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Meta-Learning from Learning Curves for Budget-Limited Algorithm Selection

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Abstract

Training a large set of machine learning algorithms to convergence in order to select the best-performing algorithm for a dataset is computationally wasteful. Moreover, in a budget-limited scenario, it is crucial to carefully select an algorithm candidate and allocate a budget for training it, ensuring that the limited budget is optimally distributed to favor the most promising candidates. Casting this problem as a Markov Decision Process, we propose a novel framework in which an agent must select in the process of learning the most promising algorithm without waiting until it is fully trained. At each time step, given an observation of partial learning curves of algorithms, the agent must decide whether to allocate resources to further train the most promising algorithm (exploitation), to wake up another algorithm previously put to sleep, or to start training a new algorithm (exploration). In addition, our framework allows the agent to metalearn from learning curves on past datasets along with dataset meta-features and algorithm hyperparameters. By incorporating meta-learning, we aim to avoid myopic decisions based solely on premature learning curves on the dataset at hand. We introduce two benchmarks of learning curves that served in international competitions at WCCI'22 and AutoMLconf'22, of which we analyze the results. Our findings

show that both meta-learning and the progression of learning curves enhance the algorithm selection process, as evidenced by methods of winning teams and our DDQN baseline, compared to heuristic baselines or a random search. Interestingly, our cost-effective baseline, which selects the best-performing algorithm w.r.t. a small budget, can perform decently when learning curves do not intersect frequently.

Keywords: algorithm selection, meta-learning, learning curves, reinforcement learning, REVEAL games, challenge

1 Introduction

In a typical Machine Learning (ML) task, given a dataset, one is asked to build a model for the dataset w.r.t. an objective (e.g., classification). The model is often defined as the output of training an ML algorithm (e.g., neural network weights) on the dataset, capturing the learned data distribution. However, selecting the best-suited algorithm for a particular dataset is challenging, especially for non-experts with limited ML knowledge. This *algorithm selection* problem becomes even more challenging in a *budget-limited* scenario, where evaluating a large set of algorithms becomes costly if each of them must be trained or optimized to convergence. As a consequence, a common practice in the ML community is early stopping or discarding unpromising algorithms

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based on their *learning curves* during training [[14]]. A learning curve evaluates an algorithm's incremental performance improvement, as a function of time, number of epochs, or number of training examples. Learning how to effectively leverage such information to boost algorithm selection is the focus of this paper.

In the literature, a common approach is to invest time in collecting premature learning curves of algorithm candidates and extrapolate them to select the most promising algorithm [[7, 14, 21, 15]]. Notably, several existing works use neural networks for this purpose. For example, [10] use Bayesian neural networks for modeling and predicting learning curves, while [3] use prior-data fitted networks trained to extrapolate artificial right-censored learning curves generated from a parametric prior. However, these approaches often require Parametric Learning Curve Models and some of them rely on the assumption of learning curve concavity. Moreover, they suffer from myopia due to extrapolations based solely on partially observed curves without considering metaknowledge.

Meta-learning can be incorporated to address these Meta-learning has shown great potential issues. in learning from previous tasks to solve new ones more efficiently [[29, 30]]. In scenarios where metaknowledge, such as features of datasets or past performances of algorithms, is available, meta-learning can help improve the algorithm selection process [[4, 6, 8]]. For instance, [2] uses meta-level information acquired in past experiments to construct an average ranking of algorithms and apply active testing. [28] exploit the similarity of the partiallyobserved rankings, and use the most similar learning curve as surrogates. [31] propose a method that learns to rank learning curves by optimizing a pairwise ranking loss. More recent works use LSTM networks and transformer-based models to learn embeddings of dataset meta-features and algorithm candidates' learning behavior observed on other datasets [13, 20]]. However, these works often require a complex learning pipeline and do not specifically target budget-limited scenarios.

In this work, we seek to address the budget-limited algorithm selection problem from a different perspective. We frame this problem as a special type of Markov Decision Process, paving the way for Reinforcement Learning methods. In this setting, an agent actively requests to train and test algorithms to reveal their performances on a given dataset, which implies an "active meta-learning" setting. The agent should interrupt the training of less promising algorithms based on partial learning curves, rather than waiting until all algorithm candidates are fully trained to evaluate. This idea is inspired by the concept of "freezing" and "thawing" algorithms proposed by [25]. Our framework allows meta-learning to improve the algorithm selection process. We focus on First-level meta-learning, which involves algorithm evaluations (i.e., learning curves), dataset meta-features, and/or algorithm hyperparameters; in the same line of work by [[16, 23, 24]]. The meta-trained agent should balance two aspects: (1)exploration-exploitation trade-offs between continuing to train an already tried good candidate and trying a new candidate; and (2) *multi-fidelity* trade-offs between querying high-fidelity data with higher cost and low-fidelity data with lower cost.

