

Automatic Exploration of Machine Learning Experiments on OpenML

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Abstract

Understanding the influence of hyperparameters on the performance of a machine learning algorithm is an important part of finding a well performing and adequately tuned algorithm for a given dataset. As to date no dataset exists to support this required understanding for state of the art algorithms like xgboost or random forest, this paper presents a large and open dataset for this problem (see [Probst and Kühn, 2018] to access the dataset). The dataset contains the performance results (AUC, accuracy and Brier score) of six different machine learning algorithms, the used hyperparameters that were set by a random search, runtimes and meta-data for each dataset. It can be used for meta-learning, finding good defaults, measuring the tunability of algorithms and hyperparameters, benchmarking of algorithms and other tasks mainly related with hyperparameters.

1 Introduction

When applying machine learning on real world datasets, users have to choose from a large selection of different machine learning algorithms with many of these algorithms offering a set of hyperparameters, which can be specified by the user and can have a significant influence on the performance of the algorithm. Since there is no free lunch in algorithm selection and one can not expect one algorithm to outperform all the others [Wolpert, 2001], a crucial question practitioners have to face on a daily basis therefore is the selection of the "right" algorithm with the "right" hyperparameters for a given dataset. This problem is not easy to solve, because choices are many and the evaluation of a single machine learning run usually is computationally expensive and the hyperparameter-space is complex [Claesen and Moor, 2015]. A usual approach is to run a tuning algorithm like bayesian optimization to find the best hyperparameter setting. While showing promising results, bayesian optimization and other hyperparameter optimization techniques require a large overhead.

Meta-learning tries to decrease this overhead [Feurer et al., 2015], by using information of previous algorithm runs on other datasets. A requirement for this, is to have a meta-learning dataset, that contains the information of previous runs. With this paper we provide a open accesible dataset that contains information of previous runs of six different machine learning algorithms on 38 classification datasets. As large datasets like Imagenet [Deng et al., 2009] have shown to improve the progress of machine learning, we hope to support the development of new meta-learning algorithms with this dataset.

We first describe how we created such a dataset by executing random machine learning experiments and storing the results on OpenML [Vanschoren et al., 2013], an open source database for machine learning problems. Then the possibilities of accessing this dataset are shortly presented. Finally we briefly discuss potential usage of the dataset.

2 Related literature

Other related projects and papers (e.g. AutoWeka) Dataset repositories: - [Dheeru and Karra Taniskidou, 2017]

Similar datasets: - [Reif, 2012]

3 Creating the dataset

To create the dataset different supervised machine learning algorithms were defined with ranges for their relevant hyperparameters and run on different classification tasks. The following six frequently used algorithms were chosen from their respective R-packages: elastic net (`glmnet` package), decision tree (`rpart`), k-nearest neighbors (`knn`), support vector machines (`svm`), random forest (`ranger`) and gradient boosting (`xgboost`). These algorithms cover a broad range of approaches to machine learning and therefore should explore most datasets reasonably well. *Was heißt explore well?* For each algorithm the available hyperparameters were explored in a predefined range (see table 1). Values of some of these ranges were transformed by the function found in column *trafo* to explore the range in a non-uniform manner. This is useful, if, for example, minor changes in a hyperparameter are not expected to have a significant impact on the performance of an algorithm.

These algorithms are run on a subset of the OpenML100 Benchmark suite [Bischl et al., 2017], which consists of 100 classification datasets carefully curated from the thousands of datasets available on OpenML. We only include datasets without missing data and with binary outcome resulting in 38 datasets. The datasets with their specific characteristics can be found in table 3.

