Multi-Step Budgeted Bayesian Optimization with Unknown Evaluation Costs

Anonymous Author(s)

Affiliation

Address

email

Abstract

Bayesian optimization (BO) is a sample-efficient approach to optimizing costly-to-evaluate black-box functions. Most BO methods ignore how evaluation costs may vary over the optimization domain. However, these costs are highly heterogeneous and often unknown in advance in many practical settings, such as hyperparameter tuning of machine learning algorithms, or physics-based simulation optimization. Moreover, those few existing methods that acknowledge cost heterogeneity do not naturally accommodate a budget constraint on the total evaluation cost. This combination of unknown costs and a budget constraint introduces a new dimension to the exploration-exploitation trade-off, where learning about the cost incurs a cost itself. Existing approaches do not reason about the various trade-offs of this problem in a principled way, leading often to poor performance. We formalize this claim by proving that the expected improvement and the expected improvement per unit of cost, arguably the two most widely used acquisition functions in practice, can be arbitrarily inferior with respect to the optimal non-myopic policy. To overcome the shortcomings of existing approaches, we propose the *budgeted multi-step expected improvement*, a non-myopic acquisition function that generalizes classical expected improvement to the setting of heterogeneous and unknown evaluation costs. We show that our acquisition function outperforms existing BO methods in a variety of synthetic and realistic problems.

1 Introduction

Bayesian optimization (BO) [23, 7] is a family of algorithms for optimizing black-box functions that performs well when the number of evaluations is limited [24, 4, 10]. However, most BO algorithms ignore the fact that evaluation costs may vary substantially across the optimization domain and are often unknown. Failing to account for this can lead one to evaluate an expensive point when another less expensive one would provide equal benefit towards finding the optimum.

We consider *budgeted* Bayesian optimization of a black-box objective function, whose evaluation costs are unknown and possibly heterogeneous across the domain. The goal is to find a point with the largest possible objective value by querying the function at a sequence of adaptively chosen points, where the total evaluation cost is subject to a budget constraint. (This cost only affects evaluation, and not a point's quality upon implementation.) Problems of this form arise commonly in practice. For instance, in the context of hyperparameter optimization of machine learning algorithms [26, 33], certain values of hyperparameters such as the learning rate yield significantly longer training times (see Fig. 1). Similarly, in materials design and robotics, simulation experiments can take longer for certain parameter configurations [6].

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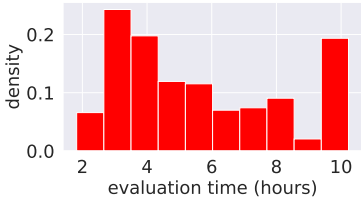


Figure 1: Evaluation times of the latent Dirichlet allocation problem (described in Section 5.2) over a uniform grid of points. These evaluations times are highly heterogeneous, with each evaluation taking between 2 and 10 hours.

While some existing approaches do address heterogeneity of evaluation costs, all do so heuristically, e.g. by maximizing a traditional cost-agnostic acquisition function divided by the (expected) cost of evaluation [24, 21, 33, 20]. Importantly, these approaches accommodate neither budget constraints nor uncertainty about the cost function as part of the exploration-exploitation trade-off in a principled way. As we argue theoretically and demonstrate empirically in our experiments, this can lead to poor performance.

Main Contributions. Motivated by the above shortcomings in existing work, we provide a principled approach to budgeted BO. Our main contributions are:

- We propose a Markov decision process (MDP) formulation of the budgeted BO problem with unknown and heterogeneous evaluation costs. Our formulation allows for a random time horizon (i.e., the first time that the budget is depleted) and accounting for costs, going beyond the fixed-horizon MDPs formulated in existing work on nonmyopic BO.
- *Budgeted multi-step expected improvement* (B-MS-EI), a novel look-ahead acquisition function that generalizes classical expected improvement to the budgeted cost-heterogeneous setting. B-MS-EI can be seen as a principled approximation of the optimal policy of the MDP formulation.
- We theoretically show that expected improvement and its cost-normalized variant, two popular existing approaches, can be arbitrarily inferior with respect to the optimal non-myopic policy.
- An empirical evaluation on a number of synthetic and real-world experiments demonstrate that B-MS-EI performs favorably with respect to other cost-aware acquisition functions that are widely-used in settings with heterogeneous costs.

The remainder of this work is organized as follows: In Section 2, we review related work. Our problem setup is formalized in Section 3. In Section 4 we introduce B-MS-EI and discuss its efficient maximization via one-shot multi-step Monte Carlo trees. Numerical experiments are presented in Section 5. Finally, we discuss directions of future work and conclude in Section 6.

2 Related Work

Our work falls within the Bayesian optimization framework [7], whose origins date back to the seminal work of [17], and which has been successful in a wide range of applications such as hyperparameter tuning of machine learning algorithms [24, 33], materials design [37], drug discovery [10], and robot locomotion [4, 29].