We summarize our contributions in this work as follows:

- (i) We formulate the limited-budget algorithm selection problem using Markov Decision Processes (MDP). Our framework neither requires explicit extrapolation of learning curves nor does it necessitate parametric and concavity assumptions. (Section 2)
- (ii) We discuss our challenge series design, including the novel benchmark datasets we created and used in the challenges. We present the challenge results compared to several baseline methods instantiated from our framework. (Section 3)
- (iii) We perform a comprehensive result analysis with a comparison of data usage and policy types of methods (Section 3.3.1). To see the benefits of meta-learning and learning from learning curves, we conduct an ablation study for a specific baseline method (Section 4.2). We examine in-depth the strategies learned by the winning methods, comparing them with



Figure 1: **Our problem setup**. Given a dataset, an agent (meta-learner) \mathcal{M} takes an action to start or continue training an algorithm using a budget, based on an observation containing partially revealed training and validation learning curves. The corresponding test learning curves are kept hidden and used for computing a reward to be returned to the agent. This interaction is repeated until the given total budget is exhausted.

the baselines and offering diverse effective approaches. (Section 4.3)

Code for reproducing the challenge results, as well as the analysis results presented in this paper, is publicly available in our repositories. $^{1-2}$.

2 Problem Setup

We formally describe the budget-limited algorithm selection problem. Let \mathcal{D} represent a set of datasets, and Ω denote a set of algorithms of interest. Given a dataset $d_i \in \mathcal{D}$, the goal is to identify the bestperforming algorithm $\omega_{j^*} \in \Omega$ for d_i . During the selection process, a computational resource budget \mathcal{T}_i is provided for training and evaluating algorithms on dataset d_i . We are interested in learning a selection policy π that efficiently utilizes budget \mathcal{T}_i to find the best-performing algorithm for any given dataset in \mathcal{D} .

We formulate this problem as a Markov Decision Process (MDP) and define its components as follows. In an episode, a dataset d_i is given. At time step t, a state s_t contains current information about learning curves of algorithms in Ω , on the training set d_i^{train} and validation set d_i^{val} , denoted by $\mathcal{L}_{ij}^{train}(\tau_j)$ and $\mathcal{L}_{ij}^{val}(\tau_j)$, respectively. Here, a learning curve is a function of cost τ_j ($0 \leq \tau_j \leq \mathcal{T}_i$), which returns the performance of algorithm ω_i on dataset d_i after spending τ_j for training and evaluation, w.r.t. a certain metric (e.g., classification accuracy). The cost τ_i can be time spent, the percentage of training data used, etc. Thus, the learning curve of algorithm ω_i is only partially revealed up until τ_i . The state s_t also contains meta-features of dataset d_i and hyperparameters of algorithms in Ω . An agent \mathcal{M} observes state s_t and takes an action $a_t = (\omega_i, \Delta_i, \widehat{\omega_{i^*}})$. In this tuple, ω_i is an algorithm to be continually trained and evaluated using a budget increment Δ_i (hence, we update $\tau_j = \tau_j + \Delta_j$), and $\widehat{\omega_{j^*}}$ is the predicted best performing algorithm on the test set d_i^{test} given observations. Once action a_t is executed, learning curves $\mathcal{L}_{ij}^{train}(\tau_j)$ and $\mathcal{L}_{ij}^{val}(\tau_j)$ are updated and revealed to the agent in the next time step. In contrast, learning curves on the test set $\mathcal{L}_{ij}^{test}(\tau_{j^*})$ are kept hidden from the agent and used for computing a reward r_t . Concretely, r_t is defined as the improvement on the test set, weighted by the normalized remaining budget:

$$r_{t} = \left[\mathcal{L}_{ij_{t}^{*}}^{test}(\tau_{j_{t}^{*}}) - \mathcal{L}_{ij_{t-1}^{*}}^{test}(\tau_{j_{t-1}^{*}}) \right] \left[1 - \tilde{t} \right]$$
(1)

with the normalized time:

$$\tilde{t} = \frac{\log(1 + \sum_{j=1}^{|\Omega|} \tau_j / \sigma)}{\log(1 + \mathcal{T}_i / \sigma)}$$
(2)

where $\sum_{j=1}^{|\Omega|} \tau_j$ denotes the total budget spent up to time step t. The hyperparameter σ controls the emphasis on performance importance at the beginning of the episode. The goal is to encourage the agent \mathcal{M} to discover good algorithms as quickly as possible. In this way, even if the agent is stopped early, we will get as good performance as possible. This is known as

 $[\]label{eq:linear} \ensuremath{^1https://github.com/LishengSun/metaLC-post-challenge-analysis-1st-round$

 $^{^{2}} https://github.com/LishengSun/metaLC-post-challenge-analysis-2n-round$

an "Any-time Learning" setting. An episode is terminated when the total budget \mathcal{T}_i is exhausted. By integrating the learning curve using horizontal rectangles, in the style of Lebesgue integrals, the accumulated reward during the episode is equal to the area under the learning curve (ALC) of the agent. Figure 1 illustrates our problem setup.

