Enhancing Explainability of Hyperparameter Optimization via Bayesian Algorithm Execution

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Abstract
Despite all the benefits of automated hyperparameter optimization (HPO), most modern HPO algorithms are black-boxes themselves. This makes it difficult to understand the decision process which lead to the selected configuration, reduces trust in HPO, and thus hinders its broad adoption. Here, we study the combination of HPO with interpretable machine learning (IML) methods such as partial dependence plots. However, if such methods are naively applied to the experimental data of the HPO process in a post-hoc manner, the underlying sampling bias of the optimizer can distort interpretations. We propose a modified HPO method which efficiently balances the search for the global optimum w.r.t. predictive performance and the reliable estimation of IML explanations of an underlying black-box function by coupling Bayesian optimization and Bayesian Algorithm Execution. On benchmark cases of both synthetic objectives and HPO of a neural network, we demonstrate that our method returns more reliable explanations of the underlying black-box without a loss of optimization performance.

1 Introduction
The performance of machine learning (ML) models usually depends on many decisions, such as the choice of a learning algorithm and its hyperparameter configurations. Manually reaching these decisions is usually a tedious trial-and-error process. Automated machine learning (AutoML), e.g., hyperparameter optimization (HPO), can support developers and researchers in this regard. By framing these decisions as an optimization problem and solving them using efficient black-box optimizers such as Bayesian optimization (BO), HPO is demonstrably more efficient than manual tuning and grid or random search [Bergstra et al., 2011, Snoek et al., 2012, Turner et al., 2020, Bischl et al., 2021]. However, due to the lack of insight into the internal decisions of the HPO process, there is a lack of confidence in AutoML systems and a reluctance to trust the returned best configuration [Drozdal et al., 2020]. Some practitioners even prefer manual tuning because they feel they understand the process better [Hasebrook et al., 2022].

Desirable insights into the HPO process could be generated by applying methods of interpretable machine learning (IML) to experimental data from the HPO process. Examples include marginal effects of individual hyperparameters or their importance. However, these methods – even though possible from a technical perspective and used before [Van Rijn and Hutter, 2018] – should be used with caution in this context. The main reason for this is a sampling bias caused by the desire for efficient optimization during HPO: Efficient optimizers typically sample more configurations in promising regions with potentially well-performing hyperparameter configurations, while other regions are completely underrepresented. This sampling bias introduces a model bias in under-
explored regions as the model is subject to high uncertainty in this region. Consequently, explanations of HPO runs, such as partial dependence plots (PDPs) [Friedman, 2001], can be misleading as they also rely on artificially created evaluations in under-explored regions [Moosbauer et al., 2021].

To anticipate the unintended effects of this sampling bias as effectively as possible already during the HPO process, we propose a modified BO algorithm that efficiently searches for the global optimum and reliable explanations of the underlying black-box function at the same time. We build on the concept of Bayesian Algorithm Execution (BAX) [Neiswanger et al., 2021] to estimate the expected information gain (EIG) [Lindley, 1956] of sampled configurations w.r.t. the output of an explanation method. We ultimately couple BO with BAX and propose BOBAX as an efficient method that searches for reliable explanations without a relevant loss of optimization performance. Our proposed method is generic as it is applicable to any BO variant (e.g., different acquisition functions or probabilistic surrogate models) and also to different IML methods (e.g., marginal effects of hyperparameters via PDPs).

In our benchmark study, we demonstrate how BOBAX consistently yields more reliable estimates for marginal effects estimated via the partial dependence method while maintaining the same level of optimization efficiency as state-of-the-art methods. Finally, we demonstrate how BOBAX can give reliable insights into hyperparameter effects of a neural network during tuning yielding state-of-the-art performance. We believe that through our generic method, the potential of IML methods can be unlocked in the context of HPO, thus paving the way for more explainability of and trust into HPO.

Specifically, our contributions include:

1. The direct optimization for interpretability via marginal effects as part of BO for HPO to make HPO interpretable and more trustworthy;
2. The combination of BO and Bayesian Algorithm Execution (BAX), dubbed BOBAX, where BAX is used to guide the search towards better interpretability;
3. Thorough study of different variants of BOBAX and baselines on synthetic functions; and
4. Empirical evidence that improved interpretability does not come at the expense of optimization performance on a deep learning HPO benchmark.

2 Background

In this section, we formalize HPO and BO as the context of our work. We also give an overview of Bayesian Algorithm Execution (BAX) as it serves as basis for our work.

Hyperparameter Optimization The aim of HPO is to efficiently find a well-performing configuration of a learning algorithm. HPO is therefore commonly formalized as finding the minimizer \( \lambda^* \in \arg\min_{\lambda \in \Lambda} c(\lambda) \) of a black-box cost function \( c : \Lambda \to \mathbb{R} \) which maps a hyperparameter configuration \( \lambda = (\lambda_1, \ldots, \lambda_d) \in \Lambda \) to the validation error by a learning algorithm run using \( \lambda \). The hyperparameter space \( \Lambda = \Lambda_1 \times \ldots \times \Lambda_d \) can be mixed, containing categorical and continuous hyperparameters. Particularly in the context of AutoML, where whole machine learning pipeline configurations are optimized over, \( \Lambda \) may even contain hierarchical dependencies between hyperparameters [Thornton et al., 2013, Olson and Moore, 2016].

