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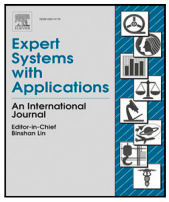

AutoMLBench: A comprehensive experimental evaluation of automated machine learning frameworks

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ABSTRACT

With the booming demand for machine learning applications, it has been recognized that the number of knowledgeable data scientists cannot scale with the growing data volumes and application needs in our digital world. In response to this demand, several automated machine learning (AutoML) frameworks have been developed to fill the gap of human expertise by automating the process of building machine learning pipelines. Each framework comes with different heuristics-based design decisions. In this study, we present a comprehensive evaluation and comparison of the performance characteristics of six popular AutoML frameworks, namely, `AutoWeka`, `AutoSKlearn`, `TPOT`, `Recipe`, `ATM` and `SmartML` across 100 data sets from established AutoML benchmark suites. Our experimental evaluation considers different aspects for its comparison, including the performance impact of several design decisions, including *time budget*, *size of search space*, *meta-learning*, and *ensemble construction*. The results of our study reveal various interesting insights that can significantly guide and impact the design of AutoML frameworks.

1. Introduction

We are witnessing tremendous interest in artificial intelligence applications across governments, industries and research communities with a yearly cost of around 12.5 billion US dollars (International Data Corporation, 2017). The driver for this interest is the advent and increasing popularity of machine learning (ML) and deep learning (DL) techniques. The rise of generated data from different sources, processing capabilities, and ML algorithms opened the way for adopting ML in a wide range of real-world applications (Zomaya & Sakr, 2017). This situation is increasingly contributing towards a potential *data science crisis*, similar to the software crisis (Fitzgerald, 2012), due to the crucial need to have an increasing number of data scientists with solid knowledge and good experience so that they can keep up with harnessing the power of the massive amounts of data produced daily. Thus, we are witnessing a growing interest in automating the process of building ML pipelines where the presence of a human in the loop can be dramatically reduced. Research in the area of AutoML aims to alleviate both the computational cost and human expertise required for developing ML pipelines through automation with efficient algorithms. In particular, AutoML techniques enable the widespread use of ML techniques by domain experts and non-technical users.

Applying ML to real-world problems is a multi-stage process and highly iterative exploratory process. It aims to automatically produce the optimal ML pipeline that maximizes the predictive performance over the validation set of a dataset within a fixed computational budget (See Fig. 1). The problem of AutoML for supervised task can be formally stated as follows: For $i = 1, \ldots, n'+m'$, let $x_i \in \mathbf{R}$ denote a feature vector and $y_i \in Y$ the corresponding target value. Given a training dataset $D_{train} = \{(x_1, y_1), \ldots, (x_{n'}, y_{n'})\}$ and the feature vectors $x_{n'+1}, \ldots, x_{n'+m'}$ of a test dataset $D_{test} = \{(x_{n'+1}, y_{n'+1}), \ldots, (x_{n'+m'}, y_{n'+m'})\}$ drawn from the same underlying data distribution, as well as a resource budget b and a loss metric $L(.,.)$, the AutoML problem is to automatically produce test set predictions $\hat{y}_{n'+1}, \ldots, \hat{y}_{n'+m'}$ while minimizing the loss (L). The loss of a solution $\hat{y}_{n'+m'}$ to the AutoML problem is given by $\frac{1}{m'} \sum_{j=1}^{m'} L(\hat{y}_{n'+j}, y_{n'+j})$.

The budget b would comprise computational resources (e.g., CPU and/or wallclock time, memory usage). In particular, solving the AutoML problem aims to select and tune an ML algorithm from a defined search space to achieve (near)-optimal performance in terms of the

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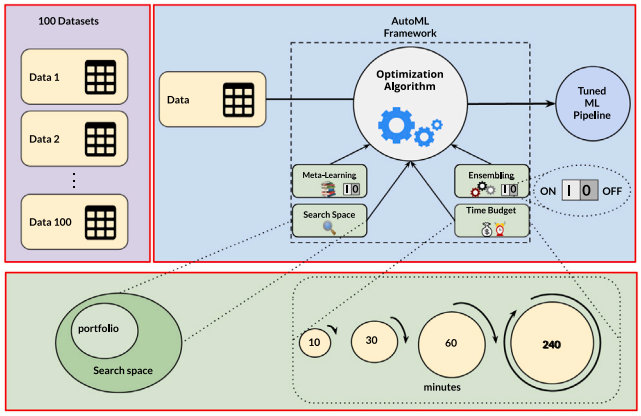


Fig. 1. The general Workflow of the benchmark design and AutoML process.

user-defined evaluation metric (e.g., accuracy, sensitivity, specificity, F1-score) within the user-defined budget for the search process, as shown in Fig. 1. Additionally, different AutoML frameworks consider various design decisions. For example, `SmartML` (Maher & Sakr, 2019) adopts a *meta-learning* based mechanism to improve the performance of the automated search process by starting with the most promising classifiers that performed well with similar datasets in the past. Another example, `AutoSKlearn` (Feurer et al., 2015) employs an option to take a weighted average of the predictions of an ensemble composed of the top trained models during the optimization process. Auto-Tuned Models (`ATM`) (Swearingen et al., 2017) restricts the default search space into only three classifiers, namely, decision tree, K-nearest neighbors, and logistic regression. Nevertheless, there is no clear understanding of the impact of various design decisions of the different AutoML frameworks on the performance of the output pipeline. In this work, we aim to answer the following four questions:

(1) What is the impact of the time budget on the performance of different AutoML frameworks? Given more time budget, can AutoML frameworks guarantee consistent performance improvement?

(2) What is the impact of the search space size of the AutoML framework on the performance? How does limiting the search space to a predefined portfolio affect the predictive performance?

(3) Does meta-learning always yield a consistent performance improvement across different time budgets? Is there a relationship between the characteristics of the datasets and the improvement caused by employing the meta-learning version of the AutoML framework?

(4) Does ensemble construction yield better performance than single learners across different time budgets? Is there a relationship between the characteristics of the datasets and the improvement caused by employing the ensembling version of the AutoML framework?

This work is an extension of our initial work (Eldeeb et al., 2021) that mainly focused on studying the impact of different design decisions on the performance of `AutoSKlearn`. More specifically, in this work, we follow a holistic approach to design and conduct a comparative study of six AutoML frameworks, namely `AutoWeka` (Kotthoff et al., 2017), `AutoSKlearn`, `TPOT` (Olson & Moore, 2016), `Recipe` (de Sá et al., 2017), `ATM` and `SmartML`, focusing on comparing their general performance under various design decisions including *time budget*, *size of search space*, *meta-learning* and *ensembling*. For ensuring reproducibility as one of the main targets of this work, we provide access to the source codes and the detailed results for the experiments of our studies.[1]

The remainder of this paper is organized as follows. The related work is reviewed in Section 2. Section 3 provides an overview of the evaluated frameworks included in our study. Section 4 describes our benchmark design. The evaluation of the general performance of the benchmark frameworks and the evaluation of the different design decisions on the performance of the benchmark frameworks are presented in Section 5. We discuss the results and future direction in Section 6 before we finally conclude the paper in Section 7.

2. Related work

Recently, few research efforts have attempted to tackle the challenge of benchmarking different AutoML frameworks (Gijsbers et al., 2019; He et al., 2019; Shawi et al., 2019; Truong et al., 2019; Zöller & Huber, 2021). In general, most experimental evaluation and comparison studies show no framework always performed the best, as some trade-offs always need to be considered and optimized according to user-defined objectives. For example, Gijsbers et al. (2022) conducted a study to compare the performance of 9 AutoML frameworks, namely, Autogluon-tabular (Erickson et al., 2020), `AutoSKlearn`, `AutoSKlearn 2` (Feurer et al., 2020), `FLAML` (Wang et al., 2021), `GAMA` (Gijsbers & Vanschoren, 2020), `H2O AutoML` (LeDell & Poirier, 2020), `LightAutoMLs` (Vakhrushev et al., 2021), `MLjar` (Płońska & Płoński, 2021), and `TPOT`, across 71 classification and 33 regression tasks. The study includes techniques for comparing AutoML frameworks, including final model accuracy, inference time trade-offs, and failure analysis. Autogluon has a consistently higher average performance in this benchmark. Additionally, an interactive visualization tool is supported to explore further the results and reproducibility of the analyses performed. Gijsbers et al. (2019) have conducted an experimental study to compare the performance of 4 AutoML frameworks, namely, `AutoWeka`, `AutoSKlearn`, `TPOT` and `H2O` on 39 datasets across two time budgets (60 min and 240 min). The results showed that no single AutoML framework outperformed others across all time budgets. Surprisingly, on some datasets, none of the frameworks outperformed the Random Forest model within 4 h time budget. Truong et al. (2019) compared the performance of 7 AutoML frameworks, namely, `H2O`, `Auto-keras` (Jin et al., 2019), `AutoSKlearn`, `Ludwig`,[2] `Darwin`,[3] `TPOT` and `Auto-ml`[4] on 300 datasets across different time budgets. The results showed that no single framework outperformed all others on a plurality of tasks. Across the various evaluations and benchmarks, `H2O`, `Auto-keras` and `AutoSKlearn` performed better than the rest of the frameworks. In particular, `H2O` slightly outperformed other frameworks for binary classification and regression tasks while achieving poor performance on multi-class classification tasks. `Auto-keras` showed a stable performance across all tasks and slightly outperformed other frameworks on multi-class classification tasks while achieving poor performance on binary classification tasks.

Zöller and Huber (2021) compared the performance of different optimization techniques, namely, *Grid Search*, *Random Search*, *RObust Bayesian Optimization* (ROBO) (Klein et al., 2017), *Bayesian Tuning and Bandits* (BTB) (Smith et al., 2020), *hyperopt* (Bergstra et al., 2013b), *SMAC* (Hutter et al., 2011), *BOHB* (Falkner et al., 2018) and *Optunity* (Smith et al., 2020). The results showed that all optimization techniques achieved comparable performance, and a simple search algorithm such as random search did not perform worse than other techniques. Thus, the study suggested that ranking optimization techniques on pure performance measures are not reasonable, and other aspects like scalability should also be considered. The study also compared the performance of 5 AutoML frameworks, namely, `TPOT`, `hpsklearn` (Komer et al., 2014), `AutoSKlearn`, `ATM`, and `H2O` on 73 real datasets. The study considered `AutoSKLearn` once with the default optimizer *SMAC* and once replacing *SMAC* with the random

[1] https://datasystemsgrouput.github.io/AutoMLBench/

[2] https://github.com/uber/ludwig

[3] https://www.sparkcognition.com/product/darwin/

[4] https://github.com/ClimbsRocks/auto_ml

Table 1
Comparison table of the functionality of the AutoML frameworks considered in this study as of Jul 9, 2023.

	Release date	Popularity (#of stars on GitHub)	Optimization technique	ML tool box	Meta-Learning	Post-processing	GUI	Data pre-processing
AutoWeka	2013	314	Bayesian optimization	Weka	×	×	✓	✓
AutoSKlearn	2015	7k	Bayesian optimization	Scikit-Learn	✓	Ensemble selection	×	✓
TPOT	2016	9.1k	Evolutionary optimization	Scikit-Learn	×	×	×	×
Recipe	2017	50	Grammar-based genetic algorithm	Scikit-Learn	×	×	×	✓
ATM	2017	522	Distributed Random search & Tree-Parzen estimators	Scikit-Learn	×	×	×	✓
SmartML	2019	23	Bayesian optimization	mlr, RWeka & other R packages	✓	Voting ensembles	×	✓

search while ensemble building and meta-learning options are disabled. The comparison results showed that, on average, all AutoML frameworks performed quite similar with a maximum performance difference of 2.2%.

To the best of our knowledge, our study is the first to investigate the impact of different AutoML design decisions on predictive performance. We benchmark six open-source, centralized, and distributed AutoML frameworks, namely, `AutoWeka`, `AutoSKlearn`, `TPOT`, `Recipe`, `ATM` and `SmartML` on 100 datasets from established AutoML benchmark suites. Differently from the previous benchmark studies focused only on comparing the performance of different AutoML frameworks, we take a holistic approach to studying the impact of various design decisions, including the size of the search space, time budget, meta-learning, and ensembling construction on the performance of the AutoML frameworks.

3. AutoML frameworks

This section provides an introduction to the evaluated AutoML frameworks used in this study in terms of popularity (measured in terms of the number of stars on GitHub), ML tool-box used, optimization technique, whether they use meta-learning to learn from previous experience, whether they perform post-processing (e.g., ensemble construction), whether they use Graphical User Interface (GUI), or whether they perform pre-processing. Table 1 briefly summarizes the comparison across the AutoML frameworks considered in this study. More detailed comparisons between these frameworks follow in the rest of this section.

`AutoWeka` is implemented in Java on top of `Weka`, a popular ML library with a wide range of ML algorithms. `AutoWeka` employs Bayesian optimization using `SMAC` (Hutter et al., 2011) and `TPE` (Bergstra et al., 2013a) for algorithm selection and hyperparameter tuning. In particular, `SMAC` draws the relationship between algorithm performance and a given set of hyperparameters by estimating the predictive mean and variance of their performance along with the trees of a random forest model. `TPE` is a robust technique that separates low-performing parameter configurations from the best-performing ones.

`AutoSKlearn` is a tool for automating the process of building ML pipelines for classification and regression tasks. `AutoSKlearn` is implemented on top of `Scikit-Learn` (Buitinck et al., 2013), a popular Python ML package, and uses `SMAC` for algorithm selection and hyperparameter tuning. `AutoSKlearn` uses meta-learning to initialize the optimization procedure. Additionally, ensemble selection is implemented by combining the best pipelines to improve the performance of the output model. `AutoSKlearn` supports different execution options including the *vanilla* version (`AutoSKlearn-v`), the meta-learning version (`AutoSKlearn-m`), the ensembling selection version (`AutoSKlearn-e`), and the full version (`AutoSKlearn`), where all options are enabled.

`TPOT` is an AutoML framework for building classification and regression pipelines based on a genetic algorithm. ML pipelines can be expressed as a computational graph, with different branches representing different preprocessing pipelines. These pipelines are then optimized using a multi-objective optimization technique to minimize pipeline complexity while optimizing for performance to reduce overfitting caused by the large search space (Olson et al., 2016).

`Recipe` is an AutoML framework for building machine learning pipelines for classification tasks. `Recipe` follows the same optimization procedure as `TPOT`, exploiting the advantages of a global search. `TPOT` suffers from the unconstrained search problem in which resources can be spent on generating and evaluating invalid solutions. `Recipe` handles this problem by adding a grammar that reduces the generation of invalid pipelines and hence accelerates the optimization process.

`ATM` is a collaborative service for optimizing ML pipelines for classification tasks. In particular, `ATM` supports parallel execution through multiple nodes/cores with a shared model hub storing the results out of these executions and improving the selection of pipelines that may outperform the currently chosen ones. `ATM` is based on a hybrid Bayesian and multi-armed bandit optimization technique to traverse the search space and report the target pipeline.

`SmartML` is the first AutoML `R` package for classification tasks. In the algorithm selection phase, `SmartML` employs a meta-learning approach to identify the best-performing algorithms on similar datasets. The hyperparameter tuning of `SmartML` is based on `SMAC`. `SmartML` maintains the results of the new runs to continuously enrich its knowledge base to further improve the performance and robustness of future runs. `SmartML` supports two execution options which are the base version `SmartML-m` that employs meta-leaning for warm-starting, and the ensemble version `SmartML-e` that additionally employs a voting ensemble mechanism.