The proposed MDP framework was tested as follows. During the meta-training phase, participants could employ any learning method using all available resources, including training, validation, and test learning curves, as well as meta-features for all meta-training datasets, to develop the agent's policy. This policy determines the probability of taking specific actions under certain circumstances. In the meta-testing phase, the agent, using the developed policy, interacts with the environment. The environment provides a new dataset from the meta-test datasets along with observations containing partially revealed training and validation learning curves based on the agent's actions. The corresponding test learning curves remain hidden within the environment and are used solely to compute the reward returned to the agent, contributing to the calculation of the agent's final ALC score.

In this MDP, the agent's action does not influence how underlying states and rewards are generated, which distinguishes it from a standard MDP. Consequently, both states and rewards can be precomputed at the beginning of an episode. Thus, the problem becomes a REVEAL game, a special MDP discussed in prior works by [23] and [16].

3 MetaLC Challenge

We investigated the potentials of meta-learning from learning curves for improving budget-limited algorithm selection, by creating a series of challenges, namely, *MetaLC*. The main objective of these challenges was to train an agent \mathcal{M} (also referred to as a meta-learner) that is capable of meta-learning from learning curves on other datasets and efficiently identify the best-performing algorithm for a new dataset within a limited budget. The challenge series comprised two rounds.

3.1 Benchmark meta-datasets

At the time of organizing this challenge, there were limited meta-datasets of learning curves available in the machine learning (ML) community, despite their widespread use. To facilitate benchmarking, we created a new meta-dataset comprising learning curves of Automated Machine Learning (AutoML) algorithms on 30 cross-domain AutoML datasets provided by [9]. The application domains of these datasets include medical diagnosis, text classification, customer satisfaction prediction, speech recognition, object recognition. The datasets have been preprocessed into suitable fixed-length vectorial representations.

We created a set of algorithms by modifying an AutoML baseline provided in the AutoML challenge by [9], and varying its hyperparameters.³ Concretely, we changed only the core algorithm of the AutoML method and kept the rest of its components unchanged. In round 1, we used tree-based algorithms (Random Forest, Gradient Boosting) as the core algorithm. To compute a learning curve, we incrementally increased the number of estimators and repeated evaluation. In round 2, we used Nearest Neighbors, Multilayer Perceptron, Adaboost, and Stochastic Gradient Descent algorithms; we computed a learning curve by increasing the training data size (i.e., from 10%, 20%, ..., 100%). In the first round, we had a total of 600 learning curves (20 algorithms \times 30 datasets). In the second round, we had 1200 learning curves (40 algorithms \times 30 datasets). In both rounds, meta-features of datasets and hyperparameters of algorithms were also provided. A starter kit with a synthetic meta-dataset created by [17, 18], was given to participants for practice.

3.2 Evaluation protocol

Participants were asked to develop an agent \mathcal{M} and submit it to be executed on our Codalab competition websites.⁴⁵. Each round had two phases: meta-training and meta-testing. We split \mathcal{D} into

 $^{^3 \}rm https://github.com/ch-imad/AutoMl_Challenge/blob/master/Starting_kit <math display="inline">^4 1 \rm st$ round: https://codalab.lisn.upsaclay.fr/competitions/753

 $^{^52\}mathrm{nd}$ round: https://codalab.lisn.upsaclay.fr/competitions/4894

Table 1: Data usage and policy type of the top-3 teams in each round vs. five baselines. The \checkmark symbol corresponds to the method that meta-learned from learning curves in meta-training, represented by a blue bar in Figure 2. A *combined* policy refers to a combination of learned and hard-coded policies.