Bayesian Optimization BO is a black-box optimization algorithm which has become increasingly popular in the context of HPO [Jones et al., 1998, Snoek et al., 2012]. The approach sequentially chooses configurations \( \lambda^{(1)}, \ldots, \lambda^{(T)} \) that are evaluated \( c_{\lambda^{(1)}}, \ldots, c_{\lambda^{(T)}} \) to obtain an archive \( A_T = \{ (\lambda^{(i)}, c_{\lambda^{(i)}}) \}_{i=1, \ldots, T} \). To choose the next configuration \( \lambda^{(T+1)} \) as effective as possible, a surrogate model \( \tilde{c} \) is estimated on the archive \( A_T \), and a new point is proposed based on an acquisition function that leverages information from the surrogate model \( \tilde{c} \). Typically, we chose a probabilistic model and estimate a distribution over \( c \), denoted by \( p(c \mid A_T) \). A common choice are Gaussian processes \( c \sim \mathcal{GP}(\mu, k) \), characterized by a mean function \( \mu : \Lambda \to \mathbb{R} \) and a covariance function \( k : \Lambda \times \Lambda \to \mathbb{R} \). Acquisition functions usually trade off exploration (i.e., sampling in regions with few data points and high posterior uncertainty) and exploitation (i.e., sampling in regions with low mean). Common examples are the expected improvement (EI) [Jones et al., 1998], the lower confidence bound (LCB) [Jones, 2001, Srinivas et al., 2010], entropy search [Hennig and Schuler, 2012, Hernandez-Lobato et al., 2014] and knowledge gradient [Wu et al., 2017].
Marginal Effects of Hyperparameters Users of HPO are often interested in whether and how individual hyperparameters affect performance. Not only is there a desire to understand, also such insights can influence decisions, for example whether to tune a hyperparameter or not [Probst et al., 2019], or modify hyperparameter ranges. Therefore, one quantity of interest for practitioners is the marginal effect of one or multiple hyperparameters \( \lambda_S \), \( S \subset \{1, 2, ..., d\} \), which is defined as

\[
c^S(\lambda_S) := E_{\lambda_C}[c(\lambda)] = \int_{\lambda_C} c(\lambda_S, \lambda_C) \, d\Pi(\lambda_C).
\]  

In the context of HPO, \( \Pi \) is typically assumed to be the uniform distribution over \( \Lambda_C \) since we are interested in how hyperparameter values \( \lambda_S \) impact model performance uniformly across the hyperparameter space [Hutter et al., 2014, Moosbauer et al., 2021]. Since computing Eq. (1) exactly is usually not computationally feasible in the context of HPO for an expensive black-box \( c \), the PDP method [Friedman, 2001] approximates the integral, as in Eq. (1), by Monte Carlo approximation.  

Information-based Bayesian Algorithm Execution Information-based Bayesian Algorithm Execution (BAX) extends the idea of using entropy search for estimating global optima to estimating other properties of a function \( f : \mathcal{X} \rightarrow \mathbb{R} \) [Neiswanger et al., 2021]. Similar to BO, BAX tries to sequentially choose points \( x^{(i)} \in \mathcal{X} \) in order to estimate the quantity of interest as precisely as possible with as few evaluations as possible. It is assumed that the quantity of interest can be computed as the output \( O_A := O_A(f) \) of running an algorithm \( A \) on \( f \), e.g. top-k estimation on a finite set, computing level sets or finding shortest paths. 

Similarly to BO, BAX sequentially builds a probabilistic model \( p(f \mid A_T) \), e.g., a GP, over an archive of evaluated points \( A_T \). Based on \( p(f \mid A_T) \), they derive the posterior distribution over the algorithm output \( p(O_A \mid A_T) \). To build the archive \( A_T \) as efficiently as possible, they choose to evaluate the point \( x^{(T+1)} \) which maximizes the expected information gain about the algorithm output \( O_A \)

\[
EIG_T(x) = \mathbb{H}[O_A|A_T] - E_{p(f_A|A_T)} \left[ \mathbb{H}[O_A|A_T \cup \{(x, f_x)\}] \right].
\]  

Here, \( f_x \) denotes the (unrevealed) value of \( f \) at \( x \), and \( \mathbb{H} \) denotes the entropy. Neiswanger et al. [2021] propose an acquisition function to approximate the EIG as presented in Eq. (2). In its simplest form, the algorithm output \( O_A \) in the EIG is replaced by the algorithm’s execution path \( e_A \), i.e., the sequence of all evaluations the algorithm \( A \) traverses, which thus gives full information about the output. The expected information gain estimated based on the execution path \( e_A \) is given by

\[
EIG'_T(x) = \mathbb{H}[e_A|A_T] - E_{p(f_x|A_T)} \left[ \mathbb{H}[e_A|A_T \cup \{(x, f_x)\}] \right)
\]  

where they used the symmetry of the mutual information to come up with the latter expression. The first term \( \mathbb{H}[f_x|A_T] \) is the entropy of the posterior predictive distribution at an input \( x \) and can be computed in closed form. The second term can be estimated as follows: A number of \( n_{\text{path}} \) samples \( \tilde{f} \sim p(f \mid A_T) \) is drawn from the posterior process. The algorithm \( A \) is run on each of the samples \( \tilde{f} \) to produce sample execution paths \( \tilde{e}_A \), yielding samples \( \tilde{e}_A \sim p(e_A \mid A_T) \), used to estimate the second term as described by Neiswanger et al. [2021].

3 Related Work

Explainability in AutoML refers either to (1) the explanation of the resulting model output by an AutoML system [Xanthopoulos et al., 2020, Binder et al., 2020, Carmichael et al., 2021, Coors et al., 2021], or (2) the interpretation of the HPO process itself [Moosbauer et al., 2021]. We focus on the latter, contributing to more transparency, understanding and trust in AutoML Drozdal et al. [2020].

To keep notation simple, we denote \( c(\lambda) \) as a function of two arguments \((\lambda_S, \lambda_C)\) to differentiate components in the index set \( S \) from those in the complement \( C = \{1, 2, ..., d\} \setminus S \). The integral shall be understood as a multiple integral of \( c \) where \( \lambda_j \), \( j \in C \), are integrated out.
There are HPO frameworks and AutoML systems that provide visualisations and explainability statistics as additional outputs, e.g., Google Vizier [Golovin et al. 2017] and AutoML [Zöller et al. 2022] provide an interactive dashboard visualizing the progress of the optimization and insights via parallel coordinate plots and MDS on the optimizer footprint. Similarly, the HPO frameworks optuna [Akiba et al. 2019] or scikit-optimize [Head et al. 2018] allow for quick and simple visualization of optimization progress and results. However, these relatively simple visualization tools do not provide deeper insights into the HPO process.

