LAMDA: TWO-PHASE MULTI-FIDELITY HPO VIA LEARNING PROMISING REGIONS FROM DATA

ABSTRACT

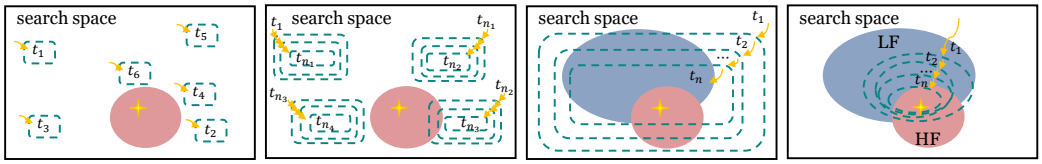
Hyperparameter Optimization (HPO) plays a critical role in machine learning, aiming to automatically find the best hyperparameter configurations to maximize model performance. Existing multi-fidelity HPO methods combine data from both high-fidelity (HF) and low-fidelity (LF) problems during the optimization process, aiding in effective sampling or preliminary screening. Despite this, their sampling strategies are conducted across the whole search space. Additionally, while approaches that incorporate prior knowledge can constrain the search space, such knowledge is not always accessible. We have observed that high-quality solutions in HPO exhibit some overlapping between high- and low-fidelity problems. Bearing the above consideration in mind, this paper proposes a simple yet effective two-phase search framework named `Lamda` to streamline multi-fidelity HPO. Specifically, in the first phase, it searches in the LF landscape to identify the promising region therein. Thereafter, in the second phase, we transfer such promising regions to navigate the HPO. Further, the `Lamda` framework is integrated with various HPO techniques to boost their performance. We demonstrate the rational of the framework by showcasing theoretical analysis towards the prior-based Bayesian optimization and bandit-based Hyperband. Empirically, we demonstrate the efficiency of this method across a range of HPO tasks.

1. INTRODUCTION

The performance of machine learning models, deep learning in particular, highly depend on the choice of hyperparameters (Bischl et al., 2023). As a result, hyperparameter optimization (HPO) has emerged as a popular research area in both academia and industry (Li et al., 2022a). However, the cost of HPO becomes prohibitively high when dealing with large models or datasets. For instance, the training time for a single hyperparameter configuration on a large dataset can range from several hours to even days (Krizhevsky et al., 2012).

A variety of HPO methods have been developed to identify well-performing hyperparameter configurations (Bischl et al., 2023). These include random search (RS) (Bergstra & Bengio, 2012), grid search (Montgomery, 2017) and Bayesian optimization (BO) (Kandasamy et al., 2018; Bergstra et al., 2011; McLeod et al., 2017). However, these techniques rely on expensive evaluations to explore the whole search space as shown in Figure 1(a). Methods based on localized search strategies such as trust region Bayesian optimization (TuRBO) (Eriksson et al., 2019) have also been proposed. However, they require iterated local searches across the whole search space to ensure coverage of optimal regions as shown in Figure 1(b). Consequently, the above methods are constrained to exploring a finite set of configurations when computational resources are limited.

To address the high cost associated with performance evaluations of hyperparameter configurations, a variety of multi-fidelity optimization methods have been devised. These methods employ a variety of techniques to control the fidelity of HPO problems, including the use of subsets of the dataset (Klein et al., 2017), the selection of specific features (Li et al., 2017), and the reduction in the number of training epochs (Falkner et al., 2018). Low-fidelity (LF) problems are generated by using these strategies, which approximate the high-fidelity (HF) problem but require less computational cost. Multi-fidelity methods try to reduce the overall cost by using the LF problems to assist the optimization of HF problems (Swersky et al., 2013; Klein et al., 2017; Kandasamy et al., 2017; Poloczek et al., 2017; Li et al., 2020b). Multi-fidelity Bayesian optimization (MFBO) (Swersky et al., 2013) and bandit-based methods (Li et al., 2017) are two widely adopted multi-fidelity approaches for HPO. In the realm of MFBO, previous research primarily leverages the data from LF problems to construct a multi-fidelity model for sampling new configurations (Swersky et al., 2013; Poloczek et al., 2017; Kandasamy et al., 2019; Mikkola et al., 2022; Li et al., 2020b). How-



(a) Global search methods (b) Local search methods: TuRBO (c) Bandit based methods (d) Methods using promising area

Figure 1: A conceptual demonstration of how different search methods explore the whole search space in HPO. The red area represents regions of high-quality solutions for an HF problem, while the yellow stars denote its optimal solution. The blue areas indicate regions of high-quality solutions for the LF problem. The dashed lines in panel (a) show the locations of sampled points at each iteration and represent the search space of the sampling function depicted in panels (b) through (d). t represents the iteration number, illustrating the progression of each method's search strategy.

ever, the optimization of the acquisition function is still conducted within the entire search space. Bandit-based methods, on the other hand, utilize data from LF problems to identify promising configurations for the HF (Falkner et al., 2018; Li et al., 2022b; Awad et al., 2021). They continuously utilize data from both high- and low-fidelity problems to explore the whole search space, systematically narrowing down the exploration space until the search process stops, as shown in Figure 1(c). However, it always sample the entire space in both low- and high-fidelity levels (Mallik et al., 2023).

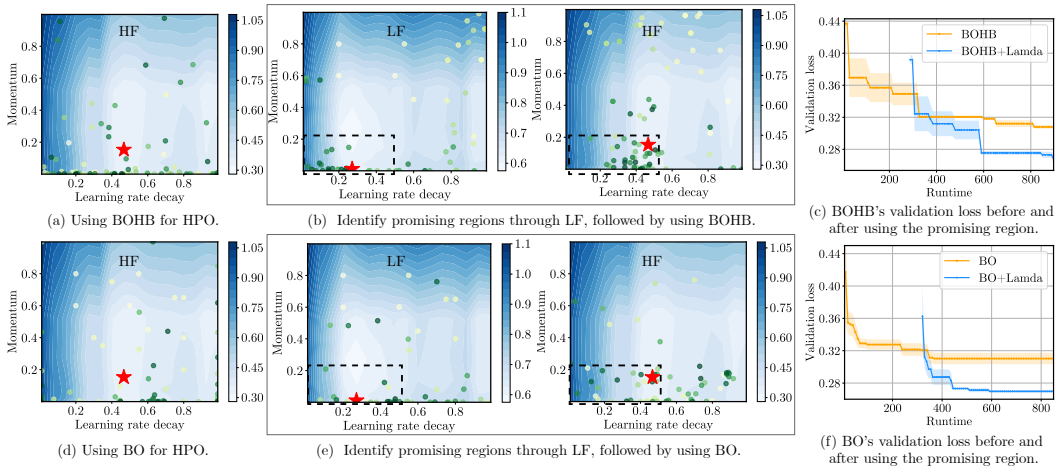
In addition to the multi-fidelity methods, another approach addressing the challenges of sampling in the whole search space is to leverage expert knowledge or information from similar tasks to constrain the search space. As shown in Figure 1(d), these methods focus on promising areas to reduce resource consumption. One such technique involves integrating prior information about the locations of optimal solutions into the standard probabilistic model of BO, forming a pseudo-posterior that has been proven to be more sample-efficient than standard BO approaches (Souza et al., 2021; Li et al., 2020a). Moreover, prior Gaussian distributions of the optimal solutions are utilized in the acquisition function to expedite the HPO (Hvarfner et al., 2022). However, obtaining accurate prior knowledge remains a challenge for these methods.

Table 1: Existing methods in addressing the challenges of HPO. Methods that successfully address a challenge are marked with a checkmark (✓), while those that do not are marked with a cross (✕).

Challenges	RS	BO	TuRBO	MFBO	Bandit-based	BO with prior	Transfer search space	Priorband	Ours
Expensive evaluation	✕	✕	✕	✓	✓	✕	✕	✓	✓
Sampling space	✕	✕	✓	✕	✕	Use expert prior	Use similar tasks	Use expert prior	Use LF

Table 1 shows a comparison of existing HPO methods in addressing the challenges of *expensive evaluation* and *sampling space exploration*. It can be seen that using expert prior and similar tasks are two methods to constrain sampling space. However, both approaches rely on prescribed knowledge or experience from domain experts, which may not always be readily available. To address the reliance on expert knowledge while simultaneously improving sampling efficiency, we propose leveraging LF problems to identify promising regions for the HF problem. The optimization of the HF problems are focused on these identified promising regions, thereby accelerating optimization by reducing resource consumption in less promising regions. This strategy is inspired by the potential overlap of promising regions between high- and low-fidelity HPO problems. We show the the effectiveness of our method through hyperparameter optimization of a WideResNet on the CIFAR-100 dataset, using BOHB (Falkner et al., 2018) and BO (Bergstra et al., 2011), both before and after incorporating promising regions (denoted as with or without `Lamda`). In this case, the promising regions for both high and low-fidelity problems were primarily concentrated within regions bounded by momentum values between [0, 0.5] and learning rate decay values between [0.2, 0.8], as shown in Figure 2(b) and (e). Algorithms with `Lamda` can quickly explore the real promising regions in the high fidelity (right panel of Figure 2(b) and (e)). The performance curves in Figure 2(c) and (f) further demonstrate the efficiency gains after leveraging promising regions.

Overall, we propose a novel framework for HPO named `Lamda` (**Le**arning pro**m**ising regions from **da**ta), which utilizes LF problems to learn promising regions, then leverages these priors to guide optimization of HF problems. The contributions are threefold:



(a) Using BOHB for HPO. (b) Identify promising regions through LF, followed by using BOHB. (c) BOHB's validation loss before and after using the promising region.

(d) Using BO for HPO. (e) Identify promising regions through LF, followed by using BO. (f) BO's validation loss before and after using the promising region.

Figure 2: Using BOHB and BO for hyperparameter optimization of a WideResNet on CIFAR-100, before and after employing promising regions (denoted as with or without `Lamda`). The pentagrams mark the optimal solutions. In (a) and (b), the points represent sampled solutions by BOHB, while in (d) and (e), they represent sampled solutions by BO. The color gradient from yellow to green indicates the progression of sampling over time. The points represent samples from BOHB in (a) and (b), and from BO in (d) and (e), with colors transitioning from yellow to green indicating the progression of sampling over time.

- Building on the overlapping promising regions between LF and HF landscapes, we design a framework that leverages LF problems to identify the promising regions of HF problems, thereby accelerating the HPO process. In addition, an overlapping coefficient is introduced to quantitatively measure the extent of overlapping.
- We integrate the framework with existing HPO techniques, ranging from prior- and bandit-based methods, as well as multi-fidelity BO, to further augment their performance. Moreover, we demonstrate the rational of this augmentation by showcasing theoretical analysis towards the prior-based Bayesian optimization and bandit-based Hyperband.
- We validate the competitiveness of our methods across diverse hyperparameter optimization tasks, including fully connected networks, transformers, ResNet, neural architecture search benchmarks, as well as joint architecture and hyperparameter search cases.

2. Multi-Fidelity HPO by Learning Promising Regions from Data

The HPO problem is formulated as *minimizing* an expensive-to-evaluate objective function $f : \mathcal{X} \to \mathbb{R}$, where the goal is to find

$$\mathbf{x}^* \in \arg\min_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x}). \tag{1}$$

The configuration $\mathbf{x}$ is selected from a search space $\mathcal{X}$ that may include any combination of continuous, discrete, and categorical variables. In the context of HPO, $f(\mathbf{x})$ represents the training or validation performance of a machine learning model given the hyperparameters defined by $\mathbf{x}$. In multi-fidelity HPO, $f_z(\cdot)$ with $z \in \{\ell, \ell+1, \ldots, h\}$ is introduced to denote a computation of $f(\cdot)$ at the fidelity level z, e.g., the validation loss of a model trained for z epochs. Define f_h and f_ℓ with $\ell < h$ as the HF and LF objectives, respectively.

In this paper, we propose a multi-fidelity HPO framework by exploiting promising regions from data (dubbed `Lamda`). It comprises a two-phase search strategy: ▶ the *first-phase search* initially identifies promising regions in the LF landscape; ▶ the *second-phase search* leverages the learned information to guide the search in the HF landscape. In the subsequent sections, we will introduce the search strategies at different phases by addressing two key questions.

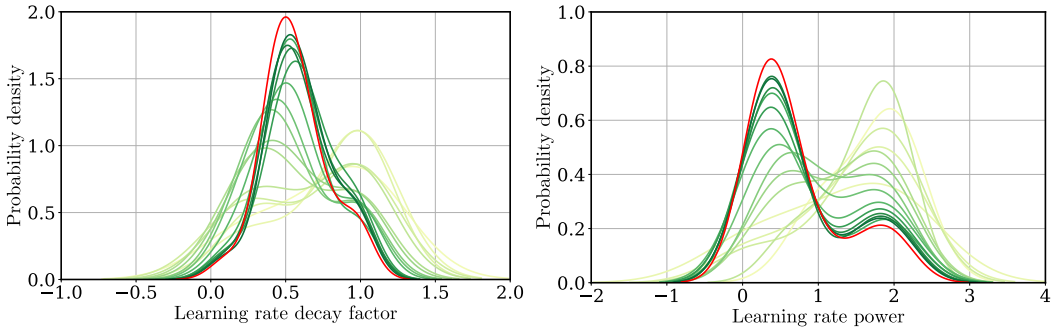


Figure 3: This figure shows the progression of PDFs for promising regions during hyperparameter optimization on a transformer model for the LM1B dataset, focusing on the LF problem. We display PDFs for two out of four hyperparameters, with colors changing from yellow to green to indicate iteration progress. The red line represents the true PDF of the promising solutions in the LF problem.

2.1 How to Identify the Promising Regions in the Low-fidelity Landscape?

Our basic idea of the *first-phase search* is to divide the LF landscape into two parts: one consists of the promising regions while the other represents the inferior ones. This can be implemented as a binary classification problem. To train such classifier, we leverage the configurations visited so far during the HPO process in the LF landscape, denoted as $\mathcal{S} = \{\langle \mathbf{x}^i, f_\ell(\mathbf{x}^i)\rangle\}_{i=1}^t$ where $f_\ell(\cdot)$ is the LF objective function and t is the current number of function evaluations. In particular, this paper adopts the classic tree-structured Parzen estimator (TPE) method (Bergstra et al., 2011; Gramacki, 2018) as the classifier, given the scalability and supports for both mixed continuous and discrete spaces. It uses the quantile of $\{f_\ell(\mathbf{x}) | \mathbf{x} \in \mathcal{S}\}$ to determine the classification boundary. Specifically, we divide $\mathcal{S}$ into: $\mathcal{S}_{\text{pro}} = \{\mathbf{x} \mid f_\ell(\mathbf{x}) \leq y^*, \mathbf{x} \in \mathcal{S}\}$ containing promising solutions, and $\mathcal{S}_{\text{inf}} = \{\mathbf{x} \mid f_\ell(\mathbf{x}) > y^*, \mathbf{x} \in \mathcal{S}\}$ containing inferior solutions, where y^* is determined from $\alpha = \Pr(f_\ell(\mathbf{x}) < y^*)$ quantile of $\{f_\ell(\mathbf{x}) | \forall \mathbf{x} \in \mathcal{S}\}$. Then we denote

$$\varphi_{\text{pro}}(\mathbf{x}) = p(\mathbf{x} \mid \mathcal{S}_{\text{pro}}), \quad \varphi_{\text{inf}}(\mathbf{x}) = p(\mathbf{x} \mid \mathcal{S}_{\text{inf}}), \tag{2}$$

where $\varphi_{\text{pro}}(\mathbf{x})$ is the probability density function (PDF) of the promising solutions, and $\varphi_{\text{inf}}(\mathbf{x})$ is the PDF of the inferior solutions. We will adopt the kernel density estimation for $\varphi_{\text{pro}}(\mathbf{x})$ and $\varphi_{\text{inf}}(\mathbf{x})$, given its non-parametric nature and applicability to complicated distributions (Chen, 2017).

Instead of searching for the optimal configurations in the LF landscape, the purpose of the *first-phase search* is to identify the promising regions. In practice, the targeted regions are relatively scattered at the beginning and will gradually become focused around the regions that potentially cover the optima (see an illustrative example in Figure 3). Based on this observation, we hypothesize that the *first-phase search* can be terminated when the distribution of promising regions becomes stable. To keep track of the progression of such distribution, we propose to use the overlapping coefficient (OVL) (Anderson et al., 2012) as a metric to quantify the similarity between two distributions.

Definition 1 (Overlapping coefficient)**.** *Let $\varphi_1(\mathbf{x})$ and $\varphi_2(\mathbf{x})$ be two PDFs on the search space $\mathcal{X}$. The overlapping coefficient ρ of the two functions is defined as:*

$$\rho(\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})) = \int_{\mathbf{x} \in \mathcal{X}} \min\{\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})\} \, d\mathbf{x}. \tag{3}$$

Note that $\rho(\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x}))$ ranges from 0 to 1, where $\rho = 1$ if and only if the two distributions are fully overlapped, and $\rho = 0$ if there is no intersection at all. The *first-phase search* is terminated either if the allocated computational budget is exhausted or the OVL of estimated distributions between $\Delta \in \mathbb{N}$ iterations is close enough:

$$1 - \rho\left(\varphi_{\text{pro}}^t(\mathbf{x}), \varphi_{\text{pro}}^{t+\Delta}(\mathbf{x})\right) \leq \gamma, \tag{4}$$

where γ denotes the threshold. The calculation of ρ involves a multidimensional integral, which can be numerically intractable. In practice, we employ the Monte Carlo method to estimate ρ as

$$\begin{aligned} \rho(\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})) &= \int_{\mathbf{x} \in \mathcal{X}} \min\{\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})\} \, d\mathbf{x} = \int_{\mathbf{x} \in \mathcal{X}} \min\left\{1, \frac{\varphi_2(\mathbf{x})}{\varphi_1(\mathbf{x})}\right\} \varphi_1(\mathbf{x}) d\mathbf{x} \\ &= \mathbb{E}\left[\min\left\{1, \frac{\varphi_2(\mathbf{x})}{\varphi_1(\mathbf{x})}\right\}\right] \approx \frac{1}{N} \sum_{i=1}^{N} \min\left\{1, \frac{\hat{\varphi}_2(\mathbf{x})}{\hat{\varphi}_1(\mathbf{x})}\right\}, \end{aligned} \tag{5}$$

where N is the number of samples used in the Markov Chain Monte Carlo sampling, and $\hat{\varphi}(\cdot)$ is an approximation of $\varphi(\cdot)$ such as using the kernel density estimation.

2.2 How to Leverage LF Promising Regions in the High-fidelity Landscape?

With the identified promising regions in the LF landscape, we hypothesize that such information can be used to define the promising regions in the HF landscape. Instead of searching among the entire search space, the *second-phase search* is more focused within the regions defined below:

$$\tilde{\varphi}_{\text{pro}}(\mathbf{x}) = (1 - w) \cdot \varphi(\mathbf{x}) + w \cdot \varphi_{\text{pro}}(\mathbf{x}), \tag{6}$$

where $\varphi(\mathbf{x})$ is the probability distribution used to guide the HPO process in the HF landscape, $\varphi_{\text{pro}}(\mathbf{x})$ is the probability distribution of the promising regions identified from the *first-phase search* in the LF landscape, and $w \in [0, 1)$ with is a hyperparameter that controls the trade-off between the importance of $\varphi(\mathbf{x})$ learned *on-the-fly* and $\varphi_{\text{pro}}(\mathbf{x})$ learned in the *first-phase search*. Figure 4 provides a conceptual visualization of leveraging equation (6) during the second-phase search. The redefined promising regions will be closer to the true optimal solution if the promising regions learned in the first phase are closer to the optimum than those before the redefinition, as proven in Proposition 1. Note that since $\varphi(\mathbf{x})$ is progressively updated during the HPO process with new configurations evaluated and added to the dataset, it is expected that $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ will experience a similar trend as $\varphi_{\text{pro}}(\mathbf{x})$ in the *first-phase search*.

