree, a Logistic Regression and a
168
   Neural Network are built. Similar to the models before, a
169
   model-specific wrapper approach is applied before the model
170
   building process.
171
172
   For reproduction of the results, the output of the wrapper
173
174
   functions can again be accessed directly.
175
176
   177
   source("dt_wrapper.R")
178
179
180
   # For replication purposes: dt_wrapper results
181
   vars$dt <- c("customer", "account_status", "credit_history",</pre>
                    "savings", "number credits")
182
183
   184
   source("logit_wrapper.R")
185
186
187
   # For replication purposes: logit_wrapper results
   vars$logit
              <- c("customer", "duration", "credit_history",</pre>
188
                    "purpose", "amount", "installment_rate",
189
                    "status_sex", "residence_duration", "age",
190
                    "installment_plans", "number_credits",
191
                    "liable_people", "telephone", "foreign_worker")
192
193
   194
195
   source("nnet_wrapper.R")
196
   # For replication purposes: nnet_wrapper results
197
   vars$nnet <- c("customer", "account_status", "credit_history")</pre>
198
199
   200
201
   source("gb_wrapper_stacking.R")
202
   # For replication purposes: gb_wrapper results
203
   vars$gb2 <- c("customer", "account_status.A11",</pre>
204
                    "account_status.A14", "credit_history.A34",
205
                    "purpose.A41", "savings.A65",
206
207
                    "employment_duration.A74", "status_sex.A94",
                    "other_debtors.A103", "installment_plans.A143")
208
209
   210
   source("rf_wrapper_stacking.R")
211
212
   # For replication purposes: rf_wrapper results
213
             <- c("customer", "account_status", "duration",</pre>
214
                    "credit_history", "purpose", "savings",
215
                    "employment_duration", "other_debtors",
216
217
                    "residence_duration", "age",
218
                    "installment_plans", "housing", "job",
219
                    "liable_people", "foreign_worker")
220
221
```

```
#-----
222
223
  # Model Building
224
225
226
  'In the following, the models are built, parameters are tuned and
  predictions on the test dataset are made. Each model uses the
227
  optimal subset of features from the corresponding wrapper approach.'
228
229
  230
^{231}
  source("rf_model.R")
232
233
  234
  source("gb_model.R")
235
236
237
238
  239
  # Partitioning the dataset for the Stacking into five equally
240
  # sized disjoint sets
241
  set.seed(2610)
242
  idx2 <- sample(rep(1:5, each = nrow(train)/5))</pre>
243
  train_sets <- lapply(split(1:nrow(train), idx2),</pre>
244
               function(i) creditdata[i,])
245
246
247
  source("dt_model.R")
248
249
250
  251
252
  # No tuning necessary
253
  source("logit_model.R")
254
255
  256
  source("nnet_model.R")
257
258
  260
  source("gb_model_stacking.R")
261
262
263
  264
  source("rf_model_stacking.R")
265
266
267
  268
  source("st_model.R")
269
270
271
272
273
  # Model evaluation
274
  #-----
275
276
  'After having built all the models, they can now be compared and
  evaluated with regard to a variety of evaluation metrics.'
277
278
```

```
# Create empty lists to store the measure values in
279
280
    auc
                <- list() # Area under curve performance measure
                <- list() # Accuracy performance measure
281
    acc
                <- list() # Kappa performance measure
282
    kappa
    logloss
                <- list() # Logarithmic Loss measure
283
                <- list() # Brier score measure
    brier
284
285
    # AUC
286
287
    auc$rf
                <- mlr::performance(yhat$rf,</pre>
288
                                       measures = mlr::auc); auc$rf
289
    auc$gb
                <- mlr::performance(yhat$gb,</pre>
                                      measures = mlr::auc); auc$gb
290
    auc$dt
                <- mlr::performance(yhat$dt_test,</pre>
291
                                      measures = mlr::auc); auc$dt
292
293
    auc$logit <- mlr::performance(yhat$logit_test,</pre>
294
                                       measures = mlr::auc); auc$logit
295
    auc$nnet
                <- mlr::performance(yhat$nnet_test,</pre>
                                      measures = mlr::auc); auc$nnet
296
                <- mlr::performance(yhat$gb2_test,</pre>
    auc$gb2
297
298
                                      measures = mlr::auc); auc$gb2
    auc$rf2
                 <- mlr::performance(yhat$rf2_test,</pre>
299
300
                                      measures = mlr::auc); auc$rf2
301
    auc$st1
                 <- measureAUC(probabilities = yhat$st1$prob.good,</pre>
                             truth = yhat$st1$truth, positive = "1",
302
                             negative = "2"); auc$st1
303
304
    auc$st2
                 <- measureAUC(probabilities = yhat$st2$prob.good,</pre>
                             truth = yhat$st2$truth, positive = "1",
305
                             negative = "2"); auc$st2
306
                 <- measureAUC(probabilities = yhat$st3[,3],</pre>
    auc$st3
307
308
                                truth = yhat$st3[,2], positive = "1",
309
                                negative = "2"); auc$st3
310
    auc$st4
                 <- measureAUC(probabilities = yhat$st4[,3],</pre>
311
                                truth = yhat$st4[,2], positive = "1",
                                negative = "2"); auc$st4
312
313
314
    # Accuracy
315
    acc$rf
                <- mlr::performance(yhat$rf,</pre>
316
                                       measures = mlr::acc); acc$rf
                <- mlr::performance(yhat$gb,</pre>
317
    acc$gb
                                      measures = mlr::acc); acc$gb
318
                <- mlr::performance(yhat$dt_test,
    acc$dt
319
                                      measures = mlr::acc); acc$dt
320
    acc$logit
                <- mlr::performance(yhat$logit_test,</pre>
321
322
                                      measures = mlr::acc); acc$logit
323
    acc$nnet
                <- mlr::performance(yhat$nnet_test,</pre>
                                      measures = mlr::acc); acc$nnet
324
325
    acc$gb2
                 <- mlr::performance(yhat$gb2_test,</pre>
                                       measures = mlr::acc); acc$gb2
326
327
    acc$rf2
                 <- mlr::performance(yhat$rf2_test,</pre>
                                      measures = mlr::acc); acc$rf2
328
                 <- measureACC(response = round(yhat$st1$prob.good),</pre>
329
    acc$st1
                                truth = yhat$st1$truth); acc$st1
330
331
    acc$st2
                 <- measureACC(response = round(yhat$st2$prob.good),</pre>
332
                                truth = yhat$st2$truth); acc$st2
333
    acc$st3
                <- measureACC(response = round(yhat$st3[,3]),</pre>
                                truth = yhat$st3[,2]); acc$st3
334
    acc$st4 <- measureACC(response = round(yhat$st4[,3]),</pre>
335
```