In the context of HPO, hyperparameter importance and hyperparameter effects are particularly informative and suitable for drawing meaningful conclusions, e.g., hyperparameter importance via functional ANOVA [Hutter et al. 2014], ablation studies [Biedenkapp et al. 2017], or tunability [Probst et al. 2019]. Hyperparameter effects are still less established as statistic with exceptions of [Hutter et al. 2014], even though they contain more information than an importance score. While all these approaches have their merits, none of them discusses the impact of a sampling bias, who particularly raise the danger of biased interpretations caused by sampling bias. So far, only Moosbauer et al. [2021] explicitly proposed a post-hoc method that is able to yield reliable PDPs in the presence of a sampling bias via a partitioning of the configuration space.

All of the above methods are post-hoc methods, i.e., they are applied to experimental data produced by an HPO run, but they are not designed to guide the optimization process in order to enhance interpretability. To our knowledge, we are the first to propose an ex-ante method, i.e., a method that adapts the sampling process of HPO to yield reliable explanations instead of correcting for a sampling bias in a post-hoc manner.

4 BOBAX: A Method to Enhance Interpretability of HPO

Now, we present our main contribution: BOBAX that efficiently searches for reliable marginal effect estimates of hyperparameters while maintaining competitive HPO performance.

4.1 Expected Information Gain for Partial Dependence

We first derive the information gained with regards to the estimate of a marginal effect of a hyperparameter $\lambda_S$ if we observe performance $c_{\lambda(S)}^{(T+1)}$ for a hyperparameter configuration $\lambda^{(T+1)}$. To this end, we quantify and analyze how a marginal effect is estimated in the context of HPO. We perform two types of approximations: First, instead of estimating the marginal effect with regards to the true, but unknown and expensive objective $c$, we estimate the marginal effect of the surrogate model $\hat{c}$, with $\hat{c}$ denoting the posterior mean of a probabilistic model $p(c \mid A_T)$. Secondly, we use the partial dependence method [Friedman 2001] for efficient estimation of marginal effects of $\hat{c} : \Lambda \rightarrow \mathbb{R}$, which estimates Eq. (4) by Monte-Carlo sampling:

$$\varphi_{\lambda_S} = \frac{1}{n} \sum_{i=1}^{n} \hat{c} \left( \lambda_S, \lambda_C^{(i)} \right), \quad (5)$$

with $\lambda_S$ fixed and $\lambda_C^{(i)} \sim \mathbb{P}(\lambda_C)$ a Monte-Carlo sample drawn from a uniform distribution $\mathbb{P}$. To bound the computational effort to compute the PDP, Eq. (5) is evaluated for a (typically equidistant) set of grid points $\{\lambda_C^{(j)}\}_{j=1,..,G}$. The PDP visualizes $\varphi_{\lambda_S}$ against $\lambda_S$.

To define the expected information gain for partial dependence $\text{ElG}_{\text{PDP}}$, we have the partial dependence method in terms of a formal execution path (see also Algorithm 1 in the Appendix): We iterate over all grid points, and compute the mean prediction $\hat{c}^{(g,i)}$. The execution path $e_A$ thus corresponds to the Cartesian product $\left( \lambda_S^{(g)}, \lambda_C^{(i)} \right)$ for $g \in \{1, \ldots, G\}$ and $i \in \{1, \ldots, n\}$ of all grid points $\lambda_S^{(g)}$ and the Monte-Carlo samples $\lambda_C^{(i)}$.

As proposed by Neiswanger et al. [2021] as one variant, we estimate the information gained with regards to the execution path of $e_A$ instead of estimating the execution path with regards to the algorithm output $O_A$. Note that Neiswanger et al. [2021] argue that the criterion in Eq. (4) is in general suboptimal, if for example large parts of the execution path $e_A$ do not have an influence on
We additionally propose adaptive BOBAX (a-BOBAX), which takes the desired precision of a PD into account. To keep the notion of desired precision as user-friendly as possible, we define it as the desired average width of a \( \alpha \)-confidence interval. Once the desired precision is reached, we transition to pure optimization (i.e., we stop interleaving EIG by the average width of the confidence interval). From a practitioner’s point of view, it may be reasonable to consider interpretability rather as a constraint than an objective function to optimize for. To be more precise, a user could specify a desired level of precision of an interpretation method as input to a HPO system. We propose to assess the precision of PD estimates via estimated \( \alpha \)-confidence intervals adapting BOBAX as described above in a first stage, we continuously monitor the precision of a PD estimated on a surrogate model \( \hat{c} \) that is fitted on the archive \( A_T \).

Algorithm 1: Partial dependence

\[
\begin{align*}
\text{Input} & \quad G, \hat{c}, \left( \lambda^{(1)}_S, \ldots, \lambda^{(G)}_S \right) \sim i.i.d. \quad \mathbb{P}(\lambda_C) \\
\left( \lambda^{(1)}_S, \ldots, \lambda^{(G)}_S \right) & \leftarrow \text{equidistant grid on } \Lambda_S \\
& \text{for } g \in \{1, 2, \ldots, G\} \text{ do} \\
& \quad \text{for } i \in \{1, 2, \ldots, n\} \text{ do} \\
& \quad \quad \lambda^{(g,i)} \leftarrow \left( \lambda^{(g)}_S, \lambda^{(i)}_C \right) \\
& \quad \quad \hat{c}^{(g,i)} = \hat{c}(\lambda^{(g,i)}) \\
& \quad \quad e_A \leftarrow e_A \cup \left( \lambda^{(g,i)}, \hat{c}^{(g,i)} \right) \\
& \quad \text{end for} \\
& \quad \varphi^{(g)} \leftarrow \frac{1}{n} \sum_{i=1}^{n} \hat{c}^{(g,i)} \\
& \text{end for} \\
& \text{Return} \quad \left( \lambda^{(g)}_S, \varphi^{(g)} \right), \quad g = 1, \ldots, G 
\end{align*}
\]

Figure 1: \textbf{Left:} Partial dependence algorithm highlighting the execution path \( e_A \). \textbf{Right:} Shows the elements execution path \( e_A \), i.e., the configurations used to estimate the partial dependence plot based on a surrogate model \( \hat{c} \) that is fitted on the archive \( A_T \).

4.2 BOBAX: Efficient Optimization and Search for Explainability

Given the EIG\(_{\text{PDP}}\) for PD, the optimization for interpretability of hyperparameter effects as part of BO is possible by using the EIG\(_{\text{PDP}}\) as acquisition function. However, interpretability alone is rarely of primary interest in practice; rather, the goal is to identify well-performing configurations and obtaining reasonable interpretations at the same time. We propose a method, dubbed BOBAX, that allows to efficiently search for explanations without a relevant loss of optimization efficiency.

