MASIF: Meta-learned Algorithm Selection using Implicit Fidelity Information

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Abstract

Selecting a well-performing algorithm for a given task or dataset can be time-consuming and tedious, but is crucial for the successful day-to-day business of developing new AI & ML applications. Algorithm Selection (AS) mitigates this through a meta-model leveraging meta-information about previous tasks. However, most of the available AS methods are error-prone because they characterize a task by either cheap-to-compute properties of the dataset or evaluations of cheap proxy algorithms, called landmarks. In this work, we extend the classical AS data setup to include multi-fidelity information and empirically demonstrate how meta-learning on algorithms' learning behaviour allows us to exploit cheap test-time evidence effectively and combat myopia significantly. We further postulate a budget-regret trade-off w.r.t. the selection process. Our new selector MASIF is able to jointly interpret online evidence on a task in form of varying-length learning curves without any parametric assumption by leveraging a transformer-based encoder. This opens up new possibilities for guided rapid prototyping in data science on cheaply observed partial learning curves.

$_{\scriptscriptstyle 14}$ 1 Introduction

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Data scientists typically spend most of their time with data engineering and thus often have less time for choosing a well-performing algorithm for a given task (Anaconda, 2020). This selection process is typically powered by both the experience of the data scientist w.r.t. the performance of algorithms on previous tasks and datasets as well as a limited number of partial evaluations of the candidate algorithms on the task at hand. In doing so, a data scientist inherently carefully trades off (i) time invested into actively gathering performance information on the new task to make an informed decision and (ii) the regret in terms of performance incurred by possibly not selecting the best algorithm.

On one extreme end of this trade-off lie classical AS (Rice, 1976; Kerschke et al., 2019) approaches which characterize a task using handcrafted meta-features (Vanschoren, 2018) of the corresponding dataset. These 23 24 features are supposed to be informative w.r.t. the performance of an algorithm on that particular dataset. These approaches aim at learning a mapping from these characteristics to the pool of algorithms, allowing 25 them to recommend an algorithm for a new task at hand. In practice, such dataset meta-features may show limited association with the performance of the considered classes of algorithms (Pfahringer et al., 2000; 27 J. Fürnkranz, 2001). In particular, so-called dataset meta-features, corresponding to cheaply-computable 28 properties of the dataset (including simple, statistical, information-theoretic, complexity- and model-based properties (Vanschoren, 2018)), are known to be only indicative of algorithm performance to a limited 30 degree (Pfahringer et al., 2000). Similarly, the correlation of landmarking meta-features, i.e., performances of 31 cheap proxy algorithms computed on the new dataset, can be limited, as they hinge on how well the proxy 32 algorithms' performances are associated with those of the pool of candidates. For instance, the performance of a decision stump might not be informative on how well a deep neural network will perform.

On the other extreme end of this trade-off lie existing learning curve approaches (Mohr & van Rijn, 2021),
which exclusively invest time into gathering information on potentially well-performing algorithms from the
pool of candidates on the new dataset. They utilize cheap but premature approximations of the candidates
performances, such as training models only for a limited amount of epochs or only on parts of the training

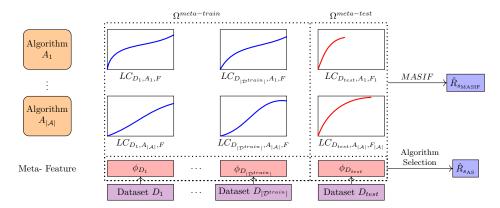


Figure 1: In contrast to classical algorithm selection trained only on meta-features, MASIF utilizes the information from both meta-features and learning curve values to predict the best performing algorithms.

data, and extrapolate to converged training on all the data. As such, learning curve approaches invest comparatively more budget on obtaining information naturally associated with the final performance of the classes of algorithms. A common downside to these approaches lies in their extrapolation strategy. Observing only premature approximations of the performance data with little or no meta-knowledge about an algorithm's learning behavior, learning curve methods often resort to strong parametric assumptions (Mohr & van Rijn, 2022) and are myopic in the sense that an extrapolated estimate of the final performance can only be based on the observed premature performance values. Further, with few exceptions, such as (van Rijn et al., 2015; Klein et al., 2017; Baker et al., 2018; Long et al., 2020), they only extrapolate each algorithm independently, ignorant of possible existing relations in learning behaviors to other algorithms.

In this work, we propose MASIF (Meta-learned Algorithm Selection using Implicit Fidelity)¹, an approach designed to support data scientists in the AS process in a much more intuitive manner. It supports a data scientist's active discovery process on a new dataset, as it allows refining the expectation on the final ranking over algorithms based on his/hers incremental budget allocation. This provides the user with full flexibility in different trade-offs between invested budgets and regret of the final ranking. It is however also a limitation in the sense that a user has to make this decision. As alleviation, we later provide an exemplary solution but note that this opens up a new area for research.

MASIF is powered by a transformer-based model accounting for the sequential nature of learning curves and interpreting their (partial) informational content. It learns to interpret them based on the meta-knowledge w.r.t. the candidates' learning behavior obtained from observing them on other datasets. Using this encoder and the available meta-knowledge, our model neither requires explicitly extrapolating the curves nor does it necessitate assumptions on their parametric shapes. Learning a latent representation of each curve respectively, a subsequent transformer and MLP merge the gathered test-time evidence in the form of observed premature performances. This allows learning cross-correlations between the algorithms' learning behaviors (cf. Figure 1).

Overall, we make the following contributions:

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- 1. From a practical perspective, we formalize a meta-learning multi-fidelity setup that closely resembles a data scientist's workflow. Based on this we discuss the budget-regret trade-off that contemporary algorithm selectors implicitly make.
- 2. We introduce MASIF, a learning curve interpreter living in this framework, leveraging both dataset meta-features and formulating a well-informed meta-prior on the candidates' learning behaviors. It mitigates the fallacies of classical AS and learning curve-based approaches; namely, as the first of its kind, it jointly interprets multiple learning curves of varying lengths and, utilizing meta-knowledge to combat myopia, leading to a better-informed ranking with less compute on a new dataset.

¹MASIF's code is published on https://anonymous.4open.science/status/MASIF-824D

- 3. Since we open up a new framework for AS with multi-fidelity information, we propose a new evaluation scheme based on fidelity slices.
 - 4. We demonstrate the usage of this novel learning curve interpreter as an algorithm selector based on a user's budgetary and regret preferences, and evaluate its performance against other baselines on several benchmarks.

77 2 Preliminaries

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As we seek to unify classical AS, multi-fidelity, and learning curves, we re-examine them and offer a notation, with which we later detail how selectors behave. Particularly, this notation is aimed at highlighting both the available meta-knowledge and the associated cost of acquiring information on a new dataset.

