Szkic artykułu

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1 zarys wstępu: wypisanie źródeł, które będą zacytowane we wstępie wraz z komentarzem pod jakim kątem będą opisane

In the introduction we would like to present (below some main thoughts),

- the main differences between traditional approach and autoML approach,
- why AutoML can be beneficial in solving ML problems,
- the different approaches to AutoML,
- introduction to why we choose AutoSklearn2.0

Some ideas considering first bullet point

- autoML gives you opportunity to use automated algorithms to build predictive models,
- traditional approach requires some domain knowledge and time to build and compare over a dozen models.

Another ideas considering why AutoML can be beneficial

- it allows to automates time-consuming, iterative tasks,
- can product models with high scale, efficiency while maintaining quality,
- it doesn't require any significant domain knowledge.

The different approaches to AutoML (citations)

- Gama [3] - different approach into an AutoML (it uses genetic algorithms to optimize score) (lower exemplary text, which can be used)
  Gama uses different approach to optimize scores. There are three optimization algorithms, which search for optimal machine learning pipelines: random search, an asychronous successive halving algorithm and an asynchronous multi-objective evolutionary algorithm.
- Autosklearn [2] - using meta-learning for initializing the Bayesian optimizer and automated ensemble construction. (lower some example text, which can be used)
  It uses meta-features (i.e characteristics of the dataset), which can be computed efficiently, to choose which algorithm to use on a new dataset. These meta-features are complimentary to Bayesian optimization. They can quickly suggest some ML algorithms that are likely to perform well. But they don't work well with the high dimensional configuration spaces.
- Autosklearn2.0 [1] - the improvement of autosklearn (lower exemplary text, which can be used)
  Autosklearn2.0 presents two new parts, which improved performance of package. One of them was Portfolio Successive Halving. Another one of them was proposal of model-base policy selector to automatically chose the best optimization policy for an AutoML system for a given dataset.

2 opis wybranego frameworku autoML (w oparciu o prezentację z KM1)

Auto-sklearn is an automated machine learning toolkit and a drop-in replacement for a scikit-learn estimator. It allows its users to automate:

- data preprocessing
- feature preprocessing
- hyperparameter optimization
- model selection
- model evaluation

Auto-sklearn is currently suitable only for classification. It chooses from sklearn-based models. The space of possible models currently spans 16 classifiers. Auto-sklearn performs following preprocessing techniques:

- Balances the dataset using class weights
- For categorical features it chooses between One Hot Encoding and no preprocessing. It also coerces rarely occurring categories, by default these smaller than 0.01 of the observations
- It imputes missing values using mean, median or mode
- Rescales the data, by default using standardization.
- Performs quantile Transformation by defult with 1000 quantiles and uniform output distribution
- Handles otliers removing the median and scaling the data according to the quantile range

After data pre-processing, features may be optionally pre-processed with one or more of the following categories of feature pre-processors:

- Matrix decomposition using PCA, truncated SCV, kernel PCA or ICA
- Univariate feature selection
- Classification-based features selection
- Feature clustering
- Kernel approximations
- Polynomial feature expansion
- Feature embeddings
- Sparse representation and transformation