BOBAX is an interleaving strategy which performs BO, and iterates between using the EI (or any other suited acquisition function) and the EIG\(_{\text{PDP}}\) as acquisition function. Although we have investigated also more complex variants (see Appendix A.2), interleaving EIG\(_{\text{PDP}}\) in every \( k \)-th is simple yet efficient. The smaller \( k \) is, the higher is the weight of optimization for interpretability in a BO run. We note that this strategy can replace other interleaving exploration strategies, such as random samples [Hutter et al. 2011], since optimizing for interpretability can be seen as another strategy to cover the entire space in an efficient manner.

From a practitioner’s point of view, it may be reasonable to consider interpretability rather as a constraint than an objective function to optimize for. To be more precise, a user could specify a desired level of precision of an interpretation method as input to a HPO system. We propose to assess the precision of PD estimates via estimated \( \alpha \)-confidence intervals \( \varphi^{(g)} \) denoting the uncertainty of a PD estimate for a grid point \( g \) as proposed by [Moosbauer et al. 2021].

We additionally propose adaptive BOBAX (a-BOBAX), which takes the desired precision of a PD estimate as given by a user into account. To keep the notion of desired precision as user-friendly as possible, we define it as the desired average width of a \( \alpha \)-confidence interval in relation to the range of the function (e.g., \([0, 1]\) for validation accuracy). While performing the interleaving strategy in BOBAX as described above in a first stage, we continuously monitor the precision of a PD estimated by the average width of the confidence interval. Once the desired precision is reached, we transition to pure optimization (i.e., we stop interleaving EIG\(_{\text{PDP}}\)).

4.3 Theoretical and Practical Considerations

Runtime Complexity Since BOBAX comes with additional overhead, we discuss this here in more detail. The computation of the expectation requires posterior samples of the execution path \( e_A \sim p(e_A \mid A_T) \). This is achieved by sampling from the posterior GP \( \hat{c} \sim p(c \mid A_T) \) and execution of \( O_A \) on those samples, which may produce a computational overhead depending on the costs of
running $O_A$. We assume that executing $O_A$ is negligible in terms of runtime. However, to compute the entropy $\mathbb{H}[c_A|A_T, e_A]$, the posterior process needs to be trained based on $A_T \cup e_A$ (which has size $T + n \cdot G$). Thus, the overall runtime complexity is dominated by $O\left(n_{\text{path}} \cdot (T + n)^3\right)$, as we compute the entropy $n_{\text{path}}$ times to approximate the expectation and since training a GP is cubic in the number of data points. Therefore, we recommend to keep an eye on the runtime overhead of the calculation of $\text{EIG}_{\text{PD}}$ in relation to evaluating $c$ (e.g., training and evaluating an ML algorithm). Especially in the context of deep learning, the evaluation of a single configuration is usually by orders of magnitude higher than that of computing the $\text{EIG}_{\text{PD}}$.

Also, we would like to emphasize that the implementation of our method is based on GPflow [Matthews et al., 2017], which allows fast execution of GPs on GPUs. Since GPUs are typically in use for training in the context of DL anyway, they can easily be leveraged in between iterations to speed up the computation of the $\text{EIG}_{\text{PD}}$.

### Marginal Effects for Multiple Hyperparameters
Until now we have assumed that a user specifies a single hyperparameter of interest $\lambda_S$ for which we will compute the PD. However, it is difficult to prioritize the hyperparameter of interest a-priori. Fortunately, it is possible to extend the execution path to compute $\text{EIG}_{\text{PD}}$ by the respective execution paths of the PDs with regards to all variables $e_A = e_{A, \lambda_1} \cup e_{A, \lambda_2} \cup ... \cup e_{A, \lambda_d}$. This adaption is investigated in more detail in Appendix B.

### 5 Benchmark
In this section, we present experiments to demonstrate the validity of our method. In particular, we aim at supporting the following two hypotheses:

**Hypothesis H1 (Optimization for Interpretability):** It is possible to optimize more efficiently than random search for interpretability – measured by the error of the PDP w.r.t. the true marginal effect – by using the EIG as in Eq. (4) as acquisition function in BO.

**Hypothesis H2 (Enhanced Interpretability at no Relevant Loss of Optimization Efficiency):**

BOBAX enhances quality of marginal effect interpretations – measured by the error of the PDP w.r.t. the true marginal effect – without a significant loss of optimization performance.

The investigation of additional hypotheses is described in Appendix B.

#### 5.1 Experimental Setup

**Objective Functions** We first apply our method to synthetic functions which are treated as black-box function during optimization, including Branin ($d = 2$), Camelback ($d = 2$), Stylistsinki-Tang ($d = 3$), Hartmann3 ($d = 3$) and Hartmann6 ($d = 6$).

**Algorithms** To investigate H1, we consider BO with $\text{EIG}_{\text{PD}}$ as acquisition function. For H2, we consider BOBAX as described in Algorithm 2, where we iterate evenly ($k = 2$) between EI and $\text{EIG}_{\text{PD}}$ as acquisition function. In both variants we follow the recommendation of Neiswanger et al. [2021] and set the number of execution path samples to 20 to approximate the expectation in Eq. (4). As baselines we consider random search (RS), BO with EI (EI), and BO with the posterior variance as acquisition function (PVAR) as a pure exploration case of LCB. Further variants of our methods (e.g., different frequencies of interleaving) and additional baselines (such as BO with LCB with different exploration factors, or BO with EI and random interleaving) are described in Appendix B.

