Incremental Search Space Construction for Machine Learning Pipeline Synthesis

Marc-André Zöller¹, Tien-Dung Nguyen², and Marco F. Huber^{3,4}

¹ USU Software AG, Rüppurrer Str. 1, Karlsruhe, Germany marc.zoeller@usu.com
² University of Technology Sydney, Sydney, Australia
TienDung.Nguyen-2@student.uts.edu.au

³ Institute of Industrial Manufacturing and Management IFF, University of Stuttgart
⁴ Center for Cyber Cognitive Intelligence CCI, Fraunhofer IPA, Nobelstr. 12,
Stuttgart, Germany marco.huber@ieee.org

Abstract. Automated machine learning (AutoML) aims for constructing machine learning (ML) pipelines automatically. Many studies have investigated efficient methods for algorithm selection and hyperparameter optimization. However, methods for ML pipeline synthesis and optimization considering the impact of complex pipeline structures containing multiple preprocessing and classification algorithms have not been studied thoroughly. In this paper, we propose a data-centric approach based on meta-features for pipeline construction and hyperparameter optimization inspired by human behavior. By expanding the pipeline search space incrementally in combination with meta-features of intermediate data sets, we are able to prune the pipeline structure search space efficiently. Consequently, flexible and data set specific ML pipelines can be constructed. We prove the effectiveness and competitiveness of our approach on 28 data sets used in well-established AutoML benchmarks in comparison with state-of-the-art AutoML frameworks.

Keywords: Pipeline Structure Search · Meta-Learning · AutoML.

1 Introduction

AutoML promises to automate the synthesis of ML pipelines, handling hyperparameter optimization (HPO), algorithm selection and pipeline structure search. Many publications have proven the superiority of Bayesian optimization for HPO and algorithm selection, formulated as combined algorithm selection and hyperparameter optimization (CASH), over classic approaches like grid or random search [2,10]. More recently, methods for composing complete ML pipelines from a set of algorithms have been proposed. Those methods have a holistic view on pipeline synthesis: pipeline structure search is considered as an extension of CASH where, instead of a single algorithm, a combination of multiple algorithms is selected and optimized simultaneously. Due to the exponential growth in complexity, the pipeline structure space is usually not evaluated thoroughly.

In contrast to current AutoML approaches, data scientists often create an ML pipeline in several small distinct steps. Starting from an empty pipeline, data

scientists add algorithms to an ML pipeline incrementally by taking a detailed look at how the data set evolves in a pipeline in combination with their profound experience. Only if a pipeline structure performs well enough, a fine-tuning via hyperparameters is performed.

In this paper, we propose an alternative data-centric view on pipeline structure synthesis inspired by human behavior that allows an adaption of a pipeline to a specific data set. Through extensive use of meta-learning, we are able to dynamically prune the pipeline structure search space depending on meta-features of intermediate data sets. Intermediate data sets are the outputs of the execution of each individual step in a pipeline. Furthermore, the HPO of a pipeline candidate is boosted via knowledge-sharing between different pipelines. The main contributions of this paper are as follows:

- We reformulate the CASH and pipeline synthesis problem to enable efficient measures to reduce the pipeline search space and warm-starting CASH.
- We present a data-centric approach for incremental pipeline synthesis and hyperparameter optimization without expert knowledge inspired by human behavior called DSWIZARD.
- To ensure reproducibility of the results, we publish our meta-learning base consisting of 13.5 million unique ML pipelines on 28 data sets.

In Section 2 related work regarding pipeline structure synthesis and metalearning in AutoML is discussed. Section 3 describes how we model the pipeline synthesis and the creation of the meta-learning base. The effectiveness of this approach is evaluated in Section 4 followed by a short conclusion in Section 5.