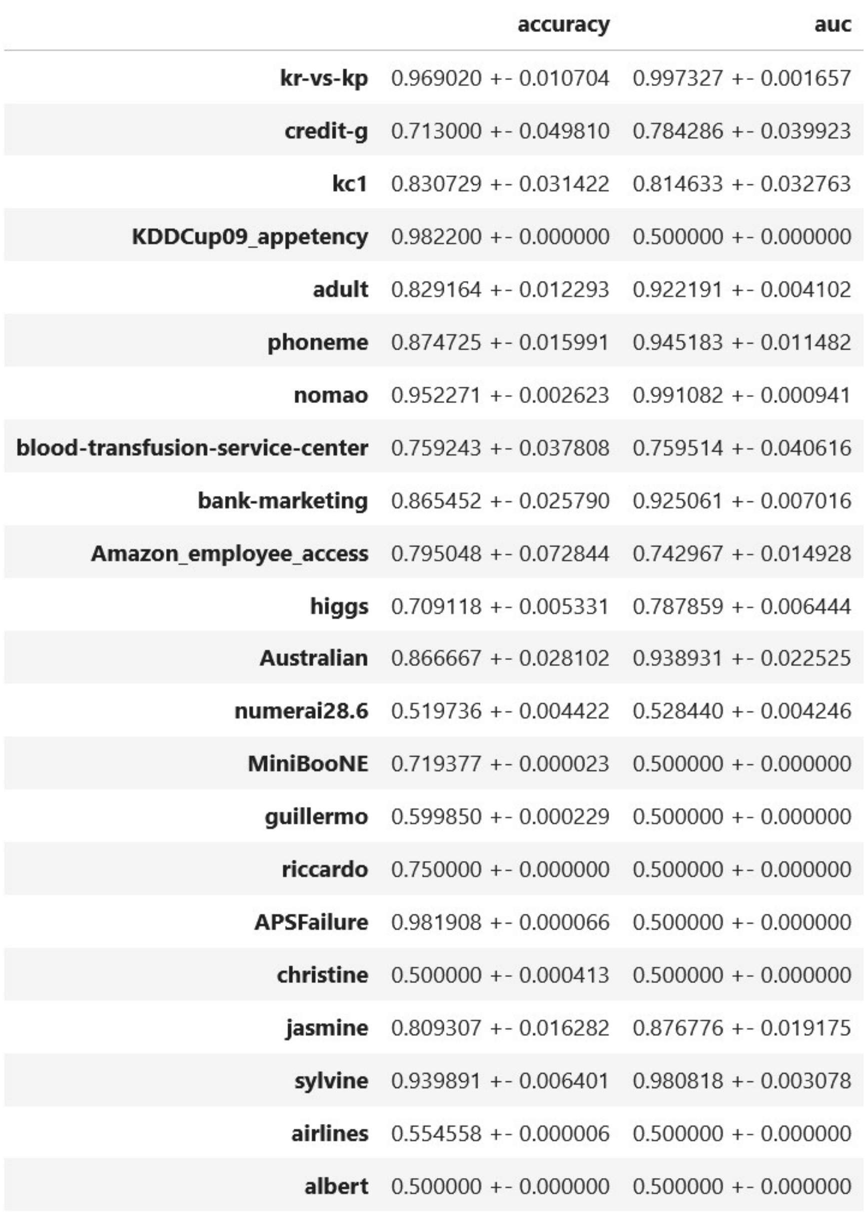
For Auto-sklearn to find the best performing pipeline in given time from vast searching space the authors constructed a portfolio consisting of high-performing and complementary ML pipelines to perform well on as many datasets as possible offline. Then for a dataset at hand all pipelines in this portfolio are simply evaluated one after the other and if there is time left afterwards, the algorithm continues with pipelines suggested by Bayesian Optimization warmstarted with the evaluated portfolio pipelines. Auto-sklearn uses use an early-stopping strategy inside the whole search space which performs well on large datasets, but it's mostly useful for tree-based classifiers. To improve model selection the framework uses a multi-fidelity optimization method such as BOHB and several different strategies, including holdout and cross-validation. It also builds an automated policy selection on top of the previous improvements to select the best strategy.

3 Preprocessing

We made some functions responsible for the whole preprocessing and we store them in separate .py file. It is worth mentioning that we assume every column including data connected with dates in given set is in Datetime type. First step of preprocess is to make some changes in Datetime columns. We can not leave them without a change, because Auto sklearn 2.0 would treat them as a categorical column, thus it would be One Hot Encoded. This kind of operation creates many columns, which does not really contribute to any predictions. That is why we divide values in each row into three new columns, first of them is a day, second one is month and last of them is the year of the Datetime object. Then the original column is removed from data set. Second step is to change numerical columns which contains no more than 10 unique values to categorical type. Our framework does not know how to operate on columns with type object, so we decided to convert every object type column into categorical type. Sometimes we can come across a column in a data set which contains only NA or NaN values. It does not give us any information, that is why we remove them before giving the data to our framework.

