AutoML project: Tuning a majority voting ensemble pipeline consisting of a random forest classifier, a gradient boosting classifier and a SVM classifier using DEHB

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Abstract The AutoML system tunes a ML pipeline consisting of an imputer, an optional sampler, an optional scaler and a choice of three models. Since the tasks are imbalanced tabular datasets, a random forest classifier, a gradient boosting classifier and a SVM classifier are reasonable choices, which should yield a good overall prediction by majority voting. I used DEHB as an optimizer, which combines the advantages of differential evolutions and hyperband, i.e., generating promising new hyperparameter configurations for more costly evaluations based on initial cheap evaluations. Overall, the improvement in performance compared to the untuned random forest classifier baseline is 0.8% and 25.9% as measured by balanced accuarcy. Thus the AutoML system outperforms the baseline across all datasets and the algorithm is significantly different for 9 out of 10 datasets by the McNemar test. The source code is available at: https://github.com/constantin-crailsheim/automl_imbalanced

1 Introduction

The objective of the AutoML system is to yield good performance as measured by the balanced accuracy on imbalanced tabular datasets and to be able to deal with missing values. Thus, it optimizes a ML pipeline consisting of five elements. First, a choice of two imputers replaces missing values. Then, an optional sampling method is applied to deal with imbalance in the targets, which can be under- and/or oversampling methods. Next, the pre-processed integer features are rounded such that they do not take values that would not appear in the original data. After optionally normalizing all features, three different models were fitted, i.e., a random forest classifier, a gradient boosting classifier and a SVM classifier. The pre-processing choices and the hyperparameters of the model were optimized by DEHB, which is a computationally cheap optimizer that works well on discrete search spaces. The final predictions are derived by majority voting over the individual predictions of the best pipelines for each model. This means that the overall predictions should be in particular good if the errors of the models are not too correlated.

2 Method

This section outlines the specific choices of the AutoML system and how it will be optimized and evaluated. The choices of sklearn.impute for the imputation strategy are:

- The SimpleImputer is an univariate imputer, which completes missing values with a descriptive statistic per feature. I chose the median, since it is less sensitive to outliers than the mean.
- The KNNImputer replaces missing values by the mean value of its 5 nearest neighbors as default based on Euclidian distance of their non-missing observations of the same feature.

The choices of imblearn for the data-level sampling method to yield a balanced dataset are:

• SMOTE as an oversampling approach generates new samples of the minority class by interpolating between existing observations of the minority class, where no distinction is made between easy and hard samples.

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- TomekLinks as an undersampling approach removes samples from the majority class, if they are nearest neighbors to a minority class sample, thus removing noisy borderline samples of the majority class.
- SMOTETomek combines SMOTE and Tomek links.
- No sampling method would allow algorithmic-level methods to deal with the imbalanced data.

The above pre-processing methods could generate numeric values for features that should contain only integers (e.g., ordinal categorical features), since they impute missing values by means or medians and generate new samples by interpolation. Thus, I added another layer to the pipeline, which rounds all observations of these features to the closest integer.

The last step of pre-processing is the choice of whether to apply the StandardScaler of sklearn.preprocessing to standardize the features. This will be in particular useful for the SVM, since an RBF kernel assumes features centered around zero and similar variance across features.

Subsequently, the hyperparameters of the three models of the ensemble were optimized, where I defined the search space with the ConfigSpace package. For almost all hyperparameters, the default was set to the default specified for each model. I chose the search space mostly such that it is centered around the default while accounting for log scale. In those cases where the default would be a the lower end of a reasonable search space, I chose the upper bound reasonably higher.

The first model in the ensemble is a RandomForestClassifier from sklearn.ensemble. It can handle all data types well and generalizes well by having a low variance due to ensembling over relatively uncorrelated models. The hyperparameters, which will all be sampled uniformly, are:

Hyperparameter	Data type	Search space	Default	Other
criterion	Categorical	{gini, entropy, log_loss}	gini	
max_depth	Integer	[5,15]	10	
min_samples_split	Integer	[1, 32]	2	Log scale
min_samples_leaf	Integer	[1, 16]	1	Log scale
max_features	Integer	[0.1, 0.9]	0.5	
class_weight	Categorical	{balanced, balanced_subsample, None}	None	

The class_weight is an algorithm-level method that deals with imbalanced data by giving less frequent classes more weight. It will only have an effect if no data-level sampling method was used, since in the other case the dataset passed to the model will be balanced.

The second model in the ensemble is a GradientBoostingClassifier from sklearn.ensemble. It has strong predictive performance by iteratively fitting weak learners on the error of the previous learner and has similar advantages as the RandomForestClassifier. The hyperparameters are:

Hyperparameter	Data type	Search space	Default	Other
loss	Categorical	{log_loss, exponential}	log_loss	
learning_rate	Float	[0.01, 1]	0.1	Log scale
criterion	Categorical	<pre>{friedman_mse, squared_error}</pre>	friedman_mse	
min_samples_split	Integer	[1, 32]	2	Log scale
min_samples_leaf	Integer	[1, 16]	1	Log scale
max_depth	Integer	[2,10]	3	

The third model in the ensemble is a Support Vector Classifier (SVC) from sklearn.svm. This model works in particular well on easily to separate datasets, on small datasets and in high-dimensional spaces (GeeksforGeeks, 2023). The hyperparameters are:

]	Hyperparameter	Data type	Search space	Default	Other
	С	Float	[0.1, 10]	1.0	Log scale
	kernel	Categorical	{linear, poly, rbf, sigmoid}	rbf	
	shrinking	Boolean	{True, False}	True	
	tol	Float	[1e-4,1e-2]	1e-3	
	class_weight	Categorical	{balanced, None}	None	

To optimize the hyperparameter of the AutoML system, I used DEHB by Awad et al. (2021), which combines differential evolution and hyperband. Differential evolution constructs a new mutant vector from three random parents and then generates the offspring by randomly selecting values from the new mutant vector with probability p and otherwise from one of the corresponding parents. Hyperband allows to search the whole search space with cheap evaluations and only trains more costly models on promising areas of the search space. The algorithm starts by sampling N random hyperparameter configurations, which are evaluated at the lowest budget. Then the best $1/\eta$ of these configurations are evaluated at a η -times higher budget and this process is repeated until the highest fidelity (denoted here by f) is reached, thus $N = \eta^{f-1}$. After completing one iteration, the algorithm restarts with new instantiations and evaluates these at the second lowest fidelity, thereby hedging against bad initializations. DEHB combines both approaches by generating the hyperparameter configurations for the next fidelity by differential evolution from the lower fidelity as parent pool. The authors state that DEHB is computationally cheap with high speed-up gains compared to BOHB. Furthermore, it has strong final performance for discrete search spaces, which I have for various hyperparameters. The authors experiments have shown that DEHB also outperforms SMAC by mean ranks across all of their chosen benchmarks. For those reasons, I chose DEHB as an efficient optimizer for this problem.

For the optimization, I set $\eta=3$ and f=4, which implies an initial population of $N=3^3=27$. I set the budget for the RandomForestClassifier and the GradientBoostingClassifier, as indicated by the number of trees in the forest, to a minimum of 10 and maximum of 270. For SVC, I chose the maximum number of iterations as budget and I set it to a minimum of 500 and maximum of 13500. However, the runtime between the lowest and largest budget usually did not differ too much since the SVM optimizer most likely already converged in most cases and the evaluation was relatively cheap compared to the forest based classifiers for most datasets. Thus, the SVC mostly benefits from differential evolution and the successive halving element is not as important, since many configurations can be tested irrespecitively. Hence, I allocated 40% of the maximum cost to optimizing the forest based models and 20% to optimizing the SVC.

To evaluate the performance of the AutoML system, I used 3-fold external and 4-fold internal cross-validation. I used stratified CV to ensure that the class imbalance of the targets is preserved in each fold. Given a total budget of 3600 seconds per dataset, a total of 1200 second could be used to optimize the AutoML system in each fold. Since the budget is not that larger after accounting for cross-validation, I tuned only a selection of hyperparameters of the actual model and the hyperparameters of the preprocessing functions were kept at their default values.

After the optimization routine, all three model pipelines are passed to the VotingClassifier from sklearn.ensemble and fitted with their incumbent configurations. Then the imbalance sampling is removed from the pipeline to not sample for the test set. Thus, the final AutoML system is an ensemble of three pipelines with majority voting for the final classification.

3 Experiments

To run the optimization, I used a M1 Pro chip and 32 GB RAM from 2021. The external cross-validation performance in terms of balanced accuracy of the AutoML system vs. the untuned RandomForestClassifer baseline for each dataset id is shown below:

Model	976	980	1002	1018	1019	1021	1040	1053	1461	41160
Baseline	0.962	0.939	0.547	0.554	0.989	0.932	0.960	0.594	0.695	0.571
AutoML system	0.990	0.982	0.806	0.809	0.997	0.957	0.992	0.657	0.838	0.743
Improvement	0.027	0.043	0.259	0.254	0.008	0.025	0.032	0.063	0.143	0.172
McNemar test	37.19	30.94	927.63	906.28	8.75	11.40	1.86	287.88	660.02	117.14

Hence, the AutoML system outperforms the baseline across all datasets with an improvement between 0.8% and 25.9%. To evaluate whether the two algorithms are significantly different, I used the McNemar test, which was computed over the concatenated predictions of all folds. The reference distribution is χ_1^2 and thus the algorithms would be significantly different at the 5%-level if the test statistic is larger than 3.84, which is the case for all datasets except for dataset 1040. However, for this dataset the balanced accuracy is still 3.2% better and above 99%.

The plots of the trajectories for each dataset are shown in appendix A. For dataset 976, 980 1019, the SVC is the top performing estimator, followed by the GradientBoostingClassifier and the RandomForestClassifier. For the other datasets, the ranking is not as clear. For the last two datasets, the SVC has the worst performance, most likely since SVMs are costlier to fit given the large number of observations and less iterations to tune the hyperparameters were possible. However, the overall performance of the AutoML system is still similar to the best individual pipelines due to majority voting. The benchmarks are usually outperformed after at most 50 seconds, except for the last two datasets due to the underperforming SVC. The final externally cross-validated performance is a bit lower than the performances of the individual algorithms for a few datasets, since the performance of the individual algorithms tends to be overly optimistic due to the hyperparameters being tuned on that specific fold.