Within the BO literature, the works most closely related to ours are those that acknowledge the existence of costs for evaluating the objective function that are heterogeneous across the search space, and those that aim to devise algorithms that are cost-efficient. Much of this work has occurred in the multi-fidelity setting [26, 14, 15, 21, 25, 33], i.e., where cheaper approximations of the objective function are available. The only exceptions known to us are the works of [24] and [20], both of which consider the single-fidelity setting. The former proposes as acquisition function the expected improvement per unit of cost (EI-PUC), i.e, $\mathrm{EI}(x)/c(x)$ and the latter proposes $\mathrm{EI}(x)/c(x)^{\alpha}$, where α is the ratio between the remaining budget and the total budget.[1] The intuition of the latter is that points with high cost c should be discouraged early in the BO loop. However, neither of these formulations provides a principled way to assess the benefit of evaluating a certain point given the remaining budget, nor do they consider uncertainty in the cost function.

[1]These expressions are for the case when $c(x)$ is known. When $c(x)$ is unknown and learned, then either the expectation is taken over the distribution of improvement to cost ratios (as we do in our experiments) or the denominator is replaced by the mean cost.

This approach of dividing a cost-agnostic acquisition function by some cost term is widely used in practice for addressing heterogeneity in costs, and is closely related to the use of "value divided by cost" in knapsack problems [1]. In the knapsack problem, one selects items to include into a knapsack to maximize the sum of the selected items' values subject to a budget constraint on the sum of the items' costs. In this setting, myopically adding items to the knapsack that maximize value divided by cost has strong theoretical guarantees: this algorithm provides at least $1/2$ the optimal value [30]. However, this theoretical guarantee relies on the additive nature of value in the knapsack problem. In contrast, in BO, the value obtained from multiple evaluations is the maximum of the values of the evaluations, not their sum. Indeed, we show that in this setting the "value divided by cost" approach can perform arbitrarily worse than the optimal policy.

Heterogeneous evaluation costs have also been considered in the multi-armed bandits literature [1, 35, 34]. These works develop algorithms based on optimistic policies that maximize some form of reward-to-cost ratio. As mentioned above, this type of policy is sensible when the measure of performance is the cumulative regret but is not appropriate in an optimization or "best-arm identification" setting.

Our work is also closely related to non-myopic BO [9, 18, 36, 12, 19, 13], a class of acquisition functions that account for future evaluations when quantifying a point's acquisition value. To the best of our knowledge, no existing non-myopic BO method handles heterogeneous evaluation costs.

3 Budgeted Bayesian Optimization with Unknown Evaluation Costs

We now formally state the problem of budgeted BO with unknown, heterogeneous evaluation costs. Given a compact optimization domain $\mathbb{X} \subset \mathbb{R}^d$, our goal is to find a point $x \in \mathbb{X}$ with the largest possible objective value by querying the black-box objective function, $f : \mathbb{X} \to \mathbb{R}$, at a sequence of points $\{x_i\}_{i=1}^n$, subject to the constraint $\sum_{i=1}^n c(x_n) \leq B$, where $c(x)$ is the cost of evaluating f at x and B is the evaluation budget. The cost observation $c(x)$ is revealed immediately after the evaluation of $f(x)$ is performed. However, the actual cost function c is unknown. As is typical in BO, we endow f and c with a joint prior distribution, p. An *observation* in our setting is a triple $(x_i, y_i, z_i) \in \mathbb{X} \times \mathbb{R} \times \mathbb{R}_{>0}$, where y_i is an observation of the objective f at x_i, and z_i is an observation of the cost c at for evaluating f at x_i.

3.1 MDP Formulation of the Budgeted BO Problem

Let $\mathcal{D}_n$ denote the set of observations up to step n, for $n \geq 0$, where $\mathcal{D}_0$ is a set of initial observations. These sets are defined recursively by $\mathcal{D}_n = \mathcal{D}_{n-1} \cup (x_n, y_n, z_n)$ for $n \geq 1$. The joint posterior distribution over f and c given $\mathcal{D}_n$ is denoted by $p(\cdot \mid \mathcal{D}_n)$. The *utility* generated by a particular set $\mathcal{D}_n$ is defined as the maximum observed objective value $u(\mathcal{D}_n) = \max_{(x,y,z)\in\mathcal{D}_n} y$. Note that this utility function encodes the fact that *after evaluation*, a point with maximum objective value, regardless of its cost, is desired. We also let $s(\mathcal{D}_n) = \sum_{(x,y,z)\in\mathcal{D}_n} z$ denote the *total cost* of observed points in $\mathcal{D}_n$.

