Value-at-Risk Optimization with Gaussian Processes

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Abstract

Value-at-risk (VAR) is an established measure to assess risks in critical real-world applications with random environmental factors. This paper presents a novel VAR upper confidence bound (V-UCB) algorithm for maximizing the VAR of a black-box objective function with the first noregret guarantee. To realize this, we first derive a confidence bound of VAR and then prove the existence of values of the environmental random variable (to be selected to achieve no regret) such that the confidence bound of VAR lies within that of the objective function evaluated at such values. Our V-UCB algorithm empirically demonstrates state-of-the-art performance in optimizing synthetic benchmark functions, a portfolio optimization problem, and a simulated robot task.

1. Introduction

Consider the problem of maximizing an expensive-tocompute black-box objective function f that depends on an optimization variable \mathbf{x} and an environmental random variable Z. Due to the randomness in Z, the function evaluation $f(\mathbf{x}, \mathbf{Z})$ of f at x is a random variable. Though for such an objective function f, Bayesian optimization (BO) can be naturally applied to maximize its expectation $\mathbb{E}_{\mathbf{Z}}[f(\mathbf{x}, \mathbf{Z})]$ over Z (Toscano-Palmerin & Frazier, 2018), this maximization objective overlooks the risks of potentially undesirable function evaluations. These risks can arise from either (a) the realization of an unknown distribution of \mathbf{Z} or (b) the realization of the random Z given that the distribution of $f(\mathbf{x}, \mathbf{Z})$ can be estimated well or that of \mathbf{Z} is known. The issue (a) has been tackled by distributionally robust BO (Kirschner et al., 2020; Nguyen et al., 2020) which maximizes $\mathbb{E}_{\mathbf{Z}}[f(\mathbf{x}, \mathbf{Z})]$ under the worst-case realization of the distribution of \mathbf{Z} . To resolve the issue (b), the risk from the

uncertainty in **Z** can be controlled via the mean-variance optimization framework (Iwazaki et al., 2020), *value-at-risk* (VAR), or *conditional value-at-risk* (CVAR) (Cakmak et al., 2020; Torossian et al., 2020). The work of Bogunovic et al. (2018) has considered *adversarially robust BO*, where **z** is controlled by an adversary deterministically.¹ In this case, the objective is to find **x** that maximizes the function under the worst-case realization of **z**, i.e., $\operatorname{argmax}_{\mathbf{x}} \min_{\mathbf{z}} f(\mathbf{x}, \mathbf{z})$.

In this paper, we focus on case (b) where the distribution of Z is known (or well-estimated). For example, in agriculture, although farmers cannot control the temperature of an outdoor farm, its distribution can be estimated from historical data and controlled in an indoor environment for optimizing the plant yield. Given the distribution of \mathbf{Z} , the objective is to control the risk that the function evaluation $f(\mathbf{x}, \mathbf{z})$, for a z sampled from Z, is small. One popular framework is to control the trade-off between the mean (viewed as reward) and the variance (viewed as risk) of the function evaluation with respect to Z (Iwazaki et al., 2020). However, quantifying the risk using variance implies indifference between positive and negative deviations from the mean, while people often have asymmetric risk attitudes (Goh et al., 2012). In our problem of maximizing the objective function, it is reasonable to assume that people are risk-averse towards only the negative deviations from the mean, i.e., the risk of getting lower function evaluations. Thus, it is more appropriate to adopt risk measures with this asymmetric property, such as value-at-risk (VAR) which is a widely adopted risk measure in real-world applications (e.g., banking (Basel Committee on Banking Supervision, 2006)). Intuitively, the risk that the random $f(\mathbf{x}, \mathbf{Z})$ is less than VAR at level $\alpha \in (0,1)$ does not exceed α , e.g., by specifying a small value of α as 0.1, this risk is controlled to be at most 10%. Therefore, to maximize the function f while controlling the risk of undesirable (i.e., small) function evaluations, we aim to maximize VAR of the random function $f(\mathbf{x}, \mathbf{Z})$ over \mathbf{x} .

The recent work of Cakmak et al. (2020) has used BO to maximize VAR and has achieved state-of-the-art empirical performances. They have assumed that we are able to select both x and z to query during BO, which is motivated by

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¹We use upper-case letter \mathbf{Z} to denote the environmental random variable and lower-case letter \mathbf{z} to denote its realization or a (non-random) variable.

fact that physical experiments can usually be studied by simulation (Williams et al., 2000). In the example on agriculture given above, we can control the temperature, light and water (\mathbf{z}) in a small indoor environment to optimize the amount of fertilizer (\mathbf{x}) , which can then be used in an outdoor environment with random weather factors. Cakmak et al. (2020) have exploited the ability to select z to model the function $f(\mathbf{x}, \mathbf{z})$ as a GP, which allows them to retain the appealing closed-form posterior belief of the objective function. To select the queries x and z, they have designed a one-step lookahead approach based on the well-known knowledge gradient (KG) acquisition function (Scott et al., 2011). However, the one-step lookahead incurs an expensive nested optimization procedure, which is computationally expensive and hence requires approximations. Besides, the acquisition function can only be approximated using samples of the objective function f from the GP posterior and the environmental random variable Z. While they have analysed the asymptotically unbiased and consistent estimator of the gradients, it is challenging to obtain a guarantee for the convergence of their algorithm. Another recent work (Torossian et al., 2020) has also applied BO to maximize VAR using an asymmetric Laplace likelihood function and variational approximation of the posterior belief. However, in contrast to Cakmak et al. (2020) and our work, they have focused on a different setting where the realizations of Z are not observed.