The Algorithm Selection Problem denotes the task of finding an algorithm selector $s: \mathcal{D} \to \mathcal{A}$ from the space of algorithm selectors \mathcal{S} , which selects the presumably most suitable (machine learning) algorithm $A^* \in \mathcal{A}$ for a given dataset $D \in \mathcal{D}$. Here, suitability is expressed through a costly-to-evaluate performance metric $m: \mathcal{D} \times \mathcal{A} \to \mathbb{R}$, which quantifies how well the given algorithm performs on the given dataset at the end of its training process. Examples include the accuracy or cross-entropy loss on the test data. The (hypothetical) best algorithm selector, also called the oracle, s^* , chooses the best algorithm for every dataset D on the final performances:

$$s^*(D) = A^* \in \arg\max_{A \in \mathcal{A}} m(D, A) \tag{1}$$

Classical Algorithm Selectors seek to meta-learn across datasets, which algorithm will perform best on a new dataset. As the performance of an algorithm $A \in \mathcal{A}$ is costly to evaluate, a complete enumeration over \mathcal{A} to select the best one is often not feasible in practice, which leads to the application of machine learning to predict the best algorithm. To allow learning such a selector based on meta-training data, datasets D are 91 characterized by their dataset meta-features ϕ_D and are fed as input to the selector. In the classical setting, 92 these are quickly-computable properties of a dataset, called dataset meta-features Vanschoren (2018) such 93 as, e.g., the number of data points, number of explanatory features or the entropy of a dataset's dependent 94 variable. For the purpose of analyzing a selector's associated cost, computing ϕ_D is part of the selector's 95 computational budget on a meta-test dataset to gain information about it. Optionally, s can also take algorithm meta-features ϕ_A as input, e.g., the number of neurons in a particular layer of a neural net (Tornede 97 et al., 2020; Pulatov et al., 2022). 98

In practice, many AS approaches, either implicitly (Xu et al., 2012; Amadini et al., 2014) or explicitly (Cunha et al., 2018; Hanselle et al., 2020), compute a ranking over the algorithms \mathcal{A} and return the best one. Correspondingly, as we also rely on rankings, for the remainder of this paper, we assume that a selector returns a ranking from the ranking space $\mathcal{R}(\mathcal{A})$ over the discrete set \mathcal{A} , i.e., we consider algorithm selectors of the form $s: \mathcal{D} \to \mathcal{R}(\mathcal{A})$.

In the classical setting, the data used to train a selector is called meta-training set² to differentiate it from the actual datasets D, on which the individual algorithms are trained and evaluated. It is defined as

$$\Omega^{meta-train} = \{ \phi_D, \phi_A, m(D, A) | D \in \mathcal{D}^{train}, A \in \mathcal{A} \}, \tag{2}$$

where \mathcal{D}^{train} is a set of datasets to meta-train on.

 \mathcal{D}^{train} is used to train a selector s to predict rankings over the known set of algorithms \mathcal{A} across datasets with minimal meta-train loss $\mathcal{L}: \mathcal{R}(\mathcal{A}) \times \mathcal{R}(\mathcal{A}) \to \mathbb{R}$, when comparing the prediction s(D) against the respective ground-truth ranking $R_D^*(\mathcal{A}) \in \mathcal{R}(\mathcal{A})$. Hence, we solve the optimization problem defined as

$$\min_{s \in \mathcal{S}} \sum_{D \in \mathcal{D}^{train}} \mathcal{L}(R_D^*(\mathcal{A}), s(D)). \tag{3}$$

²We refer to this meta-training set as meta-knowledge interchangeably.

Similarly, the meta-test loss \mathcal{L}' of s is measured on the known set \mathcal{A} on hold-out datasets $D \in \mathcal{D}^{test}$.

$$\mathcal{L}^{test}(s) = \sum_{D \in \mathcal{D}^{test}} \mathcal{L}'(R_D^*(\mathcal{A}), s(D)). \tag{4}$$

While \mathcal{L} usually is a differentiable training loss, during test time, \mathcal{L}' does not need to have this restriction. For the remainder, we assume this to be a regret function. In particular, since algorithm selectors return a recommendation of the most promising algorithms on the given dataset, we use the top-k regret for the test-loss as defined in Eq. (4)

$$\mathcal{L}_k^{test}(R_D^*(\mathcal{A}), s(D)) = \min_{A \in \text{top-}k(s(D))} m(D, A^*(D)) - m(D, A), \tag{5}$$

where top-k returns the first k elements of the ranking that s recommended and $A^*(D) = \arg\max_{A \in \mathcal{A}} m(D, A)$.

The selector s is allowed to access the available test-time information $\{\phi_D, \phi_A | A \in \mathcal{A}\}$ for its prediction on D, resulting in the meta-test knowledge: $\Omega^{meta-test}|D = \{\phi_D, \phi_A | A \in \mathcal{A}\}$.

A particularly strong kind of meta-feature in classical AS is landmarking (Pfahringer et al., 2000). Landmarking 118 features report the validation performances m(D,A) of cheap algorithms that are usually not in the pool of 119 candidates $(A \notin \mathcal{A})$ as dataset meta-features. This relaxes the assumption that meta-features need to be very 120 fast to compute. The utility of classical and landmarking meta-features w.r.t. the selection task depends on the alignment of their description of the topology to the topology that the candidate algorithms' inductive 122 biases are successful on – as observed in terms of their final test performance. This is particularly true for 123 landmarking features as they apply their inductive biases to the datasets' topology. Their relevance is related 124 to the overlap in the functions that both sets of algorithms describe. For example, a shallow decision tree 125 might be partially informative regarding the performance of other tree-based algorithms, such as random 126 forests (Breimann, 2001) or xgboost (Chen & Guestrin, 2016). We refer to the question of information content 127 as the alignment problem of meta-features and algorithm performance.

Multi-Fidelity Optimization Since training a machine learning model to completion can be very expensive, multi-fidelity optimization (Li et al., 2018) aims at using cheap-to-evaluate proxies to make efficient decisions, e.g., which algorithm performs best. In automated machine learning (AutoML, Hutter et al. (2019)), these proxies can include training for a limited number of epochs, or training on a subset of the training data.

Formally, we seek to approximate a costly-to-evaluate function F by a fidelity $f_i \in \mathcal{F}$ from the space of fidelities \mathcal{F} . We note that also F is part of \mathcal{F} . Each fidelity f_i comes with a cost $c(x, f_i)$ to evaluate $f_i(x)$ at point x. The common assumption is that the approximation quality of f_i w.r.t. F gets better in proportion to its cost $c(\cdot, f_i)$, leading to a trade-off between approximation quality and cost of the fidelity.

Learning Curves form an ordered sub-case in multi-fidelity optimization, in particular \mathcal{F} is cost-ordered. In our case, we consider a learning curve of an algorithm to be the performance metric $m: \mathcal{D} \times \mathcal{A} \times \mathcal{F} \to \mathbb{R}$ observed on cost-ordered fidelities f_1, \ldots, F_A , where $c(x, F_A) \leq c(x, F)$ and F_A is the maximally observed fidelity for algorithm A. Formally, a learning curve can be defined as

$$LC_{D,A,F_A} = (m(D,A,f))_{f=f_1,\dots,F_A}$$
 (6)

Notably, we distinguish between a partial learning curve, i.e., $F_A \neq F$, and a full learning curve, i.e., $F_A = F$.

