Ranking of Classification Algorithms in AutoML

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INTELLIGENT
SYSTEMS

Intelligent Systems Group (ISG)

Bachelor's Thesis

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Abstract

Should abstract be included?

Abstract (German)

Und falls ja, dann zweisprachig?

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Contents

Introduction

This introduction emphasizes why there is a need for automation in machine learning, and how this thesis relates to that problem in that it proposes two different approaches for ranking classification algorithms. Furthermore, an overview of the thesis structure is given.

1.1 Motivation and Problem Statement

The potential of big data is evident, and an increasing amount of information is collected and available for analysis - but this potential is not utilized. In a white paper, the International Data Corporation claims that in 2012, out of the 2.8 zettabytes (ZB) of available data only 3% were tagged as to enable further processing, and only 0.5% were analyzed [GR12]. A follow-up paper in 2017 projects that in 2025, 15% of the estimated 163ZB of global data will be tagged, and approximately 3% analyzed [GR17]. While this is more optimistic, it still shows that there is a huge gap between the amount of data that could potentially be used and the amount of data actually available. This indicates that the demand of data to be analyzed cannot be covered by data scientists alone, and the process is not accessible enough to non-experts. It thus calls for automation of the process in a way that not much expertise in the field of machine learning is needed to gain insights about the collected data.

One of the most prominent machine learning tasks is classification: A class is assigned to an instance, for example clients of a bank may be either deemed creditworthy or not, based on factors like other existing credits or the job of the client. But selecting a fitting classifier for a new data set is difficult, since algorithm performances can vary substantially among data sets, and it is not feasible to simply apply a large number of them to empirically find a good match. For example, on a data set about the electricity prices in the Australian state New South Wales [Har99], the predictive accuracy for the Multilayer Perceptron[1] is 0.7887 [Cac17c]. The predictive accuracy of the Random Forest[2] algorithm on the same data set is 0.9236 [Cac17b], a much higher value. On a different data set, with the topic of vehicle silhouettes [Sie87], we get a predictive accuracy of 0.7979 for the Multilayer Perceptron [Cac17d], and

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[1] With standard hyperparameters (L:0.3,M:0.2,N:500,V:0,S:0,E:20,H:a).
[2] With standart hyperparameters (P:100,I:100,num-slots:1,K:0,M:1.0,V:0.001,S:1).

0.7518 for Random Forests [Cac17a], showing an advantage of the former on this data set[3]. So in each case, one would have picked a different algorithm in order to achieve the best results, and this example just illustrates the choice between two algorithms - in reality, the of available algorithms is much larger. In general, this means that for a different data set, a different algorithm might yield the best performance.

Since there is no one best classifier for all data sets, it is likely that how well a classifier performs on a given data set is dependent on properties of the data set, at least to some degree. Combined with the need for automated machine learning and the importance but difficulty of selecting a fitting algorithm, this calls for an approach that considers past performances of classifiers for data sets in relation to properties of these data sets to automatically suggest well-performing classifiers for a new problem.

Thus, the aim of this thesis is the implementation and evaluation of two different approaches to ranking classification algorithms based on past-performances of the algorithms and according to properties of the data set. The two approaches include one regression-based approach that breaks down the problem of predicting a ranking into predicting a single performance value for each algorithm and then ranking them accordingly, and a preference based approach that is concerned with learning the rankings directly. Especially in the case of regression based ranking there is reason to believe that such a prediction is possible, as regression models have been used successfully to predict the performance of an algorithm dependent on the hyperparameter configuration [Egg+15].

A tool that efficiently predicts which algorithms are likely to perform well compared to their alternatives regarding a specific data set simplifies the process of selecting an algorithm for inexperienced users and experts alike. A user would send a request to the tool for their specific data set at hand and then evaluate highly ranked algorithms manually, choosing the one with the best performance. The advantage is that the user does not need to know characteristics of the classification algorithms or data set in order to achieve relatively good results in a short amount of time. A further speed-up and simplification could then possibly be achieved by embedding this tool in a solution that also takes care of the sampling of selected classifiers on the data set, for example existing solutions in the context of automated machine learning (auto-ml) context.

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[3]Hyperparameters as above.

1.2 Thesis Structure

The following paragraphs give an outline of the thesis structure by providing a brief summary of each chapter.

Chapter 2 - Fundamentals

First, some preliminaries are discussed. A brief overview of tasks from the field of machine learning which are relevant to this thesis is given, and methods used for evaluation are explained.

Chapter 3 - Approach

The next chapter continues by describing the approach of this thesis for ranking classification algorithms. The two different proposed methods are contrasted.

Chapter 4 - Implementation

Following the details of the approach, the implementation thereof is presented. Used software libraries are pointed out.

Chapter 5 - Evaluation

The evaluation of the different ranking implementations is described by first clarifying the experimental setup used for the evaluation, followed by a discussion of the results.

Chapter 6 - Related Work

After the approach of this thesis has been laid out in detail, the scope is extended to related work in the area of auto-ml in general and ranking of learning algorithms more specifically. Differences and similarities in the approaches are discussed briefly.

Chapter 7 - Conclusion

In the last chapter, the results which have been achieved are revisited with the goals in mind. Finally, an outlook for possible future work extending more eval is provided.

Fundamentals

<div style="text-align: right; font-size: large;">2</div>

The core topic of this thesis falls under the category of machine learning. Thus, first the concept of machine learning and the tasks related to the approach of this thesis are explained. Second, means used for evaluation of the approach are discussed.

2.1 Machine Learning

In this section, the aspects of the field of machine learning which are relevant for this thesis are going to be introduced briefly. The core of machine learning is learning algorithms, which are used to induce a general model from a set of data samples. The concept of machine learning will be explained here with the help of an example.