```
truth = yhat$st4[,2]); acc$st4
336
337
    # Logarithmic Loss
338
                    <- mlr::performance(yhat$rf,</pre>
339
    logloss$rf
                                          measures = mlr::logloss)
340
341
    logloss$rf
    logloss$gb
                    <- mlr::performance(yhat$gb,</pre>
342
                                          measures = mlr::logloss)
343
344
    logloss$gb
345
    logloss$dt
                    <- mlr::performance(yhat$dt_test,</pre>
346
                                          measures = mlr::logloss)
    logloss$dt
347
    logloss$logit <- mlr::performance(yhat$logit_test,</pre>
348
                                          measures = mlr::logloss)
349
350
    logloss$logit
351
    logloss$nnet <- mlr::performance(yhat$nnet_test,</pre>
352
                                          measures = mlr::logloss)
    logloss$nnet
353
                   <- mlr::performance(yhat$gb2_test,
    logloss$gb2
354
355
                                          measures = mlr::logloss)
    logloss$gb2
356
    logloss$rf2
                    <- mlr::performance(yhat$rf2_test,</pre>
357
358
                                          measures = mlr::logloss)
    logloss$rf2
359
    log_loss=function(actual, predicted)
360
361
      result=-1/length(actual)*
362
363
         (sum((actual*log(predicted)+
                  (1-actual)*log(1-predicted))))
364
365
      return(result)
366
    }
367
    logloss$st1
                   <- log_loss(yhat$st1$truth, yhat$st1$prob.good)</pre>
368
    logloss$st1
    logloss$st2
                   <- log_loss(yhat$st2$truth, yhat$st2$prob.good)</pre>
369
    logloss$st2
370
                   <- log_loss(yhat$st3[,2], yhat$st3[,3])</pre>
371
    logloss$st3
372
    logloss$st3
373
    logloss$st4
                    <- log_loss(yhat$st4[,2], yhat$st4[,3])</pre>
    logloss$st4
374
375
    # MSE/Brier score
376
377
    brier$rf
                 <- mlr::performance(yhat$rf,</pre>
                                          measures = mlr::brier); brier$rf
378
379
    brier$gb
                   <- mlr::performance(yhat$gb,</pre>
                                          measures = mlr::brier); brier$gb
380
    brier$dt
                    <- mlr::performance(yhat$dt_test,</pre>
381
382
                                          measures = mlr::brier); brier$dt
    brier$logit
                    <- mlr::performance(yhat$logit_test,</pre>
383
                                          measures = mlr::brier); brier$logit
384
    brier$nnet
                    <- mlr::performance(yhat$nnet_test,</pre>
385
386
                                          measures = mlr::brier); brier$nnet
                    <- mlr::performance(yhat$gb2_test,</pre>
387
    brier$gb2
388
                                          measures = mlr::brier); brier$gb2
389
    brier$rf2
                    <- mlr::performance(yhat$rf2_test,</pre>
390
                                          measures = mlr::brier); brier$rf2
                    <- measureBrier(probabilities = yhat$st1$prob.good,</pre>
    brier$st1
391
                                    truth = yhat$st1$truth,
392
```

```
positive = 1, negative = 2); brier$st1
393
    brier$st2
                   <- measureBrier(probabilities = yhat$st2$prob.good,</pre>
394
                                     truth = yhat$st2$truth, positive = 1,
395
                                     negative = 2); brier$st2
396
397
    brier$st3
                   <- measureBrier(probabilities = yhat$st3[,3],</pre>
398
                                     truth = yhat$st3[,2], positive =1,
                                     negative = 2); brier$st3
399
    brier$st4
                   <- measureBrier(probabilities = yhat$st4[,3],</pre>
400
401
                                     truth = yhat$st4[,2], positive = 1,
402
                                     negative = 2); brier$st4
403
    # Make evaluation table
404
    eval table
                           <- cbind(auc, acc, logloss, brier)
405
    rownames(eval_table) <- c("Random Forest", "Gradient Boosting",</pre>
406
407
                                "Decision Tree (level 0)",
                                "Logit Regression (level 0)",
408
409
                                "Neural Network (level 0)",
                                "Random Forest (level 0)",
410
                                "Gradient Boosting (level 0)",
411
                                "Stacking Model 1", "Stacking Model 2",
412
                                "Stacking Model 3", "Stacking Model 4")
413
    colnames(eval_table) <- c("AUC", "Accuracy",</pre>
414
                                "Logarithmic Loss", "Brier Score")
415
416
417
418
    print(xtable(eval_table), file="tables/evaltable.txt")
419
    # Generate plot with AUC curves for all models
420
    plot(performance(prediction(yhat$rf$data$prob.good,
421
                                  labels = matrix(test$customer,
422
423
                                                    nrow = NROW(test$customer),
424
                                                    ncol = 1))
                       , "tpr", "fpr"),
425
          colorize = FALSE, col = "gray0", type = "1",
426
         lty = 1, lwd = 1.2,
427
          xlab="1 - Specificity", ylab="Senstitivity")
428
429
430
    plot(performance(prediction(yhat$gb$data$prob.good,
                                  labels = matrix(test$customer,
431
                                                    nrow = NROW(test$customer),
432
                                                    ncol = 1))
433
434
                       , "tpr", "fpr"),
          colorize = FALSE, add = TRUE, col = "gray40",
435
          type = "1", 1ty = 1, 1wd = 1.2)
436
437
    plot(performance(prediction(yhat$dt_test$data$prob.good,
438
                                   labels = matrix(test$customer,
439
                                                    nrow = NROW(test$customer),
440
441
                                                    ncol = 1))
                       , "tpr", "fpr"),
442
          colorize = FALSE, add = TRUE, col = "gray0",
443
444
          type = "1", lty = 1, lwd = 1.2)
445
446
    plot(performance(prediction(yhat$logit_test$data$prob.good,
447
                                  labels = matrix(test$customer,
                                                    nrow = NROW(test$customer),
448
                                                    ncol = 1)
449
```

```
, "tpr", "fpr"),
450
          colorize = FALSE, add = TRUE, col = "gray25",
451
          type = "1", lty = 2, lwd = 1.2)
452
453
454
    plot(performance(prediction(yhat$nnet_test$data$prob.good,
                                  labels = matrix(test$customer,
455
                                                    nrow = NROW(test$customer),
456
                                                    ncol = 1))
457
                       , "tpr", "fpr"),
458
459
          colorize = FALSE, add = TRUE, col = "gray50",
          type = "1", lty = 2, lwd = 1.2)
460
461
    plot(performance(prediction(yhat$rf2_test$data$prob.good,
462
                                  labels = matrix(test$customer,
463
464
                                                    nrow = NROW(test$customer),
465
                                                    ncol = 1))
466
                       , "tpr", "fpr"),
          colorize = FALSE, add = TRUE, col = "gray60",
467
          type = "1", 1ty = 2, 1wd = 1.2)
468
469
    plot(performance(prediction(yhat$gb2_test$data$prob.good,
470
                                  labels = matrix(test$customer,
471
472
                                                   nrow = NROW(test$customer),
                                                    ncol = 1))
473
                       , "tpr", "fpr"),
474
475
          colorize = FALSE, add = TRUE, col = "gray70",
          type = "1", lty =2, lwd = 1.2)
476
477
    plot(performance(prediction(yhat$st1$prob.good,
478
479
                                  labels = matrix(test$customer,
480
                                                   nrow = NROW(test$customer),
481
                                                   ncol = 1))
                       , "tpr", "fpr"),
482
          colorize = FALSE, add = TRUE, col = "gra0",
483
          type = "1", 1ty = 3, 1wd = 1.2)
484
485
486
    plot(performance(prediction(yhat$st2$prob.good,
487
                                  labels = matrix(test$customer,
                                                   nrow = NROW(test$customer),
488
                                                   ncol = 1))
489
                       , "tpr", "fpr"),
490
491
          colorize = FALSE, add = TRUE, col = "gray25",
          type = "1", lty = 3, lwd = 1.2)
492
493
    plot(performance(prediction(yhat$st3[,3],
494
                                  labels = matrix(test$customer,
495
                                                    nrow = NROW(test$customer),
496
                                                    ncol = 1))
497
                       , "tpr", "fpr"),
498
          colorize = FALSE, add = TRUE, col = "gray50",
499
500
          type = "1", lty = 3, lwd = 1.22)
501
502
    plot(performance(prediction(yhat$st4[,3],
503
                                  labels = matrix(test$customer,
504
                                                   nrow = NROW(test$customer),
                                                    ncol = 1))
505
                      , "tpr", "fpr"),
506
```