Each algorithm may be observed at a different maximum fidelity F_A , since a user may decide to spend different amounts of computing resources to evaluate different algorithms A.

3 MASIF: Interpreting Partial Learning Curves Jointly

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In this section, we introduce our core contributions: (i) extending the classical AS setup by adding multifidelity information, allowing for a more detailed analysis of the budget-regret trade-off of algorithm selectors; (ii) our transformer-based MASIF approach as an efficient method for this extended data setup; and (iii) a data augmentation scheme to achieve strong predictive performance and enable MASIF to accept arbitrary budget allocation strategies.

3.1 Extending Algorithm Selection by Multi-Fidelity Information

In addition to dataset meta-features, we propose to use information from learning curves as multi-fidelity information for algorithm selection. This allows inquiring about a new dataset's topology from the perspective of the candidates' inductive biases. Since this information is well aligned with the goal of AS, it opens up a new informative and cheap-to-compute information source. We summarize this setup in Figure 1.

Meta-Training Data The aforementioned idea extends our available training meta-knowledge in Eq. (2) and Eq. (3) by fidelity information, amounting to

$$\Omega^{meta-train} = \{\phi_D, \phi_A, LC_{D,A,F} | D \in \mathcal{D}^{train}, A \in \mathcal{A}\}$$
(7)

where the learning curves $LC_{D,A,F} \in \mathbb{R}^F$ replace the performance values $m(D,A) \in \mathbb{R}$ in Eq. (2). For our experiments, we observed full learning curves up to the maximal fidelity F for the meta-training dataset. This meta-knowledge as part of the meta-training dataset encodes several aspects: (i) the relation of the algorithm's performance w.r.t. the dataset's topology, (ii) how information about the algorithm's inductive bias is unrolled across fidelities and (iii) how the learning behavior of different algorithms relate to each other.

Meta-Testing Data The meta-testing phase provides partial learning curves observed on a new hold-out dataset. The set of curves provides evidence of the dataset's topology observed through the lens of the algorithms. The available information at test time for our selector s in Eq. (4) is:

$$\Omega^{meta-test} = \{\phi_D, \phi_A, LC_{D,A,F_A} | , F_A \le F, A \in \mathcal{A}, D \in \mathcal{D} \}.$$
(8)

Notably, depending on a user's budgetary preferences, some of the learning curves may be revealed nearly entirely or not at all; in general, we assume that the set of all learning curves may be incomplete. Since an algorithm selector returns a ranking over the algorithms on the given dataset, we use the top-k regret for the test-loss as defined in Eq. (4). Subsequently, we consider the performance comparison on the final fidelity F.

169 3.2 MASIF Architecture

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We choose a deep learning architecture because of its functional flexibility and its non-parametric modelling.

However, we have to exploit the little data typically available in AS without grossly over-fitting to the
meta-data. Our proposed architecture is displayed in Figure 2; it consists of five main building blocks:

Block 1 Assuming some valuable information on the topology in the classical meta-features f_D , an MLP encodes them into a latent space. Utilizing this cheap set of features, from an informational standpoint, our method can only improve over classical AS methods and further allows us to contextualize the observed learning curves to the observed dataset. If, for instance, ϕ_D conveys some information regarding the complexity of the dataset, this may be indicative of how fast an algorithm might learn, affecting the shape of the curve.

Block 2 As preprocessing of the learning curves, we apply zero-padding to fill the learning curves up to the final fidelity F and generate an according mask to store the padding information. To avoid technical issues with fully masked sequences, we append an extra learnable End Of Sequence (EOS) token (Dosovitskiy et al., 2020). We then use an MLP to embed each position of a learning curve individually, to increase the expressivity of our one-dimensional learning curve sequences into e dimensions akin to BERT's vector representations for each word (Devlin et al., 2019). Specifically, a single shared MLP is applied separately to each position of each learning curve. To overcome the transformer's native positional ignorance, we follow Vaswani et al. (2017) in encoding the positional information with sine and cosine functions and adding these

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values to the embedded learning curves. This is a crucial step in preserving the sequence information, which in our case conveys the order in learning curves.

Block 3 We use a variation of the transformerencoder proposed by Vaswani et al. (2017) on the set of partially observed learning curves LC_{D,A,F_A} of each algorithm $A \in \mathcal{A}$ to translate the (incomplete/masked) learning curve sequence into a latent vector representation enriched with the meta-knowledge of the algorithms' marginal learning behaviors.

Since the classical dataset meta-features may carry valuable information for the amount and variability of information at each position in the sequence, we introduce a mechanism we dub guided attention. Similar to the classical attention module, our encoder receives a query Q, key K, and value V tensor, containing the preprocessed learning curves from Block 2. That is, we multiply the query Q of the attention heads element-wise with a linear projection of the embedding described in Block 1 if dataset meta-features are available. The projection's role is merely to fit the shape of Q. To increase parallelism and reduce the number of learnable parameters, we use a batch trick; i.e., we only process one dataset at a time, but conceive the set of algorithms \mathcal{A} to be a batch of dimensions $[\mathcal{A}, \mathcal{F}, e]$, that is processed in parallel. The attentionguided transformer-encoder layer returns a tensor of the same dimension as its input. This layer is repeated N times. The result is a marginal summarisation of the latent representation of each of the learning curves. The order of the batch is held fixed over all datasets, s.t. the subsequent module receives the latent vector representation of an algorithm's learning curve at the exact same position every time.

Given the generated feature maps, the next step is aimed at receiving a joint representation of the evidence on D encoded in these vectors. Specifically, we reduce the $[\mathcal{A}, \mathcal{F}, e]$ -dimensional tensor along the fidelity dimension. This is done using a learnable weighted average over the fidelities \mathcal{F} applied independently over \mathcal{A} , resulting in e-dimensional vectors. Given the properties of the target dataset, the model should focus on different stages of the learning curves.

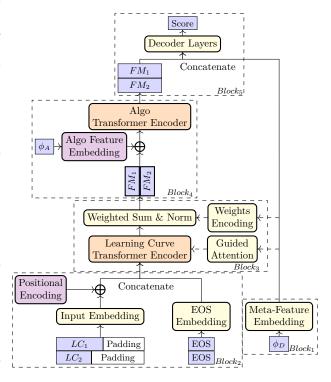


Figure 2: MASIF Architecture. Blue rectangles represent data, yellow rectangles denote MLP layers, purple rectangles indicate positional encodings, and orange rectangles are transformer layers. MASIF receives the partial learning curves of all the algorithms $LC_{D,A,F_A} \forall A \in \mathcal{A}$ (in this figure, we only show two learning curves, i.e., LC_1 and LC_2 , indicating $LC_{D,A_1,F_{A_1}}$ and $LC_{D,A_2,F_{A_2}}$). The two transformer encoder layers apply attention operations on the fidelity and the algorithm dimensions, respectively. Therefore, the output of each transformer needs to be transposed to fit the dimension. The output of the last transformer $(FM_1 \text{ and } FM_2)$ is concatenated with the embedded meta-features ϕ_D . Finally, the joint features are fed to the decoder to get the predicted ranks.