The sets of observations $\mathcal{D}_0, \mathcal{D}_1, \mathcal{D}_2, \ldots$ are random under the prior p due to the yet unobserved values of the objective and cost functions. A *policy* $\pi = \{\pi_k\}_{k=1}^\infty$ is a sequence of functions, each mapping sets of observations to points in $\mathbb{X}$, so that $x_k = \pi_k(\mathcal{D}_{k-1})$. Given an initial set of observations $\mathcal{D}_0$, we aim to find the policy that maximizes the increase in expected utility, i.e., we wish to solve

$$V^*(\mathcal{D}) = \sup_\pi \mathbb{E}^\pi_{\mathcal{D}}\big[u(\mathcal{D}_{N_B}) - u(\mathcal{D}_0)\big], \tag{1}$$

where the random stopping time $N_B = \sup\{k : s(\mathcal{D}_k) \leq B\}$ is the largest time step k for which the budget constraint is still satisfied. The notation $\mathbb{E}^\pi_{\mathcal{D}}[\,\cdot\,]$ indicates an expectation taken over sequences of observation sets $\mathcal{D}_1, \mathcal{D}_2, \ldots, \mathcal{D}_{N_B}$ selected by a policy π, starting with $\mathcal{D}_0 = \mathcal{D}$. We will also use the notation $V^\pi(\mathcal{D}) = \mathbb{E}^\pi_{\mathcal{D}}\big[u(\mathcal{D}_{N_B}) - u(\mathcal{D}_0)\big]$.

The above problem is well-defined provided that $N_B < \infty$ for all policies π. This is the case, for example, when $\ln c$ follows a Gaussian process (GP) prior, a modeling choice that we make in our numerical experiments. Since the horizon N_B is random, the formulation (1) can be viewed as a stochastic shortest path problem, rather than a standard finite or discounted infinite horizon dynamic program [3]. Note that at time step k, the set $\mathcal{D}_k$ contains all past observed costs and therefore fully captures the remaining budget. This formulation is capable of the following:

1. Through multi-step planning, it can navigate the trade-off of how to sequence high-cost and low-cost evaluations in order to make the best use of the given budget.

2. It can reason about optimal cost-learning through uncertainty estimates of the cost model, which can be expensive but also worthwhile: a seemingly high-cost point with high model uncertainty in a promising region may be worth evaluating due to the possibility that it is actually lower-cost (and therefore becomes particularly valuable in a budgeted setting).

3.2 Contrast with Value-to-Cost Ratio Methods

It is not surprising that cost-agnostic methods, such as expected improvement (EI), can perform poorly when the evaluation cost is heterogeneous. In particular, ignoring cost can lead to evaluating excessively high-cost points, depleting budget and limiting future evaluations. In an attempt to avoid this, past work has focused on using a value-to-cost ratio [24, 26, 14, 15, 21, 25, 33, 20].

We show here, however, that value-to-cost acquisition functions exhibit a complementary kind of undesirable behavior: they may repeatedly measure excessively low-cost points that are also low-value, also leading to poor overall performance. In fact, the performance can be arbitrarily bad compared with an optimal policy. Theorem 1 demonstrates this formally for the most widely-used of these policies: measuring at the point that maximizes the expected improvement divided by the expected cost of evaluation (Theorem 1 also holds for cost-agnostic EI).

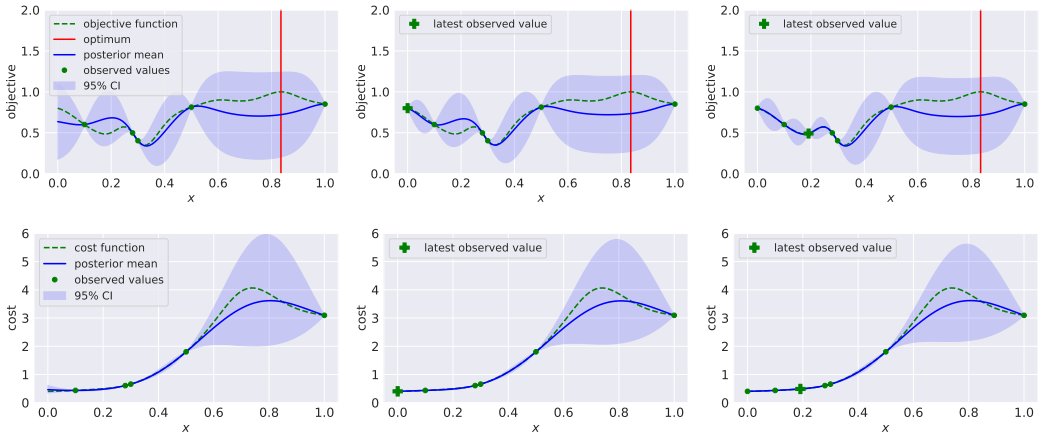
Theorem 1. *The approximation ratios provided by the* EI *and* $\mathrm{EI\text{-}PUC}$ *policies are unbounded. That is, for any* $\alpha > 0$ *and each policy* $\pi \in \{\mathrm{EI}, \mathrm{EI\text{-}PUC}\}$*, there exists a Bayesian optimization problem instance (a prior probability distribution over objective and cost functions, a budget, and a set of initial observations* $\mathcal{D}_0$*) where* $V^*(\mathcal{D}_0) > \alpha\, V^\pi(\mathcal{D}_0)$.