	Data usage						Policy type	
	in meta-training			in meta-testing				
	learning curve progression	dataset meta features	algorithm hyperparameters	learning curve progression	dataset meta features	algorithm hyperparameters	algorithm selection	budget allocation
Team MoRiHa	\checkmark	1		1	1		combined	combined
Team neptune	\checkmark	1	✓		1	1	combined	combined
Team Alpert	\checkmark	1			1		combined	combined
Team dragon_bra	 Image: A set of the set of the	1			1		combined	hard-coded
Team diaprofesser	\checkmark	1			1		combined	combined
Team carml	\checkmark	1	✓	1	1	1	combined	hard-coded
DDQN [[27]]	 Image: A second s			1			learned	hard-coded
AvgRank [[16]]							combined	hard-coded
Freeze-Thaw [[25]]				1		1	hard-coded	hard-coded
BoS [[16]]				1			hard-coded	hard-coded
RANDSEARCH							hard-coded	hard-coded

 $\mathcal{D}^{meta-train}$ and $\mathcal{D}^{meta-test}$, and use learning curves of algorithms in these sets for meta-training and meta-testing agent \mathcal{M} , respectively. In metatraining, participants were allowed to use any kind of learning on provided data. In meta-testing, the agent \mathcal{M} was evaluated by interacting with an environment as described in Section 2 and illustrated in Figure 1. The ranking of the agent on the leaderboard was determined by the average accumulated reward over datasets in $\mathcal{D}^{meta-test}$.

3.3 Baseline methods

In this section, we introduce our five baseline methods. These are methods we instantiated following our proposed framework and leveraging techniques from existing work to serve as baselines. We then compare these baselines with the methods submitted by participants in the challenges to assess whether any improvements over the baselines were achieved. Each baseline method represents a distinct solution within the proposed framework, developing its own policies for algorithm selection and budget allocation.

Double Deep Q-Network (DDQN). As the challenge is inspired by RL, we wanted to evaluate the meta-learning capabilities of RL methods. We started with DDQN, a classic RL method proposed by [27]. We used the data given in the

meta-training phase to create an RL environment for training (same setup discussed in Section 2). The agent learned a policy $\pi_{\theta,\theta'}$ with two networks, one for action selection parameterized by θ , the other for value estimation parameterized by θ' . The parameters were updated by minimizing the following loss using trajectories sampled from a replay buffer \mathbb{B} : $\theta, \theta' = \operatorname{argmin}_{\theta, \theta'} \mathbb{E}_{(s_t, a_t, r_t, s_{t+1}) \sim \mathbb{B}}[(y_t - y_t)]$ $Q(s_t, a_t; \theta))^2$ with learning target y_t defined by: $y_t = r_t + \gamma Q(s_{t+1}, \operatorname{argmax}_a Q(s_{t+1}, a; \theta); \theta')$. We used this learned policy only for choosing algorithm ω_i in the action triplet $(\omega_j, \Delta_j, \widehat{\omega_{j^*}})$, i.e. $\pi_{\theta, \theta'}(s_t) =$ ω_i . The algorithm with the highest performance revealed on the validation set so far was selected as the predicted best-performing algorithm $\widehat{\omega_{i^*}}$ with $j^* = \operatorname{argmax}_j \mathcal{L}_{ij}^{val}(\tau_j)$. For budget allocation, it used a fixed policy that starts with a pre-defined small budget and doubles the amount of budget spent for an algorithm ω_i every time it resumes training: $\tau_i = 2 * \tau_i.$

Freeze-Thaw. We considered the problem as a hyperparameter search, as our dataset of algorithms was created by varying their hyperparameters (see Section 3.1). We used the Freeze-Thaw Bayesian Optimization (FREEZE-THAW) method proposed by [25], which was adapted to become one of the winning solutions in the AutoML challenge [[9]]. It used the partial learning curve information in a Bayesian

Optimization fashion to decide which algorithm to "freeze" or "thaw" training it. Concretely, it selected algorithm ω_j that maximizes an acquisition function, i.e. $j = \operatorname{argmax}_j f_{acq}(j)$. It used an entropy search acquisition function that maximizes the expected information gain over the location of the performance maximum: $f_{acq}(j) = \int (H(P_{max}^y) - H(P_{max}))P(y|\{(j^n, y^n)\}_{n=1}^N)dy$. Here, P_{max} represents the current estimated distribution over the performance maximum, and P_{max}^y is the updated distribution given that point j yields the performance y. Nis the number of observations. Similar to DDQN, $\widehat{\omega_{j^*}}$ was set by $j^* = \operatorname{argmax}_j \mathcal{L}_{ij}^{val}(\tau_j)$. We used a fixed budget increment Δ_j in each time step. We note that FREEZE-THAW does not have a meta-learning capability.

AvgRank Inspired by existing works [[1, 5, 11, 12]], this AVGRANK baseline meta-learned an average ranking of algorithms Ω on $\mathcal{D}^{meta-train}$ during the meta-training phase. In meta-testing, only the algorithm ω_j that ranked highest was chosen to be trained and evaluated using the entire given budget $\Delta_j = \mathcal{T}_i$. The average rank of algorithm ω_j was defined as: $avg_rank(\omega_j) = [\sum_{d_i \in \mathcal{D}^{meta-train}} rank(\omega_j, d_i)] / |\mathcal{D}^{meta-train}|$. Since this baseline trained only one algorithm, hence, $\widehat{\omega_{j^*}} = \omega_j$. In a real-life scenario, this is an expensive baseline, as it requires training and testing the entire set of algorithms on all meta-training datasets to have an accurate ranking.