In this paper, we adopt the setting of Cakmak et al. (2020) which allows us to choose both x and z to query, and assume that the distribution of Z is known or well-estimated. Our contributions include:

Firstly, we propose a novel BO algorithm named Value-atrisk Upper Confidence Bound (V-UCB) in Section 3. Unlike the work of Cakmak et al. (2020), V-UCB is equipped with a no-regret convergence guarantee and is more computationally efficient. To guide its query selection and facilitate its proof of the no-regret guarantee, the classical GP-UCB algorithm (Srinivas et al., 2010) constructs a confidence bound of the objective function. Similarly, to maximize the VAR of a random function, we, for the first time to the best of our knowledge, construct a confidence bound of VAR (Lemma 2). The resulting confidence bound of VAR naturally gives rise to a strategy to select x. However, it remains a major challenge to select z to preserve the noregret convergence of GP-UCB. To this end, we firstly prove that our algorithm is no-regret as long as we ensure that at the selected z, the confidence bound of VAR *lies within* the confidence bound of the objective function. Next, we also prove that this query selection strategy is *feasible*, i.e., such values of z, referred to as lacing values (LV), exist.

Secondly, although our theoretical no-regret property allows the selection of *any* LV, we design a heuristic to select

an LV such that it improves our empirical performance over random selection of LV (Section 3.3). We also discuss the implications when z cannot be selected by BO and is instead randomly sampled by the environment during BO (Remark 1). Thirdly, we show that adversarially robust BO (Bogunovic et al., 2018) can be cast as a special case of our V-UCB when the risk level α of VAR approaches 0 from the right and the domain of z is the support of Z. In this case, adversarially robust BO (Bogunovic et al., 2018) selects the same input queries as those selected by V-UCB since the set of LV collapse into the set of minimizers of the lower bound of the objective function (Section 3.4). Lastly, we provide practical techniques for implementing V-UCB with continuous random variable \mathbf{Z} (Section 3.5): we (a) introduce local neural surrogate optimization with the pinball loss to optimize VAR, and (b) construct an objective function to search for an LV in the continuous support of Z.

The performance of our proposed algorithm is empirically demonstrated in optimizing several synthetic benchmark functions, a portfolio optimization problem, and a simulated robot task in Section 4.

2. Problem Statement and Background

Let the objective function be defined as $f : \mathcal{D}_{\mathbf{x}} \times \mathcal{D}_{\mathbf{z}} \to \mathbb{R}$ where $\mathcal{D}_{\mathbf{x}} \subset \mathbb{R}^{d_x}$ and $\mathcal{D}_{\mathbf{z}} \subset \mathbb{R}^{d_z}$ are the bounded domain of the optimization variable \mathbf{x} and the support of the environmental random variable \mathbf{Z} , respectively; d_x and d_z are the dimensions of \mathbf{x} and \mathbf{z} , respectively. The support of \mathbf{Z} is defined as the smallest closed subset $\mathcal{D}_{\mathbf{z}}$ of \mathbb{R}^{d_z} such that $P(\mathbf{Z} \in \mathcal{D}_{\mathbf{z}}) = 1$. Let $\mathbf{z} \in \mathcal{D}_{\mathbf{z}}$ denote a realization of the random variable \mathbf{Z} . Let $f(\mathbf{x}, \mathbf{Z})$ denote a random variable whose randomness comes from \mathbf{Z} . The VAR of $f(\mathbf{x}, \mathbf{Z})$ at *risk level* $\alpha \in (0, 1)$ is defined as:

$$V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \triangleq \inf\{\omega : P(f(\mathbf{x}, \mathbf{Z}) \le \omega) \ge \alpha\} \quad (1)$$

which implies the risk that $f(\mathbf{x}, \mathbf{Z})$ is less than its VAR at level α does not exceed α .

Our objective is to search for $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$ that maximizes $V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$ at a user-specified risk level $\alpha \in (0, 1)$. Intuitively, the goal is find \mathbf{x} where the evaluations of the objective function are as large as possible under most realizations of the environmental random variable \mathbf{Z} which is characterized by the probability of $1 - \alpha$.

The unknown objective function $f(\mathbf{x}, \mathbf{z})$ is modeled with a GP. That is, every finite subset of $\{f(\mathbf{x}, \mathbf{z})\}_{(\mathbf{x}, \mathbf{z}) \in \mathcal{D}_{\mathbf{x}} \times \mathcal{D}_{\mathbf{z}}}$ follows a multivariate Gaussian distribution (Rasmussen & Williams, 2006). The GP is fully specified by its *prior* mean and covariance function $k_{(\mathbf{x}, \mathbf{z}), (\mathbf{x}', \mathbf{z}')} \triangleq$ $\operatorname{cov}[f(\mathbf{x}, \mathbf{z}), f(\mathbf{x}', \mathbf{z}')]$ for all \mathbf{x}, \mathbf{x}' in $\mathcal{D}_{\mathbf{x}}$ and \mathbf{z}, \mathbf{z}' in $\mathcal{D}_{\mathbf{z}}$. For notational simplicity (and w.l.o.g.), the former is assumed to be zero, while we use the *squared exponential* (SE) kernel as its bounded maximum information gain can be used for later analysis (Srinivas et al., 2010).