Therefore, we make these weights learnable. More precisely, if dataset meta-features are available, these weights are computed by an MLP that projects the dataset meta-feature embedding to the size of \mathcal{F} . Otherwise, these weights directly become learnable parameters.

Block 4 The model up until this point is still unaware of the cross-algorithm information between different learning curves, which is essential to predict the relative ranking of each algorithm. Therefore, we build another transformer on top of the first transformer that fuses the evidence on the topology derived from the partial learning curves of all $A \in \mathcal{A}$. The rationale is that since the algorithms are always presented in the same position, the position of these vectors holds meaning. From the perspective of BERT, each algorithm vector is the embedding to a token, and the sequence of algorithms is a sentence. Therefore, we transpose the

set of representations and make the batch dimension explicit [1, A, e]. To let the transformer identify different algorithms, we encode the algorithms' features (i.e., their hyperparameters or a simple one-hot encoding when no hyperparameter is available) as positional encoding and attach them to the generated transformations.

Block 5 Yet again, we employ an MLP on the concatenation of the vectorized evidence and the dataset meta-feature embedding to fuse their information and project to the size $n_{\mathcal{A}} = |\mathcal{A}|$. The returned values are scores for the respective algorithms, corresponding to latent utility values, which are used to construct a ranking across the algorithms. As an objective, optimally, we would like to maximize the Spearman rank correlation between predicted and true algorithm ranks. In order to obtain a differentiable loss, we thus leverage a differentiable sorting algorithm (Blondel et al., 2020) to compute the training loss.

246 3.3 Data Augmentation

Since AS usually only has a limited amount of dataset-algorithm combinations in its meta-training dataset for which we observe a single learning curve instantiation, respectively, we use a data augmentation strategy. Namely, we employ random masking on the learning curves to avoid meta-overfitting. The masking strategy consists of sampling the available learning curve length F_A uniformly and independently over [0, F], where 0 indicates complete lack of information on that learning curve. This strategy also facilitates that our model can be presented with any budget allocation (combination of fidelities), i.e. $\{F_A \in \mathcal{F} \cup \{0\}\}_{A \in \mathcal{A}}$ – including the option of not evaluating a curve during test-time.

254 3.4 MASIF's Benefits

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The transformer encoding of the learning curves offers significant advantages: at no point do the learning curves require extrapolation. Instead, only their informational content is summarized and transformed into a conditioned ranking score. Our method, therefore, does not fall victim to error propagation as often encountered in time series regression or multi-label classification (Senge et al., 2012). Additionally, leveraging the meta-knowledge of having observed the learning curves of the same algorithms on meta-training datasets, we combat multi-fidelity's inherent myopia problem effectively and can be fully non-parametric in the shape of the learning curves due to a strong meta-prior encoded in the weights of our architecture. To this end, MASIF exploits extensive meta-knowledge of observing the algorithms' learning curves on multiple datasets jointly. Depending on the fidelity type and type of algorithms considered, this meta-knowledge in form of algorithms' learning curves comes almost at no cost when collecting the meta-training data in the classical AS setting. Crucially, taking a multi-fidelity lens – independent of whether or not we include classical and landmarking meta-features – its ranking ability is no longer bounded by the alignment of tediously handcrafted and highly task-specific meta-features. Instead, it is governed by the trade-off between the approximation quality of the fidelities and the induced cost of querying them. It does, however, readily consider expert knowledge in form of dataset meta-features to contextualize the observed learning curves.

Given some budget allocation, the MASIF model corresponds to an algorithm selector since it produces a ranking that takes all the available meta-knowledge and the gathered evidence on the test dataset into account. However, since any budget allocation is possible, it can be readily utilized not only as a selector but as an interpreter of the incrementally arriving performance feedback from the budget allocation. Queried continuously as more evidence arrives, users can observe the shift in expectation on the final ranking, conditioned on what has been observed so far. This application mode makes this model an actionable support system for data science practitioners facing the AS problem.

The trade-off between approximation quality and budget costs opens up the opportunity of defining a scheduler that iteratively queries the fidelities of algorithms (i.e., extending their learning curves) by exploiting our model. Since our contribution focuses on the model part and since MASIF's model works with arbitrary strategies for deciding the budget allocation, in our experiments we show exemplary results with the prominent scheduling approach of Successive Halving (SH) (Jamieson & Talwalkar, 2016). While the original SH procedure in each "bracket" retains the current top-performing algorithms, our variant, dubbed SH Scheduler retains those that based on the current observation MASIF predicts to be top-performing on the final ranking.

Experiments 284

In this section, we first introduce a new evaluation protocol for our proposed extension of the classical AS 285 meta-data setup with added fidelity information. Then, we detail our baselines along with their perks and shortcomings, briefly describe the meta-datasets we use as benchmarks and subsequently detail our findings. 287

4.1 Fidelity-Slice Evaluation Protocol

In order to assess the ability of methods to improve performance as a function of the length of the observed 289 learning curves, we introduce a standardized fidelity-slice evaluation protocol that demonstrates how a 290 method's top-k regret w.r.t. the true ranking changes as more and more fidelity information becomes available. 291 This way, we can observe the progression of an information-bounded expectation traded with the additional 292 cost incurred. In particular, this protocol computes the regret of s(D)'s prediction on the test set at a 293 gradually increasing amount of available fidelity slices; i.e. all algorithms are observed up to the same fidelity. 294

4.2 **Baselines**

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We consider several baselines to highlight different aspects of our setup and architecture ranging from simple 296 random rankings over classical AS to an extended version of successive halving. 297

Random Baseline. Consider a selector that randomly guesses the ranking. It will lead to a regret 298 distribution depending on (i) k in top-k (ii) the spread and clustering of learning curves on a single dataset. 299 indicating the hardness of the ranking task and (iii) the performance scale. This baseline averages the 300 obtainable regret of each dataset instance. It contextualizes the selectors' regrets across tasks.

