Bayesian Optimization Meets Bayesian Optimal Stopping

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Abstract

Bayesian optimization (BO) is a popular paradigm for optimizing the hyperparameters of *machine learning* (ML) models due to its sample efficiency. Many ML models require running an iterative training procedure (e.g., stochastic gradient descent). This motivates the question whether information available during the training process (e.g., validation accuracy after each epoch) can be exploited for improving the epoch efficiency of BO algorithms by early-stopping model training under hyperparameter settings that will end up under-performing and hence eliminating unnecessary training epochs. This paper proposes to unify *BO* (specifically, *Gaussian process-upper confidence bound* (GP-UCB)) *with Bayesian optimal stopping* (BO-BOS) to boost the epoch efficiency of BO. To achieve this, while GP-UCB is sample-efficient in the number of function evaluations, BOS complements it with epoch efficiency for each function evaluation by providing a principled optimal stopping mechanism for early stopping. BO-BOS preserves the (asymptotic) no-regret performance of GP-UCB using our specified choice of BOS parameters that is amenable to an elegant interpretation in terms of the exploration-exploitation trade-off. We empirically evaluate the performance of BO-BOS and demonstrate its generality in hyperparameter optimization of ML models and two other interesting applications.

1. Introduction

The state-of-the-art *machine learning* (ML) models have recently reached an unprecedented level of predictive performance in several applications such as image recognition, complex board games, among others (LeCun et al., 2015; Silver et al., 2016). However, a major difficulty faced by ML practitioners is the choice of model hyperparameters which significantly impacts the predictive performance. This calls for the need to develop hyperparameter optimization algorithms that have to be sample-efficient since the training of many modern ML models consumes massive computational resources. To this end, *Bayesian optimization* (BO) is a popular paradigm due to its high sample efficiency and strong theoretical performance guarantee (Shahriari et al., 2016). In particular, the BO algorithm based on the *Gaussian process-upper confidence bound* (GP-UCB) acquisition function has been shown to achieve no regret asymptotically and perform competitively in practice (Srinivas et al., 2010).

Many ML models require running an iterative training procedure for some number of epochs such as stochastic gradient descent for neural networks (LeCun et al., 2015) and boosting procedure for gradient boosting machines (Friedman, 2001). During BO, any query of a hyperparameter setting usually involves training the ML model for a fixed number of epochs. Information typically available during the training process (e.g., validation accuracy after each epoch) is rarely exploited for improving the epoch efficiency of BO algorithms, specifically, by early-stopping model training under hyperparameter settings that will end up under-performing, hence eliminating unnecessary training epochs.

To address this challenging issue, a number of works have been proposed to make BO more epoch-efficient: Freeze-thaw BO (Swersky et al., 2014) explores a diverse collection of hyperparameter settings in the initial stage by training their ML models with a small number of epochs, and then gradually focuses on (exploits) a small number of promising settings. Despite its promising epoch efficiency, its performance is not theoretically guaranteed and its computational cost can be excessive. Multi-fidelity BO (Kandasamy et al., 2016; 2017) reduces the resource consumption of BO by utilizing low-fidelity functions which can be obtained by using a subset of the training data or by training the ML model for a small number of epochs. However, in each BO iteration, since the fidelity (e.g., number of epochs) is determined before function evaluation, it is not influenced by information that is typically available during the training process (e.g., validation accuracy after each epoch). In addition to BO, attempts have also been made to improve the epoch efficiency of other hyperparameter optimization algorithms: Some heuristic methods (Baker et al., 2017; Domhan et al., 2015; Klein et al., 2017) have predicted the final training out-

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come based on partially trained learning curves in order to identify hyperparameter settings that are predicted to underperform and early-stop their model training. Hyperband (Li et al., 2017), which dynamically allocates the computational resource (e.g., training epochs) through random sampling and eliminates under-performing hyperparameter settings by successive halving, has been proposed and shown to perform well in practice. Both the learning curve prediction methods and Hyperband can be combined with BO to further improve the epoch efficiency (Domhan et al., 2015; Falkner et al., 2018; Klein et al., 2017), but their resulting performances are not theoretically guaranteed. Despite these recent advances, we still lack an epoch-efficient algorithm that can incorporate early stopping into BO (i.e., by exploiting information available during the training process) and yet offer a theoretical performance guarantee, the design of which is likely to require a principled decision-making mechanism for determining the optimal stopping time.

Optimal stopping is a classic research topic in statistics and operations research regarding sequential decision-making problems whose objective is to make the optimal stopping decision with a small number of observations (Ferguson, 2006). In *Bayesian optimal stopping* (BOS) or Bayesian sequential design, the decision between stopping vs. continuing is made to maximize the expected utility or, equivalently, minimize the expected loss (Powell & Ryzhov, 2012). BOS has found success in application domains such as finance (Longstaff & Schwartz, 2001), clinical design (Brockwell & Kadane, 2003; Müller et al., 2007; Wathen & Thall, 2008), and economics (Davis & Cairns, 2012). The capability of BOS in providing a principled optimal stopping mechanism makes it a prime candidate for introducing early stopping into BO in a theoretically sound and rigorous way.

This paper proposes to unify *Bayesian optimization* (specifically, GP-UCB) *with Bayesian optimal stopping* (BO-BOS) to boost the epoch efficiency of BO (Section 3). Intuitively, GP-UCB is acclaimed for being sample-efficient in the number of function evaluations while BOS can reduce the required number of epochs for each function evaluation. BO-BOS unifies the best of both worlds to yield an epoch-efficient hyperparameter optimization algorithm. Interestingly, in spite of the seemingly disparate optimization objectives of GP-UCB vs. BOS (respectively, objective function v.s. expected loss), BO-BOS can preserve the trademark (asymptotic) no-regret performance of GP-UCB with our specified choice of BOS parameters that is amenable to an elegant interpretation in terms of the exploration-exploitation trade-off (Section 4). Though the focus of our work here is on epoch-efficient BO for hyperparameter tuning, we additionally evaluate the performance of BO-BOS empirically in two other interesting applications to demonstrate its generality: policy search for reinforcement learning, and joint hyperparameter tuning and feature selection (Section 5).