4. Benchmark design

Each benchmark task consists of a dataset, a metric to optimize, and design decisions made by the user, including a specific time budget to use. We will briefly explain our choice for each.

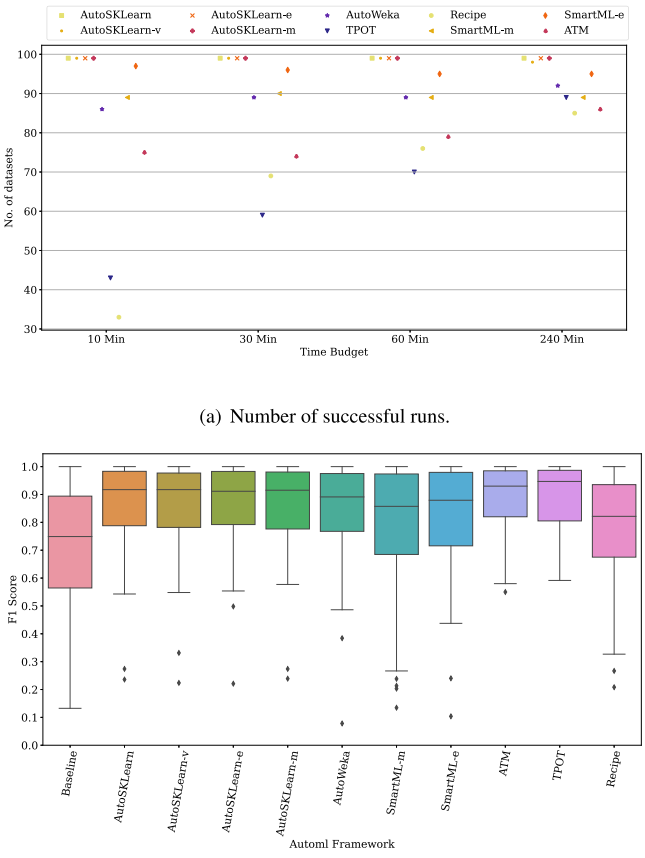
Datasets We used 100 datasets collected from the popular `OpenML` repository (Vanschoren et al., 2013), allowing users to query data for different use cases. Detailed descriptions of the datasets used in this study are given in Table A.9 in Appendix A. To evaluate the AutoML frameworks on a variety of dataset characteristics, we selected multiple datasets according to different criteria, including the number of classes, number of features, number of instances, number of categorical features per sample, number of instances with missing values, and the class entropy. The datasets represent a mix of binary (50%) and multiclass (50%) classification tasks, where the size of the largest dataset is 643MB.

Performance metrics The benchmark can be run with a wide range of measures per user's choice. The reported results in this paper are based on F1-score. AutoML frameworks are optimized for the same metric they are evaluated on. The measures are estimated with hold-out validation; each dataset is partitioned into two parts, 70% for training and 30% for testing. All AutoML frameworks are applied to the same training and testing splits on all datasets. To eliminate the effects of non-deterministic factors, the performance reported in each experiment is based on an average of 10 trials. We report a performance of 0 for any framework if the number of failed trials exceeds or is equal to 5.

Frameworks and design decisions The frameworks considered in this paper are selected based on ease of use, variety of underlying optimization techniques and ML toolboxes, popularity measured by the number of stars on GitHub, and citation count. All frameworks considered in this work are open source. A reference to the source code of each framework is given in Table B.10 in Appendix B. We do plan to include more frameworks in future work. For `AutoSKlearn`, we consider four execution options; `AutoSKlearn-v`, `AutoSKlearn-m`, `AutoSKlearn-e` and `AutoSKlearn`. For `SmartML`, we consider two execution options including `SmartML-m`, and `SmartML-e`. We examined different design decisions, including the size of the search space, meta-learning, and ensemble construction as a post-processing step. We study the impact of these design decisions for only AutoML frameworks that support configuring these decisions. It is important to highlight that the optimization technique is not consistent among all the frameworks, which prevents drawing a clear conclusion about this point in this benchmark. We consider the following versions of the frameworks: AutoSKLearn 0.11.0, AutoWeka 2.5, TPOT 0.11.6, Recipe 1.0, ATM 0.2.2, and SmartML 0.2.

Baseline method To assess the effectiveness of the different AutoML frameworks included in this work, we use a baseline method which is a simple pipeline consisting of an imputation of missing values and a random forest model (Pedregosa et al., 2011).

Time budget choice All AutoML frameworks were used with four different time budgets. Each framework is limited by a soft time budget (10, 30, 60, and 240 min) and a hard one (10% more than soft time budget). If a framework exceeds the hard time budget, the run is terminated and considered failed. Setting a time budget for all experiments is not straightforward. While it is more favorable to un-set a time limit to guarantee the best performance for each framework, however, doing so for all the six evaluated frameworks, with different configurations, across the 100 datasets, with ten trials for each, is very time-consuming. Therefore we used four time budgets which led to more than 40000 experiments to run for a total of more than 88366-hour EC2 run-time. To keep the experiment run-time and cost to practical limits, we tested the maximum cut-off timeouts of 4 and 8 h on 14 randomly selected datasets. The results are reported in Table C.11 in Appendix C. Additionally, the Wilcoxon signed-rank test was conducted to determine if a statistically significant difference in performance exists between the AutoML frameworks over the two-time budgets (See Table C.11). The results confirm that the difference is not necessarily towards the 8-hour budget, and not statistically significant. Hence, the 8-hour budget is not further considered.



(a) Number of successful runs.

(b) Performance of the final pipeline per AutoML framework for 240 minutes.

Fig. 2. General performance trends of the benchmark AutoML frameworks.

Hardware choice and resource specifications Our experiments were conducted on Google Cloud machines; each machine is configured with 2 vCPUs, 7.5 GB RAM and ubuntu-minimal-1804-bionic. Each machine uses Python 2.7.15, Python 3.6.8, scikit-learn 0.21.3, R 3.4.4, and Java 1.8. To avoid memory leakage, we have rebooted the machines after each run to ensure that each experiment has the same available memory size.

5. Experimental evaluation

This section provides empirical evaluations of the different AutoML frameworks. We first compare the general performance of the different AutoML frameworks in Section 5.1. Next, we examine the impact of various design decisions on the performance of the different AutoML frameworks in Section 5.2.

5.1. General performance evaluation

In this section, we focus on evaluating and comparing the general performance of the benchmark frameworks. Our evaluation considers different aspects for its comparison, including (a) the number of successful runs, (b) the average performance of the final pipeline per AutoML framework across all datasets, (c) the significance of the performance difference between different frameworks across different time budgets, (d) the robustness of the benchmark frameworks, and (e) the quality of the machine learning pipelines generated by the benchmark frameworks.

(a) 10 minutes time budget

(b) 30 minutes time budget

(c) 60 minutes time budget

(d) 240 minutes time budget

Fig. 3. Heatmaps show the number of datasets a given AutoML framework outperforms another in terms of predictive performance over different time budgets. Two frameworks are considered to have the same performance on a task if they achieve predictive performance with $< 1\%$ difference.

Fig. 2(a) shows the number of datasets with successful runs of each framework on different time budgets. If an AutoML framework could not generate a model for a particular dataset 5 times or more, it is considered a failed experiment. Generally, the results show that increasing the time budget for the AutoML frameworks increases the number of successful runs. `AutoSKlearn` achieves the largest number of successful runs across all time budgets, as shown in Fig. 2(a). Each of the different versions of `AutoSKlearn` successfully ran on 99 datasets across different time budgets. `SmartML-e` comes in second place in terms of the number of successful runs, followed by `AutoWeka` and `SmartML`. The genetic-based frameworks, `TPOT` and `Recipe` come in the last place, as shown in Fig. 2(a). For `Recipe` and `TPOT`, the number of successful runs achieved in the longest time budget, 240 min, is almost double that achieved for the smallest time budget of 10 min. Hence, larger budgets are preferable for `Recipe` and `TPOT`.

Fig. 2(b) reports the performances of all AutoML frameworks averaged over all datasets over 240 min budget. It is apparent that all frameworks are able to outperform the random forest baseline on average. However, single results vary significantly. D.9,D.10,D.11 in Appendix D report the performance of all AutoML frameworks and the baseline across 10, 30, 60 min, respectively. We investigate pair-wise "outperformance" by calculating the number of datasets for which one framework outperforms another across different time budgets, shown in Fig. 3. One framework outperforms another on a dataset if it has at least a 1% higher predictive performance, representing a minimal threshold for performance improvement. In terms of "outperformance", it is worth mentioning that no single AutoML framework performs best across all 100 datasets on all-time budgets. For example, for the 10 min time budget, there are 2 datasets for which `Recipe` performs better than `AutoSKlearn`, despite being the overall worst- and best-ranked algorithms, respectively, as shown in Fig. 3(a). On average, the results show that `AutoSKlearn` framework comes in the first place, outperforming other frameworks on the most significant number of datasets for different time budgets, followed by `ATM` framework, while `Recipe` comes in the last place, as shown in Fig. 3. The Wilcoxon signed-rank test (Gehan, 1965) was conducted to determine if a statistically significant difference in performance exists between the AutoML frameworks including the baseline over different time budgets, the results of which are summarized in Table 2. The results show that all AutoML frameworks except `Recipe` statistically outperform the baseline across all time budgets with a significant difference. The results of the Wilcoxon test confirm the fact that there is no dominating winner, and the statistical significance in the performance difference among the AutoML frameworks can vary from one-time budget to another. The ensembling version and the full version of `AutoSKlearn` statistically outperform most of the other frameworks across all time budgets. The results show that `SmartML-m`, `SmartML-e`, and `AutoWeka` are statistically outperformed by the majority of the frameworks, as shown in Table 2. For longer time budgets of 60 and 240 min, `TPOT` significantly outperforms `AutoWeka`, `Recipe`, `SmartML-m`, `SmartML-e`, `AutoSKlearn-m`, and `AutoSKlearn-v`.

We investigate the performance of the different AutoML frameworks based on the various characteristics of datasets and tasks. Fig. 4 reports the mean performances of the AutoML frameworks on multi-class and binary-class classification tasks across 240 min budget. Notably, the improvement achieved by all AutoML on multi-class datasets is less significant than the average improvement on whole datasets. The second subgroup of datasets where autoML frameworks struggle to boost their

Table 2
Wilcoxon pairwise test p-values for AutoML frameworks over different time budgets. Bold entries highlight significant differences ($p \leq 0.05$). Highlighted entries in each row represent a given AutoML framework (row) outperforms another AutoML framework (column).

10 Minutes

	Baseline	ATM	AutoWeka	Recipe	AutoSKLearn-e	AutoSKLearn-m	AutoSKLearn-v	AutoSKLearn	SmartML-m	SmartML-e	TPOT
Baseline		0.0	0.0	0.15	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ATM	**0.0**		**0.008**	0.088	0.768	0.516	0.299	0.587	0.064	0.062	0.879
AutoWeka	**0.0**	0.008		0.156	0.0	0.0	0.004	0.0	0.748	0.096	0.06
Recipe	0.15	0.088	0.156		0.002	0.002	0.004	0.0	0.417	0.248	0.013
AutoSKLearn-e	**0.0**	0.768	**0.0**	**0.002**		0.569	**0.014**	0.001	**0.023**	0.203	0.492
AutoSKLearn-m	**0.0**	0.516	**0.0**	**0.002**	0.569		**0.009**	0.009	**0.004**	0.1	0.33
AutoSKLearn-v	**0.0**	0.299	**0.004**	**0.004**	0.014	0.009		0.0	**0.042**	0.663	**0.026**
AutoSKLearn	**0.0**	0.587	**0.0**	**0.0**	**0.001**	**0.009**	**0.0**		**0.001**	**0.035**	0.258
SmartML-m	**0.0**	0.064	0.748	0.417	0.023	0.004	0.042	0.001		0.014	0.022
SmartML-e	**0.0**	0.062	0.096	0.248	0.203	0.1	0.663	0.035	**0.014**		0.452
TPOT	**0.0**	0.879	0.06	**0.013**	0.492	0.33	0.026	0.258	**0.022**	0.452	

30 Minutes

	Baseline	ATM	AutoWeka	Recipe	AutoSKLearn-e	AutoSKLearn-m	AutoSKLearn-v	AutoSKLearn	SmartML-m	SmartML-e	TPOT
Baseline		0.0	0.0	0.346	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ATM	**0.0**		**0.034**	**0.0**	0.898	0.408	0.159	0.85	**0.009**	**0.015**	0.902
AutoWeka	**0.0**	0.034		**0.004**	0.0	0.0	0.003	0.0	0.92	0.195	0.003
Recipe	0.346	0.0	0.004		0.0	0.0	0.0	0.0	0.134	0.007	0.0
AutoSKLearn-e	**0.0**	0.898	**0.0**	**0.0**		**0.015**	**0.0**	0.694	**0.001**	**0.005**	0.94
AutoSKLearn-m	**0.0**	0.408	**0.0**	**0.0**	0.015		**0.03**	0.152	**0.006**	0.075	0.316
AutoSKLearn-v	**0.0**	0.159	**0.003**	**0.0**	0.0	0.03		0.0	0.064	0.112	0.005
AutoSKLearn	**0.0**	0.85	**0.0**	**0.0**	0.694	0.152	**0.0**		**0.002**	**0.014**	0.337
SmartML-m	**0.0**	0.009	0.92	0.134	0.001	0.006	0.064	0.002		0.015	0.002
SmartML-e	**0.0**	0.015	0.195	**0.007**	0.005	0.075	0.112	0.014	**0.015**		0.065
TPOT	**0.0**	0.902	**0.003**	**0.0**	0.94	0.316	**0.005**	0.337	**0.002**	0.065	

60 Minutes

	Baseline	ATM	AutoWeka	Recipe	AutoSKLearn-e	AutoSKLearn-m	AutoSKLearn-v	AutoSKLearn	SmartML-m	SmartML-e	TPOT
Baseline		0.0	0.0	0.201	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ATM	**0.0**		**0.017**	**0.0**	0.075	0.358	0.424	0.149	**0.005**	**0.004**	0.064
AutoWeka	**0.0**	0.017		**0.015**	0.0	0.0	0.0	0.0	0.59	0.083	0.0
Recipe	0.201	0.0	0.015		0.0	0.0	0.0	0.0	0.054	0.003	0.0
AutoSKLearn-e	**0.0**	0.075	**0.0**	**0.0**		**0.046**	**0.003**	0.319	**0.003**	**0.011**	0.198
AutoSKLearn-m	**0.0**	0.358	**0.0**	**0.0**	0.046		0.474	0.0	**0.012**	0.052	0.067
AutoSKLearn-v	**0.0**	0.424	**0.0**	**0.0**	0.003	0.474		0.0	**0.039**	0.201	0.01
AutoSKLearn	**0.0**	0.149	**0.0**	**0.0**	0.319	**0.0**	**0.0**		**0.001**	**0.015**	0.86
SmartML-m	**0.0**	0.005	0.59	0.054	0.003	0.012	0.039	0.001		0.047	0.0
SmartML-e	**0.0**	0.004	0.083	**0.003**	0.011	0.052	0.201	0.015	**0.047**		0.007
TPOT	**0.0**	0.064	**0.0**	**0.0**	0.198	0.067	**0.01**	0.86	**0.0**	**0.007**	

4 Hours

	Baseline	ATM	AutoWeka	Recipe	AutoSKLearn-e	AutoSKLearn-m	AutoSKLearn-v	AutoSKLearn	SmartML-m	SmartML-e	TPOT
Baseline		0.0	0.0	0.039	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ATM	**0.0**		**0.046**	**0.0**	0.637	0.943	0.969	0.754	**0.002**	0.061	0.153
AutoWeka	**0.0**	0.046		**0.027**	0.0	0.001	0.002	0.0	0.773	0.389	0.0
Recipe	**0.039**	0.0	0.027		0.0	0.0	0.0	0.0	0.024	0.004	0.0
AutoSKLearn-e	**0.0**	0.637	**0.0**	**0.0**		**0.015**	**0.021**	0.447	**0.001**	**0.007**	0.152
AutoSKLearn-m	**0.0**	0.943	**0.001**	**0.0**	0.015		0.852	0.0	**0.006**	**0.043**	0.001
AutoSKLearn-v	**0.0**	0.969	**0.002**	**0.0**	0.021	0.852		0.001	**0.004**	0.06	0.0
AutoSKLearn	**0.0**	0.754	**0.0**	**0.0**	0.447	**0.0**	**0.001**		**0.0**	**0.002**	0.119
SmartML-m	**0.0**	0.002	0.773	**0.024**	0.001	0.006	0.004	0.0		0.031	0.0
SmartML-e	**0.0**	0.061	0.389	**0.004**	0.007	0.043	0.06	0.002	**0.031**		0.001
TPOT	**0.0**	0.153	**0.0**	**0.0**	0.152	**0.001**	**0.0**	0.119	**0.0**	**0.001**	

performance contains datasets with a relatively large number of features and a small number of instances as shown in D.13,D.14,D.15,D.12 in Appendix D. These figures report the mean performance of the different AutoML frameworks on datasets with various characteristics, including a large number of instances and features, a small number of features and instances, a small number of features and a large number of instances, and a large number of features and a small number of instances. Additionally, we report the mean performance of all frameworks on binary classification tasks (See Fig. 4(b) in Appendix D).