To identify the optimal $\mathbf{x}_* \triangleq \operatorname{argmax}_{\mathbf{x}\in\mathcal{D}_{\mathbf{x}}} V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$, BO algorithm selects an input query $(\mathbf{x}_t, \mathbf{z}_t)$ in the *t*-th iteration to obtain a noisy function evaluation $y_{(\mathbf{x}_t, \mathbf{z}_t)} \triangleq f(\mathbf{x}_t, \mathbf{z}_t) + \epsilon_t$ where $\epsilon_t \sim \mathcal{N}(0, \sigma_n^2)$ are i.i.d. Gaussian noise with variance σ_n^2 . Given noisy observations $\mathbf{y}_{\mathcal{D}_t} \triangleq (y_{(\mathbf{x}, \mathbf{z})})_{(\mathbf{x}, \mathbf{z})\in\mathcal{D}_t}^{\top}$ at observed inputs $\mathcal{D}_t \triangleq \mathcal{D}_{t-1} \cup \{(\mathbf{x}_t, \mathbf{z}_t)\}$ (and \mathcal{D}_0 is the initial observed inputs), the GP posterior belief of function evaluation at any input (\mathbf{x}, \mathbf{z}) is a Gaussian $p(f(\mathbf{x}, \mathbf{z})|\mathbf{y}_{\mathcal{D}_t}) \triangleq \mathcal{N}(f(\mathbf{x}, \mathbf{z})|\mu_t(\mathbf{x}, \mathbf{z}), \sigma_t^2(\mathbf{x}, \mathbf{z}))$:

$$\mu_t(\mathbf{x}, \mathbf{z}) \stackrel{\Delta}{=} \mathbf{K}_{(\mathbf{x}, \mathbf{z}), \mathcal{D}_t} \mathbf{\Lambda}_{\mathcal{D}_t \mathcal{D}_t} \mathbf{y}_{\mathcal{D}_t} , \\ \sigma_t^2(\mathbf{x}, \mathbf{z}) \stackrel{\Delta}{=} k_{(\mathbf{x}, \mathbf{z}), (\mathbf{x}, \mathbf{z})} - \mathbf{K}_{(\mathbf{x}, \mathbf{z}), \mathcal{D}_t} \mathbf{\Lambda}_{\mathcal{D}_t \mathcal{D}_t} \mathbf{K}_{\mathcal{D}_t, (\mathbf{x}, \mathbf{z})}$$

where $\mathbf{\Lambda}_{\mathcal{D}_t \mathcal{D}_t} \triangleq (\mathbf{K}_{\mathcal{D}_t \mathcal{D}_t} + \sigma_n^2 \mathbf{I})^{-1}, \ \mathbf{K}_{(\mathbf{x}, \mathbf{z}), \mathcal{D}_t} \triangleq (k_{(\mathbf{x}, \mathbf{z}), (\mathbf{x}', \mathbf{z}')})_{(\mathbf{x}', \mathbf{z}') \in \mathcal{D}_t}, \mathbf{K}_{\mathcal{D}_t, (\mathbf{x}, \mathbf{z})} \triangleq \mathbf{K}_{(\mathbf{x}, \mathbf{z}), \mathcal{D}_t}^{\top}, \mathbf{K}_{\mathcal{D}_t \mathcal{D}_t} \triangleq (k_{(\mathbf{x}', \mathbf{z}'), (\mathbf{x}'', \mathbf{z}')})_{(\mathbf{x}', \mathbf{z}'), (\mathbf{x}'', \mathbf{z}'') \in \mathcal{D}_t}, \mathbf{I}$ is the identity matrix.

3. BO of VAR

Following the seminal work (Srinivas et al., 2010), we use the *cumulative regret* as the performance metric to quantify the performance of our BO algorithm. It is defined as $R_T \triangleq \sum_{t=1}^{T} r(\mathbf{x}_t)$ where $r(\mathbf{x}_t) \triangleq$ $V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) - V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))$ is the *instantaneous regret* and $\mathbf{x}_* \triangleq \operatorname{argmax}_{\mathbf{x} \in \mathcal{D}_{\mathbf{x}}} V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$. We would like to design a query selection strategy that incurs *no regret*, i.e., $\lim_{T\to\infty} R_T/T = 0$. Furthermore, we have that $\min_{t\leq T} r(\mathbf{x}_t) \leq R_T/T$, equivalently, $\max_{t\leq T} V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z})) \geq V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) - R_T/T$. Thus, $\lim_{T\to\infty} \max_{t\leq T} V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z})) = V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z}))$ for a noregret algorithm.

The proof of the upper bound on the cumulative regret of GP-UCB is based on confidence bounds of the objective function (Srinivas et al., 2010). Similarly, in the next section, we start by constructing a confidence bound of $V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$, which naturally leads to a query selection strategy for \mathbf{x}_t .

3.1. A Confidence Bound of $V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$ and the Query Selection Strategy for \mathbf{x}_t

Firstly, we adopt a confidence bound of the function $f(\mathbf{x}, \mathbf{z})$ from Chowdhury & Gopalan (2017), which assumes that f belongs to a *reproducing kernel Hilbert space* $\mathcal{F}_k(B)$ such that its RKHS norm is bounded $||f||_k \leq B$.

