
Optimizing Conditional Value-At-Risk of Black-Box Functions

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Abstract

This paper presents two *Bayesian optimization* (BO) algorithms with theoretical performance guarantee to maximize the *conditional value-at-risk* (CVaR) of a black-box function: CV-UCB and CV-TS which are based on the well-established principle of optimism in the face of uncertainty and Thompson sampling, respectively. To achieve this, we develop an upper confidence bound of CVaR and prove the no-regret guarantee of CV-UCB by utilizing an interesting connection between CVaR and *value-at-risk* (VaR). For CV-TS, though it is straightforwardly performed with Thompson sampling, bounding its Bayesian regret is non-trivial because it requires a tail expectation bound for the distribution of CVaR of a black-box function, which has not been shown in the literature. The performances of both CV-UCB and CV-TS are empirically evaluated in optimizing CVaR of synthetic benchmark functions and simulated real-world optimization problems.

1 Introduction

A wide range of applications from Auto-ML [15] to chemistry [6] and drug design [3] require optimizing a *black-box* objective function (i.e., its closed-form expression, gradient, and convexity are unknown) through observing noisy function evaluations. To resolve this problem, an efficient class of algorithms, called *Bayesian optimization* (BO) [2, 20], has seen rapid development lately.

One of the recent developments of BO considers searching for the *optimization variable* \mathbf{x}_* that maximizes the objective function $\rho[f(\mathbf{x}, \mathbf{W})]$ [4]. Different from the classical BO, there exists an *environmental random variable* \mathbf{W} that cannot be controlled, which happens frequently in real-world problems. For example, to maximize the crop yield (i.e., $f(\mathbf{x}, \mathbf{W})$) by controlling the amount of fertilizer (i.e., \mathbf{x}), there are various uncontrollable weather conditions such as the temperature, lighting, and rainfall (i.e., \mathbf{W}) [13]. Thus, even though an amount of fertilizer \mathbf{x} increases the crop yield most of the time, there exists a risk/chance that under certain weather conditions (realizations of \mathbf{W}), the same amount of fertilizer leads to a low crop yield (an undesirable realization of the random variable $f(\mathbf{x}, \mathbf{W})$). This issue renders the optimization of $f(\mathbf{x}, \mathbf{W})$ futile, so the work of [4] proposes to optimize a risk measure, denoted as ρ , of $f(\mathbf{x}, \mathbf{W})$ such as *value-at-risk* (VaR) and *conditional VaR* (CVaR). However, its approach suffers from two main shortcomings: the computational cost of a nested optimization procedure and the lack of theoretical performance guarantee. Although these drawbacks are addressed in the work of [13], its proposed algorithm only works for optimizing VaR of a black-box function. Hence, an efficient algorithm with theoretical performance guarantee for optimizing CVaR of a black-box function remains an open question.

Nonetheless, optimizing CVaR of a black-box function is desirable, especially when the effect of optimizing CVaR cannot be obtained by optimizing VaR. A prominent property of CVaR is its sensitivity to values at the extreme tails of the random variable $f(\mathbf{x}, \mathbf{W})$, which VaR does not exhibit [19]. Let us consider two portfolio allocation schemes: one scheme has an unacceptable

worst-case value of the return and the other does not. It is possible that the two schemes have the same VaR of the return because VaR is insensitive to the extreme tails of the return (e.g., the worst-case value of the return). On the other hand, CVaR is able to distinguish the risks of the two schemes. This advantage of CVaR is further clarified in Remark 1.

In this paper, we adopt the settings of [4, 13]: the distribution of \mathbf{W} is given and we can control/select the realization \mathbf{w} of \mathbf{W} in the optimization procedure. In practice, the distribution of \mathbf{W} can be estimated from data (e.g., weather historical data in the crop yield optimization example) and we can perform BO in a laboratory or using computer simulation where \mathbf{W} is controlled [4, 13]. After the optimization, the optimal \mathbf{x}_* can be used in the real-world environment with the uncontrollable \mathbf{W} . Our main contribution is to propose two computationally efficient algorithms (Sec. 3) with theoretical performance guarantee (Sec. 4) for optimizing CVaR of a black-box function.

First, we propose *CVaR optimization with upper confidence bound* (CV-UCB) that is based on the well-established principle of optimism in the face of uncertainty. By exploiting the connection between CVaR and VaR, we are able to develop a confidence bound of CVaR (Sec. 3.1.1) and prove the no-regret guarantee of CV-UCB (Sec. 4.1).

Second, we propose *CVaR optimization with Thompson sampling* (CV-TS) which can be naturally extended to handle batch queries (i.e., gathering observations at a batch of inputs in each BO iteration). The capability of gathering observations in a batch simultaneously is often available and preferable in laboratory settings and computer simulations. Though CV-TS can be simply performed with the popular Thompson sampling (or posterior sampling) [18] (Sec. 3.1.2), bounding its Bayesian regret is challenging as the distribution of CVaR in our problem has not been investigated before and its support is unbounded. Fortunately, we are able to relate the problem of bounding the tail expectation of CVaR to that of the function evaluation $f(\mathbf{x}, \mathbf{w})$ (Sec. 4.2). The latter follows a Gaussian distribution with known tail expectation, unlike that of CVaR.

We empirically evaluate the performance of both CV-UCB and CV-TS in optimizing CVaR of synthetic benchmark functions, an optimization problem of the residuary resistance per unit weight of displacement of a yacht, a portfolio optimization problem, and a simulated robot task (Sec. 5).

Related works. Existing solutions to optimizing a black-box function $f(\mathbf{x}, \mathbf{W})$ with an environmental random variable \mathbf{W} are different in the assumptions about \mathbf{W} and the objective function. Other than the aforementioned works of [4, 13] where we adopt the assumptions that the distribution of \mathbf{W} is known and \mathbf{w} can be selected during the optimization procedure, the work of [9] also proposes an efficient algorithm with theoretical performance guarantee under the same assumptions to maximize the *probabilistic threshold robustness measure*. This measure requires a threshold of the desirable performance, instead of a *risk level* (i.e., the probability of undesirable performance) in CVaR and VaR. Another related work is *adversarially robust BO* [1] which maximizes $f(\mathbf{x}, \mathbf{w})$ with the worst-case realization \mathbf{w} of \mathbf{W} . It can be cast as an optimization problem of VaR of a black-box function [13]. The work of [10] assumes that the distribution of \mathbf{W} is given, but \mathbf{W} is sampled from its distribution during the optimization. Its objective is to balance between the mean and the variance of $f(\mathbf{x}, \mathbf{W})$ from different perspectives: multi-task learning, multi-objective optimization, and constrained optimization. The work of [22] maximizes VaR and CVaR of a black-box function, yet, it assumes \mathbf{W} is unobservable and its distribution is unknown. It suffers from an approximate posterior belief and the lack of theoretical performance guarantee. The works of [12, 14] (namely, *distributional robust BO*) assume that the unknown distribution of \mathbf{W} belongs to an uncertainty set of distributions. They maximize the mean of $f(\mathbf{x}, \mathbf{W})$ under the worst-case realization of the unknown distribution of \mathbf{W} in the uncertainty set.

2 Background

2.1 Conditional Value-at-Risk

Let the black-box function of interest be a real-valued function $f(\mathbf{x}, \mathbf{w})$ where $\mathbf{x} \in \mathbb{X} \subset \mathbb{R}^m$ and $\mathbf{w} \in \mathbb{W} \subset \mathbb{R}^n$. Let \mathbf{W} denote the *environmental random variable* whose probability distribution is specified by $p(\mathbf{W} = \mathbf{w})$ for all $\mathbf{w} \in \mathbb{W}$. Let $f(\mathbf{x}, \mathbf{W})$ denote the random variable representing the function evaluation at \mathbf{x} and a random realization of \mathbf{W} . The *conditional value-at-risk* (CVaR) of $f(\mathbf{x}, \mathbf{W})$ at *risk level* $\alpha \in (0, 1)$ is defined as:

$$c_f(\mathbf{x}; \alpha) \triangleq \mathbb{E}[f(\mathbf{x}, \mathbf{W}) | f(\mathbf{x}, \mathbf{W}) \leq v_f(\mathbf{x}; \alpha)] \quad (1)$$

which is the expectation of $f(\mathbf{x}, \mathbf{W})$ over function values that are at most the *value-at-risk* (VaR) at the same risk level α defined as $v_f(\mathbf{x}; \alpha) \triangleq \inf\{\omega : P(f(\mathbf{x}, \mathbf{W}) \leq \omega) \geq \alpha\}$.

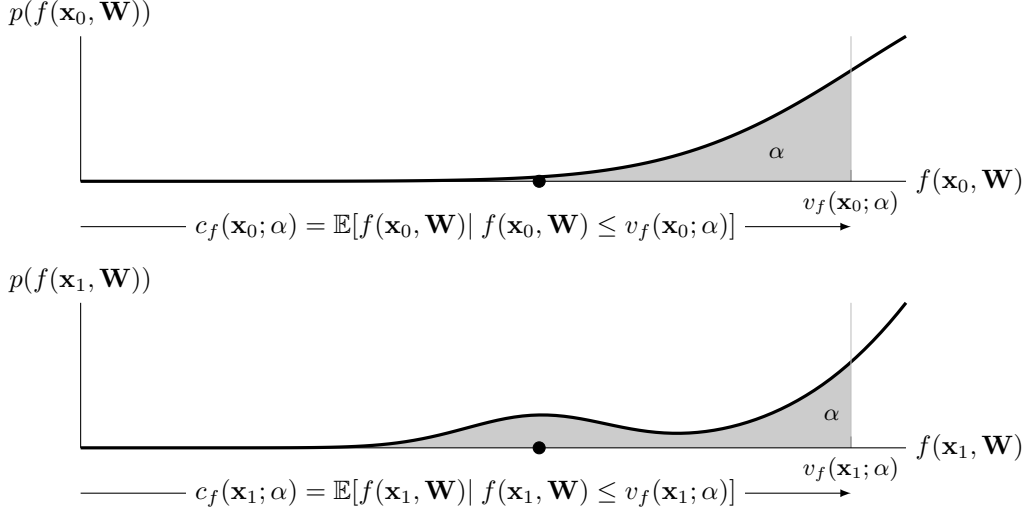


Figure 1: Plot of the lower tails of $f(\mathbf{x}_0, \mathbf{W})$ and $f(\mathbf{x}_1, \mathbf{W})$ with their VaR and CVaR at risk level α . The shaded area is α . It is observed that $v_f(\mathbf{x}_0; \alpha) = v_f(\mathbf{x}_1; \alpha)$ but $c_f(\mathbf{x}_0; \alpha) > c_f(\mathbf{x}_1; \alpha)$.

Remark 1 (CVaR vs. VaR). While VaR at α is interpreted as the α -percentile of $f(\mathbf{x}, \mathbf{W})$, CVaR is interpreted as the expectation of function values that are at most VaR. Therefore, CVaR is sensitive to the function values less than VaR, while VaR is not. Fig. 1 shows an example of function evaluations at \mathbf{x}_0 and \mathbf{x}_1 such that their VaR values (i.e., their α -percentiles) are the same. We observe that VaR is insensitive to the tails of $f(\mathbf{x}, \mathbf{W})$ which are different in this case (see the region around the black dot). In contrast, $c_f(\mathbf{x}_0; \alpha) > c_f(\mathbf{x}_1; \alpha)$ which conveys the idea that $f(\mathbf{x}_0, \mathbf{W})$ has a lower risk of low function values as the probability density of function values less than VaR concentrates in a region nearer to VaR than that of $f(\mathbf{x}_1, \mathbf{W})$. Thus, CVaR is more risk-averse than VaR, especially when the distribution of $f(\mathbf{x}, \mathbf{W})$ has a heavy lower tail, which makes it more suitable for critical applications. In the portfolio optimization problem, if the distribution of the portfolio's return has negative outliers (which are captured in CVaR), the average return in the long run can be negative even though the VaR of the return is positive.