```
colorize = FALSE, add = TRUE, col = "gray75",
507
508
          type = "1", 1ty = 3, 1wd = 1.2)
509
    lines(x = c(0,1), y = c(0,1))
510
511
    legend(xy.coords(0.6,0.57), legend = c("Random Forest",
512
                                               "Gradient Boosting",
513
                                               "Decision Tree (level 0)",
514
                                               "Logit Regression (level 0)",
515
516
                                               "Neural Network (level 0)",
                                               "Random Forest (level 0)",
517
                                               "Gradient Boosting (level 0)",
518
                                               "Stacking Model 1",
519
                                               "Stacking Model 2",
520
                                               "Stacking Model 3",
521
522
                                               "Stacking Model 4"),
523
           lty= c(1,1,2,2,2,2,2,3,3,3,3), cex=0.75, col=c("gray0", "gray40",
                                                              "gray0", "gray25",
524
                                                              "gray50", "gray60",
525
                                                              "gray70", "gray0",
526
527
                                                              "gray25", "gray50",
                                                              "gray75"),
528
529
           box.lty=0)
```

2: Gradient Boosting Model Feature Selection

```
##### Variable selection for the Gradient Boosting model. A wrapper approach #####
2
   # A model building approach with sequential forward selection is
   # established in order to find the best subset of features.
   # Each model is built with crossvalidation on the AUC measure.
6
   set.seed(2610)
7
   # One-hot-encoding of categorical features
   train_wrapper
                   <- mlr::createDummyFeatures(train,</pre>
10
                                                     target = "customer")
11
12
13
   gb_task_wrapper
                       <- makeClassifTask(data = train_wrapper,</pre>
                                           target = "customer",
14
                                           positive = "good")
15
16
   gb_learner_wrapper<- makeLearner("classif.xgboost",</pre>
17
                                       predict.type = "prob")
18
19
   gb_ctrl_wrapper <- makeFeatSelControlSequential(method = "sfs",</pre>
21
                                                         alpha = 0.00001)
22
   gb_rdesc_wrapper <- makeResampleDesc("CV", iters = 3)</pre>
23
24
                       <- selectFeatures(learner = gb_learner_wrapper,</pre>
25
   gb_sfeats
26
                                          task = gb_task_wrapper,
27
                                          resampling = gb_rdesc_wrapper,
                                          control = gb_ctrl_wrapper,
28
```

```
show.info = TRUE,
29
                                         measures = mlr::auc)
30
31
   # Performance score for each combination of features
32
   analyzeFeatSelResult(gb_sfeats)
33
34
   # Next, I define the dataset to use for the gradient
35
   # boosting model. This dataset is then used in the model
36
   # building file "gb_model.R"
37
   vars$gb <- c("customer", gb_sfeats$x)</pre>
```

3: Random Forest Model Feature Selection

```
##### Feature selection for the Random Forest model. A wrapper approach #####
2
   # A model building approach with sequential forward selection is established in order
3
   # to find the best subset of features. Each model is built with crossvalidation on
   # the AUC measure.
   set.seed(2610)
                        <- makeClassifTask(data = train,</pre>
9
   rf_task_wrapper
                                            target = "customer",
10
                                             positive = "good")
11
12
   rf_learner_wrapper <- makeLearner("classif.randomForest",</pre>
13
                                        predict.type = "prob",
14
                                         "ntree" = 300)
15
16
                        <- makeFeatSelControlSequential(method = "sfs",</pre>
17
   rf_ctrl_wrapper
                                                           alpha = 0.00001)
18
19
20
   rf_rdesc_wrapper
                        <- makeResampleDesc("CV", iters = 3)</pre>
21
   rf_sfeats
                         <- selectFeatures(learner = rf_learner_wrapper,</pre>
22
23
                                            task = rf_task_wrapper,
                                            resampling = rf_rdesc_wrapper,
24
                                            control = rf_ctrl_wrapper,
25
26
                                            show.info = TRUE,
27
                                            measures = mlr::auc)
28
   # Performance score for each combination
29
   analyzeFeatSelResult(rf_sfeats)
30
31
   # Next, I define the dataset to use for the gradient boosting model.
32
   # This dataset is then used in the model building file "rf_model.R"
   vars$rf <- c("customer", rf_sfeats$x)</pre>
```

4: Stacking: Decision Tree (level 0) Feature Selection

```
##### Feature selection for the Decision Tree model. A wrapper approach #####
1
2
   \# A model building approach with sequential forward selection is
3
   # established in order to find the best subset of features.
4
   \mbox{\tt\#} Each model is built with crossvalidation on the AUC measure.
7
   set.seed(2610)
                     <- makeClassifTask(data = train, target = "customer",</pre>
9
   dt_task_wrapper
10
                                              positive = "good")
11
   dt_learner_wrapper <- makeLearner("classif.rpart",</pre>
12
                                         predict.type = "prob")
13
14
15
   \# We set the minimum required difference to 0.0001 Euros in expected loss
16
   # per observation
                        <- makeFeatSelControlSequential(method = "sfs",</pre>
17
   dt_ctrl_wrapper
                                                            alpha = 0.00001)
18
19
                        <- makeResampleDesc("CV", iters = 3)</pre>
20
   dt_rdesc_wrapper
21
22
   dt_sfeats
                        <- selectFeatures(learner = dt_learner_wrapper,</pre>
23
                                            task = dt_task_wrapper,
                                            resampling = dt_rdesc_wrapper,
24
                                             control = dt_ctrl_wrapper,
25
26
                                             show.info = TRUE,
27
                                             measures = mlr::auc)
28
29
   # Performance score for each combination of features
   analyzeFeatSelResult(dt_sfeats)
30
31
   \mbox{\tt\#} Next, I store the optimal set of features to later use it
32
   # in the model building part file "dt_model.R"
33
   vars$dt <- c("customer", dt_sfeats$x)</pre>
34
```

5: Logistic Regression (level 0) Feature Selection

