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 scientific topic in itself and can help to improve automatic hyperparameter tuning procedures. Unfortunately, experimental meta data for this purpose is still rare. This paper presents a large, free and open dataset addressing this problem, containing results on 38 OpenML data sets, six different machine learning algorithms and many different hyperparameter configurations. Results where generated by an automated random sampling strategy, termed the OpenML Random Bot. Each algorithm was cross-validated up to 20,000 times per dataset with different hyperparameters settings, resulting in a meta dataset of around 2.5 million experiments overall.

1. Introduction
When applying machine learning algorithms on real world datasets, users have to choose from a large selection of different algorithms with many of them offering a set of hyperparameters to control algorithmic performance. Although sometimes default values exist, there is no agreed upon principle for their definition (but see our recent work in in (Probst et al., 2018) for a potential approach). Automatic tuning of such parameters is a possible solution (Claesen and Moor, 2015), but comes with a considerable computational burden.

Meta-learning tries to decrease this cost (Feurer et al., 2015), by reusing information of previous runs of the algorithm on similar datasets, which obviously requires access to such prior empirical results. With this paper we provide a freely accessible meta dataset that contains around 2.5 million runs of six different machine learning algorithms on 38 classification datasets.

Large, freely available datasets like Imagenet (Deng et al., 2009) are important for the progress of machine learning, we hope to support developments in the area of meta-learning and benchmarking, meta-learning and hyperparameter tuning with our work here.

While similar meta-datasets have been created in the past, we were not able to access them by the links provided in their respective papers: Smith et al. (2014) provides a repository with Weka-based machine learning experiments on 72 data sets, 9 machine learning algorithms, 10 hyperparameter settings for each algorithm, and several meta-features of each data set. Reif (2012) created a meta-dataset based on machine learning experiments on 83 datasets, 6 classification algorithms, and 49 meta features.

In this paper, we describe our experimental setup, specify how our meta-dataset is created by running random machine learning experiments through the OpenML platform (Vanschoren et al., 2013) and explain how to access our results.
2. Considered ML data sets, algorithms and hyperparameters

To create the meta dataset, six supervised machine learning algorithms are run on 38 classification tasks. For each algorithm the available hyperparameters are explored in a predefined range (see Table 1). Some of these hyperparameters are transformed by the function found in column \textit{trafo} of Table 1 to allow non-uniform sampling, a usual procedure in tuning.

| 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    | -     |
| kknn      | 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    | \(2^x\) |

Table 1: Hyperparameters of the algorithms. \(p\) refers to the number of variables and \(n\) to the number of observations. The used algorithms are \textit{glmnet} (Friedman et al., 2010), \textit{rpart} (Therneau and Atkinson, 2018), \textit{kknn} (Schliep and Hechenbichler, 2016), \textit{svm} (Meyer et al., 2017), \textit{ranger} (Wright and Ziegler, 2017) and \textit{xgboost} (Chen and Guestrin, 2016).