2 Preliminary and Related Work

Let a classification task—containing a data set $D = \{(\vec{x}_1, y_1), \dots, (\vec{x}_m, y_m)\}$ with $\vec{x}_i \in \mathbb{X}^d$ being the input domain and $y \in \mathbb{Y} \subset N$ the target domain and a loss function $\mathcal{L}: \mathbb{Y}^2 \to \mathbb{R}$ —be given. Furthermore, let a fixed set of algorithms be given as $\mathcal{A} = \{A^{(1)}, A^{(2)}, \dots, A^{(n)}\}$. Each algorithm $A^{(i)}$ is a transformation $\phi: \mathbb{Z} \to \mathbb{Z}'$ between two arbitrary domains. In case of $\mathbb{Z}' = \mathbb{Y}$ we denote the algorithm as a classifier, otherwise as a preprocessor. Usually $A^{(i)}$ is configured by hyperparameters $\vec{\lambda}^{(i)}$ from a domain $\Lambda_{A^{(i)}}$. $A^{(i)}$ transforming a data set D being configured by $\vec{\lambda}$ is denoted as $\phi_{\vec{\lambda}}^{(i)}(D)$. An ML pipeline \mathcal{P} is a sequential combination of algorithms mapping data from an input domain to a target domain $f_{\mathcal{P}}: \mathbb{X}^d \to \mathbb{Y}$. It consists of a pipeline structure g—usually modeled as a directed acyclic graph (DAG)—with length |g|, algorithms $\vec{A} = [A_1, \dots, A_{|g|}]$ and the according hyperparameters $\vec{\lambda} = [A_1, \dots, A_{|g|}]$. AutoML aims at generating a pipeline \mathcal{P} that optimizes

$$(g, \vec{A}, \vec{\lambda})^* \in \mathop{\arg\min}_{g \in G, \vec{A} \in \mathcal{A}^{|g|}, \vec{\lambda} \in \varLambda_{A_1} \times \dots \times \varLambda_{A_{|g|}}} \pi \left(g, \vec{A}, \vec{\lambda}, D\right)$$

with

$$\pi\left(g, \vec{A}, \vec{\lambda}, D\right) = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(\hat{y}_i, y_i)$$

with \hat{y}_i being the predicted output on the sample \vec{x}_i . We refer to this extension of the CASH problem as pipeline synthesis and optimization (PSO) problem.

The CASH notation, as originally introduced by [20], extends HPO by introducing an additional categorical meta-hyperparameter that represents an algorithm choice. This approach does not scale well as the search space grows exponentially with the length of the pipeline [12]. To counter this problem, many frameworks use a fixed pipeline structure based on best-practices reducing PSO to CASH, e.g. [13,19]. AUTOSKLEARN [7] allows the omission of single steps in a fixed pipeline, effectively replacing a fixed pipeline structure with a small set of pipeline candidates. Similarly, P4ML [9] uses a set of hand-crafted, best-practice pipelines for a wide variety of task instances. Appropriate pipeline candidates are selected based on data set meta-features followed by a fine-tuning via HPO. Yet, even when selecting from a set of fixed structures, the pipeline structure cannot be freely adapted to a specific problem instance.

TPOT [17] uses genetic programming to solve the PSO problem. RECEIPE [18] extends TPOT by incorporating a context-free grammar to guide the construction of pipeline structures. Even though this approach is able to build flexible tree-shaped pipelines, experiments have shown that genetic programming approaches tend to build pipelines using only one or two algorithms [22].

Multiple approaches that use a Monte Carlo tree search (MCTS) [5] for pipeline synthesis have been proposed. ML-Plan [15] traverses a hierarchical task network with a MCTS to perform PSO. By design, the structure is determined first followed by the HPO. To assess the score of incomplete pipelines, random path completion is used, which does not scale well to high dimensions [11]. Similarly, Alphaddm [6] uses a combination of MCTS and neural networks to build pipeline structures based on a grammar while ignoring HPO completely. These approaches are more flexible in comparison to semi-fixed pipelines but still enforce specific pipeline patterns.

Many AutoML approaches use meta-learning to warm-start CASH or find promising pairs of preprocessors and classifiers [11]. AlphaD3M uses meta-features and the algorithms in the current pipeline to predict the performance of a possible pipeline candidate. However, all those approaches only calculate meta-features of the initial data set.

3 DSWIZARD Methodology

Our approach, dubbed DSWIZARD, is inspired by the behavior of a human data scientist creating an ML pipeline. Starting from a very basic pipeline with default hyperparameters, the pipeline structure is extended gradually based on the characteristics of the intermediate data sets and the experience from previous tasks. After obtaining a combination of algorithms, a fine-tuning of the hyperparameters is performed. Fig. 1 contains an overview of our proposed approach.

Starting from an empty pipeline and a given data set, at first the meta-features of the data set are extracted. Based on these meta-features, a suited algorithm is selected using information from a pre-computed meta-learning base.

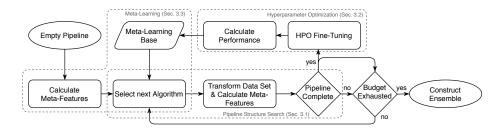


Fig. 1: General pipeline synthesis procedure in DSWIZARD.