2. Background and Notations

2.1. Bayesian Optimization (BO) and GP-UCB

Consider the problem of sequentially optimizing an unknown objective function $f : \mathcal{D} \rightarrow \mathbb{R}$ representing the validation accuracy over a compact input domain $\mathcal{D} \subseteq \mathbb{R}^d$ of different hyperparameter settings for training an ML model: In each iteration $t = 1, \ldots, T$, an input query $\mathbf{z}_t \triangleq [\mathbf{x}_t, n_t]$ of a hyperparameter setting (comprising $N_0 < n_t \leq N$ training epochs and a vector $\mathbf{x}_t$ of the other hyperparameters) is selected for evaluating the validation accuracy f of the ML model to yield a noisy observed output (validation accuracy) $y_t \triangleq f(\mathbf{z}_t) + \epsilon$ with i.i.d. Gaussian noise $\epsilon \sim \mathcal{N}(0, \sigma^2)$ and noise variance σ^2. Since every evaluation of f is costly (Section 1), our goal is to strategically select input queries to approach the global maximizer $\mathbf{z}^* \triangleq \arg\max_{\mathbf{z}\in\mathcal{D}} f(\mathbf{z})$ as rapidly as possible. This can be achieved by minimizing a standard BO objective such as the *simple regret* $S_T \triangleq f(\mathbf{z}^*) - \max_{t\in\{1,\ldots,T\}} f(\mathbf{z}_t)$. A BO algorithm is said to guarantee *no regret* asymptotically if it satisfies $\lim_{T\rightarrow\infty} S_T = 0$, thus implying that it will eventually converge to the global maximum.

To guarantee no regret, the belief of f is modeled by a *Gaussian process* (GP). Let $\{f(\mathbf{z})\}_{\mathbf{z}\in\mathcal{D}}$ denote a GP, that is, every finite subset of $\{f(\mathbf{z})\}_{\mathbf{z}\in\mathcal{D}}$ follows a multivariate Gaussian distribution (Rasmussen & Williams, 2006). Then, a GP is fully specified by its *prior* mean $\mu(z)$ and covariance $k(\mathbf{z}, \mathbf{z}')$ for all $\mathbf{z}, \mathbf{z}' \in \mathcal{D}$, which are, respectively, assumed w.l.o.g. to be $\mu(\mathbf{z}) = 0$ and $k(\mathbf{z}, \mathbf{z}') \leq 1$ for notational simplicity. Given a column vector $\mathbf{y}_T \triangleq [y_t]^\top_{t=1,\ldots,T}$ of noisy outputs observed from evaluating f at the selected input queries $\mathbf{z}_1, \ldots, \mathbf{z}_T \in \mathcal{D}$ after T iterations, the GP posterior belief of f at some input $\mathbf{z} \in \mathcal{D}$ is a Gaussian with the following *posterior* mean $\mu_T(\mathbf{z})$ and variance $\sigma^2_T(\mathbf{z})$:

$$\begin{aligned} \mu_T(\mathbf{z}) &\triangleq \mathbf{k}_T(\mathbf{z})^\top (\mathbf{K}_T + \sigma^2 I)^{-1} \mathbf{y}_T \ , \\ \sigma^2_T(\mathbf{z}) &\triangleq k(\mathbf{z}, \mathbf{z}) - \mathbf{k}_T(\mathbf{z})^\top (\mathbf{K}_T + \sigma^2 I)^{-1} \mathbf{k}_T(\mathbf{z}) \end{aligned} \tag{1}$$

where $\mathbf{K}_T \triangleq [k(\mathbf{z}_t, \mathbf{z}_{t'})]_{t,t'=1,\ldots,T}$ and $\mathbf{k}_T(\mathbf{z}) \triangleq [k(\mathbf{z}_t, \mathbf{z})]^\top_{t=1,\ldots,T}$. In each iteration t of BO, an input query $\mathbf{z}_t \in \mathcal{D}$ is selected to maximize the GP-UCB acquisition function (Srinivas et al., 2010) that trades off between observing an expected maximum (i.e., with a large GP posterior mean $\mu_{t-1}(\mathbf{z})$) given the current GP belief of f (i.e., exploitation) vs. that of high predictive uncertainty (i.e., with a large GP posterior variance $\sigma^2_{t-1}(\mathbf{z})$) to improve the GP belief of f over $\mathcal{D}$ (i.e., exploration). That is, $\mathbf{z}_t \triangleq \arg\max_{\mathbf{z}\in\mathcal{D}} \mu_{t-1}(\mathbf{z}) + \sqrt{\beta_t}\sigma_{t-1}(\mathbf{z})$ where the parameter $\beta_t > 0$ is set to trade off between exploitation vs. exploration for guaranteeing no regret asymptotically with high probability.