Classical Algorithm Selection. While AS allows for generalization over dataset instances, its limitation 302 in ranking performance lies in the limited expressivity and relevance of the employed meta-features. Therefore, 303 we seek to demonstrate the benefit of partial learning curves as an addition to classical meta-features. For 304 that purpose, we compare against SatZilla'11 (Xu et al., 2012), a portfolio-based algorithm selector, which 305 models the AS problem as a multi-class classification problem and solves it using a cost-sensitive all-pairs decomposition to single label classification by employing one random forest classifier for each subproblem. 307 The final ranking is then obtained by voting. This selector is irrespective of fidelity and will produce a 308 constant value in the slice evaluation protocol. 309

Fidelity enabled Algorithm Selection. Classical AS only considers the dataset and algorithms' meta-310 features. Considering that our method's learning curve embedding could be conceived to be a latent 311 meta-feature ϕ_D , classical AS can conceptually similarly be enabled. To achieve that, the classical ϕ_D can be extended by m(D, A, f) for some intermediate fidelities f < F observed for all $A \in \mathcal{A}$. Given $f \in \mathcal{F}'$ with $\mathcal{F}' \subset \mathcal{F}$, this implies that $|\mathcal{A}| \cdot |\mathcal{F}'|$ columns are added to the feature space. Consequently, we limit $|\mathcal{F}'|$ to a subset of evenly spaced fidelities.³ In the slice evaluation protocol, the intermediate fidelities are added only 315 up until the horizon of the protocol.

Parametric Learning Curve Predictors. Neglecting any meta-knowledge and combating myopia through strong parametric assumptions, a naive learning curve predictor can interpret any partial information available. Such a predictor fits a parametric curve to each partial curve and extrapolates it to the final performance. The selector s independently extrapolates to the final performances and ranks the algorithms according to these. To create a meaningful and more expressive selector that mimics a practitioner's attempt at extrapolating learning curves for AS, we fit all parametric curves described in Mohr et al. (2022) and select the best fitting one on the observed part for extrapolation. This baseline highlights that learning curve predictors are used as algorithm selectors by practitioners when lacking meta-knowledge. Surpassing this baseline indicates that our method's expectation of the ranking can benefit from joined meta-knowledge about an algorithm's past progressions and related learning behaviors.

³In our experiment, this amounts to the fidelity sequence [0, 0.2, 0.4, 0.6, 0.8, 1].

IMFAS (Mohan et al., 2022) Implicit Multi-Fidelity Algorithm Selection (IMFAS) utilizes an LSTMbased architecture that initializes its hidden state using an MLP encoding of the dataset meta-features and auto-regressively accepts slices of fidelity to refine the expectation of the ranking.

Successive Halving (SH). Despite its simplicity, SH (Karnin et al., 2013; Jamieson & Talwalkar, 2016) has several desirable properties to compare against in terms of its interpretation of partial learning curves. It is a meta-agnostic and therefore myopic, fidelity-aware but non-parametric method. SH naturally produces a myopic ranking, by the level at which it terminates the algorithm. Ties within this set of terminated algorithms are resolved by their relative performances on that bracket. Limiting the fidelity information horizon of the selectors implies that for every such horizon, we need to recompute the ranking induced by SH. Notably, to permit SH the same information horizon, the last available fidelity in its schedule will be the maximum fidelity in that horizon. The benefit of this convention is that SH has access to the same fidelity information and can make better decisions for the algorithms it recommends. Its drawback of SH as a baseline is that the incurred cost differs from that of our method.

340 4.3 Datasets

Where possible, we utilize training, validation, and test learning curves for the training of all approaches. These are obtained by splitting each dataset in the corresponding benchmark in training, validation, and test data, training the corresponding algorithms on the training data under each fidelity, and computing their validation and test performance corresponding to the model trained for that fidelity. While the classical AS approaches only receive the final test performance on the meta-train datasets as training data, we provide (partial) validation curves to SH, the learning curve approaches, and MASIF to train on, but measure the final regret with respect to the full fidelity test performance. The same applies when the approaches are applied to new test datasets. We then assess the performance of each approach by performing a 10-fold outer cross-validation of the meta-dataset. We use three different benchmarks (more details in Appendix A.1):

- Synthetic. We constructed the Synthetic meta-dataset based on parametric learning curves taken from Mohr et al. (2022), specifically to demonstrate the myopia of SH and learning curve predictors. Particularly, it introduces noisy curves, that exhibit crossing points. We show how MASIF alleviates myopia through strong prior knowledge w.r.t. the functional family an algorithm is adhering to.
- Task-set. Task-set (Metz et al., 2020) is a fairly noisy real-world dataset based on parameterizations of the Adam optimizer (Kingma & Ba, 2015), with a variety of learning rates, run on a large variety of modern deep learning architectures and datasets.
- Scikit-CC18. With Scikit-CC18, we evaluated multiple well-known scikit-learn (Pedregosa et al., 2011) algorithms on the classification benchmark OpenML-CC18 (Bischl et al., 2021b). Since it is the only benchmark with available meta-features ϕ_D , we can evaluate SatZilla and IMFAS only on it.

These three benchmarks differ in their availability of dataset and algorithm meta-features: while Synthetic and Task-set exhibit neither, Scikit-CC18 exhibits both. We further investigated LCBench (Zimmer et al., 2021) as a similar benchmark to Task-set that provides qualitative similar results and is shown in Appendix A.2.

4.4 Results

Summarizing our results, depicted in Figure 3, on benchmarks Task-set and Synthetic, MASIF outperforms the other methods in terms of top-1 regret, and on Scikit-CC18 it performs competitively. Since our baselines applied in the slice-evaluation protocol on their own already reveal a few features of the meta-datasets we would like to detail their implications first. Afterwards, we discuss our experiments in light of the available meta-knowledge w.r.t. myopia and parametric assumptions.

Benchmark Difficulty. First of all, paying close attention to the random baseline and SH already indicates the difficulty of a benchmark; the random baseline can be thought of as an upper regret bound for any meaningful selector. If this threshold already incurs a small regret as in Scikit-CC18, this implies that

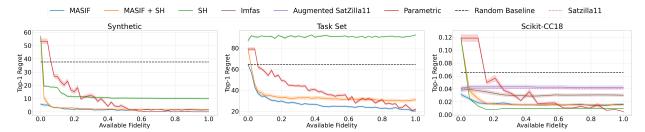


Figure 3: Average test-set top-1 regret over ten meta-dataset folds in the slice evaluation protocol. Available fidelity is expressed in share of the target fidelity's budget. The standard error bands originate from five repetitions for each of the ten folds. (right) exhibits dataset meta-features, while (left) and (mid) do not.

there is only little to gain, increasing the difficulty for a selector to improve. SH, on the other hand, pays close attention to the earlier parts of the curve. If this is already very indicative in terms of the final performance, only few crossings of the curves occur and thus decisions based on low-fidelity are good w.r.t. final performance. In this sense, Scikit-CC18 is an arguably easier meta-dataset than Task-set, as SH is close to oracle performance after a few fidelity slices in their top-3 regrets (compare with Figure A.3). SH's detrimental performance on Task-set on the other hand likely is due to the high variability and crossing of the curves, indicating the difficulty of this meta-dataset. The fact that no method obtains zero regret on Task-set at the final fidelity originates from the noisy target as indicated by the final fidelity of the parametric baseline. Moreover, parametric learning curve is (almost) guaranteed to yield oracle performance on Synthetic by construction.