Suppose an aspiring gardener wants to learn how to distinguish between different species of iris plants, a genus of ornamental plants with colorful flowers. More specifically, the focus lies on the three species iris versicolor, virginica and setosa. In order to do so, the gardener has observed four different *features*, namely the length and width of their petals and sepals, for a number of different individuals for which he knows the species, which is illustrated in Table **??**. The goal of the gardener is then to learn how to distinguish the species based on these features, that is to derive a *model* from the data that will predict which species (out of the considered three) an unknown iris plant is. The gardener decides to build a decision tree from the data with forks on the basis of feature values, so that they can determine the species of the plant without much calculation. They observe that all iris setosa plants from his sample have a petal width of ≤ 0.6 cm, and that of the plants with a petal width of > 0.6 cm, most plants with a petal width ≤ 1.7 cm are of the iris versicolor species. The remaining plants with a petal width of > 1.7 cm are mostly iris virginica plants. While this model will not correctly predict the species of all iris plants, the gardener is settles with the approximation they have found.

In formal terms, the gardener is searching for an unknown *target function* $f : X \to Y$ from the input space X to the output space Y that represents an ideal way of identifying iris species [ALM12]. X denotes the possible inputs, in this case all combinations of the four features that have been defined, whereas Y are the outputs, here the species of iris plant. The examples that the gardener recorded are samples

Feature	Sepal length	Sepal width	Petal length	Petal width	Species
	5.1	3.5	1.4	0.2	Iris setosa
	5.0	3.5	1.6	0.6	Iris setosa
	5.0	3.4	1.6	0.4	Iris setosa
	5.6	3.0	4.5	1.5	Iris versicolor
	6.7	3.1	4.4	1.4	Iris versicolor
	5.9	3.2	4.8	1.8	Iris versicolor
	7.2	3.0	5.8	1.6	Iris virginica
	5.9	3.0	5.1	1.8	Iris virginica
	6.9	3.1	5.1	2.3	Iris virginica

Tab. 2.1.: Example values for the predictive accuracy of classifiers (data set not relevant in this context). The predictive accuracy denotes the percentage of instances for which the classifier correctly perdicted the class membership.

$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ from f such that $f(x_i) = y_i$. Together, they form a data set D which is one of all possible data sets $\mathbb{D}$ for the problem. They then choose a specific approximation $g : X \to Y, g \approx f$, the decision tree they built, from the hypothesis space H, which in this case consists of possible decision trees. The learning algorithm itself thus maps a data set to a hypothesis from the hypothesis space and can be defined as $A : \mathbb{D} \to H$.

2.1.1 Supervised Learning

The problem described above has some additional properties besides being a machine learning problem in general. Firstly, it falls in the category of supervised machine learning. Supervised learning is one of the three main learning paradigms of machine learning, together with reinforcement learning and unsupervised learning [ALM12]. In the context of this thesis, the latter will be neglected as only supervised learning is used. It is characterized by the fact that the learning algorithm is provided with a set of inputs *together* with the outputs, which could be viewed as a kind of teacher, or supervisor, explaining expected results to the learner. In the other cases, no such detailed feedback is provided to the learner.

2.1.2 Classification and Regression

In addition to falling into the category of supervised learning, the problem is a classification problem. The nature of the prediction is to assign one of the three classes, or labels, 'iris setosa', iris virginica' and 'iris versicolor' to a new plant. Formally, this means that the output space Y of the target function consists of a finite set of labels $\{y_1, \ldots, y_n\}$, so that each instance of the data set is associated with a label $y_i \in Y$, in this case $Y = \{'iris - setosa', 'irisvirginica', 'irisversicolor'\}$.

Apart from classification, another important category of machine learning problems is regression problems. In the case of regression, the output space of the target function is no longer finite, but instead consist of real numbers. To reconsider the gardening example, the gardener could want to predict the height of a plant on the basis of the same features as used above. Likewise, they would have to observe a number of plants to gather feature values together with the expected target value, which instead of the species would then be the height of the plant in centimeters, that is $Y = \mathbb{R}$.

2.1.3 Preference Learning

Preference Learning is a relatively new subfield of machine learning [FH10]. It is dedicated to the problem of learning how to rank, the precise definition of what this encompasses being defined by the specific task one considers. Out of the three main tasks of preference learning, namely label ranking, instance ranking and object ranking, label ranking is the relevant one in the context of this thesis. But before going into the details of label ranking, it first has to be explained what is meant with a ranking in this context and how it is distinguished from the concept of an ordering, as it is easily confused.

Ranking and Ordering

To clarify the meaning of ranking and ordering, we return to the gardening example. After spending some time studying the different flowers, the gardener has realized he prefers certain iris species to others.

Ranking = Permutation of the actual labels! Ordering =

A ranking for a set of items defines a strict total order

The ordering sorts the labels according to their given score. It thus may also implicitly be given by ordering the items themselves, as the labels are aliases for them. Therefore, an ordering for a set of labels $\{1 \ldots k\}$ is a permutation π of the labels where $\pi(i)$ is the

It must be noted that the definitions given here are not transferable to the general case of a ranking or ordering problems, since a strict total order is not required in all contexts for either ranking or ordering.

The values in table **??** result in the ranking $[2, 3, 1]$, whereas the ordering is $[3, 1, 2]$.

Species	iris virginica	iris versicolor	iris setosa
Label	[1,	2,	3]
Score	[0.17,	0.12,	0.89]
Ranking	[2,	3,	1]
Ordering	[3,	1,	2]

Tab. 2.2.: Example values for the predictive accuracy of classifiers (data set not relevant in this context). The predictive accuracy denotes the percentage of instances for which the classifier correctly perdicted the class membership.

Label Ranking

Similar to classification, in label ranking there is a finite set of labels $Y = \{y_1, \ldots, y_n\}$, but it is not the output space. Instead, Fürnkranz and Hüllermeier define the target function for label ranking as $f : X \rightarrow S_Y$ where the output space S_Y contains all permutations over the set of labels Y [FH10]. An instance $x \in X$ therefore is assigned a permutation $y_{\pi_x^i}$

Although called label ranking actually label ordering!

original algorithms selection problem [Ric76] can be viewed as a learning problem itself

2.1.4 Meta Learning

Meta leThe previous discussion of machine learning problems has conceptually been about the fitting of different machine learning algorithms to problems in the form of data sets. In the context of meta learning, is 'possible to learn about the learning process itself, and in particular that a system could learn to profit from previous experience to generate additional knowledge that can simplify the automatic selection of efficient models summarizing the data' [**razdil2008metalearning**].