Proposition 1. *Assume the OVL between $\varphi(\mathbf{x})$ and the PDF of the true promising solutions $\varphi_*(\mathbf{x})$ is less than the overlapping between the PDF of promising region $\varphi_{\text{pro}}(\mathbf{x})$ and $\varphi_*(\mathbf{x})$. Then, the modified sampling function $\tilde{\varphi}_{\text{pro}}(\mathbf{x}) = w_1 \cdot \varphi(\mathbf{x}) + w_2 \cdot \varphi_{\text{pro}}(\mathbf{x})$, where $w_1 + w_2 = 1$, will have a greater or equal overlapping with $\varphi_*(\mathbf{x})$ compared to the overlapping of $\varphi(\mathbf{x})$ with $\varphi_*(\mathbf{x})$.*

The proof of Proposition 1 is presented in Appendix A.1. It suggests that incorporating the promising regions into the sampling distribution enhances its alignment with the distribution of the real optimal solutions.

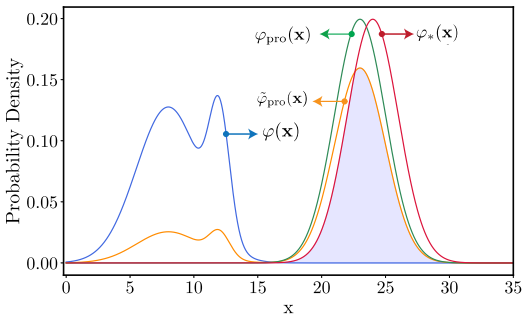


Figure 4: Conceptual visualization of leveraging promising regions: $\varphi(\mathbf{x})$, $\varphi_{\text{pro}}(\mathbf{x})$, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$, and $\varphi_*(\mathbf{x})$ represent the original sampling distribution at the t-th iteration, the density function of the promising regions, the modified density function incorporating the promising regions with a weight of $w_t = 0.8$, and the density function of the real optimum, respectively.

2.3 Integration and Comparison with Current Multi-fidelity HPO Methods

Instead of a standalone algorithm, `Lamda` plays as a booster that can be integrated with any existing multi-fidelity HPO methods with minor adaptation and thus augmenting the performance of the baseline optimizer. In a nutshell, we only need to replace the sampling strategies of the baseline optimizer with $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$. We justify this by comparing with current multi-fidelity HPO methods.

- **Prior-Based Methods:** By using `Lamda`, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ serves as *a priori* knowledge that represents a reasonable estimation of promising regions in the *second-phase search*. Unlike prior-based methods, which depend on prescribed knowledge or experience from domain experts, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ is adaptively learned from data during the *first-phase search* through the HPO process in the LF landscape. As a result, our approach is resilient to 'pathological priors'—whether misleading, lacking in informative values, or potentially adversarial—which are not uncommon when tackling new, unseen real-life black-box applications. Additionally, we expect a scenario between our data-driven priors with those elicited from experts can offer consolidated performance enhancement.
- **Bandit-Based Methods:** By using `Lamda`, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ serves as an effective alternative to the sampling distributions used in bandit-based methods. This restricts the HPO process to focus exclusively on the learned promising regions. In contrast, bandit-based methods begin with LF assessments to identify candidates for HF evaluation and then gradually shift

the search focus towards these identified areas. This process, which alternates between exploration and exploitation throughout the entire search space, often leads to inefficient use of computational resources by exploring less promising regions.

- **MFBO Methods:** Similar to bandit-based methods, MFBO methods use an acquisition function learned from data collected across multiple fidelities to explore the entire search space. This can lead to unnecessary exploration of less promising regions. By using `Lamda`, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ restricts the search space within the learned promising regions. Note that this strategy can be applied to the other BO variants.

For proof-of-concept purposes, we choose `PriorBand`, `BOHB`, `MUMBO` as representatives of the prior-, bandit-based and MFBO methods, respectively. By augmenting with `Lamda`, we have `Lamda+PriorBand`, `Lamda+BOHB`, and `Lamda+MUMBO`. In addition, it is also interesting to see whether `Lamda` can be useful for vanilla BO and even random search. To this end, we derive two other variants `Lamda+BO` and `Lamda+RS`. Furthermore, we provide theoretical analysis under both the prior-based BO framework and bandit-based Hyperband framework, indicating the rational of this augmentation. For `Lamda+BO`, it incorporates prior knowledge in the acquisition function:

$$\mathbf{x}^{n+1} = \arg\max \tilde{\varphi}_{\text{pro}}(\mathbf{x})\text{AF}(\mathbf{x}, \mathcal{D}), \tag{7}$$

where AF is the acquisition function in vanilla BO such as the expected improvement (EI) considered in this paper. $\mathcal{D} = \{\langle \mathbf{x}^i, f_h(\mathbf{x}^i)\rangle\}_{i=1}^n$ where $f_h(\cdot)$ is the HF objective function. The Gaussian process regression is employed as the surrogate model of $f_h(\cdot)$. For a solution $\tilde{\mathbf{x}}$, the predicted mean and variance of the value distribution of $f_h(\tilde{\mathbf{x}})$ are $\mu_f(\tilde{\mathbf{x}})$ and $\sigma_f^2(\tilde{\mathbf{x}})$.

In `Lamda+BO`, we apply the widely used EI as the acquisition function in equation (7) given as

$$\text{EI}(\tilde{\mathbf{x}}|\mathcal{D}) = \sigma_f(\tilde{\mathbf{x}})\big(z\Phi_f(z) + \phi_f(z)\big), \tag{8}$$

where $z = \frac{f_{\mathcal{D}}^* - \mu_f(\tilde{\mathbf{x}})}{\sigma_f(\tilde{\mathbf{x}})}$, $f_{\mathcal{D}}^* = \min_{\langle \mathbf{x}, f_h(\mathbf{x})\rangle \in \mathcal{D}} f_h(\mathbf{x})$, Φ_f and ϕ_f denote the cumulative distribution function and probability density function, respectively.

Theorem 1. *Given $\mathcal{D}_n$, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$, and applying the EI into equation (7), assume the GP models are non-degenerated. Let $\mathcal{D}$ be the collected observations with $\langle \mathbf{x}^1, f_h(\mathbf{x}^1)\rangle$ fixed while $\{\langle \mathbf{x}^i, f_h(\mathbf{x}^i)\rangle\}_{i=2}^n$ are sequentially chosen by*

$$\mathbf{x}^{n+1} = \arg\max \tilde{\varphi}_{\text{pro}}(\mathbf{x})\text{EI}(\tilde{\mathbf{x}}|\mathcal{D}). \tag{9}$$

Then, as $n \to \infty$, almost surely: the acquisition function converges to zero; and the evaluated best objective $f_{\mathcal{D}}^* \to f_h^*$, where f_h^* represents the global optimum of $f_h(\cdot)$.

The proof is given in Appendix A.2. Unlike the theory in (Hvarfner et al., 2022), the convergence property of equation (9) does not need a decaying factor to force exponentially decreasing of the priors of promising LF regions. Based on the dynamic update of $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$, it is sufficient to capture the promising regions in the HF landscape according to the overlap.

For bandit-based method, we study the `Lamda+PriorBand` in the theoretical routine of Hyperband. The algorithm involves two loops. In the outer loop, at the k-th round, the algorithm allocates $B_{k,s} = 2^k + \text{poly}(k)$ budgets and $n_{k,s} = 2^s$ configurations randomly sampled from $\tilde{\varphi}_{\text{pro}}(x)$, for $s = 0, 1, \ldots, s_{\max}$, subject to $s_{\max} + \log_2(s_{\max}) < k$, where $\text{poly}(k)$ is some polynomial function w.r.t k. In the inner loop, the successive halving algorithm is leveraged to find the best arm among the $n_{k,s}$ arms with $B_{k,s}$ budget. In the context of multi-arm bandits, each configuration $\mathbf{x}^i$ corresponds to an independent arm to pull, whose reward with the j-th pull is denoted by $l_{i,j} = f_j(\mathbf{x}^i)$. We assume there exists $\lim_{k\to\infty} l_{i,k} = \nu_i$ for all $\mathbf{x}^i \in \mathcal{X}$, and denote $\nu_* = \inf_{x\in\mathcal{X}} \nu_i$. Denote also that the distribution of v as F satisfying $P(\nu - \nu_* \le \epsilon) = F(\nu_* + \epsilon)$ for any ϵ. The inverse function is defined by $F^{-1}(y) = \inf\{x : F(x) \le y\}$. In addition, there exists a monotonically decreasing function $\gamma(t) : N \to R$ satisfying $\sup_i |l_{i,t} - \nu_i| \le \gamma(t)$.

Theorem 2. *For fixed $\delta \in (0, 1)$. Let $\hat{\nu}_B$ be the empirically best-performing arm output from successive halving of round $k_B = \log_2(B)$ of the outer loop, and let $s_B < k_B$. Then, there is:*

$$\hat{\nu}_B - \nu_* \le 3\left(F^{-1}\left(\frac{\log(4k_B^3/\delta)}{2^{s_B}} - \nu_*\right) + \gamma\left(\frac{2^{k_B-1}}{k_B}\right)\right), \tag{10}$$

where s_B satisfies $2^{k_B} + \text{poly}(k_B) > 4s_B\mathbf{H}(F, \gamma, 2^{s_B}, 2k_B^3/\gamma)$ with $\mathbf{H}(F, \gamma, n, \delta) = 2n\int_{p_n}^1 \gamma^{-1}(\frac{F^{-1}(t)-\nu^*}{4})dt + \frac{10}{3}\log(2/\delta)\gamma^{-1}\left(\frac{F^{-1}(p_n)-\nu_*}{4}\right)$ and $p_n = \frac{\log_2(2/\delta)}{n}$.

Since all configurations for successive halving tasks are sampled randomly from a probability distribution described by $\tilde{\varphi}_{\text{pro}}$, the theoretical results, specifically Corollary 3 in (Li et al., 2017), still hold in this case. Different from Hyperband that relied on non-adaptive grid search exhausting $c\log_2(B)$ overall budgets with some constant c, we sample configurations and allocate budget through both grid search and adaptive design based on $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$. Theoretically, this requires the same order of budgets as Hyperband. It will be a quite interesting question to ask how the fact of overlapping can help avoiding the grid search of Hyperband, which will be our future work.

3. Experiment Setup

3.1 Benchmark suites

Our experiments consider 36 benchmarks that cover various search spaces including mixed types and log-scaled hyperparameters. Further, they involve a wide range of downstream tasks including image classification, language modeling, tabular data processing, medical applications, and translation.

They are selected from four sources. ① Tabular benchmarks include ▶ four cases from `FCNet` (Pfisterer et al., 2022), each with 6 hyperparameters; ▶ one from `NAS-Bench-301` with 34 hyperparameters (Pfisterer et al., 2022); ▶ three from `NAS-Bench-201`, each with 6 hyperparameters (Eggensperger et al., 2021); and ▶ twenty benchmarks from `rpart` on decision tree, `glmnet` on elastic net, `ranger` on random forest, and `XGBoost` (Eggensperger et al., 2021). ② Surrogate benchmarks include ▶ four problems from `PD1 benchmarks` with 4 hyperparameters (Mallik et al., 2023; Wang et al., 2021); ▶ three problems from `JAHSBench` (Mallik et al., 2023; Bansal et al., 2022) with 14 mixed-type hyperparameters for tuning both the neural networks architecture and training hyperparameters. ③ Training two deep neural networks include LeNet on CIFAR-10, and ResNet-18 on CIFAR-10 and CIFAR-100 with 5 hyperparameters. ④ Two synthetic Hartmann functions (Mallik et al., 2023) with three and six variables respectively.

For the tabular and surrogate benchmarks, we use the number of epochs as the parameter to set the fidelity level. As for the training of deep neural networks, the size of the dataset is used as the parameter to control the fidelity level. Further detail about all benchmarks are provided in Appendix C.

3.2 Peer algorithms

We choose nine peer algorithms as the baselines to validate the effectiveness of proposed approach. They are ▶ `PriorBand` (Mallik et al., 2023) and `PFNs4BO` (Müller et al., 2023) as prior-based methods; ▶ `HyperBand` (Li et al., 2017), `BOHB` (Falkner et al., 2018), and `Hyper-Tune` (Li et al., 2022b) as bandit-based methods; ▶ `MUMBO` (Li et al., 2021a) and `DPL` (Kadra et al., 2023) as MFBO methods; and ▶ random search (`RS`), `BO` and `TuRBO` (Eriksson et al., 2019) as other popular HPO methods. During our experiments, we used the default values for these algorithms. For our algorithm, the parameter settings are as follows: $\gamma = 0.1$, $\Delta = 5$, $\alpha = 15$ and $w = 0.5$. Additionally, we allocate a computational budget of $B = 5D$ high-fidelity resources in the first-phase search, where D denotes the problem's dimensionality.

4. Experimental Results

4.1 Effective of using promising regions

Results on tabular, surrogate and synthetic benchmarks: This experiment demonstrates how our algorithm framework improves five commonly used optimizers: `PriorBand`, `BOHB`, `MUMBO`, `BO` and `RS`. For `BOHB`, `MUMBO`, `BO` and `RS`, 33 tasks from the above tabular, surrogate and synthetic benchmarks are used. For `PriorBand`, the evaluation included eight tasks: four from the original paper (PD1-LM1B, PD1-WMT, MFH3, and MFH6) and four additional tasks in FCNet. In addition, good prior are used at `PriorBand` for PD1-LM1B, PD1-WMT, MFH3, and MFH6. Table 2 presents the numbers of win/lose/tie obtained by using the Wilcoxon signed-rank test and Figure 5 shows the average rank over the HPO tasks. According to Figure 5, it can seen that using the strategy of promising regions can obtain better results on all the five algorithms. The results of the Wilcoxon signed-rank test in Table 2 also validate the efficiency of using promising regions. Using promising regions can achieve significantly better results than the baseline in more than half

of the tasks. For the remaining problems, they obtain results equal to those of the baseline. Regarding `PriorBand`, for the four tasks with prior information, `Lamda+PriorBand` achieves results comparable to those of `PriorBand`. However, for the four tasks without prior information, `Lamda+PriorBand` achieves better results. For `BOHB`, using the strategy of promising regions improves in rank as the consumed resources grow. The main reason for such slow-starting may caused by the resources needed for finding promising regions. However, it quickly takes the top rank after using about 15 HF resources. `MUMBO`, `BO` and `RS` present similar performances in the condition of using promising regions.

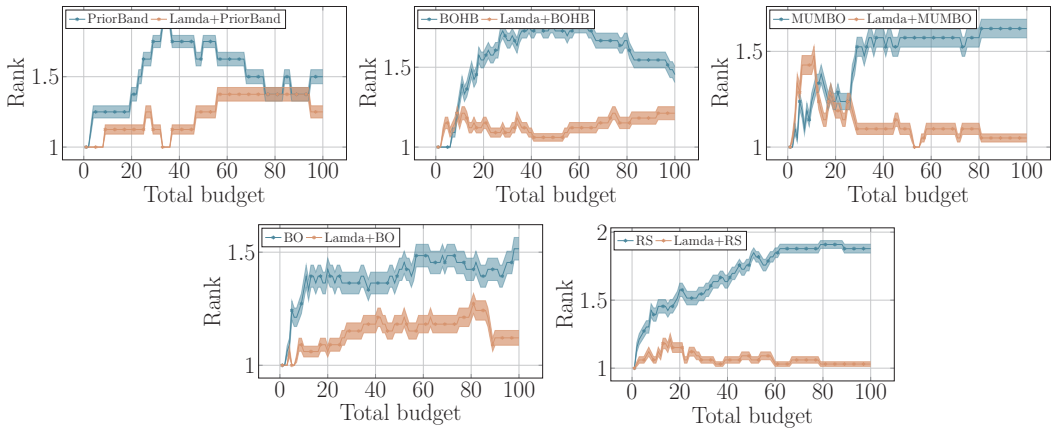


Figure 5: Comparing average relative ranks of `PriorBand`, `BOHB`, `MUMBO`, `BO` and `RS` under the proposed framework across 33 HPO tasks.

Table 2: Performance comparison (**Win**/Lose/Tie) of `Lamda+PriorBand`, `Lamda+BOHB`, `Lamda+MUMBO`, `Lamda+BO` and `Lamda+RS` against their baselines over 100 HF evaluations.

`Lamda+PriorBand`	`Lamda+BOHB`	`Lamda+MUMBO`	`Lamda+BO`	`Lamda+RS`
3/0/5	**24**/0/9	**19**/0/14	**17**/1/15	**29**/1/3

Figure 6 and Figure 17 to Figure 24 shows the performance curves for each benchmark under the framework of `Priorband`, `BOHB`, `MUMBO`, `BO` and `RS`. Within the framework of `Priorband`, `Lamda+Priorband` converge faster on all the 8 tasks as shown in Figure 6. For other four algorithms, using the promising regions accelerates the discovery of effective solutions compared to the baseline on most of the tasks. To better understand the results, we sample $10,000$ hyperparameter configurations for each benchmark and evaluate their performance at high and low fidelities. The configurations are mapped into 2D space. We visualize the top 10% solutions at the high and low fidelities, with high fidelity solutions marked in red as shown in Figure 13, Figure 14, Figure 15, and Figure 16. For FCNet, PD1, and NAS-Bench-201, the gap between `Lamda+BOHB` and the naıve `BOHB` is caused by the great overlapping between the high and low fidelities as shown in Figure 13.

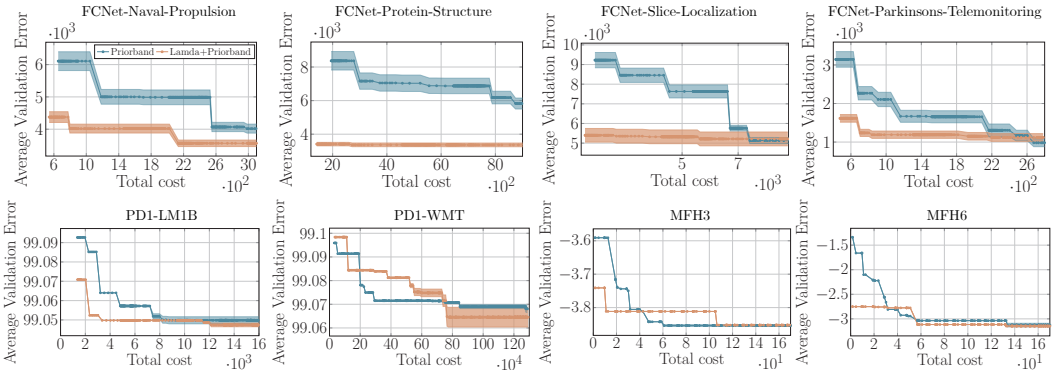


Figure 6: Validation error observed in tuning 8 HPO tasks, using `PriorBand` as the baseline.

Additionally, Figure 7 shows the found good solutions by the LF. It can be seen that these solutions are close to the good solutions of HF.

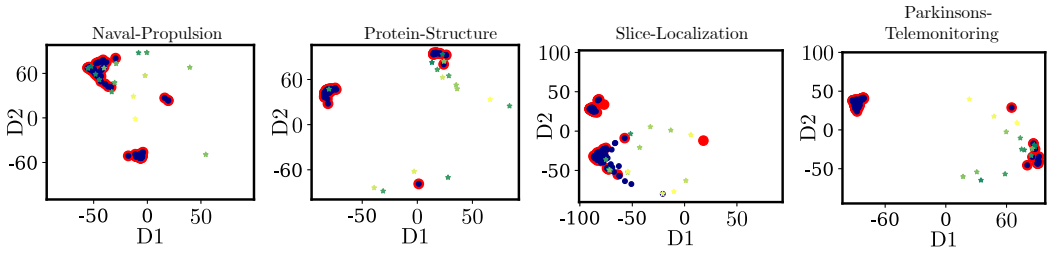


Figure 7: Visualization of good solutions identified by `Lamda+BOHB` at the first stage for FCNet. The solutions were mapped to a 2D representation for clarity. The red and blue points are the real top 10% high and low fidelity solutions from 10,000 sampling points. Stars are obtained by `Lamda+BOHB`, with a more yellow color indicating later sampling.

Results on raw problems: In this part, we evaluate `BOHB` and `Lamda+BOHB` on three raw HPO tasks. Figure 8 shows the the performance curves on three vision problems. We observe that the performance of `Lamda+BOHB` is worse than `BOHB` at the initial iteration. However, it quickly outperforms `BOHB` after some resources. The main reason is that the promising regions at the high and low fidelity have great overlapping as shown Figure 9.