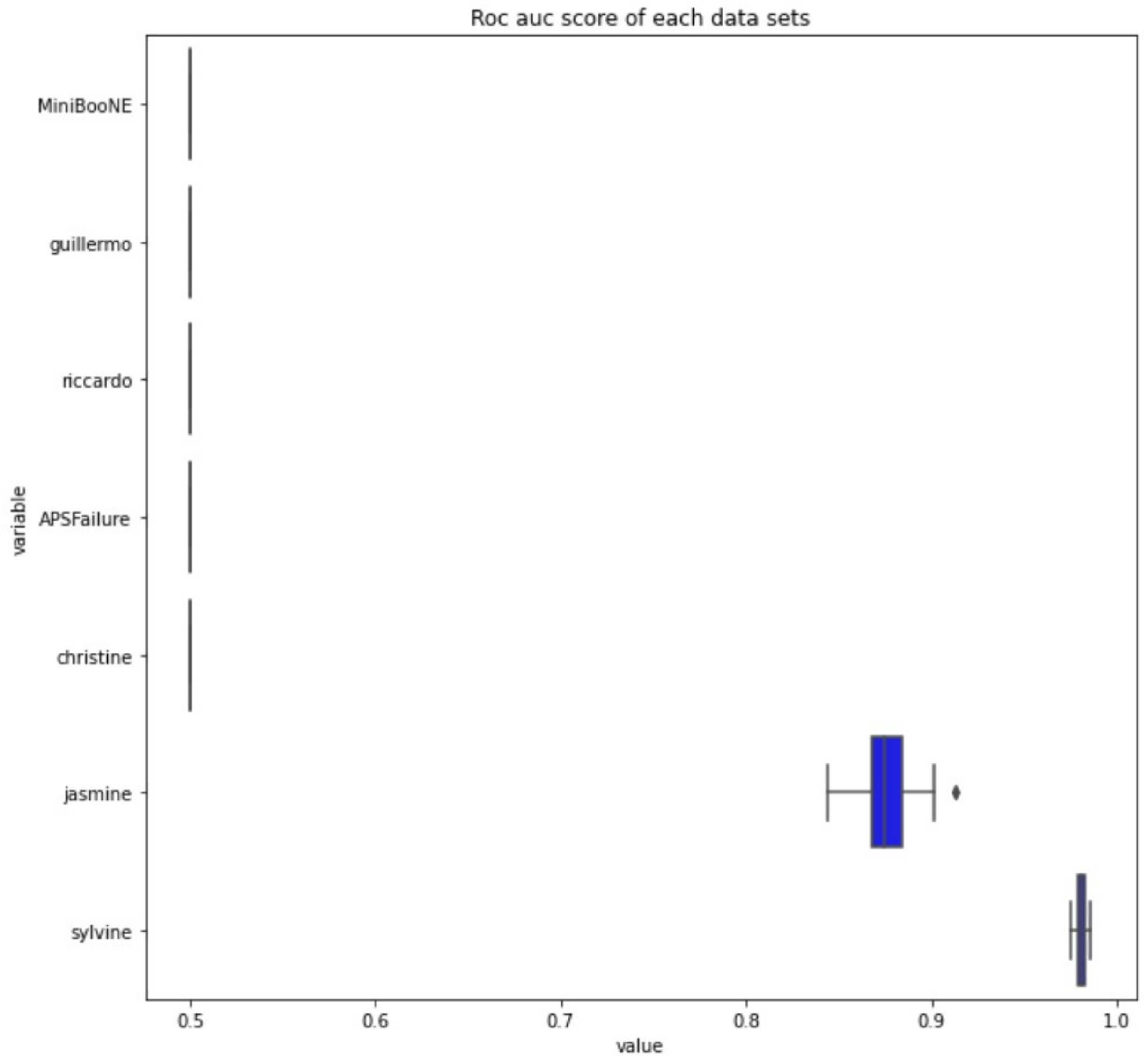
4 Evaluation scores

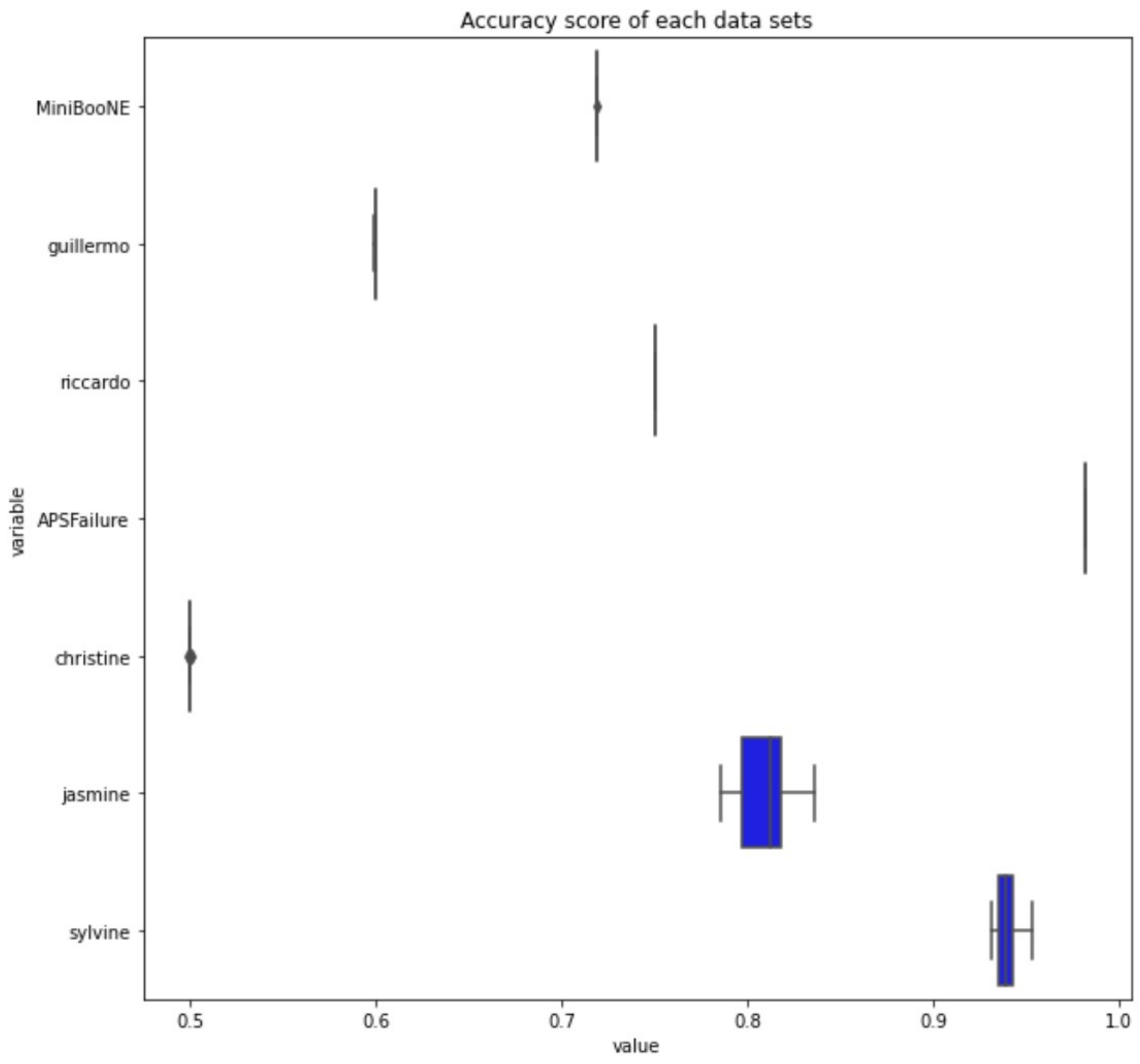
To test our framework we decided to use data sets from OpenML. We chose twenty-two sets related to binary classification issue. We used ten fold cross-validation on each set to test performance. Our first results are surely not the best one, because we gave our framework only sixty second on each fold due to an *No space left on device* error. To rate the scores received for each set we decided to use two metrics, accuracy score and roc auc score. We did not use f1 score, since we encountered a problem with finding out which value in target column is positive and which one is negative one. We would like to present our mean scores in a table:



	accuracy	auc
kr-vs-kp	0.969020 +- 0.010704	0.997327 +- 0.001657
credit-g	0.713000 +- 0.049810	0.784286 +- 0.039923
kc1	0.830729 +- 0.031422	0.814633 +- 0.032763
KDDCup09_appetency	0.982200 +- 0.000000	0.500000 +- 0.000000
adult	0.829164 +- 0.012293	0.922191 +- 0.004102
phoneme	0.874725 +- 0.015991	0.945183 +- 0.011482
nomao	0.952271 +- 0.002623	0.991082 +- 0.000941
blood-transfusion-service-center	0.759243 +- 0.037808	0.759514 +- 0.040616
bank-marketing	0.865452 +- 0.025790	0.925061 +- 0.007016
Amazon_employee_access	0.795048 +- 0.072844	0.742967 +- 0.014928
higgs	0.709118 +- 0.005331	0.787859 +- 0.006444
Australian	0.866667 +- 0.028102	0.938931 +- 0.022525
numerai28.6	0.519736 +- 0.004422	0.528440 +- 0.004246
MiniBooNE	0.719377 +- 0.000023	0.500000 +- 0.000000
guillermo	0.599850 +- 0.000229	0.500000 +- 0.000000
riccardo	0.750000 +- 0.000000	0.500000 +- 0.000000
APSFailure	0.981908 +- 0.000066	0.500000 +- 0.000000
christine	0.500000 +- 0.000413	0.500000 +- 0.000000
jasmine	0.809307 +- 0.016282	0.876776 +- 0.019175
sylvine	0.939891 +- 0.006401	0.980818 +- 0.003078
airlines	0.554558 +- 0.000006	0.500000 +- 0.000000
albert	0.500000 +- 0.000000	0.500000 +- 0.000000

After we will overcome an error with the lack of memory we will run the framework for every data set once again, this time with few minutes on each fold. But for now we can present a boxplot of scores from some sets from that shortened run.


Roc auc score of each data sets
MiniBooNE
guillermo
riccardo
APSFailure
christine
jasmine
sylvine
variable
0.5
0.6
0.7
0.8
0.9
1.0
value



References

[1] Matthias Feurer et al. “Auto-Sklearn 2.0: Hands-free AutoML via Meta-Learning”. In: (2020).

[2] Matthias Feurer et al. “Efficient and Robust Automated Machine Learning”. In: *Advances in Neural Information Processing Systems 28 (2015)*. 2015, pp. 2962–2970.

[3] Pieter Gijsbers and Joaquin Vanschoren. “GAMA: a General Automated Machine learning Assistant”. In: *CoRR* abs/2007.04911 (2020). arXiv: `2007.04911`. URL: `https://arxiv.org/abs/2007.04911`.