2.2 Evaluation

After having discussed the preliminaries that the theoretical approach of this thesis is built upon, how a data set can be split into training and test data to estimate the performance of learning algorithms and the measures that will be used in the evaluation of the different ranking methods are briefly reviewed. These include means of comparing the predicted rankings with actual rankings as well as a statistic that reveals if an advantage regarding one measure can be viewed as significant.

2.2.1 Estimation Procedures

- estimation using cross validation (monte carloMCCV)

- estimation using leave one out

2.2.2 Kendall Rank Correlation Coefficient

To evaluate the quality of the prediction that a ranker will make, a statistic is needed to compare a predicted ranking with the correct ranking. For this, the Kendall Rank Correlation Coefficient will be used here, as it expresses the similarity of two rankings.

The Kendall Rank Correlation Coefficient, also known as Kendall's tau, is a measure of association between two rankings of the same items [Ken38]. For two independent variables X and Y and and observations of values $(x_1, x_2, ..., x_m)$ for X and $(y_1, y_2, ..., y_n)$ for Y with unique x_i and y_i respectively, the coefficient is based on comparing pairs of observations. If for two pairs (x_i, y_i) and (x_j, y_j) both $x_i < x_j$ and $y_i < y_j$ (or the opposite) holds, they are viewed as concordant. If $x_i < x_j$ but $y_i > y_j$ (or the opposite), they are viewed as discordant. Other cases are not considered. The simplest version of the statistic, called T_A is then defined as

$$T_A = \frac{n_c - n_d}{n_0},$$

with
n_c, the number of concordant pairs,
n_d, the number of discordant pairs, and
$n_0 = n * (n + 1)/2$.

As we have seen in example above, can also have same rank for items. In order to account for this, a second statistic, T_B is defined as

$$T_B = \frac{n_c - n_d}{\sqrt{(n_0 - n_1)(n_0 - n_2)}},$$

with
n_c, n_d, n_0 as above,
$n_1 = \sum_i t_i(t_i - 1)/2,$
$n_1 = \sum_j t_j(t_j - 1)/2,$

t_i, the number of ties observed for X in the ith position of the ranking

u_j, the number of ties observed for Y in the ith position of the ranking

Thus, the value of the tau (for both versions) lies in the interval $[-1, 1]$, with 1 indicating a perfect agreement of rankings, -1 perfect disagreement, and 0 corresponding to no correlation. A high value is therefore desirable in this context, as it indicates that the prediction of the ranker agrees with the actual ranking of algorithms.

2.2.3 Loss

While the Kendall rank correlation coefficient is an indication as to what degree a predicted ranking agrees with the correct ranking of classifiers for a certain data set, it does not convey the difference in performance experienced by the user when choosing the first of the recommended algorithms. This difference can be expressed in measure called loss [LBV12], which is defined as the difference of the performance of the actual best algorithm and the actual performance of the first recommended algorithm.

Additionally, the ranker recommends a ranking instead of a single algorithm in order to allow a user (or automated tool) to test a few of the top-ranked algorithms, which therefore also needs to be taken into account when thinking about loss. This is done here by computing a measure called best three loss, which denotes the loss resulting in the selection of the best of the first three recommended classifiers in comparison to the actual best-performing classifier in the considered set of classifiers.

2.2.4 Mann-Whitney U Test

The measures previously presented can indicate if one alternative is superior to another regarding that measure, but one cannot conclude from those results alone whether this advantage is significant. The question is whether the null-hypothesis that two distributions [MW47]

Approach

In this chapter the two alternatives which ar

3.1 Theory

Approach of ranking classifier implementations here realized by two concepts, regression-based and preference-based ranking, which will be explained in detail. Also predicting predictive accuracy here. Thus target function of the form $metafeatures^n \rightarrow classifiers^m$. performance measure chosen predictive accuracy

Since the aim is to generate a ranking of classification algorithms, first, performance values of a number of classifiers are recorded on a few data sets. Then, meta features are computed for each data set. This is for training the ranking model. This generates a table that contains all necessary informatino for training both types of rankers. A ranking of the classifiers for a new instance is then achieved by computing the meta features for the data set and subsequently using it to query the underlying model.

MF 1	MF 2	...	MF n	PV 1	PV 2	...	PV k
v_{11}	v_{12}	...	v_{1n}	p_{11}	p_{12}	...	p_{1k}
v_{21}	v_{22}	...	v_{2n}	p_{21}	p_{22}	...	p_{2k}
...	...	...	...	...	...	...	...
v_{m1}	v_{m2}	...	v_{mn}	p_{2m}	p_{m2}	...	p_{mk}

Tab. 3.1.: This is a caption text.

One possibility to derive a ranking of classifiers from this information when given a new data set is to use regression models. The idea is to use separate regression models to predict a performance value for each classifier, and to then derive an ordering from these predictions. This is done by splitting the data set compiled beforehand into separate data sets that each contain all meta features for all data sets, but only the performance values of one classifier. The target feature on these individual data sets, the performance value of the classifier, is a numeric value, and thus a regression model can be trained on each of them. All regression models therefore try to learn the target function $metafeatures \rightarrow classifierperformancevalue$ for their respective classifier. Hence for a query instance, after computing the meta features,

these are fed into each regression model and the predicted performance value for each classifier is saved. In a second step, the classifiers are ordered according to the predictions.

Meta Feature 1	...	Meta Feature n	Performance Value 1
v_{11}	...	v_{1n}	p_{11}
v_{21}	...	v_{2n}	p_{21}
...	...	...	...
v_{m1}	...	v_{mn}	p_{m1}
Meta Feature 1	...	Meta Feature n	Performance Value 2
v_{11}	...	v_{1n}	p_{12}
v_{21}	...	v_{2n}	p_{22}
...	...	...	...
v_{m1}	...	v_{mn}	p_{m2}

...

Meta Feature 1	...	Meta Feature n	Performance Value k
v_{11}	...	v_{1n}	p_{1k}
v_{21}	...	v_{2n}	p_{2k}
...	...	...	...
v_{m1}	...	v_{mn}	p_{mk}

Tab. 3.2.: This is a caption text.