Next, the data set is transformed using the selected algorithm and its default hyperparameters. Whenever the pipeline ends in a classifier, a fine tuning via HPO is performed to obtain a performance measure. This procedure is repeated until a predefined time budget is exhausted. Finally, ensemble selection [4] is used to create an ensemble of the best performing pipelines.

More formally, we reformulate the pipeline synthesis and optimization problem as a bilevel optimization problem:

$$(g, \vec{A}, \vec{\lambda}^*)^* \in \underset{g \in G, \vec{A} \in \mathcal{A}^{|g|}}{\arg \min} \quad \pi \left(g, \vec{A}, \vec{\lambda}^*, D \right)$$
s.t.
$$\vec{\lambda}^* \in \underset{\vec{\lambda} \in \Lambda_{A_1} \times \dots \times \Lambda_{A_{|g|}}}{\arg \min} \pi \left(g, \vec{A}, \vec{\lambda}, D \right).$$

The outer optimization problem is used for pipeline structure search and algorithm selection. The inner optimization problem performs the HPO of the selected algorithms. The implementation is publicly available on ${\rm GitHub.}^5$

3.1 Incremental Pipeline Structure Search

As each pipeline has to have a finite length and the set of algorithms \mathcal{A} is finite, it is possible to enumerate the complete pipeline search space up to a depth d. The resulting search space can be interpreted as a layered DAG. Each node/state s_t represents a pipeline candidate g_{s_t} , i.e., a list of algorithms, and a vector of meta-features of the intermediate data set D_{s_t} obtained by applying the (incomplete) pipeline candidate to the input data set; each edge/action represents an algorithm $A_t \in \mathcal{A}$. All nodes in a layer have pipeline candidates with identical lengths. We use an adapted MCTS [5] to efficiently traverse the search graph. In contrast to all existing solutions, we explicitly calculate the meta-features of each intermediate data set and not only the initial data set.

The policy for MCTS's selection and expansion phase—inspired by polynomial upper confidence trees [1]—is

$$A_t \in \underset{A \in \mathcal{A}}{\operatorname{arg \, max}} \ o(s_t) \cdot \left(Q(s_t, A) + c(t) \cdot U(s_t, A) \right)$$

 $^{^5}$ See https://github.com/Ennosigaeon/dswizard.

weighting the exploitation Q and exploration U by a function c for a given action $A \in \mathcal{A}$ and state s_t . Exploitation is defined as

$$Q(s_t, A) = \frac{P(s_t, A)}{1 + N(s_t, A)} \sum_{s' \in s_t(A)} \nu(s')$$

with $P(s_t, A)$ being a prior performance estimate (see Section 3.3), $N(s_t, A)$ being the number of times action A was selected in state s_t , $s_t(A)$ the state obtained after applying action A and $\nu(s')$ a previously observed performance in state s'. Exploration, defined as

$$U(s_t, A) = \frac{\sqrt{\sum_{b \in \mathcal{A}} N(s_t, b)}}{1 + N(s_t, A)} ,$$

calculates the multiplicative inverse of the relative number of selections of A, giving a higher weight to less frequently selected actions. To account for overfitting we introduce an additional exponential term

$$o(s_t) = 1 - \frac{c^{|g_{s_t}|}}{c^{l_{\max}}}$$

that reduces the node reward depending on the current pipeline length, a maximum pipeline length l_{max} and a scaling constant c > 1.

The MCTS procedure is adapted such that selection can be aborted if the current node has a higher reward than all child nodes. Similarly, expansion can be skipped. During each expansion step the data set in s_t is transformed by A_t and stored. Usually, MCTS uses a *simulation* to calculate the reward of s_t . However, a few random simulations do not scale well in high dimensional search spaces and many simulations are prohibitively expensive [11]. Instead, expansion is repeated recursively until the pipeline candidate ends in a classifier. After e consecutive expansions the selection of a classifier is enforced. Conceptually, this is similar to a random simulation. However, as we immediately know the meta-features of each intermediate data set, the simulation can be guided by the meta-learning base explained in Section 3.3. This approach explicitly does not restrict the pipeline structure via a grammar or similar measures.

The reward $\nu(s_{t+1})$ is not directly obtained during the MCTS. Instead it is computed via the HPO procedure described in Section 3.2. Therefore, pipeline structure search and HPO can be solved independently of each other while still being tightly coupled.