In this work, we assume that $|\mathbb{W}|$ is finite to simplify the theoretical analysis (described in Sec. 4) and the evaluation of CVaR. The latter requires the computation of the cumulative probability mass of $f(\mathbf{x}, \mathbf{W})$ by enumerating all possible realizations of $f(\mathbf{x}, \mathbf{W})$ (described in [4]).

2.2 Bayesian Optimization of CVaR and Gaussian Processes

BO of CVaR. In this paper, we would like to maximize CVaR $c_f(\mathbf{x}; \alpha)$ (1) of $f(\mathbf{x}, \mathbf{W})$ given the distribution $p(\mathbf{W})$ by iteratively gathering observations as noisy function evaluations $y(\mathbf{x}, \mathbf{w}) \triangleq f(\mathbf{x}, \mathbf{w}) + \epsilon(\mathbf{x}, \mathbf{w})$ where $\epsilon(\mathbf{x}, \mathbf{w}) \sim \mathcal{N}(0, \sigma_n^2)$. The gist of BO of CVaR is a strategy to select the *input query* $(\mathbf{x}_t, \mathbf{w}_t)$ at iteration t such that the maximizer $\mathbf{x}_* \in \arg\max_{\mathbf{x} \in \mathbb{X}} c_f(\mathbf{x}; \alpha)$ is found as rapidly as possible. Note that while \mathbf{W} is controllable in BO, after the optimization, the optimal \mathbf{x}_* can be used in real-world settings where \mathbf{W} is uncontrollable. At iteration t , we have all observations at input queries in the previous $t - 1$ iterations, denote as $\mathbf{D}_{t-1} = \mathbf{D}_{t-2} \cup \{(\mathbf{x}_{t-1}, \mathbf{w}_{t-1})\}$ (\mathbf{D}_0 denotes the set of initial observed inputs). These observations $\mathbf{y}_{\mathbf{D}_{t-1}} \triangleq (y(\mathbf{x}, \mathbf{w}))_{(\mathbf{x}, \mathbf{w}) \in \mathbf{D}_{t-1}}$ are used to construct the *posterior* belief/distribution of the underlying black-box function $f(\mathbf{x}, \mathbf{w})$ which is utilized in building the query selection strategy. Let us revisit Fig. 1: $c_f(\mathbf{x}_0; \alpha) > c_f(\mathbf{x}_1; \alpha)$ implies that \mathbf{x}_0 is preferred to \mathbf{x}_1 . It is because the risk/chance of getting low function values at \mathbf{x}_0 is smaller (see the region around the black dot). In contrast, VaR cannot differentiate the risk of $f(\mathbf{x}_0, \mathbf{W})$ and that of $f(\mathbf{x}_1, \mathbf{W})$ since their VaR values are the same.

Algorithm 1 BO Algorithms for optimizing CVaR of a black-box function

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1: Input: algo,  $\mathbb{X}$ ,  $\mathbb{W}$ , initial observation  $\mathbf{y}_{\mathbf{D}_0}$ , prior  $\mu_0 = 0, \sigma_n, \kappa$ 
2: for  $t = 1, 2, \dots$  do
3:   {Selecting  $\mathbf{x}_t$ }
4:   if algo is CV-UCB then
5:     Select  $\mathbf{x}_t \in \operatorname{argmax}_{\mathbf{x}} c_{u_{t-1}}(\mathbf{x}; \alpha)$ 
6:   else if algo is CV-TS then
7:     Sample a function  $f_1$  from the GP posterior belief given  $\mathbf{y}_{\mathbf{D}_{t-1}}$ 
8:     Select  $\mathbf{x}_t \in \operatorname{argmax}_{\mathbf{x}} c_{f_1}(\mathbf{x}; \alpha)$ 
9:   end if
10:  {Selecting  $\mathbf{w}_t$ }
11:  Find  $\alpha_t \in \arg \max_{\alpha' \in (0, \alpha]} v_{u_{t-1}}(\mathbf{x}_t; \alpha') - v_{l_{t-1}}(\mathbf{x}_t; \alpha')$ 
12:  Given  $\alpha_t$ , select  $\mathbf{w}_t$  as an LV w.r.t.  $\mathbf{x}_t$ ,  $u_{t-1}$ , and  $l_{t-1}$ 
13:  {Collecting data and updating GP}
14:  Incorporate new observation at input query:  $\mathbf{y}_{\mathbf{D}_t} = \mathbf{y}_{\mathbf{D}_{t-1}} \cup \{y(\mathbf{x}_t, \mathbf{w}_t)\}$ 
15:  Update the GP posterior belief given  $\mathbf{y}_{\mathbf{D}_t}$ 
16: end for

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Gaussian process (GP). In order to obtain the posterior belief of $f(\mathbf{x}, \mathbf{w})$ given noisy observations $\mathbf{y}_{\mathbf{D}_{t-1}}$, we model the black-box function f with a GP: every finite subset of $\{f(\mathbf{x}, \mathbf{w})\}_{(\mathbf{x}, \mathbf{w}) \in \mathbb{X} \times \mathbb{W}}$ follows a multivariate Gaussian distribution [17]. Thus, GP is fully specified by its *prior* mean which is assumed to be zero and its *covariance function/kernel* $\kappa(\mathbf{x}, \mathbf{w}; \mathbf{x}', \mathbf{w}') \triangleq \operatorname{cov}[f(\mathbf{x}, \mathbf{w}), f(\mathbf{x}', \mathbf{w}')]$. Given noisy observations $\mathbf{y}_{\mathbf{D}_{t-1}}$ at iteration t , the posterior belief $p(f(\mathbf{x}, \mathbf{w}) | \mathbf{y}_{\mathbf{D}_{t-1}})$ is a Gaussian specified by the following mean and variance:

$$\begin{aligned} \mu_{t-1}(\mathbf{x}, \mathbf{w}) &\triangleq \mathbf{K}_{\mathbf{x}, \mathbf{w}; \mathbf{D}_{t-1}} \mathbf{\Lambda}_{\mathbf{D}_{t-1}} \mathbf{y}_{\mathbf{D}_{t-1}} \\ \sigma_{t-1}^2(\mathbf{x}, \mathbf{w}) &\triangleq \kappa(\mathbf{x}, \mathbf{w}) - \mathbf{K}_{\mathbf{x}, \mathbf{w}; \mathbf{D}_{t-1}} \mathbf{\Lambda}_{\mathbf{D}_{t-1}} \mathbf{K}_{\mathbf{D}_{t-1}; \mathbf{x}, \mathbf{w}} \end{aligned} \quad (2)$$

where $\kappa(\mathbf{x}, \mathbf{w}) \triangleq \kappa(\mathbf{x}, \mathbf{w}; \mathbf{x}, \mathbf{w})$, $\mathbf{K}_{\mathbf{x}, \mathbf{w}; \mathbf{D}_{t-1}} \triangleq (\kappa(\mathbf{x}, \mathbf{w}; \mathbf{x}', \mathbf{w}'))_{(\mathbf{x}', \mathbf{w}') \in \mathbf{D}_{t-1}}$, $\mathbf{K}_{\mathbf{D}_{t-1}; \mathbf{x}, \mathbf{w}} \triangleq \mathbf{K}_{\mathbf{x}, \mathbf{w}; \mathbf{D}_{t-1}}^\top$, and $\mathbf{\Lambda}_{\mathbf{D}_{t-1}} \triangleq (\mathbf{K}_{\mathbf{D}_{t-1} \mathbf{D}_{t-1}} + \sigma_n^2 \mathbf{I})^{-1}$ (\mathbf{I} is the identity matrix and $\mathbf{K}_{\mathbf{D}_{t-1} \mathbf{D}_{t-1}} \triangleq (\kappa(\mathbf{x}', \mathbf{w}'; \mathbf{x}'', \mathbf{w}''))_{(\mathbf{x}', \mathbf{w}'; \mathbf{x}'', \mathbf{w}'') \in \mathbf{D}_{t-1} \times \mathbf{D}_{t-1}}$).

Although $f(\mathbf{x}, \mathbf{w})$ follows a Gaussian distribution, CVaR $c_f(\mathbf{x}; \alpha)$ (defined in (1)) does not. Furthermore, although $|\mathbb{W}|$ is finite, the distribution of CVaR is continuous because the black-box function evaluation is real-valued. Besides, as the support of $f(\mathbf{x}, \mathbf{W})$ is unbounded, so is CVaR. These points pose challenges in deriving the following 2 algorithms and their theoretical analyses.

3 BO Algorithms for Optimizing CVaR of a Black-Box Function

In this section, we present two BO algorithms for optimizing CVaR of a black-box function $f(\mathbf{x}, \mathbf{W})$: *CVaR optimization with upper confidence bound* (CV-UCB) and *CVaR optimization with Thompson sampling* (CV-TS). These two algorithms are different in the way of handling the exploration-exploitation trade-off in the selection of \mathbf{x}_t to find $\operatorname{argmax}_{\mathbf{x} \in \mathbb{X}} c_f(\mathbf{x}; \alpha)$ (Sec. 3.1.1 and Sec. 3.1.2). On the other hand, given the selected \mathbf{x}_t , selecting \mathbf{w}_t is only about reducing the uncertainty of CVaR $c_f(\mathbf{x}_t; \alpha)$. Therefore, we would like to design a single selection strategy of \mathbf{w}_t that works for both CV-UCB and CV-TS (Sec. 3.2).

3.1 Selection Strategy of \mathbf{x}_t

3.1.1 A UCB-based Approach to Select \mathbf{x}_t in CV-UCB

In (1), CVaR $c_f(\mathbf{x}; \alpha)$ at risk level α of $f(\mathbf{x}, \mathbf{W})$ is defined as the expectation of function values that are at most VaR at risk level α [4]. While this definition (1) is interpretable, it is challenging to devise a no-regret BO algorithm based on (1). It is because (1) requires learning about not only (i) VaR $v_f(\mathbf{x}; \alpha)$ but also (ii) the probabilities of function values less than $v_f(\mathbf{x}; \alpha)$. Even though the former (i.e., VaR $v_f(\mathbf{x}; \alpha)$) can be optimized using the V-UCB algorithm in [13], it remains a challenge to learn about the latter.

Interestingly, in this section, we present an approach that does not resort to handling the above two problems (i) and (ii) separately. To achieve this, we employ an alternative definition of CVaR which is an expectation of VaR over the risk level:

$$c_f(\mathbf{x}; \alpha) = \frac{1}{\alpha} \int_0^\alpha v_f(\mathbf{x}; \alpha') d\alpha'. \quad (3)$$