The second possibility considered in this context is using preference learning to predict a ranking. Each instance of the data set generated beforehand contains meta feature information for the considered data set and performance values of all classifiers. Similarly to the regression alternative, the performance values can be converted to preference information by sorting the corresponding classifiers by their performance values. This leads to an ordering of classifiers associated with each instance, and implies that the preference learning task at hand is label ranking. In this case, there exists only one label ranking mode which is fed the computed meta data for a new data set and returns an ordering of classifiers. Thereby it attempts to learn the mapping from meta features to an ordering of classifiers directly.

MF 1	MF 2	...	MF n	PV 1	PV 2	...	PV k
v_{11}	v_{12}	...	v_{1n}	p_{11}	p_{12}	...	p_{1k}
v_{21}	v_{22}	...	v_{2n}	p_{21}	p_{22}	...	p_{2k}
...	...	...	...	...	...	...	...
v_{m1}	v_{m2}	...	v_{mn}	p_{2m}	p_{m2}	...	p_{mk}

Tab. 3.3.: This is a ranking

3.2 Implementation

META FEATURES USED!

for mann-whitney U apache commons implementation used with ties averaged and NaNs removed before

Implementation

4

4.0.1 Frameworks used

4.0.2 jPL framework

The jPL framework is a java framework for the evaluation of preference learning algorithms. It implements several tasks from the context of preference learning, including label ranking. Furthermore, the framework introduces the Generic Preference Representation Format (GPRF) to store preference information.

4.0.3 WEKA

4.1 Generating Performance Values

Performance values generated by

4.2 Stuff

Rankers trained with data set of the following form, so each ranking algorithm can derive its on performance

Evaluation

5

This chapter is dedicated to the evaluation of the proposed ranking approaches. First, the oracle and baseline against which the rankers are compared are explained. Second, the experimental setup, that is conditions under which the evaluation was conducted, is set forth. Last, results are presented and discussed.

5.1 Baseline and Oracle

In order to evaluate the implemented rankers, their outputs are compared to a perfect output generated by an oracle. The oracle is implemented as a ranker that, after having been trained on a meta data - performance data set returns correct rankings when queried for any instance of that data set. The correct ranking is implied by the performance values (highest first, as the measure used here is predictive accuracy), with ties being handled in a sequential manner, i.e. for the same performance values, the algorithm that was encountered first when constructing the ranking will be ranked before all others with the same value.

As rankings returned by this oracle represent the ideal solution, the predicted rankings are compared with them through the measures presented in chapter **??**. These include the Kendall rank correlation coefficient, loss and best three loss. The regression based rankers pose a special case: internally, they predict a performance value for each classifier, which therefore can be compared to the actual performance values to show how well they are predicted. This is done by computing the root mean square error between the predicted and actual performance values. In summary, it is desirable for the rankers to come as close as possible to the correct ranking, which is reflected by a high rank correlation and a low loss and root mean square error.

Furthermore, we are interested in the question as to what degree knowing about the properties of a data set influences the quality of rankings. Therefore, a ranker that is agnostic of the meta features of a query data set, that is that will always return the same ranking for any data set, is used as a baseline. More specifically, a best algorithm strategy that iteratively determines a ranking by counting the number of data sets where an algorithm is the best choice, is implemented. That means the first algorithm in the best algorithm ranking is the classifier that performs best

on most data sets, the second is the best on most data sets when only rankings excluding the first algorithm are considered, and so forth. This baseline is evaluated in the same way as the preference rankers; as it does not predict performance values, the root mean square error of predicted performance values cannot bet computed. Ideally, rankings returned by the preference and regression based rankers should then be statistically significant better than the baseline, which will be determined by calculating the Mann-Whitney U and determining whether its P-value.

5.2 Experimental Setup

In the following paragraphs, it is briefly summarized under which conditions the experiments which led to the results discussed in the next section where observed. This includes which classifiers and data sets where chosen in the evaluation, what the specifications of the machines the evaluation was executed on where, how the evaluation was carried out, and which specific regression based and preference based implementations where used.

The classifiers considered for a recommended ranking were the learning algorithms implemented in WEKA that are fit for classification, excluding meta and ensemble methods. The full list of the 22 classifiers can be gathered from Table **??**. They where all used in their default configurations as specified by WEKA.

datasets

The performance data of the classifiers for the selected data sets was generated on [MACHINE DETAILS]. [TIMEOUT AND HARDWARE ALLOCATION DETAILS]. For each of the classifiers, the predictive accuracy (the percentage of correctly classified instances in the data set) was recorded on each data set by means of five times stratified Monte-Carlo cross validation with a 70/30 split in training and test data. When a timeout occurred, the predictive accuracy was set to 0.

All other experiments where carried out on a Windows Machine running Windows 10 Education (version 1709) with a Intel(R) Core(TM) i5-4200U CPU running at 1.60GHz (2.30GHz max) and 12 GB RAM. It is notable that especially the time-related results are to be viewed in regard to this setup. No timeouts where used in this evaluation, and the rankers where evaluated on the training data by means of leave-one-out estimation, that is for the n data sets for which performance values where recorded, they where trained with the meta data - performance examples for $n - 1$ data sets, and queried for the remaining data set. As $n = 448$ in this case, the full results are not included in the discussion of the results. They can, however, be

found in the supplementary material, offering clues to how each ranker performed in the prediction of a ranking for each of the used data sets, identified by their ID on OpenML.

Furthermore, four alternatives where selected for a regression based and preference based alternative each, to get a general idea of how well the respective approach might be suited for the problem. For the regression based approach, the algorithms chosen where random forest, REPTree, M5P, and linear regression. For all of them, the WEKA implemenation [Hal+09] was used, and the algorithms where used with the standard hyperparameters set by WEKA. As the preference based ranking falls under the category of label ranking, and in the jPL-framework, which was used for the implementation of the label ranking algorithms and data set representations, only two alternatives for label ranking are implemented [Int17], the other two alternatives where generated by modifying the hyperparameters. The implemented alternatives are label ranking by pairwise comparison and instance based label ranking. As in early tests it became apparent that the instance based approach might hold more potential, for label ranking by pairwise comparison, only the default configuration dictated by jPL was used. For instance based label ranking, the default configuration, a configuration where the rank aggregation algorithm used by the label ranker was set to Kemeny-Young, and a configuration with Kemeny-Young rank aggregation and the number of neighbors of the base learner of the label ranker, namely k nearest neighbor (kNN), set to the square root of the number of instances in the training data set. In the following section, these eight variants are compared with the baseline and oracle mentioned in the previous section, and among each others.