Sketch of Proof. To show that EI-PUC has an unbounded approximation ratio, the detailed proof of Theorem 1 (provided in the supplementary material) constructs a problem instance with a prior that is independent across a discrete domain with a known cost function. There are two kinds of points: high-cost points with large prior variance; and low-cost points with low variance. To support analysis, all points have the same mean. The variance of the low-cost points is low enough that spending the entire budget on low-cost points earns only a fraction of the value, in expectation, compared to evaluating a single high cost point. The acquisition function EI-PUC, however, does not understand this. Its greedy nature leads it to overvalue these points. As a result, EI-PUC spends its entire budget on these low-cost points, earning almost no value. In contrast, the optimal policy spends its entire budget on a single evaluation of the high-cost point, obtaining substantially more value in expectation. □

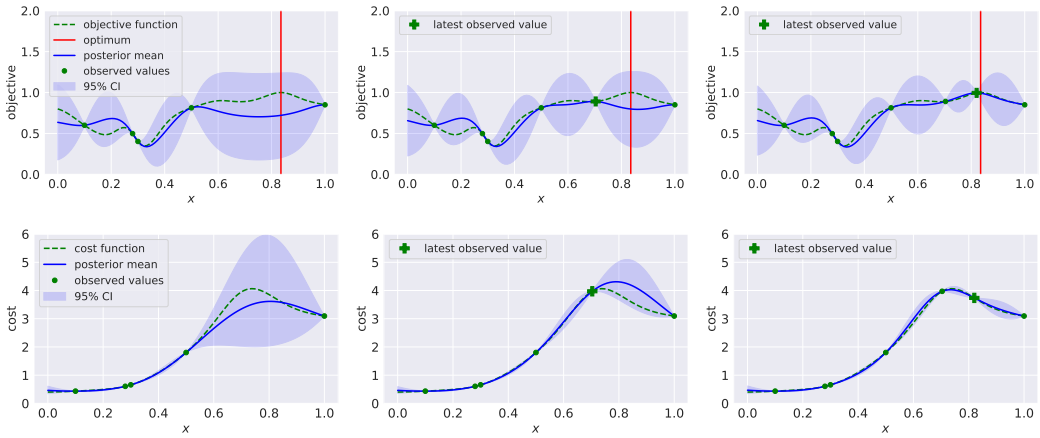
Indeed, the EI value for evaluating at x, $\mathbb{E}[(f(x) - f^*)^+]$, assumes that f^*, the best previously observed function value, is the best value attainable without evaluating $f(x)$. But when we look multiple steps ahead, we may realize that we are likely to find other points substantially better than f^* in future evaluations. This should lead us to value points that are likely to improve, not with respect to the *current* best known point, but with respect to values we are likely to discover in the future. As a result, non-myopic strategies place more weight on evaluations that will lead to improvements above and beyond this more ambitious bar.

Fig. 2 illustrates this phenomenon in a continuous one-dimensional setting with a Gaussian process prior. Under the posterior in the first time slice, there is a lower-cost region on the left ($x < 0.5$) with low-variance and a mean that is substantially below the best point observed. There is a higher-cost region on the right ($x > 0.5$) where the mean and variance are both much larger. These means and variances are such that the global maximum of the function is likely to be in the right-hand region. In its first two measurements, the EI-PUC strategy measures at two low-cost points, which results in reduction of variance in this region but (as expected) no values that contend with the likely value of the global maximum on the right. In contrast, in its first two measurements, our multi-step B-MS-EI strategy evaluates on the right, finding values that are close to the global optimum.

In this example, EI-PUC encounters the same difficulty it faces in the proof of Theorem 1: It overvalues low-cost points that improve relative to the status quo but not relative to where we hope to be near the end of the budget. While some budget remains to evaluate on the right after these evaluations, the evaluations on the left are likely unproductive toward the goal of finding a global maximum.



(a) EI-PUC



(b) B-MS-EI

Figure 2: The top six panels show the EI-PUC strategy and the bottom six show our B-MS-EI strategy. In each group, the top row shows the objective function and the bottom shows the cost, using 95% confidence intervals. Time moves from left to right, where the first column shows the initial posterior, and the second and third columns show the posterior after one and two evaluations by the algorithm, respectively. EI-PUC evaluates low-variance, low-mean points that are low-cost but unlikely to reveal values near the global optimum. In contrast, B-MS-EI discovers a point near this global optimum within budget and with two evaluations.