The chosen incumbents for each model pipeline for all datasets are shown in appendix B. Some key trends are as following: The preferred sampling method for RandomForestClassifier and SVC is quite mixed, but for the GradientBoostingClassifier only oversampling or mixed methods were selected. As expected, SVC uses the StandardScaler for all datasets, except 1019. If no sampling method was chosen, the imbalance was always accounted for by class weights. Lastly, the RandomForestClassifier prefers on average deeper trees than the GradientBoostingClassifier.

4 Conclusion

The AutoML system outperforms the benchmark across all datasets and has thus has proven to be useful. However, some improvements are still possible if a larger budget would be available. The hyperparameters of the pre-processing methods could be also tuned to fit better to each dataset and algorithm. Furthermore, a stacking classifier could be trained on the three algorithms, which would allow to find the best weighted combination of the predictions of each individual algorithm for the final prediction of the AutoML system. I conducted experiments with stacking, but the training on the final incumbents with the highest budgets took fairly long, thus I decided to use the budget rather to improve the performance of the individual estimators. Overall, however, this AutoML system is capable of tuning well performing pipelines for imbalanced classification tasks.

References

Awad, N., Mallik, N., and Hutter, F. (2021). DEHB: Evolutionary hyberband for scalable, robust and efficient hyperparameter optimization. In Zhou, Z., editor, *Proceedings of the Thirtieth International Joint Conference on Artificial Intelligence, IJCAI-21*, pages 2147–2153. ijcai.org.

GeeksforGeeks (2023). Support vector machine in machine learning. https://www.geeksforgeeks.org/support-vector-machine-in-machine-learning/.

A Trajectories

The following plots show the trajectories of the incumbent performance of all three model pipelines (RandomForestClassifier (RFC), RandomForestClassifier (GBC), SVC) evaluated with internal CV in each fold, over runtime. Furthermore, the external CV of the untuned RFC baseline is plotted as grey horizontal line and the external CV of the final performance of the AutoML system is plotted as purple dot at the maximum runtime per model in each fold.

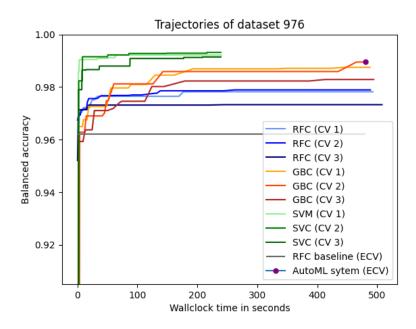


Figure 1: Trajectories for dataset 976 with 9961 observations and 14 features.

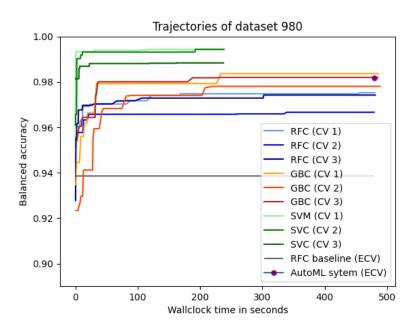


Figure 2: Trajectories for dataset 980 with 5620 observations and 64 features.

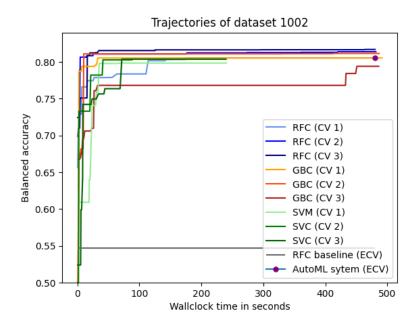


Figure 3: Trajectories for dataset 1002 with 7485 observations and 55 features.

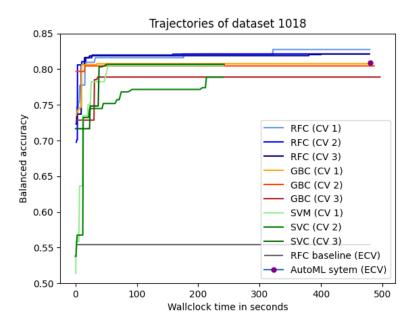


Figure 4: Trajectories for dataset 1018 with 8844 observations and 56 features.

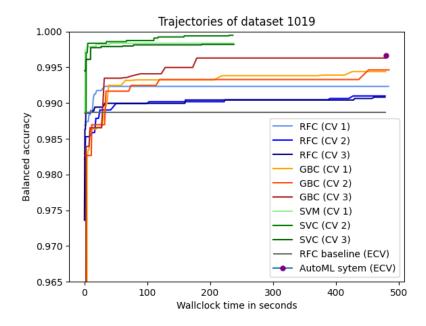


Figure 5: Trajectories for dataset 1019 with 10992 observations with 16 features

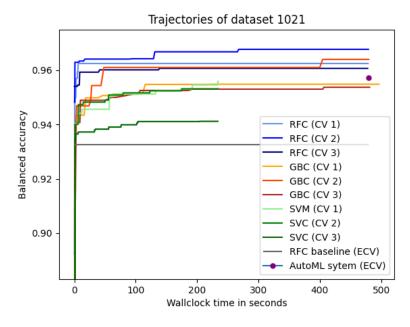


Figure 6: Trajectories for dataset 1021 with 5473 observations and 10 features.