The Role of Meta-knowledge. We highlight the fact that zero-fidelity corresponds to the classical AS setup and expresses the prior belief of a selector in the final performance based on the meta-knowledge. Baring this in mind, the fact that MASIF is almost constant and already top-performing on Synthetic indicates that the strong prior derived from meta-knowledge is already sufficient – which in the case of Synthetic is by construction. A decrease in regret indicates that the additional test-time fidelity information up to F_{max} refines this meta-knowledge-based belief and thus is indicative of the benefit of fidelity information.

The trajectory of parametric learning curve is a strong myopic baseline to demonstrate the effect of meta-knowledge, as more fidelity becomes available. SH similarly acts as a myopic baseline, but its schedule's path dependency may deny it to recover from early mistakes and hence result in sub-optimal states even when full fidelity is available. The steep decay in regret of MASIF at the beginning of its regret curves on Task-set and the minor adjustments on Scikit-CC18 demonstrate, that MASIF's prior can be improved based on incoming fidelity information, which corroborates that this intended property does indeed work in practice. Similarly, IMFAS (Mohan et al., 2022) exhibits, albeit far less pronounced, such a decay indicating that fidelity information also helps it. Its dependence on classical dataset meta-features as initialization and its autoregressive nature prevent it from excelling at fidelity information. This strong dependence on classical dataset meta-features also prevents it from being runnable on Synthetic and Task-set.

A direct comparison of MASIF with the parametric learning curve baseline on Synthetic and Task-set in terms of reduced variability and consistent superiority – already – in the early stages highlights the benefit of having meta-learned the algorithms' learning behaviour to combat myopia effectively. The SH Scheduler observed on Task-set supports this fact. When comparing SH against SH Scheduler on this noisy dataset it is apparent, that the gained meta-knowledge becomes the main driver of the regret curve. Notably, the SH Scheduler's curve appears inferior at first to MASIF's trajectory, until we factor in that MASIF follows the slice evaluation protocol very closely and the SH Scheduler has considerably less overall budget available due to the SH's budget allocation strategy. It also suffers from its path dependency, yielding slightly inferior results to MASIF, but at considerably less cost. This regret gap diminishes with lower benchmark difficulty in terms of accuracy of the meta-knowledge, as can be observed on Synthetic and Scikit-CC18, when strong prior beliefs facilitate making good decisions early on. This most prominently demonstrates the budget-regret trade-off a scheduler incurs. A comparison of Satzilla11 and our variants on Scikit-CC18 similarly highlights this trade-off; Satzilla11 incurs zero additional cost at test time over the computation of dataset meta-features

which are available to all three. Its prediction must fully rely on its prior, but MASIF can reduce Satzilla11's regret at a small additional cost during test time, having learned the algorithms' learning behaviors.

To our surprise, fidelity-enabled Satzilla11 performs similarly to that without fidelity information on Scikit-CC18. This fidelity-aware but non-parametric baseline ignores the naturally occurring sequential nature and fails to improve over its fidelity-agnostic variant. It remains unclear as to why this occurs in our experiments. We conjecture that it grossly overfits the meta-training data due to its sizable feature space.

As the ablation results in Appendix A.4 suggest, the usefulness of the raw dataset & algorithm meta-features in the two datasets is negligible at best. This has two implications: first, the meta-learned multi-fidelity information is the definite driver of our model and well outperforms the classical meta-feature-based approaches. A small caveat to the results of classical methods is their handcrafted nature. Considerable time investment into the generation and preprocessing of task-specific meta-features may yield improved regret performances for all models accepting dataset meta-features. This is why, despite the lack of strong evidence for its improvement, we keep the dataset- and algorithm meta-features as an optional part of our architecture.

5 Related Work

Classical AS approaches are based on the assumption that dataset instances (tasks) can be represented using 425 meta-features. They learn mappings between datasets and algorithms w.r.t. performance based on such 426 pre-computed meta-features. Most methods to learn such mappings in the literature either leverage regression 427 techniques (Xu et al., 2008; Bischl et al., 2016), ranking techniques (Cunha et al., 2018; Abdulrahman et al., 428 2018), collaborative filtering (Stern et al., 2010; Fusi et al., 2018), instance-based learning approaches (Amadini et al., 2014; Kadioglu et al., 2010) or mixtures of the aforementioned techniques (Hanselle et al., 2020; Fehring 430 et al., 2022). All of these approaches, however, suffer from the same limitation: Pre-computed meta-features, 431 as mentioned earlier, can have trouble sufficiently characterizing the datasets and algorithms due to the 432 alignment problem discussed in Section 2. Our approach circumvents the alignment issue by landmarking 433 datasets directly based on the candidate algorithms' inductive biases, as unrolled in their partial learning 434 curves, and predicts a rank over the set of candidate algorithms. 435

The idea of exploiting partial learning curves has previously been explored in some works. SAM (Leite & Brazdil, 2004) non-parametrically matched partial learning curves to the closest in terms of shape from the 437 observed meta-learning curves using kNN, while van Rijn et al. (2015) reduced the cost of cross-validation by exploiting the similarity of the partially-observed rankings with those of the meta-datasets and using the 439 most similar learning curve as surrogates. Mohr & van Rijn (2021) extended this approach by terminating 440 less promising candidates early on based on their predicted learning curves modelled in a semi-parametric 441 way under the assumption of concavity. In contrast to this explicit prediction of the missing parts of the learning curves, MASIF implicitly meta-learns correlations between the partial performances of algorithms to 443 predict a ranking. Leite & Brazdil (2010) pursue a cheaper and meta-informed alternative to cross-validation that evaluates the collection of fidelities using SAM, and then actively schedules them in a cost-aware manner. 445 Similarly, in hyperparameter optimization (Bischl et al., 2021a) the majority of approaches leverage learning 446 curves or ideas from multi-fidelity in one way or the other (Swersky et al., 2014; Li et al., 2018; Falkner et al., 447 2018; Awad et al., 2021). 448

Two approaches orthogonal to ours, although bearing some resemblances in terms of setup, are Meta-REVEAL (Nguyen et al., 2021) and MetaBu (Rakotoarison et al., 2021). Meta-REVEAL focuses on scheduling the 450 algorithms and fidelities through a Reinforcement Learning perspective by modelling it as a REVEAL game. 451 The agent acts on a discrete action space that does not account for the correlations between learning curves. 452 As we do not focus on scheduling but on learning cross-correlations on the learning behaviour, we refrain 453 from a comparison. Consequently, using the estimates produced by MASIF can provide a pre-processed 454 action space for their problem. MetaBu extends the classical AS idea by relating dataset meta-features 455 and algorithms' hyperparameters using a learned optimal transport map. They, however, ignore that the 456 dataset meta-features cannot sufficiently characterize the dataset, thus, subsequently falling victim to the 457 same fallacies as the methods mentioned before.