```
##### Feature selection for the Logit model. A wrapper approach #####
1
2
   # A model building approach with sequential forward selection is
   # established in order to find the best subset of features.
   # Each model is built with crossvalidation on
   # the AUC measure.
6
7
   set.seed(2610)
   logit_task_wrapper <- makeClassifTask(data = train[, -1], target = "customer",</pre>
10
                                              positive = "good")
11
12
   logit_learner_wrapper <- makeLearner("classif.logreg",</pre>
13
                                         predict.type = "prob")
14
15
16 | logit_ctrl_wrapper <- makeFeatSelControlSequential(method = "sfs",
```

```
alpha = 0.00001)
17
18
   logit_rdesc_wrapper <- makeResampleDesc("CV", iters = 3)</pre>
19
20
21
   logit_sfeats
                           <- selectFeatures(learner = logit_learner_wrapper,</pre>
22
                                              task = logit_task_wrapper,
                                              resampling = logit_rdesc_wrapper,
23
                                              control = logit_ctrl_wrapper,
24
25
                                               show.info = TRUE,
                                              measures = mlr::auc)
26
   # Performance score for each combination
28
   analyzeFeatSelResult(logit_sfeats)
29
30
31
   # Next, I store the optimal set of features to later use it
   # in the model building part file "logit_model.R"
   vars$logit <- c("customer", logit_sfeats$x)</pre>
```

6: Stacking: Neural Network (level 0) Feature Selection

```
##### Feature selection for the Neural Network. A wrapper approach ######
1
2
   # A model building approach with sequential forward selection is
3
   # established in order to find the best subset of features.
   # Each model is built with crossvalidation on the AUC measure.
   set.seed(2610)
                         <- makeClassifTask(data = train,</pre>
9
   nnet_task_wrapper
                                                target = "customer",
10
                                                positive = "good")
11
12
   nnet_learner_wrapper <- makeLearner("classif.nnet",</pre>
13
                                            predict.type = "prob",
14
                                            "trace" = FALSE)
15
16
17
   nnet_ctrl_wrapper
                           <- makeFeatSelControlSequential(method = "sfs",</pre>
                                                              alpha = 0.00001)
18
19
                           <- makeResampleDesc("CV", iters = 3)</pre>
20
   nnet_rdesc_wrapper
21
22
   nnet_sfeats
                           <- selectFeatures(learner = nnet_learner_wrapper,</pre>
23
                                               task = nnet_task_wrapper,
24
                                               resampling = nnet_rdesc_wrapper,
25
                                               control = nnet_ctrl_wrapper,
                                               show.info = TRUE,
26
                                               measures = mlr::auc)
27
28
   # Performance score for each combination
   analyzeFeatSelResult(nnet_sfeats)
30
31
   \mbox{\tt\#} Next, I store the optimal set of features to later use it
32
   # in the model building part file "nnet_model.R"
33
   vars$nnet <- c("customer", nnet_sfeats$x)</pre>
```

7: Gradient Boosting (level 0) Feature Selection

```
##### Feature selection for the Gradient Boosting model. A wrapper approach #####
1
3
   # A model building approach with sequential forward selection is
   # established in order to find the best subset of features.
   # Each model is built with crossvalidation on the AUC measure.
   # One-hot-encoding of categorical features
                          <- mlr::createDummyFeatures(train, target = "customer")</pre>
   train_wrapper2
9
   gb_task_wrapper
                         <- makeClassifTask(data = train_wrapper2,</pre>
10
                                               target = "customer",
11
                                               positive = "good")
12
13
                        <- makeLearner("classif.xgboost",</pre>
14
   gb_learner_wrapper
                                           predict.type = "prob")
15
16
                          <- makeFeatSelControlSequential(method = "sfs",</pre>
17
   gb_ctrl_wrapper
                                                             alpha = 0.00001)
18
19
   gb_rdesc_wrapper
                          <- makeResampleDesc("CV", iters = 3)</pre>
20
21
   gb_sfeats
                           <- selectFeatures(learner = gb_learner_wrapper,</pre>
22
                                              task = gb_task_wrapper,
23
                                              resampling = gb_rdesc_wrapper,
24
25
                                              control = gb_ctrl_wrapper,
26
                                              show.info = TRUE,
27
                                              measures = mlr::auc)
28
   # Performance score for each combination of features
29
30
   analyzeFeatSelResult(gb_sfeats)
31
   # Next, I store the optimal set of features to later use it
32
   # in the model building part file "gb_model_stacking.R"
33
   vars$gb2 <- c("customer", gb_sfeats$x)</pre>
```

8: Stacking: Random Forest (level 0) Feature Selection

```
##### Feature selection for the Random Forest model. A wrapper approach #####
   # A model building approach with sequential forward selection is
3
   # established in order to find the best subset of features.
   # Each model is built with crossvalidation on the AUC measure.
   set.seed(2610)
7
                      <- makeClassifTask(data = train,</pre>
9
   rf_task_wrapper
10
                                           target = "customer",
11
                                           positive = "good")
12
```

```
rf_learner_wrapper <- makeLearner("classif.randomForest",</pre>
                                         predict.type = "prob",
14
                                         "ntree" = 300)
15
16
   rf_ctrl_wrapper <- makeFeatSelControlSequential(method = "sfs",</pre>
17
                                                          alpha = 0.00001)
18
19
   rf_rdesc_wrapper <- makeResampleDesc("CV", iters = 3)</pre>
20
^{21}
   rf_sfeats
                       <- selectFeatures(learner = rf_learner_wrapper,</pre>
22
                                          task = rf_task_wrapper,
23
                                          resampling = rf_rdesc_wrapper,
24
                                          control = rf_ctrl_wrapper,
25
                                          show.info = TRUE,
26
27
                                          measures = mlr::auc)
28
29
   # Performance score for each combination
   analyzeFeatSelResult(rf sfeats)
30
31
   # Next, I store the optimal set of features to later use it
32
   # in the model building part file "rf_model_stacking.R"
   vars$rf2 <- c("customer", rf_sfeats$x)</pre>
```

9: Random Forest Model Building

```
2
   set.seed(2610)
3
   # Define task
5
   rf_task <- makeClassifTask(data = train[, c(vars$rf)],</pre>
6
                             target = "customer", positive = "good")
7
8
9
   # Define learner: decision tree
   rf_learner <- makeLearner("classif.randomForest",</pre>
10
                            predict.type = "prob",
11
                            par.vals = list("replace" = TRUE,
12
                                            "importance" = FALSE,
13
                                            "ntree" = 800))
14
15
   # Tuning the hyperparameters of the random forest
16
   rf_parms <- makeParamSet(</pre>
17
     # Number of features selected at each node
18
     makeIntegerParam("mtry", lower = 2, upper = 12),
19
     # Bootstrap sample size
20
    makeDiscreteParam("sampsize", values = c(30, 50, 70, 100, 130)),
21
22
     # Node size
     makeIntegerParam("nodesize", lower = 2, upper = 12)
23
24
^{25}
   rf_tunecontrol <- makeTuneControlGrid(resolution = 7, tune.threshold = FALSE)
26
   # Cross validation
27
   rf_rdesc <- makeResampleDesc(method = "CV", iters = 3, stratify = TRUE)
28
29
```