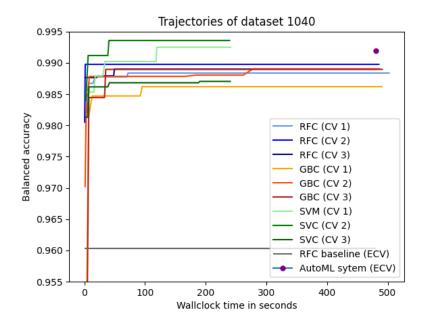


Figure 7: Trajectories for dataset 1040 with 14395 observations and 108 features.

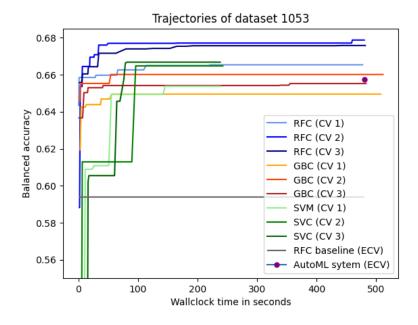


Figure 8: Trajectories for dataset 1053 with 10885 observations and 21 features.

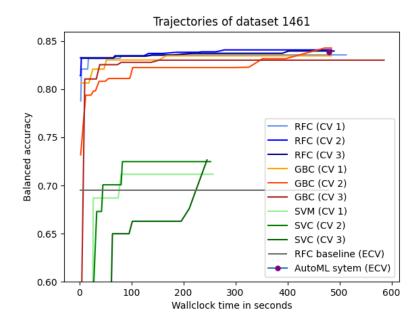


Figure 9: Trajectories for dataset 1461 with 45221 observations and 16 features.

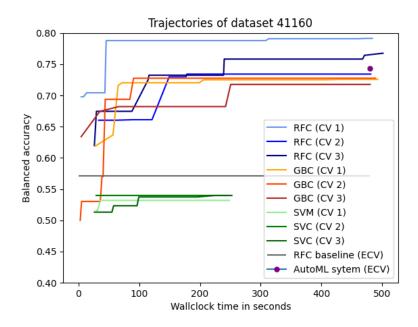


Figure 10: Trajectories for dataset 41660 with 31406 observations and 22 features.

B Incumbent hyperparameters

The following tables shows the incumbent hyperparameter configurations for each algorithm and each dataset in each fold.

Table 1: Incumbent hyperparameters configurations for the random forest classifier $% \left(1\right) =\left\{ 1\right\} =\left\{ 1\right\}$

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2 Simple Tomek True gini 12 24 4 1 Simple None False entropy 11 5 16 2 Simple None False gini 9 10 1 3 KNN Tomek False log_loss 12 28 11 2 Simple Tomek False gini 10 3 5 2 Simple Tomek False gini 10 3 5 3 KNN None True gini 12 5 9	1053	1	KNN	Tomek	False	log_loss	8	10	16	0.590	balanced_subsample
3 KNN Tomek False entropy 25 9 14 2 Simple None False entropy 11 5 16 1 Simple None False entropy 15 8 15 1 Simple Tomek False log_loss 12 28 11 2 Simple Tomek False gini 10 3 5 3 KNN None True gini 12 5 9	1053	2	Simple	Tomek	True	gini	12	24	4	0.400	balanced
1 Simple Simple None False False entropy gini 1 5 16 2 Simple Tomek False False entropy gini 15 8 15 1 Simple Tomek False False gini 10 3 5 2 Simple Tomek True gini 10 3 5 3 KNN None True gini 12 5 9	1053	3	KNN	Tomek	False	entropy	25	6	14	0.555	balanced
2 Simple symple None False shrropy 15 10 1 1 Simple Tomek False simple Tomek False simple Tomek False simple Tomek 10 3 5 3 KNN None True simil simple Tomek 12 5 9	1461	1	Simple	None	False	entropy	11	5	16	0.628	balanced
3 KNN Tomek False entropy 15 8 15 1 Simple Tomek False log_loss 12 28 11 2 Simple Tomek False gini 10 3 5 3 KNN None True gini 12 5 9	1461	2	Simple	None	False	gini	6	10	1	0.390	balanced
1 Simple Tomek False log_loss 12 28 11 2 Simple Tomek False gini 10 3 5 3 KNN None True gini 12 5 9	1461	3	KNN	Tomek	False	entropy	15	8	15	0.765	balanced_subsample
2 Simple Tomek False gini 10 3 5 3 KNN None True gini 12 5 9	41160	1	Simple	Tomek	False	log_loss	12	28	11	0.811	balanced
3 KNN None True gini 12 5 9	41160	2	Simple	Tomek	False	gini	10	3	5	0.379	balanced
	41160	3	KNN	None	True	gini	12	2	6	0.851	balanced

Table 2: Incumbent hyperparameters configurations for the gradient boosting classifier