2.2. Bayesian Optimal Stopping (BOS)

BOS provides a principled mechanism for making the Bayes-optimal stopping decision with a small number of

observations. As shall be seen in Algorithm 1, in each iteration t of BO-BOS, BOS is used to early-stop model training under the selected input hyperparameters $\mathbf{x}_t$ that will end up under-performing, hence reducing the required number of training epochs. In a BOS problem, the goal is to decide whether to stop and conclude either hypothesis/event $\theta_t = \theta_{t,1}$ or $\theta_t = \theta_{t,2}$ corresponding to terminal decision d_1 or d_2, or to gather one more observation via the continuation decision d_0. Let $y_{t,n'}$ be the noisy output (validation accuracy) observed in epoch n' and $\mathbf{y}_{t,n} \triangleq [y_{t,n'}]^\top_{n'=1,\ldots,n}$ be a vector of noisy outputs observed up till epoch n in iteration t. Recall from Section 2.1 that in iteration t, the ML model is trained using the selected input hyperparameter setting $[\mathbf{x}_t, n_t]$ to yield the noisy observed output (validation accuracy) y_t. So, $y_t = y_{t,n_t}$ for $t = 1, \ldots, T$. After each epoch n, the posterior belief of event θ_t is updated to $\Pr(\theta_t|\mathbf{y}_{t,n})$ which will be used to compute the expected losses of terminal decisions d_1 and d_2. Such a loss function l has to encode the cost of making a wrong decision. Define $\rho_{t,n}(\mathbf{y}_{t,n})$ as the minimum expected loss among all decisions in epoch n:

$$\rho_{t,n}(\mathbf{y}_{t,n}) \triangleq \min\{\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,n}}[l(d_1,\theta_t)],\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,n}}[l(d_2,\theta_t)],\ c_{d_0} + \mathbb{E}_{y_{t,n+1}|\mathbf{y}_{t,n}}[\rho_{t,n+1}(\mathbf{y}_{t,n+1})]\ \} \tag{2}$$

for $n = 1, \ldots, N-1$ where the first two terms are the expected losses of terminal decisions d_1 and d_2, the last term sums the immediate cost c_{d_0} and expected future loss of making the continuation decision d_0 to continue model training in the next epoch $n+1$ to yield the noisy observed output (validation accuracy) $y_{t,n+1}$, and $\rho_{t,N}(\mathbf{y}_{t,N}) \triangleq \min\{\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,N}}[l(d_1,\theta_t)],\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,N}}[l(d_2,\theta_t)]\ \}$. Since $\rho_{t,n}$ depends on $\rho_{t,n+1}$, it naturally prompts the use of backward induction to solve the BOS problem (2) exactly, which is unfortunately intractable due to an uncountable set of possible observed outputs $y_{t,n+1}$. This computational difficulty can be overcome using approximate backward induction techniques (Brockwell & Kadane, 2003; Müller et al., 2007) whose main ideas include using summary statistics to represent the posterior belief, discretizing the space of summary statistics, and estimating the expectation terms via sampling. Appendix A describes a commonly-used approximate backward induction algorithm (Müller et al., 2007).

Solving the BOS problem (2) yields a Bayes-optimal decision rule in each epoch n: Take the Bayes-optimal stopping decision if the expected loss of either terminal decision d_1 or d_2 is at most that of the continuation decision d_0, that is, $\min\{\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,n}}[l(d_1,\theta_t)],\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,n}}[l(d_2,\theta_t)]\ \} \leq c_{d_0} + \mathbb{E}_{y_{t,n+1}|\mathbf{y}_{t,n}}[\rho_{n+1}(\mathbf{y}_{t,n+1})]$. Otherwise, continue model training to yield the noisy observed output (validation accuracy) $y_{t,n+1}$ and repeat this rule in the next epoch $n+1$.

3. BO-BOS Algorithm

In this section, we will describe our proposed BO-BOS algorithm (Section 3.1) and define the loss function l in BOS (2) such that it can serve as an effective early-stopping mechanism in BO (Section 3.2). We focus on problem settings where the objective function f is bounded and monotonically increasing in n:

Assumption 1. *(a)* $f(\mathbf{z}) \in [0,1]$ *for all* $\mathbf{z} \in \mathcal{D}$ *and (b)* $f([\mathbf{x},n]) \leq f([\mathbf{x},n+1])$ *for all* $\mathbf{x}$ *and* $n = 1,\ldots,N-1$.

Assumption 1a is not restrictive since it applies to any bounded f with a proper transformation. Assumption 1b holds reasonably well in a number of important ML problems: (a) f represents the validation accuracy of ML models and n denotes the number of training epochs or the number of selected features during feature selection, and (b) f represents the (discounted) cumulative rewards in reinforcement learning (assuming non-negative rewards) and n denotes the number of steps taken by the agent in the environment. Our experiments in Section 5 will demonstrate that BO-BOS outperforms the state-of-the-art hyperparameter optimization algorithms in these ML problems.

3.1. Algorithm Description

In each iteration t of BO-BOS (Algorithm 1), the input hyperparameters $\mathbf{x}_t$ are selected to maximize the GP-UCB acquisition function with the input dimension of training epochs fixed at N (line 2). The ML model is trained using $\mathbf{x}_t$ for N_0 initial training epochs to yield the noisy observed outputs (validation accuracies) $\mathbf{y}_{t,N_0}$ (line 3). After that, the BOS problem is solved (line 5) to obtain Bayes-optimal decision rules (see Sections 2.2 and 3.2). Then, in each epoch $n > N_0$, model training continues under $\mathbf{x}_t$ to yield the noisy observed output (validation accuracy) $y_{t,n}$ (line 8). If both of the following conditions are satisfied (line 9),

C1. BOS decision rule in epoch n outputs stopping decision;

C2. $\sigma_{t-1}([\mathbf{x}_t,n]) \geq \sigma_{t-1}([\mathbf{x}_t,N])/\kappa$,

then model training is early-stopped in epoch $n_t = n$. Otherwise, the above procedure is repeated in epoch $n+1$. If none of the training epochs $n = N_0+1,\ldots,N-1$ satisfy both C1 and C2, then $n_t = N$ (i.e., no early stopping). Finally, the GP posterior belief (1) is updated with the selected input hyperparameter setting $\mathbf{z}_t = [\mathbf{x}_t, n_t]$ and the corresponding noisy observed output (validation accuracy) $y_t = y_{t,n_t}$ (line 11). BO-BOS then proceeds to the next iteration $t+1$.