**Evaluation** We evaluate the quality of the interpretation given by a PD estimate by comparing it against the true marginal effect computed on the ground-truth objective function. As measure we use $d_L := \frac{1}{G} \sum_{g=1}^{G} \left| \phi^{(g)}_S - c_S(\Lambda^{(g)}_S) \right|$, which is the average $L_1$ distance between our estimate $\phi^{(g)}_S$ and the ground truth $c_S(\Lambda^{(g)}_S)$ averaged over all grid points. Additionally, we report the mean confidence (MC) of a PD estimate as $d_L := \frac{1}{G} \sum_{g=1}^{G} s(\Lambda^{(g)}_S)$ to evaluate the confidence in the estimate. To assess optimization performance, we report the optimization simple regret $c(\hat{\lambda}) - c(\lambda^*)$, where $\lambda^*$ denotes the theoretical optimum of a function, and $\hat{\lambda} \in \text{argmin} \{c_\lambda \mid (\lambda, c_\lambda) \in A_T\}$ is the best found configuration during optimization.

**Further Configurations** For BO variants, we use a Gaussian process with a squared exponential kernel with a nugget effect as surrogate model. For these methods, the partial dependence is computed on the surrogate model used by the BO procedure. For RS, a GP is fitted on the $A_T$ and a PDP

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2In our case, the computation of the $\text{EIG}_{\text{PD}}$ was ranging from the order of a few seconds to a few minutes.
is computed thereon. Acquisition function optimization is performed by randomly sampling 1500 configurations, evaluating the respective acquisition function and returning the best. Each (BO) run is given a maximum number of $30 \cdot d$ function evaluations.

**Reproducibility and Open Science** The implementation of methods as well as reproducible scripts for all experiments are publicly made available. Each experiment is replicated 20 times based on 20 different seeds fixed across all variants. More details on the code can be found in Appendix D.

### 5.2 Optimization for Interpretability (H1)

Our experiments support hypothesis H1, i.e., we can achieve more accurate PD estimates more efficiently through targeted sampling via the EI$_{PDP}$ both with BAX and BOBAX. An example run on the Branin function shown in Figure 2 illustrates the behavior of the methods that is observable across all experiments: BO with EI$_{PDP}$ is yielding clearly more accurate PDPs than the BO with EI already after few iterations. As expected, this comes to the cost of optimization efficiency. Aggregated results for both accuracy of PD estimates and optimization regret across all problems and replications confirm this behavior on a broader scale, see Table 1. BAX is producing more accurate PDPs than RS (which can be assumed to converge against the true marginal effect) already at early stages, and is strongly significantly ($\alpha = 5\%$) outperforming RS with less iterations. So we conclude that both BAX and PV AR can contribute to approximating the true marginal effect well, but BAX is converging faster. In addition, BO with EI improvement is significantly outperformed in terms of accuracy of PDPs, which supports our assumption of lowered quality caused through a heavy sampling bias. A more detailed view on the results of the experiments can be found in Appendix B.2.

Table 1: **Left:** $L_1$ error of the estimated PDP w.r.t. the ground truth PDP, relative to RS as baseline. Negative values mean a relative reduction of the $L_1$ error compared to random search. **Right:** Optimization relative to EI as baseline. Results are averaged across all 20 replications. Best values are bold, and values are underlined if not significantly worse than the best based on a Post-Hoc Friedman test ($\alpha = 5\%$), see also Demsar [2006], García et al. [2010] and Appendix B.1 for more details.

| Relative $d_{L_1}$ (PDP) after Max. iterations spent | Relative optimization regret after Max. iterations spent |
|------------------------------------------------------|-------------------------------------------------------|
| RS 0.00 0.00 0.00 0.00 | Rs 2.42 160.99 530.70 951.47 |
| EI 0.18 0.39 0.47 0.67 | EI **0.00 0.00 0.00 0.00** |
| PVAR 0.13 -0.08 0.08 0.14 | PVAR 3.38 232.14 741.69 1887.22 |
| BAX -0.17 -0.20 -0.07 **0.00** | BAX 2.27 242.062 602.15 1408.62 |
| BOBAX -0.14 -0.16 -0.04 0.03 | BOBAX 1.68 5.04 4.73 3.26 |

We note that the different functions live on different scales s.t. we normalized it by showing relative metrics w.r.t. baselines, such RS for PDP estimates and EI for optimization regret.

Figure 2: The first three plots show the estimated PD with 95% confidence interval (blue) based on the surrogate model $\hat{c}$ after $T = 30$ iterations vs. the true marginal effect (black). BAX and BOBAX yield more accurate estimates for the PD as compared the BO with EI. The right plot shows the cumulative regret for the three methods. BAX, which is not performing optimization at all, is also clearly outperformed in optimization performance. BOBAX reaches the optimization result of BO with EI only after a few more iterations.
5.3 Enhanced Interpretability at no Relevant Loss of Optimization Efficiency (H2)

Our experiments also support hypothesis H2, i.e., with BOBAX we can achieve clearly more accurate PD estimates while maintaining a competitive level of optimization efficiency. Figure 3 compares accuracy of a PD (measured via $d_{L1}$) and optimization regret for the Hartmann3 objective function as an example. BOBAX allows for more accurate PDPs than the other methods, with diminishing relative distance to RS, while BO with EI is clearly outperformed. On the other hand, it can be observed that BOBAX is giving optimization performance comparable to BO with EI throughout the course of optimization, whereas RS is clearly outperformed. This conclusion is also supported by Table 1 aggregating results for all five objective functions. So, BOBAX combines the best of both worlds: good interpretability (even better than RS) and efficient optimization (on par with BO-EI). We conclude that our experiments support that BOBAX makes no (or only little) compromises in optimization performance, but yields clearly better estimates of marginal effects at the same time.

Figure 3: **Left:** Accuracy of PD estimates, measured by $d_{L1}$ on the Hartmann3 function. BOBAX is outperforming both BO with EI and RS, even though BOBAX and RS seem to converge. **Right:** Optimization regret. While RS is clearly outperformed in terms of optimization efficiency, BOBAX and BO with EI perform comparable on this problem instance.

6 Practical HPO Application

We demonstrate our method on a concrete HPO scenario, following the setup of Moosbauer et al. [2021]. We tune common hyperparameters of a neural network with regards to balanced validation accuracy on five different datasets representing different domains: Australian (167104), cnae-9 (167185), higgs (167200), Fashion-MNIST (189908), KDDCup09_appetency (3945), based on Zimmer et al., 2021, see Table 5 in the Appendix, using the interface provided by YAHPO gym [Pfisterer et al., 2021]. We compare RS, EI, BAX, and adaptive BOBAX (a-BOBAX) with a desired precision of $\pm 1.5\%$ for 95% confidence intervals (i.e., a confidence band around balanced accuracy with width $\pm 0.015$ covers the true marginal effect with a likelihood of 95%). For the latter two variants, we are computing the EIGPDP jointly for the PDPs of learning rate, dropout, max. number of units, weight decay, and momentum as described in Section 4.3. The respective methods ran under the same conditions as in Section 5.