Finally, it remains to decide how many HPO samples are drawn to determine the reward of a state. To quickly discard unpromising structures, we wrap the complete structure search procedure in a multi-fidelity approach similar to Hyperband [14]. Yet, instead of deterministically calculated budgets—the number of HPO iterations—we adapt the greediness of the policy depending on the remaining optimization time

$$c(t) = w \cdot \left(\exp\left(\frac{t_{\text{max}} - t}{t_{\text{max}}}\right) - 1 \right) ,$$

with t_{max} being the total optimization time and w a non-negative weighting constant. For each pipeline candidate a small fixed number of HPO iterations is performed leading to more HPO iterations on well-performing candidates.

Using this procedure, the pipeline structure search space is incrementally expanded whenever a new layer of the graph is visited. Simultaneously, ineffective—the algorithm does not modify the data set—incompatible or bad performing transformations can be identified quickly. Consequently, the search graph is pruned efficiently, often even without any HPO.

3.2 Hyperparameter Optimization

After fixing the pipeline structure, its actual performance has to be assessed. In general, this step is computationally equally expensive as optimizing the hyperparameter for a fixed pipeline. Consequently, an efficient HPO procedure is key to evaluating various pipeline structures.

Traditional CASH procedures model the problem for a fixed structure g with—for simplicity—only one algorithm as

$$\vec{\lambda}^* \in \operatorname*{arg\,min}_{A^{(i)} \in \mathcal{A}, \vec{\lambda} \in \Lambda_{A^{(i)}}} \pi_g \left(A^{(i)}, \vec{\lambda}, D \right).$$

selecting the actual algorithm and its hyperparameters simultaneously, configuring all algorithms accordingly and finally evaluating the performance on the input data set. This approach has three major drawbacks: 1. The transformation of the data set being processed is not considered. 2. The algorithms in a pipeline may be incompatible with each other due to implicit requirements of the used algorithms on the input data. Selecting and fitting all algorithms at once may lead to wasted optimization time as incompatibilities are only detected during fitting [16]. 3. Sharing knowledge about well performing configurations between different pipeline structures using the same subset of algorithms is not possible. Instead we propose, to use a distinct optimization instance

$$\vec{\lambda}_i^* \in \underset{\vec{\lambda} \in A_{A(i)}}{\operatorname{arg\,min}} \ \pi\left(A^{(i)}, \vec{\lambda}, D\right)$$

for each algorithm only considering HPO. To prevent an improper impact of previous algorithms and their hyperparameter on the optimization, we additionally require that all meta-features of the transient data set D have to be similar. Otherwise, a new HPO instance is created. This allows sharing knowledge about well-performing hyperparameters between identical algorithms in different pipeline candidates, given that the pipeline prefixes yielded similar data sets.

The hyperparameters of each algorithm can be selected "on-the-fly" in order of appearance of the algorithms. After selecting the hyperparameters for each algorithm, the final performance is back-propagated to update each optimizer leading to a formulation compatible with current CASH formulations

$$\vec{\lambda}^* \in \mathop{\arg\min}_{\vec{\lambda}_1 \in A_1, \dots, \vec{\lambda}_{|g|} \in A_{|g|}} \pi \left(A_{|g|}, \vec{\lambda}_{|g|}, \phi_{\vec{\lambda}_{|g|}}^{(|g|)} \left(\phi_{\vec{\lambda}_{|g-1|}}^{(|g-1|)} \left(\dots \phi_{\vec{\lambda}_1}^{(1)}(D) \right) \right) \right)$$

with $\vec{\lambda}^* = \vec{\lambda}_1 \cup \cdots \cup \vec{\lambda}_{|g|}$ and \vec{A} being provided via the previously described structure search. Consequently, the hyperparameter search space for a single algorithm is significantly smaller than the complete CASH search space. This imposes two major benefits: 1. Bayesian optimization methods have been proven to be more powerful for low dimensional search spaces [12]. 2. The small search space improves the applicability of warm-starting. Based on the meta-features of the intermediate data set, samples for warm-starting can be extracted from previously evaluated configurations on different pipeline structure candidates. Each individual optimization problem can be solved via standard procedures like SMAC or HYPEROPT. In the context of this work tree Parzen estimators [2] are used. Each instance of this procedure yields a new performance measure $\nu(s_{t+1})$ for the MCTS procedure.

3.3 Meta-Learning

Traditional MCTS uses *simulations* to determine the score of an unvisited node. As extensive simulations are prohibitively expensive in the context of ML, current AutoML tools use a small number of random completions, potentially restricted by a grammar, to estimate the reward of a state, e.g. [15]. We propose to guide the random completions by considering intermediate meta-features.