5.3 Results

In the results mainly as so many data sets only taked about mean values but the full results with related to the specific data set id are included in supplementary material.

5.3.1 Accuracy

Ranker	Kendall's Rank Correlation				Loss				BestThreeLoss			
	Min	Max	Stdv	Mean	Min	Max	Stdv	Mean	Min	Max	Stdv	Mean
LinearRegression	-0.255	0.896	0.221	0.473	0	86.667	7.244	3.469	0	31.220	3.011	1.267
M5P	-0.29	0.870	0.219	0.470	0	82.353	6.535	3.78	0	82.353	4.757	1.508
RandomForest	-0.281	0.922	0.228	0.495	0	60	5.745	3.097	0	34.634	3.150	1.308
REPTree	-0.229	0.896	0.213	0.412	0	82.353	7.948	4.829	0	34.634	3.515	1.759
InstanceBased	-0.429	0.870	0.249	0.221	0	82.353	9.44	5.401	0	82.353	8.540	3.62
InstanceBased[1]	-0.429	0.887	0.252	0.340	0	98.367	10.323	5.437	0	82.353	8.367	3.294
InstanceBased[2]	-0.429	0.870	0.249	0.335	0	82.353	9.402	5.382	0	82.353	8.493	3.511
PairwiseComparison	-0.870	0.576	0.234	0.014	0	97.822	13.135	9.762	0	82.353	8.600	4.001
BestAlgorithm	-0.437	0.489	0.159	0.057	0	82.353	10.168	6.480	0	82.353	8.195	3.420
LinearRegression	-0.255	0.896	0.221	0.473	0	86.667	7.244	3.469	0	31.220	3.011	1.267
M5P	-0.29	0.870	0.219	0.470	0	82.353	6.535	3.78	0	82.353	4.757	1.508
RandomForest	-0.281	0.922	0.228	0.495	0	60	5.745	3.097	0	34.634	3.150	1.308
REPTree	-0.229	0.896	0.213	0.412	0	82.353	7.948	4.829	0	34.634	3.515	1.759
InstanceBased	-0.429	0.870	0.249	0.221	0	82.353	9.44	5.401	0	82.353	8.540	3.62
InstanceBased[1]	-0.429	0.887	0.252	0.340	0	98.367	10.323	5.437	0	82.353	8.367	3.294
InstanceBased[2]	-0.429	0.870	0.249	0.335	0	82.353	9.402	5.382	0	82.353	8.493	3.511
PairwiseComparison	-0.870	0.576	0.234	0.014	0	97.822	13.135	9.762	0	82.353	8.600	4.001
BestAlgorithm	-0.437	0.489	0.159	0.057	0	82.353	10.168	6.480	0	82.353	8.195	3.420

Tab. 5.1.: Evaluation results with full meta data (top) and no probing (bottom)

[1] Rankaggregation: Kemeny-Young
[2] Rankaggregation: Kemeny-Young, Baselearner KNN with $n = \sqrt{\text{number of instances}}$

??

Meta Feature Group	Computation Time (ms)			
	Min	Max	Mean	Stdv

Computation Times for Groups of Meta Features

??

Ranker	Kendall's Rank Correlation		Loss		BestThreeLoss	
	Mann-Whitney U	P-Value	Mann-Whitney U	P-Value	Mann-Whitney U	P-Value
LinearRegression	186381.5	2.702E-109	126861.5	7.694E-12	129028.0	1.327E-13
M5P	186236.0	6.230E-109	118828.5	1.840E-6	126379.5	1.821E-11
RandomForest	187750.5	9.737E-113	128853.5	1.861E-13	129037.0	1.304E-13
REPTree	181228.0	8.094E-97	111850.0	0.003	118793.0	1.926E-6
InstanceBased	142665.5	8.818E-28	109372.0	0.020	104279.0	0.311
InstanceBased[3]	166460.5	2.583E-65	111940.5	0.003	109211.0	0.022
InstanceBased[4]	166031.0	1.715E-64	110675.5	0.008	106223.0	0.130
PairwiseComparison	110610.0	0.008	120547.5	1.848E-7	107728.0	0.057
LinearRegression	186381.5	2.702E-109	126861.5	7.694E-12	129028.0	1.327E-13
M5P	186236.0	6.230E-109	118828.5	1.840E-6	126379.5	1.821E-11
RandomForest	187750.5	9.737E-113	128853.5	1.861E-13	129037.0	1.304E-13
REPTree	181228.0	8.094E-97	111850.0	0.003	118793.0	1.926E-6
InstanceBased	142665.5	8.818E-28	109372.0	0.020	104279.0	0.311
InstanceBased[5]	166460.5	2.583E-65	111940.5	0.003	109211.0	0.022
InstanceBased[6]	166031.0	1.715E-64	110675.5	0.008	106223.0	0.130
PairwiseComparison	110610.0	0.008	120547.5	1.848E-7	107728.0	0.057

Significance of Results Regarding Kendall Rank Correlation Coefficient

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[5]Rankaggregation: Kemeny-Young