Lemma 1 (Chowdhury & Gopalan (2017)). Pick $\delta \in (0, 1)$ and set $\beta_t = (B + \sigma_n \sqrt{2(\gamma_{t-1} + 1 + \log 1/\delta)})^2$. Then, $f(\mathbf{x}, \mathbf{z}) \in I_{t-1}[f(\mathbf{x}, \mathbf{z})] \triangleq [l_{t-1}(\mathbf{x}, \mathbf{z}), u_{t-1}(\mathbf{x}, \mathbf{z})] \forall \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \geq 1$ holds with probability $\geq 1 - \delta$ where

$$l_{t-1}(\mathbf{x}, \mathbf{z}) \triangleq \mu_{t-1}(\mathbf{x}, \mathbf{z}) - \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{z})$$

$$u_{t-1}(\mathbf{x}, \mathbf{z}) \triangleq \mu_{t-1}(\mathbf{x}, \mathbf{z}) + \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}, \mathbf{z}) .$$
(3)

As the above lemma holds for both finite and continuous \mathcal{D}_x and \mathcal{D}_z , it is used to analyse the regret in both cases. On the other hand, the confidence bound can be adopted to the Bayesian setting by changing only β_t following the work of Srinivas et al. (2010) as noted by (Bogunovic et al., 2018).

Then, we exploit this confidence bound on the function evaluations (Lemma 1) to formulate a confidence bound of $V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$ as follows.

Lemma 2. Similar to the definition of $f(\mathbf{x}, \mathbf{Z})$, let $l_{t-1}(\mathbf{x}, \mathbf{Z})$ and $u_{t-1}(\mathbf{x}, \mathbf{Z})$ denote the random function over \mathbf{x} where the randomness comes from the random variable \mathbf{Z} ; l_{t-1} and u_{t-1} are defined in (3). Then, $\forall \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, t \geq 1$,

$$V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \in I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \\ \triangleq [V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})), V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))]$$

holds with probability $\geq 1 - \delta$ for δ in Lemma 1, where $V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z}))$ and $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ are defined as (1).

The proof is in Appendix A. Given the confidence bound $I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \triangleq [V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})), V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ in Lemma 2, we follow the the well-known "optimism in the face of uncertainty" principle to select $\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x} \in \mathcal{D}_{\mathbf{x}}} V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$. This query selection strategy for \mathbf{x}_t leads to an upper bound of $r(\mathbf{x}_t)$:

$$r(\mathbf{x}_t) \le V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \ \forall t \ge 1$$
(4)

which holds with probability $\geq 1 - \delta$ for δ in Lemma 1, and is proved in Appendix B.

As our goal is $\lim_{T\to\infty} R_T/T = 0$, given the selected query \mathbf{x}_t , a reasonable query selection strategy of \mathbf{z}_t should gather informative observations at $(\mathbf{x}_t, \mathbf{z}_t)$ that improves the confidence bound $I_{t-1}[V_\alpha(f(\mathbf{x}_t, \mathbf{Z}))]$ (i.e., $I_t[V_\alpha(f(\mathbf{x}_t, \mathbf{Z}))]$ is a proper subset of $I_{t-1}[V_\alpha(f(\mathbf{x}_t, \mathbf{Z}))]$ if $I_{t-1}[V_\alpha(f(\mathbf{x}_t, \mathbf{Z}))] \neq \emptyset$) which can be viewed as the uncertainty of $V_\alpha(f(\mathbf{x}_t, \mathbf{Z}))$.

Assume that there exists $\mathbf{z}_l \in \mathcal{D}_{\mathbf{z}}$ such that $l_{t-1}(\mathbf{x}_t, \mathbf{z}_l) =$ $V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z}))$ and $\mathbf{z}_u \in \mathcal{D}_{\mathbf{z}}$ such that $u_{t-1}(\mathbf{x}_t, \mathbf{z}_u) =$ $V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z}))$. Lemma 2 implies that $V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z})) \in$ $I_{t-1}[V_{\alpha}(f(\mathbf{x}_{t}, \mathbf{Z}))] = [l_{t-1}(\mathbf{x}_{t}, \mathbf{z}_{l}), u_{t-1}(\mathbf{x}_{t}, \mathbf{z}_{u})]$ with high probability. Hence, we may naïvely want to query for observations at $(\mathbf{x}_t, \mathbf{z}_l)$ and $(\mathbf{x}_t, \mathbf{z}_u)$ to reduce $I_{t-1}[V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))]$. However, these observations may not always reduce $I_{t-1}[V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))]$. The insight is that $I_{t-1}[V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))]$ changes (i.e., shrinks) when either of its boundary values (i.e., $l_{t-1}(\mathbf{x}_t, \mathbf{z}_l)$ or $u_{t-1}(\mathbf{x}_t, \mathbf{z}_u)$) changes. Consider $u_{t-1}(\mathbf{x}_t, \mathbf{z}_u)$ and finite $\mathcal{D}_{\mathbf{z}}$ as an example, since $u_{t-1}(\mathbf{x}_t, \mathbf{z}_u) = V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z})),$ a natural cause for the change in $u_{t-1}(\mathbf{x}_t, \mathbf{z}_u)$ is when \mathbf{z}_u changes. This happens if there exists $\mathbf{z}' \neq \mathbf{z}_u$ such that the *ordering* of $u_{t-1}(\mathbf{x}_t, \mathbf{z}')$ relative to $u_{t-1}(\mathbf{x}_t, \mathbf{z}_u)$ changes given more observations. Thus, observations that are capable of reducing $I_{t-1}[V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))]$ should be able to *change the*

relative ordering in this case. We construct the following counterexample where observations at \mathbf{z}_u (and \mathbf{z}_l) are not able to change the relative ordering, so they do not reduce $I_{t-1}[V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))]$.