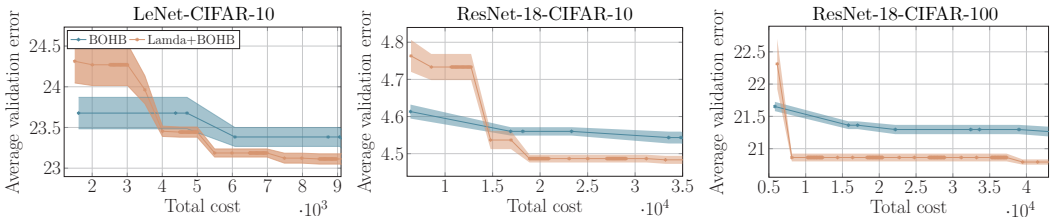


Figure 8: Validation error observed in tuning raw problems.

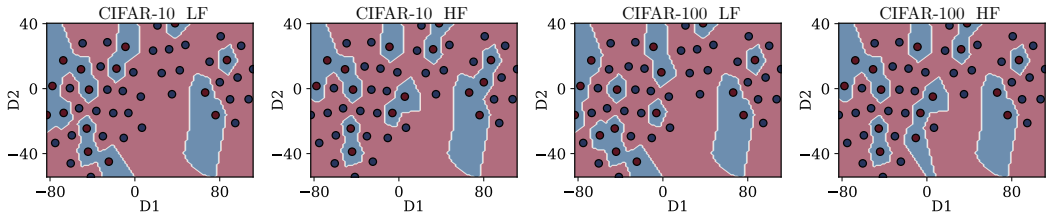


Figure 9: Visualizing the top 30% of solutions (represented by blue regions) in both high and low fidelity while optimizing the hyperparameters of ResNet-18 on CIFAR-10 and CIFAR-100 datasets. The data, originally in a higher-dimensional space, has been dimensionally reduced to a 2D representation for clarity.

4.2 Peer Comparison

Results on tabular and surrogate benchmarks: This experiment demonstrates how the performance of the proposed algorithm framework compared to the other methods over the number of evaluations. Figure 10 shows the average rank over the 33 tasks. According to Figure 10, we observe that `Lamda+BO` and `Lamda+MUMBO` consistently quickly take the top and keep the rank until the end. It also can be seen that `Hyperband` and `RS` are the two worst algorithms, which may be due to the random sampling strategy.

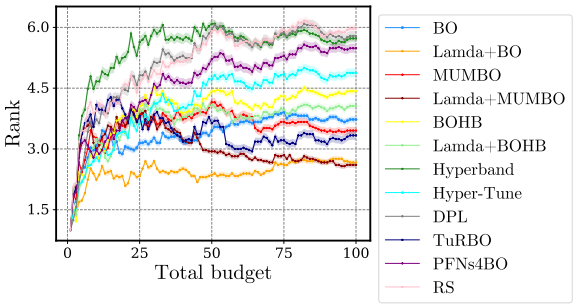


Figure 10: Comparing average relative ranks of peer algorithms across 33 HPO tasks.

4.3 PARAMETER ANALYSIS

We investigate the impact of parameters in `Lamda` within the `BOHB` framework, including different budgets (B) and thresholds (γ) for stopping the first phase, the interval for calculating the overlapping coefficient (Δ), the quantile (α) used in the TPE, and the initial weight (w_0). Four tasks at the XGBoost benchmark, each involving a 10-dimensional hyperparameter optimization problem, are used for the experiments. The budgets are varied as $B = D, 4D, 8D, 10D$, and $20D$, and γ values are tested at $0.5, 0.2$, and 0.1. As shown in Figure 27, the choice of B influences algorithm performance, where too high a budget ($B > 8D$) leads to excessive resource consumption in the first phase. The impact of γ on the algorithm is relatively minor as shown in Figure 28, likely due to the constraints imposed by the maximum budget B. Additionally, we investigate the influence of the parameter Δ on the algorithm's performance, as illustrated in Figure 29. The settings for Δ are $3, 5, 15, 35$, and 50. The results indicate that both excessively large and excessively small values of Δ slightly affect the algorithm's performance. Specifically, values of Δ that are too low may cause the algorithm to erroneously determine that promising regions have stabilized, whereas excessively high values of Δ can lead to considerable delays in the algorithm's capacity to verify the stability of these regions. We also analyze the influence of parameter α using the values 5, 15, and 25. The results in Figure 30 indicate no significant impact on the algorithm's performance.

Regarding the initial weight w_0, we examine settings of $1, 0.8, 0.5, 0.3$, and 0.1. The results, illustrated in Figure 31, suggest that while the optimal w_0 slightly vary across tasks, its overall impact on the algorithm's performance is minimal. In addition, values above 0.1 consistently outperform the original `BOHB`. Further analysis of rankings show that settings with $w > 0.1$ achieve better results compared to $w = 0.1$. Notably, a setting of $w = 1$ shows superior performance during the early stages of the optimization. These results also indicate the efficiency of using the promising regions.

5. LIMITATIONS AND FUTURE WORK

In this work, we only consider two fidelities for a proof-of-concept purpose. Our next step is to extend the current `Lamda` framework for tackling multiple fidelity levels. In addition, there is a gap on theoretical underpinnings about how the involved parameters, such as the quantile threshold in LF problems and the overlapping coefficient between LF and HF landscape, impact the convergence rate or regret of the HBO methods augmented with `Lamda`. Last but not the least, this paper is mainly designed for multi-fidelity hyperparameter optimization. It will be interesting to explore its applications to a broader range of black-box optimization problems where multi-fidelity experiments and data are prevalent (e.g., computational fluid dynamics optimization in engineering design (Barrett et al., 2006; Liu et al., 2017), and new material (Goldfeld et al., 2005; Khatamsaz et al., 2021), or drug design (Fare et al., 2022; Greenman et al., 2021) in scientific discovery).

6. CONCLUSIONS

This paper highlights a common limitation in existing HPO algorithms, which often searches across the whole search space. While some methods leverage prior knowledge to constrain the search space, accessibility to the knowledge is not always guaranteed. To address this challenge, we have developed an algorithmic framework that enables algorithms to autonomously identify promising regions from the LF to accelerate the HPO process, based on the the potential overlap of promising regions between high- and low-fidelity HPO landscape. This framework is integrated with a variety of existing HPO techniques, including prior- and bandit-based methods, as well as multi-fidelity BO, to enhance their efficacy. We support the rationale behind this augmentation through theoretical analysis focused on prior-based Bayesian optimization and bandit-based Hyperband. Our empirical evaluations across diverse hyperparameter optimization tasks—such as fully connected networks, transformers, ResNets, and neural architecture search benchmarks, including joint architecture and hyperparameter searches—demonstrate the competitiveness of our methods.

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A. Theoretical Analysis

A.1 Proofs of Proposition 1

Proof. Using the definition of $\rho(\varphi_1, \varphi_2)$ in equation (3), the OVL between $\varphi(\mathbf{x})$, $\varphi_{\text{pro}}(\mathbf{x})$, $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ and $\varphi_*(\mathbf{x})$ are computed as follows:

$$\begin{aligned}
\rho(\varphi(\mathbf{x}), \varphi_*(\mathbf{x})) &= 1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x}, \\
\rho(\varphi_{\text{pro}}(\mathbf{x}), \varphi_*(\mathbf{x})) &= 1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x}, \\
\rho(\tilde{\varphi}_{\text{pro}}(\mathbf{x}), \varphi_*(\mathbf{x})) &= 1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\tilde{\varphi}_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x}.
\end{aligned} \tag{11}$$

where

$$\rho(\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})) = \int_{\mathbf{x}\in\mathcal{X}} \min\{\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})\}\, d\mathbf{x} = 1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi_1(\mathbf{x}) - \varphi_2(\mathbf{x})|\, d\mathbf{x}. \tag{12}$$

Given that thus $\varphi(\mathbf{x})$ has a smaller overlap with $\varphi_*(\mathbf{x})$ than $\varphi_{\text{pro}}(\mathbf{x})$, it follows that:

$$\begin{aligned}
&\rho(\varphi(\mathbf{x}), \varphi_*(\mathbf{x})) - \rho(\varphi_{\text{pro}}(\mathbf{x}), \varphi_*(\mathbf{x})) \\
&= 1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} - \left(1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x}\right) \\
&= \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} \\
&= \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})| - |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} \leq 0
\end{aligned} \tag{13}$$

Given the above, if $\rho(\varphi(\mathbf{x}), \varphi_*(\mathbf{x})) < \rho(\tilde{\varphi}_{\text{pro}}(\mathbf{x}), \varphi_*(\mathbf{x}))$, it implies that $\varphi(\mathbf{x})$ has a smaller overlap with $\varphi_*(\mathbf{x})$ than $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$. This can be further analyzed as:

$$\begin{aligned}
&\rho(\varphi(\mathbf{x}), \varphi_*(\mathbf{x})) - \rho(\tilde{\varphi}_{\text{pro}}(\mathbf{x}), \varphi_*(\mathbf{x})) \\
&= 1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} - \left(1 - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |w_1\cdot\varphi(\mathbf{x}) + w_2\cdot\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x}\right) \\
&= \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |w_1\cdot\varphi(\mathbf{x}) + w_2\cdot\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} - \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} \\
&\leq \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} w_1\cdot|\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})| + w_2\cdot|\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})| - |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} \\
&= \frac{1}{2}\int_{\mathbf{x}\in\mathcal{X}} w_2\cdot|\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})| - w_2\cdot|\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} \\
&= \frac{w_2}{2}\int_{\mathbf{x}\in\mathcal{X}} |\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})| - |\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})|\, d\mathbf{x} \leq 0
\end{aligned} \tag{14}$$

where the inequality is obtained with the following formula:

$$\begin{aligned}
&|w_1\cdot\varphi(\mathbf{x}) + w_2\cdot\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})| \\
&= |w_1\cdot\varphi(\mathbf{x}) - w_1\cdot\varphi_*(\mathbf{x}) + w_2\cdot\varphi_{\text{pro}}(\mathbf{x}) - w_2\cdot\varphi_*(\mathbf{x})| \\
&\leq w_1\cdot|\varphi(\mathbf{x}) - \varphi_*(\mathbf{x})| + w_2\cdot|\varphi_{\text{pro}}(\mathbf{x}) - \varphi_*(\mathbf{x})|
\end{aligned} \tag{15}$$

This implies that $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ has a greater overlap with $\varphi_*(\mathbf{x})$ than $\varphi(\mathbf{x})$ does. □

A.2 Proofs of Theorem 1

In the context of sequential design, let $\mathcal{F}_N$ denote the σ-algebra generated by the random variables $\mathbf{x}^1, Z^1, \ldots, \mathbf{x}^N, Z^N$ where Z^i is the observation of $f_l(\mathbf{x}^i)$. Additionally, let $\mathcal{F}_{N,\tilde{\mathbf{x}}}$ be the σ-algebra

generated by $\mathbf{x}^1, Z^1, \ldots, \mathbf{x}^N, Z^N, \tilde{\mathbf{x}}, \tilde{Z}$ with $\tilde{Z}$ the observation of $f_h(\tilde{\mathbf{x}})$. Then, the EI-based sequential design of `Lamda+BO` takes the following form:

$$\mathbf{x}_{N+1} = \arg\max_{\tilde{\mathbf{x}} \in \Omega} \mathbb{E}_N \left[M_N^0 - M_{N,\tilde{\mathbf{x}}}^\rho \right], \tag{16}$$

in which y_h^* is the threshold of promising solutions in HF problems lower bounded by the α quantile of $\{f_\ell(\mathbf{x}) | \forall \mathbf{x} \in \mathcal{S}\}$ due to the overlapping between HF and LF landscape, and

$$M_{N,\tilde{\mathbf{x}}}^\rho = \min_{\mathbf{x} \in \mathcal{X},\, \mathbb{P}(f_h(\mathbf{x}) < y_h^* | \mathcal{F}_{N,\tilde{\mathbf{x}}}) = 1,\, \sigma_f(\mathbf{x} | \mathcal{F}_{N,\tilde{\mathbf{x}}}) = 0} \tilde{f}(\mathbf{x}), \tag{17}$$

$$M_N^0 = \min_{\mathbf{x} \in \mathcal{X},\, \mathbb{P}(f_h(\mathbf{x}) < y_h^* | \mathcal{F}) = 1,\, \sigma_f(\mathbf{x} | \mathcal{F}_N) = 0} \tilde{f}(\mathbf{x}). \tag{18}$$

When GPs are non-degenerate, i.e., $\sigma_f = 0$ only if $\mathbf{x} \in \mathcal{D}$ equation (16) becomes equivalent to equation (9). Specifically, M_N^0 will be equal to $f_{\mathcal{D}}^*$ in equation (8), while $M_{N,\tilde{\mathbf{x}}}^\rho$ will be the predicted promising HF objective value under threshold y_h^* implicitly defined by equation (6). Next, we present the criteria for *asymptotic convergence* of `Lamda+BO`. The proof of the first statement, i.e., the convergence of the acquisition function, compromises three steps.

Step 1. `Lamda+BO` serves as a stepwise uncertainty reduction (SUR) sequential design. For $N \geq 2$, a minimization version of equation (16) can be given as

$$\mathbf{x}_{N+1} = \arg\min_{\tilde{\mathbf{x}} \in \mathcal{X}} \mathbb{E}_N \left[H_{N,\tilde{\mathbf{x}}} \right], \tag{19}$$

in which

$$H_{N,\tilde{\mathbf{x}}} = M_{N,\tilde{\mathbf{x}}}^\rho - M_N^0 = \mathbb{E}_{N,\tilde{\mathbf{x}}} \left[M_{N,\tilde{\mathbf{x}}}^\rho - \min_{\mathbf{x} \in \mathcal{X},\, \mathbb{P}(f_h(\mathbf{x}) < y_h^*)} \tilde{f}(\mathbf{x}) \right].$$

The above equation holds since: $i)$ M_N^0 is independent from $\tilde{\mathbf{x}}$, and $ii)$ $\mathbb{E}_{N,\tilde{\mathbf{x}}} \left[M_{N,\tilde{\mathbf{x}}}^\rho \right] = M_{N,\tilde{\mathbf{x}}}^\rho$ for minimum operation. Therefore this strategy can be transformed into an equivalent SUR sequential design strategy for $H_{N,\tilde{\mathbf{x}}}$. Likewise, we define

$$H_N = \mathbb{E}_N \left[M_N^\rho - \min_{\mathbf{x} \in \mathcal{X},\, f_h(\mathbf{x}) < y_h^*} \tilde{f}(\mathbf{x}) \right]. \tag{20}$$

Step 2. (H_N) is a supermartingale. For well-structured GP models and well-defined smooth functions ρ^i, we have: $i)$ $\sigma_f(\mathbf{x} | \mathcal{F}_{N+1}) \leq \sigma_f(\mathbf{x} | \mathcal{F}_N)$ (based on the definition of GP predicted variance), and $ii)$ $\mathbb{P}(f_h(\mathbf{x}) < y_h^*(\mathbf{x}) | \mathcal{F}_N) = 1$ is sufficient for $\mathbb{P}(f_h(\mathbf{x}) < y_h^*(\mathbf{x}) | \mathcal{F}_{N+1}) = 1$ based on the non-increasing property of density estimation on an evaluated solution $\mathbf{x}^N$. Therefore, the following inequality holds:

$$H_N - \mathbb{E}_N[H_{N+1}] = \mathbb{E}_N \left[M_N^\rho - M_{N+1}^\rho \right] \geq 0, \tag{21}$$

which implies that $(H_N)_{N \in \mathbb{N}}$ is a supermartingale. Consequently, there is $H_N - \mathbb{E}_N[H_{N+1}] \to 0$ as $N \to \infty$, and also

$$\sup_{\tilde{\mathbf{x}} \in \mathcal{X}} \left[H_N - \mathbb{E}_N[H_{N,\tilde{\mathbf{x}}}] \right] \to 0. \tag{22}$$

Step 3. The acquisition function of `Lamda+BO` converges to zero almost surely. Due to the lower bound, according to equation (21), as evaluations of HF objective increase, $\tilde{\varphi}_{\text{pro}}$ tends to converge to φ. Note that for $N \to \infty$, $M_N^\rho = M_N^0$ as this convergence appears. Additionally, we also have

$$\sup_{\tilde{\mathbf{x}} \in \mathcal{X}} \mathbb{E}_N \left[M_N^\rho - M_{N,\tilde{\mathbf{x}}}^\rho \right] \geq \sup_{\tilde{\mathbf{x}} \in \mathcal{X}} \mathbb{E}_N \left[M_N^0 - M_{N,\tilde{\mathbf{x}}}^\rho \right] \geq \sup_{\tilde{\mathbf{x}} \in \mathcal{X}} \tilde{\varphi}_{\text{pro}}(\mathbf{x}) \text{EI}(\tilde{\mathbf{x}} | \mathcal{D}). \tag{23}$$

Therefore, with the same proof as that of Proposition 2.9 (Bect et al., 2019), for $N \to \infty$, equation 22 and equation 23 yield $\tilde{\varphi}_{\text{pro}}(\mathbf{x}) \text{EI}(\tilde{\mathbf{x}} | \mathcal{D}) \to 0$. This completes the proof for the first statement.

The second statement stands according to the global search ability of EI and corresponding dense evaluated solutions in $\mathcal{X}$. We complete the proof by providing the following facts: $i)$ $\tilde{\varphi}_{\text{pro}}(\mathbf{x}) \sigma_f(\tilde{\mathbf{x}}) \to 0$ holds from the first statement; $ii)$ the lower bound y_h^* will be tight when $N \to \infty$; and $iii)$ $\sigma_f(z | \mathcal{F}_N) \to 0$ for all sequences accordingly. Based on these facts, the sequence is almost surely dense in $\mathcal{X}$. As a result, $f_{\mathcal{D}}^*$ from any sequence converges to $f_{\mathcal{X}}^*$ almost surely when $N \to \infty$.

B. Related Works

B.1 Multi-fidelity Bayesian optimization

In the realm of MFBO, previous research primarily leverages LF to construct an accurate MF model for guiding the sampling process (Swersky et al., 2013; Poloczek et al., 2017; Kandasamy et al., 2019; Mikkola et al., 2022; Li et al., 2020b). One challenge in these methods is to model performance using data from various fidelities. Solutions include employing Gaussian process regression (GPR) models tailored to each fidelity level (Kandasamy et al., 2019), multi-task GPR models for discrete fidelity levels (Swersky et al., 2013; Poloczek et al., 2017; Mikkola et al., 2022; Li et al., 2020b), and GPR models for a continuous fidelity space (Klein et al., 2017; Kandasamy et al., 2017). While Gaussian processes are commonly used for modelling the surrogate function, Li et al. (Li et al., 2020b; 2021a) have implemented deep neural networks to represent the relationships across different fidelities. In terms of sampling, entropy search methods (Swersky et al., 2013; Poloczek et al., 2017; Takeno et al., 2020) are utilized, which take into account both the information gain and the associated costs of each fidelity level. These techniques enable the sampling of new solutions at either low or high fidelity levels, gradually leading to improved hyperparameters in the HF space.

B.2 Bandit based method

Bandit-based methods employ LF for identifying promising solutions for HF evaluations (Falkner et al., 2018; Li et al., 2022b; Awad et al., 2021). In pioneering work in the field, Li et al. (2017) introduced Hyperband, a method that improves upon the Successive Halving (SH) algorithm by integrating various early stopping strategies across multiple SH brackets. Each bracket starts with a different number of solutions at varied fidelity levels. However, Hyperband's approach of randomly sampling solutions doesn't utilize previous sample information (Falkner et al., 2018). To enhance this, Falkner et al. (2018) developed BOHB, which combines BO with Hyperband, using the tree Parzen estimator (TPE) (Bergstra et al., 2011) to build surrogate models for each fidelity level. While BOHB is effective, it struggles with discrete dimensions and scaling to high-dimensional problems. Addressing these challenges, Awad et al. (2021) enhanced BOHB with differential evolution for better candidate sampling. Additionally, Li et al. (2021b) developed an MF ensemble model that integrates information from all fidelity levels to more accurately estimate the highest fidelity. Nevertheless, despite their utilization of LF data, these approaches still demand extensive exploration throughout the entire search space.