3.3 Decomposition and Truncation

We now discuss how we can additively decompose and then truncate the problem in (1) so that it is more amenable as a BO acquisition function. Let $r(\mathcal{D}_{n-1}, \mathcal{D}_n) = u(\mathcal{D}_n) - u(\mathcal{D}_{n-1})$ be the increase in utility between successive observation sets. We can write

$$V^*(\mathcal{D}) = \sup_{\pi \in \Pi} \mathbb{E}^{\pi}_{\mathcal{D}} \left[\sum_{n=1}^{N_B} r(\mathcal{D}_{n-1}, \mathcal{D}_n) \right] = \sup_{\pi \in \Pi} \mathbb{E}^{\pi}_{\mathcal{D}} \left[\sum_{n=1}^{\infty} r(\mathcal{D}_{n-1}, \mathcal{D}_n) \, \mathbf{1}_{\{n \le N_B\}} \right].$$

Note that $\{n \le N_B\} = \{s(\mathcal{D}_n) \le B\}$. For any fixed N,

$$V^*(\mathcal{D}) = \sup_{\pi \in \Pi} \mathbb{E}^{\pi}_{\mathcal{D}} \left[\sum_{n=1}^{N} r(\mathcal{D}_{n-1}, \mathcal{D}_n) \, \mathbf{1}_{\{n \le N_B\}} + r_N(\mathcal{D}_N) \right],$$

where $r_N(\mathcal{D}_N) = V^*(\mathcal{D}_N)\,\mathbf{1}_{\{N \le N_B\}}$. Define

$$V_N(\mathcal{D}) = \sup_{\pi \in \Pi} \mathbb{E}^{\pi}_{\mathcal{D}} \left[\sum_{n=1}^{N} r(\mathcal{D}_{n-1}, \mathcal{D}_n)\,\mathbf{1}_{\{n \le N_B\}} \right], \tag{2}$$

a standard finite-horizon dynamic program. When for each c drawn from its prior, there exists a lower bound on $c(x)$ over $\mathbb{X}$ so that (1) is well-defined, it follows that the truncation becomes more accurate when N becomes large: $\lim_{N\to\infty} r_N(\mathcal{D}_N) = 0$ and $\lim_{N\to\infty} V_N(\mathcal{D}) = V^*(\mathcal{D})$. This serves as the motivation for our acquisition function described below.

4 Budgeted Multi-Step Expected Improvement

We now derive the *budgeted multi-step expected improvement* (B-MS-EI) acquisition function, where the main idea is to solve the truncated problem given in (2). Accordingly, the acquisition function is parameterized by N, the maximum number of look-ahead steps. In Section 4.2, we discuss how to approximately optimize this acquisition function using a scenario tree, leveraging the technique developed in [13], and in Section 4.3, we discuss how to set the budget that defines our acquisition function when the actual remaining budget is too large to be meaningfully taken into account by a computationally feasible number of look-ahead steps.

4.1 Dynamic Programming on the Truncated Problem

Our derivation of B-MS-EI starts with applying Bellman recursion to (2). To this end, we define the one-step marginal value of a measurement at point x given an arbitrary set of observations $\mathcal{D}$ to be

$$v_1(x \mid \mathcal{D}) = \mathbb{E}_{y,z}\left[r(\mathcal{D}, \mathcal{D} \cup \{(x,y,z)\})\right] = \mathbb{E}_{y,z}\left[(y - u(\mathcal{D}))^+\,\mathbf{1}_{\{s(\mathcal{D})+z \le B\}}\right].$$

Proposition 1 below shows that, when f and $\ln c$ are drawn from independent GPs, v_1 admits an analytic expression similar to the one of constrained expected improvement [22, 8]. The proof of this result can be found in the supplementary material.

Proposition 1. *Suppose that f and $\ln c$ are drawn from independent Gaussian processes and that $\mathcal{D}$ is an arbitrary set of observations. Define $\mu^f_{\mathcal{D}}(x) = \mathbb{E}[f(x) \,|\, \mathcal{D}]$, $\mu^{\log c}_{\mathcal{D}}(x) = \mathbb{E}[\ln c(x) \,|\, \mathcal{D}]$, $\sigma^f_{\mathcal{D}}(x) = \mathrm{Var}[f(x) \,|\, \mathcal{D}]^{1/2}$, and $\sigma^{\ln c}_{\mathcal{D}}(x) = \mathrm{Var}[\ln c(x) \,|\, \mathcal{D}]^{1/2}$. Then,*

$$v_1(x \mid \mathcal{D}) = \mathrm{EI}^f(x \,|\, \mathcal{D})\,\Phi(\zeta)\,\mathbf{1}_{\{s(\mathcal{D}) \le B\}}$$

where EI^f is the classical expected improvement computed with respect to f, $\zeta = \big(\ln(B - s(\mathcal{D})) - \mu^{\ln c}_{\mathcal{D}}(x)\big)/\sigma^{\ln c}_{\mathcal{D}}(x)$, and Φ is the standard normal cdf.

In contrast with homogeneous-budget non-myopic formulations, the indicator $\mathbf{1}_{\{s(\mathcal{D}) \le B\}}$ truncates our reward sequence at the random time when we first exceed our budget.