To understand the rationale of our choices of C1 and C2, the BOS decision rule in C1 recommends the stopping decision to early-stop model training in epoch n if it concludes that model training under $\mathbf{x}_t$ for N epochs will produce a validation accuracy not more than the currently found maximum in iterations $1,\ldots,t-1$; this will be formally described in Section 3.2. On the other hand, C2 prefers to evaluate the validation accuracy f of the ML model with the input query $[\mathbf{x}_t,n]$ of fewer training epochs $n < N$ than $[\mathbf{x}_t,N]$ if the predictive uncertainty of $f([\mathbf{x}_t,n])$ is higher

Algorithm 1 BO-BOS

for $t = 1, 2, \ldots, T$ **do**
  $\mathbf{x}_t \leftarrow \arg\max_{\mathbf{x}} \mu_{t-1}([\mathbf{x}, N]) + \sqrt{\beta_t}\sigma_{t-1}([\mathbf{x}, N])$
  Train model using $\mathbf{x}_t$ for N_0 epochs to yield $\mathbf{y}_{t,N_0}$
  $n \leftarrow N_0$
  Solve BOS problem (2) to obtain decision rules
  repeat
    $n \leftarrow n + 1$
    Continue model training using $\mathbf{x}_t$ to yield $y_{t,n}$
  until $(n = N) \vee (\text{C1} \wedge \text{C2})$
  $n_t = n$
  Update GP posterior belief (1) with $\mathbf{z}_t = [\mathbf{x}_t, n_t]$ and $y_t = y_{t,n_t}$

than that of $f([\mathbf{x}_t, N])$ being scaled down by a factor of $\kappa \geq 1$, hence better improving the GP belief of f (i.e., exploration) along the input dimension of training epochs (i.e., $\{[\mathbf{x}_t, n']\}_{n'=1,\ldots,N}$); the degree of preference/exploration is controlled by parameter κ. The requirement to satisfy both C1 and C2 thus reflects two complementary principles of early stopping in BO: (a) exploiting BOS's capability to early-stop model training under hyperparameter settings that will end up under-performing and (b) exploring to improve the GP belief along the input dimension of training epochs. Both C1 and C2 are necessary for theoretically guaranteeing the no-regret performance of BO-BOS (Section 4).

3.2. BOS for Early Stopping in BO

In iteration t, let the currently found maximum or incumbent value be denoted as $y^*_{t-1} \triangleq \max_{t' \in \{1,\ldots,t-1\}} y_{t'}$. In the context of early stopping in BO, BOS has to determine whether model training under $\mathbf{x}_t$ for N epochs will produce a validation accuracy not more than the incumbent value, i.e., $f([\mathbf{x}_t, N]) \leq y^*_{t-1} - \xi_t$ given the noisy outputs (validation accuracies) $\mathbf{y}_{t,n}$ observed up till epoch $n < N$ where $y^*_0 \triangleq 0$ and ξ_t is defined later in Theorem 1. To achieve this, we model it with the following three decisions: (a) d_1: stop and conclude that $f([\mathbf{x}_t, N]) \leq y^*_{t-1} - \xi_t$, (b) d_2: stop and conclude that $f([\mathbf{x}_t, N]) > y^*_{t-1} - \xi_t$, and (c) d_0: continue to train for one more epoch. Based on this setting, the event θ (Section 2.2) can be defined as

$$\theta_t \triangleq \begin{cases} \theta_{t,1} & \text{if } f([\mathbf{x}_t, N]) > y^*_{t-1} - \xi_t \ , \\ \theta_{t,2} & \text{otherwise} \ ; \end{cases}$$

about which we are uncertain due to the uncertainty regarding the value of $f([\mathbf{x}_t, N])$ when $n < N$, and the objective of BOS is to determine whether $\theta_t = \theta_{t,1}$ or $\theta_t = \theta_{t,2}$. We adopt the $0-K$ loss function commonly used in clinical designs (Lewis & Berry, 1994; Jiang et al., 2013) due to its simplicity and interpretablility:

$$l(d_1, \theta_t) \triangleq K_1 \mathbb{1}_{\theta_t = \theta_{t,1}} \ , \quad l(d_2, \theta_t) \triangleq K_2 \mathbb{1}_{\theta_t = \theta_{t,2}} \ , \quad (3)$$

in which the cost parameters $K_1 > 0$ and $K_2 > 0$ represent how much we would like to penalize falsely making the corresponding terminal decisions. As a result, the expected losses of the terminal decisions, d_1 and d_2 can be calculated:

$$\begin{aligned} \mathbb{E}_{\theta_t|\mathbf{y}_{t,n}}[l(d_1, \theta_t)] &= K_1 \Pr(\theta_t = \theta_{t,1}|\mathbf{y}_{t,n}) \ , \\ \mathbb{E}_{\theta_t|\mathbf{y}_{t,n}}[l(d_2, \theta_t)] &= K_2 \Pr(\theta_t = \theta_{t,2}|\mathbf{y}_{t,n}) \ . \end{aligned} \quad (4)$$

Note that if a cost parameter is set to $+\infty$, the corresponding expected loss is taken as $+\infty$ and the corresponding terminal decision is never taken; e.g., if $K_1 = +\infty$, decision d_1 is never selected. Based on these definitions, the expected loss at step n is defined as the minimum expected losses among all decisions in the same way as (2):