B.3 Using Priors for Optimization

These methods concentrate on promising regions to reduce the consumed resources by leveraging prior information. A line of work uses prior information about locations of optimal solutions to accelerate the process of HPO. For instance to reduce evaluations on bad regions, Souza et al. (2021) injected priors about which parts of the input space will yield the best performance into BO's standard probabilistic model to form a pseudo-posterior, which was shown to be more sample-efficient than BO baselines. Further, Li et al. (2020a) incorporated Gaussian distributions of optimal solutions into the posterior distribution of observed data and used Thompson sampling to obtain the next solution. Ramachandran et al. (2020) used the prior distribution of optimal solutions to warp the search space, expanding around high-probability regions of optimal solutions and shrinking around low-probability regions. Truncated normal and gamma distributions were used to form the prior distributions. Additionally, Hvarfner et al. (2022) incorporated prior Gaussian distributions about locations of optimal solutions into the acquisition function, achieving competitive results across a wide range of benchmarks. Mallik et al. (2023) also integrated prior knowledge of optimal hyperparameters to enhance the efficiency of Hyperband. Although using prior distributions of locations of optimal solutions can accelerate optimization, accessing the prior for a specific task may not always be accessible.

B.4 Transfer search space

In addition to leveraging experts' prior, this method used information from previous tasks to reduce search space. For instance, Wistuba et al. (2015) pruned the bad regions of search space according

to the results from previous tasks. Perrone & Shen (2019) and Li et al. (2022a) utilized previous tasks to design a sub-region of the entire search space for a new task. While these approaches have demonstrated efficiency in using promising regions instead of the entire space, they require the preparation of source tasks and the evaluation of task similarities to effectively select relevant tasks for learning promising regions, which can be challenging (Perrone & Shen, 2019).

C. BENCHMARKS

C.1 TABULAR BENCHMARKS

FCNet: We utilized benchmarks for FCNet from Yahpo-Gym (Pfisterer et al., 2022), detailed in Table 3. The selected tasks include FCNet-Naval-Propulsion, FCNet-Protein-Structure, FCNet-Slice-Localization, and FCNet-Parkinsons-Telemonitoring.

NAS-Bench-301: Our NAS-Bench-301 benchmarks, also sourced from Yahpo-Gym (Pfisterer et al., 2022), focus on CIFAR-10. For hyperparameter details, refer to (Pfisterer et al., 2022).

NAS-Bench-201: This benchmark encompasses 6 hyperparameters for neural architecture search. It includes statistics from 15,625 CNN models across three datasets: CIFAR-10-valid, CIFAR-100, and ImageNet16-120 (Eggensperger et al., 2021). We simplify their name as CIFAR-10, CIFAR-100, and ImageNet in this paper.

Table 3: Hyperparameter ranges for FCNet.

Parameter	Name	Type	Range
Fidelity	epoch	int	$[1, 100]$
Hyperparameter	batch size	int	$[8, 64]$ (log-scale)
	initial learning rate	con	$[5e-04, 0.1]$ (log-scale)
	dropout 1	con	$[0.0, 0.6]$
	dropout 2	con	$[0.0, 0.6]$
	number of units 1	int	$[16, 512]$
	number of units 2	int	$[16, 512]$

C.2 SURROGATE BENCHMARKS

We utilized four problems from the PD1 benchmarks and three from the JAHSBench surrogate benchmarks. Detailed information about these benchmarks is available in (Mallik et al., 2023).

C.3 RAW PROBLEMS

The hyperparameters for the deep neural networks, LeNet and ResNet-18, are detailed in Table 4.

Table 4: Hyperparameter ranges for LeNet and ResNet-18.

Parameter	Name	Type	Range
Fidelity	datasize	con	$[0.3, 1]$
Hyperparameter	batch size	int	$[64, 512]$ (log-scale)
	initial learning rate	con	$[5e-3, 0.1]$ (log-scale)
	momentum	con	$[0.5, 0.99]$
	weight decay	con	$[1e-5, 1e-2]$
	nesterov	cat	{True, False}

C.4 PARAMETERS OF LF PROBLEMS

Table 5 shows parameters of LF problems used in the first phase and the corresponding OVL between high- and low-fidelity problems.

Table 5: Parameters of LF problems used in the first phase and the corresponding OVL between high- and low-fidelity problems.

Tasks	LF parameter	OVL	Tasks	LF parameter	OVL
MFH3	epoch=4	0.713	MFH6	epoch=4	0.728
XGBoost-40981	datasize=0.3	0.885	FCNet-Naval-Propulsion	epoch=4	0.901
XGBoost-41146	datasize=0.3	0.933	FCNet-Protein-Structure	epoch=4	0.694
XGBoost-1489	datasize=0.3	0.805	FCNet-Slice-Localization	epoch=4	0.731
XGBoost-1067	datasize=0.3	0.883	FCNet-Parkinsons-Telemonitoring	epoch=4	0.854
rpart-40981	datasize=0.3	0.167	NAS-Bench-301-CIFAR-10	epoch=20	0.712
rpart-41146	datasize=0.3	0.488	NAS-Bench-201-CIFAR-10	epoch=20	0.760
rpart-1089	datasize=0.3	0.89	NAS-Bench-201-CIFAR-100	epoch=20	0.727
rpart-1067	datasize=0.3	0.642	NAS-Bench-201-ImageNet	epoch=20	0.696
ranger-40981	datasize=0.3	0.711	JAHS-CIFAR-10	epoch=4	0.574
ranger-41146	datasize=0.3	0.782	JAHS-Colorectal-Histology	epoch=4	0.523
ranger-1489	datasize=0.3	0.77	JAHS-Fashion-MNIST	epoch=4	0.532
ranger-1067	datasize=0.3	NAN	PD1-LM1B	epoch=30	0.934
glmnet-40981	datasize=0.3	0.294	PD1-WMT	epoch=4	0.926
glmnet-41146	datasize=0.3	0.962	PD1-CIFAR-100	epoch=45	0.797
glmnet-1489	datasize=0.3	0.918	PD1-ImageNet	epoch=20	0.727
glmnet-1067	datasize=0.3	0.648	NAN	NAN	NAN

D. OVL BETWEEN LOW AND HIGH FIDELITY

Figure 11 presents the overlapping coefficients between good solutions in high- and low-fidelity settings across various HPO tasks. The overlapping coefficients are computed using equation (3) and are visualized over epochs or datasets for different benchmarks. It can be observed that the overlap generally increases with the number of iterations (e.g., epochs or dataset size), especially for FCNet, NAS-Bench-201, and RecNet-18. However, for NAS-Bench-301 and JAHS, the overlap exhibits a trend of decreasing in the middle stages before rising again. Specifically:

- FCNet and RecNet-18 show an overlap that is already close to or greater than 0.7 even at smaller iteration parameters (e.g., fewer epochs or smaller datasets), indicating strong LF-HF consistency and stability at earlier stages.
- For PD1 and NAS-Bench-201, the overlap reaches or exceeds 0.7 at specific points, such as epoch = 10 for PD1 and epoch = 20 for NAS-Bench-201, suggesting that these tasks achieve good LF-HF agreement relatively early in the optimization process.
- NAS-Bench-301 and JAHS, on the other hand, maintain relatively low overlap in the initial and middle stages. The overlap only increases significantly as the settings approach the HF level, indicating that these tasks require longer training or higher fidelity to achieve substantial LF-HF alignment.

E. DISTRIBUTION OF SOLUTIONS IN THE HF AND LF.

In this section, we present the distribution of solutions in the HF and LF settings. Figure 12 shows good solutions identified by `Lamda+BOHB` at the first phase for NAS-Bench-301 and JAHS. It can be observed that there is an overlap between the good solutions in the HF and LF settings, and the good solutions found in the first phase are close to these overlapping regions.

Moreover, Figure 13, Figure 14, Figure 15 and Figure 16 show the distribution of good solutions in the HF and LF. Across all 15 problems, a clear overlap is observed between the good solutions identified in both fidelity levels.

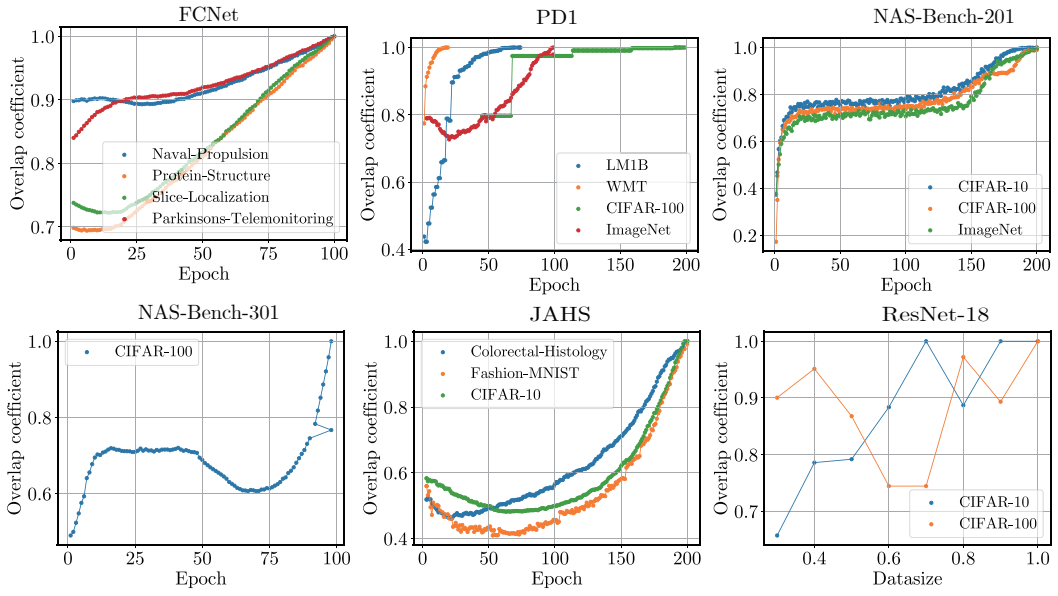

Figure 11: The overlapping coefficient of the HPO tasks.

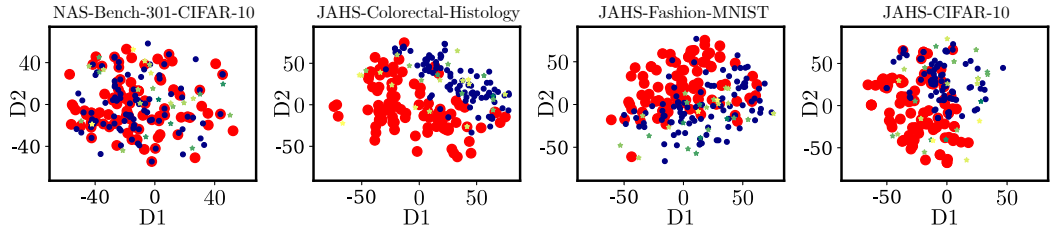

Figure 12: Visualization of good solutions identified by `Lamda+BOHB` at the first phase for NAS-Bench-301 and JAHS. The solutions were mapped to 2D. The red and blue points are the real top 10% high and low fidelity solutions from $10,000$ sampling points. Stars are obtained by `Lamda+BOHB`, with a more yellow color indicating later sampling.

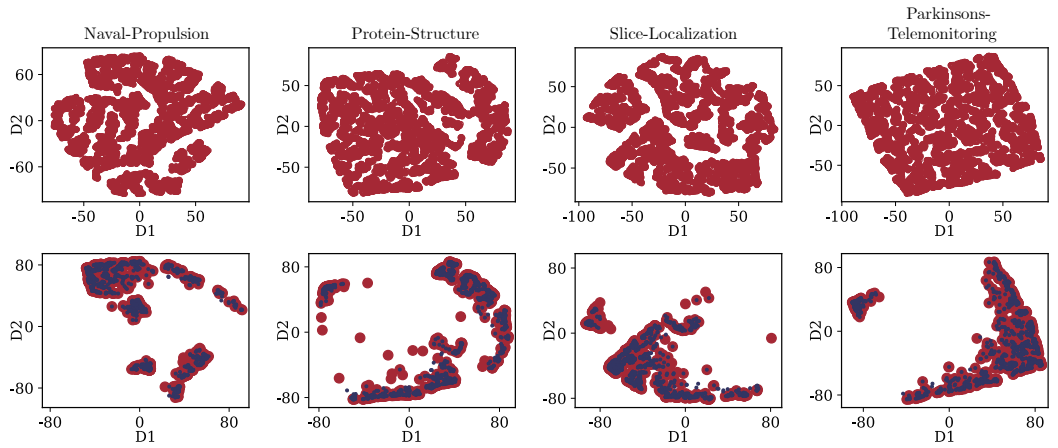

Figure 13: (Top) The visualization of $10,000$ hyperparameter configurations in the 2D space for FCNet. (Bottom) The visualization of the top 10% solutions at the high and low fidelity, with high fidelity solutions marked in red. In this case, LF is obtained by setting the epoch number as four.

F. Experimental Results

F.1 Convergence Curves

This section presents the convergence curves of the proposed algorithm and its peer methods. The convergence performance of `Lamda` under different algorithms, including `BOHB`, `MUMBO`, `BO`, and

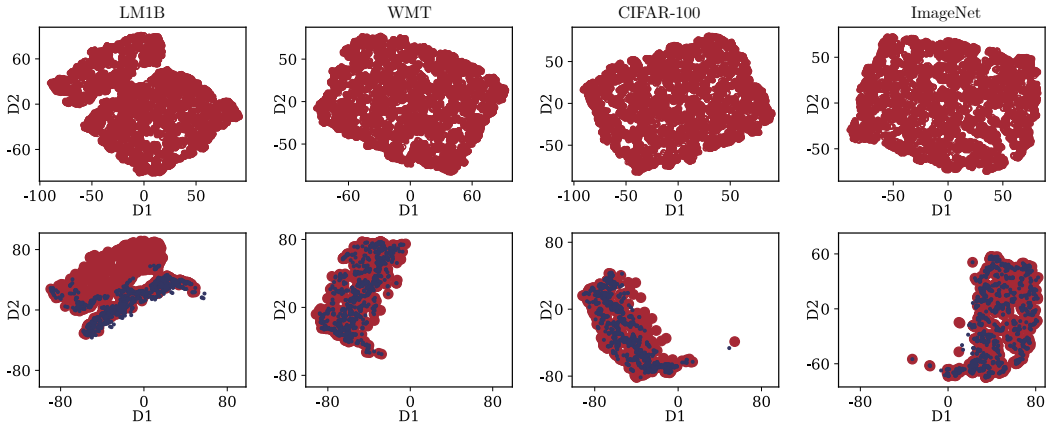

Figure 14: (Top) The visualization of the $10,000$ hyperparameter configurations in the 2D space for PD1. (Bottom) The visualization of the top 10% solutions at the high and low fidelity, with high fidelity solutions marked in red. In this case, LF is obtained by setting the epoch number as 30, 4, 45, and 20 for the four tasks.

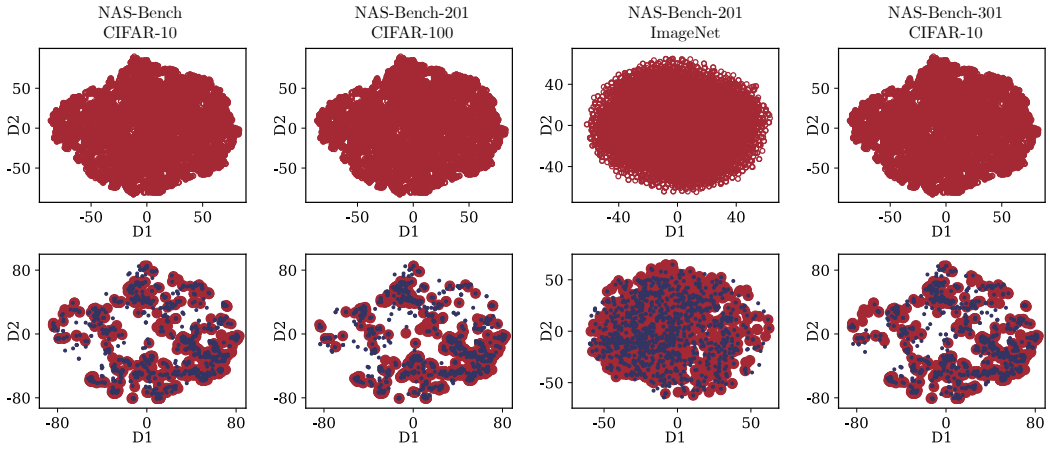

Figure 15: (Top) The visualization of $10,000$ hyperparameter configurations in the 2D space for NAS-Bench-201 and NAS-Bench-301. (Bottom) The visualization of the top 10% solutions at the high and low fidelity, with high fidelity solutions marked in red. In this case, LF is obtained by setting the epoch number as 20.

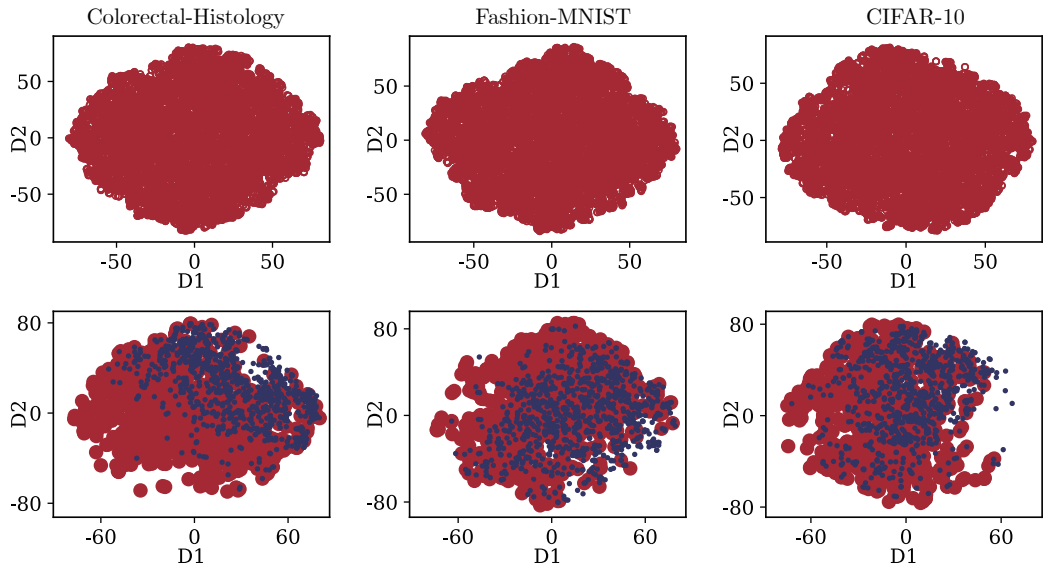

Figure 16: (Top) The visualization of $10,000$ hyperparameter configurations in the 2D space for JASH. (Bottom) The visualization of the top 10% solutions at the high and low fidelity, with high fidelity solutions marked in red. In this case, LF is obtained by setting the epoch number as 20.

RS, is illustrated in Figure 17, Figure 18, Figure 19, Figure 20, Figure 21, Figure 22, Figure 23 and Figure 24. The experimental results demonstrated that using Lamda can enhance peformanc of the baseline algorithms. The convergence curves of peer algorithms are presented in Figure 25 and Figure 26. Lamda also performs good compared with peer algorithms.

Figure 27, Figure 28, Figure 29, Figure 30 and Figure 31 depict the results of parameter analysis including budget (B), thresholds (γ) for stopping the first phase, the interval for calculating the overlapping coefficient (Δ), the quantile (α) used in the TPE, and the initial weight (w_0). These results indicate that the algorithm's performance is robust to the hyperparameter settings.

F.2 Table results of peer algorithms

Table 6 shows the peer algorithms' final validation errors of the current incumbent at 100 HF evaluations horizons.