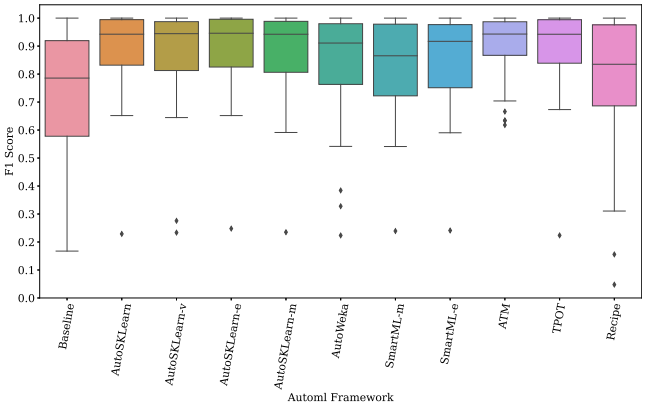
We test the robustness of the AutoML frameworks evaluated by the ability of the framework to achieve the same results across different runs on the same input dataset. For a randomly selected dataset, we run each AutoML framework for 10 different times on 10 min time budget. Fig. 5 shows the robustness of the AutoML frameworks. The results show that the four versions of `AutoSKlearn` have the most stable runs, and `Recipe` and `AutoWeka` comes second. on contrast, the two versions of `SmartML` achieve the least stable runs.

In our evaluation of machine learning (ML) pipelines generated by AutoML frameworks, we employ a set of well-defined evaluation metrics to provide a comprehensive understanding of the factors that significantly affect the practicality and utility of ML pipelines produced by AutoML frameworks. Following the approach outlined in (Ali et al., 2017), we establish quality metrics with the goal of offering a new perspective on the assessment of AutoML frameworks. These metrics particularly focus on evaluating the frameworks' efficiency during training, performance during inference, model stability, and robustness to noise. In Table 3, we present the average performance of AutoML frameworks using these metrics across all datasets. Definitions for these metrics are provided below.

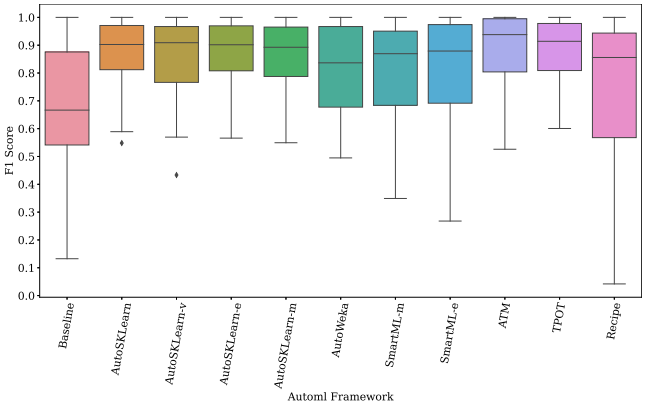
- **Training Efficiency:** assesses the training efficiency of an ML model, measuring the CPU wall-clock time required for model training. This metric provides insights into the computational resources consumed during the training process. Table 3 shows

Table 3
Performance evaluation of benchmark AutoML frameworks using key metrics: training efficiency, inference performance, robustness to noise and model stability.

Framework	Training efficiency (s)	Inference performance (s)	Robustness to noise	Model stability
ATM	43.25 ± 1.17	0.100 ± 0.007	0.07	0.0014
AutoWeka	46.85 ± 1.28	0.103 ± 0.008	0.05	0.0016
Recipe	43.10 ± 0.95	0.098 ± 0.007	0.04	0.0013
AutoSKLearn-e	66.50 ± 1.11	0.106 ± 0.007	0.10	0.0017
AutoSKLearn-m	45.20 ± 0.98	0.099 ± 0.007	0.10	0.0015
AutoSKLearn-v	44.80 ± 1.15	0.101 ± 0.008	0.06	0.0018
AutoSKLearn	67.20 ± 1.02	0.105 ± 0.007	0.07	0.0016
SmartML-m	53.00 ± 0.93	0.098 ± 0.007	0.04	0.0014
SmartML-e	73.50 ± 1.10	0.107 ± 0.008	0.07	0.0017
TPOT	48.80 ± 1.19	0.104 ± 0.008	0.09	0.0015



(a) Performance of the final pipeline on multi-class classification tasks.



(b) Performance of the final pipeline on binary classification tasks.

Fig. 4. Performance of the different AutoML frameworks based on the various characteristics of datasets and tasks over 240 min.

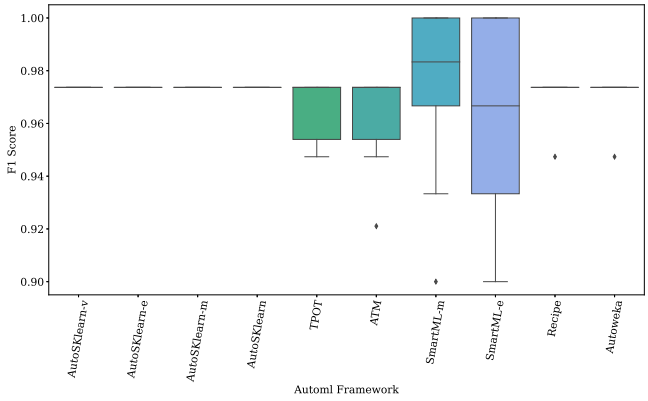


Fig. 5. Evaluation of AutoML frameworks for robustness on (dataset_61_iris).

that ATM and Recipe offer the shortest training periods among the benchmarked frameworks. This is particularly advantageous for applications with limited computational resources or for scenarios where rapid model development is essential. On the other hand, AutoSKLearn and SmartML-e require significantly more time for training.

- **Inference Performance:** measures the inference speed of an ML model by quantifying the CPU wall-clock time required to produce a single prediction. The results in Table 3 highlight that SmartML-m and Recipe stand out with shorter inference times. This information is vital for use cases where quick decisions or predictions are necessary, such as online recommendation systems or autonomous vehicles. Conversely, SmartML-e lags behind, as it records the longest inference time.
- **Model Stability:** assesses the consistency of an ML model by calculating the standard deviation when the model is retrained on the same dataset. Notably, Recipe, SmartML-m, and ATM exhibit the most stable performance among all frameworks, as evidenced by their lower standard deviation.
- **Robustness to Noise:** evaluates the resilience of an ML model to noise introduced into the data. Robustness is assessed by observing how the model's behavior changes when noise is introduced to the test set. Greater variations in a model's behavior in response to noise indicate lower robustness. The difference in behavior is quantified using the Cohen's Kappa metric (Landis & Koch, 1977). More specifically, we use Kappa as a measure of similarity between a model's predictions on the original and perturbed test sets. Instances in the test sets are perturbed by modifying their feature values within a range of possible values. For continuous features, we introduce Gaussian noise with level 10 (Beerenwinkel & Siebourg, 2012). For categorical features, random uniform noise is added, implying that all categories, except the original one, have an equal probability $(1/n - 1)$ of being selected as noise, where n is the number of categories.
  The results in Table 3 reveal that AutoSKLearn-e and AutoSKLearn-m exhibit the highest levels of robustness among the frameworks, while Recipe and SmartML-m demonstrate comparatively lower levels of robustness.

5.2. Performance evaluation of different design decisions

In this section, we study the impact of different design decisions including time budget (Section 5.2.1), size of search space (Section 5.2.2),

Table 4
$Mean_{Succ}$, Mean and standard deviation of the predictive performance of AutoML frameworks per time budget. Bold entries highlight highest $Mean_{Succ}$, mean and lowest standard deviation.

Time budget	Framework	$Mean_{Succ}$	Mean	SD	Time budget	Framework	$Mean_{Succ}$	Mean	SD
	ATM	0.664	0.886	0.126		**ATM**	0.700	**0.886**	**0.132**
	AutoWeka	0.724	0.842	0.165		**AutoWeka**	0.743	0.835	0.167
	Recipe	0.252	0.764	0.221		**Recipe**	0.568	0.748	0.247
	AutoSKLearn-e	**0.859**	0.868	0.145		**AutoSKLearn-e**	**0.870**	0.879	0.138
	AutoSKLearn-m	0.855	0.864	0.153		**AutoSKLearn-m**	0.861	0.870	0.144
10 Min	**AutoSKLearn-v**	0.853	0.862	0.151	**60 Min**	**AutoSKLearn-v**	0.861	0.870	0.142
	AutoSKLearn	**0.859**	0.868	0.152		**AutoSKLearn**	0.868	0.877	0.137
	SmartML-m	0.806	0.799	0.212		**SmartML-m**	0.790	0.816	0.194
	SmartML-e	0.711	0.831	0.176		**SmartML-e**	0.726	0.832	0.0172
	TPOT	0.383	**0.890**	**0.121**		**TPOT**	0.620	0.885	0.137
	ATM	0.665	**0.899**	**0.121**		**ATM**	0.768	**0.893**	**0.124**
	AutoWeka	0.747	0.839	0.166		**AutoWeka**	0.771	0.838	0.166
	Recipe	0.516	0.748	0.254		**Recipe**	0.645	0.759	0.248
	AutoSKLearn-e	**0.866**	0.875	0.141		**AutoSKLearn-e**	0.874	0.883	0.132
	AutoSKLearn-m	0.859	0.868	0.152		**AutoSKLearn-m**	0.864	0.873	0.141
30 Min	**AutoSKLearn-v**	0.858	0.867	0.149	**240 Min**	**AutoSKLearn-v**	0.850	0.867	0.156
	AutoSKLearn	0.862	0.871	0.148		**AutoSKLearn**	**0.875**	0.884	0.132
	SmartML-m	0.804	0.808	0.199		**SmartML-m**	0.798	0.826	0.169
	SmartML-e	0.727	0.838	0.159		**SmartML-e**	0.735	0.840	0.165
	TPOT	0.518	0.878	0.144		**TPOT**	0.790	0.888	0.131

meta-learning (Section 5.2.3), and ensembling (Section 5.2.4) on the performance of the different AutoML frameworks across different time budgets. For each framework, the performance reported in each experiment is based on an average of 10 runs.

5.2.1. Impact of time budget

Tuning the time budget is a crucial and challenging task in AutoML, as it requires a balance between the available computational resources and the desired level of performance. It is a task that involves careful consideration of trade-offs between generalization and over-fitting of the AutoML frameworks. We investigate the impact of time budget on the performance of various AutoML frameworks, examining the speed at which they can generate ML pipelines and their ability to consistently improve performance given more time. We assess each framework's performance on successful runs under four different time budgets: 10, 30, 60, and 240 min. Table 4 presents the mean (`Mean`) and standard deviation (`SD`) of performance for all successful runs at each time budget. Furthermore, we report the mean predictive performance weighted by the percentage of successful runs ($Mean_{succ}$).

$$Mean_{succ} = Mean \times \frac{N}{T} \tag{1}$$

where N is the number of successful runs and T is the total number of runs.

The results show that for the 10 and 240 min budgets, `AutoSKlearn` and `AutoSKlearn-e` have comparable $Mean_{succ}$, while `AutoSKlearn-e` has the highest $Mean_{succ}$ over the rest of time budgets. In contrast, `Recipe` achieves the lowest mean performance and $\texttt{Mean}_{\texttt{succ}}$ over all time budgets, as shown in Table 4. Notably, the performance of genetic-based tools, i.e., `Recipe` and `TPOT`, improves over time as the $Mean_{succ}$ values show. G.18, G.19, G.20, G.21, G.22, G.23, G.24, G.25, G.26, G.27 in Appendix G show the impact of increasing the time budget for each AutoML framework on 100 datasets.

Extended time budgets do not necessarily lead to better performance, in contrast to the prior assumptions, as shown in Table 5. We report the gain (g) or loss (l) in the predictive performance of the frameworks when increasing the time budget. The gain is measured by the mean and maximum predictive performance improvement over all improved/declined datasets. When increasing the time budget from 10 to 30 min, `Recipe` achieves the highest mean gain of 19.3 on 2 datasets, followed by `SmartML-m`, while `AutoSKlearn` comes in the last place achieving a mean gain of 3.5 on 17 datasets. It is noticeable that `Recipe` has the smallest number of datasets that witnessed performance improvement and performance degradation when increasing the time budget. `AutoSKlearn-v` have the largest number of datasets that witnessed performance improvement when increasing the time budget from 30 to 60 min and from 60 to 240 min, while `AutoSKlearn-e` witnessed performance improvement across the largest number of datasets when increasing the time budget from 10 to 30 min. In contrast, `ATM` has the most significant number of datasets with performance degradation when increasing the time budget from 10 to 30 min and from 30 to 60 min.

The Wilcoxon signed-rank test is conducted to determine if the average performance difference when extending the time budget is statistically significant, as shown in Table 6. The impact of increasing the time budget varies from one framework to another. For example, `AutoSKlearn-m`, `Recipe`, `ATM`, `SmartML-m` and `SmartML-e` does not witness significant performance difference. While in most of the cases of `AutoWeka`, `TPOT` and all versions of `AutoSKlearn` except `AutoSKlearn-m`, the differences are statistically significant. These results show that end-users should always carefully consider the trade-off between time budget and performance for the benchmark frameworks based on their specific goals.