[6]Rankaggregation: Kemeny-Young, Baselearner KNN with $n = \sqrt{\text{number of instances}}$
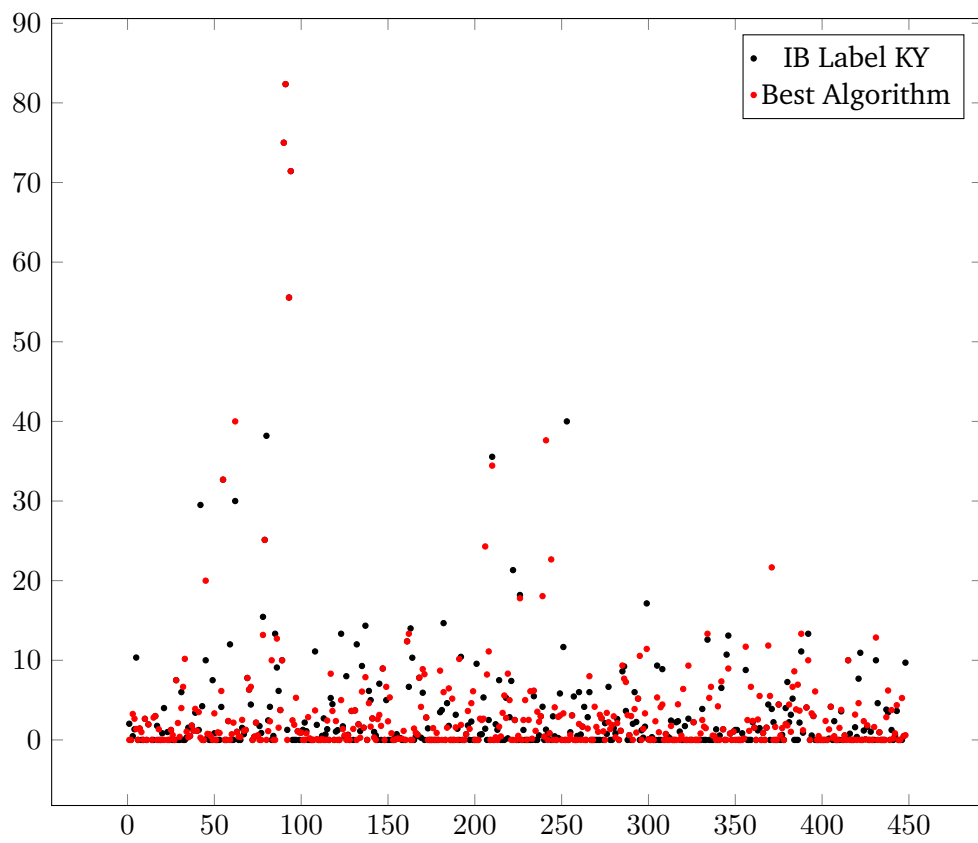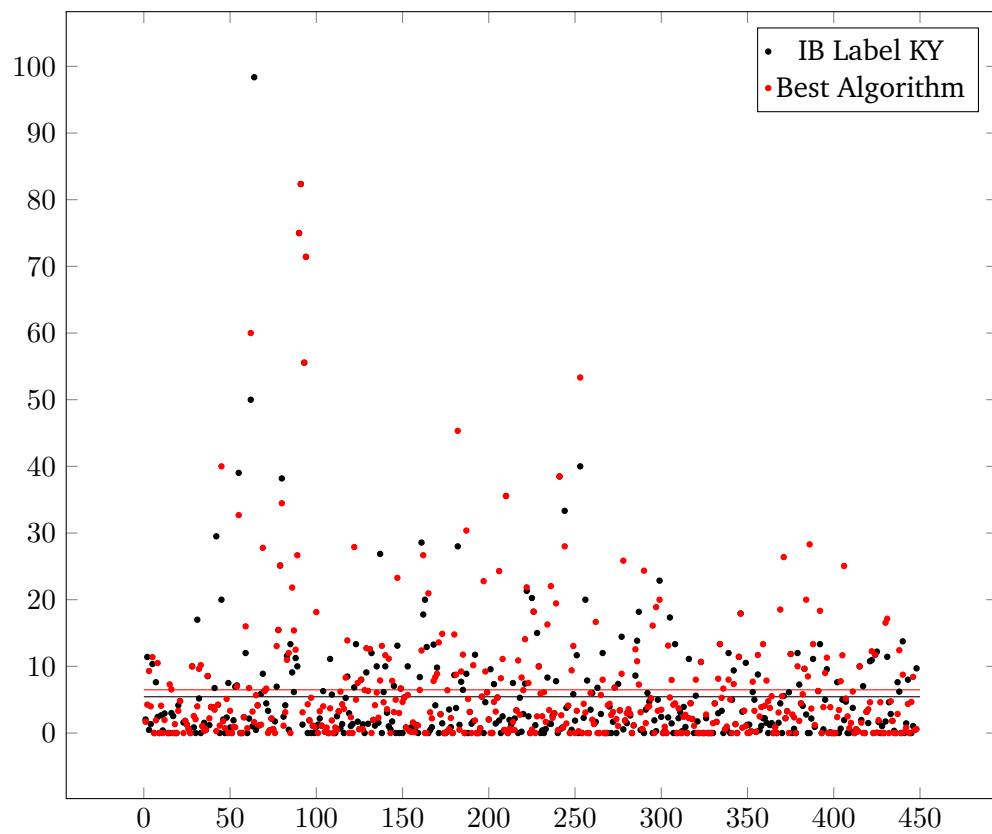
5.3.2 Build and Prediction Times

Ranker	Ranker Build Time (ms)				Ranker Prediction Time (ms)			
	Min	Max	Mean	Stdv	Min	Max	Mean	Stdv
LinearRegression	1454	2060	1580	36	0	1	0	0
M5P	3145	4916	3226	89	0	16	0	1
RandomForest	6048	9720	6236	259	0	16	3	2
REPTree	599	1264	629	38	0	16	1	16
InstanceBased	66	550	90	25	0	47	5	8
InstanceBased[7]	66	138	88	12	0	19	1	3
InstanceBased[8]	66	163	87	12	0	16	1	2
PairwiseComparison	11784	15096	12623	348	0	0	9.762	13.135
BestAlgorithm	193	321	221	23	0	0	0	0
LinearRegression	1454	2060	1580	36	0	1	0	0
M5P	3145	4916	3226	89	0	16	0	1
RandomForest	6048	9720	6236	259	0	16	3	2
REPTree	599	1264	629	38	0	16	1	16
InstanceBased	66	550	90	25	0	47	5	8
InstanceBased[9]	66	138	88	12	0	19	1	3
InstanceBased[10]	66	163	87	12	0	16	1	2
PairwiseComparison	11784	15096	12623	348	0	0	9.762	13.135
BestAlgorithm	193	321	221	23	0	0	0	0

Tab. 5.4.: Build and Prediction Times of the Rankers rounded to Full Milliseconds (Full Meta Data)

??