```
# Tuning with parallel computing
   no cores
                  <- detectCores() - 1
31
32
   parallelStartSocket(no_cores, level = "mlr.tuneParams")
33
   system.time(
34
35
     rf_tuning
                   <- tuneParams(rf_learner, task = rf_task,</pre>
                                  resampling = rf_rdesc,
36
                                  par.set = rf_parms,
37
38
                                  control = rf_tunecontrol,
                                  measures = mlr::auc)
39
40
   parallelStop()
41
42
   # Results for the different choices of hyperparameters
43
   rf_tuning_results <- generateHyperParsEffectData(rf_tuning, partial.dep = TRUE)</pre>
45
   rf_tuning_results$data
46
   # Detailed investigation
47
   tapply(rf_tuning_results$data$auc.test.mean,
48
          INDEX = c(rf_tuning_results$data$mtry), mean)
49
   tapply(rf_tuning_results$data$auc.test.mean,
          INDEX = c(rf_tuning_results$data$sampsize), mean)
51
   tapply(rf_tuning_results$data$auc.test.mean,
52
          INDEX = c(rf_tuning_results$data$nodesize), mean)
53
54
   # Choose the optimal hyperparameters and update the learner
55
                 <- setHyperPars(rf_learner, par.vals = rf_tuning$x)
56
   rf_tuned
57
58
59
   # Now we train the model on the full training data
   model_lib$rf <- mlr::train(rf_tuned, task = rf_task)</pre>
60
61
62
   # Prediction on current test data
   yhat$rf <- predict(model_lib$rf, newdata = test)</pre>
63
```

Q 10: Gradient Boosting Model Building

```
1
2
   set.seed(2610)
   # Define task
   gb_task <- makeClassifTask(data = train_wrapper[, c(vars$gb)],</pre>
6
                              target = "customer", positive = "good")
7
   # Define learner: gradient boosting model consisting of trees
   gb_learner <- makeLearner("classif.xgboost",</pre>
10
                          predict.type = "prob",
11
                          par.vals = list("booster" = "gbtree",
12
                                         "silent" = 0)
13
14
15
   # Tuning the hyperparameter of the model
   gb_parms <- makeParamSet(</pre>
16
17 # Learning rate
```

```
makeDiscreteParam("eta", values = c(0.15, 0.25, 0.3, 0.6)),
18
     # Maximum depth of a tree
19
     makeIntegerParam("max_depth", lower = 3, upper = 10),
20
     # Minimum number of observations to have in a node
21
     makeIntegerParam("min_child_weight", lower = 1, upper = 4),
22
     # Number of iterations through data
23
     makeIntegerParam("nrounds", lower = 4, upper = 12),
24
     # L2 regularization on weights
25
     makeDiscreteParam("lambda", values = c(0.05, 0.1, 0.2)),
26
     # Minimum loss reduction
27
     makeDiscreteParam("gamma", values = c(0.5, 0.9, 1.5)),
28
     # Subsample size
29
     makeDiscreteParam("subsample", values = c(1))
30
   )
31
32
33
   # Define how dense the parameters are selected from the defined ranges
34
   gb_tunecontrol <- makeTuneControlGrid(resolution = 3,</pre>
                                           tune.threshold = FALSE)
35
36
   # Sampling strategy: cross validation
37
                 <- makeResampleDesc(method = "CV",</pre>
38
39
                                        iters = 3.
                                        stratify = TRUE)
40
41
   # Tuning
42
   no_cores
                   <- detectCores() - 1 # Detect number of cores
43
44
   parallelStartSocket(no_cores, level = "mlr.tuneParams")
45
   system.time(
46
47
     gb_tuning
                   <- tuneParams(gb_learner,</pre>
48
                                  task = gb_task,
                                  resampling = gb_rdesc,
49
                                  par.set = gb_parms,
50
                                  control = gb_tunecontrol,
51
                                  measures = mlr::auc)
52
53
54
   parallelStop()
55
   # Results for the different choices of hyperparameters
56
   gb_tuning_results <- generateHyperParsEffectData(gb_tuning,</pre>
57
                                                       partial.dep = TRUE)
58
   gb_tuning_results$data
59
60
   # Detailed investigation
61
   tapply(gb_tuning_results$data$auc.test.mean,
62
           INDEX = c(gb_tuning_results$data$eta), mean)
63
64
   tapply(gb_tuning_results$data$auc.test.mean,
           INDEX = c(gb_tuning_results$data$min_child_weight), mean)
65
66
    tapply(gb_tuning_results$data$auc.test.mean,
           INDEX = c(gb_tuning_results$data$nrounds), mean)
67
   tapply(gb_tuning_results$data$auc.test.mean,
68
69
           INDEX = c(gb_tuning_results$data$lambda), mean)
70
   tapply(gb_tuning_results$data$auc.test.mean,
71
           INDEX = c(gb_tuning_results$data$gamma), mean)
   tapply(gb_tuning_results$data$auc.test.mean,
72
          INDEX = c(gb_tuning_results$data$subsample), mean)
73
   tapply(gb_tuning_results$data$auc.test.mean,
```

```
INDEX = c(gb_tuning_results$data$max_depth), mean)
75
76
   # Choose the optimal hyperparameters and update the learner
77
                <- setHyperPars(gb_learner, par.vals = gb_tuning$x)</pre>
78
   gb_tuned
   gb_tuned
79
80
   # Now we train the model on the full training data
81
   model_lib$gb <- mlr::train(gb_tuned, task = gb_task)</pre>
82
83
   # Prediction on current (one hot encoded) test dataset
84
   test_onehot <- mlr::createDummyFeatures(test, target = "customer")</pre>
85
               <- predict(model_lib$gb, newdata = test_onehot[, c(vars$gb)])</pre>
86
   yhat$gb
```

11: Stacking: Decision Tree (level 0) Model Building

```
1
2
3
   set.seed(2610)
   pred <- list()</pre>
5
   # Define dataset
6
   for (i in 1:5) {
7
     test_st <- train_sets[[i]]
     train_st <- train[-as.numeric(rownames(train_sets[[i]])), ]</pre>
10
11
     # Define task
     dt_task <- makeClassifTask(data = train_st[, c(vars$dt)],</pre>
12
                                    target = "customer",
13
                                    positive = "good")
14
15
     # Define learner: decision tree
16
     dt_learner <- makeLearner("classif.rpart",</pre>
17
18
                              predict.type = "prob")
19
     # Tuning the hyperparameter of the tree
20
     dt_parms <- makeParamSet(</pre>
21
       # Complexity parameter
22
       makeNumericParam("cp", lower = 0.00005, upper = 0.001),
23
       # Minimum number of observation in a node for a split
^{24}
       makeDiscreteParam("minsplit", values = c(5, 7, 10, 12, 15, 17,
25
                                                 20, 23, 25, 27, 30)),
26
       # Minimum number of observation to keep in terminal nodes
27
       makeDiscreteParam("minbucket", values = c(5, 8, 10, 12,
28
                                                 15, 18, 21, 25))
29
     )
30
31
32
     # Grid density
     dt_tunecontrol <- makeTuneControlGrid(resolution = 10,</pre>
33
                                            tune.threshold = FALSE)
34
35
     # Sampling strategy: cross validation
36
37
                   <- makeResampleDesc(method = "CV",</pre>
38
                                         iters = 3,
                                        stratify = TRUE)
39
```