BestOnSamples (BoS). This baseline, inspired by the work of [19], selected the algorithm that performed best within a fixed small budget α . More specifically, at the beginning of each episode, it trained every algorithm with the same budget $\Delta_j = \alpha$. Based on the observed results, it selected algorithm ω_j that achieved the highest performance with $j = \operatorname{argmax}_j \mathcal{L}_{ij}^{val}(\alpha)$, and spent the entire remaining budget (now, $\Delta_j = \mathcal{T}_i - \alpha * |\Omega|$). Again, the predicted best-performing algorithm $\widehat{\omega_{j^*}}$ was set by $j^* = \operatorname{argmax}_j \mathcal{L}_{ij}^{val}(\tau_j)$. This baseline does not have a meta-learning capability.

RandSearch. This simple baseline performs a random search over the given algorithm set Ω . It uniformly sampled an algorithm $\omega_j \sim \mathcal{U}(\Omega)$ and uniformly assigned an amount of budget for training

and evaluating the algorithm, $\Delta_j \sim \mathcal{U}(\Delta_{min}, \Delta_{max})$. Again, $\widehat{\omega_{j^*}}$ is set by $j^* = \operatorname{argmax}_j \mathcal{L}_{ij}^{val}(\tau_j)$. Due to its high variance, we ran this baseline five times internally and reported its average performance. This baseline was implemented solely for comparison purposes and is not realistic, as one would not average several runs of an algorithm in practice.

3.3.1 Results

Table 1 provides a summary of winning teams' methods and baselines. We found that learning curves and dataset meta-features were more frequently utilized than algorithm hyperparameters. In each round, only one team made use of partially revealed learning curves during meta-testing. Surprisingly, only a few participants employed RL to train their agents, despite the challenge setting being designed as an RL problem. Figure 2 presents the challenge results, showing the average accumulated reward of each method over meta-test datasets for both the "Any-time learning" and "Fixed-time learning" settings. In the "Fixed-time learning" setting, the accumulated reward is equivalent to the highest performance found during an episode, regardless of when it is found.

In the first round at WCCI 2022, the top-3 teams outperformed the best baseline DDQN in the Anytime learning setting; while in the Fixed-time learning setting, DDQN slightly surpassed the thirdranked team. These teams used a combination of learned and hard-coded policies for algorithm selection and budget allocation (Table 1). Only team "MoRiHa", which ranked first, utilized partially revealed learning curves during meta-testing and achieved the highest ALC score on 21/30 datasets. Notably, they performed better than other teams in some multi-label and multi-class classification tasks, such as *tania*, *robert*, *newsgroups*, and *marco*. One of their key findings was that switching the explored algorithm more than once is rarely beneficial due to the high cost associated.

In the second round at *AutoML-Conf 2022*, among the top-3 teams, only one team ("dragon_bra") beat DDQN in Any-time learning, while two teams ("dragon_bra" and "diaprofesser") outper-



(a) 1st Round - Any-time (b) 1st Round - Fixed-time (c) 2nd Round - Any-time (d) 2nd Round - Fixed-time Learning Learning Learning Learning

Figure 2: MetaLC challenge results. Comparison of top-3 teams and five baselines. Blue bars represent methods that meta-learned from learning curves in meta-training (corresponds to \checkmark in the first column of Table 1). We highlight RANDSEARCH in plain gray, a special baseline with internally averaged performance over several runs. Results for fixed-time learning are included for analysis purposes only and were not officially used in our challenges. The reported results are from the worst run out of three runs with different seeds, and the error bar indicates the standard deviation across meta-test datasets.

formed DDQN in Fixed-time learning. All winners meta-learned from learning curves in metatraining. A combined policy for algorithm selection was used by all winners, while 2/3 winners used hardcoded rules for distributing the given budget. Team "dragon_bra" obtained the highest average ALC by winning in 6/15 datasets. They had two key findings: (i) At the beginning of an episode, the agent should spend only a small budget to grab a "base score", which would make the area under the agent's learning curve larger; and (ii) if a small budget is used near the end of an episode, it is unlikely that substantial improvement will be made.

4 Discussions

Our series of challenges was the first of its kind in the ML community when we introduced it. We delve into important considerations during benchmark creation and challenge design, along with notable observations and investigations.