Figure 4 shows how the accuracy of the partial dependence estimate increases over time for BO with EI vs. BAX. We observe that BAX is clearly more efficient in returning an accurate estimate, which is in line with the results we observed in Section 5. As motivated in Section 4.2, a practitioner might prefer to rather ensure a minimum level of interpretability, and therefore, handle interpretability rather as a constraint than as an objective. Table 2 is showing the time to reach the desired precision of $\pm 1.5\%$ for the PDP for learning rate as well as final optimization performance. For a more granular representation of results, please refer to Appendix C.2. We observe that a-BOBAX is reaching the desired level of precision clearly faster and comes at almost no loss of final optimization performance.

7 Discussion and Conclusion

**Findings** We proposed (adaptive) BOBAX, modifying Bayesian Optimization (BO) for black-box optimization and HPO to enhance interpretability of the optimization problem at hand. We achieved this by adapting BAX to optimize for marginal effects and then interleaved BO and BAX. We further
showed that BOBAX can significantly enhance the estimation of marginal effects for PDPs during an optimization procedure, while not losing optimization performance.

**Usage** If a user already has some desired confidence level of the interpretations in mind, adaptive BOBAX allows them to make use of BAX only until this level is not reached yet and will focus only on the optimization quality afterwards. This simple, yet efficient strategy allows to get the most out of the overall optimization budget.

**Critical View and Limitations** Even though the usage of EIG is beneficial to the quality of a PDP estimate, there are also examples where it does not really give a significant improvement. Based on a more detailed look into the results, we assume that this particularly holds for hyperparameters that have a simple (and therefore easy-to-learn) effect on performance. As a consequence, the marginal effect is easily learned for any of the methods. In addition to using the adaptive version of BOBAX, we recommend dropping these simple-to-learn hyperparameters from the joint computation of the EIG as soon as the PDPs are sufficiently certain. Furthermore, our method comes at a computational overhead, being slightly larger than traditional BO since computing EIG with BAX costs a bit more compute time. In terms of application to HPO, we expect that the cost for training and validating hyperparameter configurations or architectures of neural networks will be much larger than BOBAX’s overhead in most relevant cases.

**Outlook** We believe that BOBAX will contribute in particular towards a more human-centered approach to HPO, where developers can start inspecting intermediate results as soon as desired confidence was reached and then adapt the configuration space if necessary. Although we focused on PDPs as an interpretability method, extending our BOBAX idea to other interpretability approaches (e.g., permutation feature importance) would be straightforward and opens up new follow up directions. As one of the next steps, we envision extending BOBAX to the multi-fidelity setting [Li et al., 2017, Falkner et al., 2018] which is required for more expensive HPO and AutoML problems. Last but not least, we emphasize that we developed BOBAX primarily for HPO problems, but it can also be applied to any kind of black-box optimization problem, e.g., in engineering, chemistry or biology.
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A Additional methodological aspects

A.1 Interpretability methods beyond the PDP

BOBAX is generic in the sense that it can be applied to other IML methods than the PDP that are of interest to the user, as long as the execution path of the respective method is accessible to BOBAX. While we considered the partial dependence method to estimate main effects (i.e., the marginal effect of a single hyperparameter $\lambda_s$ on estimated performance) in our experiments, Algorithm 1 can be extended to estimate interaction effects of two hyperparameters $S = \{s, s'\}$. This is done by simply replacing the grid points in Algorithm 1 by a two-dimensional grid $\left(\lambda_s^{(g)}, \lambda_{s'}^{(g')}\right)$ for all pairs $g, g' \in \{1, 2, ..., G\}$ with $\left(\lambda_s^{(1)}, ..., \lambda_s^{(G)}\right)$ and $\left(\lambda_{s'}^{(1)}, ..., \lambda_{s'}^{(G)}\right)$ representing equidistant grids. With this modified execution path our method is be straightforwardly applied to estimate interaction effects.

Also, other methods within IML can be optimized for with BOBAX; for example, the hyperparameter importance via permutation feature importance (PFI) [Fisher et al., 2019]. Importance of a single hyperparameter $\lambda_S$ is computed by shuffling the values of this hyperparameter in the $A_T$, resulting in a modified archive $A_{T,\lambda_S}$ and the difference in errors of the model $\hat{c}$ on $A_T$ and on $A_{T,\lambda_S}$ is compared. The respective execution path $e_A$ is the joint set of all shuffled versions of the archive $\hat{A}_T, A_{T, \lambda_1} \cup \hat{A}_T, A_{T, \lambda_2} \cup ... \cup \hat{A}_T, A_{T, \lambda_k}$.

A.2 BOBAX and Variants

Algorithm 2: BOBAX

```
Input $k, n_{\text{init}}, O_A$

$A_T \leftarrow$ Sample initial design of size $n_{\text{init}}$ over $\Lambda$

while stopping criterion not met do
  if $T \mod k = 0$ then
    $\lambda^{(T+1)} \leftarrow \arg\max_{\lambda \in \Lambda} \text{EI}_{\text{PDP}}(\lambda)$
  else
    $\lambda^{(T+1)} \leftarrow \arg\max_{\lambda \in \Lambda} \text{EI}(\lambda)$
  end if
  $c_{\lambda^{(T+1)}} \leftarrow c(\lambda^{(T+1)})$
  $A_{T+1} \leftarrow A_T \cup \{(\lambda^{(T+1)}, c_{\lambda^{(T+1)}})\}$
  $T \leftarrow T + 1$
end while

Return $A_T, O_A(\hat{c})$
```