Although (1) is more interpretable and is often used to evaluate CVaR, the above definition (3) paves the way to our selection strategy of \mathbf{x}_t in CV-UCB: by utilizing (3), we are able to construct an upper confidence bound of CVaR relying on that of VaR. Recall that the work of [13] proposes a confidence bound of VaR at iteration t , denoted as $I_{t-1}[v_f(\mathbf{x}; \alpha')]$:

$$I_{t-1}[v_f(\mathbf{x}; \alpha')] \triangleq [v_{l_{t-1}}(\mathbf{x}; \alpha'), v_{u_{t-1}}(\mathbf{x}; \alpha')] \quad \forall \mathbf{x} \in \mathbb{X} \quad \forall \alpha' \in (0, 1) \quad (4)$$

where $v_{l_{t-1}}(\mathbf{x}; \alpha')$ and $v_{u_{t-1}}(\mathbf{x}; \alpha')$ are VaR (due to the randomness in \mathbf{W}) of $l_{t-1}(\mathbf{x}, \mathbf{W})$ and $u_{t-1}(\mathbf{x}, \mathbf{W})$, respectively. At iteration t , for all $(\mathbf{x}, \mathbf{w}) \in \mathbb{X} \times \mathbb{W}$, $[l_{t-1}(\mathbf{x}, \mathbf{w}), u_{t-1}(\mathbf{x}, \mathbf{w})]$ is a confidence bound of $f(\mathbf{x}, \mathbf{w})$ (due to the uncertainty in the unknown black-box function f) depending on an *exploration parameter* β_t [13]:

$$\begin{aligned} l_{t-1}(\mathbf{x}, \mathbf{w}) &\triangleq \mu_{t-1}(\mathbf{x}, \mathbf{w}) - \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{w}) \\ u_{t-1}(\mathbf{x}, \mathbf{w}) &\triangleq \mu_{t-1}(\mathbf{x}, \mathbf{w}) + \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{w}) \end{aligned} \quad (5)$$

where $\mu_{t-1}(\mathbf{x}, \mathbf{w})$ and $\sigma_{t-1}(\mathbf{x}, \mathbf{w})$ are defined in (2). The exploration parameter β_t is to balance between exploitation (based on the GP posterior mean $\mu_{t-1}(\mathbf{x}, \mathbf{w})$) and exploration (based on the GP posterior standard deviation $\sigma_{t-1}(\mathbf{x}, \mathbf{w})$), which is specified later in Lemma 1. From (3), a confidence bound $I_{t-1}[c_f(\mathbf{x}; \alpha)]$ of CVaR follows the confidence bound $I_{t-1}[v_f(\mathbf{x}; \alpha')]$ of VaR (4):

$$I_{t-1}[c_f(\mathbf{x}; \alpha)] \triangleq [c_{l_{t-1}}(\mathbf{x}; \alpha), c_{u_{t-1}}(\mathbf{x}; \alpha)] \triangleq \left[\frac{1}{\alpha} \int_0^\alpha v_{l_{t-1}}(\mathbf{x}; \alpha') d\alpha', \frac{1}{\alpha} \int_0^\alpha v_{u_{t-1}}(\mathbf{x}; \alpha') d\alpha' \right]. \quad (6)$$

Given the above upper confidence bound $c_{u_{t-1}}(\mathbf{x}; \alpha)$ of CVaR, we select \mathbf{x}_t as its maximizer (line 5 of Algorithm 1). The time complexity of the selection strategy of \mathbf{x}_t in CV-UCB is $\mathcal{O}(|\mathbf{D}_{t-1}|^3 + n_{\text{train}}(|\mathbb{W}||\mathbf{D}_{t-1}|^2 + |\mathbb{W}| \log |\mathbb{W}|))$ where n_{train} is the number of gradient descent steps to find $\arg\max_{\mathbf{x}} c_{u_{t-1}}(\mathbf{x}; \alpha)$, $\mathcal{O}(|\mathbf{D}_{t-1}|^3)$ is to compute $\Lambda_{\mathbf{D}_{t-1}}$ in (2), $\mathcal{O}(|\mathbb{W}||\mathbf{D}_{t-1}|^2)$ is the GP prediction time complexity, and $\mathcal{O}(|\mathbb{W}| \log |\mathbb{W}|)$ is to evaluate CVaR.

3.1.2 A Thompson Sampling Approach to Select \mathbf{x}_t in CV-TS

An alternative approach to select \mathbf{x}_t is based on Thompson sampling [18]: \mathbf{x}_t is selected as a sample of the maximizer \mathbf{x}_* of CVaR $c_f(\mathbf{x}; \alpha)$. Unlike the selection strategy of \mathbf{x}_t in CV-UCB that requires an exploration parameter β_t (Sec. 3.1.1), the exploration-exploitation trade-off in Thompson sampling is naturally handled by the randomness in the sampling of the maximizer of $c_f(\mathbf{x}; \alpha)$. This approach can also be extended to handle a batch query at each BO iteration by drawing a batch of samples of the maximizer of $c_f(\mathbf{x}; \alpha)$. While unexplored for BO of CVaR, batch queries are popular in BO literature [8, 11].

A sample of the maximizer of $c_f(\mathbf{x}; \alpha)$ is obtained by the following 2 steps (lines 7-8 of Algorithm 1). First, we draw a function sample f_1 from the GP posterior belief by using random Fourier feature approximation [16] which is also employed in classical BO works [7, 23] (line 7 of Algorithm 1). Second, given f_1 , we maximize CVaR $c_{f_1}(\mathbf{x}; \alpha)$ to obtain its maximizer. This is a sample of the maximizer of $c_f(\mathbf{x}; \alpha)$ which is assigned to \mathbf{x}_t in CV-TS (line 8 of Algorithm 1). The time complexity of the selection strategy of \mathbf{x}_t in CV-TS is $\mathcal{O}(|\mathbf{D}_{t-1}|^3 + n_{\text{train}}(n_{\text{feature}}^2 + |\mathbb{W}| \log |\mathbb{W}|))$ where n_{feature} is the number of random Fourier samples, n_{train} is the number of gradient descent steps to find $\arg\max_{\mathbf{x}} c_{f_1}(\mathbf{x}; \alpha)$, $\mathcal{O}(|\mathbf{D}_{t-1}|^3)$ is to compute $\Lambda_{\mathbf{D}_{t-1}}$ in (2) (which dominates the time complexity to draw a function f_1 from the GP posterior belief), $\mathcal{O}(n_{\text{feature}}^2)$ is the time complexity to evaluate f_1 , and $\mathcal{O}(|\mathbb{W}| \log |\mathbb{W}|)$ is to evaluate CVaR.

3.2 Selection Strategy of \mathbf{w}_t Shared by Both CV-UCB & CV-TS

Given the selected \mathbf{x}_t at iteration t , we would like to propose a single strategy of selecting \mathbf{w}_t to reduce the uncertainty of CVaR $c_f(\mathbf{x}_t; \alpha)$ for both CV-UCB and CV-TS that still guarantees no-regret for both algorithms as shown in Sec. 4.

Our main idea is to prioritize learning about VaR at risk level α_t which has the *highest uncertainty* among VaR $v_f(\mathbf{x}; \alpha')$ at risk levels $\alpha' \in (0, \alpha]$. In turn, it reduces the uncertainty of CVaR from (3). We quantify the uncertainty of VaR by the size of its confidence bound (4). Thus, α_t is defined as (line 11 of Algorithm 1)

$$\alpha_t \in \arg \max_{\alpha' \in (0, \alpha]} v_{u_{t-1}}(\mathbf{x}_t; \alpha') - v_{l_{t-1}}(\mathbf{x}_t; \alpha'). \quad (7)$$

To reduce the uncertainty of $v_f(\mathbf{x}_t; \alpha_t)$ quantified by the size of its confidence bound $v_{u_{t-1}}(\mathbf{x}_t; \alpha_t) - v_{l_{t-1}}(\mathbf{x}_t; \alpha_t)$, let us view $v_f(\mathbf{x}_t; \alpha_t)$ as the α_t -percentile of $f(\mathbf{x}_t, \mathbf{W})$. There is no uncertainty in the α_t -percentile of $f(\mathbf{x}_t, \mathbf{W})$ if the set of \mathbf{w} where $f(\mathbf{x}_t, \mathbf{w})$ is at most the α_t -quantile of $f(\mathbf{x}_t, \mathbf{W})$ (i.e., the lower tail of $f(\mathbf{x}_t, \mathbf{W})$ upper bounded by its α_t -percentile) remains unchanged under different realizations of f , especially its lower confidence bound l_{t-1} and its upper confidence bound u_{t-1} . On the contrary, if there exists \mathbf{w}_{LV} that violates the above statement due to the uncertainty of $f(\mathbf{x}_t, \mathbf{w}_{LV})$ (due to the unknown f), we would like to gather observation at $(\mathbf{x}_t, \mathbf{w}_{LV})$ to reduce the uncertainty of its function evaluation. Such \mathbf{w}_{LV} is formally defined as the *lacing value* (LV) which is shown to exist in [13].¹

Definition 1 (Lacing values [13]). *Lacing values* (LV) with respect to $\alpha \in (0, 1)$, $\mathbf{x} \in \mathbb{X}$, l_{t-1} , and u_{t-1} are $\mathbf{w}_{LV} \in \mathbb{W}$ that satisfies $l_{t-1}(\mathbf{x}, \mathbf{w}_{LV}) \leq v_{l_{t-1}}(\mathbf{x}; \alpha) \leq v_{u_{t-1}}(\mathbf{x}; \alpha) \leq u_{t-1}(\mathbf{x}, \mathbf{w}_{LV})$, equivalently, $I_{t-1}[v_f(\mathbf{x}; \alpha)] \subset [l_{t-1}(\mathbf{x}, \mathbf{w}_{LV}), u_{t-1}(\mathbf{x}, \mathbf{w}_{LV})]$.

Thus, we select \mathbf{w}_t as an LV w.r.t. α_t , \mathbf{x}_t , l_{t-1} , and u_{t-1} . If there are multiple LVs, we select the LV with the maximum probability $p(\mathbf{W})$. It is a heuristic to improve the performance suggested by [13]. For CV-TS, to avoid repeating inputs in the batch query, we can select \mathbf{w}_t as a sample of the random variable \mathbf{W} by restricting its support to the LVs (if there are multiple LVs).

4 Theoretical Analysis

This section presents our theoretical analyses of CV-UCB and CV-TS. We choose the exploration parameter β_t in (5) following a lemma in [21]. We assume a discrete domain \mathbb{X} for simplicity (and $|\mathbb{W}|$ is finite).

Lemma 1 (Lemma 5.1 in [21]). Pick $\delta \in (0, 1)$ and set $\beta_t = 2 \log(|\mathbb{X}||\mathbb{W}|\pi_t/\delta)$, where $\sum_{t \geq 1} \pi_t^{-1} = 1$, $\pi_t > 0$. Then,

$$|f(\mathbf{x}, \mathbf{w}) - \mu_{t-1}(\mathbf{x}, \mathbf{w})| \leq \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{w}) \quad \forall (\mathbf{x}, \mathbf{w}) \in \mathbb{X} \times \mathbb{W} \quad \forall t \geq 1 \quad (8)$$

holds with probability $\geq 1 - \delta$.

Thus, given the above β_t , the function evaluation, VaR, and CVaR are in their confidence bounds (in (5), (4), and (6), respectively) with probability $\geq 1 - \delta$.

4.1 CV-UCB

The performance of CV-UCB is measured by the *cumulative regret* adopted from existing BO works, e.g., in [21, 13]: $R_T \triangleq \sum_{t=1}^T r_t$ which is the sum over *instantaneous regrets*, denoted as $r_t \triangleq c_f(\mathbf{x}_*; \alpha) - c_f(\mathbf{x}_t; \alpha)$ where $\mathbf{x}_* \in \arg \max_{\mathbf{x} \in \mathbb{X}} c_f(\mathbf{x}; \alpha)$ is the optimal value of the optimization variable. In this section, we would like to show that the cumulative regret of CV-UCB is sublinear so that $\lim_{T \rightarrow \infty} R_T/T = 0$.

Since CV-UCB selects \mathbf{x}_t as the maximizer of the upper confidence bound of CVaR (line 5 of Algorithm 1), it can be shown in Appendix A that the instantaneous regret is bounded by

$$r_t \leq c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha) \quad (9)$$

with probability $\geq 1 - \delta$. Then, by exploiting the relationship between CVaR and VaR in (3) and the fact that the average of a set of values is at most the maximum value of the set, the bound on r_t can be simplified to the size of a confidence bound of VaR at risk level α_t (7) in Appendix A:

$$r_t \leq v_{u_{t-1}}(\mathbf{x}_t; \alpha_t) - v_{l_{t-1}}(\mathbf{x}_t; \alpha_t) \quad (10)$$

¹Shrewd readers may notice a difference between the intuition and definition of LV (\leq vs. $<$). It is to handle the case when there is only 1 LV.

holds with probability $\geq 1 - \delta$. Furthermore, utilizing the property of \mathbf{w}_t as an LV in Definition 1, it can be shown in Appendix A that

$$r_t \leq 2\beta_t^{1/2}\sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \quad (11)$$

with probability $\geq 1 - \delta$. Then, we follow [21] to construct the following theorem which shows a sublinear regret bound for CV-UCB (detailed in Appendix B).