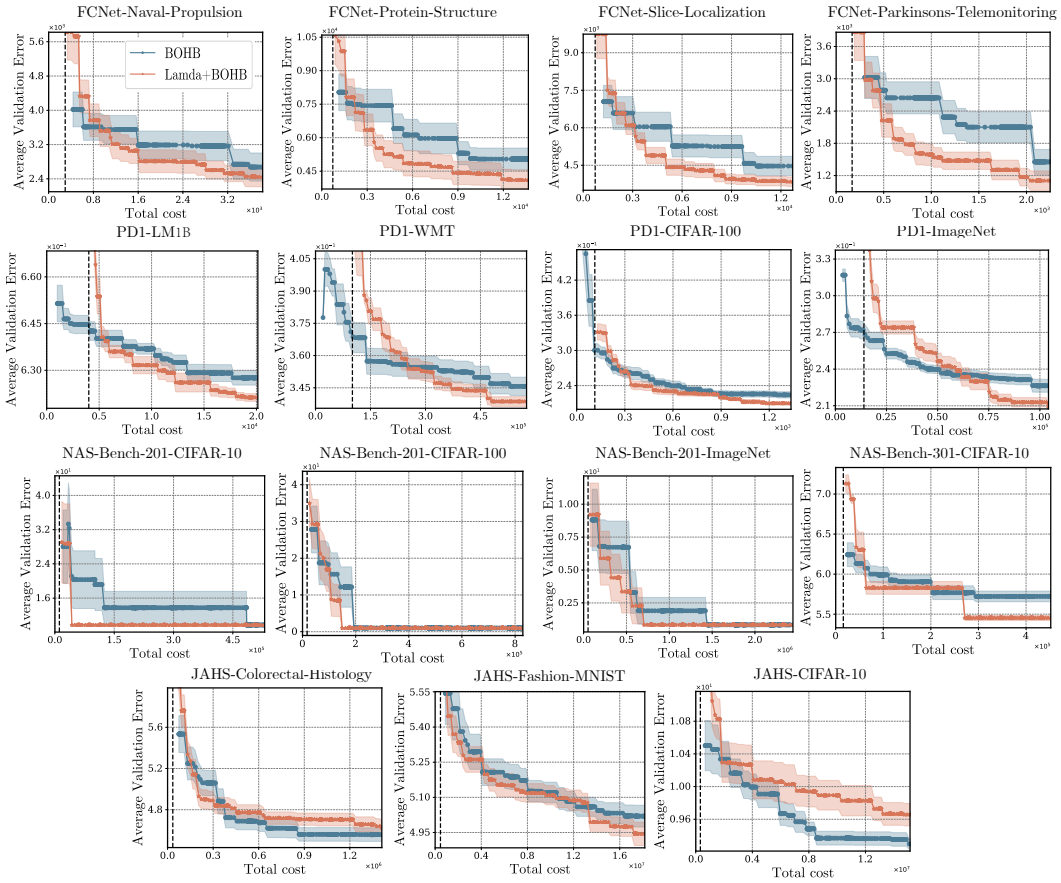

Figure 17: Validation error observed in tuning 15 HPO tasks, using BOHB as the baseline.

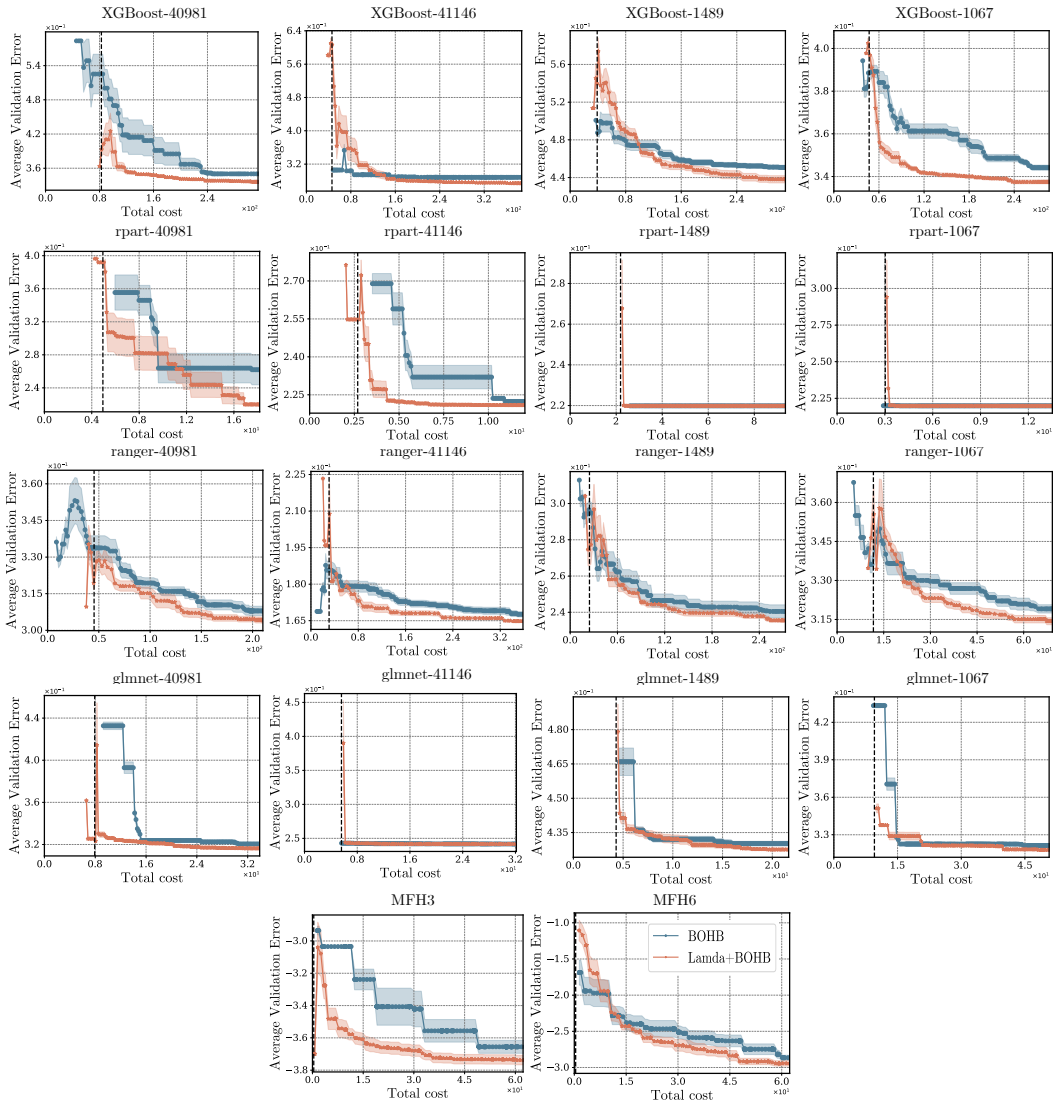

Figure 18: Validation error observed in tuning 18 HPO tasks, using BOHB as the baseline.

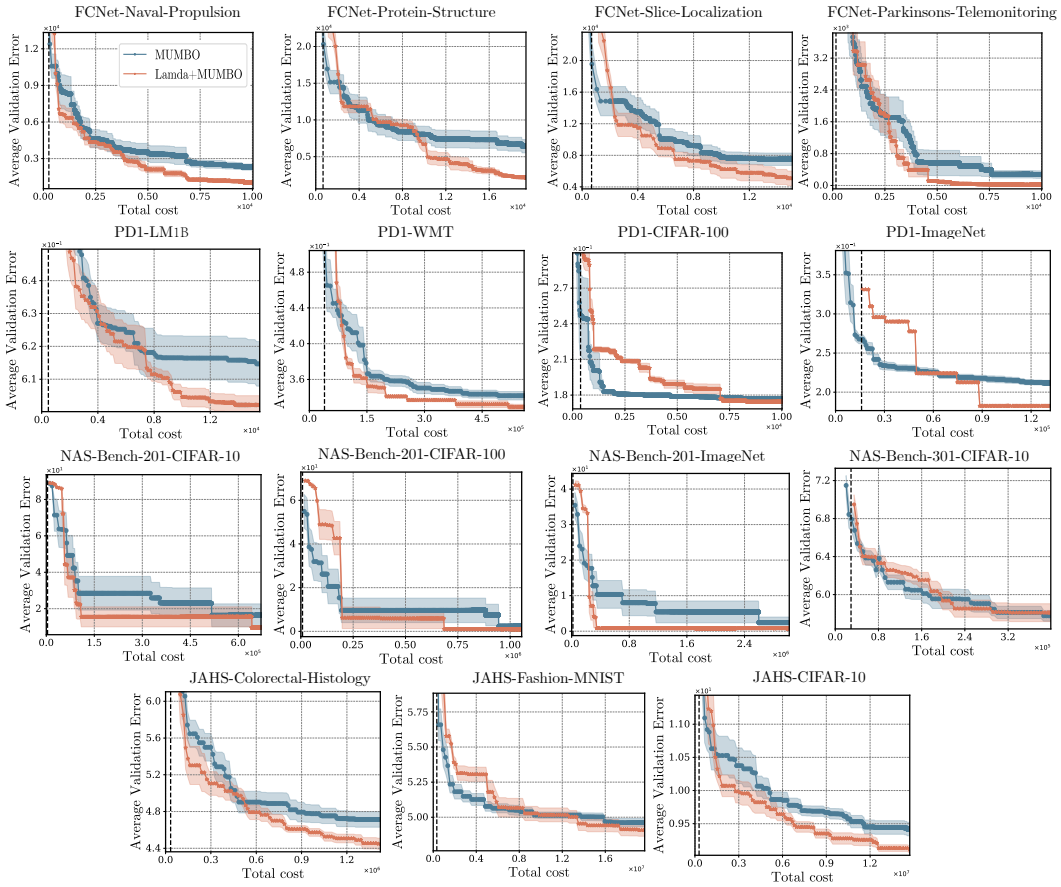

Figure 19: Validation error observed in tuning 15 HPO tasks, using MUMBO as the baseline.

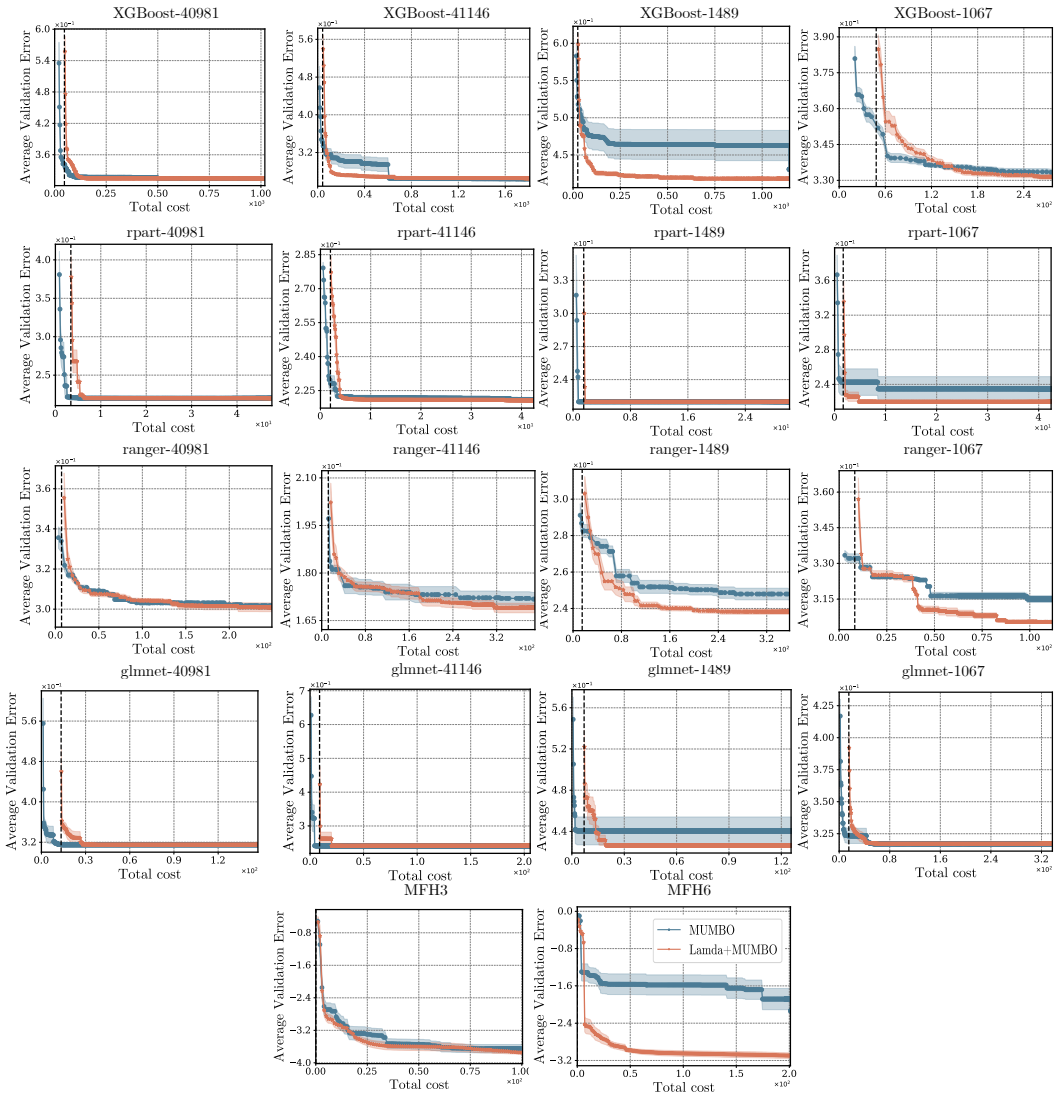

Figure 20: Validation error observed in tuning 18 HPO tasks, using MUMBO as the baseline.

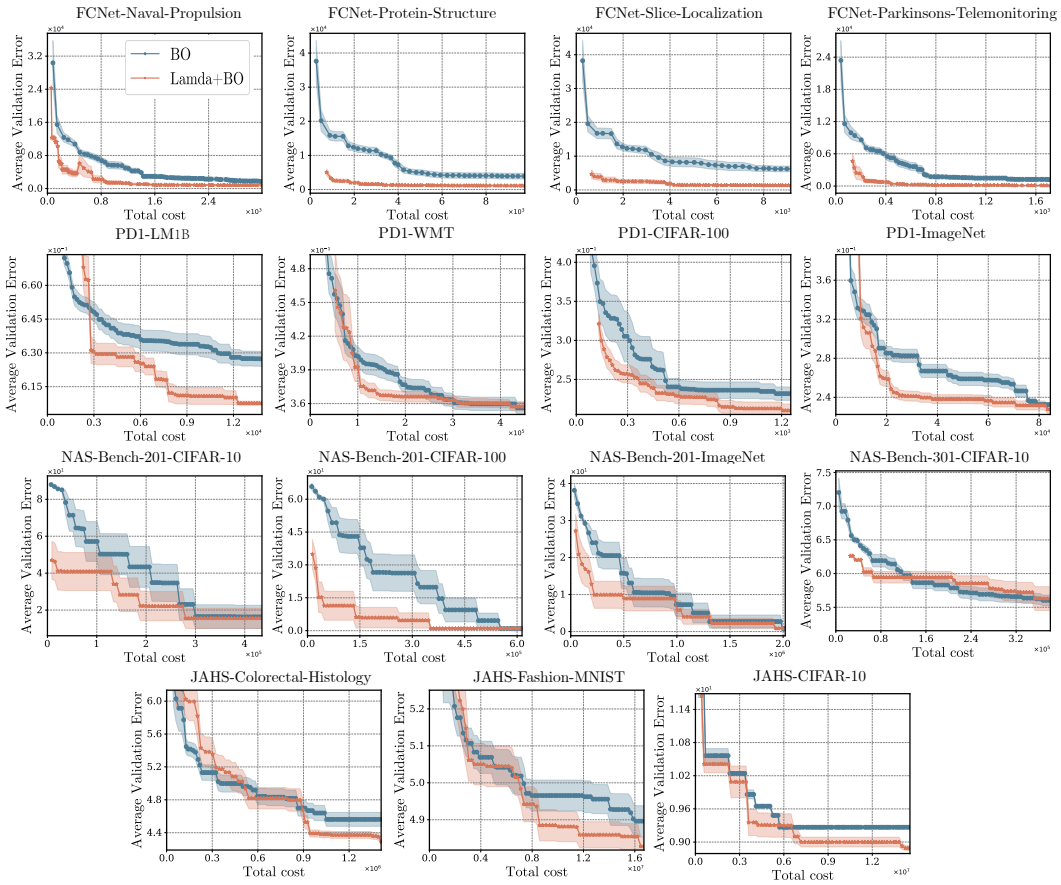

Figure 21: Validation error observed in tuning 15 HPO tasks, using BO as the baseline.

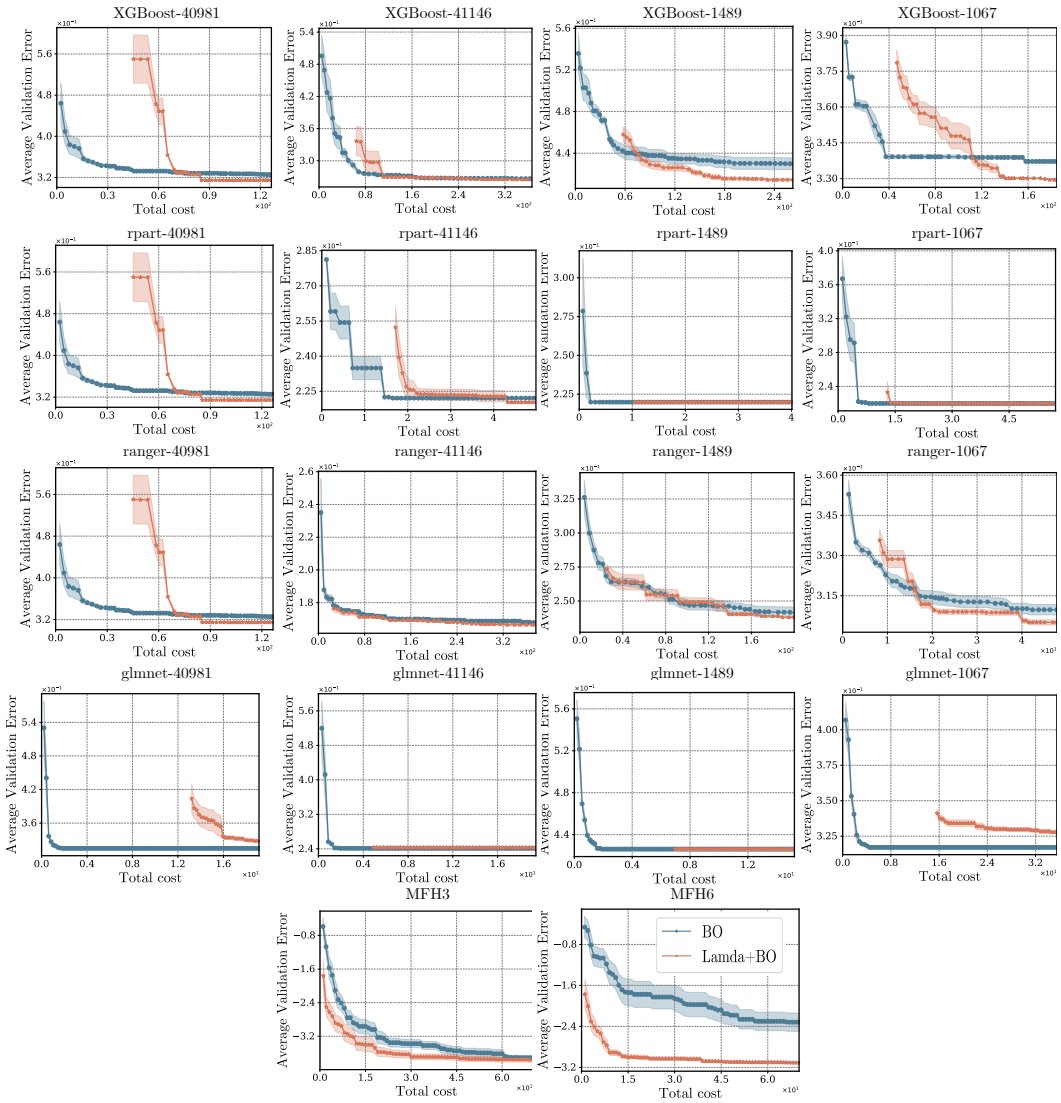

Figure 22: Validation error observed in tuning 18 HPO tasks, using BO as the baseline.