Algorithm 2 shows the BOBAX algorithm as introduced and discussed in the main paper. We have investigated two more alternative acquisition functions to trade-off interpretability and optimization efficiency. One is a probabilistic variant of interleaving $\text{EI}_{\text{PDP}}$, where in every iteration

$$
\lambda^{(T+1)} = \arg\max_{\lambda \in \Lambda} \begin{cases} 
\text{EI}_{\text{PDP}}(\lambda) & \text{if } p \leq \pi \\
\text{EI}(\lambda) & \text{if } p > \pi 
\end{cases}
$$

where $p \sim \text{Unif}(0, 1)$ and $\pi$ is a threshold set by a user. If $\pi$ is set to 0.5 this corresponds to the probabilistic variant of Algorithm 2 with $k = 2$. We call this variant BOBAX$^{\text{prob}}$. This method also opens up the possibility to reduce the relative amount search for interpretability (as a kind of exploration) over time by an annealing strategy where the probability $\pi$ is lowered over time. As a second variant, we investigated a multiplicative variant of $\text{EI}_{\text{PDP}}$ and EI inspired by [Hvarfner et al., 2022]:

$$
\text{EIBAX}^\beta(\lambda) = \text{EI}(\lambda) \cdot \text{EI}_{\text{PDP}}(\lambda)^{\beta/T},
$$

where the values of a sampled batch of $\text{EI}_{\text{PDP}}(\lambda)$ are min-max-scaled to $[0, 1]$. Note that in comparison to the interleaving strategy, this method has a computational disadvantage since it requires to compute the $\text{EI}_{\text{PDP}}$ in every iteration.

Note that in any of the variants above, the EI can be replaced by any other acquisition function.
B Benchmark

B.1 Additional Details

Details on evaluation We performed a statistical test to allow for conclusions as to whether the methods compared (RS, EI, BAX, BOBAX) are performing significantly differently in terms of (1) quality of the PD estimate measured by $d_{L1}$, (2) optimization performance as measured by regret in Table 1. We applied a Friedman aligned ranks test as described in [García et al., 2010] on the respective performance values on different objective functions and replications to conclude whether there is a difference between methods. Note that the chosen test is recommended over the Friedman test by García et al. [2010] in particular if the number of algorithms is low (four to five) because of an increased power. We applied a post hoc test with Hommel correction for multiple testing, and report statistical significance based on corrected p-values. We rely on the implementation scmamp.

Comparison with additional baselines As additional baselines, we are running BO with LCB $\hat{c}(\lambda) + \tau \cdot \hat{s}^2(\lambda)$ acquisition function with different values of $\tau \in \{1, 2, 5\}$, denoted by LCB$^1$, LCB$^2$, LCB$^5$. Also, we are running BO with interleaved random configurations every $k \in \{2, 5, 10\}$ iterations, denoted by BO-RS$^2$, BO-RS$^5$, BO-RS$^{10}$. We are in addition considering different variations of the BOBAX method as described in Section A.2: We consider EIBAX$^{20}$, EIBAX$^{50}$, EIBAX$^{10}$, as well as BOBAX$^{0.5}$. Also, we have run BOBAX for different degrees of random interleaving $k \in \{2, 5, 10\}$, denoted by BOBAX$^2$, BOBAX$^5$, BOBAX$^{10}$. Note that all (BAX) variants optimize for a PD for one variable only; we have chosen the first variable as default. To support our claims in Section 4.3 that our method can be easily applied to jointly compute the PDP for multiple variables, we are also comparing to one variant which computes the PDP for all variables, denoted by BAX$^\text{all}$ and compare it to BAX.

Technical details All experiments only require CPUs (and no GPUs) and were computed on a Linux cluster (see Table 3).

| Computing Infrastructure |
|--------------------------|
| Type                     | Linux CPU Cluster |
| Architecture             | 28-way Haswell-EP nodes |
| Cores per Node           | 1 |
| Memory limit (per core)  | 2.2 GB |

Implementation details Our implementation of BOBAX is based on the implementation provided by [Neiswanger et al., 2021] which in turn is based on the GPflow [Matthews et al., 2017] implementation for Gaussian processes.

Note that we are not optimizing the hyperparameters of the GP (lengthscale, kernel variance, and nugget effect) during BOBAX to eliminate one source of variance between methods. Instead, similarly to [Neiswanger et al., 2021], we are setting those parameters to sensible default values. These are determined by the following heuristic executed prior to all experiments: For every objective function, we perform maximum likelihood optimization of these GP hyperparameters based on 200 randomly sampled points, and choose the configuration with the highest likelihood. This configuration is fixed across all replications and methods. While this heuristic does not impact the expressiveness of our statements since all methods are based on the same kernel hyperparameters, we emphasize that choosing appropriate hyperparameters is crucial for the performance of our method; therefore, a stable implementation (as done in established BO libraries) is regarded a necessary requirement for practical usage.

B.2 Additional Results

To evaluate many different algorithms based on two criteria (1) error in PDP estimate $d_{L1}$, and (2) optimization regret in a compressed way, we are looking at the ranks of different methods with regards to both metrics, resulting in two ranks rank$_{d_{L1}}$, rank$_{\text{regret}}$. For the sake of evaluation we

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1. https://github.com/b0rxa/scmamp
2. https://github.com/willieneis/bayesian-algorithm-execution
Table 4: The table shows the combined ranks $\frac{1}{2} \cdot \text{rank}_{\text{data}} + \frac{1}{2} \cdot \text{rank}_{\text{regret}}$ of different methods introduced in Section 4 as well as additional baselines introduced in Appendix B.1. Results are averaged across 20 replications and across all problems. We observe that BOBAX$^2$ is best in terms of the combined rank.

| Method      | 25% | 50% | 75% | 100% |
|-------------|-----|-----|-----|------|
| BOBAX$^2$  | 6.30| 5.24| 4.88| 4.88 |
| BOBAX$^5$  | 6.36| 5.91| 5.23| 5.08 |
| BOBAX$^{10}$ | 6.51| 6.10| 5.46| 5.14 |
| BO-RS$^2$ | 7.65| 7.02| 5.88| 5.49 |
| BOBAX$^{0.5}_{\text{prob}}$ | 6.96| 6.39| 5.92| 5.72 |
| BO-RS$^5$ | 7.24| 6.60| 5.92| 5.73 |
| BO-RS$^{10}$ | 7.37| 6.64| 6.18| 5.78 |
| EIBAX$^{100}$ | 6.71| 6.40| 6.00| 5.94 |
| BAX | 6.77| 6.95| 6.32| 6.18 |
| EIBAX$^{20}$ | 6.91| 6.79| 6.10| 6.20 |
| LCB$^9$ | 8.93| 6.65| 6.09| 6.22 |
| EI | 7.53| 7.44| 6.67| 6.28 |
| EIBAX$^{50}$ | 6.83| 6.45| 6.21| 6.49 |
| RS | 8.82| 9.19| 7.74| 6.92 |
| PVAR | 9.80| 8.01| 7.18| 7.00 |
| LCB$^2$ | 8.94| 7.30| 7.30| 7.54 |
| LCB$^1$ | 8.36| 7.99| 8.20| 8.10 |