Theorem 1. By selecting \mathbf{x}_t as the maximizer of the upper confidence bound $c_{u_{t-1}}(\mathbf{x}; \alpha)$ (line 5 of Algorithm 1) and selecting \mathbf{w}_t as an LV w.r.t. α_t (7), \mathbf{x}_t , l_{t-1} , and u_{t-1} (line 12 of Algorithm 1),

$$R_T \leq \sqrt{C_1 T \beta_T \gamma_T} \quad (12)$$

holds with probability $\geq 1 - \delta$ where $C_1 \triangleq 8/\log(1 + \sigma_n^2)$, γ_T is the maximum information gain about f that can be obtained by observing any set of T observations (which is bounded in [21] for several commonly used kernels), β_T and δ are defined in Lemma 1.

4.2 CV-TS

The performance of CV-TS is measured by the *Bayesian cumulative regret* [18]: $R_T^{\text{Bayes}} \triangleq \mathbb{E} \left[\sum_{t=1}^T c_f(\mathbf{x}_*; \alpha) - c_f(\mathbf{x}_t; \alpha) \right]$ where the expectation includes the randomness in the GP prior of f , the observation noise, and \mathbf{x}_t . Let us denote $r_t^{\text{Bayes}} \triangleq \mathbb{E}[c_f(\mathbf{x}_*; \alpha) - c_f(\mathbf{x}_t; \alpha) | \mathbf{y}_{\mathbf{D}_{t-1}}]$ where the expectation includes the randomness in the GP posterior of f given $\mathbf{y}_{\mathbf{D}_{t-1}}$ and \mathbf{x}_t , then $R_T^{\text{Bayes}} = \mathbb{E} \left[\sum_{t=1}^T r_t^{\text{Bayes}} \right]$. In this section, we would like to show that the Bayesian cumulative regret of CV-TS is sublinear so that $\lim_{T \rightarrow \infty} R_T^{\text{Bayes}}/T = 0$. Following [18], we can decompose r_t^{Bayes} into (to ease the notation, we omit $\mathbf{y}_{\mathbf{D}_{t-1}}$):

$$r_t^{\text{Bayes}} \leq \mathbb{E}[\Delta_c^{\text{lower}}(\mathbf{x}_t; \alpha)] + \mathbb{E}[\Delta_c^{\text{upper}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha)] \quad (13)$$

where $\Delta_c^{\text{lower}}(\mathbf{x}_t; \alpha) \triangleq \max(0, c_{l_{t-1}}(\mathbf{x}_t; \alpha) - c_f(\mathbf{x}_t; \alpha))$ and $\Delta_c^{\text{upper}}(\mathbf{x}_*; \alpha) \triangleq \max(0, c_f(\mathbf{x}_*; \alpha) - c_{u_{t-1}}(\mathbf{x}_*; \alpha))$ (shown in Appendix C).

From Appendix A, $c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha)$ is bounded by $2\beta_t^{1/2}\sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t)$ provided that \mathbf{w}_t is an LV w.r.t. α_t (7), \mathbf{x}_t , l_{t-1} , and u_{t-1} (line 12 of Algorithm 1). Thus, we are able to obtain a bound on the last term of the decomposed r_t^{Bayes} (13):

$$\mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha)] \leq 2\beta_t^{1/2}\sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t). \quad (14)$$

However, the challenge remains in bounding the first two terms (i.e., $\mathbb{E}[\Delta_c^{\text{lower}}(\mathbf{x}_t; \alpha)]$ and $\mathbb{E}[\Delta_c^{\text{upper}}(\mathbf{x}_*; \alpha)]$) of the decomposed r_t^{Bayes} (13). These terms are the expectations over the tails of CVaR. As suggested by the seminal work of [18], bounding these terms may require CVaR to have a bounded support or a strong tail decay. However, in our BO formulation where f is modelled with a GP, the support of CVaR is unbounded. Thus, to derive the bound of the tail expectation of the unfamiliar distribution of CVaR, our key idea is to relate it to the tail expectation of a Gaussian distribution through 3 steps: **first**, relating this tail expectation of CVaR to that of VaR in Lemma 2, **second**, relating the tail expectation of VaR to the tail probability of VaR in (16), and **third**, relating the tail probability of VaR to that of function evaluation $f(\mathbf{x}, \mathbf{w})$ in Lemma 3. As $f(\mathbf{x}, \mathbf{w})$ follows a Gaussian distribution, we can bound its tail expectation.

Lemma 2 (From tail expectation of CVaR to that of VaR). For all $\mathbf{x} \in \mathbb{X}$,

$$\mathbb{E}[\Delta_c^{\text{lower}}(\mathbf{x}; \alpha)] \leq \frac{1}{\alpha} \int_0^\alpha \mathbb{E}[\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')] d\alpha' \quad (15)$$

where $\Delta_v^{\text{lower}}(\mathbf{x}; \alpha') \triangleq \max(0, v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha'))$ (shown in Appendix D).

Furthermore, as $\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')$ is a non-negative random variable, its expectation in (15) can be expressed as an integration over the tail probabilities: $\forall \alpha' \in (0, 1)$, $\mathbf{x} \in \mathbb{X}$,

$$\mathbb{E}[\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')] = \int_0^\infty P(\Delta_v^{\text{lower}}(\mathbf{x}; \alpha') > \omega) d\omega = \int_0^\infty P(v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha') > \omega) d\omega. \quad (16)$$

Then, we are able to relate the tail probability $P(v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha') > \omega)$ to the tail probability of the function evaluation $f(\mathbf{x}, \mathbf{w})$ using our key observation on the relationship between the 2 events: (a) VaR $v_f(\mathbf{x}; \alpha')$ falls below its lower confidence bound $v_{l_{t-1}}(\mathbf{x}; \alpha')$ by $\omega \geq 0$ and (b) the function evaluation $f(\mathbf{x}, \mathbf{w})$ falls below its lower confidence bound $l_{t-1}(\mathbf{x}, \mathbf{w})$ by ω in the following lemma (proved in Appendix E).

Lemma 3. Consider a realization f_1 of the black-box function f following the GP posterior belief given $\mathbf{y}_{\mathbf{D}_{t-1}}$ that satisfies

$$v_{l_{t-1}}(\mathbf{x}; \alpha') - v_{f_1}(\mathbf{x}; \alpha') > \omega$$

for $\alpha' \in (0, 1)$, $\mathbf{x} \in \mathbb{X}$, and $\omega \geq 0$. Let $\mathbb{W}_{l_{t-1}}^{\text{upper}} \triangleq \{\mathbf{w} \in \mathbb{W} : l_{t-1}(\mathbf{x}, \mathbf{w}) \geq v_{l_{t-1}}(\mathbf{x}; \alpha')\}$. Then,

$$\exists \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, l_{t-1}(\mathbf{x}, \mathbf{w}_0) - f_1(\mathbf{x}, \mathbf{w}_0) > \omega.$$

As the tail expectation of the Gaussian random variable $f(\mathbf{x}, \mathbf{w})$ can be evaluated, we can utilize the above results ((15), (16), and Lemma 3) to obtain a bound of $\mathbb{E}[\Delta_c^{\text{lower}}(\mathbf{x}; \alpha)]$ (and similarly, a bound of $\mathbb{E}[\Delta_c^{\text{upper}}(\mathbf{x}; \alpha)]$) for all $\mathbf{x} \in \mathbb{X}$. These bounds and (14) lead to the following theorem on the Bayesian cumulative regret bound (proved in Appendix F).

Theorem 2. Assuming a bounded GP prior standard deviation: $\kappa(\mathbf{x}, \mathbf{w}) \leq 1 \forall (\mathbf{x}, \mathbf{w}) \in \mathbb{X} \times \mathbb{W}$, by selecting \mathbf{x}_t as a sample of the maximizer of $c_f(\mathbf{x}; \alpha)$ (lines 7-8 of Algorithm 1) and selecting \mathbf{w}_t as an LV w.r.t. α_t (7), \mathbf{x}_t , l_{t-1} , and u_{t-1} (line 12 of Algorithm 1), then the Bayesian cumulative regret is bounded by

$$R_T^{\text{Bayes}} \leq \frac{\delta\sqrt{2}}{|\mathbb{X}|\sqrt{\pi}} + \sqrt{C_1 T \beta_T \gamma_T} \quad (17)$$

where $C_1 \triangleq 8/\log(1 + \sigma_n^{-2})$, γ_T is the maximum information gain about f that can be obtained by observing any set of T observations, β_T and δ are defined in Lemma 1.

Remark 2. We can extend CV-TS to select a batch query of size k (instead of a single query) at each BO iteration by drawing k samples of the maximizer of CVaR and finding their corresponding α_t and LVs (detailed in Appendix G). We can also show that the difference between the average (over the number of observations) of the Bayesian cumulative regret bound of CV-TS with batch queries and that of CV-TS with single queries is small for a large number of observations (Appendix G), which is similar to a result in [11] for the classical BO with Thompson sampling. However, with a larger batch size k , more observations can be obtained given the same number of BO iterations. Thus, the use of CV-TS with a large batch size k is advantageous if obtaining observations at the batch query is feasible, e.g., by running multiple simulations in parallel.

Remark 3. Our CV-TS algorithm and its theoretical analysis can be utilized to construct a BO algorithm to optimize VaR of a black-box function. Like CV-TS, this algorithm is also capable of handling batch queries. Since it is beyond the scope of this work (which is about CVaR), we refer readers interested in optimizing VaR of a black-box function to Appendix H.

5 Experiments

We empirically evaluate the performance of CV-UCB and CV-TS by comparing them with the work of [4]. To the best of our knowledge, it is the only existing work that optimizes CVaR of a black-box function by selecting both \mathbf{x} and \mathbf{w} . In particular, the $\rho\text{KG}^{\text{apx}}$ algorithm is selected as a baseline thanks to its time efficiency and competitive empirical performance as demonstrated in [4]. There are 2 variants of CV-TS in the experiments: *CV-TS* $k = 1$ which selects 1 input query at each iteration and *CV-TS* $k = 3$ which selects 3 input queries at each iteration. Each experiment is repeated 10 times with different random seeds to account for the randomness in the observation noise, the set of initial observations, and the sampling from the GP posterior belief. Both the average and the confidence interval of the logarithm of the inference regret (taken from [7, 23]) are reported. The hyperparameters of GP and the noise variance are learned from the observations using maximum likelihood estimation [17]. Further details on the experiments are described in Appendix I.²

Figs. 2a-d show the results of optimizing CVaR of synthetic benchmark functions with low input dimensions (the dimension of \mathbf{x} is $m = 1$ and of \mathbf{W} is $n = 1$): Branin-Hoo and Goldstein-Price; and

²The code is available at <https://github.com/qphong/BayesOpt-LV>.