The approach that comes closest to ours in terms of its setting is the Multi-LCNet (Jawed et al., 2021). While they use a related $\Omega^{meta-train}$ and $\Omega^{meta-test}$ data setup, the work has substantial differences and rigid assumptions, which make us abstain from an experimental comparison of MASIF to it, as a fair comparison is not possible. The core differences are threefold; 1. they consider a hyperparameter optimization multi-fidelity problem 2. their model can assume the existence of auxiliary curves for a single algorithm, because of the narrow definition of an algorithm and 3. they use this multi-modal data in an autoregressive way for the explicit extrapolation of a single curve at a time. A more detailed discussion is deferred to Appendix A.5.

466 6 Conclusion

In this work, we revisited classical meta-learning- and learning curve-based approaches to AS from the 467 perspective of a trade-off between the budget they invest in inquiring information about a new dataset and the corresponding regret of choosing an inferior algorithm. Doing so, we argued that both of these selector classes 469 are on opposite ends of the spectrum in this trade-off and both suffer from severe limitations, likely leaving data scientists with an inferior selected algorithm. To alleviate this, we present MASIF, an algorithm selector 471 designed to support data scientists in the selection process in a far more native manner, whose position in the spectrum can be controlled by the data scientist depending on their budgetary constraints. MASIF leverages 473 a transformer-encoder-based architecture to model the performance of algorithms across both, fidelities and 474 algorithms in the form of learning curves of varying lengths. As such, it alleviates the myopia of many 475 existing learning curve-based approaches while making no parametric assumptions on the learning curves it 476 can model. Crucially, our selector utilizes computation from previous selections as meta-knowledge. In an 477 extensive experimental study on four different benchmarks, we showed that MASIF outperforms existing 478 meta-learning-based approaches in terms of the regret of the selected algorithm and learning curve-based 479 algorithm selectors in terms of regret for the invested budget. As such, MASIF is not only an AS approach 480 designed to support the data scientist in practice by leaving the concrete instantiation of the trade-off to 481 their preference but also yields state-of-the-art AS performance. 482

7 Future Work

The aforementioned budget-regret trade-off leads to a multi-objective view of the AS problem, where both 484 the budget invested and the regret of the corresponding algorithm selector are rivaling objectives. This holistic view naturally suggests tackling the problem with multi-objective methods to be able to present a 486 Pareto front of selectors to choose from, suited to a data scientist's budget-regret preferences in the face of uncertainty. This line of work is orthogonal to previous multi-objective work in Algorithm Selection 488 (Bossek & Trautmann, 2018). Any instance on this Pareto front is a scheduler of sorts. Determining how a scheduler knowledgeable in learning behaviors should choose its budget allocation sequentially and in the 490 face of uncertainty inspires research on its own. Lastly, in the current form of this work, the algorithms are 491 predominantly represented through their learning curves and we use algorithm meta-features in a relatively 492 limited manner. Multi-LCNet (Jawed et al., 2021) presumes that using hyperparameters among other 493 informative algorithm meta-features may also be beneficial in contextualizing a learning curve. In that sense, 494 a natural extension to the scope of this work is the transition from tackling the AS problem to tackling the 495 hyperparameter optimization problem. In contrast to existing approaches, we will seek to extract the joint 496 topology evidence derived from the observed partial learning curves in order to tackle this problem. 497

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653 A Appendix

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A.1 Meta-Datasets

Synthetic To make the task even more challenging, we add random noises to the generated curves. A snapshot of the synthetic curve meta-dataset can be found under Figure 4. To demonstrate that MASIF is a non-myopic approach, we create a synthetic function meta-dataset. To break the myopic algorithms, we force the curves in one dataset to intersect at least another curve in an incrementally way. We initialize by randomly picking a parametric curve. Subsequent curves are generated by first sampling a parametric family as described by Mohr et al. (2022) and then computing its parametrization such that it is ensured to intersect with its predecessor. In more detail, we want to ensure that the intersections

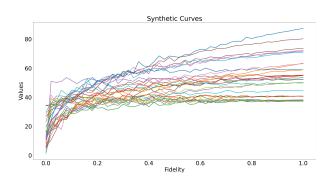


Figure 4: A snapshot of a Synthetic dataset

occur at different stages of the training procedure. This is obtained by randomly selecting one of a few preset intervals in which the intersection is supposed to take place. Repeating this process for $|\mathcal{A}| - 1$ times produces a single dataset. To obtain strong meta-knowledge across datasets originating from the shape of an algorithm's curve, a new dataset is generated by perturbing the parametrization of the existing curves. Therefore, these datasets contain similar but non-identical curves, that yield variability in the final ranking. This dataset does not provide dataset meta-features. Overall, we collect 22 datasets each containing 30 learning curves with 51 fidelities.

Task-set Task-set (Metz et al., 2020) is a meta-dataset that consists of over a thousand tasks ranging from image classification with fully connected or convolutional neural networks to variational autoencoders on a variety of datasets. Each task is characterized by 1. an initialization function 2. data split 3. loss function 4. gradients

On these tasks, the training, validation, and test curves of multiple optimizer settings have been recorded. For our experiments, we sub-sample the tasks that consist of curves generated from fully-connected networks run

on image recognition tasks. Additionally, we sample the set of algorithms to be the different configurations of the Adam optimizer (Kingma & Ba, 2015) with only the learning rate varying. This allows us to create a meta-dataset of 1000 configurations on 100 tasks. This meta-dataset does not provide dataset meta-features. The rationale is that given the noise in the curves sampled from realistic tasks, the performance on initial fidelities is not indicative of the final ranks, making it hard for methods like Successive Halving to get a good regret value without any form of meta-knowledge.

Scikit-CC18 OpenML-CC18 (Bischl et al., 2021b) is a curated classification benchmark featuring 72 carefully selected datasets from OpenML (Vanschoren et al., 2014) with a variety of desirable properties for a benchmark (see (Bischl et al., 2021b) for details). We generated learning curves on these datasets for 16 classifiers from Scikit-learn (Pedregosa et al., 2011), namely (i) ExtraTreeClassifier (ii) DecisionTreeClassifier (iii) MLPClassifier (iv) KNeighborsClassifier (v) SGDClassifier (vi) RidgeClassifier (vii) PassiveAggressiveClassifier (viii) GradientBoostingClassifier (ix) ExtraTreesClassifier (x) BernoulliNB (xi) LinearSVC (xii) LogisticRegression (xiii) MultinomialNB (xiv) NearestCentroid (xv) Perceptron (xvi) SVC.

We collect their learning curves performing the following procedure for every dataset and learner pair: We performed three-fold cross-validation and for each of these folds again split 20% off of the training data as validation data. We then trained the classifier on $5\%, 10\%, \ldots, 100\%$ of the training data and evaluated it on the train, test, and validation data using accuracy as a loss function. As preprocessing, we imputed missing feature values with the most frequent one in the training data and one-hot encoded categorical features. Correspondingly, the budgeted resource is the dataset subset size for this meta-dataset. This dataset provides dataset meta-features.