Example 1. This example is described by Fig. 1. We reduce notational clutter by removing \mathbf{x}_t and t since they are fixed in this example, i.e., we use $f(\mathbf{z})$, $f(\mathbf{Z})$, and $l(\mathbf{z})$ to denote $f(\mathbf{x}_t, \mathbf{z})$, $f(\mathbf{x}_t, \mathbf{Z})$, and $l_{t-1}(\mathbf{x}_t, \mathbf{z})$ respectively. We condition on the event $f(\mathbf{z}) \in I[f(\mathbf{z})] \triangleq [l(\mathbf{z}), u(\mathbf{z})]$ for all $\mathbf{z} \in \mathcal{D}_{\mathbf{z}}$ which occurs with probability $\geq 1 - \delta$ in Lemma 1. In this example, $\mathbf{z}_l = \mathbf{z}_1$ and $l(\mathbf{z}_1) = u(\mathbf{z}_1)$, so there is no uncertainty in $f(\mathbf{z}_l) = f(\mathbf{z}_1)$. Similarly, there is no uncertainty in $f(\mathbf{z}_u) = f(\mathbf{z}_2)$. Thus, new observations at \mathbf{z}_l and \mathbf{z}_u change neither $l(\mathbf{z}_l)$ nor $u(\mathbf{z}_u)$, so these observations do not reduce the confidence bound $I[V_{\alpha=0.4}(f(\mathbf{Z}))] = [l(\mathbf{z}_l), u(\mathbf{z}_u)]$ (plotted as the doubleheaded arrow in Fig. 1b). In fact, to reduce $I[V_{\alpha=0.4}(f(\mathbf{Z}))]$, we should gather new observations at z_0 which potentially change the ordering of $u(\mathbf{z}_0)$ relative to $u(\mathbf{z}_2)$ (which is $u(\mathbf{z}_n)$ without new observations). For example, after getting new observations at z_0 , if $u(z_0)$ is improved to be in the white region between A and B $(u(\mathbf{z}_0) > u(\mathbf{z}_2))$ in Fig. 1b changes to $u(\mathbf{z}_0) < u(\mathbf{z}_2)$ in Fig. 1c), then $I[V_{\alpha=0,4}(f(\mathbf{Z}))]$ is reduced to $[l(\mathbf{z}_1), u(\mathbf{z}_0)]$ because now $\mathbf{z}_u = \mathbf{z}_0$. Thus, as the confidence bound $I[f(\mathbf{z}_0)]$ is shortened with more and more observations at z_0 , the confidence bound $I[V_{\alpha=0.4}(f(\mathbf{Z}))]$ reduces (the white region in Fig. 1 is 'laced up').

In the next section, we define a property of z_0 in Example 1 and prove the existence of z's with this property. Then, we prove that along with the optimistic selection of x_t , the selection of z_t such that it satisfies this property leads to a no-regret algorithm.

3.2. Lacing Value (LV) and the Query Selection Strategy for z_t

We note that in Example 1, as long as the confidence bound of the function evaluation at z_0 contains the confidence bound of VAR, observations at z_0 can reduce the confidence bound of VAR. We name the values of z satisfying this property as *lacing values* (LV):

Definition 1 (Lacing values). Lacing values (LV) with respect to $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$ and $t \geq 1$ are $\mathbf{z}_{\text{LV}} \in \mathcal{D}_{\mathbf{z}}$ that satisfies $l_{t-1}(\mathbf{x}, \mathbf{z}_{\text{LV}}) \leq V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z})) \leq u_{t-1}(\mathbf{x}, \mathbf{z}_{\text{LV}})$, equivalently, $I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \subset [l_{t-1}(\mathbf{x}, \mathbf{z}_{\text{LV}}), u_{t-1}(\mathbf{x}, \mathbf{z}_{\text{LV}})]$.

Recall that the support $\mathcal{D}_{\mathbf{z}}$ of \mathbf{Z} is defined as the smallest closed subset $\mathcal{D}_{\mathbf{z}}$ of \mathbb{R}^{d_z} such that $P(\mathbf{Z} \in \mathcal{D}_{\mathbf{z}}) = 1$ (e.g., $\mathcal{D}_{\mathbf{z}}$ is a finite subset of \mathbb{R}^{d_z} and $\mathcal{D}_{\mathbf{z}} = \mathbb{R}^{d_z}$). The following theorem guarantees the existence of lacing values and is proved in Appendix C.

Algorithm 1 The V-UCB Algorithm

1: Input: $\mathcal{D}_{\mathbf{x}}, \mathcal{D}_{\mathbf{z}}$, prior $\mu_0 = 0, \sigma_0, k$

2: for i = 1, 2, ... do

- 3: Select $\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x} \in \mathcal{D}_{\mathbf{x}}} V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$
- 4: Select \mathbf{z}_t as a *lacing value* w.r.t. \mathbf{x}_t (Definition 1)
- 5: Obtain observation $y_t \triangleq f(\mathbf{x}_t, \mathbf{z}_t) + \epsilon_t$
- 6: Update the GP posterior belief to obtain μ_t and σ_t
- 7: end for

Theorem 1 (Existence of lacing values). $\forall \alpha \in (0, 1), \forall \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \forall t \geq 1$, there exists a lacing value in $\mathcal{D}_{\mathbf{z}}$ with respect to \mathbf{x} and t.