To get a diverse foundation for the meta-learning base, we collected 30 unique data sets from OPENML [21]. Starting from the input data set, each available algorithm is applied using its default hyperparameters. The transformed data set is added to the meta-learning base—in case of a classifier, the transformed data set consists of the input data set with the prediction added as a new feature. This procedure is repeated exhaustively until the maximum pipeline length of five algorithms is reached. For each data set in the meta-learning base, 40 meta-features are extracted. As the meta-feature extraction has to be applied in each stage of the MCTS, a fast calculation of the meta-features is important, which limits the available meta-features to general, statistical, information-theoretical and simple model-based meta-features.⁶

If the applied algorithm comprises a classifier, the current performance is evaluated. For preprocessing algorithms the performance is estimated using all subsequent classification algorithms. Using this approach, we extracted the performance of over 13.5 million unique pipelines on 30 diverse data sets.

To account for the stochastic environment, the performance prediction of an algorithm for a given state is modeled by a normal distribution

$$P(s_t, A) \sim \mathcal{N}\left(RF_{\mu}(s_t, A), RF_{\sigma}(s_t, A)\right)$$

with RF_{μ} and RF_{σ} being two random forest regression models trained on the mean and standard deviation of the performance, respectively. The complete meta-learning base, namely the raw data and trained models, is publicly available alongside the source code but we also plan to publish all pipelines on OPENML.

⁶ The complete list of all data sets, algorithms and used meta-features is available in the online Appendix alongside the source code at https://git.io/JIOaJ.

4 Experiments

To prove the effectiveness and efficiency of our approach, DSWIZARD is compared with the two best established AutoML tools: AUTOSKLEARN and TPOT. Additionally, we perform an ablation study in which we test a variation of DSWIZARD without meta-learning, dubbed DSWIZARD*, to get a better impression of the impact of meta-learning during structure synthesis on the final performance.

4.1 Experiment Setup

To ensure fair and comparable results, the existing OPENML AutoML benchmark framework [8] is used for all experiments. We reuse the predefined constraints of a 60 minute optimization timeout per fold. Experiments are conducted on e2-standard-4 virtual machines on Google Cloud Platform equipped with Intel Xeon E5 processors with 4 cores and 16 GB memory.

All frameworks are evaluated on 28 publicly available binary and multiclass classification data sets from established and curated AutoML benchmark suits [3,8]. More specifically, OPENML tasks are used for each data set. A task provides information about a data set, for example how train-test splits have to be done or which loss function to use, to enable comparable results. The performance of each final configuration is computed using a hold-out validation data set. For binary and multiclass tasks AUC and logloss are used as metric, respectively.

To eliminate the impact of different search spaces on the final performance, the existing TPOT and AUTOSKLEARN adapters are adopted to use the same search space as DSWIZARD. This includes the available algorithms, hyperparameters per algorithm as well as search ranges. The complete search space consists of 35 algorithms with 38 categorical and 62 numerical hyperparameters. A short summary of the configuration space is provided in the online Appendix.

To prevent a leaking of information via meta-learning in DSWIZARD, we construct an individual meta-learning base for each data set excluding the data set under evaluation. The OPENML AutoML benchmark's AUTOSKLEARN adapter always performs label encoding before passing the data to the optimization routine. Similarly, the TPOT adapter always performs label encoding and an imputation of missing data. As these algorithms are not obtained via an optimization procedure, they are not further considered.

4.2 Experiment Results

Table 1 and 2 contain the final test performances of all evaluations. For each data set, the mean performance and standard deviation over 10 folds is reported. Bold face represents the best mean value for each data set. Results not significantly worse than the best result, according to a two-sided Wilcoxon signed-rank test with p=0.05, are underlined. If a framework consistently failed to yield results for at least three folds, the performance for that data set is not recorded.

⁷ At least if supported by the frameworks. For example, TPOT can only handle discretized continuous hyperparameters.

Table 1: Final test performance for all tested binary classification data sets using AUC as metric. Larger values are better.