Analogously, we can define the n-step value function evaluated at x, $v_n(x \mid \mathcal{D})$, as the expected difference in utility after using the optimal policy to evaluate n additional points, among which x is the first of them. Using the Bellman recursion, one can write $v_n(x \mid \mathcal{D})$ as

$$v_n(x \mid \mathcal{D}) = v_1(x \mid \mathcal{D}) + \mathbb{E}_{y,z}\Big[\max_{x \in \mathbb{X}} v_{n-1}\left(x \mid \mathcal{D} \cup \{(x,y,z)\}\right)\Big],$$

which holds for all n. Our acquisition function B-MS-EI is defined as v_N, meaning that at every step our sampling policy evaluates $x_{n+1} \in \operatorname{argmax}_{x \in \mathbb{X}} v_N(x \mid \mathcal{D}_n)$.

4.2 Optimizing B-MS-EI via Budgeted Multi-Step Trees

Maximizing our acquisition function is challenging as, in principle, this requires nested stochastic optimization over a continuous domain. We build upon the multi-step scenario tree approach of [13] and devise an optimization method based on a sample average approximation of $\max_{x \in \mathbb{X}} v_N(x \mid \mathcal{D}_n)$. In our approach, each scenario is associated with its own decision variable, allowing the problem to be cast as a single deterministic optimization problem over a higher-dimensional domain instead of a sequence of nested stochastic optimization problems. We tackle the higher-dimensional problem

using modern tools of automatic differentiation and batched linear algebra operations [2]. We begin by noting that, if we apply Bellman recursion repeatedly, v_N can be rewritten as

$$v_N(x \mid \mathcal{D}) = v_1(x \mid \mathcal{D}) + \mathbb{E}_{y,z}\Big[\max_{x_2}\big\{v_1\left(x_2 \mid \mathcal{D}_1\right) + \mathbb{E}_{y,z}\big[\max_{x_3}\big\{v_1\big(x_3 \mid \mathcal{D}_2\big) + \cdots\big\}\big]\big\}\Big].$$

Now we consider the Monte Carlo approximation of $v_N(x \mid \mathcal{D})$ given by

$$\widehat{v}_N(x|\mathcal{D}) = v_1(x|\mathcal{D}) + \frac{1}{m_1}\sum_{j_1}^{m_1}\left[\max_{x_2^{j_1}}\left\{v_1(x_2^{j_1}|\mathcal{D}_1^{j_1}) + \frac{1}{m_2}\sum_{j_2}^{m_2}\left[\max_{x_3^{j_1 j_2}}\left\{v_1(x_3^{j_1 j_2}|\mathcal{D}_2^{j_1 j_2}) + \cdots\right\}\right]\right\}\right],$$

where $m_i,\ i = 1, \ldots, N-1$, is the number of samples used in step i, and the sets of observations are defined recursively by the equations $\mathcal{D}_i^{j_1} = \mathcal{D} \cup \left\{\left(x, y_i^{j_1}, z_i^{j_1}\right)\right\}$ and

$$\mathcal{D}_i^{j_1 \cdots j_i} = \mathcal{D}_i^{j_1 \cdots j_{i-1}} \cup \left\{\left(x_i^{j_1 \cdots j_{i-1}}, y_i^{j_1 \cdots j_i}, z_i^{j_1 \cdots j_i}\right)\right\},$$

with *fantasy* samples $(y_i^{j_1 \cdots j_i}, z_i^{j_1 \cdots j_i}) \sim p(\cdot \mid x_i^{j_1 \cdots j_i}, \mathcal{D}_i^{j_1 \cdots j_{i-1}})$ obtained via the *reparametrization trick*[2] [16, 31].

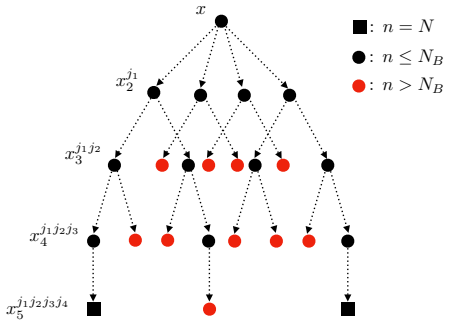


Figure 3: An illustration of the scenario tree representation of our acquisition function for $N = 5$ stages, where $m_1 = 4$, $m_2 = 2$, $m_3 = 2$, and $m_4 = 1$. Some sample paths down the tree may stop accumulating value earlier than others due to the budget being exhausted, i.e., when $s(\mathcal{D}_i^{j_1 \cdots j_i}) > B$ (ending in red nodes). Others paths may terminate due to the maximum look-ahead N before the budget is exhausted (black square nodes), representing some approximation error due to the truncation.

4.3 Budget Scheduling via Rollout of Base Sampling Policy

Let $B_n = B - \sum_{i=1}^{n} z_i$ be the remaining budget at time n. Since the number of look-ahead steps, N, that can be performed in practice is relatively small due to computational limits, B_n may be too large to be taken into account by our acquisition function in a meaningful way, especially during the first few evaluations. At a high level, this can be understood as follows: if the remaining budget is too large relative to the number of look-ahead steps, then the evaluation costs have little effect in our sampling decisions. Therefore, instead of using the actual remaining budget at step n, our acquisition function uses a budget set by a heuristic rule.