Dataset ID	CV fold	Imputer	Sampler	Scaler	Loss	Learning rate	Criterion	Min samples per split	Min samples per leaf	Max depth
926	1	Simple	SMOTE	False	exponential	0.603	squared_error	2	7	9
926	2	Simple	SMOTETomek	True	log_loss	0.522	squared_error	23	3	2
926	3	Simple	SMOTETomek	True	exponential	0.815	squared_error	5	3	3
086	1	Simple	SMOTE	True	log_loss	0.598	squared_error	7	4	4
086	2	KNN	SMOTETomek	True	log_loss	0.432	friedman_mse	6	7	3
086	3	Simple	SMOTETomek	True	exponential	0.322	squared_error	9	1	2
1002	1	KNN	SMOTETomek	True	log_loss	0.010	squared_error	3	7	2
1002	2	KNN	SMOTETomek	False	log_loss	0.013	squared_error	7	9	2
1002	3	KNN	SMOTE	True	exponential	0.021	friedman_mse	12	7	4
1018	1	KNN	SMOTETomek	True	log_loss	0.061	friedman_mse	9	1	3
1018	2	Simple	SMOTETomek	True	log_loss	0.185	squared_error	9	12	3
1018	3	KNN	SMOTE	True	exponential	0.054	friedman_mse	2	1	3
1019	1	Simple	SMOTE	True	exponential	0.398	squared_error	31	4	4
1019	2	Simple	SMOTETomek	True	log_loss	0.158	friedman_mse	7	1	3
1019	3	Simple	SMOTE	False	exponential	999.0	friedman_mse	5	9	4
1021	1	KNN	SMOTETomek	True	exponential	0.018	friedman_mse	7	9	5
1021	2	Simple	SMOTE	False	log_loss	0.034	squared_error	3	4	5
1021	3	KNN	SMOTETomek	True	log_loss	0.141	friedman_mse	7	3	9
1040	1	KNN	SMOTETomek	True	log_loss	0.048	friedman_mse	5	3	4
1040	2	Simple	SMOTE	False	exponential	0.588	friedman_mse	4	3	3
1040	3	Simple	SMOTE	False	log_loss	0.410	friedman_mse	20	7	3
1053	1	KNN	SMOTETomek	True	exponential	0.014	squared_error	15	1	3
1053	2	Simple	SMOTETomek	False	exponential	0.021	squared_error	7	3	3
1053	3	KNN	SMOTETomek	True	log_loss	0.270	squared_error	8	8	2
1461	1	KNN	SMOTETomek	False	exponential	0.092	squared_error	7	4	7
1461	2	KNN	SMOTETomek	False	log_loss	0.035	friedman_mse	4	7	5
1461	3	Simple	SMOTETomek	False	log_loss	0.111	friedman_mse	8	5	8
41160	1	Simple	SMOTE	False	log_loss	0.023	friedman_mse	16	2	11
41160	2	Simple	SMOTE	False	exponential	0.043	friedman_mse	30	2	6
41160	3	Simple	SMOTETomek	False	log_loss	0.058	squared_error	5	3	111