Data Set	Autosklearn	ТРОТ	DSWIZARD	DSWIZARD*
Australian	0.9337 ± 0.0186	0.9380 ± 0.0180	0.9660 ± 0.0125	0.9461 ± 0.0219
ada_agnostic	0.9046 ± 0.0161	0.9034 ± 0.0136	60.9138 ± 0.0140	0.9121 ± 0.0171
adult	$\textbf{0.9279}\pm\textbf{0.0052}$	_	0.8933 ± 0.0121	0.8921 ± 0.0103
bank-marketing	$\textbf{0.9350}\pm\textbf{0.0068}$	_	0.9172 ± 0.0302	0.9090 ± 0.0132
blood-transfusion	0.7288 ± 0.0544	0.7601 ± 0.0664	0.7885 ± 0.0649	0.7310 ± 0.0632
credit-g	0.7719 ± 0.0318	0.7731 ± 0.0517	0.8527 ± 0.0260	0.8050 ± 0.0315
eeg-eye-state	$\textbf{0.9909}\pm\textbf{0.0033}$	_	0.9903 ± 0.0041	
higgs	$\textbf{0.8084}\pm\textbf{0.0061}$	0.7902 ± 0.0123	0.7263 ± 0.0844	0.7667 ± 0.0345
jasmine	0.8814 ± 0.0167	0.8880 ± 0.0167	0.9073 ± 0.0177	0.8977 ± 0.0209
kc2	0.8162 ± 0.0931	0.8252 ± 0.1599	0.8911 ± 0.0447	0.7867 ± 0.0522
kr-vs-kp	0.9992 ± 0.0014	0.9975 ± 0.0046	60.9995 ± 0.0009	0.9979 ± 0.0057
nomao	0.9956 ± 0.0009	0.9936 ± 0.0044	0.9939 ± 0.0015	0.9935 ± 0.0018
numerai28.6	0.5291 ± 0.0053	0.5267 ± 0.0042	0.5311 ± 0.0116	0.5286 ± 0.0081
phoneme	0.9629 ± 0.0101	0.9656 ± 0.0082	0.9662 ± 0.0086	$\overline{0.9638 \pm 0.0087}$
sa-heart	0.7586 ± 0.0485	0.7551 ± 0.1196	0.7968 ± 0.1065	0.8321 ± 0.0651
sylvine	0.9899 ± 0.0037	0.9855 ± 0.0075	0.9903 ± 0.0032	0.9865 ± 0.0042

Table 2: Final test performance for all tested multiclass classification data sets using *logloss* as metric. Smaller values are better.

Data Set	Autosklearn	TPOT	DSWIZARD	DSWIZARD*
Helena	3.0091 ± 0.1153	_	3.0226 ± 0.0829	3.2283 ± 0.2200
Jannis	0.7016 ± 0.0235	0.7297 ± 0.0417	0.7582 ± 0.0524	0.7861 ± 0.0856
Shuttle	0.0006 ± 0.0004	_	0.0011 ± 0.0013	S —
$analcatdata_auth$	0.0691 ± 0.1285	0.0123 ± 0.0210	0.0182 ± 0.0378	0.0073 ± 0.0090
$analcatdata_dmft$	1.7520 ± 0.0233	8—	1.7147 ± 0.0288	1.7498 ± 0.0676
car	0.0045 ± 0.0075	0.0033 ± 0.0035	0.0122 ± 0.0295	0.0450 ± 0.1028
connect-4	0.4181 ± 0.0685	_	0.6831 ± 0.1107	0.6989 ± 0.0745
jungle_chess_2pc	0.1786 ± 0.0350	0.2390 ± 0.0106	i —	_
mfeat-factors	0.1061 ± 0.0388	30.1160 ± 0.0488	$3\ 0.0615\ \pm\ 0.0387$	0.1122 ± 0.0533
mfeat-morphologic	0.6183 ± 0.0687	0.6560 ± 0.1035	$6.0.5599 \pm 0.0780$	$\overline{0.5916 \pm 0.0821}$
segment	0.0737 ± 0.0692	20.0596 ± 0.0379	0.0511 ± 0.0293	0.0696 ± 0.0362
vehicle	0.4525 ± 0.0495	$\overline{0.4407 \pm 0.0898}$	30.3889 ± 0.0576	$\overline{0.4329 \pm 0.0378}$

It is apparent that, on average, DSWIZARD outperforms the other frameworks. However, absolute performance differences are small and, especially for *logloss*, often not significant. TPOT and DSWIZARD/DSWIZARD* struggled with some data sets. For TPOT, single configuration evaluations often exceeded the global timeout leading to an aborted evaluation. In contrast, DSWIZARD/DSWIZARD* exceeded the available memory leading to a crash. The results for DSWIZARD* show that meta-learning is able to significantly boost the results of DSWIZARD for 16 of 28 data sets. Yet, even without meta-learning the more thoroughly eval-

uation of the pipeline search space yielded configurations outperforming either TPOT or AUTOSKLEARN on 13 data sets.