4.1 Challenge design

Learning Curve. Our benchmark meta-datasets contained pre-recorded learning curves to avoid any on-the-fly computational issues during the challenges. In ML community, there are various types of learning curves, such as Iteration Learning Curve, and Observation Learning Curve to name a few: see more types in prior work by [14]. As mentioned in Section 3.1, we leveraged the AutoML challenge to collect the learning curves. In the first round, a learning curve was represented as a function of time. The points on the learning curves were irregularly spaced and chosen by the learning algorithms themselves (as set by the AutoML challenge). When a participant's method requested points between two recorded points, we interpolated the requested points using the closest previously recorded point. However, this approach did not provide new information on the learning curve while still incurring a cost. To address this, we introduced a new type of learning curve based on training data size in the second round. Participants' methods could choose a training data size from a fixed given set, query an algorithm's performance w.r.t. the chosen size, and pay the associated cost.

Data splitting. In the first round, we kept vali-



Figure 3: Ablation study of DDQN baseline. Meta-learning and progression of learning curves improved DDQN's performance in both challenge rounds.

dation and test learning curves separate, using them for the feedback phase and final testing phase, respectively. This was to prevent overfitting on the test learning curves. However, it was pointed out in the first round that the test learning curves were highly correlated with the validation curves. Therefore, one could overfit the former by simply overfitting the latter. To mitigate this issue, we divided our dataset into two equal portions in the second round, using one half for the feedback phase and keeping the other half completely private for the final testing phase.

4.2 Ablation study of DDQN baseline

We conducted an ablation study to examine the benefits of using learning curves and meta-learning in tackling the budget-limited algorithm selection problem. Figure 3 shows a performance comparison of the DDQN baseline with certain components removed. First, we compared the performance of DDQN with and without meta-learning by omitting the metatraining phase. In the latter case, the policy network $\pi_{\theta,\theta'}$ of DDQN was randomly initialized and did not go through any tuning using meta-learning. Second, we compared the performance of DDQN with learning from the entire progression of learning curves (all points on the learning curves) versus learning solely from the final evaluations (last points on the learning curves). In the latter case, an agent selects only ω_i , and the last points on the pre-computed learning curves $\mathcal{L}_{ij}^{train,val}$ are returned, with an associated cost Δ_j the agent must pay. The results showcased that both meta-learning and learning curve progression highly contributed to the performance of DDQN. This finding also explains the success of the top-3 teams in both challenge rounds, as their methods meta-learned from learning curve progression.

4.3 Agent policy and action trajectory

We investigated the learned policies of agents by examining their action trajectories during the metatesting phase. Figure 4 shows an example dataset, *Flora*, where we compare trajectories generated by our best baseline, DDQN, and the top-3 teams' methods. We focus on segments that emphasize moments of algorithm transition, particularly near the beginning of the episode. (1) DDQN's policy: The agent started with algorithm no. 37, a top-performing candidate in meta-training (ranked 3rd/40 algorithms in terms of average performance). It then transitioned to train a new algorithm, no. 36 (ranked 6th), and ultimately to algorithm no. 32 (ranked 7th) upon observing a performance plateau. This pattern demonstrated DDQN's ability to metalearn effective initial candidates, ensuring a strong starting position. Subsequently, it switched to a new candidate or resumed training a previously paused candidate when the current one reached a performance plateau, guaranteeing efficient any-time learning for which it was meta-trained. (2) Winning teams' policies: In contrast to DDQN, the winning teams' policies prioritized optimal any-time learning performance through a strategy characterized by less repetition of choices and a greater emphasis on exploration. Specifically, team "Dragon_bra" is noted for its cautious approach, thoroughly assessing algorithms, particularly its initial choice, and choosing from different algorithm families like AdaBoost (algorithm no. 7 and no. 1 in orange) to SGD (algorithm no. 37 in blue). Meanwhile, team "carml" and team "Diaprofesser" favored a more exploratory approach within the most promising regions according to average performance in meta-training (SGD family, algorithm no. 30 to 39, shown in blue mark-



Figure 4: Trajectories of baseline DDQN and winning teams' methods on dataset *Flora*, capturing moments of algorithm transitions. Each marker corresponds to a choice of algorithm ω_j , with the chosen algorithm's family denoted by the marker's color: SGD in blue, AdaBoost in orange, and KNN in purple. Transitions between algorithms are marked with red lines. (a) The DDQN agent began with a strong candidate and consistently selected it. It made a transition only when a performance plateau was reached. (b, c, d) Winning teams' agents exhibited less repetition in their choices and placed a greater emphasis on exploration to achieve better results. The different time ranges on the x-axis were chosen near the beginning of the episode, specifically targeting moments of transition.