Following the search paradigm of random search the bot iteratively executes several steps:

1. Randomly draw one of the six algorithms

algorithm	hyperparameter	type	lower	upper	trafo
glmnet	alpha	numeric	0	1	-
	lambda	numeric	-10	10	2^x
rpart	cp	numeric	0	1	-
	maxdepth	integer	1	30	-
	minbucket	integer	1	60	-
	minsplit	integer	1	60	-
kkn	k	integer	1	30	-
svm	kernel	discrete	-	-	-
	cost	numeric	-10	10	2^x
	gamma	numeric	-10	10	2^x
	degree	integer	2	5	-
ranger	num.trees	integer	1	2000	-
	replace	logical	-	-	-
	sample.fraction	numeric	0	1	-
	mtry	numeric	0	1	$x \cdot p$
	respect.unordered.factors	logical	-	-	-
	min.node.size	numeric	0	1	n^x
xgboost	nrounds	integer	1	5000	-
	eta	numeric	-10	0	2^x
	subsample	numeric	0	1	-
	booster	discrete	-	-	-
	max_depth	integer	1	15	-
	min_child_weight	numeric	0	7	2^x
	colsample_bytree	numeric	0	1	-
	colsample_bylevel	numeric	0	1	-
	lambda	numeric	-10	10	2^x
	alpha	numeric	-10	10	2^x

Table 1: Hyperparameters of the algorithms. p refers to the number of variables and n to the number of observations

2. Randomly draw a hyperparameter setting of the chosen algorithm
3. Randomly draw one of the benchmark datasets
4. Download the dataset from OpenML
5. Benchmark the specified algorithm on the specified dataset with 10-fold cross-validation
6. Upload the benchmark results with time measurements to OpenML with the identification tag `mlrRandomBot`

The code for the bot can be found on GitHub (<https://GitHub.com/ja-thomas/OMLbots>), the R packages `mlr` [Bischl et al., 2016] and `OpenML` [Casalicchio et al., 2017] were used for the whole process.

Data.id	Name	nObs	nFeat	majPerc	numFeat	catFeat
3	kr-vs-kp	3196	37	0.52	0	37
31	credit-g	1000	21	0.70	7	14
37	diabetes	768	9	0.65	8	1
44	spambase	4601	58	0.61	57	1
50	tic-tac-toe	958	10	0.65	0	10
151	electricity	45312	9	0.58	7	2
312	scene	2407	300	0.82	294	6
333	monks-problems-1	556	7	0.50	0	7
334	monks-problems-2	601	7	0.66	0	7
335	monks-problems-3	554	7	0.52	0	7
1038	gina_agnostic	3468	971	0.51	970	1
1046	mozilla4	15545	6	0.67	5	1
1049	pc4	1458	38	0.88	37	1
1050	pc3	1563	38	0.90	37	1
1063	kc2	522	22	0.80	21	1
1067	kc1	2109	22	0.85	21	1
1068	pc1	1109	22	0.93	21	1
1120	MagicTelescope	19020	12	0.65	11	1
1570	wilt	4839	6	0.95	5	1
1510	wdbc	569	31	0.63	30	1
1489	phoneme	5404	6	0.71	5	1
1494	qsar-biodeg	1055	42	0.66	41	1
1504	steel-plates-fault	1941	34	0.65	33	1
1479	hill-valley	1212	101	0.50	100	1
1480	ilpd	583	11	0.71	9	2
1485	madelon	2600	501	0.50	500	1
1486	nomao	34465	119	0.71	89	30
1487	ozone-level-8hr	2534	73	0.94	72	1
1467	climate-model-simulation-crashes	540	21	0.91	20	1
1471	eeg-eye-state	14980	15	0.55	14	1
1462	banknote-authentication	1372	5	0.56	4	1
1464	blood-transfusion-service-center	748	5	0.76	4	1
1461	bank-marketing	45211	17	0.88	7	10
4134	Bioresponse	3751	1777	0.54	1776	1
1220	Click_prediction_small	39948	12	0.83	11	1
4534	PhishingWebsites	11055	31	0.56	0	31
4135	Amazon_employee_access	32769	10	0.94	0	10
1036	sylva_agnostic	14395	217	0.94	216	1
1043	ada_agnostic	4562	49	0.75	48	1
1176	Internet-Advertisements	3279	1559	0.86	1558	1
40509	Australian	690	15	0.56	14	1

Table 2: Included datasets with meta-data. *nFeat* are the number of Features, *majPerc* the percentage of observations with the most common class, *numFeat* the number of numeric features and *catFeat* the number of categorical features.