A.2 Results on LCBench

LCBench (Zimmer et al., 2021) is a meta-dataset, that consists of 2000 hyperparameter configurations of a funnel-shaped neural net on 35 datasets. To meet the AS setup, we choose a subset of size 170 of these configurations using a Latin Hypercube design. Presuming, that hyperparameters change the inductive bias of a model, we conceive for the purpose of our analysis these configurations as independent algorithms. Notably because of this, the hyperparameter optimization usually resorts to assuming similarity of performance w.r.t. hyperparameters. By extension, we expect that we can assume some similarity in the learning behaviors encoded in their learning curves, that MASIF should be able to exploit. This meta-dataset provides dataset meta-features.

Inspired by Multi-LCNet, which uses LCBench as its sole benchmark, we also computed our experiments on LCBench. The results of these experiments are depicted in Figure 5. Overall on top-1 the results follow those tendencies described in Section 4.4. Considering the wide and overlapping confidence bounds centred around the already very small regret of 0.02 and the fact that all of the meta-aware selectors do not require additional fidelity information to adjust their prior suggests, that LCBench is not a strong Benchmark for this new data setup. This is strongly supported by the relatively steep regret-decay and strong final performances of SH and the parametric learning curve baseline. An interesting observation here lies in IMFAS's slightly deteriorating performance. We attribute this behaviour to its autoregressive interpretation of the learning curves.

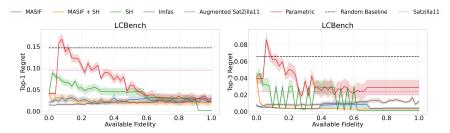


Figure 5: Average test-set top-1 (left) and top-3 (right) regret over ten meta-dataset folds in the slice evaluation protocol for LCBench. Available fidelity is expressed in the share of the target fidelity's budget. The standard deviation originates from five repetitions for each fold.

9 A.3 Top-3 results

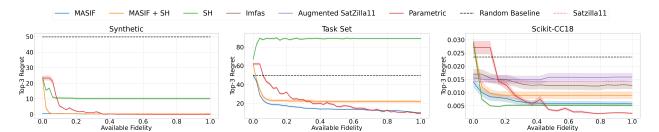


Figure 6: Average test-set top-3 regret over ten meta-dataset folds in the slice evaluation protocol. Available fidelity is expressed in the share of the target fidelity's budget. The standard deviation originates from five repetitions for each fold. Scikit-CC18 exhibits dataset meta-features, while Synthetic and Task-set do not.

As increasing k in top-k is a hedge, the overall regret is reduced compared to those results of top-1, because it is more likely to pick the best performer in this enlarged set. The overall tendencies in Figure 6 are however exactly the same as described in Section 4.4

723 A.4 Ablations

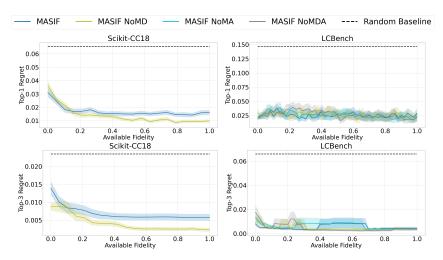


Figure 7: Ablation of MASIF w.r.t. whether or not meta-features are available on Scikit-CC18 (Left) and LCBench (Right) benchmarks. 'NoM' indicates that the subsequently detailed meta-feature information is hidden to the model. In particular, 'D' stands for dataset meta-features, 'A' for algorithm meta-features.

The results in Figure 7 indicate that the regret difference in whether or not the meta-features are present have – if any – only negligible effect for the Scikit-CC18 and LCBench dataset, once the scale of this difference is considered. On the other hand, the results in Figure 8 detail, the regret gap, when using a secondary transformer over the sequence of algorithms rather than an MLP, supporting our design choice for the former. The vector representation of the learning curves as output to the first transformer holds positional information since an algorithm is presented always in the same order irrespective of the dataset. The secondary transformer picks up on this positional information more easily than an MLP.

A.5 Discussion on Multi-LCNet

As it is conceptually the closest to our model, we will discuss the differences summarized in 5 more thoroughly. First, their method considers hyperparameters, which allows exploiting the similarities in that space to interpolate between algorithms - which eases our assumption of a discrete and rigidly observed \mathcal{A} in the meta-training set and therefore is rather hyperparameter optimization than AS. Second, they leverage

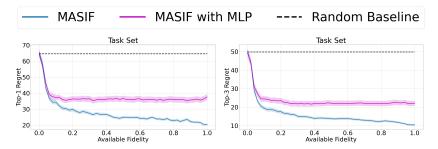


Figure 8: Ablation of MASIF on Task-set benchmark, switching out the second transformer for a simple MLP on the reduced output as joint interpretation module.

multi-modal data; i.e. multiple auxiliary curves such as e.g. the layer's gradient information are tracked during training. These curves are only accessible for all configurations, because they limit themselves to a single class of algorithms, in their case funnel-shaped neural nets. These secondary curves are not necessarily available for all candidate algorithms considered in an AS model and as such, the method cannot be applied in our setting. Besides, considering SH's almost oracle performance on LCBench in Appendix 5 with a sizeable subset of 170 algorithm configurations in our experiments, the multi-modal nature of their analysis may not be a driver for their performance on this particular dataset. Third, their focus is on explicitly extrapolating single learning curves at a higher fidelity in an auto-regressive manner based on the meta-learned weights of their Gated Recurrent Units (Cho et al., 2014) that only combine the information from the partial learning curves of the same algorithm observed from multiple modes of data. Instead, our method leverages the joint evidence of all invested computations in addition to the meta-knowledge and avoids explicit extrapolation. Fourth, their handcrafted loss metric is intended at fostering good predictions early on, which, despite working with rather small budgets, might yield suboptimal decisions. Similarly to the SH baseline, this seems to express and favour a particular budgetary preference over the resulting regret. In contrast, as mentioned several times, MASIF is much more flexible regarding the budget-regret trade-off.

A.6 Reproducibility Statement

- Where can the code be found? MASIF's code is published on https://anonymous.4open.science/status/MASIF-824D
- What hardware did we use for the experiments? All the experiments are executed on 4 Intel Xeon E5 cores with 8000MB RAM.
- What hyperparameter settings did we use? How did we get to those? Where can they be found? Using Hydra (hydra.cc) as base package for all our experiment pipelines including the preprocessing of dataset & algorithm meta-features as well as those for the learning curves, all of the configurations detailing the used models and their configurations can be found in the "configs" folder in the linked repository.
- What are the requirements in terms of packages and version numbers? The packages & version numbers are available in the setups file of the linked repository.
- Where can you download our benchmark datasets? We added the newly created Scikit-CC18 benchmark as supplementary material. LCBench can be downloaded from https://github.com/automl/LCBench. Task-set can be obtained from https://github.com/google-research/google-research/tree/master/task_set. We provide the Synthetic and Scikit-CC18 benchmarks as supplementary.
- How many seeds/splits etc. did we perform? We used five seeds and ten folds for each benchmark. A crucial detail regarding the split in the algorithms' learning curves is described in the dataset section.