Corollary 1.1. Lacing values with respect to $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$ and $t \geq 1$ are in $\mathcal{Z}_{l}^{\leq} \cap \mathcal{Z}_{u}^{\geq}$ where $\mathcal{Z}_{l}^{\leq} \triangleq \{\mathbf{z} \in \mathcal{D}_{\mathbf{z}} : l_{t-1}(\mathbf{x}, \mathbf{z}) \leq V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z}))\}$ and $\mathcal{Z}_{u}^{\geq} \triangleq \{\mathbf{z} \in \mathcal{D}_{\mathbf{z}} : u_{t-1}(\mathbf{x}, \mathbf{z}) \geq V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))\}.$

As a special case, when $\mathbf{z}_l = \mathbf{z}_u$, $I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] = I_{t-1}[f(\mathbf{x}, \mathbf{z}_l)]$ which means $\mathbf{z}_l = \mathbf{z}_u$ is an LV. Based on Theorem 1, we can always select \mathbf{z}_t as an LV w.r.t \mathbf{x}_t defined in Definition 1. This strategy for the selection of \mathbf{z}_t , together with the selection of $\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x} \in \mathcal{D}_{\mathbf{x}}} V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ (Section 3.1), completes our algorithm: VAR Upper Confidence Bound (V-UCB) (Algorithm 1).

Upper Bound on Regret. As a result of the selection strategies for \mathbf{x}_t and \mathbf{z}_t , our V-UCB algorithm enjoys the following upper bound on its instantaneous regret (proven in Appendix D):

Lemma 3. By selecting \mathbf{x}_t as a maximizer of $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ and selecting \mathbf{z}_t as an LV w.r.t \mathbf{x}_t , the instantaneous regret is upper-bounded by:

$$r(\mathbf{x}_t) \le 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \ \forall t \ge 1$$

with probability $\geq 1 - \delta$ for δ in Lemma 1.

Lemma 3, together with Lemma 5.4 from Srinivas et al. (2010), implies that the cumulative regret of our algorithm is bounded (Appendix E): $R_T \leq \sqrt{C_1 T \beta_T \gamma_T}$ where $C_1 \triangleq 8/\log(1 + \sigma_n^{-2})$, and γ_T is the maximum information gain about f that can be obtained from any set of T observations. Srinivas et al. (2010) have analyzed γ_T for several commonly used kernels such as SE and Matérn kernels, and have shown that for these kernels, the upper bound on R_T grows sub-linearly. This implies that our algorithm is *no-regret* because $\lim_{T\to\infty} R_T/T = 0$.

Inspired by Bogunovic et al. (2018), at the *T*-th iteration of V-UCB, we can recommend $\mathbf{x}_{t_*(T)}$ as an estimate of the maximizer \mathbf{x}_* of $V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$, where $t_*(T) \triangleq \operatorname{argmax}_{t \in \{1, \dots, T\}} V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z}))$. Then, the instantaneous regret $r(\mathbf{x}_{t_*(T)})$ is upper-bounded by $\sqrt{C_1\beta_T\gamma_T/T}$ with high probability as we show in Appendix F. In our experiments in Section 4, we recommend



Figure 1. A counterexample against selecting \mathbf{z}_u and \mathbf{z}_l as input queries. Here \mathbf{z} follows a discrete uniform distribution over $\mathcal{D}_{\mathbf{z}} \triangleq \{\mathbf{z}_0, \mathbf{z}_1, \mathbf{z}_2\}$. (a) shows the mappings of \mathbf{z} to the upper bound $u(\mathbf{z})$ and lower bound $l(\mathbf{z})$. The VAR at $\alpha = 0.4$ of $u(\mathbf{Z})$ and $l(\mathbf{Z})$ are $u(\mathbf{z}_2)$ and $l(\mathbf{z}_1)$, respectively, i.e., $\mathbf{z}_u = \mathbf{z}_2$ and $\mathbf{z}_l = \mathbf{z}_1$. (b) shows the values of $l(\mathbf{z})$ and $u(\mathbf{z})$ for all \mathbf{z} on the same axis, as well as the confidence bounds of $f(\mathbf{z})$ and $V_{\alpha}(f(\mathbf{Z}))$. The gray areas A and B indicate the intervals of values $\omega \in \mathbb{R}$ where $\omega \leq l(\mathbf{z}_l) = l(\mathbf{z}_1)$ and $\omega \geq u(\mathbf{z}_u) = u(\mathbf{z}_2)$, respectively. (c) shows a hypothetical scenario when $I[f(\mathbf{z}_0)]$ is shortened with more observations at \mathbf{z}_0 .

 $\operatorname{argmax}_{\mathbf{x}\in\mathcal{D}_T} V_{\alpha}(\mu_{t-1}(\mathbf{x}, \mathbf{Z}))$ (where $\mu_{t-1}(\mathbf{x}, \mathbf{Z})$ is a random function defined in the same manner as $f(\mathbf{x}, \mathbf{Z})$) as an estimate of \mathbf{x}_* due to its empirical convergence.