Table 3: Incumbent hyperparameters configurations for the SVM classifier $\,$

976 1 KNN SMOTETomek True 8.489 rhf True 0.005 976 2 Simple None True 8.670 rhf False 0.0001 976 3 Simple None True 4.036 rhf False 0.0001 980 1 Simple SNOTETomek True 0.190 False 0.0004 980 2 KNN None False 1.061 rhf 7.001 1.000 1002 1 KNN None True 0.190 linear False 0.0001 1002 2 KNN Tomek True 0.190 linear False 0.000 1019 3 Simple SMOTETomek True 0.190 Irue 0.000 1019 4 3 Simple None True 0.190 Irue 0.000 1011 5 Simple Tomek True <th>Dataset ID</th> <th>CV fold</th> <th>Imputer</th> <th>Sampler</th> <th>Scaler</th> <th>၁</th> <th>Kernel</th> <th>Shrinking</th> <th>Tolerance</th> <th>Class weight</th>	Dataset ID	CV fold	Imputer	Sampler	Scaler	၁	Kernel	Shrinking	Tolerance	Class weight
2 Simple None True 8.670 rhf False 3 Simple None True 4.036 rhf False 2 KNN Tomek True 0.893 poly False 1 KNN Tomek True 0.893 poly True 2 KNN Nome True 0.160 linear False 2 KNN Tomek True 0.169 linear False 3 Simple SMOTETomek True 0.169 linear False 2 Simple SMOTETomek True 0.131 linear True 3 Simple None True 0.131 linear True 4 Simple None True 0.136 rhf True 5 Simple None True 0.136 rhf True 6 Simple None True 0.136	926	1	KNN	SMOTETomek	True	8.489	rbf	True	0.0085	balanced
3 Simple None True 4.036 rbf False 2 KNN Tomek True 2.230 poly False 2 KNN Tomek True 0.893 poly True 2 KNN Tomek True 0.161 linear False 2 KNN Tomek True 0.169 linear False 2 KNN Tomek True 0.169 linear False 2 KNN SMOTETomek True 0.169 linear False 2 Simple Tomek True 0.131 linear True 2 Simple Tomek True 0.131 linear True 3 Simple Tomek True 0.131 linear True 4 Simple Tomek True 0.131 linear True 5 Simple Tomek True 0.213	926	2	Simple	None	True	8.670	rbf	False	0.0016	balanced
1 Simple SMOTETomek True 0.893 poly False 2 KNN Tomek True 0.893 poly True 2 KNN SMOTETomek True 0.161 linear False 2 KNN Tomek True 0.19 linear False 2 KNN Tomek True 0.19 linear False 2 Simple SMOTETomek True 0.13 linear False 2 Simple Tomek True 0.13 linear True 2 Simple Mone True 0.13 linear True 2 Simple None True 0.13 linear True 2 Simple Tomek True 0.13 linear True 3 Simple Tomek True 0.14 rbf True 4 KNN SMOTE True 0.13	926	3	Simple	None	True	4.036	rbf	False	0.0005	balanced
2 KNN Tomek True 0.893 poly True 3 KNN SMOTETomek True 0.161 linear False 2 KNN Tomek True 0.199 linear False 1 KNN Tomek True 0.199 linear False 2 Simple SMOTETomek True 0.131 linear False 2 Simple Tomek True 0.621 poly True 2 Simple Tomek True 0.131 linear True 2 Simple None True 0.132 rbf True 2 Simple Tomek True 0.134 rbf True 2 Simple Tomek True 0.143 linear True 3 Simple Tomek True 0.143 linear True 4 KNN SMOTE True 0.218	086	1	Simple	SMOTETomek	True	2.230	poly	False	0.0040	balanced
3 KNN None False 1.061 rbf True 2 KNN Tomek True 0.169 linear False 3 Simple SMOTETomek True 0.169 linear False 1 Simple SMOTETomek True 0.621 poly True 2 Simple SMOTETomek True 0.621 poly True 3 Kinn SMOTETomek True 0.621 poly True 1 Simple SMOTETomek True 0.113 linear True 2 Simple Tomek True 0.143 linear True 3 Simple Tomek True 0.244 rbf True 4 KNN SMOTE True 0.234 rbf True 5 KNNN SMOTE True 0.138 sigmoid False 6 Simple Tomek True <t< td=""><td>086</td><td>2</td><td>KNN</td><td>Tomek</td><td>True</td><td>0.893</td><td>poly</td><td>True</td><td>0.0030</td><td>balanced</td></t<>	086	2	KNN	Tomek	True	0.893	poly	True	0.0030	balanced
1 KNNN SMOTETomek Tue 0.161 linear False 2 KNNN Tomek True 0.199 linear False 1 Simple SMOTETomek True 0.213 sigmoid True 2 Simple Tomek True 0.621 poly True 3 KNN SMOTETomek True 0.131 linear True 1 Simple None False 6.871 rhf True 2 Simple None True 6.803 rhf True 3 Simple Tomek True 6.803 rhf True 4 Simple Tomek True 6.803 rhf True 5 Simple Tomek True 6.803 rhf True 6 Simple Tomek True 6.803 rhf True 7 KNNN SMOTE True 6.244	086	3	KNN	None	False	1.061	rbf	True	900000	balanced
2 KNN Tomek True 0.199 linear False 3 Simple SMOTE True 0.169 linear False 2 Simple Tomek True 0.213 sigmoid True 3 KNN SMOTETomek True 0.113 linear True 1 Simple None False 2.186 poly True 2 Simple None False 6.871 rbf True 2 Simple Tomek True 6.871 rbf True 2 Simple Tomek True 6.871 rbf True 2 Simple Tomek True 6.244 rbf True 2 Simple None True 0.133 infmoid False 3 Simple None True 0.384 rbf False 4 NNN Tomek True 0.363	1002	1	KNN	SMOTETomek	True	0.161	linear	True	0.0017	balanced