5.3.3 Further Insights

Ranker	Root Mean Square Error			
	Min	Max	Mean	Stdv
LinearRegression	1454	2060	1580	36
M5P	3145	4916	3226	89
RandomForest	6048	9720	6236	259
REPTree	599	1264	629	38
LinearRegression	1454	2060	1580	36
M5P	3145	4916	3226	89
RandomForest	6048	9720	6236	259
REPTree	599	1264	629	38

Tab. 5.5.: Root Mean Square Error of Predicted Performance Values for the Regression-Based Rankers (full meta data)

??

??

[9]Rankaggregation: Kemeny-Young
[10]Rankaggregation: Kemeny-Young, Baselearner KNN with n$=\sqrt{}$number of instances

Classifier	Number of Data Sets Placed First
Logistic	28
Naive Bayes	29
IBk	23
KStar	24
LMT	17
VotedPerceptron	16
ZeroR	14
J48	13
NaiveBayesMultinomial	6
RandomTree	2
SimpleLogistic	1
DecisionStump	1
MultilayerPerceptron	1
RandomForest	1
DecisionTable	1
PART	1
SGD	1
BayesNet	1
REPTree	1
JRip	1
SMO	313
OneR	448

Tab. 5.6.: The Ranking of Classifiers returned by the Best Algorithm Baseline

Related Work

6

The demand for aid in the process of selecting an algorithm has already led to the development of numerous solutions that automate machine-learning (AutoML). In the following sections, the workings of a few such tools that are related to this work are outlined briefly, loosely organized by their scope of operation. Each tool's usage of meta knowledge is discussed shortly.

6.1 Predicting Rankings

In contrast to ranking solely based on classifier performances, Abdulrahman et al. investigated an approach to extend existing ranking methods by incorporating the time needed for the evaluation of the classifier [Abd+18]. They call this combined measure of accuracy and time A3R, and integrate it into to different ranking approaches.

One of those two approaches is called average-ranking. It utilizes meta knowledge to suggest a ranking of classifiers for a new data sets, which in this case consist of recorded past performances of classifiers on data sets. That means this algorithms aggregates the performances of classifiers on all rankings once and then always recommends the same ranking. The new measures is integrated here by, instead of ordering only according to performance values, the classifiers are ordered according to the combined measure A3R.

6.2 Algorithm and Hyperparameter Selection

Taking it a step further than predicting rankings of classification algorithms with fixed hyperparameters are tools that in addition two selecting an algorithm also optimize its hyperparameters, which has been defined as 'the combined algorithm selection and hyperparameter optimization problem (short: CASH)' [Tho+13]. Two widely used approaches of this kind are AUTO-WEKA and AUTO-SKLEARN. It has to be noted that thus these approaches also go further than the solution proposed

in this thesis, which currently only takes into account one fixed hyperparameter configuration for each classification algorithm.

Auto-WEKA is an AutoML tool that both selects a machine learning algorithm and optimizes its hyperparameters by using Bayesian optimization [Tho+13]. It was first released in 2013 as an extension to the popular data mining software WEKA [Hal+09], which also offers a user-friendly GUI in addition to a command-line interface and an API, to assist the large number of novice users of the software in selecting parameterized algorithms for their problems. The tool has since grown in popularity and is in version 2.0 as of March 2016 [Kot+16]. In Auto-WEKA, the problem of selecting an algorithm and its hyperparameters is combined by treating the algorithm itself as a hyperparameter and searching the joint space of algorithms and hyperparameters for the best solution. An input data set is first preprocessed by means of feature selection. Then, Sequential Model-Based Optimization for General Algorithm Configuration (SMAC) is used to 'iterate[...] between fitting models and using them to make choices about which configurations to investigate' [HHL11]. In the case of Auto-WEKA, this means that during the optimization process, a model is built, a configuration of hyperparameters that is promising regarding the current model and training data is tried out, and the result is fed back to the model. This cycle is then repeated until the allocated time has run out. Auto-WEKA exploits meta-knowledge, that is considering past performances of algorithms, to make decisions by always trying algorithms like Random Forest, which perform well on a large number of data sets, first.

AUTO-SKLEARN has been described as a sister-package to Auto-WEKA and is an AutoML tool which is based on scikit-learn, a machine learning library for Python [Feu+15]. It works very similar to AutoML but extends it by adding a meta-learning pre-processing step to warmstart the Bayesian optimization and automatically constructing ensembles during optimization. During the pre-processing phase, performance values for the classifiers available in AUTO-SKLEARN are recorded on a set of data sets. For each data set, the algorithm which shows the best empirical performance is noted. Then, certain meta-features are calculated for each data set. The first step of the tool when given a new problem is to calculate meta-features of the data set. Then, the Manhattan distance to the other data sets is determined according to the meta-features, and the algorithms that are associated with the k-nearest data sets are used as a starting point for further optimization. The authors observe that the additional meta-learning and ensemble construction result in a more efficient and robust application. Their results show that meta-learning can be used to improve the overall AutoML process.

6.3 Constructing pipelines

Before a classifier is evaluated on a data set, often a number of pre-processing steps are executed first. These could include selecting promising features and discarding other and normalizing the data. The 'sequence of tasks that need to be performed to classify instances belonging to a given dataset into a set of predefined categories' [Sá+17] can therefore be defined as a machine learning pipeline. Two tools which construct such complete pipelines for data sets are MP-Plan and the RECIPE framework.

ML-Plan is an AutoML tool that instead of concentrating on hyperparameter optimization, aims to optimize the whole machine-learning pipeline [WMH]. This is achieved by viewing machine-learning as a task, building a hierarchical task network out of those tasks, and then searching for a solution in the induced tree structure. In the tree, the root node contains the complex task of building a machine learning pipeline, inner nodes represent incomplete pipelines consisting of complex and possibly also primitive tasks, and leaf nodes are complete pipelines that include only primitive tasks. An example of this might be 'classify' as the root node, with an intermediate node on some level that contains the tasks 'build NN', 'train NN' and 'predict from NN'. The complex task 'build NN' would then further be decomposed, and could lead to a leaf node with n tasks 'Add layer', 'build NN' and 'predict from NN', which are all primitive tasks that do not need to be further decomposed. A best-first search algorithm in a modified variant is then used to find good solutions in this task network. For the actual implementation of the learning algorithms, WEKA is used. While this variant does not use meta-learning in the process of optimizing the pipeline, the authors find that their results exceed those achieved by Auto-WEKA.