5.2.2. Impact of the size of search space

Search space defines the structural paradigm that the different optimization methods can explore; thus, designing a good search space is a vital but challenging problem. Fig. 6 provides an overview of the most frequent ML models commonly used by the different AutoML frameworks. By analyzing the returned best-performing models, it is notable that there is no single ML algorithm that dominates all AutoML frameworks; however, it is apparent the tree-based models are the most frequent across all frameworks for all time budgets. For example, the returned pipelines by `AutoWeka`, `AutoSKlearn-v`, and `SmartML-m` show that *random forest* is the most frequently used classifier, as shown in Figs. 6(a), 6(c), and 6(e). The most frequent classifier for `AutoSKlearn-m`, `TPOT`, and `Recipe` is *gradient boosting*, as shown in Figs. 6(d), 6(f), and 6(g), respectively. To efficiently utilize the time budget, `ATM` limits its default search space to only three classifiers, namely, *k-nearest neighbors*, *decision tree*, and *logistic regression*, while *decision tree* is the most frequently used one, as shown in Fig. 6(b).

Finding an optimal solution to the time-bounded optimization problem of AutoML requires defining the underlying search space and

Table 5
Summary of the impact of increasing the time budget. Bold entries highlight the highest mean gain, highest maximum gain, smallest mean loss, smallest maximum loss, and maximum and minimum number of datasets with gain > 1 and loss >1, respectively.

Time Budget	Framework	Gain (g)		#datasets with			Loss (l)	
in minutes		Mean	Max	$g > 1\%$	$g \approx 0\%$	$l > 1\%$	Mean	Max
10 → 30	**ATM**	4.3	21.0	19	33	15	−4.7	**−21.4**
	AutoWeka	5.8	20.1	16	62	7	−3.8	−11.9
	Recipe	**19.3**	36.6	2	17	2	−4.4	−6.2
	AutoSKLearn-e	3.6	13.5	24	67	8	−2.7	−6.8
	AutoSKLearn-m	3.6	13.3	21	65	13	−2.6	−10.7
	AutoSKLearn-v	3.9	22.1	23	63	13	−3.1	−7.4
	AutoSKLearn	3.5	15.2	17	72	10	−2.6	−4.8
	SmartML-m	8.0	33.3	13	64	11	−3.6	−8.3
	SmartML-e	7.9	**85.2**	18	67	11	**−6.3**	−16.9
	TPOT	6.2	17.0	7	29	4	−2.2	−3.7
30 → 60	**ATM**	5.0	16.5	15	34	20	−6.7	−28.6
	AutoWeka	9.1	**66.6**	14	61	13	−9.6	−56.7
	Recipe	4.7	17.2	6	58	3	**−19.2**	−29.1
	AutoSKLearn-e	4.9	19.6	16	66	17	−2.2	−5.7
	AutoSKLearn-m	4.9	23.4	16	67	16	−4.1	−13.3
	AutoSKLearn-v	4.1	14.2	23	62	14	−4.6	−13.9
	AutoSKLearn	4.1	32.0	22	65	12	−2.4	−6.8
	SmartML-m	**12.2**	40.0	10	73	6	−6.2	−18.3
	SmartML-e	6.5	18.2	21	54	20	−9.0	**−84.3**
	TPOT	3.7	8.7	6	42	8	−2.8	−7.7
60 → 240	**ATM**	5.6	31.1	21	39	17	−3.4	−12.0
	AutoWeka	4.1	8.7	17	61	8	−3.8	−11.5
	Recipe	13.5	38.2	4	69	2	**−20.5**	**−40.0**
	AutoSKLearn-e	4.3	39.0	21	62	16	−3.8	−12.7
	AutoSKLearn-m	4.0	13.3	20	59	20	−2.7	−6.0
	AutoSKLearn-v	3.6	12.5	22	63	13	−8.7	−25.3
	AutoSKLearn	4.8	36.5	22	63	14	−3.2	−9.9
	SmartML-m	**10.6**	**59.6**	19	59	10	−6.6	−19.4
	SmartML-e	9.1	22.3	23	53	19	−6.9	−18.8
	TPOT	2.6	5.6	18	47	5	−4.1	−7.7

searching for well-performing ML pipelines as efficiently as possible. Often these search spaces are chosen arbitrarily without any validation, sometimes leading to bloated spaces and the inability to find optimal results (Zöller & Huber, 2021). In the following, we examine the impact of a budget allocation strategy as a complementary design decision for AutoML frameworks. The strategy is based on using a static portfolio (Kotthoff, 2016) – a set of configurations that covers as many diverse datasets as possible and minimizes the risk of failure when facing a new task. So, we construct a portfolio consisting of the top three performing classifiers over the 100 datasets and supported by all AutoML frameworks. These classifiers are *support vector machine*, *random forest*, and *decision tree*. Then for a dataset at hand, all algorithms in this portfolio based on different hyperparameters are evaluated. For the AutoML frameworks included in this work that allows configuring the search space, `ATM`, `AutoSKlearn`, and `TPOT`, we compare the performance of using the full search space including all available classifiers (FC) to the performance when using the static portfolio ($3C$) on 30 min time budget, the results of which are summarized in Fig. 7.

For `AutoSKlearn`, the results show that the performance of the FC outperforms $3C$ on 28 datasets with an average predictive performance gain of 3.3%. However, the performance achieved using the $3C$ outperforms that achieved using the FC on 21 datasets by 5.9%, as shown in Fig. 7(a). This performance discrepancy is attributed to the AutoML framework's focus on tuning classifiers that have yielded good performance, thereby evaluating more hyperparameters of these classifiers. Hence, AutoML frameworks concentrate on promising regions in the search space while disregarding unimportant ones. The performance of both FC and $3C$ is comparable on 50 datasets, with predictive performance differences of less than 1%. For `TPOT`, 23 datasets failed to run using the $3C$, while 20 failed using the FC. Both search spaces failed to produce results for 12 datasets, as shown in Fig. 7(b). For successful runs, the FC outperformed the $3C$ on 21 datasets, with an average predictive performance improvement of 9.6%. In contrast, the performance of both search spaces was comparable on 18 datasets. Notably, the $3C$ search space achieved better performance than the FC search space on six datasets, with an average predictive performance difference of 8.8%. For `ATM`, the $3C$ outperformed the FC search space on 17 datasets, with an average predictive performance improvement of 4%. In contrast, the FC search space outperformed the $3C$ search space on 15 datasets, with an average performance improvement of 9.3%. Both search spaces achieved comparable performance on 22 datasets, as depicted in Fig. 7(c). Notably, the FC failed to produce results for 19 datasets in which the $3C$ search space succeeded. In contrast, the $3C$ failed for ten datasets that the FC was successful. The Wilcoxon signed-rank test was conducted to determine if a statistically significant difference in performance exists between the FC and $3C$ across all datasets. For `TPOT`, the test results show that the difference in performance between the two search spaces is statistically significant with more than 95% level of confidence (p-value=0.003). However, no statistically significant difference in performance exists between the two search spaces for `AutoSKlearn` and `ATM`.

5.2.3. Impact of meta-learning

One way to define meta-learning is the process of learning from previous experience gained during applying various learning algorithms on different ML tasks, reducing the time needed to learn new tasks (Vanschoren, 2018). In the following, we study the impact of meta-learning on the performance of AutoML frameworks. The only framework that supports configuring meta-learning is `AutoSKlearn`. Furthermore, we investigate the relationship between the characteristics of the different datasets and the improvement caused by employing the vanilla version or the meta-learning version of the `AutoSKlearn`.

Table 6
Wilcoxon test p-values for all the AutoML frameworks over different time budgets. Bold entries highlight significant difference.

Framework	Time budget 1	Time budget 2	Avg. acc. diff	*P* value	Framework	Time budget 1	Time budget 2	Avg. acc. diff	*P* value
AutoWeka	30	10	0.008	**0.016**	**AutoSKLearn**	30	10	0.003	0.338
	60	10	0.003	**0.034**		60	10	0.010	**0.001**
	60	30	0.000	0.885		60	30	0.007	**0.034**
	240	10	0.009	**0.000**		240	10	0.016	**0.004**
	240	30	0.005	**0.039**		240	30	0.013	**0.018**
	240	60	0.005	**0.042**		240	60	0.006	0.129
TPOT	30	10	0.009	0.117	**AutoSKLearn-v**	30	10	0.005	0.175
	60	10	0.008	0.388		60	10	0.008	**0.001**
	60	30	0.001	0.428		60	30	0.003	0.088
	240	10	0.013	**0.016**		240	10	0.005	**0.000**
	240	30	0.006	**0.035**		240	30	0.000	**0.040**
	240	60	0.004	**0.008**		240	60	-0.003	0.099
Recipe	30	10	0.014	0.866	**AutoSKLearn-e**	30	10	0.008	**0.000**
	60	10	-0.002	0.955		60	10	0.012	**0.000**
	60	30	-0.004	0.535		60	30	0.004	0.904
	240	10	0.023	0.093		240	10	0.015	**0.000**
	240	30	0.003	0.067		240	30	0.007	**0.038**
	240	60	0.002	0.345		240	60	0.003	0.291
ATM	30	10	0.001	0.583	**AutoSKLearn-m**	30	10	0.004	0.156
	60	10	−0.007	0.254		60	10	0.006	0.105
	60	30	−0.008	0.499		60	30	0.002	0.873
	240	10	0.003	0.585		240	10	0.009	0.210
	240	30	−0.001	0.799		240	30	0.004	0.920
	240	60	0.008	0.394		240	60	0.003	0.660
SmartML-m	30	10	0.007	0.636	**SmartML-e**	30	10	0.008	0.521
	60	10	0.009	0.832		60	10	0.003	0.589
	60	30	0.009	0.597		60	30	−0.004	0.672
	240	10	0.026	0.121		240	10	0.011	0.092
	240	30	0.025	**0.050**		240	30	0.004	0.182
	240	60	0.015	0.071		240	60	0.008	0.305

`AutoSKlearn` applies a meta-learning mechanism based on a knowledge base storing the meta-features of datasets as well as the best-performing pipelines on these datasets. `AutoSKlearn` uses 38 meta-features, including statistical, information-theoretic and simple meta-features. In an offline phase, the meta-features and the empirically best-performing pipelines are stored for each dataset in their repository (140 datasets from the OpenML repository). In an online phase, for any new dataset, the framework extracts the meta-features of the new dataset and searches for the most similar datasets in the knowledge base. It returns the top k best-performing pipelines on these similar datasets. These k pipelines are used as a warm start for the Bayesian optimization algorithm used in the optimization process. To assess the impact of the meta-learning mechanism, we compare the performance of `AutoSKlearn-v` and `AutoSKlearn-m` on 100 datasets across different time budgets, as shown in Fig. 8. The results show that using meta-learning is not necessarily associated with performance improvement. On average, the performance of the vanilla and the meta-learning versions is very comparable on the 4 time budgets. In particular, both versions perform similarly on 64, 55, 65, and 69 datasets for 10 min, 30 min, 60 min and 240 min, respectively. Table 7 summarizes the performance of both of `AutoSKlearn-m` and `AutoSKlearn-v`, in addition to the number of datasets achieved improvement in performance by employing `AutoSKlearn-m` over `AutoSKlearn-v` on different time budgets. The improvement achieved by employing the meta-learning version decreases for extended time budgets. For example, the number of datasets that achieved performance improvement by using meta-learning dropped from 28 for the 30 min budget to 14 for the 240 min budget, as shown in Table 7. We use `Wilcoxon` statistical test to assess the significance of the performance difference between the vanilla version and the meta-learning version. The results show that the impact of the meta-learning is statistically significant only for the tiniest time budget of 10 min with more than 95% level of confidence (pvalue=0.004).

In the following, we explore the relationship between the characteristics of datasets and the improvement achieved by utilizing the meta-learning version of `AutoSKlearn` over different time budgets. We train a model that takes as input the meta-features of datasets, i.e., their characteristics, and predicts whether meta-learning can improve the performance. To develop this model, we label each dataset as `Class 1` if utilizing meta-learning improves performance over the vanilla version and `Class 0` otherwise. We implement a total of 42 meta-features from the literature, including simple, information-theoretic, and statistical meta-features (Kalousis, 2002; Mitchell et al., 1990), such as statistics about the number of data points, features, and classes, as well as data skewness and entropy of the targets. All meta-features are listed in Appendix E, Table E.12. Using the extracted information from the knowledge base, for our 100 datasets, we fit a shallow decision tree of depth 4 using the meta-feature variables as predictors. We considered decision tree classifier due to its interpretable nature, that allows rules to be derived from a root–leaf path in the tree. Given a new dataset, we compute its meta-features and use the decision tree model to recommend whether meta-learning is likely to improve performance or not. Our model achieves the following performance metrics: Recall = 0.85 and F1 Score = 0.85. Rules for `Class 1` and `Class 0` can be represented as follows, where $\wedge$ is the logical AND:

- **R1:** $min(\frac{c}{n}) > 0.5 \implies$ `Class1`
- **R2:** $min(\frac{c}{n}) < 0.27 \wedge$ *noise-signal ratio* $> 8.57 \wedge p < 845 \implies$ `Class1`
- **R3:** $0.1 < min(\frac{c}{n}) < 0.27 \wedge$ *noise-signal ratio* $< 8.57 \implies$ `Class1`
- **R4:** $0.27 < min(\frac{c}{n}) < 0.5 \implies$ `Class0`
- **R5:** $min(\frac{c}{n}) < 0.27 \wedge$ *noise-signal ratio* $> 8.57 \wedge p > 845 \implies$ `Class0`
- **R6:** $min(\frac{c}{n}) < 0.1 \wedge$ *noise-signal ratio* $< 8.57 \implies$ `Class0`

It is clear from the extracted rules that the number of features p, the percentage of the minority class to the number of instances ($min(\frac{c}{n})$),

(a) AutoWeka (b) ATM

(c) AutoSKlearn-v (d) AutoSKlearn-m

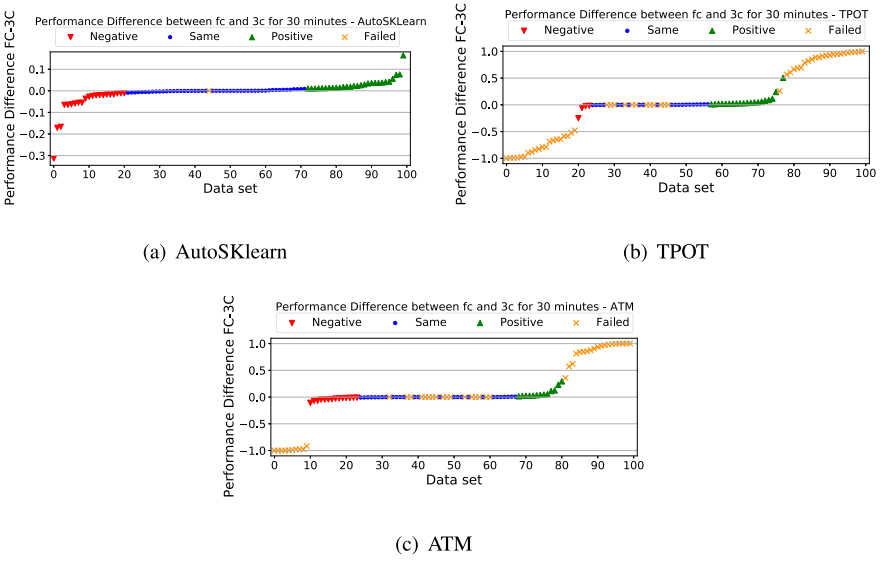
(e) SmartML-m (f) TPOT

(g) Recipe

Fig. 6. The frequency of using different machine learning models by the different AutoML frameworks.

Table 7
The performance of `AutoSklearn-v` and `AutoSklearn-m` and the gain in performance achieved by employing the meta-learning on 100 datasets over different time budgets.