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 (Vanschoren et al., 2013). We only include datasets without missing data and with a binary outcome resulting in 38 datasets. The datasets and their respective characteristics can be found in Table 2.
| Data_id | Task_id | Name            | n   | p    | majPerc | numFeat | catFeat |
|---------|---------|-----------------|-----|------|---------|---------|---------|
| 3       | 336     | kr-vs-kp        | 3196| 37   | 0.52    | 0       | 37      |
| 31      | 31      | credit-g        | 1000| 21   | 0.70    | 0       | 14      |
| 37      | 37      | diabetes        | 768 | 9    | 0.65    | 8       | 1       |
| 44      | 43      | spam.base       | 4001| 50   | 0.61    | 57      | 1       |
| 50      | 49      | tic-tac-toe     | 958 | 10   | 0.50    | 0       | 10      |
| 151     | 219     | electricity     | 45312| 3770 | 0.58    | 7       | 2       |
| 312     | 3485    | scene           | 2407| 300  | 0.82    | 294     | 6       |
| 333     | 3492    | monks-problems-1| 556 | 7    | 0.50    | 0       | 7       |
| 334     | 3493    | monks-problems-2| 601 | 7    | 0.66    | 0       | 7       |
| 335     | 3494    | monks-problems-3| 554 | 7    | 0.52    | 0       | 7       |
| 1036    | 3889    | sylvia_agnostic | 14395| 217  | 0.94    | 216     | 1       |
| 1038    | 3891    | gina_agnostic   | 3468| 971  | 0.51    | 970     | 1       |
| 1043    | 3896    | ada_agnostic    | 4562| 49   | 0.75    | 48      | 1       |
| 1046    | 3899    | mozilla4        | 15545| 6    | 0.67    | 5       | 1       |
| 1049    | 3902    | pc4             | 1458| 38   | 0.88    | 37      | 1       |
| 1050    | 3903    | pc3             | 1563| 38   | 0.90    | 37      | 1       |
| 1063    | 3913    | kc2             | 522 | 22   | 0.80    | 21      | 1       |
| 1067    | 3917    | kc1             | 2109| 22   | 0.85    | 21      | 1       |
| 1068    | 3918    | pc1             | 1109| 22   | 0.93    | 21      | 1       |
| 1120    | 3954    | MagicTelescope  | 19020| 12   | 0.65    | 11      | 1       |
| 1461    | 14965   | bank-marketing  | 45211| 17   | 0.88    | 7       | 10      |
| 1462    | 10093   | banknote-authentication | 1372 | 5 | 0.56 | 4 | 1 |
| 1464    | 10101   | blood-transfusion-service-center | 748 | 5 | 0.76 | 4 | 1 |
| 1467    | 9980    | climate-model-simulation-crashes | 540 | 21 | 0.91 | 20 | 1 |
| 1471    | 9983    | org-eye-state   | 14880| 15  | 0.55    | 14      | 1       |
| 1479    | 9970    | hill-valley     | 1212101 | 100 | 0.50    | 100     | 1       |
| 1480    | 9971    | ilpd            | 583 | 11   | 0.71    | 9       | 2       |
| 1485    | 9976    | madelon         | 2600 | 501 | 0.50    | 500     | 1       |
| 1486    | 9977    | nomao           | 34465| 119 | 0.71  | 89      | 30      |
| 1487    | 9978    | ozone-level-8hr | 2534 | 73 | 0.94 | 72 | 1 |
| 1489    | 9952    | phoneme         | 5404 | 6 | 0.71 | 5 | 1 |
| 1494    | 9957    | quasar-bioseg   | 1055 | 42 | 0.66 | 41 | 1 |
| 1504    | 9967    | steel-plates-fault | 1941 | 34 | 0.65 | 33 | 1 |
| 1510    | 9946    | wilbc           | 569 | 31   | 0.63    | 30      | 1       |
| 1570    | 9944    | wilt            | 4839| 6    | 0.95    | 5       | 1       |
| 4134    | 14966   | Bioresponse     | 37511777 | 0.54 | 1776 | 1 |
| 4534    | 34537   | PhishingWebsites | 11055| 81 | 0.56 | 0 | 31 |

Table 2: Included datasets and respective characteristics. $n$ are the number of observations, $p$ the number of features, $maj\text{class}$ the percentage of observations in the largest class, $num\text{Feat}$ the number of numeric features and $cat\text{Feat}$ the number of categorical features.

### 3. Random Experimentation Bot

To conduct a large number of experiments a bot was implemented to automatically plan and execute runs, following the paradigm of random search. The bot iteratively executes these steps:

1. Randomly sample a task $T$ (with an associated data set) from Table 2.
2. Randomly sample one ML algorithm $A$.
3. Randomly sample a hyperparameter setting $\theta$ of algorithm $A$, uniformly from the ranges specified in Table 1, then transform, if a transformation function is given.
4. Obtain task $T$ (and dataset) from OpenML and store it locally.
5. Evaluate algorithm $A$ with configuration $\theta$ on task $T$, with associated 10-fold cross-validation from OpenML.
6. Upload run results to OpenML, including hyperparameter configuration and time measurements.
7. OpenML now calculates various performance metrics for the uploaded cross-validated predictions.
8. The OpenML-ID of the bot (2702) and the tag **mlrRandomBot** is used for identification.

A clear advantage of random sampling is that all bot runs are completely independent of each other, making all experiments embarrassingly parallel. Furthermore, more experiments can easily and conveniently added later on, without introducing any kind of bias into the sampling method.
The bot is developed open source in R and can be found on GitHub\(^1\). The bot is based on the R packages \texttt{mlr} (Bischl et al., 2016) and \texttt{OpenML} (Casalicchio et al., 2017) and written in modular form such that it can be extended with new sampling strategies for hyperparameters, algorithms and datasets in the future. Parallelization was performed with R package \texttt{batchtools} (Lang et al., 2017).

After more than 6 million benchmark experiments the results of the bot are downloaded from OpenML. For each of the algorithms 500000 experiments are used to obtain the final dataset. The experiments 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. The threshold value $B$ is chosen for each algorithm separately to exactly obtain in total 500000 results for each algorithm.

For \texttt{kknn} we only execute 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 $k \in \{1, \ldots, 30\}$) appropriately, resulting in 1140 experiments. All in all this results in around 2.5 million experiments.