Fig. 2 shows the structure of the final pipelines aggregated over all data sets and folds. For better readability we substituted each used algorithm by an abstract algorithm class, namely balancing, classifier, decomposition, discretization, encoding, filtering, generation, imputation, scaling and selection. The assignment of algorithm to algorithm class is available in the online Appendix. Additionally, we treat ensembles of pipelines as sets of individual pipelines. Possible pipeline starts are indicated by rounded corners. The frequency of node and edge visits is encoded using a color scheme. Darker colors represent a more frequent usage. For better readability, edges and nodes that appear in less than 1% of all pipelines are excluded.

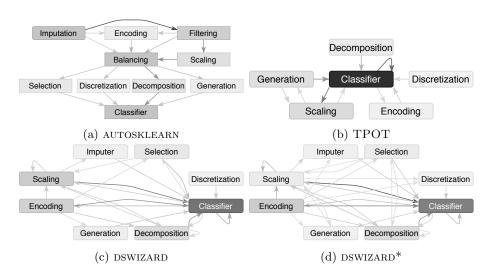


Fig. 2: Schematic representation of final structures

In Fig. 2a it is clearly visible that AUTOSKLEARN uses a semi-fixed pipeline structure where single steps can be omitted. A strict order of algorithms exists, from the top left of the graph to the bottom. *Imputation*, balancing and classifier are present in each pipeline and the remaining algorithms are roughly selected with identical frequencies. On average, each pipeline contains 5.48 algorithms. Due to the semi-fixed structure of AUTOSKLEARN, often ineffective algorithms are present in pipelines, e.g. imputation even though the data set does not contain missing values. TPOT is able to construct pipelines with highly varying shapes. However, each pipeline, on average, only contains 1.66 algorithms, mostly classifiers. Even though more complex pipelines are constructed, those complex pipelines represent less than 15% of all pipelines leading to the heavily pruned graph depicted in Fig. 2b. DSWIZARD constructs more diverse pipelines

in terms of selected algorithms and transitions between algorithms. Without meta-learning (compare Fig. 2c and 2d), structure search is less guided leading to longer pipelines (2.85 vs. 3.07 algorithms) and a more uniform distribution of the selected algorithms. Yet, as DSWIZARD* performs worse than DSWIZARD, the guidance seems to be helpful to find well performing pipeline structures.

Finally, we take a more detailed look at *credit-g* and *higgs*, two data sets where DSWIZARD performs especially well and badly, respectively. For *credit-g* 71% of the pipelines in the final ensemble have a long complex structure that can not be created by AUTOSKLEARN. Most pipelines combine stacked classifiers with multiple preprocessors. For *higgs* the meta-learning directs the structure search in a wrong direction leading to many ineffective transformations. As a result, only very basic pipelines containing combinations of the same four algorithms are constructed. Even with HPO, these simple pipelines do not perform well.

In summary, DSWIZARD significantly outperforms either AUTOSKLEARN or TPOT on 42% of the data sets. Moreover, it has a similar performance to the state-of-the-art on 32% of the data sets.

5 Conclusion

We presented a data-centric approach for solving the PSO problem inspired by human behaviour using MCTS in combination with Bayesian optimization. The possibility to expand the search space incrementally allows for a dynamic adaptation of the pipeline structure to a specific data set. Unpromising regions of the pipeline search graph can be identified and discarded quickly—often even without HPO—through the extensive use of meta-features allowing an efficient traversal of the growing search space. Furthermore, sharing knowledge between pipeline structures is implemented for warm-starting HPO. This allows a more thorough exploration of the pipeline structure search space with a dynamic adaptation to a specific data set while still obtaining competitive results.

References

- Auger, D., Couetoux, A., Teytaud, O.: Continuous Upper Confidence Trees with Polynomial Exploration – Consistency. In: Joint European Conference on Machine Learning and Knowledge Discovery in Databases. pp. 194–209 (2013)
- 2. Bergstra, J., Yamins, D., Cox, D.D.: Hyperopt: A python library for optimizing the hyperparameters of machine learning algorithms. In: Python in Science Conference. pp. 13–20 (2013)
- 3. Bischl, B., Casalicchio, G., Feurer, M., Hutter, F., Lang, M., Mantovani, R.G., van Rijn, J.N., Vanschoren, J.: OpenML Benchmarking Suites and the OpenML100. arXiv preprint arXiv:1708.03731v1 (2017)
- 4. Caruana, R., Niculescu-Mizil, A., Crew, G., Ksikes, A.: Ensemble Selection from Libraries of Models. International Conference on Machine Learning p. 18 (2004)
- 5. Coulom, R.: Efficient Selectivity and Backup Operators in Monte-Carlo Tree Search. 5th International Conference on Computer and Games (2006)