With this formulation, the resulting BOS problem can be solved with an adapted approximate backward induction algorithm. To take into account Assumption 1b, we use a kernel with prior bias towards exponentially decaying learning curves (Swersky et al., 2014) to fit a GP model on the initial N_0 validation accuracies and draw samples from the resulting GP model, which are then plugged into approximate backward induction as the forward simulation samples mainly for the estimation of $\Pr(\theta_t = \theta_{t,1}|\mathbf{y}_{t,n})$ and $\Pr(y_{t,n+1}|\mathbf{y}_{t,n})$. Following some applications of BOS (Müller et al., 2007; Jiang et al., 2013), we use the average validation accuracies as the summary statistics. A detailed description of the approximate backward induction algorithm is presented in Appendix B. After the BOS problem is solved, a set of decision rules are obtained and used by C1 in the BO-BOS algorithm. Specifically, after the n-th validation accuracy is observed, we first calculate the updated summary statistics $\sum_{n'=1}^{n} y_{t,n'}/n$, and then take the corresponding optimal decision suggested by the BOS decision rules. If the suggested decision is d_1 (i.e., the optimal decision now is to stop the current experiment since we believe $\mathbf{x}_t$ will end up having smaller validation accuracy than the incumbent), we immediately terminate the training of $\mathbf{x}_t$ (assuming C2 is satisfied); otherwise, we train for one more epoch, and repeat the process until $n = N$. Note that taking decision d_2 (i.e., early-stopping because we believe $\mathbf{x}_t$ will perform better than the incumbent) does not align with the objective of BO, which is to sequentially maximize the objective function. Therefore, when decision d_2 is suggested by BOS, to conform to the decision-making principle of BO, we do not early-stop the experiment and instead continue the training.

4. Theoretical Analysis

The goal of the theoretical analysis is to characterize the growth of the *simple regret* S_T of the proposed BO-BOS algorithm and thus show how the algorithm should be designed in order for S_T to asymptotically go to 0, i.e., for the algorithm to be *no regret*. To account for the addi-

tional uncertainty introduced by BOS, we analyze the expected regret, in which the expectation is taken with respect to the posterior probabilities from the BOS algorithms: $\Pr(f([\mathbf{x}_t, N]) > y^*_{t-1} - \xi_t | \mathbf{y}_{t,n_t})$.

We make the following assumption on the smoothness of the objective function f:

Assumption 2. *Assume for the kernel k, for some a and b,*

$$Pr(\sup_{\mathbf{z}\in\mathcal{D}} |\partial f/\partial z_j| > L) \leq a \exp(-(L/b)^2)$$

for $j = 1, \ldots, d$ where z_j is the j-th component of input $\mathbf{z}$.

Assumption 2 is satisfied by some commonly used kernels such as the Square Exponential kernel and Matérn kernel with $v > 2$ (Srinivas et al., 2010). For simplicity, we assume that the underlying domain $\mathcal{D}$ is discrete, i.e. $|\mathcal{D}| < \infty$. However, it is straightforward to extend the analysis to general compact domain by following similar analysis strategies as those in Appendix A.2. of (Srinivas et al., 2010). Theorem 1 below shows an upper bound on the expected simple regret of the BO-BOS algorithm.

Theorem 1. *Suppose that Assumptions 1 and 2 hold. Let $\delta, \delta', \delta'' \in (0, 1)$, $\beta_t \triangleq 2\log(|\mathcal{D}|t^2\pi^2/(6\delta))$, and $\tau_T \triangleq \sum_{t=1}^{T} \mathbb{1}_{n_t<N}$ be the number of BO iterations in which early stopping happens from iterations 1 to T. Let κ be the parameter used in C2. At iteration t, the BOS algorithm is run with the corresponding fixed cost parameters K_2 and c_{d_0}, as well as iteration-dependent cost parameter $K_{1,t}$, $\xi_1 \triangleq 0$, and $\xi_t \triangleq \sqrt{2\sigma^2 \log(\pi^2 t^2 (t-1)/(6\delta''))}$ for $t > 1$. Then $\forall T \geq 1$, with probability of at least $1 - \delta - \delta' - \delta''$,*

$$\mathbb{E}[S_T] \leq \frac{\kappa\sqrt{TC_1\beta_T\gamma_T}}{T} + \frac{\sum_{t=1}^{T}\eta_t}{T} + \frac{1}{T}Nb\sqrt{\log\frac{da}{\delta'}}\tau_T$$

in which $\eta_t \triangleq \frac{K_2 + c_{d_0}}{K_{1,t}}$, $C_1 = 8/log(1+\sigma^{-2})$, γ_T is the maximum information gain about the function f from any set of observations of size T, and the expectation is w.r.t. $\prod_{t\in\{t'|t'=1,\ldots,T,n_{t'}<N\}} Pr(f([\mathbf{x}_t, N]) > y^*_{t-1} - \xi_t|\mathbf{y}_{t,n_t})$ used in the BOS algorithm.

Theorem 2 below states how the BOS parameters should be chosen to make BO-BOS asymptotically no-regret.

Theorem 2. *In Theorem 1, if $K_{1,t}$ is an increasing sequence such that $K_{1,1} \geq K_2 + c_{d_0}$ and that $K_{1,t}$ goes to $+\infty$ in finite number of BO iterations, then, with probability of at least $1 - \delta - \delta' - \delta''$, $\mathbb{E}[S_T]$ goes to 0 asymptotically.*

The proof of both theorems is presented in Appendix C. The first term in the upper bound of $\mathbb{E}[S_T]$ in Theorem 1 matches that of the simple regret of the GP-UCB algorithm (up to the constant κ). Note that the theoretical results rely on the exact solution of the BOS problems; however, in practice, a trade-off exists between the quality of the approximate backward induction and the computational efficiency. In particular, increasing the number of forward simulation samples and making the grid of summary statistics more fine-grained both lead to better approximation quality, while increasing the computational cost. Recommended approximation parameters that work well in all our experiments and thus strike a reasonable balance between these two aspects are given in Section 5.