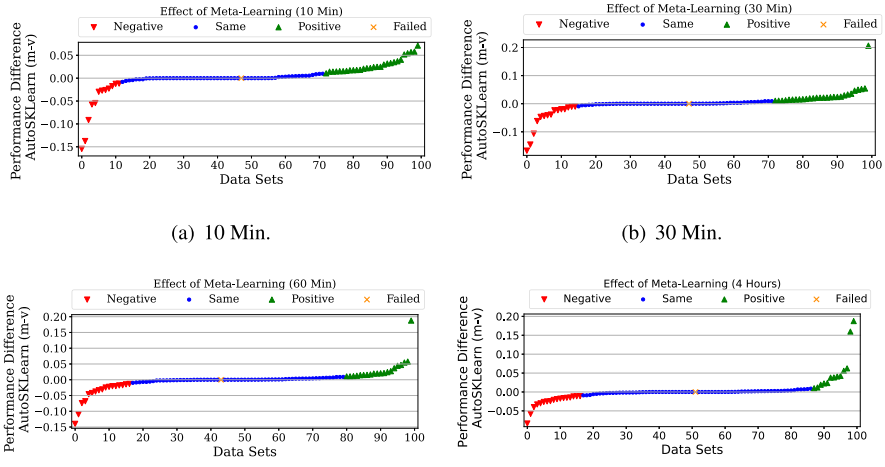
Time budget	Framework	Predictive performance		Performance gain			#datasets with
		Mean	SD	Min	Mean	Max	gain > 1%
10	AutoSKlearn-m	0.864	0.153	1.1%	2.9%	7.1%	28
	AutoSKlearn-v	0.862	0.151	1.1%	5.4%	15.5%	12
30	AutoSKlearn-m	0.868	0.152	1.1%	3.1%	20.6%	28
	AutoSKlearn-v	0.8867	0.149	1.1%	5.1%	16.7%	15
60	AutoSKlearn-m	0.870	0.144	1.1%	3.3%	18.8%	20
	AutoSKlearn-v	0.870	0.142	1.1%	4.3%	14.0%	17
240	AutoSKlearn-m	0.873	0.141	1.1%	7.7%	31.6%	14
	AutoSKlearn-v	0.867	0.156	1.1%	2.7%	8.4%	20



(a) AutoSKlearn (b) TPOT

(c) ATM

Fig. 7. The impact of using a static portfolio on each AutoML framework. Green markers represent better performance with FC search space, blue markers represent comparable performance with a difference less than 1%, red markers represent better performance with $3C$ search space, yellow markers on the left represent failed runs with FC but successful with $3C$, yellow markers on the right represent failed runs with $3C$ but successful with FC, and yellow markers in the middle represent failed runs with both FC and $3C$.



(a) 10 Min. (b) 30 Min.

(c) 60 Min. (d) 240 Min.

Fig. 8. The impact of meta-learning over all time budgets. Green markers represent better performance with `AutoSKlearn-m`, blue markers represent comparable performance with a difference less than 1%, red markers represent better performance using `AutoSKlearn-v`, and yellow markers represent failed runs with both runs with both FC and 3C.

and noisiness of data (*noise-signal ratio*) are quite important features for the prediction.

5.2.4. Impact of ensembling

Ensembling (Dietterich, 2000) is the process of combining multiple ML base models for the same task to produce a better predictive model. These base models can be combined in different techniques, including simple voting (averaging), weighted voting, bagging, and boosting (Dietterich, 2000). In the following, we explore the impact of ensembling on the performance of the AutoML frameworks allowing enabling and disabling post-processing ensemble. Such frameworks include `AutoSKlearn` and `SmartML-m`. Furthermore, we investigate whether there is a relationship between the characteristics of the different datasets and the improvement caused by employing the vanilla version or the ensembling version of the AutoML framework. During the optimization process of `AutoSKlearn` and `SmartML`, the frameworks store the generated models instead of just keeping the best-performing one. These models are used in a post-processing phase to construct an ensemble model. This automatic ensemble construction avoids relying on a single hyperparameter setting which makes the generated model more robust to overfitting. `AutoSKlearn` uses the ensemble selection methodology introduced by Caruana et al. (2004), while `SmartML` uses majority voting (Lam & Suen, 1997). Ensemble selection is a greedy technique that starts with an empty ensemble and iteratively adds base models to the ensemble in a way that maximizes the validation performance. The technique uses uniform weights; however, it allows repetitions. Majority voting is considered the simplest scheme. It adheres to democratic principles, i.e., the class with the most votes wins. We kept the default setting of `AutoSKlearn` and `SmartML` using 50 and 5 base models in the ensemble, respectively.

To assess the impact of the ensembling, we compare the mean performance of vanilla/base version of each of `AutoSKlearn` and `SmartML` to their ensembling versions across different time budgets, as shown in Table 8. More detailed performance comparisons over all datasets across all time budgets are given in Figs. F.16 and F.17 in Appendix F.

AutoSKlearn: The results show that ensembling does not always contribute to better performance than the vanilla version. However, it

Table 8
Performance comparison between vanilla/base version vs ensembling version of AutoSKlearn and SmartML different time budgets.

Time budget	Framework	Predictive performance		Performance gain			#datasets with
		Mean	SD	Min	Mean	Max	gain > 1%
10	AutoSKlearn-e	0.868	0.145	1.1%	3.9%	16.7%	24
	AutoSKlearn-v	0.868	0.151	1.1%	3.2%	8.9%	14
	SmartML-e	0.831	0.176	1.1%	12.6%	64.2%	30
	SmartML	0.176	0.176	1.1%	10.2%	36.1%	14
30	AutoSKlearn-e	0.875	0.141	1.1%	3.2%	13.9%	32
	AutoSKlearn-v	0.867	0.149	1.1%	2.9%	11.1%	11
	SmartML-e	0.838	0.159	1.1%	12.5%	73.2%	33
	SmartML	0.838	0.199	1.1%	10.6%	39.4%	16
60	AutoSKlearn-e	0.879	0.138	1.1%	4.7%	12.7%	25
	AutoSKlearn-v	0.870	0.142	1.1%	2.6%	6.1%	13
	SmartML-e	0.832	0.172	1.1%	11.2%	55.8%	28
	SmartML	0.816	0.194	1.1%	10.5%	31.1%	18
240	AutoSKlearn-e	0.883	0.132	1.1%	8.0%	69.7%	24
	AutoSKlearn-v	0.867	0.156	1.1%	3.1%	8.4%	14
	SmartML-e	0.842	0.165	1.1%	10.2%	34.5%	28
	SmartML	0.826	0.169	1.1%	11.9%	37.2%	16

achieved mean improvement of 3.9%, 3.2%, 4.7%, and 8.0% on 24, 32, 25 and 24 datasets over 10, 30, 60, and 240 min budgets, respectively, as shown in Table 8. We use Wilcoxon statistical test to assess the significance of the performance difference between AutoSKlearn-e and AutoSKlearn-v. The results show that ensembling enhances the performance with a statistically significant gain of more than 95% level of confidence (p value < 0.05) on the 4 time budgets. The level of confidence is almost 99% over all the time budgets combined.

SmartML: SmartML-e slightly improved the performance over the SmartML-m by average performance of 12.6%, 12.5%, 11.2%, and 10.2% on 30, 33, 28, and 28 datasets for 10, 30, 60, and 240 min time budgets, respectively, as shown in Table 8. We also use Wilcoxon statistical test to assess the significance of the performance difference between the base (meta-learning) and the ensembling versions of SmartML. The results show that the ensembling version enhance the performance with a statistically significant gain of more than 95% level of confidence (p value < 0.05) on the 4 time budgets.

In the following, we explore the relationship between the characteristics of the datasets and the improvement achieved by utilizing the ensembling version of AutoSKlearn over different time budgets. To this end, we followed the same approach in Section 5.2.3 and trained a decision tree of depth 3 that takes the meta-features of 100 datasets as input and provides prediction to whether using ensembling can improve the performance (Class 1) or not (Class 0). So, given a new dataset, we compute its meta-features and use the decision tree model to recommend whether ensembling will likely improve performance. Our model for AutoSKlearn has achieved the following performance: Recall = 0.70 and F1 Score = 0.70. AutoSKlearn rules for Class 1 and Class 0 can be represented as follows:

- **R1:** $\mu(\rho) > 0.13 \ \wedge \ \sigma(\rho) > 0.27 \ \wedge \ max(\rho) > 0.98 \implies$ Class1
- **R2:** $\mu(\rho) > 0.13 \ \wedge \ \sigma(\rho) \leq 0.27 \ \wedge \ min(\rho) > 0.44 \implies$ Class1
- **R3:** $\mu(\rho) \leq 0.13 \ \wedge \ \mu(\pi_i) > 3.11 \ \wedge \ \sigma(\frac{n}{p}) > 0.03 \implies$ Class1
- **R4:** $\mu(\rho) \leq 0.13 \ \wedge \ \mu(\pi_i) \leq 3.11 \ \wedge \ min(Mutual\ inform.) > 0.03 \implies$ Class1
- **R5:** $\mu(\rho) > 0.13 \ \wedge \ \sigma(\rho) > 0.27 \ \wedge \ max(\rho) \leq 0.98 \implies$ Class0
- **R6:** $\mu(\rho) > 0.13 \ \wedge \ \sigma(\rho) \leq 0.27 \ \wedge \ min(\rho) \leq 0.44 \implies$ Class0
- **R7:** $\mu(\rho) \leq 0.13 \ \wedge \ \mu(\pi_i) > 3.11 \ \wedge \ \sigma(\frac{n}{p}) \leq 0.03 \implies$ Class0
- **R8:** $\mu(\rho) \leq 0.13 \ \wedge \ \mu(\pi_i) \leq 3.11 \ \wedge \ min(Mutual\ inform.) \leq 0.03 \implies$ Class0

Clearly, the following features are important to the prediction of the model; the mean of the pairwise correlation between features ($\mu(\rho)$), standard deviation of the pairwise correlation between features ($\sigma(\rho)$), maximum of the pairwise correlation between features ($\max(\rho)$), minimum of the pairwise correlation between features ($\min(\rho)$), the standard deviation of the ratio between number of instances and the number of features ($\sigma(\frac{n}{p})$), the minimum of the mutual information between features and class ($Mutual\ inform.$), and the mean of the unique categorical values of features ($\mu(\pi_i)$).

For SmartML, we trained multiple models; however, none of the models could capture the relation of the meta-features and the performance improvement caused by employing ensembling.

6. Discussion and future direction

The global average performance, weighted by the percentage of successful runs, shows that Auto-SKlearn-e and AutoSKlearn achieve the highest performance, while Recipe comes in the last place. Overall, AutoSklearn achieves the highest number of successful runs across different time budgets and witnessed performance improvement over the most significant number of datasets when increasing the time budget. Our analysis reveals that the impact of meta-learning declines over longer time budgets (i.e., 60 mins, 240 mins). In contrast, ensembling achieves consistent performance improvement across all time budgets. For AutoSKlearn, the analysis reveals a relationship between the characteristics of the datasets (e.g., number of features, noisiness of data, mutual information between features and class) and the improvement achieved by utilizing meta-learning or ensembling. Generally, AutoML frameworks considered in this work build pipelines with an average length of 2. TPOT yields the shortest pipelines with an average length of 1.5. A possible explanation could be that TPOT generates pipelines that optimize both the pipelines' performance and complexity. Additionally, AutoSKlearn, ATM, and TPOT achieve the highest performance on multi-class classification tasks. For datasets with a large number of instances and a small number of features, ATM is a clear winner.

Our comprehensive evaluation, guided by a set of well-defined metrics, offers a comprehensive perspective on AutoML framework performance. Notably, training efficiency emerges as a vital factor, particularly in resource-constrained environments and scenarios that demand rapid model development. Here, ATM and Recipe excel, making them compelling choices for applications characterized by limited computational resources or a need for swift model iteration. In terms of inference times, SmartML-m and Recipe emerge as standout performers, with better efficiency. Moreover, Recipe, SmartML-m, and ATM

demonstrate exceptional model stability, underscoring their reliability. These attributes make them particularly well-suited for applications where consistent model performance is paramount. Furthermore, the robustness to noise metric reveals valuable insights. AutoSKLearn-e and AutoSKLearn-m exhibit high levels of robustness, making them well-suited for scenarios dealing with unpredictable, noisy real-world data.

For some datasets, the performance of the different versions of `AutoSKlearn` varies significantly across different iterations. These datasets are characterized by having far fewer instances than features. Analyzing the pipelines of the different versions of `AutoSKlearn` on these datasets across multiple iterations shows that data preprocessing component is responsible for the significant performance variance between the different pipelines. For example, the performance difference between `AutoSKlearn-v` and `AutoSKlearn-m` on `phpdo58hj` varies significantly between 6% to 13% across different iterations. The two generated pipelines for `Auto- SKlearn-v` and `AutoSKlearn-m` used the same model (LDA) with the same set of hyperparameters but different preprocessors. For large datasets, meta-learning shows significant performance improvement. For example, `AutoSKlearn-m` achieves significantly better performance than `AutoSKlearn-v` on CovPokElec. A possible explanation is that meta-learning warm-starts the optimization process and increases the chances of finding a well-performing configuration in the limited attempts during the defined time budget.

Specifying the time budget needs to be considered carefully as significantly increasing the time budget for the search process (e.g., from 60 min to 240 min) may not significantly improve the predictive performance. This decision varies from one scenario/application to another. For some applications, spending a long time to achieve an additional predictive performance of 1% could be crucial while less important for other applications. However, more extended time budgets may lead to over-fitting. Carefully selecting a small search space with few top-performing classifiers can lead to a comparable performance with a search space that includes many classifiers, which is the case for `AutoSKlearn` and `ATM` frameworks.

Intuitively, an extensive systematic search for a well-performing machine learning pipeline should bear a high risk of over-fitting, and previous AutoML frameworks have confirmed this intuition (Thornton et al., 2013). AutoML tools are on the right extreme of the bias–variance spectrum as they choose among all learners and even construct new and arbitrary large ones using ensemble methods (Mohr et al., 2018). Notably, `SmartML` and `AutoWeka` witnessed performance degradation when increasing the time budget from 30 to 60 min. One possible explanation is that the data available for the search process is not sufficiently substantial and representative of "real" data. Hence, the danger of over-fitting is higher than for basic learning algorithms. This insight calls for developing novel and more efficient mechanisms to prevent over-fitting.

While AutoML frameworks optimize predictive performance, many exceed the specified time budget by more than 10%. This violation of the time constraints caused many runs to be terminated and considered as failed. This problem is observed in all frameworks except for AutoSKLearn, which calls for a robust implementation and careful consideration of the time constraint.

Most of the current work on AutoML considered automating the preprocessing, algorithm selection and hyperparameter tuning while ignoring the feature engineering part. In practice, the feature engineering part consumes most of the Engineer's time to build ML pipelines and significantly affects the performance. The proper feature engineering phase could turn the feature space into a linearly separable space, so even naive classifiers could achieve relatively high predictive performance. On the other hand, skipping this phase or using the wrong feature engineering preprocessors makes it harder to achieve relatively high predictive performance, even for the most efficient classifiers. Hence, further research in this area can improve the overall performance of the resulting AutoML pipelines.