Assume that interpretability and optimization efficiency are of equal importance and therefore assign each method a combined rank of $\frac{1}{2} \cdot \text{rank}_{\text{data}} + \frac{1}{2} \cdot \text{rank}_{\text{regret}}$. We average the combined ranks of every method across replications and problem instances. Table 4 shows the combined ranks for our proposed methods BAX and BOBAX (introduced in Section 2) as well as all baselines.

As addition to the results presented in Section 5, we present progress diagrams for the methods compared in Figure 5 as well as box plots for the remaining objective functions in Figure 6. Figure 7 compares the EIG$_{\text{PDP}}$ computed w.r.t. the PD of a single variable vs. jointly for the PDs of all variables. We observe that there is no drop in performance; in particular, we observe that the joint computation performs comparably to the computation for a single variable when evaluated on a single variable; and the joint computation performs better, if the accuracy of all PDPs is considered.

C Practical HPO Application

C.1 Additional Details

Table 5: Hyperparameter space of the LCBench [Zimmer et al., 2021] benchmark suite within YAHPO gym [Pfisterer et al., 2021]; batch size and maximum number of layers have been set to defaults 512 and 5, respectively.

| Name                        | Range         | log | type |
|------------------------------|---------------|-----|------|
| Max. number of units         | [64, 512]     | yes | int  |
| Learning rate (SGD)          | [1e$^{-4}$, 1e$^{-1}$] | yes | float|
| Weight decay                 | [1e$^{-5}$, 1e$^{-1}$] | no  | float|
| Momentum                     | [0.1, 0.99]   | no  | float|
| Max. dropout rate            | [0.0, 1.0]    | no  | float|

As practical HPO application we have chosen the use case of tuning hyperparameters of a neural network (as shown in Table 5) on the different classification tasks (listed in Table 6) with regards to Balanced accuracy as performance measures. In BAX / a-BOBAX, we are computing the EIG$_{\text{PDP}}$
Table 6: Datasets accessed via the *lcbench* suite of YAHPO gym [Pfisterer et al., 2021]; the underlying data for the surrogate benchmark was made available by [Zimmer et al., 2021].

| ID     | Name          | Usecase                        | $n$  | $d$  |
|--------|---------------|--------------------------------|------|------|
| 167104 | Australian    | Credit approval                | 690  | 15   |
| 167185 | cnae-9        | Classification of free text    | 1080 | 857  |
| 167200 | higgs         | Higgs boson detection          | 98050| 29   |
| 189908 | Fashion-MNIST | Classification of Zalando’s article images | 70000 | 785 |
| 3945  | KDDCup09_appetency | Prediction of customer behavior | 50000 | 231 |

Jointly for the PDPs of all hyperparameters listed in Table 5. Each run is replicated 10 times. Otherwise, all other settings correspond to the settings in Sections 5 and Appendix B. Note that the benchmark provided via Yahpo Gym [Pfisterer et al., 2021] is a surrogate benchmark, which not only supports efficient execution of a benchmark, but also gives access to a (reasonably cheap-to-evaluate) empirical performance model as ground truth objective; allowing us to compute the ground-truth PDP (and thus, any measure of error of the PDP) based on this empirical performance model.

C.2 Additional Results

Figure 8 shows a more granular representation of results for the HPO usecase.

D Code and Implementation

All code and data needed to reproduce the benchmark will be made publicly available via a Github repository after completion of the review process. During review phase, all code is uploaded as a supplementary material, or can alternatively be downloaded from [https://figshare.com/s/d6ef1b8f4c9c1e844229](https://figshare.com/s/d6ef1b8f4c9c1e844229). Please refer to the README.md file for further information about how to use the code to reproduce results.

Note that our implementation is based on the implementation provided by [Neiswanger et al., 2021](https://github.com/willieneis/bayesian-algorithm-execution). Raw and processed results can be downloaded from [https://figshare.com/s/4e1808644f8452d40680](https://figshare.com/s/4e1808644f8452d40680).
Figure 5: **Left**: Progress of error in PDP as measured by $d_{L_1}$ vs. the number of iterations. **Right**: Progress of optimization regret vs. number of iterations. In both figures, the 95% confidence intervals around the mean are shown.
Figure 6: Error of PD estimates measured via $d_{L_1}$ (left) and optimization regret (right) for the different synthetic objectives. While RS is clearly outperformed in terms of optimization efficiency, BOBAX and BO with EI perform comparable on this problem instance.
Figure 7: The performance of BOBAX with EIG\textsubscript{PDP} computed with regards to the first variable only (blue) vs. the performance of BOBAX when EIG\textsubscript{PDP} is computed for the joint execution paths of PD estimates with regards to all variables (orange). **Left:** Error of the PD estimate for the first variable (measured via $d_{l_1}$). **Right:** Error of the PD estimate for the all variables (measured via $d_{l_1}$). We observe that the joint computation delivers more accurate PDs over all variables. However, we also observe that the difference is not dramatically big.
Figure 8: The figure compares error of the PDP estimate after the full budget spent (in terms of $dL_1$; shown in the first row), the percentage of iterations needed to reach the desired level of confidence (middle row), as well as the final regret (last row) for the different methods a-BOBAX, EI, and RS on the different datasets (columns) that we tuned for. In most cases, a-BOBAX has a final error in PDP comparable to RS, but clearly better than with EI, and reaches the desired level of confidence faster than the two other methods. In terms of optimization performance, a-BOBAX and EI perform comparably, and both clearly outperform RS.