```
40
      # Tuning using parallelization
41
                    <- detectCores() - 1 # Detect number of cores
42
     no_cores
43
      parallelStartSocket(no_cores, level = "mlr.tuneParams")
44
      system.time(
45
        dt_tuning
                     <- tuneParams(dt_learner,</pre>
46
                                     task = dt task,
47
48
                                     resampling = dt_rdesc,
49
                                     par.set = dt_parms,
                                     control = dt_tunecontrol,
50
                                     measures = mlr::auc)
51
52
53
     parallelStop()
54
55
      # Results for the different choices of hyperparameters
56
      dt_tuning_results <- generateHyperParsEffectData(dt_tuning,</pre>
                                                          partial.dep = TRUE)
57
     dt_tuning_results$data
58
59
      # Detailed investigation
60
     tapply(dt_tuning_results$data$auc.test.mean,
61
             INDEX = c(dt_tuning_results$data$cp), mean)
62
      tapply(dt_tuning_results$data$auc.test.mean,
63
             INDEX = c(dt_tuning_results$data$minsplit), mean)
64
65
      tapply(dt_tuning_results$data$auc.test.mean,
             INDEX = c(dt_tuning_results$data$minbucket), mean)
66
67
      # Choose the optimal hyperparameters and update the learner
68
69
     dt_tuned
                   <- setHyperPars(dt_learner, par.vals = dt_tuning$x)</pre>
70
     dt_tuned
71
      # Now the model is trained on the corresponding training data
72
     model_lib$dt <- mlr::train(dt_tuned, task = dt_task)</pre>
73
74
75
     # Prediction on current test_st data
76
      pred[[i]]
                   <- predict(model_lib$dt, newdata = test_st)</pre>
77
78
   # Combine subset predictions to obtain prediction on train dataset
79
   yhat$dt_train <- rbind(pred[[1]]$data, pred[[2]]$data, pred[[3]]$data,</pre>
80
                             pred[[4]]$data, pred[[5]]$data)
81
83
   # Prediction on test data
   yhat$dt_test <- predict(model_lib$dt, newdata = test)</pre>
84
```

12: Stacking: Logistic Regression (level 0) Model Building

```
for (i in 1:5) {
      test_st <- train_sets[[i]]</pre>
8
                    <- train[-as.numeric(rownames(train_sets[[i]])), ]</pre>
9
      train_st
10
11
      # Define task
12
      logit_task
                  <- makeClassifTask(data = train_st[, c(vars$logit)],</pre>
                                          target = "customer",
13
                                          positive = "good")
14
15
16
      # Define learner: logistic regression
      logit_learner <- makeLearner("classif.logreg",</pre>
^{17}
                                     predict.type = "prob")
18
19
      \ensuremath{\text{\#}} No tuning of hyperparameters necessary for logit model
20
^{21}
22
      # Train the model on the full corresponding training data
23
      model_lib$logit <- mlr::train(logit_learner, task = logit_task)</pre>
24
      # Prediction on current test_st data
25
      pred[[i]] <- predict(model_lib$logit, newdata = test_st)</pre>
26
   }
27
28
29
   # Combine subset predictions to obtain full prediction on train data
   yhat$logit_train <- rbind(pred[[1]]$data, pred[[2]]$data, pred[[3]]$data,</pre>
30
                                 pred[[4]]$data, pred[[5]]$data)
31
32
33
   # Prediction on test data
34
   yhat$logit_test <- predict(model_lib$logit, newdata = test)</pre>
```

13: Stacking: Neural Network (level 0) Model Building

```
1
2
3
   set.seed(2610)
   pred <- list()</pre>
5
   # Define dataset
6
   for (i in 1:5) {
     test_st <- train_sets[[i]]
                 <- train[-as.numeric(rownames(train_sets[[i]])), ]</pre>
10
     # Define task
11
                  <- makeClassifTask(data = train_st[, c(vars$nnet)],</pre>
     nnet_task
12
                                    target = "customer",
13
                                    positive = "good")
14
15
16
     # Define learner: neural net
     nnet_learner <- makeLearner("classif.nnet",</pre>
17
                                predict.type = "prob",
18
                                par.vals = list("trace" = FALSE,
19
                                                "maxit" = 400,
20
                                                "MaxNWts" = 3500))
21
22
     # Tuning the hyperparameters of the random forest
23
```

```
nnet_parms <- makeParamSet(</pre>
24
25
        makeDiscreteParam("decay", values = c(0, 0.1, 0.2, 0.3,
                                                0.4, 0.5, 0.6)),
26
        makeDiscreteParam("size", values = c(2, 4, 5, 6, 7, 8,
27
                                               9, 10, 11, 12))
28
29
30
     nnet_tunecontrol <- makeTuneControlGrid(resolution = 8,</pre>
31
32
                                                tune.threshold = FALSE)
33
      # Sampling strategy: cross validation
34
      nnet_rdesc
                      <- makeResampleDesc(method = "CV",</pre>
35
                                             iters = 3,
36
                                             stratify = TRUE)
37
38
39
      # Tuning with parallel computing
40
                       <- detectCores() - 1 # Detect number of cores
41
      parallelStartSocket(no_cores, level = "mlr.tuneParams")
42
43
      system.time(
       nnet_tuning
                     <- tuneParams(nnet_learner,</pre>
44
45
                                       task = nnet_task,
                                       resampling = nnet_rdesc,
46
                                       par.set = nnet_parms,
47
                                       control = nnet_tunecontrol,
48
49
                                       measures = mlr::auc)
50
      parallelStop()
51
52
53
     # Results for the different choices of hyperparameters
54
     nnet_tuning_results <- generateHyperParsEffectData(nnet_tuning,</pre>
                                                            partial.dep = TRUE)
55
     nnet_tuning_results$data
56
57
     # Detailed investigation
58
59
      tapply(nnet_tuning_results$data$auc.test.mean,
60
             INDEX = c(nnet_tuning_results$data$decay), mean)
61
      tapply(nnet_tuning_results$data$auc.test.mean,
             INDEX = c(nnet_tuning_results$data$size), mean)
62
63
     # Choose the optimal hyperparameters and update the learner
64
65
     nnet_tuned
                    <- setHyperPars(nnet_learner, par.vals = nnet_tuning$x)</pre>
66
     nnet_tuned
67
     # Now we train the model on the full corresponding training data
68
     model_lib$nnet <- mlr::train(nnet_tuned, task = nnet_task)</pre>
69
70
      # Prediction on current test_st data
71
                 <- predict(model_lib$nnet, newdata = test_st)</pre>
72
     pred[[i]]
   }
73
74
75
   # Combine subset predictions to obtain prediction on train dataset
76
   yhat$nnet_train <- rbind(pred[[1]]$data, pred[[2]]$data, pred[[3]]$data,</pre>
77
                         pred[[4]]$data, pred[[5]]$data)
78
   # Prediction on test data
79
   yhat$nnet_test <- predict(model_lib$nnet, newdata = test)</pre>
80
```

14: Stacking: Gradient Boosting (level 0) Model Building