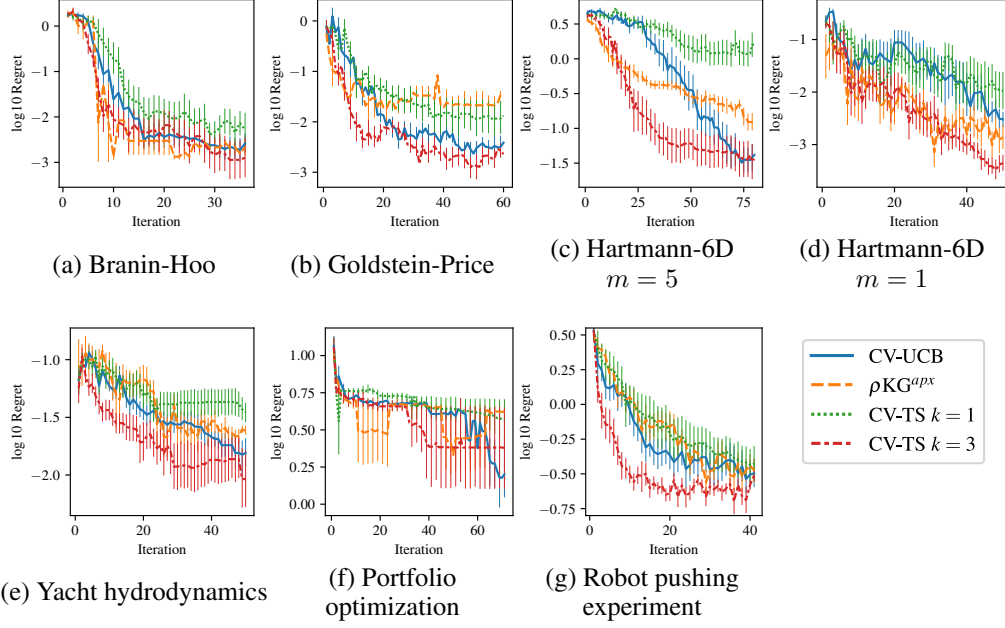


Figure 2: Plots of the regret against the BO iteration in (a-d) experiments that optimize CVaR of synthetic benchmark functions, (e-g) simulated real-world optimization problems.

with moderate input dimensions ($m = 5, n = 1$; and $m = 1, n = 5$): Hartmann-6D. The risk level α is set to 0.1. We observe that CV-UCB achieves comparable performance to the baseline ρKG^{apx} in the Branin-Hoo experiment, while it outperforms ρKG^{apx} in the Goldstein-Price and Hartmann-6D ($m = 5$) experiments. It is because the evaluation of ρKG^{apx} is approximated with samples of f and the nested optimization procedure involved in ρKG^{apx} is simplified. CV-TS $k = 1$ does not perform as well as other algorithms do. It is because with few observations, CV-TS $k = 1$ tends towards randomly exploring \mathbb{X} so the maximizer is not accurately located. Furthermore, as the GP hyperparameters are assumed to be unknown in our experiments, they can be incorrectly estimated with few observations, which affects the performance of CV-TS $k = 1$. When we increase the size of the batch query to 3 in CV-TS $k = 3$, the number of observations increases. In turn, the estimation of the GP hyperparameters and the exploration-exploitation trade-off are improved. Thus, CV-TS $k = 3$ achieves a superior performance. It suggests that CV-TS with a large batch query should be preferred when multiple observations can be obtained, e.g., by running multiple simulations in parallel. In contrast, CV-UCB should be preferred if only one observation is obtained at each BO iteration.

Figs. 2e-g show the results of optimizing CVaR in an optimization problem using the yacht hydrodynamics dataset [5], a portfolio optimization problem [4], and a simulated robot pushing experiment [23]. In the experiment with the yacht hydrodynamics dataset, we would like to minimize the residuary resistance per unit weight of displacement of a yacht by searching for the optimal hull geometry coefficients of the yacht in the face of the uncertainty in the Froude number (the Froude number depends on the real-world environment and we assume that it can be simulated with computers during the optimization). The ground truth function is constructed using the yacht hydrodynamics data set [5]. The dimension of the input variables \mathbf{x} and \mathbf{W} are $m = 5$ and $n = 1$ (the Froude number), respectively. The risk level of CVaR is set to $\alpha = 0.3$. While CV-TS $k = 3$ outperforms the other algorithms significantly thanks to its batch queries, CV-UCB converges to a lower regret than ρKG^{apx} does. The portfolio optimization problem is taken from the work of [4] where the evolution of a portfolio over 4 years is simulated and optimized using open-source market data. The optimization variables (i.e., \mathbf{x}) include the risk, the trade aversion, and the holding cost multiplier, while the environmental random variables (i.e., \mathbf{W}) include the bid-ask spread and the borrow cost [4]. The risk level of CVaR in this problem is set to $\alpha = 0.2$. We observe that CV-UCB and CV-TS $k = 3$ achieve the best performance by converging to lower regret values than the other algorithms. The simulated robot pushing experiment is taken from [23] whose task is to minimize the distance of a pushed object to a fixed goal location by controlling the robot location and the pushing duration (i.e., \mathbf{x}). We adopt the setting of [13] to introduce random perturbations to the robot location (i.e.,

W). The risk level of CVaR is set to $\alpha = 0.1$. While all algorithms converge to roughly the same value of the regret in this experiment, we observe that CV-TS $k = 3$ shows its advantage in acquiring more observations by converging faster than the others. Besides, CV-UCB also converges faster than ρKG^{apx} in this experiment.

6 Conclusion

We propose two BO algorithms to optimize CVaR of a black-box function with theoretical performance guarantee: CV-UCB and CV-TS by taking advantage of a connection between CVaR and VaR and establishing a link between the tail expectation of (non-Gaussian and unbounded support) CVaR and that of the Gaussian-distributed function evaluation. The competitive empirical performance of CV-UCB and CV-TS with batch queries are shown in optimizing CVaR of synthetic benchmark functions and simulated real-world optimization problems. These results recommend the use of CV-UCB to optimize CVaR of a black-box function when only an observation is obtained at each BO iteration and the use of CV-TS with large batch queries when multiple observations can be obtained at each BO iteration.

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A Instantaneous Regret Bound

Conditioned on the event that (8) in Lemma 1 holds (with probability $\geq 1 - \delta$), it follows that

$$\begin{aligned} c_f(\mathbf{x}_*; \alpha) &\leq c_{u_{t-1}}(\mathbf{x}_*; \alpha) \\ c_f(\mathbf{x}_t; \alpha) &\geq c_{l_{t-1}}(\mathbf{x}_t; \alpha). \end{aligned}$$

Therefore, with probability $\geq 1 - \delta$,

$$\begin{aligned} r_t &\triangleq c_f(\mathbf{x}_*; \alpha) - c_f(\mathbf{x}_t; \alpha) \\ &\leq c_{u_{t-1}}(\mathbf{x}_*; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha) \\ &\leq c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha) \end{aligned} \tag{18}$$

where the last inequality is because $\mathbf{x}_t \in \operatorname{argmax}_{\mathbf{x}} c_{u_{t-1}}(\mathbf{x}; \alpha)$.

Based on the relationship between CVaR and VaR in (3),

$$\begin{aligned} c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha) &= \frac{1}{\alpha} \int_0^\alpha v_{u_{t-1}}(\mathbf{x}_t; \alpha') - v_{l_{t-1}}(\mathbf{x}_t; \alpha') d\alpha' \\ &\leq \frac{1}{\alpha} \int_0^\alpha v_{u_{t-1}}(\mathbf{x}_t; \alpha_t) - v_{l_{t-1}}(\mathbf{x}_t; \alpha_t) d\alpha' \\ &= v_{u_{t-1}}(\mathbf{x}_t; \alpha_t) - v_{l_{t-1}}(\mathbf{x}_t; \alpha_t) \end{aligned} \tag{19}$$

where $\alpha_t \in \operatorname{argmax}_{\alpha' \in (0, \alpha]} v_{u_{t-1}}(\mathbf{x}_t; \alpha') - v_{l_{t-1}}(\mathbf{x}_t; \alpha')$ (7).

As \mathbf{w}_t is selected as an LV w.r.t. α_t , \mathbf{x}_t , l_{t-1} , and u_{t-1} ,

$$l_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \leq v_{l_{t-1}}(\mathbf{x}_t; \alpha_t) \leq v_{u_{t-1}}(\mathbf{x}_t; \alpha_t) \leq u_{t-1}(\mathbf{x}_t, \mathbf{w}_t).$$

Therefore,

$$\begin{aligned} v_{u_{t-1}}(\mathbf{x}_t; \alpha_t) - v_{l_{t-1}}(\mathbf{x}_t; \alpha_t) &\leq u_{t-1}(\mathbf{x}_t, \mathbf{w}_t) - l_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \\ &= 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \end{aligned} \tag{20}$$

where the last equality is due to (5).

From (18), (19), and (20), we obtain (9), (10), and (11), respectively.

B Proof of Theorem 1

From (11) and the nondecreasing property of β_t , with probability $\geq 1 - \delta$,

$$\begin{aligned} R_T &= \sum_{t=1}^T r_t \leq \sum_{t=1}^T 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \\ &\leq 2\beta_T^{1/2} \sum_{t=1}^T \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \\ &\leq 2\beta_T^{1/2} \sqrt{T \sum_{t=1}^T \sigma_{t-1}^2(\mathbf{x}_t, \mathbf{w}_t)} \end{aligned}$$

where the last inequality is due to the Cauchy-Schwarz inequality. Assuming $\kappa(\mathbf{x}, \mathbf{w}) \leq 1$ for all $\mathbf{x} \in \mathbb{X}$ and $\mathbf{w} \in \mathbb{W}$, Lemma 5.3 and Lemma 5.4 in [21] show that

$$2\beta_T^{1/2} \sqrt{T \sum_{t=1}^T \sigma_{t-1}^2(\mathbf{x}_t, \mathbf{w}_t)} \leq \sqrt{C_1 T \beta_T \gamma_T} \tag{21}$$

where $C_1 = 8/\log(1 + \sigma_n^{-2})$ and γ_T is the maximum information gain about f that can be obtained by observing any set of T observations. Therefore,

$$R_T \leq \sqrt{C_1 T \beta_T \gamma_T}$$

holds with probability $\geq 1 - \delta$.

C Decomposition of r_t^{Bayes}

By selecting \mathbf{x}_t as a sample from the posterior belief of \mathbf{x}_* given $\mathbf{y}_{\mathbf{D}_{t-1}}$, it is noted that the distribution of \mathbf{x}_t and \mathbf{x}_* are the same, i.e., $p(\mathbf{x}_t|\mathbf{y}_{\mathbf{D}_{t-1}}) = p(\mathbf{x}_*|\mathbf{y}_{\mathbf{D}_{t-1}})$. Furthermore, given $\mathbf{y}_{\mathbf{D}_{t-1}}$, u_{t-1} is a deterministic function, so $p(c_{u_{t-1}}(\mathbf{x}_*; \alpha)|\mathbf{y}_{\mathbf{D}_{t-1}}) = p(c_{u_{t-1}}(\mathbf{x}_t; \alpha)|\mathbf{y}_{\mathbf{D}_{t-1}})$ and

$$\mathbb{E}[c_{u_{t-1}}(\mathbf{x}_*; \alpha)] = \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha)] \quad (22)$$

Therefore, following [18], we can decompose r_t^{Bayes} as follows:

$$\begin{aligned} r_t^{\text{Bayes}} &\triangleq \mathbb{E}[c_f(\mathbf{x}_*; \alpha) - c_f(\mathbf{x}_t; \alpha)] \\ &= \mathbb{E}[c_f(\mathbf{x}_*; \alpha)] - \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha)] - \mathbb{E}[c_f(\mathbf{x}_t; \alpha)] \quad \text{from (22)} \\ &= \mathbb{E}[c_f(\mathbf{x}_*; \alpha)] - \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha)] - \mathbb{E}[c_{l_{t-1}}(\mathbf{x}_t; \alpha)] \\ &\quad + \mathbb{E}[c_{l_{t-1}}(\mathbf{x}_t; \alpha)] - \mathbb{E}[c_f(\mathbf{x}_t; \alpha)] \\ &= \mathbb{E}[c_{l_{t-1}}(\mathbf{x}_t; \alpha) - c_f(\mathbf{x}_t; \alpha)] + \mathbb{E}[c_f(\mathbf{x}_*; \alpha) - c_{u_{t-1}}(\mathbf{x}_*; \alpha)] \\ &\quad + \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha)] \end{aligned}$$

Since $\mathbb{E}[Z] \leq \mathbb{E}[\max(0, Z)]$ for a random variable Z , it follows that

$$\begin{aligned} r_t^{\text{Bayes}} &\leq \mathbb{E}[\max(0, c_{l_{t-1}}(\mathbf{x}_t; \alpha) - c_f(\mathbf{x}_t; \alpha))] + \mathbb{E}[\max(0, c_f(\mathbf{x}_*; \alpha) - c_{u_{t-1}}(\mathbf{x}_*; \alpha))] \\ &\quad + \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha)] \\ &= \mathbb{E}[\Delta_c^{\text{lower}}(\mathbf{x}_t; \alpha)] + \mathbb{E}[\Delta_c^{\text{upper}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[c_{u_{t-1}}(\mathbf{x}_t; \alpha) - c_{l_{t-1}}(\mathbf{x}_t; \alpha)] \end{aligned}$$

where $\Delta_c^{\text{lower}}(\mathbf{x}_t; \alpha) \triangleq \max(0, c_{l_{t-1}}(\mathbf{x}_t; \alpha) - c_f(\mathbf{x}_t; \alpha))$ and $\Delta_c^{\text{upper}}(\mathbf{x}_*; \alpha) \triangleq \max(0, c_f(\mathbf{x}_*; \alpha) - c_{u_{t-1}}(\mathbf{x}_*; \alpha))$.