ers). This indicates a targeted exploration strategy within these high-potential areas. For a comprehensive view, the complete trajectories for all datasets and a heatmap illustrating algorithm rankings (aiding in identifying promising candidates) can be found in our public repository.⁶

We observed that a simple method like BEST ON SAMPLES (BOS) showed decent performance and occasionally surpassed DDQN when algorithms' learning curves do not intersect often, i.e. algorithm ranking does not change significantly w.r.t. the budget spent. Figure 5 shows datasets where this phenomenon was observed. More concretely, BOS beat DDQN in 9/30 and 5/15 datasets in the first round and the second round, respectively. This method can serve as a cost-effective yet competitive baseline solution, especially in situations where the implementation of meta-learning is overly complex or resourceintensive.

5 Conclusions

We addressed the machine learning algorithm selection problem under budget constraints. Our proposed framework, based on MDP, enables simultaneous algorithm selection and budget allocation by leveraging learning curves during the learning process. We organized challenges using novel learning curve datasets, allowing agents to meta-learn from knowledge gained on other datasets. The challenges' results demonstrated that agents using meta-learned knowledge of learning curve progressions outperformed those without this capability, demonstrated by their action trajectories. The challenges will remain open for post-challenge submissions and serve as long-lasting benchmarks. Promising future directions include the meta-training of more sophisticated Reinforcement Learning (RL) methods, such as Proximal Policy Optimization by [22], and the expansion of our benchmarks to encompass a wider variety of algorithms and types of learning curves. Another future research direction is to train multiple metalearning agents to collaboratively select algorithms and budgets, motivated by the demonstrated efficacy of ensembles of algorithm selectors by [26].

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 $^{^{6}} https://github.com/LishengSun/metaLC-post-challenge-analysis-2nd-round/tree/main/figs/ddqn_trajectory$



Figure 5: Algorithms' learning curves with their final rankings. We show some datasets where the baseline BoS beats the baseline DDQN. First round: (a-g); second round: (h-p). Algorithms are color-coded based on their final ranking (i.e., by comparing the last points on their learning curves). In these datasets, the learning curves do not cross each other very often, and the algorithm that ranked first early tends to maintain a very high rank at the end. This illustrates scenarios where BoS beats DDQN. However, in practice, one cannot know in advance if the learning curves of algorithms will cross each other often on a given dataset.

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References

- S. Abdulrahman, P. Brazdil, J. van Rijn, and J. Vanschoren. Speeding up algorithm selection using average ranking and active testing by introducing runtime. *Machine Learning*, 107, 01 2018.
- [2] S. M. Abdulrahman, P. Brazdil, J. N. van Rijn, and J. Vanschoren. Algorithm selection via meta-learning and sample-based active testing. In Proceedings of the 2015 International Workshop on Meta-Learning and Algorithm Selection co-located with ECMLPKDD 2015, volume 1455 of CEUR Workshop Proceedings, pages 55–66, 2015.
- [3] S. Adriaensen, H. Rakotoarison, S. Müller, and F. Hutter. Efficient bayesian learning curve extrapolation using prior-data fitted networks. In *NeurIPS 2023*, 2023.
- [4] P. Brazdil and C. G. Giraud-Carrier. Metalearning and algorithm selection: progress, state of the art and introduction to the 2018 special issue. *Machine Learning*, 107, 2018.
- [5] P. Brazdil and C. Soares. A comparison of ranking methods for classification algorithm selection. In *ECML 2000*, volume 1810 of *Lecture Notes in Computer Science*, pages 63–74, 2000.
- [6] P. Brazdil, J. N. van Rijn, C. Soares, and J. Vanschoren. *Metalearning Approaches for Algorithm Selection II*, pages 77–102. Springer International Publishing, Cham, 2022.
- [7] T. Domhan, J. T. Springenberg, and F. Hutter. Speeding up automatic hyperparameter op-

timization of deep neural networks by extrapolation of learning curves. In *IJCAI 2015*, pages 3460–3468, 2015.