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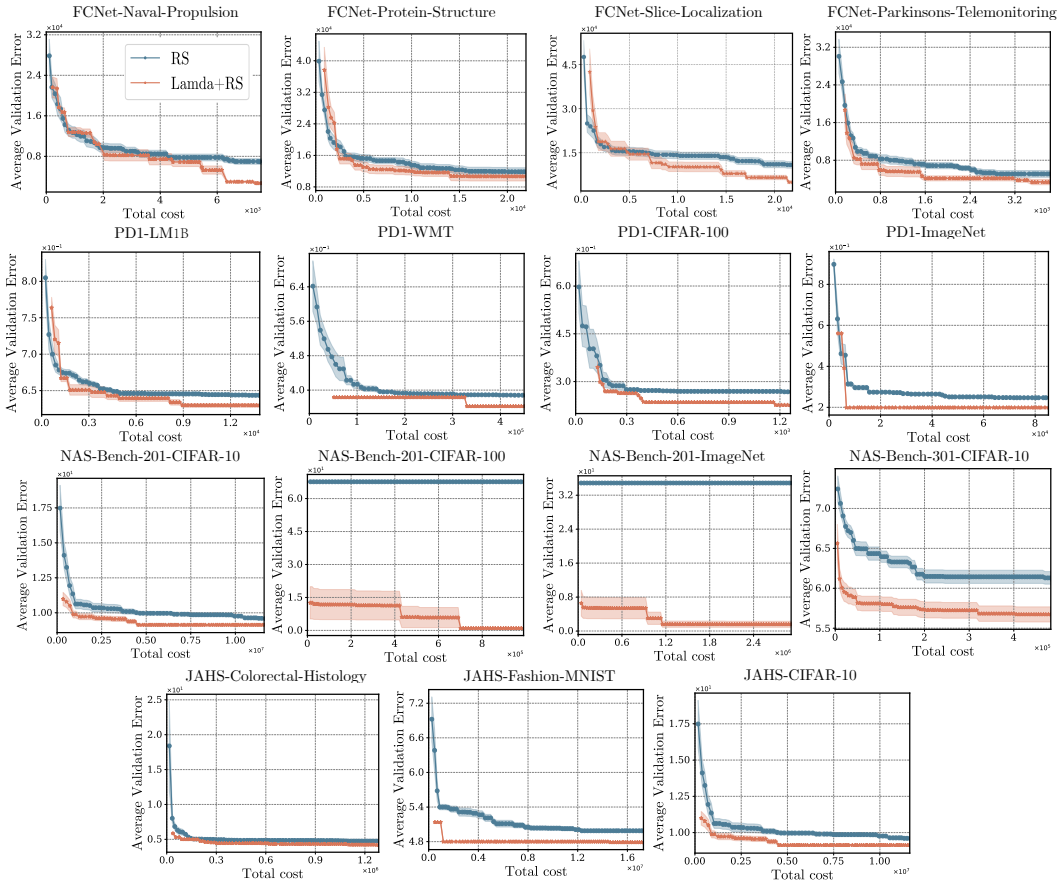

Figure 23: Validation error observed in tuning 15 HPO tasks, using RS as the baseline.

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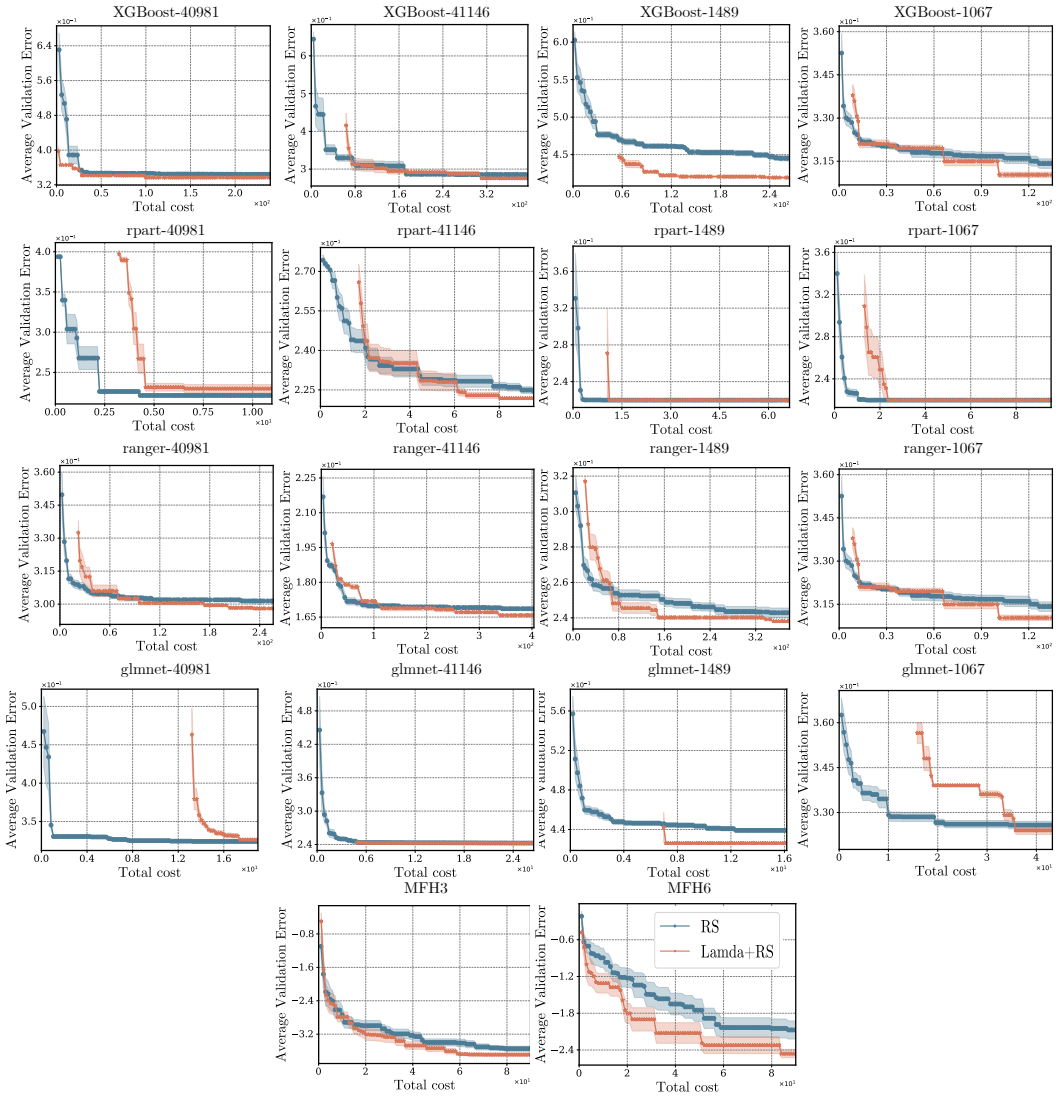

Figure 24: Validation error observed in tuning 18 HPO tasks, using RS as the baseline.

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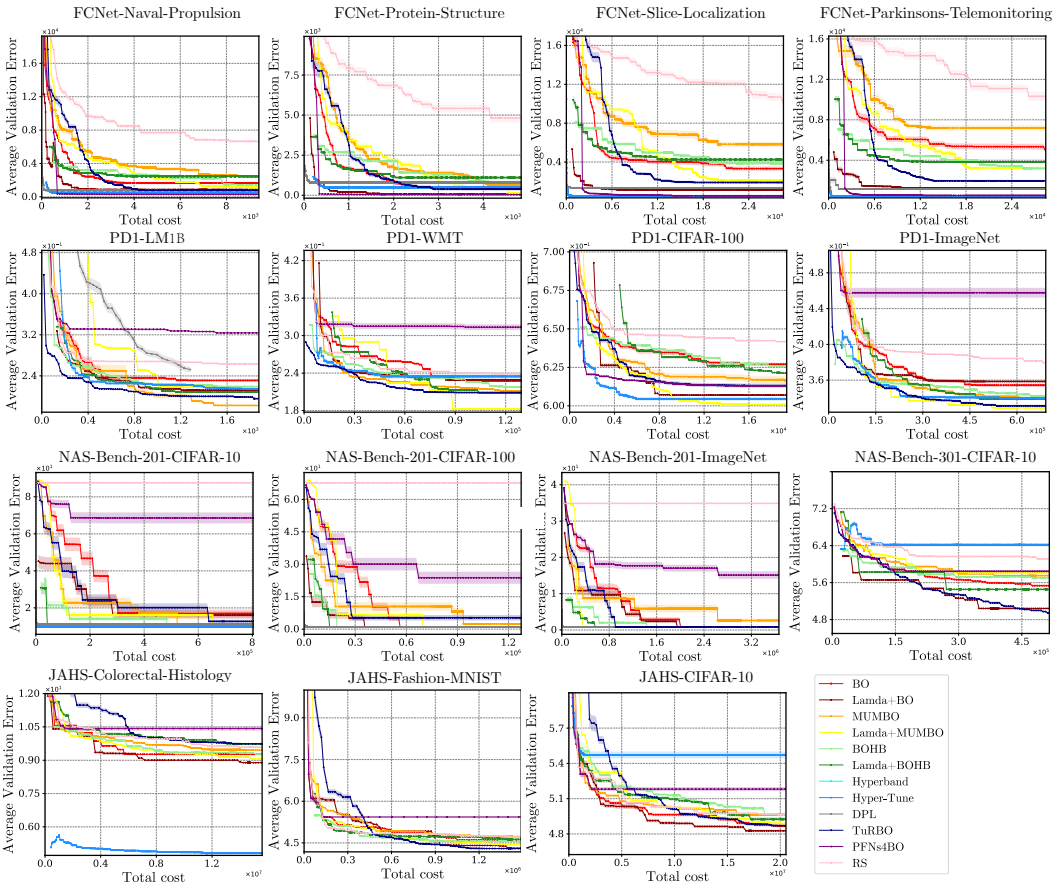

Figure 25: Validation error observed in tuning 15 HPO tasks, comparing peer algorithms.

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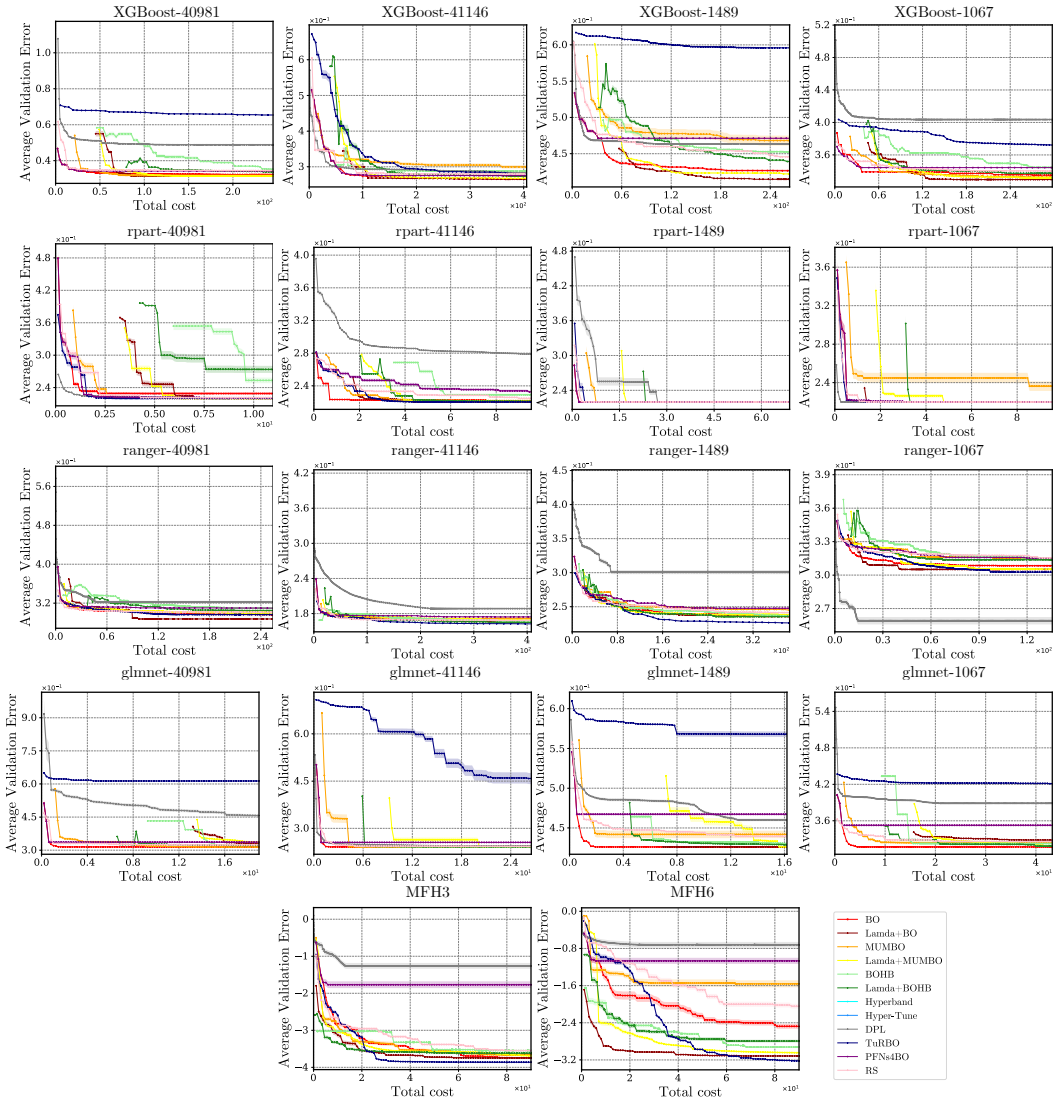

Figure 26: Validation error observed in tuning 18 HPO tasks, comparing peer algorithms.

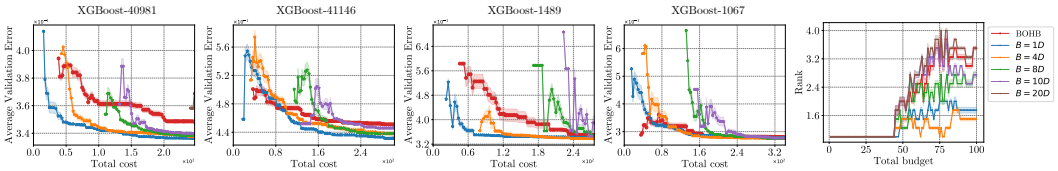

Figure 27: Validation errors of `Lamda+BOHB` under different parameters B used at the first phase.

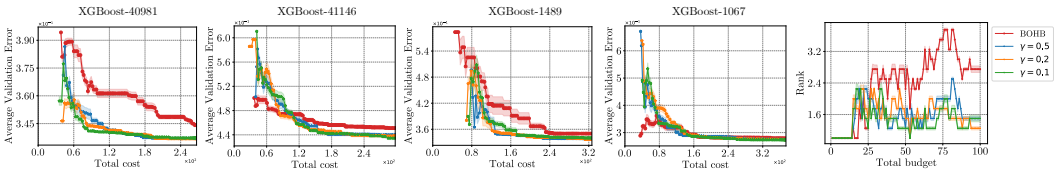

Figure 28: Validation error observed of `Lamda+BOHB` under different parameter γ at the first phase.

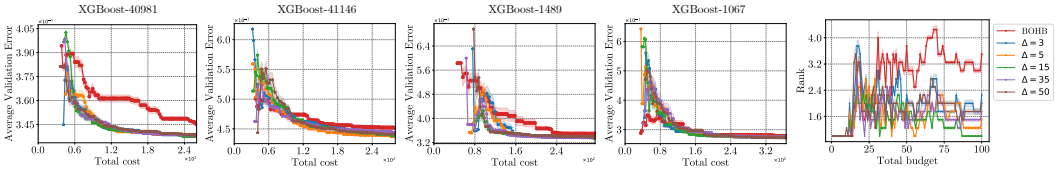

Figure 29: Validation error observed of `Lamda+BOHB` under different parameter Δ at the first phase.

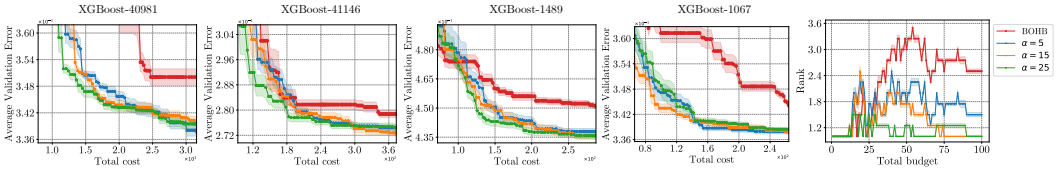

Figure 30: Validation error observed of `Lamda+BOHB` under different parameter α at the first phase.

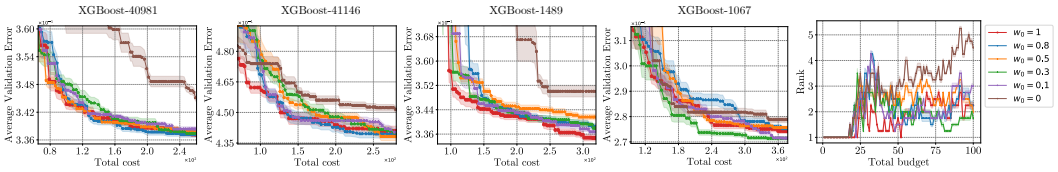

Figure 31: Validation error observed of `Lamda+BOHB` under different parameter w at the first phase.

Table 6: Comparing peer algorithms' final validation errors of the current incumbent at 100 HF evaluations horizons. Runs are averaged over 31 seeds. (The bolded part indicates: "under the Wilcoxon rank-sum test, methods incorporating priors significantly outperform their baselines.")