Interestingly, the choice of an increasing $K_{1,t}$ sequence as required by Theorem 2 is well justified in terms of the exploration-exploitation trade-off. As introduced in section 3.2, K_1 represents how much we would like to penalize the BOS algorithm for falsely early-stopping (taking decision d_1). Therefore, increasing values of K_1 implies that, as the BO-BOS algorithm progresses, we become more and more cautious at early-stopping. In other words, the preference of BOS for early stopping diminishes over BO iterations. Interestingly, this corresponds to sequentially shifting our preference from exploration (using small number of epochs) to exploitation (using large number of epochs) throughout all runs of the BOS algorithms, which is an important decision-making principle followed by many sequential decision-making algorithms such as BO, multi-armed bandit, reinforcement learning, among others.

Another intriguing interpretation of the theoretical results is that the growth rate of the $K_{1,t}$ sequence implicitly determines the trade-off between faster convergence of the BO algorithm (smaller number of BO iterations) and more computational saving in each BO iteration (smaller number of training epochs on average). In particular, if $K_{1,t}$ grows quickly, the second and third terms in the upper bound in Theorem 1 both decay fast, since η_t is inversely related to $K_{1,t}$ and large penalty for early stopping results in small τ_T; as a result, a large number of hyperparameters are run with N epochs and the resulted BO-BOS algorithm behaves similarly to GP-UCB, which is corroborated by the upper bound on $\mathbb{E}[S_T]$ in Theorem 1 since the first term dominates. On the other hand, if the $K_{1,t}$ sequence grows slowly, then the second and third terms in Theorem 1 decay slowly; consequently, these two terms dominate the regret and the resulted algorithm early-stops very often, thus leading to smaller number of epochs on average, at the potential expense of requiring more BO iterations. Furthermore, the constant κ used in C2 also implicitly encodes our relative preference for early-stopping. Specifically, large values of κ favor early stopping by relaxing C2: $\sigma_{t-1}([\mathbf{x}_t, n]) \geq \sigma_{t-1}([\mathbf{x}_t, N])/\kappa$; however, more early-stopped function evaluations might incur larger number of required BO iterations as can be verified by the fact that larger κ increases the first regret term in Theorem 1 (which matches the regret of GP-UCB). In practice, as a result of the above-mentioned trade-offs, the best choices of the BOS parameters and κ are application-dependent. In addition, to avoid abnormal behaviors of the BOS algorithms, the BOS parameters should be chosen with

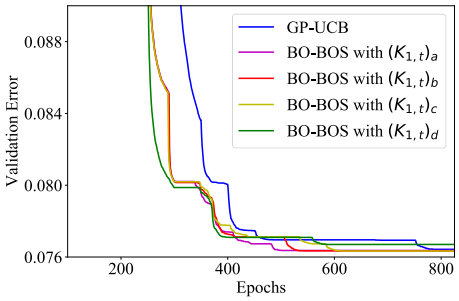


Figure 1. Best-found validation error of logistic regression v.s. the total number of epochs (averaged over 10 random initializations). $K_2 = 99$ and $c_{d_0} = 1$ are fixed; $K_{1,1} = 100$ for all four BO-BOS algorithms; for $t > 1$, the different $K_{1,t}$ sequences are: $(K_{1,t})_a = \frac{K_{1,t-1}}{0.89}$; $(K_{1,t})_b = \frac{K_{1,t-1}}{0.95}$; $(K_{1,t})_c = \frac{K_{1,t-1}}{0.99}$; $(K_{1,t})_d = \frac{K_{1,t-1}}{1.0} = K_{1,1}$.

additional care. In particular, c_{d_0} should be small, whereas K_2 and the K_1's should be chosen to be of similar order to ensure that the penalties BOS gives to different false decisions don't deviate excessively. In Section 5, we recommend some parameters that work well in all our experiments and thus are believed to perform robustly in practice.

5. Experiments and Discussion

The performance of BO-BOS is empirically compared with that of four other hyperparameter optimization algorithms: GP-UCB (Srinivas et al., 2010), Hyperband (Li et al., 2017), multi-fidelity BO algorithm called *BO with continuous approximations* (BOCA) (Kandasamy et al., 2017), and GP-UCB with learning curve prediction using an ensemble of Bayesian parametric regression models (LC Prediction) (Domhan et al., 2015). Freeze-thaw BO is not included in the comparison here since its implementation details are complicated and not fully available. We empirically evaluate the performance of BO-BOS in hyperparameter optimization of *logistic regression* (LR) and *convolutional neural networks* (CNN), respectively, in Sections 5.1 and 5.2, and demonstrate its generality in two other interesting applications in Section 5.3. Due to lack of space, additional details of the experimental setup are deferred to Appendix D.

5.1. Hyperparameter Optimization of LR

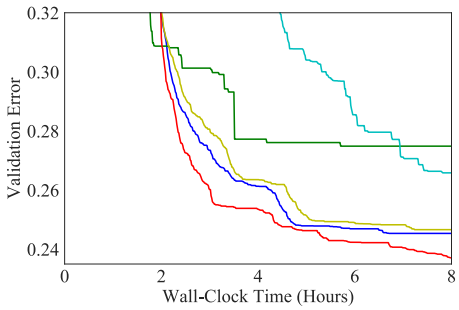
We first tune three hyperparameters of LR trained on the MNIST image dataset. Although both the $K_{1,t}$ sequence and κ determine the trade-off between the number of BO iterations and the number of epochs on average as mentioned in section 4, for simplicity, we fix $\kappa = 2$ and investigate the impact of different sequences of $K_{1,t}$ values.