D Proof of Lemma 2

$$\begin{aligned} \mathbb{E}[\Delta_c^{\text{lower}}(\mathbf{x}; \alpha)] &= \mathbb{E}[\max(0, c_{l_{t-1}}(\mathbf{x}; \alpha) - c_f(\mathbf{x}; \alpha))] \\ &= \mathbb{E}\left[\max\left(0, \frac{1}{\alpha} \int_0^\alpha (v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha')) \, d\alpha'\right)\right] \\ &\leq \mathbb{E}\left[\frac{1}{\alpha} \int_0^\alpha \max(0, v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha')) \, d\alpha'\right] \\ &= \frac{1}{\alpha} \int_0^\alpha \mathbb{E}[\max(0, v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha'))] \, d\alpha' \\ &= \frac{1}{\alpha} \int_0^\alpha \mathbb{E}[\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')] \, d\alpha' \end{aligned}$$

where $\Delta_v^{\text{lower}}(\mathbf{x}; \alpha') \triangleq \max(0, v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha'))$.

E Proof of Lemma 3

We prove the following Lemma 4 which is then used to prove Lemma 5. Lemma 3 follows from Lemma 5.

Lemma 4. Let $\mathbb{W}_{l_{t-1}}^{\text{upper}} \triangleq \{\mathbf{w} \in \mathbb{W} : l_{t-1}(\mathbf{x}, \mathbf{w}) \geq v_{l_{t-1}}(\mathbf{x}; \alpha')\}$, then $P(\mathbf{W} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}) > 1 - \alpha'$.

Proof. By contradiction, if $P(\mathbf{W} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}) \leq 1 - \alpha'$, then

$$P(\mathbf{W} \in \mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}) = 1 - P(\mathbf{W} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}) \geq \alpha'.$$

Furthermore, we assume that $|\mathbb{W}|$ is finite, so the above implies that

$$P\left(l_{t-1}(\mathbf{x}, \mathbf{W}) \leq \max_{\mathbf{w} \in \mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}} l_{t-1}(\mathbf{x}, \mathbf{w})\right) \geq \alpha'.$$

Therefore, from the definition of VaR,

$$\max_{\mathbf{w} \in \mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}} l_{t-1}(\mathbf{x}, \mathbf{w}) \geq v_{l_{t-1}}(\mathbf{x}; \alpha').$$

From the definition of $\mathbb{W}_{l_{t-1}}^{\text{upper}}$, the above implies that

$$\max_{\mathbf{w} \in \mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}} l_{t-1}(\mathbf{x}, \mathbf{w}) \in \mathbb{W}_{l_{t-1}}^{\text{upper}}.$$

However, $\max_{\mathbf{w} \in \mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}} l_{t-1}(\mathbf{x}, \mathbf{w}) \in \mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}.$

Thus, $\mathbb{W}_{l_{t-1}}^{\text{upper}} \cap (\mathbb{W} \setminus \mathbb{W}_{l_{t-1}}^{\text{upper}}) \neq \emptyset$

which is a contradiction. \square

Lemma 5. Consider a realization f_1 of the black-box function f following the GP posterior belief given $\mathbf{y}_{\mathbf{D}_{t-1}}$ that satisfies

$$v_{l_{t-1}}(\mathbf{x}; \alpha') - v_{f_1}(\mathbf{x}; \alpha') > \omega \quad (23)$$

for $\alpha' \in (0, 1)$, $\mathbf{x} \in \mathbb{X}$, and $\omega \geq 0$. Let $\mathbb{W}_{l_{t-1}}^{\text{upper}} \triangleq \{\mathbf{w} \in \mathbb{W} : l_{t-1}(\mathbf{x}, \mathbf{w}) \geq v_{l_{t-1}}(\mathbf{x}; \alpha')\}$. Then,

$$\exists \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, v_{l_{t-1}}(\mathbf{x}; \alpha') - f_1(\mathbf{x}, \mathbf{w}_0) > \omega.$$

Proof. By contradiction, if $\forall \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, v_{l_{t-1}}(\mathbf{x}; \alpha') - f_1(\mathbf{x}, \mathbf{w}_0) \leq \omega$, i.e., $\forall \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, f_1(\mathbf{x}, \mathbf{w}_0) + \omega \geq v_{l_{t-1}}(\mathbf{x}; \alpha')$. Furthermore, from (23), $v_{l_{t-1}}(\mathbf{x}; \alpha') > v_{f_1}(\mathbf{x}; \alpha') + \omega$. Therefore,

$$\forall \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, f_1(\mathbf{x}, \mathbf{w}_0) + \omega > v_{f_1}(\mathbf{x}; \alpha') + \omega.$$

Equivalently,

$$\forall \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, f_1(\mathbf{x}, \mathbf{w}_0) > v_{f_1}(\mathbf{x}; \alpha'). \quad (24)$$

By Lemma 4, we have

$$P\left(f_1(\mathbf{x}, \mathbf{W}) \geq \min_{\mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}} f_1(\mathbf{x}, \mathbf{w})\right) = P(\mathbf{W} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}) > 1 - \alpha'. \quad (25)$$

Therefore,

$$\begin{aligned} 1 &= P(\mathbf{W} \in \mathbb{W}) \\ &\geq P(f_1(\mathbf{x}, \mathbf{W}) \leq v_{f_1}(\mathbf{x}; \alpha')) + P\left(f_1(\mathbf{x}, \mathbf{W}) \geq \min_{\mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}} f_1(\mathbf{x}, \mathbf{w})\right) \text{ due to (24)} \\ &> \alpha' + 1 - \alpha' \text{ due to (25) and the definition of VaR} \\ &= 1 \end{aligned}$$

which is a contradiction. \square

Recall that $\mathbb{W}_{l_{t-1}}^{\text{upper}} \triangleq \{\mathbf{w} \in \mathbb{W} : l_{t-1}(\mathbf{x}, \mathbf{w}) \geq v_{l_{t-1}}(\mathbf{x}; \alpha')\}$. Therefore, $\forall \mathbf{w}_0 \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, l_{t-1}(\mathbf{x}; \alpha') - f_1(\mathbf{x}, \mathbf{w}_0) \geq v_{l_{t-1}}(\mathbf{x}; \alpha') - f_1(\mathbf{x}, \mathbf{w}_0)$. Thus, Lemma 5 implies Lemma 3.

F Proof of Theorem 2

Recall f is considered as a random variable, Lemma 3 implies that

$$\begin{aligned} P(v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha') > \omega) &\leq P(\exists \mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}, l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w}) > \omega) \\ &\leq \sum_{\mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}} P(l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w}) > \omega). \end{aligned} \quad (26)$$

From (16),

$$\begin{aligned}
\mathbb{E} [\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')] &= \int_0^\infty P(v_{l_{t-1}}(\mathbf{x}; \alpha') - v_f(\mathbf{x}; \alpha') > \omega) d\omega \\
&\leq \int_0^\infty \sum_{\mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}} P(l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w}) > \omega) d\omega \quad \text{from (26)} \\
&\leq \sum_{\mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}} \int_0^\infty P(l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w}) > \omega) d\omega \\
&= \sum_{\mathbf{w} \in \mathbb{W}_{l_{t-1}}^{\text{upper}}} \mathbb{E} [\max(0, l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w}))]. \tag{27}
\end{aligned}$$

Since $l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w})$ is a Gaussian random variable with mean $l_{t-1}(\mathbf{x}, \mathbf{w}) - \mu_{t-1}(\mathbf{x}, \mathbf{w}) = -\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{w})$ and variance $\sigma_{t-1}^2(\mathbf{x}, \mathbf{w})$, it follows that

$$\begin{aligned}
&\mathbb{E} [\max(0, l_{t-1}(\mathbf{x}, \mathbf{w}) - f(\mathbf{x}, \mathbf{w}))] \\
&= \int_0^\infty \frac{\omega}{\sigma_{t-1}(\mathbf{x}, \mathbf{w}) \sqrt{2\pi}} \exp\left(-\frac{(\omega + \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{w}))^2}{2\sigma_{t-1}^2(\mathbf{x}, \mathbf{w})}\right) d\omega \\
&\leq \frac{\sigma_{t-1}(\mathbf{x}, \mathbf{w})}{\sqrt{2\pi}} \exp\left(\frac{-\beta_t}{2}\right) \\
&= \frac{\sigma_{t-1}(\mathbf{x}, \mathbf{w})}{\sqrt{2\pi}} \frac{\delta}{|\mathbb{X}||\mathbb{W}|\pi_t} \quad \text{since } \beta_t = 2 \log(|\mathbb{X}||\mathbb{W}|\pi_t/\delta) \text{ in Lemma 1} \\
&\leq \frac{\delta}{|\mathbb{X}||\mathbb{W}|\sqrt{2\pi}} \pi_t^{-1} \tag{28}
\end{aligned}$$

where the last inequality is due to the assumption $\kappa(\mathbf{x}, \mathbf{w}) \leq 1 \forall (\mathbf{x}, \mathbf{w}) \in \mathbb{X} \times \mathbb{W}$.

From (27) and (28),

$$\mathbb{E} [\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')] \leq |\mathbb{W}_{l_{t-1}}^{\text{upper}}| \frac{\delta}{|\mathbb{X}||\mathbb{W}|\sqrt{2\pi}} \pi_t^{-1} \leq \frac{\delta}{|\mathbb{X}|\sqrt{2\pi}} \pi_t^{-1}. \tag{29}$$

Similar to the bound of $\Delta_v^{\text{lower}}(\mathbf{x}; \alpha')$, we can bound $\Delta_v^{\text{upper}}(\mathbf{x}; \alpha')$ by considering the set $\mathbb{W}_{u_{t-1}}^{\text{lower}} \triangleq \{\mathbf{w} \in \mathbb{W} : u_{t-1}(\mathbf{x}, \mathbf{w}) \leq v_{u_{t-1}}(\mathbf{x}; \alpha')\}$:

$$\mathbb{E} [\Delta_v^{\text{upper}}(\mathbf{x}; \alpha')] \leq |\mathbb{W}_{u_{t-1}}^{\text{lower}}| \frac{\delta}{|\mathbb{X}||\mathbb{W}|\sqrt{2\pi}} \pi_t^{-1} \leq \frac{\delta}{|\mathbb{X}|\sqrt{2\pi}} \pi_t^{-1}. \tag{30}$$

From (15), (29) and (30), we have

$$\mathbb{E} [\Delta_c^{\text{lower}}(\mathbf{x}; \alpha)] \leq \frac{\delta}{|\mathbb{X}|\sqrt{2\pi}} \pi_t^{-1} \tag{31}$$

$$\mathbb{E} [\Delta_c^{\text{upper}}(\mathbf{x}; \alpha)] \leq \frac{\delta}{|\mathbb{X}|\sqrt{2\pi}} \pi_t^{-1}. \tag{32}$$

From (13), (14), (31), and (32), r_t^{Bayes} can be bounded:

$$r_t^{\text{Bayes}} \leq \frac{\delta\sqrt{2}}{|\mathbb{X}|\sqrt{\pi}} \pi_t^{-1} + 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \tag{33}$$