Computational Complexity. To compare our computational complexity with that of the ρ KG algorithm from Cakmak et al. (2020), we exclude the common part of training the GP model (line 6) and assume that $\mathcal{D}_{\mathbf{z}}$ is finite. Then, the time complexity of V-UCB is dominated by that of the selection of \mathbf{x}_t (line 3) which includes the time complexity $\mathcal{O}(|\mathcal{D}_{\mathbf{z}}||\mathcal{D}_{t-1}|^2)$ for the GP prediction at $\{\mathbf{x}\} \times \mathcal{D}_{\mathbf{z}}$, and $\mathcal{O}(|\mathcal{D}_{\mathbf{z}}| \log |\mathcal{D}_{\mathbf{z}}|)$ for the sorting of $u_{t-1}(\mathbf{x}, \mathcal{D}_{\mathbf{z}})$ and searching of VAR. Hence, our overall complexity is $\mathcal{O}(n|\mathcal{D}_{\mathbf{z}}| (|\mathcal{D}_{t-1}|^2 + \log |\mathcal{D}_{\mathbf{z}}|))$, where *n* is the number of iterations to maximize $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ (line 3). Therefore, our V-UCB is more computationally efficient than ρ KG and its variant with approximation ρ KG^{*apx*}, whose complexities are $\mathcal{O}(n_{\text{out}}n_{\text{in}}K|\mathcal{D}_{\mathbf{z}}| (|\mathcal{D}_{t-1}|^2 + |\mathcal{D}_{\mathbf{z}}||\mathcal{D}_{t-1}| + |\mathcal{D}_{\mathbf{z}}|^2 + M|\mathcal{D}_{\mathbf{z}}|))$ of ρ KG and $\mathcal{O}(n_{\text{out}}|\mathcal{D}_{t-1}|K|\mathcal{D}_{\mathbf{z}}| (|\mathcal{D}_{t-1}|^2 + |\mathcal{D}_{\mathbf{z}}||\mathcal{D}_{t-1}| + |\mathcal{D}_{\mathbf{z}}|^2 + |\mathcal{D}_{\mathbf{z}}||\mathcal{D}_{t-1}| + |\mathcal{D}_{\mathbf{z}}|^2 + M|\mathcal{D}_{\mathbf{z}}|))$, respectively.²

3.3. On the Selection of z_t

Although Algorithm 1 is guaranteed to be no-regret with any choice of LV as \mathbf{z}_t , we would like to select the LV that can reduce a large amount of the uncertainty of $V_{\alpha}(f(\mathbf{x}_t, \mathbf{Z}))$. However, relying on the information gain measure or the knowledge gradient method often incurs the expensive one-step lookahead. Therefore, we use a simple heuristic by choosing the LV \mathbf{z}_{LV} with the maximum probability mass (or probability density if \mathbf{Z} is continuous) of \mathbf{z}_{LV} . We motivate this heuristic using an example with $\alpha = 0.2$, i.e., $V_{\alpha=0.2}(f(\mathbf{x}_t, \mathbf{Z})) = \inf \{ \omega : P(f(\mathbf{x}_t, \mathbf{Z}) \leq \omega) \geq 0.2 \}$.

Suppose $\mathcal{D}_{\mathbf{z}}$ is finite and there are 2 LV's \mathbf{z}_0 and \mathbf{z}_1 with $P(\mathbf{z}_0) \geq 0.2$ and $P(\mathbf{z}_1) = 0.01$. Then, because $P(f(\mathbf{x}_t, \mathbf{Z}) \leq f(\mathbf{x}_t, \mathbf{z}_0)) \geq P(\mathbf{z}_0) \geq 0.2$, it follows that $V_{\alpha=0.2}(f(\mathbf{x}_t, \mathbf{Z})) \leq f(\mathbf{x}_t, \mathbf{z}_0)$, i.e., querying \mathbf{z}_0 at \mathbf{x}_t gives us information about an explicit upper bound on $V_{\alpha=0.2}(f(\mathbf{x}_t, \mathbf{Z}))$ to reduce its uncertainty. In contrast, this cannot be achieved by querying \mathbf{z}_1 due to its low probability mass. This simple heuristic can also be implemented when \mathbf{Z} is a continuous random variable which we will introduce in Section 3.5.

Remark 1. Although we assume that we can select both \mathbf{x}_t and \mathbf{z}_t during our algorithm, Corollary 1.1 also gives us some insights about the scenario where we cannot select \mathbf{z}_t . In this case, in each iteration t, we select \mathbf{x}_t while \mathbf{z}_t is randomly sampled by the environment following the distribution of **Z**. Next, we observe both \mathbf{z}_t and $y_{(\mathbf{x}_t, \mathbf{z}_t)}$ and then update the GP posterior belief of f. Of note, Corollary 1.1 has shown that all LV lie in the set $\mathcal{Z}_{l}^{\leq} \cap \mathcal{Z}_{u}^{\geq}$. However, the probability of this set is usually small, because $P(\mathbf{Z} \in \mathcal{Z}_l^{\leq} \cap \mathcal{Z}_u^{\geq}) \leq P(\mathbf{Z} \in \mathcal{Z}_l^{\leq}) \leq \alpha$ and small values of α are often used by real-world applications to manage risks. Thus, the probability that the sampled z_t is an LV is small. As a result, we suggest sampling a large number of \mathbf{z}_t 's from the environment to increase the chance that an LV is sampled. On the other hand, the small probability of sampling an LV motivates the need for us to select z_t .