As shown in Fig. 1, the sequences $(K_{1,t})_a$, $(K_{1,t})_b$ and $(K_{1,t})_c$ lead to similar performances, all of which outperform GP-UCB. On the other hand, the algorithm with fixed K_1 values (the $(K_{1,t})_d$ sequence), despite having fast performance improvement initially, eventually finds a worse hyperparameter setting than all other algorithms. This undesirable performance results from the fact that fixed K_1 values give constant penalty to falsely-early stopping throughout all runs of the BOS algorithms, and as the incumbent validation error decreases, the preference of the algorithm for early stopping will increase, thus preventing the resulting algorithm from beginning to exploit (running promising hyperparameter settings with N epochs). This observation demonstrates the necessity of having an increasing sequence of $K_{1,t}$ values, thus substantiating the practical relevance of our theoretical analysis (Theorem 2). The sequence $(K_{1,t})_b$, as well as the values of $K_2 = 99$ and $c_{d_0} = 1$, will be used in the following experiments if not further specified.

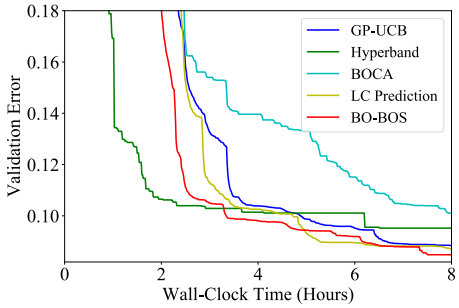
5.2. Hyperparameter Optimization of CNN

In this section, we tune six hyperparameters of CNN using two image datasets: CIFAR-10 (Krizhevsky, 2009) and Street View House Numbers (SVHN) (Netzer et al., 2011). Note that the goal of the experiments is not to compete with the state-of-the-art models, but to compare the efficiency of different hyperparameter tuning algorithms, so no data augmentation or advanced network architectures are used.

As shown in Figures 2a and 2b, BO-BOS outperforms all other algorithms under comparison in terms of the run-time efficiency. Note that the horizontal axis, which represents the wall-clock time, includes all the time spent during the algorithms, including the running time of machine learning models, the approximate backward induction used to solve BOS, etc. Although Hyperband is able to quickly reduce the validation error in the initial stage, it eventually converges to sub-optimal hyperparameter settings compared with both GP-UCB and BO-BOS. Similar findings have been reported in previous works (Klein et al., 2017; Falkner et al., 2018) and they might be attributed to the pure-exploration nature of the algorithm. Our BO-BOS algorithm, which trades off exploration and exploitation, is able to quickly surpass the performance of Hyperband and eventually converges to significantly better hyperparameter settings. In addition, we also ran the BOHB algorithm (Falkner et al., 2018) which combines Hyperband and BO; however, BOHB did not manage to reach comparable performance with the other algorithms in these two tasks. We observed that the sub-optimal behavior of Hyperband and BOHB observed here can be alleviated if the search space of hyperparameters is chosen to be smaller, in which case the advantage of pure exploration can be better manifested. The unsatisfactory performance of BOCA might be explained by the fact that it does not make use of the intermediate validation errors when selecting the number of epochs. In contrast, BO-BOS



(a) CIFAR-10.



(b) SVHN.

Figure 2. Best-found validation error of CNN v.s. run-time (averaged over 30 random initializations)

takes into account the observations after each training epoch when choosing the optimal stopping time, and thus is able to make better-informed decisions. Moreover, since BOCA is designed for general scenarios, the useful assumption of monotonic learning curve utilized by BO-BOS is not exploited; therefore, BOCA is expected to perform better if the fidelity levels result from data sub-sampling. LC Prediction performs similarly to GP-UCB, which might be because the predicted final values of the learning curves are used as real observations in the GP surrogate function (Domhan et al., 2015), thus invalidating the theoretical guarantee and deteriorating the convergence of GP-UCB, which offsets the computational saving provided by early stopping. BO-BOS, on the other hand, offers theoretically guaranteed convergence, thus allowing explicit control over the trade-off between the speed of convergence and the reduction in the average number of epochs as discussed in Section 4.

5.3. Novel Applications of the BO-BOS Algorithm

5.3.1. Policy Search for Reinforcement Learning

Thanks to its superb sample efficiency, BO has been shown to be effective for policy search in reinforcement learning (RL) (Wilson et al., 2014), especially when policy evaluation is costly such as gait optimization for robots (Lizotte et al., 2007) and vehicle navigation (Brochu et al., 2010). In policy search, the return of a policy is usually estimated by running the agent in the environment sequentially for a fixed number of steps and calculating the cumulative rewards (Wilson et al., 2014). Therefore, the sequential nature of the policy evaluation makes our BO-BOS algorithm an excellent fit to improve the efficiency of BO for policy search in RL.