```
##### Stacking: Gradient Boosting model (with mlr package) ######
1
2
   set.seed(2610)
4
   pred <- list()</pre>
5
   # Define dataset
6
   for (i in 1:5) {
     test_st <- train_sets[[i]]</pre>
     train_st <- train[-as.numeric(rownames(train_sets[[i]])), ]</pre>
10
                 <- mlr::createDummyFeatures(test_st, target = "customer")</pre>
11
     train_st <- mlr::createDummyFeatures(train_st, target = "customer")</pre>
12
     # Define task
13
               <- makeClassifTask(data = train_st[, c(vars$gb2)],</pre>
14
                                      target = "customer",
15
                                      positive = "good")
16
17
18
     # Define learner: gradient boosting model consisting of trees
     gb_learner <- makeLearner("classif.xgboost",</pre>
19
                                  predict.type = "prob",
20
                                  par.vals = list("booster" = "gbtree",
21
                                                   "silent" = 0))
22
23
24
     # Tuning the hyperparameter of the model
25
     gb_parms <- makeParamSet(</pre>
        # Learning rate
26
        makeDiscreteParam("eta", values = c(0.35, 0.45, 0.5, 0.55, 0.6)),
27
        # Maximum depth of a tree
28
        makeIntegerParam("max_depth", lower = 3, upper = 10),
29
30
        # Minimum number of obs. to have per node
        makeIntegerParam("min_child_weight", lower = 2, upper = 4),
31
        # Number of iterations through data
32
        makeIntegerParam("nrounds", lower = 8, upper = 16),
33
34
        # L2 regularization on weights
        makeDiscreteParam("lambda", values = c(0.05, 0.1, 0.15, 0.2, 0.3)),
35
36
        # Minimum loss reduction
        makeDiscreteParam("gamma", values = c(0.3, 0.4, 0.5, 0.6)),
37
        # Subsample size
38
39
        makeDiscreteParam("subsample", values = c(0.9, 0.95, 1))
40
41
     # Define how dense the parameters are selected from the defined ranges
42
     gb_tunecontrol <- makeTuneControlGrid(resolution = 3,</pre>
43
                                              tune.threshold = FALSE)
44
45
     # Sampling strategy: cross validation
46
     gb_rdesc <- makeResampleDesc(method = "CV",</pre>
47
                                           iters = 5,
48
                                           stratify = TRUE)
49
50
     # Tuning
51
                     <- detectCores() - 1 # Detect number of cores
52
     no_cores
53
```

```
parallelStartSocket(no_cores, level = "mlr.tuneParams")
54
      system.time(
55
56
        gb_tuning
                      <- tuneParams(gb_learner,</pre>
57
                                     task = gb_task,
                                     resampling = gb_rdesc,
58
                                     par.set = gb_parms,
59
60
                                     control = gb_tunecontrol,
                                     measures = mlr::auc)
61
62
      parallelStop()
63
64
      # Results for the different choices of hyperparameters
65
      gb_tuning_results <- generateHyperParsEffectData(gb_tuning,</pre>
66
67
                                                           partial.dep = TRUE)
68
      gb_tuning_results$data
69
70
      # Detailed investigation
      tapply (gb_tuning_results$data$auc.test.mean,
71
              INDEX = c(gb_tuning_results$data$eta), mean)
72
      tapply(gb_tuning_results$data$auc.test.mean,
73
             INDEX = c(gb_tuning_results$data$min_child_weight), mean)
74
75
      tapply(gb_tuning_results$data$auc.test.mean,
76
             INDEX = c(gb_tuning_results$data$nrounds), mean)
      tapply(gb_tuning_results$data$auc.test.mean,
77
             INDEX = c(gb_tuning_results$data$lambda), mean)
78
79
      tapply(gb_tuning_results$data$auc.test.mean,
80
              INDEX = c(gb_tuning_results$data$gamma), mean)
      tapply(gb_tuning_results$data$auc.test.mean,
81
              INDEX = c(gb_tuning_results$data$subsample), mean)
82
83
      tapply(gb_tuning_results$data$auc.test.mean,
84
              INDEX = c(gb_tuning_results$data$max_depth), mean)
85
      # Choose the optimal hyperparameters and update the learner
86
                     <- setHyperPars(gb_learner, par.vals = gb_tuning$x)</pre>
      gb tuned
87
      gb_tuned
88
89
90
      # Now we train the model on the full training data
91
      model_lib$gb2 <- mlr::train(gb_tuned, task = gb_task)</pre>
92
      # Prediction on current test_st data
93
      pred[[i]]
                    <- predict(model_lib$gb2, newdata = test_st[, c(vars$gb2)])</pre>
94
95
    }
    # Combine subset predictions to obtain full prediction on train data
97
    yhat$gb2_train <- rbind(pred[[1]]$data, pred[[2]]$data, pred[[3]]$data,</pre>
98
                              pred[[4]]$data, pred[[5]]$data)
99
100
    # Performance measured on one-hot encoded test data
101
102
    test_onehot <- mlr::createDummyFeatures(test, target = "customer")</pre>
    yhat$gb2_test <- predict(model_lib$gb2, newdata = test_onehot[, c(vars$gb2)])</pre>
103
```

15: Stacking: Random Forest (level 0) Model Building

```
set.seed(2610)
3
   pred <- list()</pre>
4
   # Define dataset
6
   for (i in 1:5) {
7
     test_st <- train_sets[[i]]
8
                     <- train[-as.numeric(rownames(train_sets[[i]])), ]</pre>
     train st
9
10
11
     # Define task
                     <- makeClassifTask(data = train_st[, c(vars$rf2)],</pre>
12
                                         target = "customer",
13
                                         positive = "good")
14
15
16
     # Define learner: decision tree
17
     rf_learner <- makeLearner("classif.randomForest",</pre>
18
                                     predict.type = "prob",
                                     par.vals = list("replace" = TRUE,
19
                                                      "importance" = FALSE,
20
                                                      "ntree" = 800))
21
22
     # Tuning the hyperparameters of the random forest
23
24
     rf_parms <- makeParamSet(
       # Number of features selected at each node.
25
       makeIntegerParam("mtry", lower = 2, upper = 12),
26
27
       # Bootstrap sample size
       makeDiscreteParam("sampsize", values = c(30, 50, 70, 100, 130)),
28
29
       # Size of nodes
       makeIntegerParam("nodesize", lower = 2, upper = 12)
30
31
     )
32
     # Grid density
33
     rf_tunecontrol <- makeTuneControlGrid(resolution = 7,</pre>
34
                                             tune.threshold = FALSE)
35
     # Sampling strategy: cross validation
36
     rf_rdesc <- makeResampleDesc(method = "CV",</pre>
37
38
                                          iters = 3,
39
                                           stratify = TRUE)
40
     # Tuning with parallel computing
41
                    <- detectCores() - 1 # Detect number of cores
42
     no_cores
43
     parallelStartSocket(no_cores, level = "mlr.tuneParams")
44
45
     system.time(
                   <- tuneParams(rf_learner, task = rf_task,</pre>
46
       rf_tuning
                                    resampling = rf_rdesc,
47
48
                                    par.set = rf_parms,
                                    control = rf_tunecontrol,
49
                                    measures = mlr::auc)
50
51
52
     parallelStop()
53
54
     # Results for the different choices of hyperparameters
55
     rf_tuning_results <- generateHyperParsEffectData(rf_tuning,</pre>
                                                         partial.dep = TRUE)
56
     rf_tuning_results$data
57
58
```