Algorithm 2 CV-TS with batch queries for optimizing CVaR of a black-box function

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1: Input:  $k, \mathbb{X}, \mathbb{W}$ , initial observation  $\mathbf{y}_{\mathbf{D}_0}$ , prior  $\mu_0 = 0, \sigma_n, \kappa$ 
2: for  $t = 1, 2, \dots$  do
3:   Sample  $k$  functions  $(f_j)_{j=1}^k$  from the GP posterior belief given  $\mathbf{y}_{\mathbf{D}_{k(t-1)}}$ 
4:   for  $j = 1, 2, \dots, k$  do
5:     Select  $\mathbf{x}_{k(t-1)+j} \in \arg\max_{\mathbf{x}} c_{f_j}(\mathbf{x}; \alpha)$ 
6:     Find  $\alpha_{k(t-1)+j} \in \arg \max_{\alpha' \in (0, \alpha]} v_{u_{k(t-1)}}(\mathbf{x}_t; \alpha') - v_{l_{k(t-1)}}(\mathbf{x}_t; \alpha')$ 
7:     Given  $\alpha_{k(t-1)+j}$ , select  $\mathbf{w}_{k(t-1)+j}$  as an LV w.r.t.  $\mathbf{x}_{k(t-1)+j}$ ,  $u_{k(t-1)}$ , and  $l_{k(t-1)}$ .
8:   end for
9:   Incorporate new observations at the batch query:  $\mathbf{y}_{\mathbf{D}_{kt}} = \mathbf{y}_{\mathbf{D}_{k(t-1)}} \cup \{y(\mathbf{x}_i, \mathbf{w}_i)\}_{i=k(t-1)+1}^{kt}$ 
10:  Update the GP posterior belief given  $\mathbf{y}_{\mathbf{D}_{kt}}$  to obtain  $\mu_{kt}$  and  $\sigma_{kt}^2$ 
11: end for

```

Therefore, the Bayesian cumulative regret is bounded by:

$$\begin{aligned}
R_t^{\text{Bayes}} &= \mathbb{E} \left[\sum_{t=1}^T r_t^{\text{Bayes}} \right] \\
&\leq \mathbb{E} \left[\frac{\delta \sqrt{2}}{|\mathbb{X}| \sqrt{\pi}} \sum_{t=1}^T \pi_t^{-1} + \sum_{t=1}^T 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \right] \\
&\leq \frac{\delta \sqrt{2}}{|\mathbb{X}| \sqrt{\pi}} + \sqrt{C_1 T \beta_T \gamma_T}
\end{aligned} \tag{34}$$

where the last inequality is because $\sum_{t=1}^T \pi_t^{-1} \leq \sum_{t \geq 1} \pi_t^{-1} = 1$ (in Lemma 1) and $\sum_{t=1}^T 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \leq \sqrt{C_1 T \beta_T \gamma_T}$ shown in Appendix B.

G CV-TS with Batch Queries

Let us consider CV-TS with a batch query of size k at each iteration. To simplify the notation, let us assume that the set of initial observations is empty, i.e., $\mathbf{D}_0 = \emptyset$. Following the indexing of observed inputs from [11], inputs in the first batch query (at BO iteration $t = 1$) are indexed by $i = 1, \dots, k$, inputs in the second batch query (at BO iteration $t = 2$) are indexed by $i = k + 1, \dots, 2k$, and so on. We denote $\mathbf{D}_i \triangleq \{\mathbf{x}_j\}_{j=1}^i$. Then, the set of observed inputs at index i is $\mathbf{D}_{k \lfloor \frac{i-1}{k} \rfloor}$ where $\lfloor \frac{i-1}{k} \rfloor$ is the greatest integer less than or equal to $\frac{i-1}{k}$. At BO iteration t , CV-TS selects a batch query $\{\mathbf{x}_i\}_{i=k(t-1)+1}^{kt}$ by drawing k samples of the maximizer of $c_f(\mathbf{x}; \alpha)$ given observations at $\{\mathbf{x}_j\}_{j=1}^{k(t-1)}$ (i.e., $\mathbf{D}_{k(t-1)}$).

Since at index i we only have access to observations $\mathbf{y}_{\mathbf{D}_{k \lfloor \frac{i-1}{k} \rfloor}}$, the confidence bound of $f(\mathbf{x}, \mathbf{w})$ at index i is

$$\left[l_{k \lfloor \frac{i-1}{k} \rfloor}(\mathbf{x}, \mathbf{w}), u_{k \lfloor \frac{i-1}{k} \rfloor}(\mathbf{x}, \mathbf{w}) \right].$$

At index i , given $\mathbf{D}_{k \lfloor \frac{i-1}{k} \rfloor}$, the distribution of \mathbf{x}_i is the same that that of \mathbf{x}_* (due to the selection strategy of CV-TS), so $\mathbb{E} \left[c_{u_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_*; \alpha) \right] = \mathbb{E} \left[c_{u_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_i; \alpha) \right]$. Let us use T to denote the total number of observations. Then, T is a multiple of k because there are k observations at each BO iteration and we assume that $|\mathbf{D}_0| = \emptyset$. We can decompose the Bayesian cumulative regret of CV-TS

with a batch query of size k , denoted as $R_T^{\text{Bayes}}(k)$:

$$\begin{aligned}
R_T^{\text{Bayes}}(k) &= \mathbb{E} \left[\sum_{i=1}^T c_f(\mathbf{x}_*; \alpha) - c_f(\mathbf{x}_i; \alpha) \right] \\
&= \mathbb{E} \left[\sum_{i=1}^T \underbrace{\mathbb{E} \left[c_f(\mathbf{x}_*; \alpha) - c_{u_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_*; \alpha) | \mathbf{y}_{\mathbf{D}_{k \lfloor \frac{i-1}{k} \rfloor}} \right]}_{A_0} \right] \\
&\quad + \mathbb{E} \left[\underbrace{\sum_{i=1}^T c_{u_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_i; \alpha) - c_{l_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_i; \alpha)}_B \right] \\
&\quad + \mathbb{E} \left[\sum_{i=1}^T \underbrace{\mathbb{E} \left[c_{l_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_i; \alpha) - c_f(\mathbf{x}_i; \alpha) | \mathbf{y}_{\mathbf{D}_{k \lfloor \frac{i-1}{k} \rfloor}} \right]}_{A_1} \right].
\end{aligned}$$

Similar to (31) and (32), A_0 and A_1 can be bounded by the tail expectations of CVaR which are bounded by $\frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \pi_{k \lfloor \frac{i-1}{k} \rfloor}^{-1}$. Then,

$$\mathbb{E} \left[\sum_{i=1}^T A_0 \right] \leq \mathbb{E} \left[\sum_{i=1}^T \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \pi_{k \lfloor \frac{i-1}{k} \rfloor}^{-1} \right] = \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \sum_{i=1}^T \pi_{k \lfloor \frac{i-1}{k} \rfloor}^{-1} \leq \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \sum_{t \geq 1} \pi_t^{-1} = \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \quad (35)$$

$$\mathbb{E} \left[\sum_{i=1}^T A_1 \right] \leq \mathbb{E} \left[\sum_{i=1}^T \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \pi_{k \lfloor \frac{i-1}{k} \rfloor}^{-1} \right] = \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \sum_{i=1}^T \pi_{k \lfloor \frac{i-1}{k} \rfloor}^{-1} \leq \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}} \sum_{t \geq 1} \pi_t^{-1} \leq \frac{\delta}{|\mathbb{X}| \sqrt{2\pi}}. \quad (36)$$

The term B is bounded as follows.

$$\begin{aligned}
B &= \mathbb{E} \left[\sum_{i=1}^T c_{u_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_i; \alpha) - c_{l_{k \lfloor \frac{i-1}{k} \rfloor}}(\mathbf{x}_i; \alpha) \right] \\
&\leq \mathbb{E} \left[\sum_{i=1}^T 2\beta_{k \lfloor \frac{i-1}{k} \rfloor + 1}^{1/2} \sigma_{k \lfloor \frac{i-1}{k} \rfloor}(\mathbf{x}_i, \mathbf{w}_i) \right] \quad (37)
\end{aligned}$$

$$\begin{aligned}
&= \mathbb{E} \left[\sum_{i=1}^k 2\beta_{k \lfloor \frac{i-1}{k} \rfloor + 1}^{1/2} \sigma_{k \lfloor \frac{i-1}{k} \rfloor}(\mathbf{x}_i, \mathbf{w}_i) + \sum_{i=k+1}^T 2\beta_{k \lfloor \frac{i-1}{k} \rfloor + 1}^{1/2} \sigma_{k \lfloor \frac{i-1}{k} \rfloor}(\mathbf{x}_i, \mathbf{w}_i) \right] \\
&\leq \mathbb{E} \left[\sum_{i=1}^k 2\beta_1^{1/2} + \sum_{i=k+1}^T 2\beta_{k \lfloor \frac{T-1}{k} \rfloor + 1}^{1/2} \sigma_{i-k-1}(\mathbf{x}_i, \mathbf{w}_i) \right] \quad (38)
\end{aligned}$$

$$\begin{aligned}
&\leq 2k\beta_1^{1/2} + \mathbb{E} \left[2\beta_{k \lfloor \frac{T-1}{k} \rfloor + 1}^{1/2} \sum_{i=1}^{T-k} \sigma_{i-1}(\mathbf{x}_i, \mathbf{w}_i) \right] \\
&\leq 2k\beta_1^{1/2} + \mathbb{E} \left[2\beta_{k \lfloor \frac{T-1}{k} \rfloor + 1}^{1/2} \sqrt{(T-k) \sum_{i=1}^{T-k} \sigma_{i-1}^2(\mathbf{x}_i, \mathbf{w}_i)} \right] \quad (39)
\end{aligned}$$

$$\leq 2k\beta_1^{1/2} + \sqrt{\frac{8(T-k)\beta_{k \lfloor \frac{T-1}{k} \rfloor + 1} \gamma_{T-k}}{\log(1 + \sigma_n^{-2})}} \quad (40)$$

$$\leq 2k\beta_1^{1/2} + \sqrt{C_1(T-k)\beta_{T-k+1} \gamma_{T-k}} \quad (41)$$

where

- (37) is because of (19) and (20).
- (38) is because β_t is nondecreasing, $\kappa(\mathbf{x}, \mathbf{w}) \leq 1$ (our assumption), and $\sigma_{i-k-1} \geq \sigma_{k \lfloor \frac{i-1}{k} \rfloor}$ for $i = k+1, \dots, T$ (since $\mathbf{D}_{i-k-1} \subset \mathbf{D}_{k \lfloor \frac{i-1}{k} \rfloor}$).
- (39) is because of the Cauchy-Schwarz inequality.
- (40) is because of Lemma 5.3 and Lemma 5.4 in [21] and our assumption $\kappa(\mathbf{x}, \mathbf{w}) \leq 1$.

From (35), (36), and (41), the Bayesian cumulative regret is bounded by:

$$R_T^{\text{Bayes}}(k) \leq \frac{\delta\sqrt{2}}{|\mathbb{X}|\sqrt{\pi}} + 2k\beta_1^{1/2} + \sqrt{C_1(T-k)\beta_{T-k+1}\gamma_{T-k}}. \quad (42)$$

Recall the Bayesian cumulative regret bound for CV-TS with single queries (i.e., $k = 1$) in (34):

$$R_T^{\text{Bayes}} \leq \frac{\delta\sqrt{2}}{|\mathbb{X}|\sqrt{\pi}} + \sqrt{C_1 T \beta_T \gamma_T}. \quad (43)$$

Hence, the average of the Bayesian cumulative regret for CV-TS with single queries, R_T^{Bayes}/T , and batch queries, $R_T^{\text{Bayes}}(k)/T$, are similar, especially when the number of observations T is large (so that $2k\beta_1^{1/2}/T$ vanishes).

H A Thompson Sampling Approach to Optimize VaR of Black-Box Functions

H.1 Algorithm

We present an algorithm to optimize VaR $v_f(\mathbf{x}; \alpha)$ of a black-box function $f(\mathbf{x}, \mathbf{W})$. Unlike the existing V-UCB algorithm in [13] that is based on the upper confidence bound, this algorithm is based on the Thompson sampling approach which is called V-TS (Algorithm 3).

Following the popular Thompson sampling approach (or posterior sampling [18]), V-TS selects \mathbf{x}_t as a sample of the maximizer of VaR $v_f(\mathbf{x}; \alpha)$ by: (line 4 of Algorithm 3) using the random Fourier feature approximation method [16] to draw a function sample f_1 from the GP posterior belief given $\mathbf{y}_{\mathbf{D}_{t-1}}$ and (line 5 of Algorithm 3) assigning the maximizer of $v_{f_1}(\mathbf{x}; \alpha)$ to \mathbf{x}_t .

Given the selected \mathbf{x}_t , we select \mathbf{w}_t to reduce the uncertainty of VaR $v_f(\mathbf{x}_t; \alpha)$ quantified by the size of its confidence bound $v_{u_{t-1}}(\mathbf{x}_t; \alpha) - v_{l_{t-1}}(\mathbf{x}_t; \alpha)$. Following the same approach in Sec. 3.2, we select \mathbf{w}_t as an LV w.r.t. α , \mathbf{x}_t , l_{t-1} , and u_{t-1} (line 7 of Algorithm 3). If there are multiple LVs, we select the LV with the maximum probability $p(\mathbf{W})$. It is a heuristic to improve the empirical performance suggested by [13].

Like CV-TS with batch queries (Appendix G), V-TS can also be extended to handle a batch query of size k , i.e., V-TS selects a batch of k inputs to query for their observations at each BO iteration. This batch of k inputs are obtained by: drawing k samples of the maximizer of $v_f(\mathbf{x}; \alpha)$ given $\mathbf{y}_{\mathbf{D}_{t-1}}$ and finding the corresponding k LVs w.r.t. these k samples, α , l_{t-1} , and u_{t-1} .

H.2 Theoretical Analysis

Let us consider V-TS that selects a single query at each BO iteration (Algorithm 3). We would like to show that the Bayesian cumulative regret of V-TS is sublinear. Let $\mathbf{x}_* \in \arg\max_{\mathbf{x} \in \mathbb{X}} v_f(\mathbf{x}; \alpha)$. The Bayesian cumulative regret can be expressed as

$$\begin{aligned} R_T^{\text{Bayes}} &= \mathbb{E} \left[\sum_{t=1}^T v_f(\mathbf{x}_*; \alpha) - v_f(\mathbf{x}_t; \alpha) \right] \\ &= \mathbb{E} \left[\sum_{t=1}^T \mathbb{E} [v_f(\mathbf{x}_*; \alpha) - v_f(\mathbf{x}_t; \alpha) | \mathbf{y}_{\mathbf{D}_{t-1}}] \right]. \end{aligned}$$

Algorithm 3 V-TS: A BO Algorithm for optimizing VaR of a black-box function

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1: Input:  $\mathbb{X}, \mathbb{W}$ , initial observation  $\mathbf{y}_{\mathbf{D}_0}$ , prior  $\mu_0 = 0, \sigma_n, \kappa$ 
2: for  $t = 1, 2, \dots$  do
3:   {Selecting  $\mathbf{x}_t$ }
4:   Sample a function  $f_1$  from the GP posterior belief given  $\mathbf{y}_{\mathbf{D}_{t-1}}$ 
5:   Select  $\mathbf{x}_t \in \underset{\mathbf{x}}{\operatorname{argmax}} v_{f_1}(\mathbf{x}; \alpha)$ 
6:   {Selecting  $\mathbf{w}_t$ }
7:   Select  $\mathbf{w}_t$  as an LV w.r.t.  $\alpha, \mathbf{x}_t, u_{t-1}$ , and  $l_{t-1}$ 
8:   {Collecting data and updating GP}
9:   Incorporate new observation at input query:  $\mathbf{y}_{\mathbf{D}_t} = \mathbf{y}_{\mathbf{D}_{t-1}} \cup \{y(\mathbf{x}_t, \mathbf{w}_t)\}$ 
10:  Update the GP posterior belief given  $\mathbf{y}_{\mathbf{D}_t}$ 
11: end for