3 Simple SMOTE one True 0.169 linear False 2 Simple SMOTETomek True 0.213 sigmoid True 2 Simple Tomek True 0.621 poly True 1 Simple None False 2.186 poly True 2 Simple Tomek False 2.186 poly True 2 Simple Tomek False 2.186 poly True 2 Simple Tomek True 6.871 rbf True 2 Simple Tomek True 6.244 rbf True 2 Simple Tomek True 6.244 rbf True 3 Simple None True 0.133 rigmoid False 4 KNN SMOTE True 0.384 rbf True 5 KNN Tomek True 0.363	1002	2	KNN	Tomek	True	0.199	linear	False	0.0003	balanced
1 Simple SMOTETomek True 0.213 sigmoid True 2 Simple Tomek True 0.621 poly True 1 Simple SMOTETomek False 2.186 poly True 2 Simple SMOTETomek False 6.871 rbf True 2 Simple Tomek True 6.803 rbf True 2 Simple Tomek True 6.244 rbf True 3 Simple Tomek True 6.244 rbf True 4 KNN SMOTE True 6.244 rbf True 5 KNN SMOTETOmek True 6.244 rbf True 1 KNN SMOTE True 6.244 rbf True 2 KNN SMOTE True 6.244 rbf True 3 Simple None True 6.384	1002	33	Simple	SMOTE	True	0.169	linear	False	0.0025	balanced
2 Simple Tomek True 0.621 poly True 3 KNN SMOTETomek True 0.113 linear True 1 Simple None False 2.186 poly True 2 Simple Tomek True 7.892 rbf True 2 Simple Tomek True 6.843 rbf True 2 Simple Tomek True 6.843 rbf True 3 Simple Tomek True 6.244 rbf True 4 KNN SMOTE True 6.244 rbf True 5 KNN SMOTE True 6.244 rbf True 6 KNN SMOTE True 6.244 rbf True 7 Simple None True 6.244 rbf True 8 Simple None True 6.244 rbf	1018	1	Simple	SMOTETomek	True	0.213	sigmoid	True	0.0007	None
3 KNN SMOTETomek True 0.113 linear True 1 Simple None False 2.186 poly True 2 Simple Tomek True 7.117 rbf True 2 Simple Tomek True 6.844 rbf True 3 Simple Tomek True 6.244 rbf True 4 Simple Tomek True 6.244 rbf True 5 KNN SMOTETomek True 6.244 rbf True 4 KNN SMOTETomek True 0.244 rbf True 5 KNN SMOTE True 0.343 rbf True 1 Simple None True 0.384 rbf False 2 KNN Tomek True 0.309 rigmoid False 3 Simple None True 0.309 r	1018	2	Simple	Tomek	True	0.621	poly	True	0.0001	balanced
1 Simple None False 2.186 poly True 2 Simple SMOTETomek False 6.871 rbf True 1 Simple Tomek True 6.893 rbf True 2 Simple Tomek True 6.244 rbf True 1 KNN SMOTE True 6.244 rbf True 2 KNN SMOTE True 6.244 rbf True 3 KNN SMOTE True 0.218 linear True 2 KNN SMOTE True 0.43 rigmoid False 2 Simple SMOTE True 0.384 rbf True 2 Simple None True 0.309 rigmoid False 2 KNN Tomek True 0.309 rigmoid False 3 Simple SMOTETomek True 0.506	1018	3	KNN	SMOTETomek	True	0.113	linear	True	0.0039	balanced
2 Simple SMOTETOMEK False 6.871 rbf True 3 Simple Tomek True 6.803 rbf True 2 Simple Tomek True 6.244 rbf True 3 Simple Tomek True 6.244 rbf True 2 KNN SMOTE True 0.218 linear True 3 KNN SMOTETOMEK True 0.143 linear True 2 KNN SMOTETOMEK True 0.384 rbf True 2 Simple SMOTE True 0.384 rbf True 3 Simple Tomek True 0.300 rbf False 4 Simple SMOTETOMEK True 0.363 sigmoid False 5 KNN Tomek True 0.399 sigmoid False 6 KNN SMOTETOMEK True 0.19	1019	1	Simple	None	False	2.186	poly	True	0.0062	balanced
3 Simple Tomek False 7.892 rhf True 2 Simple Tomek True 6.803 rhf True 3 Simple Tomek True 6.244 rhf True 1 KNN SMOTE True 0.218 linear True 2 KNN SMOTETomek True 0.384 rhf True 2 Simple None True 0.384 rhf True 3 Simple Tomek True 0.300 rhf False 4 Simple None True 0.303 sigmoid False 5 KNN Tomek True 0.363 sigmoid False 1 Simple SMOTETomek True 0.352 rhf False 2 KNN SMOTETomek True 0.363 sigmoid False 3 Simple SMOTETomek True 0.190	1019	2	Simple	SMOTETomek	False	6.871	rbf	True	0.0040	None
1 Simple None True 6.803 rbf True 2 Simple Tomek True 6.244 rbf True 1 KNN SMOTE True 0.218 linear True 2 KNN SMOTETomek True 0.143 linear True 1 Simple None True 0.851 rbf False 2 Simple SMOTE True 0.384 rbf False 3 Simple None True 0.384 rbf False 4 Simple None True 0.300 rbf False 5 KNN Tomek True 0.363 sigmoid False 6 Simple SMOTETomek True 0.526 rbf False 1 Simple SMOTETomek True 0.393 sigmoid True 2 KNN SMOTETomek True 0.365 <td>1019</td> <td>3</td> <td>Simple</td> <td>Tomek</td> <td>False</td> <td>7.892</td> <td>rbf</td> <td>True</td> <td>0.0003</td> <td>balanced</td>	1019	3	Simple	Tomek	False	7.892	rbf	True	0.0003	balanced
2 Simple Tomek True 7.117 rbf True 3 Simple Tomek True 6.244 rbf True 2 KNN SMOTE True 0.143 linear True 3 KNN SMOTE True 0.143 linear True 2 KNN SMOTE True 0.134 rbf False 3 Simple None True 0.384 rbf True 4 Simple None True 0.384 rbf False 5 KNN Tomek True 0.384 rbf False 2 KNN Tomek True 0.363 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 4 KNN SMOTETomek True 0.586 sigmoid True 5 KNN SMOTETomek True 0.586 <t< td=""><td>1021</td><td>1</td><td>Simple</td><td>None</td><td>True</td><td>6.803</td><td>rbf</td><td>True</td><td>0.0058</td><td>balanced</td></t<>	1021	1	Simple	None	True	6.803	rbf	True	0.0058	balanced