```
# Detailed investigation
59
      tapply(rf_tuning_results$data$auc.test.mean,
60
             INDEX = c(rf_tuning_results$data$mtry), mean)
61
62
      tapply(rf_tuning_results$data$auc.test.mean,
             INDEX = c(rf_tuning_results$data$sampsize), mean)
63
      tapply(rf_tuning_results$data$auc.test.mean,
64
             INDEX = c(rf_tuning_results$data$nodesize), mean)
65
66
67
     # Choose the optimal hyperparameters and update the learner
     rf_tuned
                     <- setHyperPars(rf_learner, par.vals = rf_tuning$x)</pre>
68
69
     rf_tuned
70
     # Now we train the model on the full training data
71
     model_lib$rf2 <- mlr::train(rf_tuned, task = rf_task)</pre>
72
73
     # Prediction on current test_st data
75
     pred[[i]]
                  <- predict(model_lib$rf2, newdata = test_st)</pre>
76
77
   # Combine subset predictions to obtain prediction on full train data
78
   yhat$rf2_train <- rbind(pred[[1]]$data, pred[[2]]$data, pred[[3]]$data,</pre>
80
                              pred[[4]]$data, pred[[5]]$data)
81
   # Performance measured on test data
82
   yhat$rf2_test <- predict(model_lib$rf2, newdata = test)</pre>
83
```

16: Stacking: Stacked Generalization Model Building

```
# Generate new train and test dataset with base learners' predictions as features
3
   data_stacking_train <- as.data.frame(matrix(data = c(train$customer,</pre>
4
5
                                                        yhat $dt_train $prob.good,
6
                                                        yhat$logit_train$prob.good,
                                                        yhat$nnet_train$prob.good,
7
                                                        yhat$gb2_train$prob.good,
8
                                                        yhat$rf2_train$prob.good),
9
                                               nrow = NROW(train)), row.names = rownames(
10
                                                   train))
11
12
   data_stacking_test <- as.data.frame(matrix(data = c(test$customer,</pre>
                                                        yhat$dt_test$data$prob.good,
13
                                                        yhat$logit_test$data$prob.good,
14
                                                        yhat$nnet_test$data$prob.good,
15
                                                        yhat $gb2_test $data $prob.good,
16
                                                        yhat$rf2_test$data$prob.good),
17
                                               nrow = NROW(test)), row.names = rownames(
18
                                                   test))
19
   colnames(data_stacking_train) <- c("truth", "dt",</pre>
20
                                      "logit", "nnet",
21
                                      "gb", "rf")
22
   colnames(data_stacking_test) <- c("truth", "dt",</pre>
23
                                    "logit", "nnet",
24
```

```
"gb", "rf")
25
   data stacking train$truth
                                    <- as.factor(data_stacking_train$truth)</pre>
26
   data_stacking_test$truth
                                    <- as.factor(data_stacking_test$truth)</pre>
27
28
29
30
    # Investigate correlation of predictions and plot correlation matrix
                                    <- cor(data_stacking_train[2:6,2:6])</pre>
31
    colnames(cormat) <- c("Decision Tree", "Logistic Regression",</pre>
32
                           "Neural Network", "Gradient Boosting",
33
                           "Random Forest")
34
   rownames(cormat) <- c("Decision Tree", "Logistic Regression",</pre>
35
                           "Neural Network", "Gradient Boosting",
36
                           "Random Forest")
37
   X11(width=6, height=6)
38
    corrplot(cormat, type = "lower", method = "circle", order = "hclust",
39
40
             col = rev(gray.colors(n = 90, start = 0.5, end = 1, gamma = 12)),
41
             tl.col = "black", tl.srt = 45,
             addCoef.col = "black")
42
43
   ###### Stacking Model 1: Averaging, all base learners ############
44
                      <- as.data.frame(matrix(data = c(data_stacking_test$truth,</pre>
45
46
                                                           rowMeans(data_stacking_test[,-1])),
47
                                                  ncol = 2))
    colnames(yhat$st1) <- c("truth", "prob.good")</pre>
48
49
50
    ##### Stacking Model 2: Averaging, best learners #####
51
                      <- as.data.frame(matrix(data = c(data_stacking_test$truth,</pre>
52
                                                           rowMeans(data_stacking_test[,-c(1,
53
                                                                2, 3)])),
                                                  ncol = 2))
54
   colnames(yhat$st2) <- c("truth", "prob.good")</pre>
55
56
57
   ###### Stacking Model 3: Gradient Boosting, all base learners #########
58
   set.seed(2610)
59
60
61
    control <- trainControl(method="repeatedcv", number=10,</pre>
                             repeats=3, savePredictions=TRUE,
62
                             classProbs=TRUE)
63
   algorithms <- c('glm', 'rpart', 'rf', 'nnet', 'xgbLinear')</pre>
64
   base <- caretList(customer~., data=train, trControl=control,</pre>
65
                       methodList=algorithms)
67
   # Stacker
68
   stackControl <- trainControl(method="repeatedcv", number=10,</pre>
69
                                   repeats=3, savePredictions=TRUE,
70
                                   classProbs=TRUE,
71
                                   summaryFunction = twoClassSummary)
72
   model_lib$st3 <- caretStack(base, method="gbm", metric="ROC",</pre>
73
74
                                  trControl=stackControl)
75
76
   # Prediction on test dataset
77
                     <- matrix(c(rownames(test),</pre>
                                    test$customer,
78
                                    1 - predict(model_lib$st3,
79
80
                                                 newdata=test,
```

```
type="prob")),
81
                                  ncol = 3)
82
    yhat$st3 <- apply(yhat$st3, 2, function(x) as.numeric(x))</pre>
83
    colnames(yhat$st3) <- c("id", "truth", "prob.good")</pre>
84
85
86
    ###### Stacking Model 4: Logistic Regression, all base learners ########
87
    set.seed(2610)
88
89
90
    # Stacker
91
    model_lib$st4 <- caretStack(base, method="glmnet",</pre>
                                 metric="ROC", trControl=stackControl)
92
93
    # Prediction on test dataset
94
95
    yhat$st4 <- matrix(c(rownames(test),</pre>
96
                                    test$customer,
97
                                    1 - predict(model_lib$st4,
                                                 newdata=test,
98
                                                 type="prob")),
99
                                  ncol = 3)
100
   yhat$st4 <- apply(yhat$st4, 2, function(x) as.numeric(x))</pre>
101
   colnames(yhat$st4) <- c("id", "truth", "prob.good")</pre>
102
```

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