7. Conclusion

In this paper, we present a comprehensive evaluation and comparison of the performance characteristics of six AutoML frameworks on 100 datasets from OpenML. Our analysis reveals that no single winning framework outperforms others over all time budgets. Across various evaluations, `AutoSklearn`, `ATM`, and `TPOT` are the top-performing frameworks. The results also show that genetic-based frameworks (`TPOT` and `Recipe`) have high frequent failure rates for short time budgets while their success rates are steadily increasing as the time budget increases. We also find that meta-learning has a significant impact on small-time budgets, and such impact declines as the time budget increases. In contrast, ensembling consistently improves performance significantly across all time budgets. Furthermore, carefully selecting a small search space with few top-performing classifiers can lead to a comparable performance with a search space that includes many classifiers. Furthermore, increasing the time budget does not necessarily improve predictive performance. We believe that the results of our analysis are beneficial for guiding and improving the design process of future AutoML techniques.

CRediT authorship contribution statement

Hassan Eldeeb: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing – original draft, Writing – review & editing, Visualization. **Mohamed Maher:** Software, Investigation, Data curation, Writing – review & editing. **Radwa Elshawi:** Validation, Resources, Writing – review & editing, Supervision, Project administration, Funding acquisition. **Sherif Sakr:** Conceptualization, Methodology, Resources, Writing – review & editing, Supervision, Project administration, Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The datasets generated during and/or analyzed during the current study are available in the AutoMLBench repository, https://datasystemsgrouput.github.io/AutoMLBench/datasets.

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Appendix A. Evaluated datasets

Table A.9 shows the datasets used in evaluating all the AutoML frameworks included in this work.

Appendix B. Framework and source code

Table B.10 lists the Github repositories of all the open-source AutoML frameworks considered in this work. Some frameworks are still under active development and may differ from the evaluated versions.

Table A.9
List of all tested datasets including information about (abbreviated) name and OpenML id for each data set together with the number of classes, the number of features, the number of instances, how many values are missing in total (Missing values), number of categorical features per sample, and the class entropy.

Dataset Name (openml id)	Nr features	Nr instances	Nr classes	Nr missing values	Nr categorical features	Class entropy
AirlinesCodrnaAdult (1240)	30	1 076 790	2	11 896	1	1,00
Amazon (1457)	10 001	1500	50	0	0	0,93
analcatdata_authorship (458)	71	841	4	0	0	0,99
AP_Breast_Lung (1150)	10 937	470	2	0	0	0,99
AP_Omentum_Ovary (1156)	10 937	275	2	0	1	0,93
AP_Prostate_Ovary (1152)	10 937	267	2	0	0	2,18
arrhythmia (1017)	263	452	2	0	1	1,58
audiology (999)	70	226	2	0	1	3,70
avila-tr (42932)	11	20 867	12	114	10	2,27
churn (40701)	21	5000	2	0	1	1,00
cifar-10 (40927)	3073	60 000	10	0	70	0,81
connect-4 (1591)	43	67 557	3	0	1	0,82
CovPokElec (149)	65	1 455 525	10	0	1	0,86
dataset_183_adult (179)	15	48 842	2	0	0	2,21
dataset_185_yeast (181)	9	1484	10	0	1	2,19
dataset_186_satimage (182)	37	6430	6	1668	3	1,00
dataset_187_abalone (183)	9	4177	28	0	1	0,94
dataset_189_baseball (185)	18	1340	3	0	0	3,32
dataset_194_eucalyptus (188)	20	736	5	816	1	0,99
dataset_24_mushroom (24)	22	8124	2	0	1	0,84
dataset_26_nursery (26)	9	12 960	5	0	0	4,20
dataset_28_optdigits (28)	63	5620	10	0	0	4,28
dataset_31_credit-g (31)	21	1000	2	0	1	2,58
dataset_36_segment (36)	19	2310	7	0	36	3,84
dataset_39_ecoli (39)	8	336	8	32	1	0,93
dataset_40_sonar (40)	61	208	2	896	6	2,26
dataset_42_soybean (42)	36	683	19	0	1	1,79
dataset_44_spambase (44)	58	4601	2	0	1	2,00
dataset_54_vehicle (54)	19	846	4	0	4	0,44
dataset_59_ionosphere (59)	34	351	2	0	14	0,88
dataset_6_letter (6)	17	20 000	26	0	0	4,65
dataset_60_waveform-5000 (60)	41	5000	3	0	1	0,83
dataset_61_iris (61)	5	150	3	0	0	0,92
dataset_9_autos (9)	26	205	6	2792	4	2,99
devnagari (40923)	785	92 000	46	0	0	3,17
electricity-normalized (151)	9	45 312	2	0	0	1,00
eye_movements (1044)	28	10 936	3	40	2	0,54
GCM (1106)	16 064	190	14	0	1	2,49
gina_agnostic (1038)	971	3468	2	0	1	5,64
hiva_agnostic (1039)	1618	4229	2	0	0	3,32
ipums_la_99-small (378)	60	8844	9	0	0	6,64
jm1 (1053)	22	10 885	2	0	0	1,71
jungle_chess_2pcs (40997)	45	4704	3	0	0	6,64
KDDCup99 (1113)	40	494 020	23	0	0	6,64
kin8 nm (189)	9	8192	2	0	1	2,41
leukemia (1104)	7130	72	2	0	1	0,47
lymphoma_2classes (1101)	4027	45	2	0	1	2,81
MagicTelescope (1120)	11	19 020	2	0	0	0,34
mfeat-pixel (20)	241	2000	2	0	0	1,00
mnist_784 (554)	720	70 000	10	0	0	1,53
openml_phpJNxH0q (15)	10	699	2	0	0	1,00
page-blocks (30)	11	5473	2	0	1	3,60
php0FyS2T (1492)	65	1600	100	0	0	0,22
php3CTpvq (1509)	5	149 332	22	0	0	0,97
php5OMDBD (40971)	23	1000	30	0	6	1,16
php5s7Ep8 (40982)	28	1941	7	0	0	1,86
php7KLval (1547)	21	1000	2	0	0	0,59
phpB0xrNj (300)	618	7797	26	0	0	1,58

(*continued on next page*)

Table A.9 (*continued*).

phpbL6t4U (1476)	129	13 910	6	0	1	0,11
phpchCuL5 (40966)	81	1080	8	0	0	1,71
phpCsX3fx (1491)	65	1600	100	0	1	0,48
phpdo58hj (1562)	4703	64	2	0	0	3,32
phpdRePGS (1487)	73	2534	2	0	0	2,30
phpEZ030X (1561)	3722	64	2	0	0	2,48
phpfLuQE4 (1485)	501	2600	2	0	0	1,00
phpfrJpBS (1568)	9	12 958	4	0	0	1,00
phpGReJjU (40985)	4	45 781	20	0	1	4,70
phpGUrE90 (1494)	42	1055	2	0	22	1,00
phphQEck0 (1502)	4	245 057	2	0	1	1,00
phpHyLSNF (1515)	1083	571	20	0	26	0,48
phpkIxskf (1461)	17	45 211	2	0	1	2,19
phpmcGu2X (1468)	857	1080	9	0	1	0,94
phpmPOD5A (4135)	10	32 769	2	50	0	0,71
phpn1jVwe (310)	7	11 183	2	0	0	1,57
phpN4gaxw (1477)	130	13 910	6	0	0	0,16
phpNevWWL (40477)	27	2800	5	0	0	1,71
phpoOxxNn (1493)	65	1599	100	0	9	1,72
phpoW7Dbi (1566)	101	1212	2	0	0	2,55
phpPbCMyg (1475)	52	6118	6	0	0	2,55
phprAeXmK (4535)	42	299 285	2	0	1	0,94
phpSZJq5T (1514)	1088	360	10	0	1	4,70
phptd5jYj (1501)	37	5100	2	0	1	2,64
phpTJRsqa (40498)	257	1593	10	0	0	0,32
phpvcoG8S (1169)	12	4898	7	0	9	0,52
phpVeNa5j (1497)	8	539 383	2	0	1	0,98
phpvtdNPU (1079)	25	5456	4	0	0	4,25
phpWfYmlu (1496)	21	7400	2	0	9	0,79
phpxijhaP (1507)	22 278	95	5	0	0	0,96
phpYLeydd (4538)	21	7400	2	0	0	3,32
phpZrCzJR (40900)	33	9873	5	0	0	1,22
pokerhand-normalized (155)	11	829 201	10	0	0	3,32
schizo (466)	14	340	2	0	1	5,52
shuttle (40685)	10	58 000	7	0	0	3,99
solar-flare_1 (40686)	13	315	5	0	0	0,74
synthetic_control (377)	61	600	6	0	29	0,34
tumors_C (1107)	7130	60	2	0	4	1,56
umistfacescropped (41084)	10 305	575	20	0	3	0,99
vowel (307)	14	990	2	0	0	1,42
wine-quality-red (40691)	12	1599	6	0	11	0,99
aaaData_for_UCI_named (43007)	14	10 000	2	0	0	1,59

Table B.10
Source code repositories for all used AutoML frameworks.

AutoML framework	Source code
AutoSKlearn	https://automl.github.io/auto-sklearn/
TPOT	https://github.com/EpistasisLab/tpot
ATM	https://github.com/HDI-Project/ATM
Recipe	https://github.com/laic-ufmg/Recipe
AutoWeka	https://github.com/automl/AutoWeka
SmartML	https://github.com/DataSystemsGroupUT/SmartML

Table C.11
Performance comparison between the 8 and 4 h budgets on 14 randomly selected datasets.

Framework	P value	Avg. diff
AutoSKlearn	0.084	−0.026
AutoSKlearn-e	**0.039**	−0.025
AutoSKlearn-m	0.382	−0.031
AutoSKlearn-v	0.272	−0.008
AutoWeka	0.133	−0.005
Recipe	0.480	0.007
SmartML	0.594	−0.003
SmartML-e	0.753	−0.009
TPOT	0.092	−0.050

Appendix C. Cut-off time budget

We tested the cut-off timeouts of 4 and 8 h on 14 randomly selected datasets. Table C.11 shows the mean performance difference between the 8 and 4 h (Avg. diff) over the 14 datasets. Additionally, we report the results of the Wilcoxon signed-rank test to determine if a statistically significant difference in performance exists between the AutoML frameworks over the two-time budgets.

Appendix D. General performance evaluation

D.9,D.10,D.11 show the average performance of all frameworks for time budgets 10, 30, and 60 min compared the average performance of the baseline. 4(b),D.13,D.14,D.15 show the AutoML frameworks' average performance on subsets of the datasets with special characteristics, namely binary-class, large number of features and instances, small number of features and instances, and small number of features and large number of instances.

Appendix E. Impact of meta learning

Table E.12 lists a total of 42 meta-features including simple, information-theoretic and statistical meta-features.

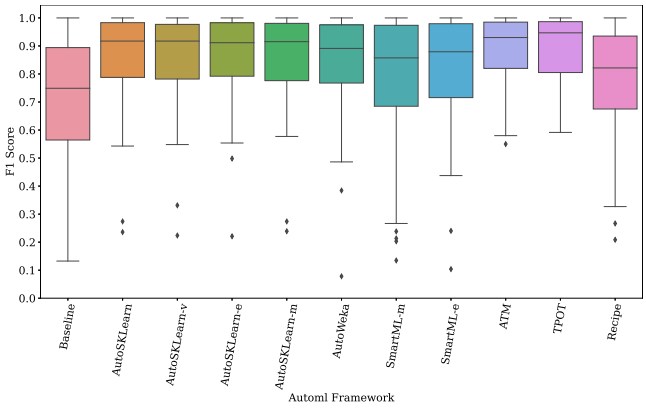


Fig. D.9. Average performance of all frameworks (10 Min) compared to the baseline.

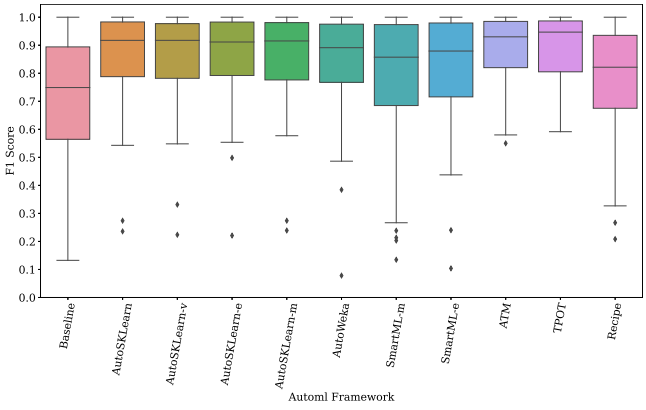


Fig. D.10. Average performance of all frameworks (30 Min) compared to the baseline.

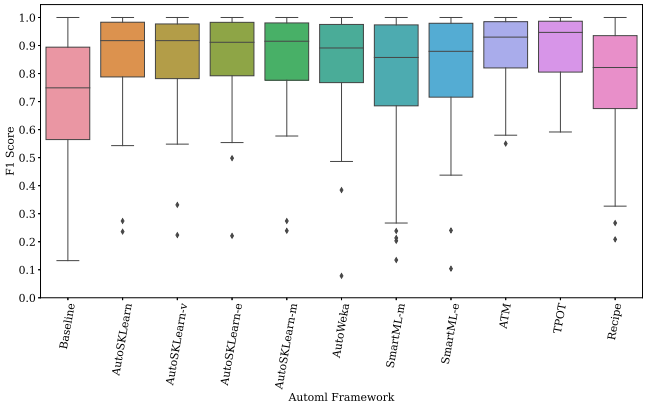


Fig. D.11. Average performance of all frameworks (60 Min) compared to the baseline.

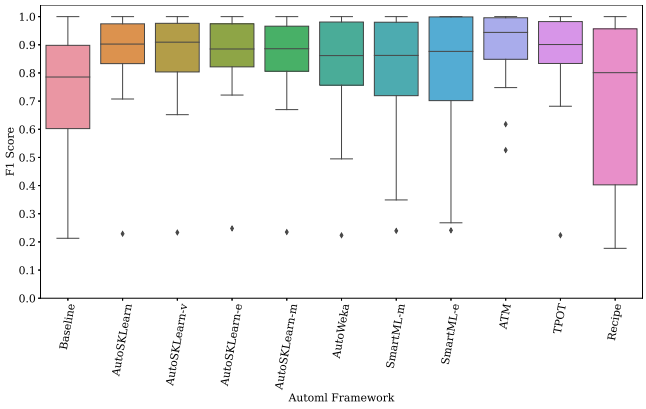


Fig. D.12. Performance of the final pipeline for datasets with large number of features and small number of instances.

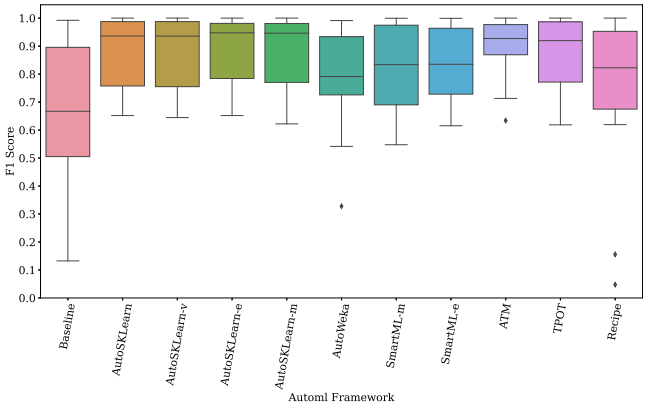


Fig. D.13. Performance of the final pipeline for datasets with large number of features and large number of instances.