```

The expectation $\mathbb{E}[v_f(\mathbf{x}_*; \alpha) - v_f(\mathbf{x}_t; \alpha) | \mathbf{y}_{\mathbf{D}_{t-1}}]$ can be decomposed into (in a similar fashion to (13) where we omit $\mathbf{y}_{\mathbf{D}_{t-1}}$ to ease the notational clutter):

$$\begin{aligned}
& \mathbb{E}[v_f(\mathbf{x}_*; \alpha) - v_{u_{t-1}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[v_{u_{t-1}}(\mathbf{x}_*; \alpha) - v_{l_{t-1}}(\mathbf{x}_t; \alpha)] + \mathbb{E}[v_{l_{t-1}}(\mathbf{x}_t; \alpha) - v_f(\mathbf{x}_t; \alpha)] \\
&= \mathbb{E}[v_f(\mathbf{x}_*; \alpha) - v_{u_{t-1}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[v_{u_{t-1}}(\mathbf{x}_t; \alpha) - v_{l_{t-1}}(\mathbf{x}_t; \alpha)] \\
&\quad + \mathbb{E}[v_{l_{t-1}}(\mathbf{x}_t; \alpha) - v_f(\mathbf{x}_t; \alpha)] \\
&\leq \mathbb{E}[\max(0, v_f(\mathbf{x}_*; \alpha) - v_{u_{t-1}}(\mathbf{x}_*; \alpha))] + \mathbb{E}[v_{u_{t-1}}(\mathbf{x}_t; \alpha) - v_{l_{t-1}}(\mathbf{x}_t; \alpha)] \\
&\quad + \mathbb{E}[\max(0, v_{l_{t-1}}(\mathbf{x}_t; \alpha) - v_f(\mathbf{x}_t; \alpha))] \\
&= \mathbb{E}[\Delta_v^{\text{upper}}(\mathbf{x}_*; \alpha)] + \mathbb{E}[v_{u_{t-1}}(\mathbf{x}_t; \alpha) - v_{l_{t-1}}(\mathbf{x}_t; \alpha)] + \mathbb{E}[\Delta_v^{\text{lower}}(\mathbf{x}_t; \alpha)]
\end{aligned} \tag{44}$$

where (44) is because we select \mathbf{x}_t as a sample of the maximizer of $v_f(\mathbf{x}; \alpha)$ given $\mathbf{y}_{\mathbf{D}_{t-1}}$ (lines 4-5 of Algorithm 3), i.e., the distribution of \mathbf{x}_t is the same as that of \mathbf{x}_* given $\mathbf{y}_{\mathbf{D}_{t-1}}$.

The bounds of $\mathbb{E}[\Delta_v^{\text{lower}}(\mathbf{x}_*; \alpha)]$ and $\mathbb{E}[\Delta_v^{\text{upper}}(\mathbf{x}_t; \alpha)]$ are obtained from (29) and (30), while the bound of $\mathbb{E}[v_{u_{t-1}}(\mathbf{x}_t; \alpha) - v_{l_{t-1}}(\mathbf{x}_t; \alpha)]$ is obtained from (20) (since \mathbf{w}_t is selected as an LV w.r.t. $\alpha, \mathbf{x}_t, l_{t-1}$, and u_{t-1}). Therefore,

$$R_T^{\text{Bayes}} \leq \mathbb{E} \left[\sum_{t=1}^T \frac{\delta \sqrt{2}}{|\mathbb{X}| \sqrt{\pi}} \pi_t^{-1} + 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{w}_t) \right] \tag{45}$$

$$\leq \frac{\delta \sqrt{2}}{|\mathbb{X}| \sqrt{\pi}} + \sqrt{C_1 T \beta_T \gamma_T} \tag{46}$$

where $C_1, \beta_T, \delta, \gamma_T$ are elaborated in Theorem 2.

I Experimental Details

We use the Matérn 5/2 kernel,

$$\kappa(\mathbf{x}, \mathbf{w}; \mathbf{x}', \mathbf{w}') = \sigma_s^2 \left(1 + \sqrt{5}r + \frac{5r^2}{3} \right) \exp(-\sqrt{5}r) \tag{47}$$

where $r^2 \triangleq (\mathbf{x} - \mathbf{x}')^\top \mathbf{L}_x^{-2} (\mathbf{x} - \mathbf{x}') + (\mathbf{w} - \mathbf{w}')^\top \mathbf{L}_w^{-2} (\mathbf{w} - \mathbf{w}')$ is the squared scaled Euclidean distance between $[\mathbf{x}, \mathbf{w}]$ and $[\mathbf{x}', \mathbf{w}']$, $\mathbf{L}_x \triangleq \text{diag}[l_1, \dots, l_m]$ and $\mathbf{L}_w \triangleq \text{diag}[l_{m+1}, \dots, l_{m+n}]$ are the length-scales.

At BO iteration t , the GP hyperparameters (i.e., σ_s^2, \mathbf{L}_x , and \mathbf{L}_w) and the noise variance σ_n^2 are learned by maximizing the likelihood of the observations $\mathbf{y}_{\mathbf{D}_{t-1}}$. We impose a Gamma prior distribution of shape 1.1 and scale 0.5 over the noise variance and initialize the noise variance σ_n^2 at the mode of its prior distribution, i.e., 0.05 (which is adopted from the implementation of [4]).

The domains of all input dimensions in the experiments are standardized to the range $[0, 1]$. There are 3 initial observations for the experiments with the Branin-Hoo and Goldstein-Price functions, and 20 initial observations for the experiment with the Hartmann-6D function with $m = 5$ and 10 initial

observations for the experiment with the Hartmann-6D function with $m = 1$. The sizes $|\mathbb{W}|$ in the experiments with Branin-Hoo, Goldstein-Price, Hartmann-6D $m = 5$, and Hartmann-6D $m = 1$ are 30, 50, 15, and 243, respectively. We perform experiments with both uniform distributions of \mathbf{W} (in the experiments with Branin-Hoo and Goldstein-Price) and a non-uniform distribution of \mathbf{W} (in the experiment with Hartmann-6D). The non-uniform distribution is a discretized Gaussian distribution with mean 0.5 and standard deviation 0.2 over the support of \mathbf{W} .

In the yacht hydrodynamics experiment, we would like to minimize the residuary resistance per unit weight of displacement of a yacht by searching for the optimal hull geometry coefficients of the yacht in the face of the uncertainty in the Froude number (the Froude number depends on the real-world environment and we assume that it can be simulated with computers during the optimization). The ground truth function is constructed using the yacht hydrodynamics data set [5]. The dimension of the input variables \mathbf{x} and \mathbf{W} are $m = 5$ and $n = 1$ (the Froude number), respectively. The environmental random variable \mathbf{W} follows a discrete uniform random variable over the support of 15 values.

The simulated robot pushing experiment is taken from [23]. The simulation returns the location of a pushed object given the robot’s location and the pushing duration, i.e., \mathbf{x} . The locations are 2 dimensional and standardized in $[0, 1]^2$. We follow the setting in [13] to perturb the robot’s location with \mathbf{W} following a discrete uniform distribution over 64 points in $[0, 1]^2$. The location of the pushed object returned by the simulation is added with a Gaussian noise of variance 0.0001 to generate noisy observations. There are 30 initial observations, i.e., $|\mathbf{D}_0| = 30$.

The portfolio optimization problem is taken from [4]. The objective function is the average daily return over a period of 4 years (obtained by a simulation) given the risk and trade aversion parameters, and the holding cost multiplier. The environmental random variables \mathbf{W} include the bid-ask spread and the borrow cost. The distribution of \mathbf{W} is a discretized Gaussian distribution with mean 0.5 and standard deviation 0.15 over 25 points in $[0.25, 0.75]^2$. The average daily returns are added with a Gaussian noise of variance 0.0001 to generate noisy observations. There are 30 initial observations, i.e., $|\mathbf{D}_0| = 30$.