We propose a heuristic rule based on the use of a *base sampling policy* that can be computed quickly. We fantasize N sequential evaluations under this base sampling policy. More specifically, for each of the N steps, we draw fantasy objective and cost values at the point recommended by this policy using the (joint) posterior distribution, then we update the posterior distribution by incorporating these fantasy evaluations, and repeat. The sum of the resulting N fantasy costs determines a cumulative cost incurred by the base sampling policy. Our acquisition function then sets the budget to be the minimum between this cumulative cost and the true remaining budget. The intuition behind this heuristic is that our acquisition function will try to find the best non-myopic decision using the same budget as the base sampling policy, and thus should perform evaluations that are better or at least as good as those of the base sampling policy. In our experiments, we use EI-PUC-CC as base policy.

[2]Note that since we employ Monte Carlo sampling to approximate $v_N(x \mid \mathcal{D}_n)$, the independence assumption between f and c in Proposition 1 is not necessary for our approach, and one can jointly model f and c (e.g. with a multi-task GP) if there is reason to believe that these functions are correlated, as is often the case in practice. For instance, randomness in training jobs based on variations in test-train splits or weight initialization may interact with adaptive learning rate scheduling and thus affect both model performance and training time.

5 Experiments

We demonstrate the efficacy of B-MS-EI on three synthetic and three real-world experiments. We report the performance of two variants of our acquisition function, the main variant that uses multiple fantasy samples per step, and the *multi-step path* variant [13], which is based on a degenerate tree with one fantasy sample per step. For each of these variants, we consider the resulting acquisition function obtained by taking $N = 2$ and $N = 4$ look-ahead steps. We denote the multi-step path variant with N steps as N-B-MS-EI$_\text{p}$ and the former simply as N-B-MS-EI.

In addition, we report the performance of three baseline acquisition functions from the literature: expected improvement (EI), expected improvement per unit of cost (EI-PUC) [24, 20], and expected improvement per unit of cost with cost cooling (EI-PUC-CC) [20]. EI-PUC and EI-PUC-CC are currently the de-facto standard approach to cost-aware BO. Since [20] assumes that the cost is known (while our experiments are run in the setting of unknown costs), we also integrate with respect to the uncertainty on the cost when computing these acquisition functions. Closed form analytical expressions for these acquisition functions can be found in the supplement.

Fig 4 plots a 95% confidence interval on log-regret versus the budget used. We perform experiments using a single budget in each problem, and so our non-myopic budget-aware algorithm's goal is to minimize regret at the point when the budget is fully exhausted at the right-hand edge of each plot. To focus attention on these budgets, we plot results over the range from 20% to 100% of this overall budget. The results for the variants of our algorithm with $N = 2$ look-ahead steps are deferred to the appendix to improve readability and also because they are outperformed by their $N = 4$ counterparts for most problems. All algorithms are implemented in BoTorch [2] and the objective function and the log-cost are modeled using independent GPs. Additional details, runtimes and code can be found in the supplement.

5.1 Synthetic Test Problems

The first three problems use as their objective functions synthetic test functions commonly used in the literature: Dropwave, Alpine1, Shekel5, and Ackley (defined in the supplement). Each objective function is accompanied by a cost function of the form $c(x) = \exp\big[\frac{\alpha}{d}\sum_{i=1}^{d}\cos\big(\beta(x_i - x_i^* + \gamma)\big)\big]$, where x^* is the objective function's maximizer. In each replication we use a different cost function, obtained by sampling α, β, and γ uniformly at random over appropriate intervals. Our results thus average over a variety of cost functions. As these parameters vary, cost functions with different characteristics arise. More concretely, α controls the magnitude of the difference between the minimum and maximum costs; β controls the variability of the cost; and γ controls the cost at the optimum. In particular, if $\gamma = 0$, then x^* is the most expensive point, whereas if $\gamma = \pi$, then x^* is the cheapest point. This family of cost functions emulates a wide range of possible scenarios.

5.2 AutoML

Our AutoML benchmark problems use publicly available data sets from the HPOLib [27] and HPOLib1.5 [28] hyperparameter optimization libraries. Following [5] we use surrogates of the underlying objective and cost functions to emulate the computationally expensive process of training the corresponding models. Details on the construction of the surrogates can be found in the supplementary material. The first data set, originally introduced by [11], was obtained by evaluating an online latent Dirichlet allocation algorithm for topic modeling with 3 hyperparameters. These evaluations are extremely expensive and highly heterogeneous, ranging from 2 to 10 hours each (see Fig. 1). The second data set was obtained by training a 3-layer convolutional neural network with 5 hyperparameters.