Similar to ML-PLAN, the RECIPE framework constructs whole classification pipelines for new problems [Sá+17]. However, this is done by means of grammar-based genetic programming: the tasks that the pipeline is composed of are represented by a grammar, which 'is used to generate the initial population, as well as to constraint the crossover and mutation operations, which always need to be valid according to the grammar' [Sá+17]. This means that generated individuals representing complete pipelines can never be invalid. So for a new data set combined with a grammar that represents the valid pipelines, the tool first initializes the first generation according to the grammar. The fitness of individuals is then evaluated by mapping them to their respective implementations in the scikit-learn framework, and a new generation is created that takes this newly gained information into account. Evaluation by the authors indicates that the RECIPE framework is able to compete with AUTO-
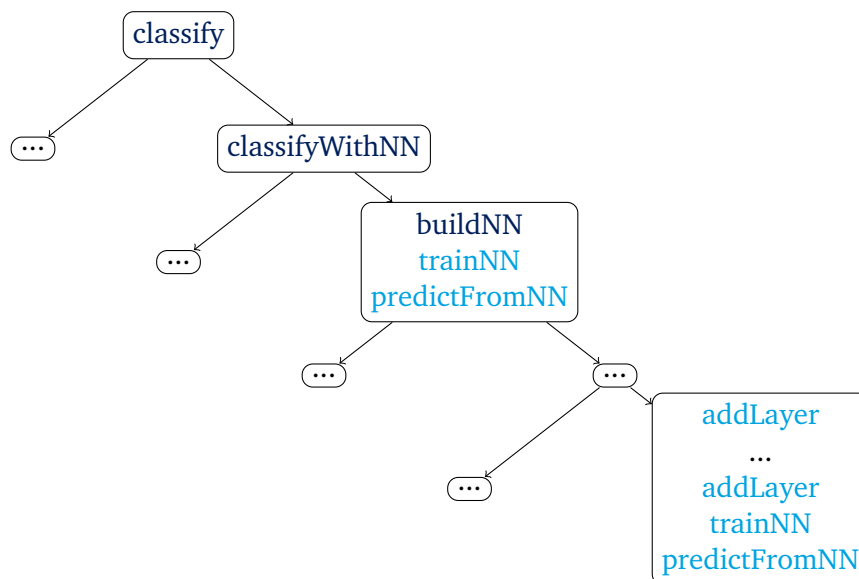
Fig. 6.1.: An example for how the complex task 'classify' might be broken down by ML-Plan. The figure is loosely adapted from [WMH]. Nodes containing '...' represent an undefined number of subtrees. Complex tasks and primitive tasks are distinguished by their color.

SKLEARN and a different evolutionary approach, although it does not incorporate meta-knowledge in the search.

Conclusion

In this thesis, the problem of predicting a ranking of classification algorithms for a new data set on the basis of meta features of the data set and past performances of the algorithms has been considered. Being able to predict a ranking of such algorithms is desirable since this potentially speeds up and simplifies the process of algorithm selection, which is important due to a rapidly increasing amount of available data, and more importantly, data that is available but has not yet been analyzed. This problem has been addressed by implementing two different approaches, regression-based and preference-based ranking. Both have been evaluated extensively against a baseline and an oracle.

- Results -

On the basis of these results, it can be concluded that a causal connection exists between certain meta features of a data set and the predictive accuracy of classification algorithms for this data set, which can be exploited to a degree by regression models and label ranking models to predict a ranking of classification algorithms. A practical application of these findings, apart from the direct use as a ranker, may be to incorporate the implementation or parts of it in another Auto-ML tool as a search heuristic, similar to how some Auto-ML solutions like AUTO-SKLEARN already benefits from meta learning [Feu+15]. However, some additional work may have to be done in extension to this thesis in order for a sensible integration.

7.1 Future Work

As the results have shown that the approach taken in this thesis has worked out reasonably well, for example when considering the regression based approach using random forests, many possibilities for additional work arise. An intuitive thought would be to extend the evaluation of the tool, for instance in terms of meta features. Different sets of meta features could be evaluated, like adding implementations for additional meta features, or considering using only light probing by incorporating the performance values for usually cheap algorithms in the meta features.

Furthermore, more insights could be gained about whether this approach is competitive by comparing it with other ranking approaches, for example like the one proposed by Abdulrahman et al. [Abd+18]. In this regard it would also be interesting to implement the loss - and time - loss curves proposed by the authors, which show how loss decreases as one advances in the predicted ranking and tries out the recommended algorithms, and at what cost in the sense of time the sampling of algorithms comes respectively.

Additionally, so far the evaluation of the tool has been confined to predicting algorithms for classification. Since this has been relatively successful, it could be tested whether similar predictions can also be made for other machine learning tasks like regression or clustering with the same approach by extending the tool to handling these functions. Also, one could try to include a few parameterized versions of algorithms, as so far only one variant of each classifier with standard hyperparameters has been used.

In a similar manner to extending the algorithms for which a performance measure is predicted, one could use the tool to predict different performance measures. For this, the tool does not even need to be adapted, as it is agnostic to the semantics behind the measure it predicts, it only needs to be numeric. One possibility for this would be the prediction of build or prediction times of learning algorithms, or a measure that combines time and accuracy [Abd+18].

Depending on the fact whether one is willing to trade-off longer build and prediction times, it would also be possible to fit more sophisticated regression models for the regression based approach. This could include feature pre-processing, automating the choice of regression algorithm with one of the available tools [Tho+13] [Feu+15], or even using a whole pipeline prediction tool [WMH] [Sá+17]. Furthermore, the building and predictions for the regression models could be parallelized and evaluated on a cluster to simulate and test the usage of the ranking tool in a productive environment.

Last, it could be interesting to implement an additional baseline that averages ranks instead of counting how many times an algorithm is ranked first. This would help to determine if the surprising ranking returned by the best algorithm baseline (see Fig. **??**) still holds when using a different baseline. Naturally this new baseline then could also be used to re-evaluate the implemented ranking concepts.

Appendix

A.1 Appendix Section 1

Alpha	Beta	Gamma
0	1	2
3	4	5

Tab. A.1.: This is a caption text.

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Paderborn, January 5, 2018

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Helena Graf