Extraction of results

After having run more than 6 million benchmark experiments the results of the bot are downloaded from OpenML. Because of technical reasons on one dataset (data.id = 4135) all algorithms except of **rpart** and **ranger** provide errors, so we exclude it and 38 datasets are left.

For each of the algorithms we only take 500000 experiments for building surrogate models. They are chosen by the following procedure: for each algorithm, a threshold B is set (see below) and, if the number of results for a dataset exceeds B , we draw randomly B of the results obtained for this algorithm and this dataset. For each algorithm, the threshold value B is chosen for each algorithm separately to exactly obtain 500000 results for each algorithm.

For **kknn** we only executed 30 experiments per dataset because this number of experiments is high enough to cover the hyperparameter space (that only consists of the parameter k for $k \in 1, \dots, 30$) appropriately, resulting in 1140 experiments. In total this results in around 2.5 million experiments.

The distribution of the runs on the datasets and algorithms can be seen in table 3.

Data_id	glmnet	rpart	kknn	svm	ranger	xgboost
3	15547	14633	30	19644	15139	16867
31	15547	14633	30	19644	15139	16867
37	15546	14633	30	15985	15139	16866
44	15547	14633	30	19644	15139	16867
50	15547	14633	30	19644	15139	16866
151	15547	14632	30	2384	12517	16866
312	6613	13455	30	18740	12985	15886
333	15546	14632	30	19644	15139	16867
334	15547	14633	30	19644	14492	16867
335	15547	14633	30	15123	15139	10002
1038	15547	5151	30	5716	4827	1370
1046	15547	14633	30	5422	8842	11812
1049	7423	14632	30	12064	15139	4453
1050	15547	14633	30	19644	11357	13758
1063	15547	14633	30	19644	7914	16866
1067	15546	14632	30	10229	7386	16866
1068	15546	14633	30	13893	8173	16866
1120	15531	7477	30	3908	9760	8143
1461	6970	14073	30	2678	14323	2215
1462	8955	14633	30	6320	15139	16867
1464	15547	14632	30	19644	15139	16867
1467	15547	14633	30	4441	15139	16866
1471	15547	14633	30	9725	13523	16866
1479	15546	14633	30	19644	15140	16867
1480	15024	14633	30	19644	15139	16254
1485	8247	10923	30	10334	15139	9237
1486	3866	11389	30	1490	15139	5813
1487	15547	6005	30	19644	15139	11194
1489	15547	14633	30	17298	15139	16867
1494	15547	14632	30	19644	15139	16867
1504	15547	14633	30	19644	15140	16867
1510	15547	14633	30	19644	15139	16867
1570	15546	14632	30	19644	15139	16867
4134	1493	3947	30	560	14516	2222
4534	2801	3231	30	2476	15139	947

Table 3: Results by dataset and algorithm

4 Access to the benchmark results

The results of the benchmarks can be accessed in different ways:

- The easiest way to access them is to go to the figshare repository [Probst and Kühn, 2018] and download the .csv files or the .RData file.
- Alternatively the code for the extraction of the data from the nightly database snapshot of OpenML can be found here: https://github.com/ja-thomas/OMLbots/blob/master/snapshot_database/database_extraction.R

5 Potential usage of the results

The results can be used to discover effects of the hyperparameters on performances of the different algorithms on different datasets.

This can be used to:

- Find good defaults for the algorithms that work well on many datasets
- Measure differences between the algorithms
- Optimize tuning algorithms:
 - Measure the tunability of algorithms and find out which parameters should be tuned [see Probst et al., 2018]
 - Use the results to get priors for tuning algorithms - in which regions of the hyperparameter space should be searched with higher probability?
- Meta-Learning: Train models that based on dataset characteristics and possibly time limitations propose hyperparameter settings that perform good on a specific dataset

Weaknesses: Dimension is too high, e.g., for xgboost. The best regions are not explored enough. The datasets are not chosen to be *representative* for a specific domain.

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