Tasks	BOHB	Lamda+BOHB	MUMBO	Lamda+MUMBO	BO	Lamda+BO	RS	Lamda+RS	PriorBand	Lamda+PriorBand
MFH3	-3.655e+00(1.339e-01)	**-3.716e+00(1.056e-01)**	-3.860e+00(3.569e-01)	-3.846e+00(2.174e-01)	-3.822e+00(2.172e-01)	-3.843e+00(5.508e-02)	**-3.572e+00(2.529e-01)**	**-3.718e+00(1.323e-01)**	-3.857e+00(3.553e-03)	-3.852e+00(2.401e-03)
MFH6	-2.864e+00(1.364e-01)	**-2.935e+00(1.427e-01)**	-1.872e+00(0)	**-3.178e+00(2.752e-01)**	-2.138e+00(9.286e-01)	**-3.112e+00(8.129e-02)**	-2.260e+00(6.577e-01)	**-2.396e+00(2.627e-01)**	-3.187e+00(1.506e-01)	-3.167e+00(5.198e-02)
XGBoost-40981	3.456e-01(9.817e-03)	3.337e-01(9.490e-03)	3.147e-01(2.235e-07)	3.147e-01(2.235e-07)	3.337e-01(4.953e-03)	**3.147e-01(1.028e-05)**	3.442e-01(1.143e-03)	**3.367e-01(1.528e-03)**	NA	NA
XGBoost-41146	2.883e-01(1.238e-03)	**2.783e-01(6.558e-03)**	2.634e-01(1.694e-03)	2.635e-01(1.063e-03)	2.660e-01(1.620e-03)	**2.646e-01(1.823e-03)**	2.824e-01(8.990e-03)	**2.768e-01(4.922e-04)**	NA	NA
XGBoost-1489	4.477e-01(8.205e-03)	**4.330e-01(2.073e-02)**	4.616e-01(5.269e-02)	**4.116e-01(1.450e-02)**	4.164e-01(1.462e-02)	4.116e-01(5.029e-03)	4.415e-01(1.642e-02)	**4.187e-01(5.514e-03)**	NA	NA
XGBoost-1067	3.453e-01(5.331e-03)	**3.377e-01(3.775e-03)**	3.345e-01(5.656e-03)	**3.301e-01(5.028e-03)**	3.357e-01(7.962e-04)	**3.298e-01(1.182e-04)**	3.399e-01(0)	**3.345e-01(0)**	NA	NA
rpart-40981	2.200e-01(6.758e-02)	**2.199e-01(8.859e-06)**	2.199e-01(7.525e-06)	2.199e-01(1.937e-06)	2.199e-01(3.759e-06)	2.200e-01(2.866e-04)	2.213e-01(8.945e-04)	**2.199e-01(1.214e-05)**	NA	NA
rpart-41146	2.222e-01(1.529e-03)	**2.210e-01(9.219e-04)**	2.210e-01(4.312e-04)	2.205e-01(3.331e-04)	2.210e-01(1.799e-03)	**2.204e-01(1.356e-04)**	2.233e-01(3.626e-03)	**2.216e-01(1.541e-03)**	NA	NA
rpart-1089	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	NA	NA
rpart-1067	2.198e-01(0)	2.198e-01(0)	2.388e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	2.198e-01(0)	NA	NA
ranger-40981	3.087e-01(4.186e-03)	**3.038e-01(6.079e-03)**	2.993e-01(2.547e-03)	3.022e-01(3.181e-03)	3.024e-01(7.710e-03)	**2.835e-01(1.074e-02)**	3.019e-01(1.860e-03)	**2.967e-01(2.828e-03)**	NA	NA
ranger-41146	1.645e-01(6.803e-03)	1.645e-01(2.341e-03)	1.683e-01(2.645e-03)	**1.679e-01(4.282e-03)**	1.670e-01(3.795e-03)	1.673e-01(1.883e-03)	1.685e-01(1.981e-03)	**1.641e-01(2.814e-03)**	NA	NA
ranger-1489	2.328e-01(5.845e-03)	2.358e-01(2.925e-03)	2.440e-01(1.350e-03)	2.372e-01(2.984e-03)	2.336e-01(2.404e-03)	**2.316e-01(1.231e-03)**	2.464e-01(4.325e-03)	**2.381e-01(1.180e-03)**	NA	NA
ranger-1067	3.182e-01(6.926e-03)	**3.136e-01(6.902e-03)**	3.138e-01(5.727e-03)	**3.055e-01(5.693e-04)**	3.142e-01(5.990e-03)	**3.061e-01(5.558e-03)**	3.180e-01(2.325e-03)	**3.089e-01(3.449e-03)**	NA	NA
glmnet-40981	3.200e-01(2.952e-03)	**3.161e-01(4.786e-04)**	3.149e-01(0)	3.149e-01(0)	3.149e-01(0)	3.269e-01(6.331e-03)	3.241e-01(4.395e-04)	**3.247e-01(1.148e-03)**	NA	NA
glmnet-41146	2.415e-01(3.053e-04)	2.413e-01(5.809e-04)	2.411e-01(0)	2.411e-01(0)	2.411e-01(0)	2.430e-01(3.797e-04)	2.425e-01(4.839e-04)	**2.429e-01(5.945e-04)**	NA	NA
glmnet-1489	4.290e-01(2.869e-03)	**4.274e-01(5.247e-04)**	4.392e-01(0)	**4.262e-01(0)**	4.262e-01(0)	4.262e-01(0)	4.392e-01(6.759e-03)	**4.262e-01(0)**	NA	NA
glmnet-1067	3.214e-01(4.097e-04)	**3.178e-01(7.455e-05)**	3.171e-01(0)	3.171e-01(0)	**3.171e-01(0)**	3.282e-01(6.786e-03)	3.232e-01(5.589e-03)	**3.210e-01(4.693e-03)**	NA	NA
FCNet-Naval-Propulsion	2.537e+03(1.014e+03)	**2.411e+03(6.557e+02)**	2.458e+03(7.802e+02)	**1.002e+03(5.606e+02)**	2.627e+02(2.871e+02)	**2.121e+02(2.884e+02)**	6.766e+03(6.833e+02)	**3.370e+03(1.043e+03)**	4.461e+03(8.544e+02)	**3.956e+03(4.427e+02)**
FCNet-Protein-Structure	5.030e+03(2.183e+03)	**4.334e+03(2.098e+03)**	6.529e+03(4.761e+03)	**2.015e+03(6.318e+02)**	2.764e+03(3.452e+03)	**1.156e+03(1.424e+02)**	1.367e+04(6.222e+03)	**1.097e+04(5.827e+03)**	6.273e+03(4.760e+03)	**3.501e+03(1.508e+02)**
FCNet-Slice-Localization	4.418e+03(5.756e+02)	**4.006e+03(3.853e+02)**	8.197e+03(4.281e+03)	**3.475e+03(2.819e+03)**	4.825e+03(5.299e+03)	**1.378e+03(1.161e+02)**	1.368e+04(1.960e+03)	**5.048e+03(3.287e+03)**	5.275e+03(1.709e+03)	**4.269e+03(5.377e+03)**
FCNet-Parkinsons-Telemonitoring	1.580e+05(4.104e+02)	**1.139e+03(7.311e+02)**	1.364e+02(2.477e+02)	**1.197e+01(9.573e+00)**	4.236e+02(7.323e+02)	**2.623e-05(6.821e+01)**	**5.333e+03(5.352e+03)**	4.275e+03(3.180e+03)	3.997e+02(8.256e+02)	4.041e+02(1.419e+03)
NAS-Bench-301-CIFAR-10	5.760e+00(2.620e-01)	**5.454e+00(1.091e-01)**	5.761e+00(1.368e-01)	**5.787e+00(3.964e-01)**	5.492e+00(2.995e-01)	5.629e+00(5.881e-01)	6.201e+00(4.134e-01)	**5.538e+00(4.347e-01)**	NA	NA
NAS-Bench-201-CIFAR-10	9.712e+00(8.138e-10)	**9.712e+00(2.543e-10)**	9.792e+00(6.103e-10)	**9.712e+00(1.272e-10)**	9.712e+00(1.424e-09)	9.712e+00(9.664e-10)	**8.760e+01(0)**	9.712e+00(1.017e-09)	NA	NA
NAS-Bench-201-CIFAR-100	1.000e+00(0)	**1.000e+00(0)**	1.000e+00(0)	1.000e+00(0)	1.000e+00(0)	1.000e+00(0)	6.764e+01(0)	**1.000e+00(0)**	NA	NA
NAS-Bench-201-ImageNet	8.333e-01(3.709e-10)	**8.333e-01(2.914e-10)**	8.333e-01(1.854e-10)	**8.133e-01(0)**	8.333e-01(2.384e-10)	8.333e-01(3.444e-10)	3.487e+01(0)	**8.333e-01(4.239e-10)**	NA	NA
JAHS-CIFAR-10	9.252e+00(1.828e-01)	9.495e+00(5.682e-01)	9.340e+00(5.540e-01)	**9.002e+00(1.398e-01)**	9.268e+00(1.037e-01)	**9.118e+00(2.973e-01)**	9.536e+00(3.553e-01)	**9.201e+00(1.504e-01)**	NA	NA
JAHS-Colorectal-Histology	4.467e+00(3.072e-01)	4.542e+00(1.801e-01)	4.596e+00(3.287e-01)	**4.451e+00(2.517e-01)**	4.576e+00(2.848e-01)	**4.288e+00(5.159e-02)**	4.940e+00(3.295e-01)	**4.209e+00(5.453e-02)**	NA	NA
JAHS-Fashion-MNIST	4.966e+00(9.998e-02)	4.960e+00(2.068e-01)	5.006e+00(1.478e-01)	**4.904e+00(2.414e-01)**	4.850e+00(1.387e-01)	4.864e+00(8.280e-02)	4.980e+00(0)	**4.788e+00(0)**	NA	NA
PD1-LM1B	6.255e-01(6.187e-03)	**6.209e-01(4.692e-03)**	6.092e-01(3.626e-02)	**6.042e-01(1.300e-02)**	6.277e-01(1.818e-02)	**6.063e-01(2.018e-04)**	6.459e-01(1.125e-02)	**6.315e-01(9.575e-03)**	9.905e+01(0)	9.905e+01(3.879e-03)
PD1-WMT	3.438e-01(1.379e-02)	**3.394e-01(1.243e-02)**	3.357e-01(4.336e-03)	**3.326e-01(8.931e-03)**	3.578e-01(1.671e-02)	3.579e-01(2.453e-02)	3.762e-01(0)	**3.624e-01(0)**	9.907e+01(2.832e-03)	9.906e+01(0)
PD1-CIFAR-100	2.141e-01(3.115e-02)	**2.097e-01(1.186e-02)**	1.767e-01(2.363e-03)	**1.743e-01(4.328e-04)**	2.345e-01(4.867e-02)	**1.946e-01(4.658e-02)**	2.722e-01(5.905e-03)	**2.269e-01(8.842e-03)**	NA	NA
PD1-ImageNet	2.282e-01(3.206e-02)	**2.050e-01(1.184e-02)**	1.942e-01(0)	**1.824e-01(0)**	2.263e-01(1.753e-03)	**2.145e-01(1.641e-02)**	2.360e-01(0)	**1.986e-01(0)**	NA	NA

F.3 Analyzing the Impact of Promising Regions Overlap in LF and HF Landscapes on Algorithm Performance

To better illustrate the solution distributions across low- and high-fidelity problems, we visualized the distributions in a 2D space. We sampled $10,000$ hyperparameter configurations and computed their fitness values under both low- and high-fidelity settings. The data was then compressed into 2D using the UMAP McInnes & Healy (2018) algorithm. To further enhance interpretability, we applied linear interpolation to generate a continuous landscape surface. Figure 32, Figure 33, Figure 34, and Figure 35 present the landscapes of FCNet, PD1, NAS-Bench-201, NAS-Bench-301, and JAHS under both high- and low-fidelity settings. The overlap between high- and low-fidelity problems is also shown in the figures.

From these visualizations, we observe that FCNet and PD1 exhibit a high overlap (ranging from 0.7 to 0.9) in their promising regions across fidelity levels, with the promising regions being relatively concentrated. In contrast, while NAS-Bench-201 and NAS-Bench-301 have moderate OVL values (ranging from 0.67 to 0.76), their solution distributions are more dispersed. JAHS demonstrates lower OVL values (ranging from 0.52 to 0.57) and also shows a more scattered solution distribution.

The results indicate that for problems where the promising regions of LF and HF landscape have varying levels of overlaps, our method (`Lamda`) achieves better performance than the original algorithms under the frameworks of `BOHB`, `MUMBO`, `BO`, and `RS`, as illustrated in the convergence curves (Figure 17, Figure 19, Figure 21, and Figure 23). In particular, we would like highlight the results on JAHS-CIFAR-10, JAHS-Colorectal-Histology, and JAHS-Fashion-MNIST, whose overlaps are low. `Lamda` consistently enhance the baseline algorithms.

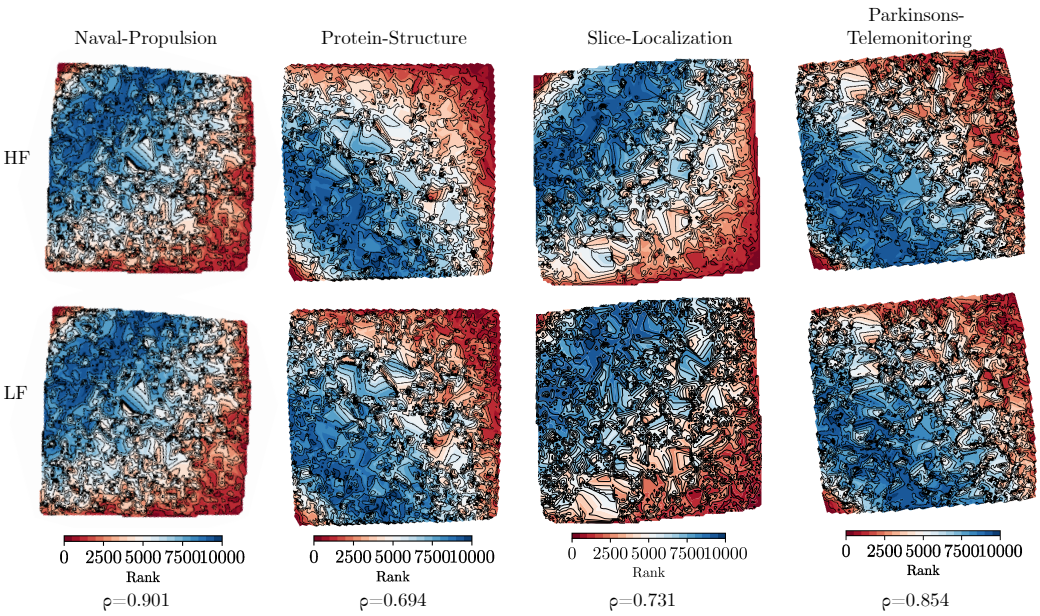

Figure 32: 2D visualization of landscapes of FCNet at high and low fideliteis.

F.4 Peer comparison on hyperparameter optimization for fine-tuning pretrained image classification models

In this section, we additionally adopt the hyperparameter optimization from (Pineda-Arango et al., 2024) for fine-tuning pretrained image classification models on different datasets. A total of 20 problems are used to evaluate the performance of the algorithms, and the results are presented in Table 7. It can be observed that texttLamda+BOHB achieves the best performance across all problems. The overall ranking of the algorithms during the optimization process is illustrated in the Figure 37, showing that `Lamda+BOHB` consistently ranks first after consuming a portion of the resources. The convergence curves in Figure 38 further highlight its superiority in the second phase,

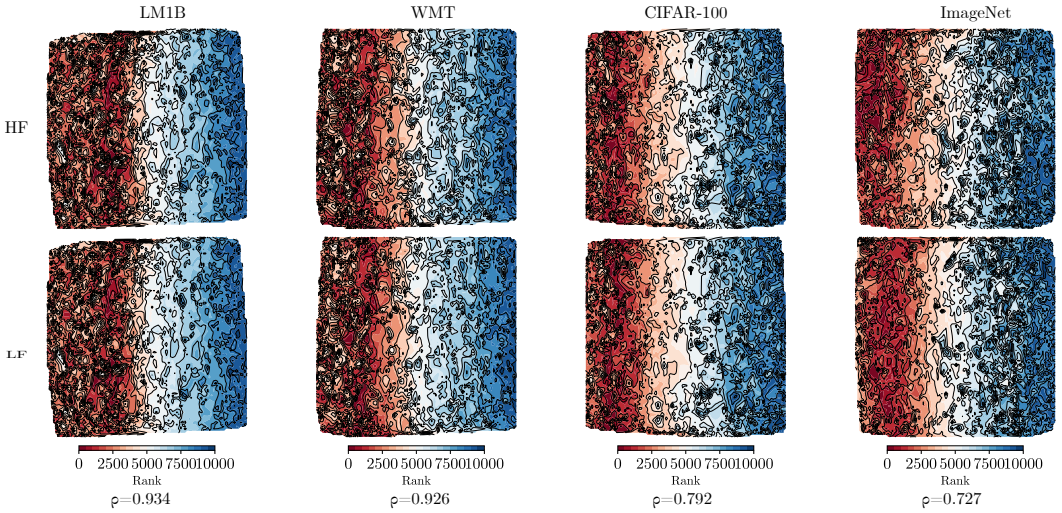

Figure 33: 2D visualization of landscapes of PD1 at high and low fideliteis.

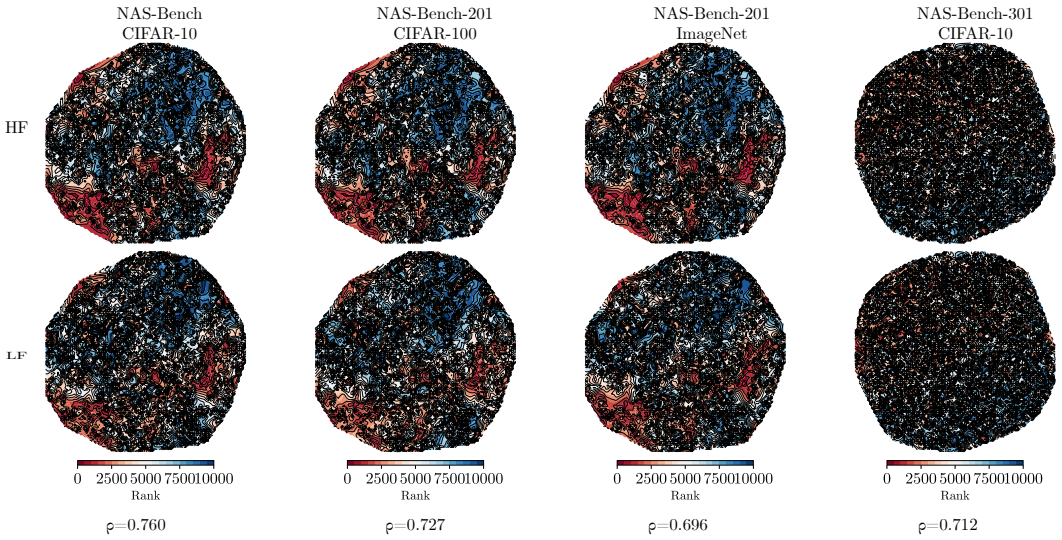

Figure 34: 2D visualization of landscapes of NAS-Banch-201 and 301 at high and low fideliteis..

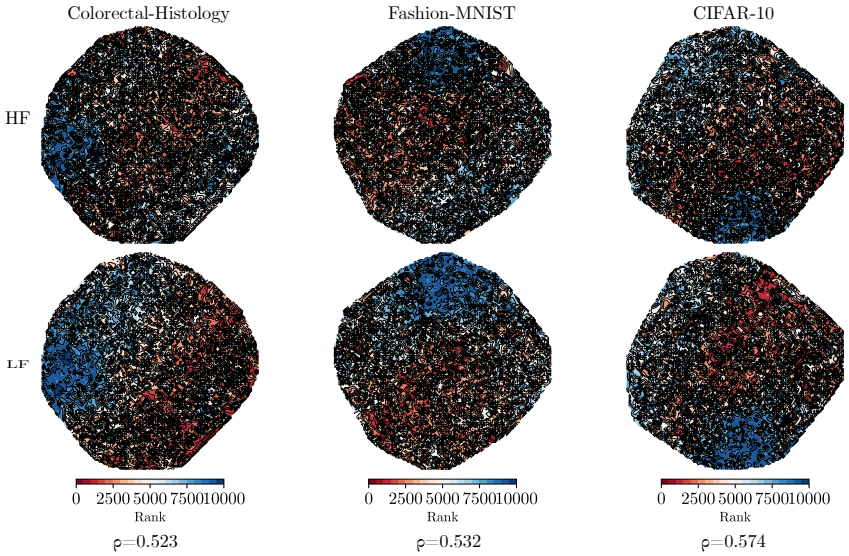

Figure 35: 2D visualization of landscapes of JAHS at high and low fideliteis.

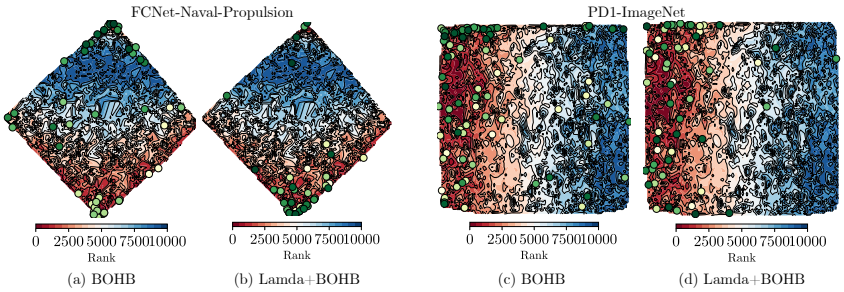

Figure 36: 2D visualization of the sampling points during the optimization process of Lamda+BOHB and BOHB on FCNet-Naval-Propulsion and PD1-ImageNet. The contour represents the dimensionality-reduced landscape of the HF problem, while the points indicate the HF samples collected during optimization. The color gradient from green to yellow indicates the order of sampling, with yellow representing later sampling stages.

where it quickly identifies high-quality solutions and accelerates the optimization process. The experimental results further demonstrate that `Lamda` consistently enhances `BOHB`.

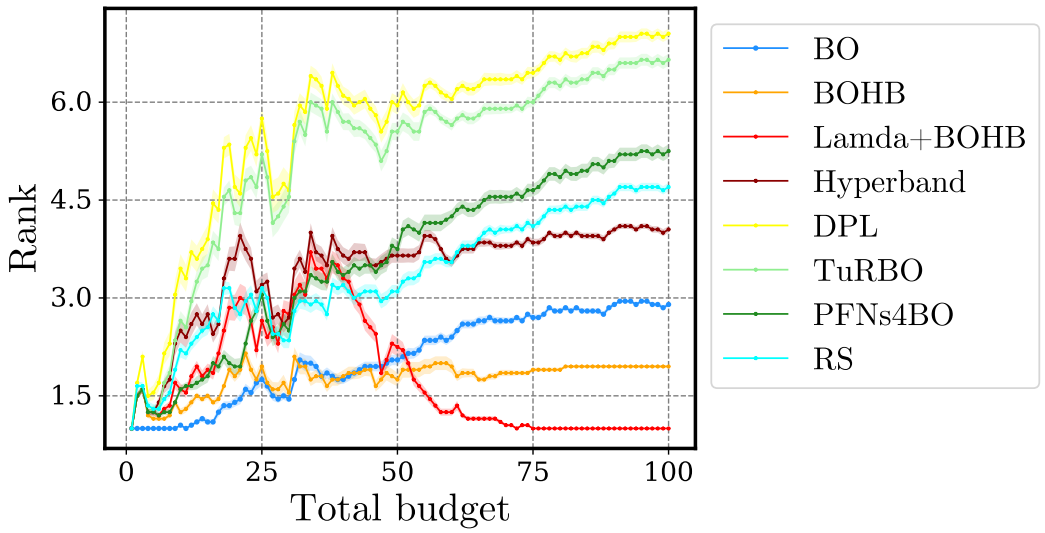

Figure 37: Comparing average relative ranks of peer algorithms across 20 HPO tasks for fine-tuning pretrained image classification models.