- [8] M. Feurer, K. Eggensperger, S. Falkner, M. Lindauer, and F. Hutter. Auto-sklearn 2.0: Handsfree automl via meta-learning. *Journal of Machine Learning Research*, 23:261:1–261:61, 2022.
- [9] I. Guyon, L. Sun-Hosoya, M. Boullé, H. J. Escalante, S. Escalera, Z. Liu, D. Jajetic, B. Ray, M. Saeed, M. Sebag, A. R. Statnikov, W. Tu, and E. Viegas. Analysis of the automl challenge series 2015-2018. In *Automated Machine Learning - Methods, Systems, Challenges*, The Springer Series on Challenges in Machine Learning, pages 177–219. 2019.
- [10] A. Klein, S. Falkner, J. T. Springenberg, and F. Hutter. Learning curve prediction with bayesian neural networks. In *ICLR 2017*, 2017.
- [11] R. Leite, P. Brazdil, and J. Vanschoren. Selecting classification algorithms with active testing. In *MLDM 2012*, volume 7376 of *Lecture Notes* in Computer Science, pages 117–131. Springer, 2012.
- [12] S. Lin. Rank aggregation methods. Wiley Interdisciplinary Reviews: Computational Statistics, 2:555 - 570, 09 2010.
- [13] A. Mohan, T. Ruhkopf, and M. Lindauer. Towards meta-learned algorithm selection using implicit fidelity information. *CoRR*, abs/2206.03130, 2022.
- [14] F. Mohr and J. N. van Rijn. Learning curves for decision making in supervised machine learning - A survey. *CoRR*, abs/2201.12150, 2022.
- [15] F. Mohr and J. N. van Rijn. Fast and informative model selection using learning curve crossvalidation. *IEEE Transactions on Pattern Anal*ysis and Machine Intelligence, 45(8):9669–9680, 2023.

- [16] M. H. Nguyen, I. Guyon, L. Sun-Hosoya, and N. Grinsztajn. Metareveal: Rl-based metalearning from learning curves. In *Interac*tive Adaptive Learning Workshop co-located with ECML PKDD 2021, volume 3079 of CEUR Workshop Proceedings, 2021.
- [17] M. H. Nguyen, L. Sun-Hosoya, N. Grinsztajn, and I. Guyon. Meta-learning from learning curves: Challenge design and baseline results. In *IJCNN 2022*, 2022.
- [18] M. H. Nguyen, L. Sun-Hosoya, N. Grinsztajn, and I. Guyon. Meta-learning from learning curves challenge: Lessons learned from the first round and design of the second round. In *Complex Feedback in Online Learning Workshop colocated with ICML 2022*, 2022.
- [19] J. Petrak. Fast subsampling performance estimates for classification algorithm selection. In Proceedings of the ECML-00 Workshop on Meta-Learning: Building Automatic Advice Strategies for Model Selection and Method Combination, pages 3–14, 2000.
- [20] T. Ruhkopf, A. Mohan, D. Deng, A. Tornede, F. Hutter, and M. Lindauer. MASIF: metalearned algorithm selection using implicit fidelity information. *Transactions on Machine Learning Research*, 2023, 2023.
- [21] M. Schmidt, J. Gastinger, S. Nicolas, and A. Schülke. HAMLET - A learning curveenabled multi-armed bandit for algorithm selection. In *IJCNN 2020*, pages 1–8. IEEE, 2020.
- [22] J. Schulman, F. Wolski, P. Dhariwal, A. Radford, and O. Klimov. Proximal policy optimization algorithms. *CoRR*, abs/1707.06347, 2017.
- [23] L. Sun-Hosoya. Meta-Learning as a Markov Decision Process. (Meta-Learning en tant que processus de décision Markovien). PhD thesis, University of Paris-Saclay, France, 2019.
- [24] L. Sun-Hosoya, I. Guyon, and M. Sebag. Activmetal: Algorithm recommendation with active meta learning. In *Interactive Adap*tive Learning Workshop co-located with ECML

PKDD 2018, volume 2192 of *CEUR Workshop Proceedings*, pages 48–59, 2018.

- [25] K. Swersky, J. Snoek, and R. P. Adams. Freeze-thaw bayesian optimization. CoRR, abs/1406.3896, 2014.
- [26] A. Tornede, L. Gehring, T. Tornede, M. Wever, and E. Hüllermeier. Algorithm selection on a meta level. *Machine Learning*, 112(4):1253– 1286, 2023.
- [27] H. van Hasselt, A. Guez, and D. Silver. Deep reinforcement learning with double q-learning. In AAAI 2016, 2016.
- [28] J. N. van Rijn, S. M. Abdulrahman, P. Brazdil, and J. Vanschoren. Fast algorithm selection using learning curves. In *IDA 2015*, volume 9385 of *Lecture Notes in Computer Science*, pages 298– 309. Springer, 2015.
- [29] J. Vanschoren. Meta-learning: A survey. CoRR, abs/1810.03548, 2018.
- [30] A. Vettoruzzo, M.-R. Bouguelia, J. Vanschoren, T. Rognvaldsson, and K. Santosh. Advances and challenges in meta-learning: A technical review. *IEEE Transactions on Pattern Analysis* and Machine Intelligence, 2024.
- [31] M. Wistuba and T. Pedapati. Learning to rank learning curves. In *ICML 2020*, volume 119, pages 10303–10312. PMLR, 2020.