3 Simple Tomek True 6.244 rbf True 1 KNN SMOTE True 0.218 linear True 2 KNN SMOTETomek True 0.143 linear True 1 Simple None True 0.851 rbf True 2 Simple Tomek True 0.900 rbf False 1 Simple None True 0.363 sigmoid False 2 KNN Tomek True 0.369 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 4 KNN SMOTETomek True 0.506 sigmoid True 5 KNN SMOTETomek True 0.526 rbf False 2 KNN SMOTETomek True 0.526 rbf False 3 KNN SMOTETomek True 0	1021	2	Simple	Tomek	True	7.117	rbf	True	0.0011	balanced
1 KNN SMOTE Tomek True 0.218 linear True 2 KNN SMOTE Tomek True 0.143 linear True 1 Simple None True 0.851 rbf True 2 Simple SMOTE True 0.304 rbf False 1 Simple None True 0.363 sigmoid False 2 KNN Tomek True 0.363 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 4 Simple SMOTETomek True 0.190 sigmoid True 5 KNN SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.190 sigmoid True 3 KNN SMOTETomek True 0.190 sigmoid True 4 True 0.190 sigmo	1021	3	Simple	Tomek	True	6.244	rbf	True	0.0005	balanced
2 KNN SMOTETomek True 0.143 linear True 3 KNN SMOTE True 0.851 rbf False 2 Simple SMOTE True 0.384 rbf True 3 Simple None True 0.300 rbf False 2 KNN Tomek True 0.363 sigmoid False 2 KNN Tomek True 0.399 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 4 KNN SMOTETomek True 0.190 sigmoid True 5 KNN SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.190 sigmoid True 3 KNN SMOTETomek True 0.190 sigmoid True 4 KNN SMOTETomek True	1040	1	KNN	SMOTE	True	0.218	linear	True	0.0019	None
3 KNN SMOTE True 1.384 sigmoid False 1 Simple None True 0.851 rbf True 2 Simple SMOTE True 0.384 rbf True 1 Simple None True 0.363 sigmoid False 2 KNN Tomek True 0.363 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 4 KNN SMOTETomek True 0.190 sigmoid True 5 KNN SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.190 sigmoid True 3 KNN SMOTETomek True 0.190 sigmoid True 3 KNN SMOTETomek True 0.190 sigmoid True	1040	2	KNN	SMOTETomek	True	0.143	linear	True	0.0001	balanced
1 Simple None True 0.851 rbf True 2 Simple Tomek True 0.384 rbf True 1 Simple None True 0.363 sigmoid False 2 KNN Tomek True 0.399 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 1 Simple SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.586 sigmoid True 3 KNN SMOTETomek True 0.586 sigmoid True 3 KNN SMOTETomek True 0.190 sigmoid True	1040	33	KNN	SMOTE	True	1.384	sigmoid	False	0.0012	balanced
2 Simple SMOTE True 0.384 rbf True 1 Simple None True 0.303 sigmoid False 2 KNN Tomek True 0.399 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 1 Simple SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.586 sigmoid True 3 KNN SMOTETomek True 0.586 sigmoid True	1053	1	Simple	None	True	0.851	rbf	True	0.0009	balanced
3 Simple Tomek True 0.900 rbf False 1 Simple None True 0.363 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 1 Simple SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.586 sigmoid True 3 KNN SMOTETomek True 1.275 rbf False	1053	2	Simple	SMOTE	True	0.384	$^{\mathrm{rpt}}$	True	0.0000	balanced
1 Simple KNN None Tomek True O.363 sigmoid sigmoid False 2 KNN Tomek True O.399 sigmoid False 1 Simple SMOTETomek KNN True O.190 sigmoid True True O.386 True O.386 2 KNN SMOTETomek True O.386 True O.386 sigmoid True False	1053	3	Simple	Tomek	True	0.900	rbf	False	0.0012	balanced
2 KNN Tomek True 0.399 sigmoid False 3 Simple SMOTETomek True 0.526 rbf False 1 Simple SMOTETomek True 0.190 sigmoid True 2 KNN SMOTETomek True 0.586 sigmoid True 3 KNN SMOTETomek True 1.275 rbf False	1461	1	Simple	None	True	0.363	sigmoid	False	0.0004	balanced
3 Simple SMOTETomek True 0.526 rbf False 1 Simple SMOTETomek True 0.190 sigmoid True 2 KNN SMOTE True 0.586 sigmoid True 3 KNN SMOTETomek True 1.275 rbf False	1461	2	KNN	Tomek	True	0.399	sigmoid	False	0.0004	balanced
1 Simple SMOTETomek True 0.190 sigmoid True 2 KNN SMOTE True 0.586 sigmoid True 3 KNN SMOTETomek True 1.275 rbf False	1461	3	Simple	SMOTETomek	True	0.526	rbf	False	0.0003	balanced
2 KNN SMOTE True 0.586 sigmoid True 3 KNN SMOTETomek True 1.275 rbf False	41160	1	Simple	SMOTETomek	True	0.190	sigmoid	True	0.0002	balanced
3 KNN SMOTETomek True 1.275 rbf False	41160	2	KNN	SMOTE	True	0.586	sigmoid	True	0.0007	balanced
	41160	3	KNN	SMOTETomek	True	1.275	rbf	False	0.0037	None

C Information about datasets

Table 4: Meta data of each dataset

Dataset ID	Observations	Features	Share of underrepresented class	Total missing values
976	9961	14	0.162	0
980	5620	64	0.102	0
1002	7485	55	0.106	0
1018	8844	56	0.064	0
1019	10992	16	0.104	0
1021	5473	10	0.102	0
1040	14395	108	0.062	0
1053	10885	21	0.193	25
1461	45211	16	0.117	0
41160	31406	22	0.095	29756