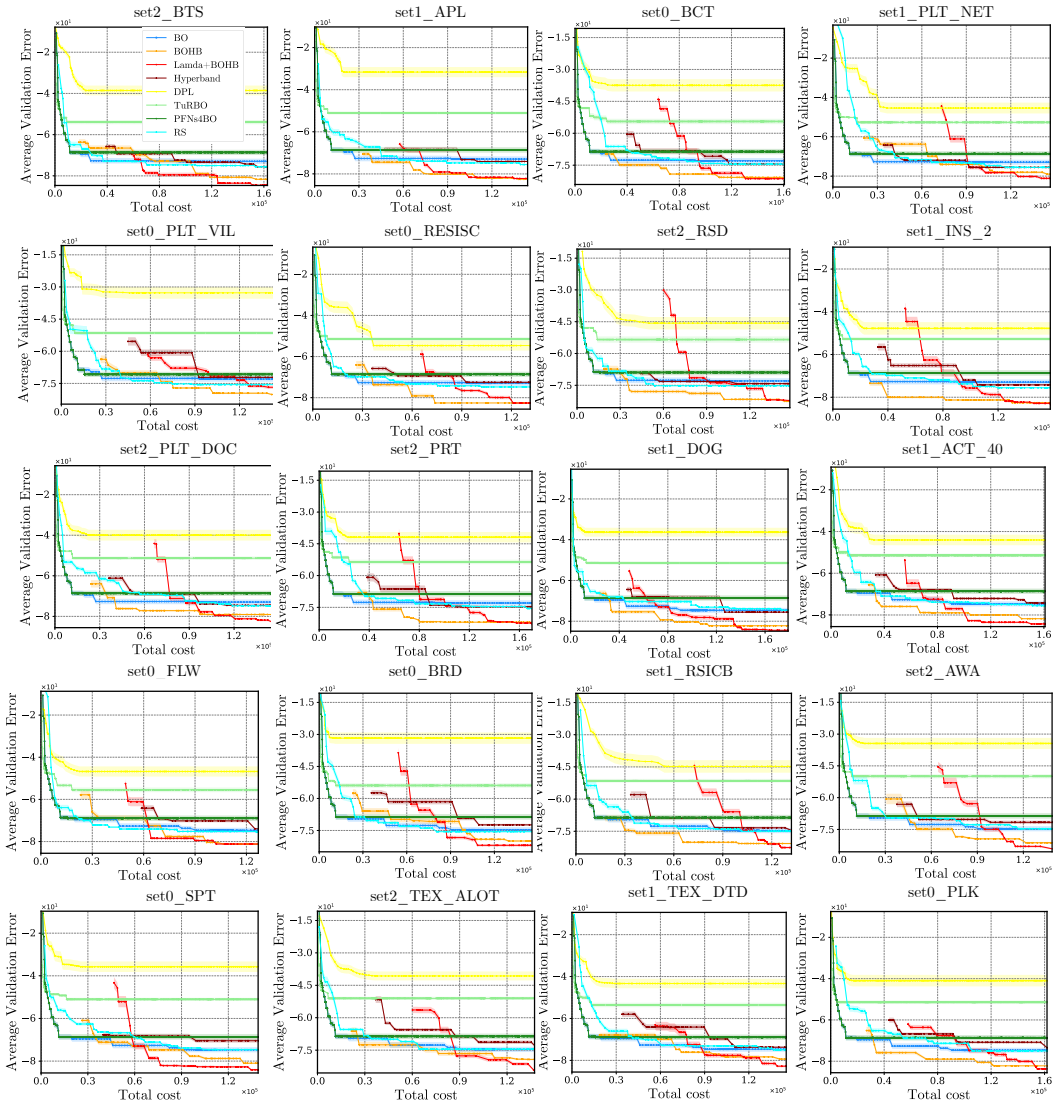

Figure 38: Validation error observed in tuning 20 HPO tasks for fine-tuning pretrained image classification models, comparing peer algorithms.

Table 7: Comparing peer algorithms' final validation errors of the current incumbent at 100 HF evaluations horizons (20 HPO tasks for fine-tuning pretrained image classification models). Runs are averaged over 31 seeds. (The bolded part indicates: "under the Wilcoxon rank-sum test, methods incorporating priors significantly outperform their baselines.")

Data Name	BO	BOHB	Lamda+BOHB	Hyperband	DPL	TuRBO	PFNs4BO	RS
mtlbm_extended_set2_BTS	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.466e+01(2.709e+00)**	-7.556e+01(0.000e+00)	-3.857e+01(2.394e+01)	-5.392e+01(1.042e+01)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set1_APL	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-3.164e+01(2.416e+01)	-5.105e+01(7.422e+00)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set0_BCT	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.409e+01(3.032e+00)**	-7.556e+01(0.000e+00)	-3.747e+01(2.900e+01)	-5.446e+01(1.274e+01)	-6.862e+01(1.273e+01)	-7.455e+01(3.034e+00)
mtlbm_extended_set1_PLT_NET	-7.295e+01(1.282e+01)	-8.166e+01(2.709e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.541e+01(2.757e+01)	-5.270e+01(8.711e+00)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set0_PLT_VIL	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.466e+01(2.709e+00)**	-7.556e+01(0.000e+00)	-3.273e+01(2.761e+01)	-5.142e+01(8.522e+00)	-7.078e+01(1.197e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set0_RESISC	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-5.465e+01(2.450e+01)	-5.142e+01(8.522e+00)	-6.862e+01(1.273e+01)	-7.478e+01(2.349e+00)
mtlbm_extended_set2_RSD	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.570e+01(2.934e+01)	-5.342e+01(1.467e+01)	-6.896e+01(1.288e+01)	-7.523e+01(9.984e-01)
mtlbm_extended_set1_INS_2	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.778e+01(2.946e+01)	-5.270e+01(8.980e+00)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set2_PLT_DOC	-7.295e+01(1.282e+01)	-8.223e+01(9.984e-01)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-3.996e+01(2.678e+01)	-5.131e+01(8.203e+00)	-6.862e+01(1.273e+01)	-7.478e+01(2.349e+00)
mtlbm_extended_set2_PRT	-7.295e+01(1.282e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.190e+01(2.468e+01)	-5.356e+01(1.065e+01)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set1_DOG	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.489e+01(1.331e+00)**	-7.556e+01(0.000e+00)	-3.633e+01(2.196e+01)	-5.142e+01(8.522e+00)	-6.862e+01(1.273e+01)	-7.462e+01(2.825e+00)
mtlbm_extended_set1_ACT_40	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.404e+01(2.534e+01)	-5.142e+01(8.392e+00)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set0_FLW	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.677e+01(2.420e+01)	-5.547e+01(1.106e+01)	-6.896e+01(1.288e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set0_BRD	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.500e+01(1.694e+00)**	-7.556e+01(0.000e+00)	-3.176e+01(2.669e+01)	-5.392e+01(1.042e+01)	-6.862e+01(1.273e+01)	-7.556e+01(0.000e+00)
mtlbm_extended_set1_RSICB	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.478e+01(2.931e+01)	-5.146e+01(8.506e+00)	-6.862e+01(1.273e+01)	-7.500e+01(1.694e+00)
mtlbm_extended_set2_AWA	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-3.442e+01(2.638e+01)	-4.993e+01(9.759e+00)	-6.862e+01(1.273e+01)	-7.466e+01(2.709e+00)
mtlbm_extended_set0_SPT	-7.467e+01(1.215e+01)	-8.178e+01(2.349e+00)	**-8.556e+01(0.000e+00)**	-7.523e+01(9.984e-01)	-3.574e+01(2.475e+01)	-5.105e+01(7.422e+00)	-6.862e+01(1.273e+01)	-7.462e+01(2.825e+00)
mtlbm_extended_set2_TEX_ALOT	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.067e+01(2.077e+01)	-5.105e+01(7.422e+00)	-6.862e+01(1.273e+01)	-7.462e+01(2.825e+00)
mtlbm_extended_set1_TEX_DTD	-7.467e+01(1.215e+01)	-8.223e+01(9.984e-01)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.332e+01(2.276e+01)	-5.356e+01(1.065e+01)	-6.896e+01(1.288e+01)	-7.500e+01(1.694e+00)
mtlbm_extended_set0_PLK	-7.467e+01(1.215e+01)	-8.256e+01(0.000e+00)	**-8.556e+01(0.000e+00)**	-7.556e+01(0.000e+00)	-4.097e+01(2.802e+01)	-5.146e+01(8.506e+00)	-6.862e+01(1.273e+01)	-7.500e+01(1.694e+00)

G. ALGORITHM DETAILS

In this section, we outline the workflow of our Lamda framework, which operates in two phases: the first-phase low-fidelity search (dubbed as Lamda-1) and the second-phase optimization (dubbed as Lamda-2). The overall workflow is depicted in Algorithm 1.

The first phase, Lamda-1, focuses on identifying promising regions in the search space using LF evaluations. The pseudocode for Lamda-1 is provided in Algorithm 2. In particular, the sampling strategy in Lamda-1 is algorithm-agnostic and can be incorporated with most HPO algorithms.

The second phase, Lamda-2, allows the use of different algorithms to guide the search. We provide multiple pseudocode to demonstrate how Lamda-2 can be adapted to various algorithms, including PriorBand, BOHB, MUMBO, vanilla BO, and random search. The details for each integration are outlined below, with modifications from the original algorithms highlighted in red:

- For PriorBand, Lamda-2 replaces the expert prior $p_\pi(\mathbf{x})$ from (Mallik et al., 2023) with the learned prior $\varphi_{\text{pro}}(\mathbf{x})$ obtained in Lamda-1.
- For BOHB, Lamda-2 modifies the uniform sampling distribution in Steps 7 and 8 of Algorithm 3 into the incumbent distribution determined by $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$.
- For MUMBO and BO, Lamda-2 combines $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ with their acquisition functions. The pseudocode for these adaptations is shown in Algorithm 4 and Algorithm 5, respectively.
- For Random Search, Lamda-2 replaces the uniform sampling strategy by the incumbent sampling strategy defined by $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$, as illustrated in Algorithm 6.

Algorithm 1: Pseudocode for Lamda

Input: Input space $\mathcal{X}$, total budget Λ, maximum budget for the first phase B, fidelity parameter used at the first phase l.
Output: Optimized design x^*.

```
/* initialize remaining budget */;
1 Λ_r ← Λ ;
/* first-phase search with low fidelity */;
2 (φ_pro(x), S, Λ_l) ← Lamda-1 (B, l);
3 Λ_r ← Λ_r − Λ_l;
/* second-phase search */;
4 x* ← Lamda-2 (φ_pro(x), Λ_r);
5 return x*
```

Algorithm 2: Pseudocode for `Lamda-1`

Input: Input space $\mathcal{X}$, maximum budget for the first phase B, threshold y^*, Δ, γ, fidelity level l, budget function λ_z.
Output: PDF of the promising solutions $\varphi_{\text{pro}}(\mathbf{x})$, observation set S, consumed budget Λ_l.

Initialize $S \leftarrow \emptyset$, $\Lambda_l \leftarrow 0$, $t \leftarrow 0$, `isEarlyStopping`$\leftarrow$ **False**;
while $\Lambda_l < B$ **and not** *`isEarlyStopping`* **do**
  $\mathbf{x}^t \leftarrow \arg\max_{\mathbf{x}\in\mathcal{X}} \text{AF}(\mathbf{x}, \mathcal{S})$;
  $y^t \leftarrow f_\ell(\mathbf{x}^t) + \epsilon$;
  $S \leftarrow S \cup \{(\mathbf{x}^t, y^t)\}$;
  $\mathcal{S}_{\text{pro}} \leftarrow \{\mathbf{x} \mid f_\ell(\mathbf{x}) \leq y^*, \mathbf{x} \in \mathcal{S}\}$, $\mathcal{S}_{\text{inf}} \leftarrow \{\mathbf{x} \mid f_\ell(\mathbf{x}) > y^*, \mathbf{x} \in \mathcal{S}\}$;
  $\varphi^t_{\text{pro}}(\mathbf{x}) \leftarrow p(\mathbf{x} \mid \mathcal{S}_{\text{pro}})$, $\varphi^t_{\text{inf}}(\mathbf{x}) \leftarrow p(\mathbf{x} \mid \mathcal{S}_{\text{inf}})$;
  if $1 - \rho\left(\varphi^t_{\text{pro}}(\mathbf{x}), \varphi^{t+\Delta}_{\text{pro}}(\mathbf{x})\right) \leq \gamma$ **then**
    `isEarlyStopping`$\leftarrow$**True**;
  $\Lambda_l \leftarrow \Lambda_l + \lambda_z(\mathbf{x}^t, l)$;
  $t \leftarrow t + 1$;
$\varphi_{\text{pro}}(\mathbf{x}) \leftarrow \varphi^t_{\text{pro}}(\mathbf{x})$;
return $(\varphi_{\text{pro}}(\mathbf{x}), S, \Lambda_l)$

Algorithm 3: Pseudocode for sampling in `Lamda+BOHB`

Input: Observations D, fraction of random runs ρ, percentile q, number of samples N_s, minimum number of points N_{min} to build GP models, and bandwidth factor b_w
Output: next configuration to evaluate

Initilize $b \leftarrow \arg\max\{D_b : |D_b| \geq N_{\text{min}} + 2\}$, $\tilde{\rho} \leftarrow \text{Rand}(0, 1)$;
if $\tilde{\rho} < \rho$ ***or*** $b = \emptyset$ **then**
  return randomly sampled configuration;
else
  Compute $l(\mathbf{x})$ and $g(\mathbf{x})$ as Eqs. (2) and (3) in Falkner et al. (2018);
  Draw N_s configurations according to $\tilde{\varphi}_{\text{pro}}(\mathbf{x})$ in equation (6);
  return configuration with highest ratio $l(\mathbf{x})/g(\mathbf{x})$

Algorithm 4: Second-phase search with BO

Input: Input space $\mathcal{X}$, $\varphi_{\text{pro}}(\mathbf{x})$, w, N solution for the initial design of GPs, budget Λ_r, fidelity level h, budget function λ_z.
Output: Optimized design x^*.

`/* Initialization */`;
Sample $\{\mathbf{x}^i\}_{i=1}^n$ from distribution given by $\varphi_{\text{pro}}(\mathbf{x})$;
$y^i \leftarrow f_h(\mathbf{x}^i) + \epsilon^i$, where $\epsilon^i \sim \mathcal{N}(0, \sigma^2)$; $\lambda^i \leftarrow \lambda_z(\mathbf{x}^i, h)$;
$\Lambda_r \leftarrow \Lambda_r - \sum_{i=1}^n \lambda^i$;
$D \leftarrow \{(\mathbf{x}^i, y^i)\}_{i=1}^n$;
while $\Lambda_r > 0$ **do**
  $\varphi(\mathbf{x}) \leftarrow p(\mathbf{x}|D)$;
  $\tilde{\varphi}_{\text{pro}}(\mathbf{x}) \leftarrow (1 - w) \cdot \varphi(\mathbf{x}) + w \cdot \varphi_{\text{pro}}(\mathbf{x})$;
  $\mathbf{x}^{n+1} \leftarrow \arg\max_{\mathbf{x}\in\mathcal{X}} \tilde{\varphi}_{\text{pro}}(\mathbf{x})\text{AF}(\mathbf{x}, \mathcal{D})$;
  $y^{n+1} \leftarrow f_h(\mathbf{x}^{n+1}) + \epsilon$;
  Update $D \leftarrow D \cup \{(\mathbf{x}^{n+1}, y^{n+1})\}$;
  $\Lambda_r \leftarrow \Lambda_r - \lambda_z(\mathbf{x}^{n+1}, h)$;
  $n \leftarrow n + 1$;
return $x^* \leftarrow \arg\min_{(\mathbf{x}^i, y^i)\in D} y^i$

Algorithm 5: Second-phase search with MUMBO

Input: Input space $\mathcal{X}$, prior obtianed in the first phase $\varphi_{\text{pro}}(\mathbf{x})$, prior confidence parameter w, size n of the initial design, budget for first phase Λ_r.

Output: Optimized design x^*.

Sample $\{\mathbf{x}^i\}_{i=1}^n \sim \varphi_{\text{pro}}(\mathbf{x})$ and randomly assign fidelity levels $\{z^i\}_{i=1}^n$ with $z^i \sim \text{Uniform}(\{\ell, \ell+1, \ldots, h\})$;

Compute $y^i \leftarrow f_z(\mathbf{x}^i, z^i) + \epsilon^i$, where $\epsilon^i \sim \mathcal{N}(0, \sigma^2)$; $\lambda^i \leftarrow \lambda_z(\mathbf{x}^i, z^i)$;

$\Lambda_r \leftarrow \Lambda_r - \sum_{i=1}^n \lambda^i$;

Initialize $D \leftarrow \{(\mathbf{x}^i, z^i), y^i\}_{i=1}^n$;

while $\Lambda_r > 0$ **do**

- Fit GP to the collected observations D, $\varphi(\mathbf{x}) \leftarrow p(\mathbf{x}|D)$;
- Simulate N samples of $g^*|D$;
- Prepare $\alpha_{n-1}^{\text{MUMBO}}(\mathbf{x}, z)$ as given by Eq. (5) in Moss et al. (2020);
- Update $\tilde{\varphi}_{\text{pro}}(\mathbf{x}) \leftarrow (1-w) \cdot \varphi(\mathbf{x}) + w \cdot \varphi_{\text{pro}}(\mathbf{x})$;
- Find the next point and fidelity to query

$$(\mathbf{x}^{n+1}, z^{n+1}) \leftarrow \tilde{\varphi}_{\text{pro}}(\mathbf{x}) \arg\max_{(\mathbf{x},z)} \frac{\alpha_{n-1}^{\text{MUMBO}}(\mathbf{x}, z)}{\lambda_z(\mathbf{x}, z)}$$

- Collect the new evaluation $y^{n+1} \leftarrow f_z(\mathbf{x}^{n+1}, z^{n+1}) + \epsilon^{n+1}$, $\epsilon^{n+1} \sim \mathcal{N}(0, \sigma^2)$;
- Append new evaluation to observation set $D \leftarrow D \cup \{(\mathbf{x}^{n+1}, z^{n+1}), y^{n+1}\}$;
- Update spent budget $\Lambda_r \leftarrow \Lambda_r - \lambda_z(\mathbf{x}^{n+1}, z^{n+1})$;

return $x^* \leftarrow \arg\min_{\{((\mathbf{x}^i, z^i), y^i) \in D, z^i = h\}} y^i$

Algorithm 6: Second-phase search with Random Search

Input: Input space $\mathcal{X}$, prior obtianed in the first phase $\varphi_{\text{pro}}(\mathbf{x})$, prior confidence parameter w, budget for first phase Λ_r, uniform distribution p_U.

Output: Optimized design x^*.

$\varphi(\mathbf{x}) \leftarrow p_U(\mathbf{x})$;

while $\Lambda_r > 0$ **do**

- $\tilde{\varphi}_{\text{pro}}(\mathbf{x}) \leftarrow (1-w) \cdot \varphi(\mathbf{x}) + w \cdot \varphi_{\text{pro}}(\mathbf{x})$;
- Sample $\mathbf{x}^{n+1} \sim \tilde{\varphi}_{\text{pro}}(\mathbf{x})$;
- $y^{n+1} \leftarrow f_h(\mathbf{x}^{n+1}) + \epsilon$;
- Update $D \leftarrow D \cup \{(\mathbf{x}^{n+1}, y^{n+1})\}$;
- $\Lambda_r \leftarrow \Lambda_r - \lambda_z(\mathbf{x}^{n+1}, h)$;

return $x^* \leftarrow \arg\min_{(\mathbf{x}^i, y^i) \in D} y^i$