5.3 Robot Pushing

We consider a version of the robot pushing problem introduced by [29], where a robot pushes an object from its origin, $w_\text{init} = (0, 0)$, to a target $w_\text{target} \in \mathbb{R}^2$. In the our version, we draw 20 different target locations uniformly at random over $\{(w_1, w_2) \in \mathbb{R}^2 : 1 < |w_1|, |w_2| < 5\}$, which are distributed equally across the replications performed. The parameters to be optimized are the location of the robot, $z \in [-5, 5]^2$, and the duration of the push, $t \in [1, 30]$. The objective to minimize is the distance from the object's location after being pushed, $w_\text{push}(z, t)$, and the target location, i.e.,

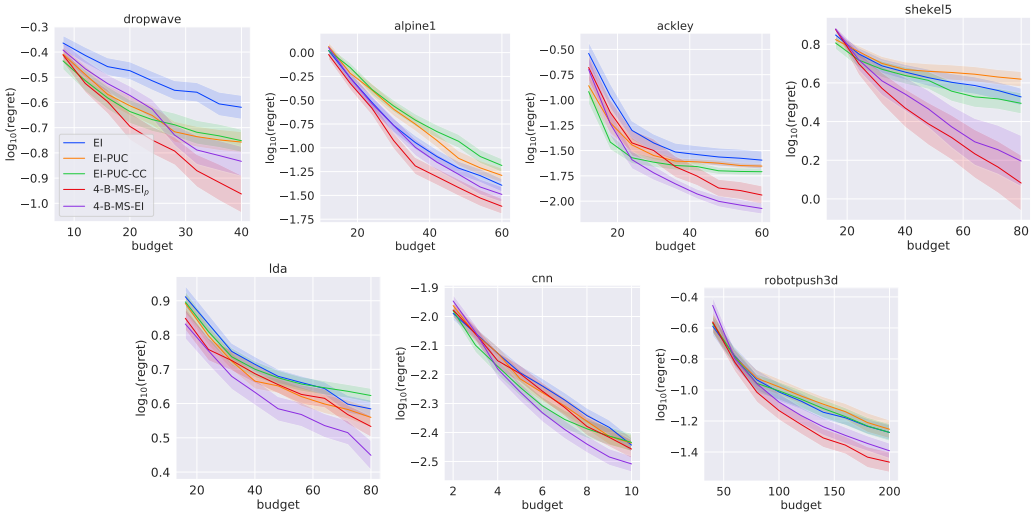


Figure 4: Log-regret of our non-myopic budget-aware BO method (4-B-MS-EI) compared with myopic benchmarks on a range of problems.

$f(z,t) = \|w_{\text{target}} - w_{\text{push}}(z,t)\|_2$. The cost function is given by $c(z,t) = \|w_{\text{push}}(z,t)\| + \epsilon$, and represents the energy spent by the robot by pushing the object.

5.4 Results and Discussion

B-MS-EI (red and purple lines) performs favorably compared to existing methods. In some cases (Dropwave and CNN) EI performs worst, while in other cases (Alpine, Shekel, LDA), one of the value-to-cost ratio methods (EI-PUC or EI-PUC-CC) performs worst.

B-MS-EI is more computationally intensive to optimize than the standard approaches. The average walltime per acquisition of 4-B-MS-EI, the most expensive variant of our algorithm, ranges from 1 to 7 minutes across the problems, whereas the average walltimes for EI, EI-PUC, and EI-PUC-CC, range from 5 to 30 seconds. However, optimization times on the order of minutes[3] is acceptable when the acquisition function is applied to real-world problems where the function evaluation often takes much longer (e.g., in Fig. 1, LDA evaluations require up to 10 hours). This point is particularly salient in cost-aware settings, where spending effort optimizing the acquisition function (that is relatively small compared to function evaluation) can significantly improve performance within a given evaluation budget. Nevertheless, there are opportunities to reduce the computational requirements of B-MS-EI; possibilities include re-using the optimized tree for multiple steps or devising better initial conditions for optimization. We leave these for future work.

6 Conclusion

We introduced the problem of budgeted BO optimization under unknown, heterogeneous evaluation costs. This arises in a wide range of practical settings where BO is applied. However, existing methods fail to account for uncertainty in the cost function as well as the presence of the budget constraint as part of the exploration-exploitation trade-off in a principled way, as we show in Theorem 1. In this work, we provided a dynamic programming formulation of this problem, along with a principled non-myopic acquisition function that addresses the shortcomings of the existing methods. Our acquisition function is derived by truncating the aforementioned dynamic program, and is approximately maximized following a one-shot multi-step tree approach. Our experiments show that our acquisition function outperforms existing methods on a number of synthetic and real-world examples that exhibit heterogeneity in evaluation costs. In the future, we hope to extend our approach to the multi-fidelity setting, where evaluation costs play an even larger role.

[3]These times are not unusual for advanced BO methods; see, e.g., Section 4 of [32])

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] Yes, in 5.4
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See supplement.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] See the supplement
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 5 and supplement.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times) [Yes]
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See supplement.
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   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]