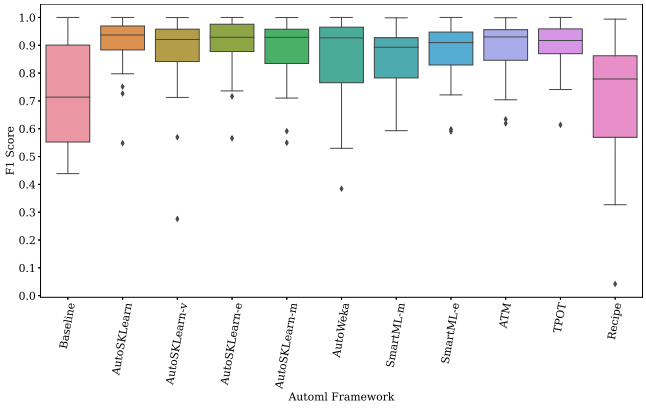


Fig. D.14. Performance of the final pipeline for datasets with small number of features and small number of instances.

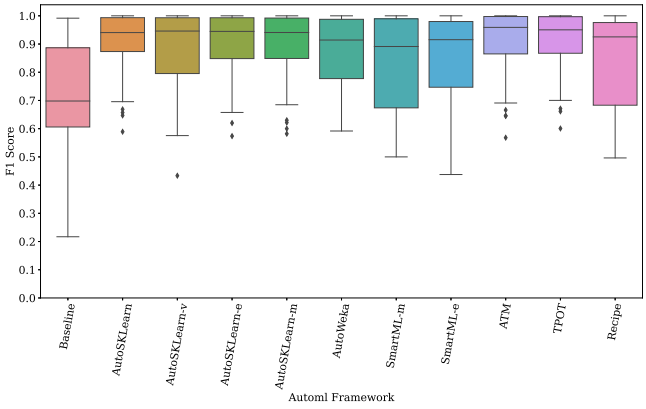
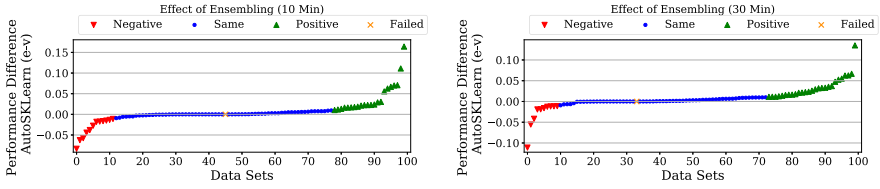


Fig. D.15. Performance of the final pipeline for datasets with small number of features and large number of instances.

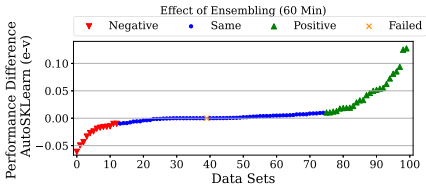
Table E.12
Overview of the used meta-features. Groups from top to bottom: simple, statistical, and information-theoretic. Continuous features X and target Y have mean μ_X, stdev σ_X, variance σ_X^2. Categorical features $\mathtt{X}$ and class $\mathtt{C}$ have categorical values π_i, conditional probabilities $\pi_{i|j}$, joint probabilities $\pi_{i,j}$, marginal probabilities $\pi_{i+} = \sum_j \pi_{ij}$, entropy $H(\mathtt{X}) = -\sum_i \pi_{i+} log_2(\pi_{i+})$. Vanschoren (2018).

Name	Formula	Rationale	Additional variants
Nr instances	n	Speed, Scalability (Michie et al., 1994)	p/n, $log(n)$
Nr features	p	Curse of dimensionality (Michie et al., 1994)	$log(p)$, Nr/$\mu/\sigma(\pi_i)$
Nr classes	c	Complexity, imbalance (Michie et al., 1994)	min/max/$\sigma(\frac{c}{n})$
Nr missing values	m	Imputation effects (Kalousis, 2002)	
Skewness	$\frac{E(X-\mu_X)^3}{\sigma_X^3}$	Feature normality (Michie et al., 1994)	min,max, μ, σ, q_1, q_3
Kurtosis	$\frac{E(X-\mu_X)^4}{\sigma_X^4}$	Feature normality (Michie et al., 1994)	min,max, μ, σ, q_1, q_3
Correlation	$\rho_{X_1X_2}$	Feature interdependence (Michie et al., 1994)	min,max, μ, σ
Class entropy	$H(\mathtt{C})$	Class imbalance (Michie et al., 1994)	$H(\mathtt{C})/\mu(MI(\mathtt{C},\mathtt{X}))$
Norm. entropy	$\frac{H(\mathtt{X})}{log_2 n}$	Feature informativeness (Castiello et al., 2005)	min,max, μ, σ
Mutual inform.	$MI(\mathtt{C},\mathtt{X})$	Feature importance (Michie et al., 1994)	min,max, μ, σ
Noise-signal ratio	$\frac{H(X)-MI(C,X)}{MI(C,X)}$	Noisiness of data (Michie et al., 1994)	

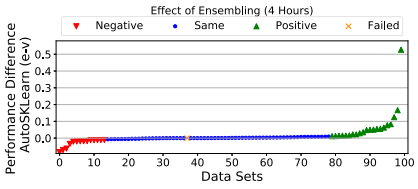


(a) 10 Min.

(b) 30 Min.

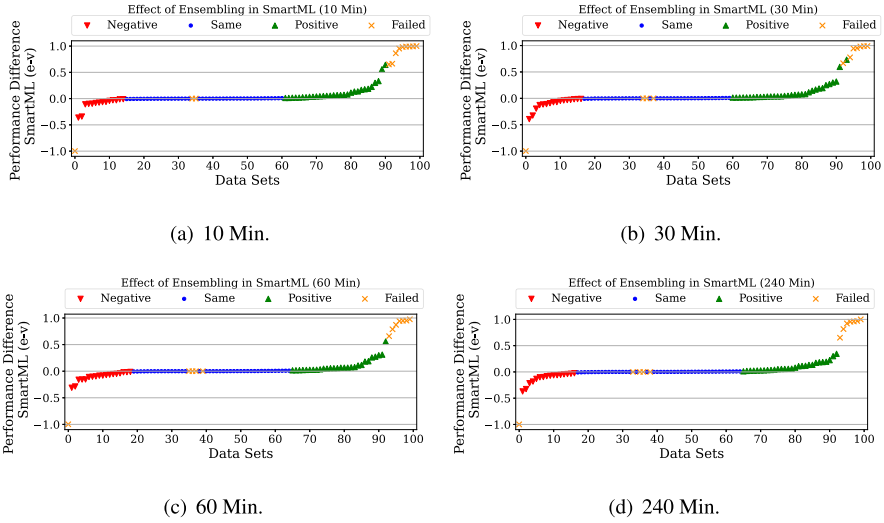


(c) 60 Min.



(d) 240 Min.

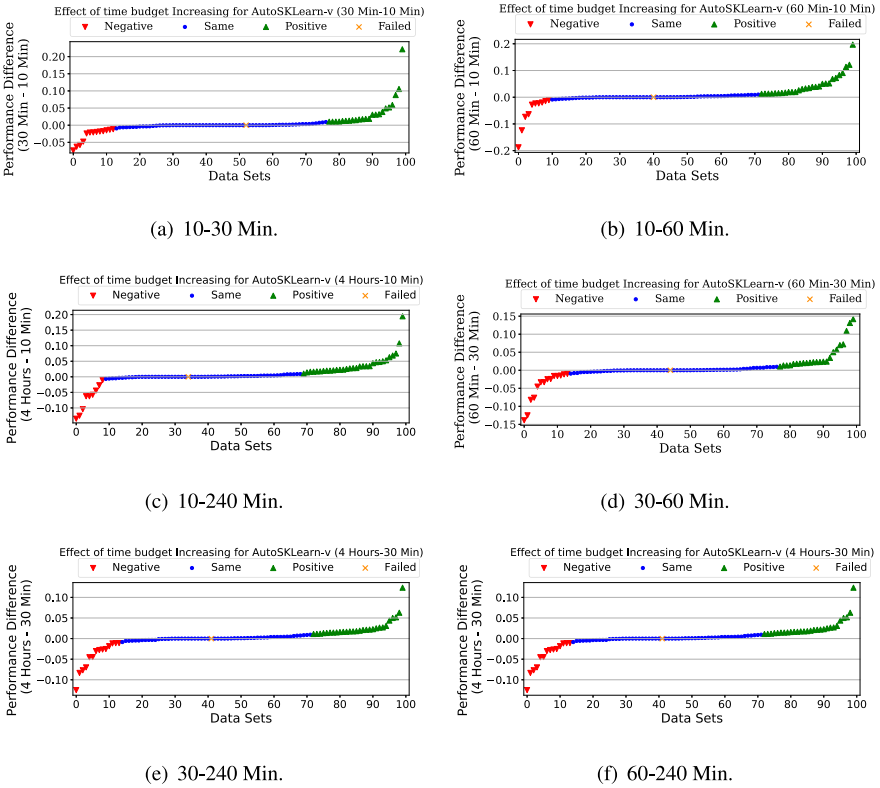
Fig. F.16. The performance difference between the `AutoSKlearn-e` and `AutoSKlearn-v` over different time budgets. Green markers represent better performance with `AutoSKlearn-e`, blue markers represent comparable performance with a difference less than 1%, red markers represent better performance with `AutoSKlearn-v`, and yellow markers represent failed runs on both versions.



(a) 10 Min. (b) 30 Min.

(c) 60 Min. (d) 240 Min.

Fig. F.17. The performance difference between the `SmartML-m` and `SmartML-e`. Green markers represent better performance with `SmartML-e`, blue markers represent comparable performance with a difference less than 1%, red markers represent better performance with `SmartML`, yellow markers on the right represent failed runs with `SmartML-m` but successful with `SmartML-e`, yellow markers on the left represent failed runs with `SmartML-e` but successful with `SmartML-m` and yellow markers in the middle represent failed runs with both `SmartML-m` and `SmartML-e`.

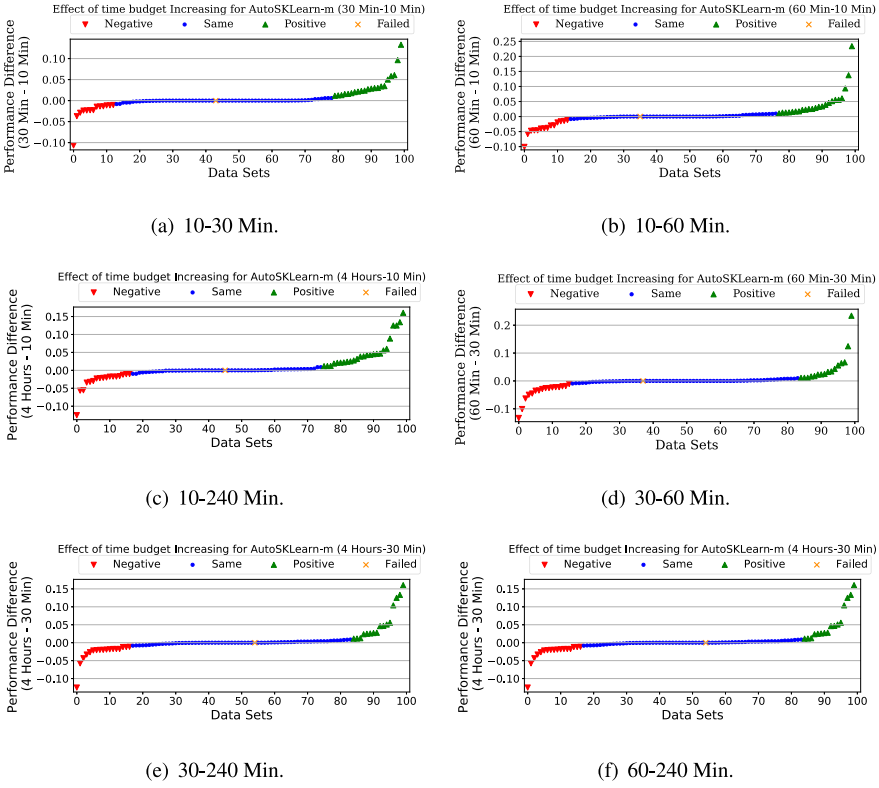


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.18. The impact of increasing the time budget on `AutoSKlearn-v` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

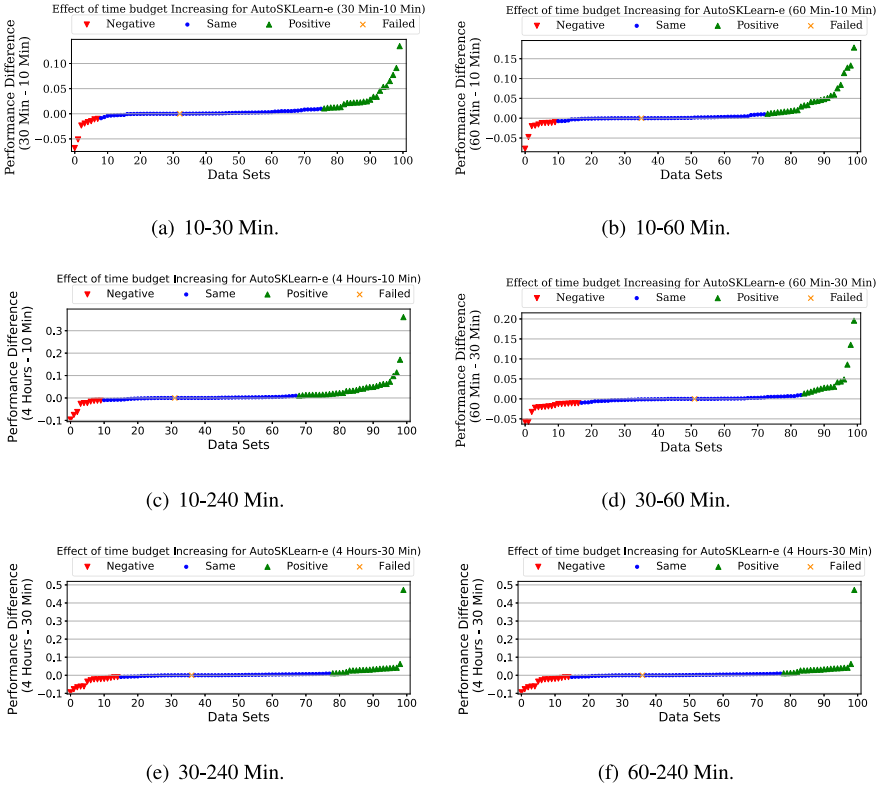


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.19. The impact of increasing the time budget on `AutoSKlearn-m` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