We apply our algorithm to the Swimmer-v2 task from OpenAI Gym, MuJoCo (Brockman et al., 2016; Todorov et al., 2012), and use a linear policy consisting of 16 parameters. Each episode consists of 1000 steps, and we treat every m consecutive steps as one single epoch such that $N = 1000/m$. Direct application of BO-BOS in this task is inappropriate since the growth pattern of cumulative rewards differs significantly from the evolution of the learning curves of ML models, as illustrated in Appendix D.3. Therefore, the rewards are discounted (by γ) when calculating the objective function, because the pattern of discounted return (cumulative rewards) bears close resemblance to that of the learning curves. Note that although the value of the objective function is the discounted return, we also record and report the corresponding un-discounted return, which is the ultimate objective to be maximized. As a result, N and γ should be chosen such that the value of discounted return faithfully aligns with its un-discounted counterpart. Fig. 3 plots the best (un-discounted) return in an episode against the total number of steps, in which BO-BOS (with $N = 50$ and $\gamma = 0.9$) outperforms GP-UCB. The observation that the solid red line shows better returns than the two dotted red lines might be because overly small γ (0.75) and overly large N (100) both enlarge the disparity between discounted and un-discounted returns since they both downplay the importance of long-term discounted rewards. Moreover, not discounting the rewards ($\gamma = 1$) leads to poor performance, corroborating the earlier analysis motivating the use of discounted rewards. The results demonstrate that even though BO-BOS is not immediately applicable in the original problem, it can still perform effectively if the problem is properly transformed, which substantiates the general applicability of BO-BOS. Moreover, we also applied Hyperband in this task, but it failed to converge to a comparable policy to the other methods (achieving an average return of around 2.5), which further supports our earlier claim stating that Hyperband under-performs when the search space is large because there are significantly more parameters (16) than the previous tasks.

Interestingly, both BO-BOS (with $N = 50$ and $\gamma = 0.9$) and GP-UCB use significantly less steps to substantially outperform the benchmarks[1] achieved by some recently developed deep RL algorithms, in which the best-performing algorithm (Deep Deterministic Policy Gradients) achieves

[1] https://spinningup.openai.com/en/latest/spinningup/bench.html

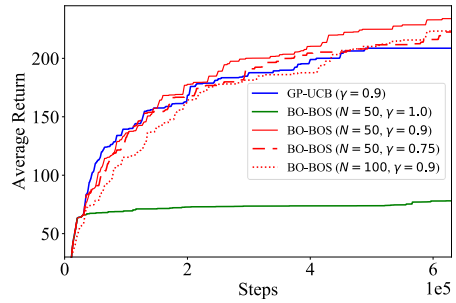


Figure 3. Best-found return (averaged over 5 episodes) v.s. the total number of steps of the robot in the environment (averaged over 30 random initializations) using the Swimmer-v2 task. The BO-BOS algorithm is run with different values of N (the maximum number of epochs) and γ (the discount factor).

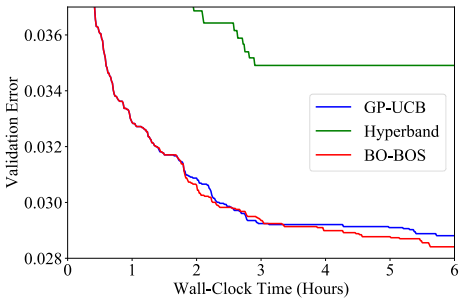


Figure 4. Best-found validation error of XGBoost v.s. run-time (averaged over 30 random initializations), obtained using joint hyperparameter tuning and feature selection.

an average return of around 120. Although the simplicity of the task might have contributed to their overwhelming performances, the results highlight the considerable potential of BO-based policy search algorithms for RL. Note that following the common practice in RL, Fig. 3 is presented in terms of the total number of steps instead of the run-time; we believe the additional computation required by BOS can be easily overshadowed in large-scale RL tasks, as demonstrated in the previous experiments. Most modern RL algorithms rely on enormous number of samples, which makes their applications problematic when sample efficiency is of crucial importance (Arulkumaran et al., 2017). As shown above, BO-BOS achieves significantly better results than popular deep RL algorithms while at the same time being far more sample-efficient, thus potentially offering practitioners a practically feasible option in solving large-scale RL problems.

5.3.2. Joint Hyperparameter Tuning and Feature Selection

Beside hyperparameter tuning, feature selection is another important pre-processing step in ML, because it can lower the computational cost and boost the model performance (Hall, 2000). There are two types of feature selection techniques: filter and wrapper methods; the wrapper methods, such as forward selection (which starts with an empty feature set and in each iteration greedily adds the feature with the largest performance improvement), have been shown to perform well, although computationally costly (Hall & Smith, 1999). Interestingly, as a result of the sequential nature of the wrapper methods, they can be naturally incorporated into BO-BOS by simply replacing the sequential training of ML models with sequential forward selection.

In this task, we tune four hyperparameters of the gradient boosting model (XGBoost (Chen & Guestrin, 2016)) trained on an email spam dataset. We additionally compare with Hyperband since it was previously applied to random feature approximation in kernel methods (Li et al., 2017). As shown in Fig. 4, BO-BOS again delivers the best performance in this application. Consistent with Fig. 2, the wall-clock time includes all the time incurred during the algorithms. The $K_{1,t}$ sequence is made smaller than before: $K_{1,t} = \frac{K_{1,t-1}}{0.99}$, because in this setting, more aggressive early stopping is needed for BO-BOS to show its advantage. Although Hyperband works well for random feature approximation (Li et al., 2017), it does not perform favourably when applied to more structured feature selection techniques. Both hyperparameter optimization and feature selection have been shown to be effective for enhancing the performance of ML models. However, performing either of them in isolation may lead to sub-optimal performance since their interaction is un-exploited. Our results suggest that BO-BOS can effectively improve the efficiency of joint hyperparameter tuning and feature selection, making the combined usage of these two pre-processing techniques a more practical choice.

6. Conclusion

In this work, we present a unifying framework, BO-BOS, that integrates BOS into BO in a natural way, to derive a principled mechanism for optimally stopping hyperparameter evaluations during BO. We analyze the regret of the algorithm, and derive the BOS parameters that make the resulting BO-BOS algorithm no-regret. Applications of BO-BOS to hyperparameter tuning of ML models, as well as two other novel applications, demonstrate the practical effectiveness of the algorithm. For future work, we plan to further exploit the generality of the BO-BOS algorithm by applying it to more applications with costly iterative function evaluations.

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