- Drori, I., Krishnamurthy, Y., de Paula Lourenco, R., Rampin, R., Kyunghyun, C., Silva, C., Freire, J.: Automatic Machine Learning by Pipeline Synthesis using Model-Based Reinforcement Learning and a Grammar. In: International Conference on Machine Learning AutoML Workshop (2019)
- Feurer, M., Klein, A., Eggensperger, K., Springenber, J.T., Blum, M., Hutter, F.: Efficient and Robust Automated Machine Learning. In: International Conference on Neural Information Processing Systems. pp. 2755–2763 (2015)
- 8. Gijsbers, P., LeDell, E., Thomas, J., Poirier, S., Bischl, B., Vanschoren, J.: An Open Source AutoML Benchmark. In: International Conference on Machine Learning AutoML Workshop (2019)
- Gil, Y., Yao, K.T., Ratnakar, V., Garijo, D., Steeg, G.V., Szekely, P., Brekelmans, R., Kejriwal, M., Luo, F., Huang, I.H.: P4ML: A Phased Performance-Based Pipeline Planner for Automated Machine Learning. In: International Conference on Machine Learning AutoML Workshop. pp. 1–8 (2018)
- Hutter, F., Hoos, H.H., Leyton-Brown, K.: Sequential Model-Based Optimization for General Algorithm Configuration. In: International Conference on Learning and Intelligent Optimization. pp. 507–523 (2011)
- Hutter, F., Kotthoff, L., Vanschoren, J.: Automated Machine Learning: Methods, Systems, Challenges. Springer (2018)
- 12. Kandasamy, K., Schneider, J., Póczos, B.: High Dimensional Bayesian Optimisation and Bandits via Additive Models. International Conference on Machine Learning pp. 295–304 (2015)
- 13. Komer, B., Bergstra, J., Eliasmith, C.: Hyperopt-Sklearn: Automatic Hyperparameter Configuration for Scikit-Learn. In: International Conference on Machine Learning AutoML Workshop. pp. 2825–2830 (2014)
- Li, L., Jamieson, K.G., DeSalvo, G., Rostamizadeh, A., Talwalkar, A.: Hyperband: A Novel Bandit-Based Approach to Hyperparameter Optimization. Journal of Machine Learning Research 18, 1–52 (2018)
- Mohr, F., Wever, M., Hüllermeier, E.: ML-Plan: Automated machine learning via hierarchical planning. Machine Learning 107, 1495–1515 (2018)
- Nguyen, T.D., Maszczyk, T., Musial, K., Zöller, M.A., Gabrys, B.: AVATAR -Machine Learning Pipeline Evaluation Using Surrogate Model. In: International Symposium on Intelligent Data Analysis. pp. 352–365 (2020)
- 17. Olson, R.S., Moore, J.H.: TPOT: A Tree-based Pipeline Optimization Tool for Automating Machine Learning. In: International Conference on Machine Learning AutoML WorkshopVa. pp. 66–74 (2016)
- de Sá, A.G.C., Pinto, W.J.G.S., Oliveira, L.O.V.B., Pappa, G.L.: RECIPE: A Grammar-Based Framework for Automatically Evolving Classification Pipelines. In: European Conference on Genetic Programming. vol. 10196, pp. 246–261 (2017)
- Swearingen, T., Drevo, W., Cyphers, B., Cuesta-Infante, A., Ross, A., Veeramachaneni, K.: ATM: A distributed, collaborative, scalable system for automated machine learning. In: IEEE International Conference on Big Data. pp. 151–162 (2017)
- Thornton, C., Hutter, F., Hoos, H.H., Leyton-Brown, K.: Auto-WEKA: Combined Selection and Hyperparameter Optimization of Classification Algorithms. In: ACM International Conference on Knowledge Discovery and Data Mining. pp. 847–855 (2013)
- Vanschoren, J., van Rijn, J.N., Bischl, B., Torgo, L.: OpenML: networked science in machine learning. ACM International Conference on Knowledge Discovery and Data Mining 15(2), 49–60 (2014)
- 22. Zöller, M.A., Huber, M.F.: Benchmark and Survey of Automated Machine Learning Frameworks. arXiv preprint arXiv:1904.12054 (2019)