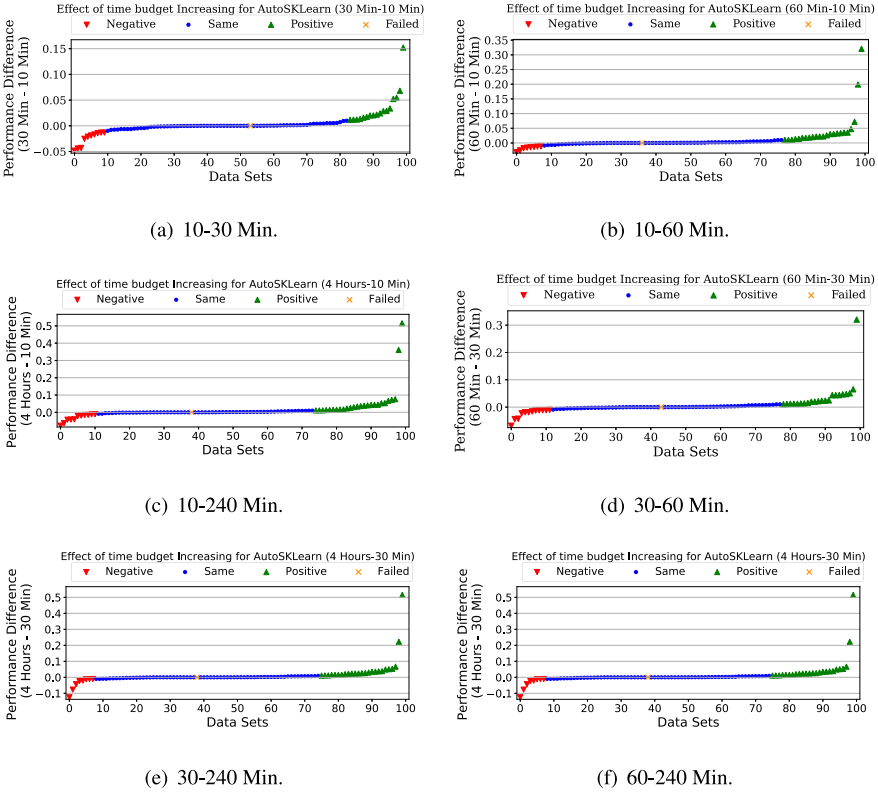


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.20. The impact of increasing the time budget on `AutoSKlearn-e` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

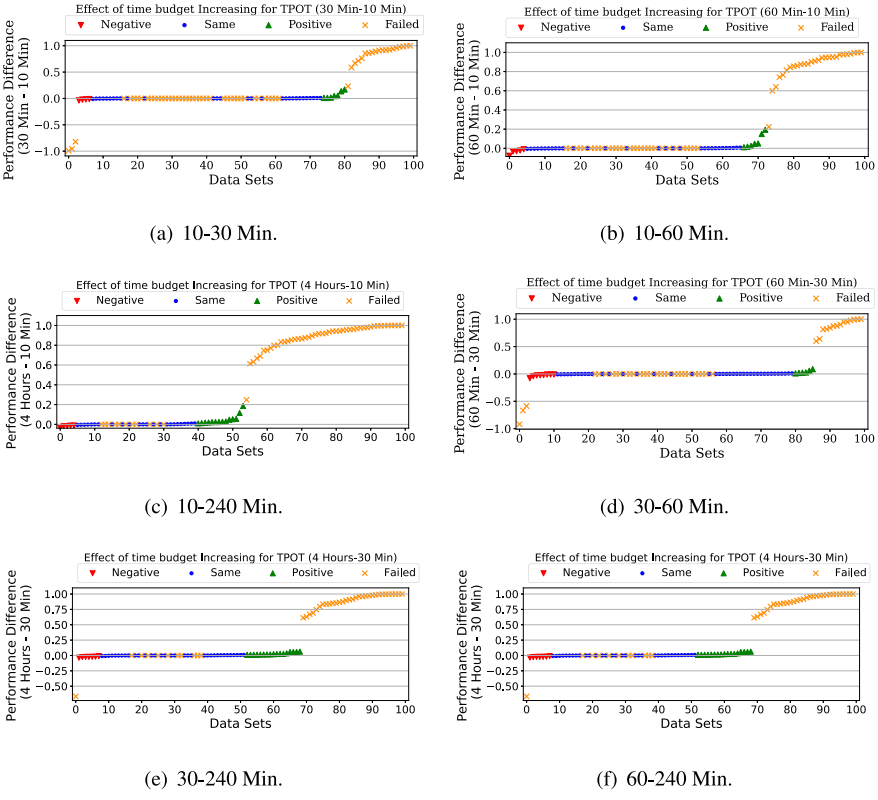


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.21. The impact of increasing the time budget on `AutoSKlearn` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

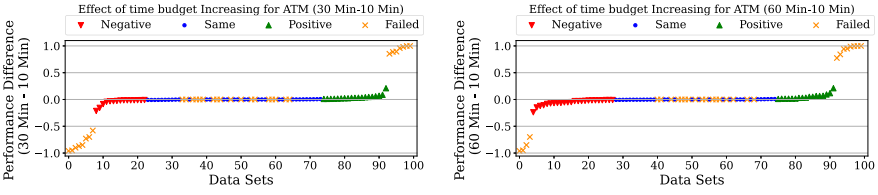


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

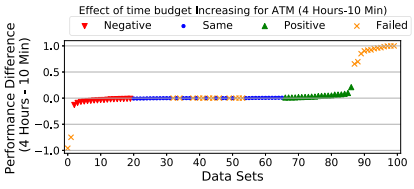
(e) 30-240 Min. (f) 60-240 Min.

Fig. G.22. The impact of increasing the time budget on `TPOT` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

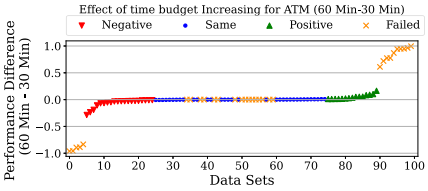


(a) 10-30 Min.

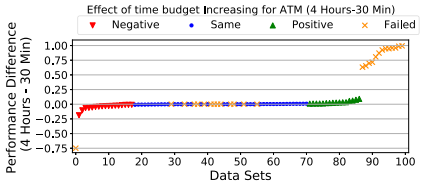
(b) 10-60 Min.



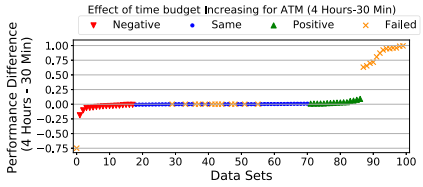
(c) 10-240 Min.



(d) 30-60 Min.

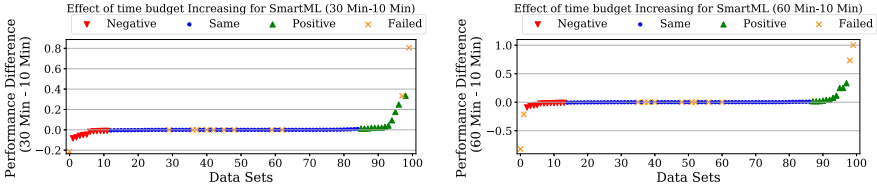


(e) 30-240 Min.



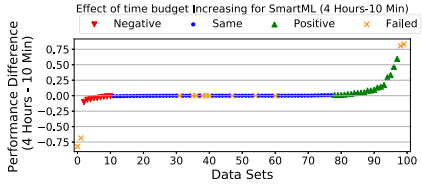
(f) 60-240 Min.

Fig. G.23. The impact of increasing the time budget on ATM performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

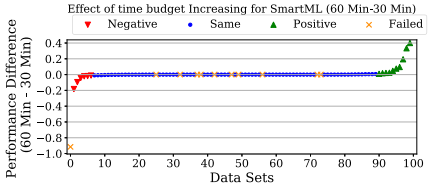


(a) 10-30 Min.

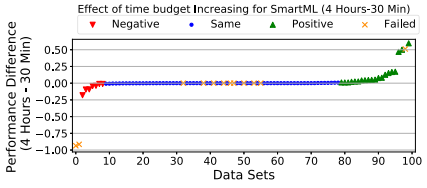
(b) 10-60 Min.



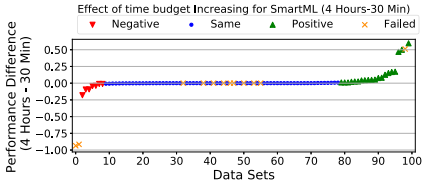
(c) 10-240 Min.



(d) 30-60 Min.

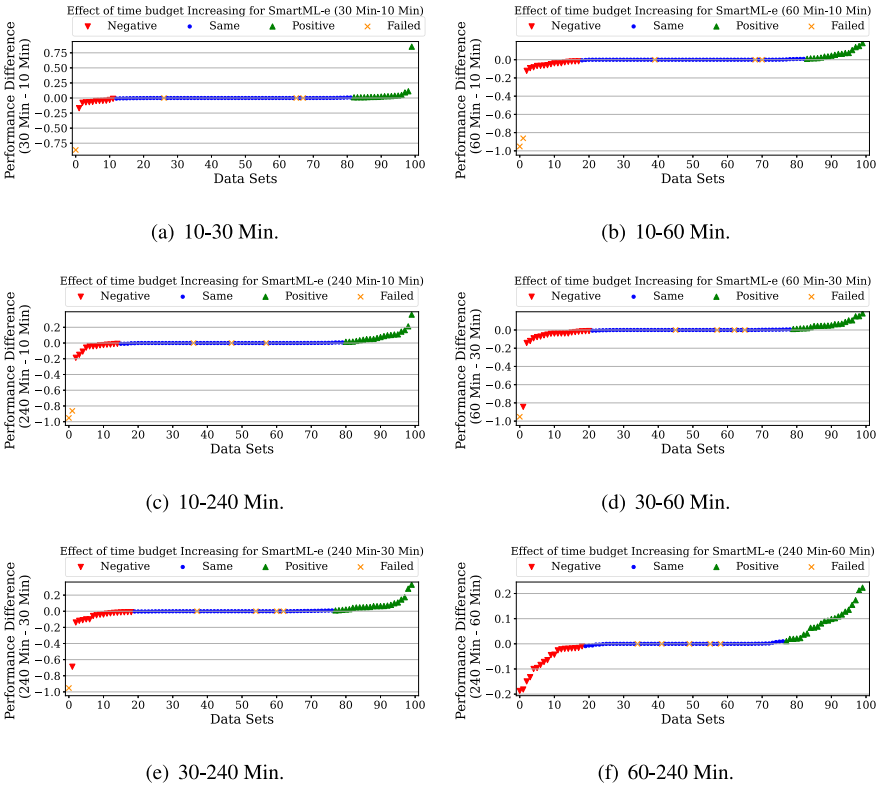


(e) 30-240 Min.



(f) 60-240 Min.

Fig. G.24. The impact of increasing the time budget on SmartML-m performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

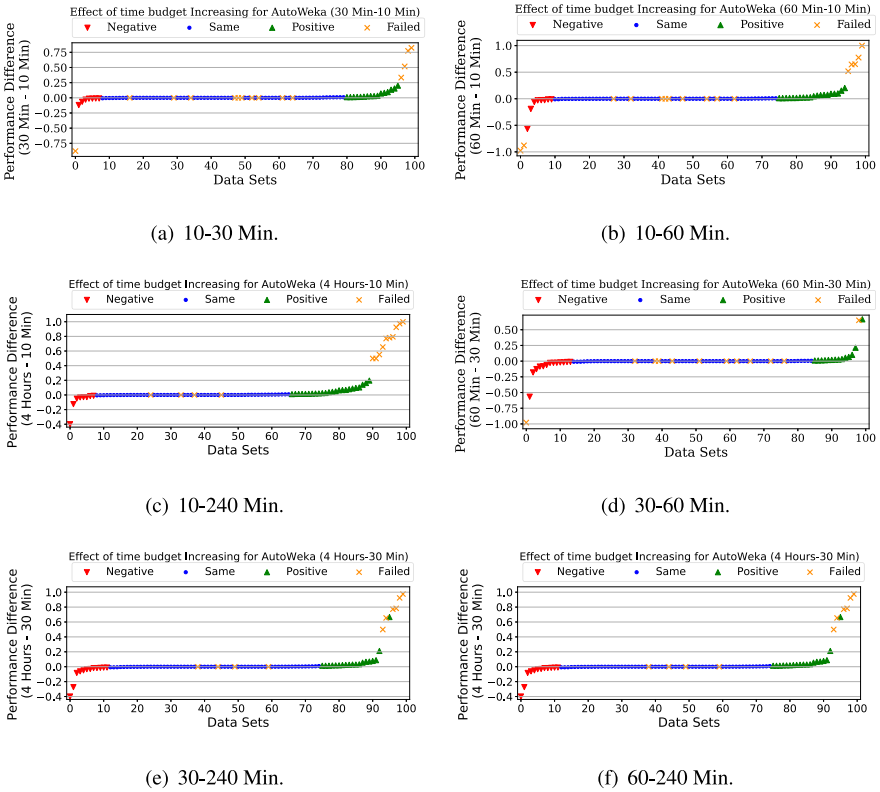


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.25. The impact of increasing the time budget on `SmartML-e` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

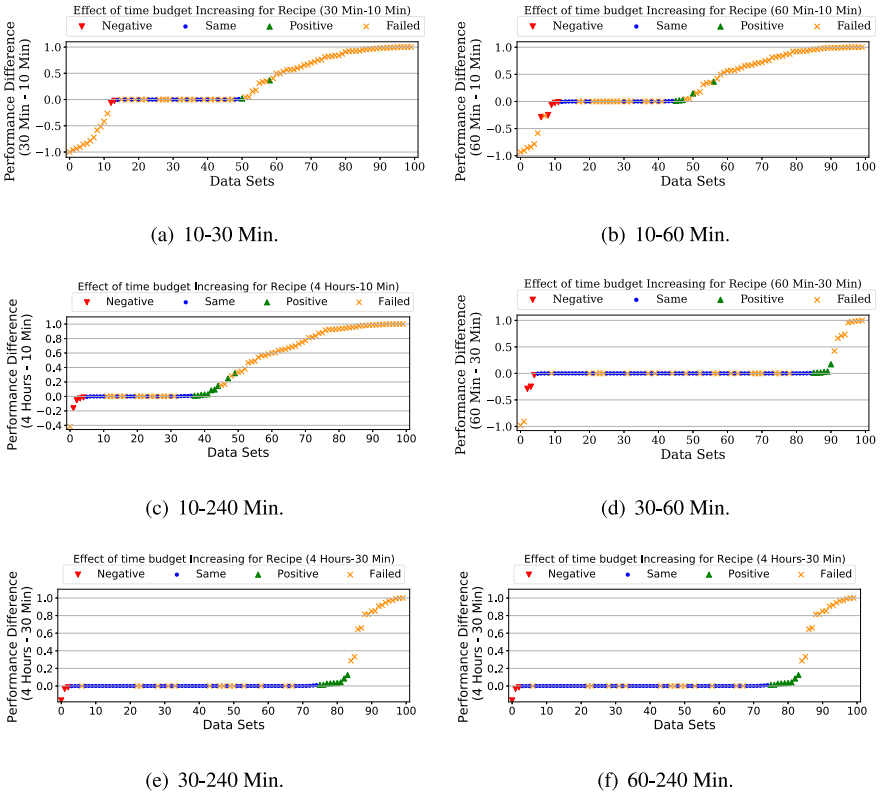


(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.26. The impact of increasing the time budget on `AutoWeka` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.



(a) 10-30 Min. (b) 10-60 Min.

(c) 10-240 Min. (d) 30-60 Min.

(e) 30-240 Min. (f) 60-240 Min.

Fig. G.27. The impact of increasing the time budget on `Recipe` performance from x to y minutes (x-y). Green markers represent better performance with y time budget, blue markers means that the difference between x and y is < 1. Red markers represent better performance on x time budget.

Appendix F. Impact of ensembling

Figs. F.16 and F.17 shows the performance difference between the ensembling version and the vanilla/base version of `AutoSKlearn` and `SmartML`, respectively over 10, 30, 60 and 240 min time budgets.

Appendix G. Impact of time budget

G.18,G.19,G.20,G.21,G.22,G.23,G.24,G.25,G.26,G.27 show the impact of increasing the time budget on the performance of the all the AutoML frameworks considered in this work.

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