The distribution of the runs on the datasets and algorithms is displayed in Table 3.

| Data_id | Task_id | glmnet | rpart | kknn | svm | ranger | xgboost | Total |
|---------|---------|--------|-------|------|-----|--------|---------|-------|
| 4       | 3       | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 31      | 36      | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 37      | 43      | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 44      | 49      | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 50      | 51      | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 151     | 219     | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 312     | 3485    | 6613   | 13455 | 30   | 18740| 12985  | 15886  | 67709 |
| 333     | 3492    | 15546  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 334     | 3493    | 15547  | 14633 | 30   | 19644| 14492  | 16867  | 61976 |
| 335     | 3494    | 15547  | 14633 | 30   | 15123| 15139  | 10002  | 70474 |
| 1036     | 3898    | 14937  | 14633 | 30   | 2338 | 7397   | 2581   | 41916 |
| 1038     | 3891    | 15547  | 5151  | 30   | 5716 | 4827   | 1370   | 32641 |
| 1043     | 3896    | 6466   | 14633 | 30   | 10121| 3788   | 16867  | 51905 |
| 1046     | 3899    | 15547  | 14633 | 30   | 5422 | 8842   | 11812  | 56286 |
| 1049     | 3902    | 7423   | 14633 | 30   | 12064| 15139  | 4453   | 53741 |
| 1050     | 3903    | 15547  | 14633 | 30   | 19644| 11357  | 13758  | 74969 |
| 1063     | 3913    | 15547  | 14633 | 30   | 19644| 7914   | 16866  | 74634 |
| 1067     | 3917    | 15546  | 14632 | 30   | 10229| 7386   | 16866  | 64689 |
| 1068     | 3918    | 15546  | 14633 | 30   | 13893| 8173   | 16866  | 69141 |
| 1120     | 3954    | 15531  | 7477  | 30   | 3908 | 9760   | 8143   | 44849 |
| 1461     | 14965   | 6970   | 14073 | 30   | 2678 | 14323  | 2235   | 60289 |
| 1462     | 10093   | 8955   | 14633 | 30   | 6320 | 15139  | 16867  | 61944 |
| 1464     | 10101   | 15547  | 14632 | 30   | 19644| 15139  | 16867  | 81859 |
| 1467     | 9980    | 15547  | 14633 | 30   | 4441 | 15139  | 16866  | 66656 |
| 1471     | 9983    | 15547  | 14633 | 30   | 9725 | 15323  | 16866  | 70324 |
| 1479     | 9970    | 15546  | 14633 | 30   | 19644| 15140  | 16867  | 81860 |
| 1480     | 9971    | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 1485     | 9976    | 8247   | 10923 | 30   | 10334| 15139  | 9237   | 35910 |
| 1486     | 9977    | 3866   | 11389 | 30   | 1490 | 15139  | 5813   | 37727 |
| 1487     | 9978    | 15547  | 6005  | 30   | 19644| 15139  | 11194  | 67559 |
| 1489     | 9952    | 15547  | 14633 | 30   | 17298| 15139  | 16867  | 79514 |
| 1494     | 9957    | 15547  | 14632 | 30   | 19644| 15139  | 16867  | 81859 |
| 1504     | 9967    | 15547  | 14633 | 30   | 19644| 15140  | 16867  | 81861 |
| 1510     | 9946    | 15547  | 14633 | 30   | 19644| 15139  | 16867  | 81860 |
| 1570     | 9914    | 15546  | 14632 | 30   | 19644| 15139  | 16867  | 81858 |
| 4134     | 14966   | 1493   | 3947  | 30   | 560 | 14516  | 2222   | 22768 |
| 4534     | 34537   | 2801   | 3231  | 30   | 2476 | 15139  | 947    | 24624 |

Total 297691 240935 455968 1149 485549 484860 486953 2430835

Table 3: Number of experiments for each combination of dataset and algorithm.

\(^1\)https://github.com/ja-thomas/OMLbots
4. Access to the results

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

- The easiest way to access them is to go to the figshare repository (Kühn et al., 2018) and to download the .csv files. For each algorithm there is a csv file that contains a row for each algorithm run with the columns Data_id, the hyperparameter settings, the performance measures (auc, accuracy and brier score), the runtime, the scimark reference runtime and some characteristics of the dataset such as the number of features or the number of observations.

- 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. With this script all results that were created by the random bot (OpenML-ID 2702) are downloaded and the final dataset is created. (Warning: As the OpenML database is updated daily, changes can occur.)

5. Discussion and potential usage of the results

The presented data can be used to study the effect and influence of hyperparameter setting on performance in various ways. Possible applications are:

- Obtaining defaults for ML algorithm that work well across many datasets (Probst et al., 2018);

- Measuring the importance of hyperparameters, to investigate which should be tuned (see van Rijn and Hutter, 2017; Probst et al., 2018);

- Obtaining ranges or priors of tuning parameters to focus on important regions of the search space (see van Rijn and Hutter, 2017; Probst et al., 2018);

- Meta-Learning;

- Investigating, debugging and improving the robustness of algorithms.

Possible weaknesses of the approach, which we would like to address in the future, are:

- For each ML algorithm, a set of considered hyperparameters and their initial ranges has to be provided. It would be much more convenient if the bot could handle the set of all technical hyperparameters, with infinite ranges.

- Smarter, sequential sampling might be required to scale to high-dimensional hyperparameter spaces. But note that we not only care about optimal configurations but much rather would like to learn as much as possible about the considered parameter space, including areas of bad performance. So simply switching to Bayesian optimization or related search techniques might not be appropriate.

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