3.4. V-UCB Approaches STABLEOPT as $\alpha \rightarrow 0^+$

Recall that the objective of adversarially robust BO is to find $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$ that maximizes $\min_{\mathbf{z}\in\mathcal{D}_{\mathbf{z}}} f(\mathbf{x}, \mathbf{z})$ (Bogunovic et al., 2018) by iteratively specifying input query $(\mathbf{x}_t, \mathbf{z}_t)$ to collect noisy observations $y_{\mathbf{x}_t, \mathbf{z}_t}$. It is different from BO of VAR since its \mathbf{z} is not random but selected by an adversary who aims to minimize the function evaluation. The work of Bogunovic et al. (2018) has proposed a no-regret algorithm

 $^{^{2}}n_{\text{out}}$ and n_{in} are the numbers of iterations for the outer and inner optimization respectively, K is the number of fantasy GP models required for their one-step lookahead, and M is the number of functions sampled from the GP posterior (Cakmak et al., 2020).

for this setting named STABLEOPT, which selects

where u_{t-1} and l_{t-1} are defined in (3).

At first glance, BO of VAR and adversarially robust BO are seemingly different problems because \mathbf{Z} is a random variable in the former but not in the latter. However, based on our key observation on the connection between the minimum value of a continuous function $h(\mathbf{w})$ and the VAR of the random variable $h(\mathbf{W})$ in the following theorem, these two problems and their solutions are connected as shown in Corollary 2.1, and 2.2.

Theorem 2. Let \mathbf{W} be a random variable with the support $\mathcal{D}_w \subset \mathbb{R}^{d_w}$ and dimension d_w . Let h be a continuous function mapping from $\mathbf{w} \in \mathcal{D}_w$ to \mathbb{R} . Then, $h(\mathbf{W})$ denotes the random variable whose realization is the function h evaluation at a realization \mathbf{w} of \mathbf{W} . Suppose $h(\mathbf{w})$ has a minimizer $\mathbf{w}_{\min} \in \mathcal{D}_w$, then $\lim_{\alpha \to 0^+} V_\alpha(h(\mathbf{W})) = h(\mathbf{w}_{\min})$.

Corollary 2.1. Adversarially robust BO which finds $\operatorname{argmax}_{\mathbf{x}} \min_{\mathbf{z}} f(\mathbf{x}, \mathbf{z})$ can be cast as BO of VAR by letting (a) α approach 0 from the right and (b) $\mathcal{D}_{\mathbf{z}}$ be the support of the environmental random variable \mathbf{Z} , i.e., $\operatorname{argmax}_{\mathbf{x}} \lim_{\alpha \to 0^+} V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$.

Interestingly, from Theorem 2, we observe that Z_l^{\leq} in Corollary 1.1 approaches the set of minimizers $\operatorname{argmin}_{\mathbf{z}\in\mathcal{D}_{\mathbf{z}}} l_{t-1}(\mathbf{x}_t, \mathbf{z})$ as $\alpha \to 0^+$. Corollary 2.2 below shows that LV w.r.t \mathbf{x}_t becomes a minimizer of $l_{t-1}(\mathbf{x}_t, \mathbf{z})$ which is same as the selected \mathbf{z}_t of STABLEOPT in (5).

Corollary 2.2. The STABLEOPT solution to adversarially robust BO selects the same input query as that selected by the V-UCB solution to the corresponding BO of VAR in Corollary 2.1.

The proof of Theorem 2 and its two corollaries are shown in Appendix G. We note that V-UCB is also applicable to the optimization of $V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$ where the distribution of \mathbf{Z} is a conditional distribution given \mathbf{x} . For example, in robotics, if there exists noise/perturbation in the control, an optimization problem of interest is $V_{\alpha}(f(\mathbf{x} + \boldsymbol{\xi}(\mathbf{x})))$ where $\boldsymbol{\xi}(\mathbf{x})$ is the random perturbation that depends on \mathbf{x} .

3.5. Implementation of V-UCB with Continuous Random Variable Z

The V-UCB algorithm involves two steps: selecting $\mathbf{x}_t = \operatorname{argmax}_{\mathbf{x} \in \mathcal{D}_{\mathbf{x}}} V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ and selecting \mathbf{z}_t as the LV \mathbf{z}_{LV} with the largest probability mass (or probability density). When $|\mathcal{D}_{\mathbf{z}}|$ is finite, given \mathbf{x} , $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ can be computed exactly. The gradient of $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ with respect to \mathbf{x} can be obtained easily (e.g., using automatic differentiation provided in the Tensorflow library (Abadi

et al., 2015)) to aid the selection of \mathbf{x}_t . In this case, the latter step can also be performed by constructing the set of all LV (checking the condition in the Definition 1 for all $\mathbf{z} \in \mathcal{D}_{\mathbf{z}}$) and choosing the LV \mathbf{z}_{LV} with the largest probability mass.

Estimation of VAR. When Z is a continuous random variable, estimating VAR by an ordered set of samples (e.g., in Cakmak et al. (2020)) may require a prohibitively large number of samples, especially for small values of α . Thus, we employ the following popular pinball (or tilted absolute value) function in quantile regression (Koenker & Bassett, 1978) to estimate VAR as a lower α -quantile:

$$\rho_{\alpha}(w) \triangleq \begin{cases} \alpha w & \text{if } w \ge 0\\ (\alpha - 1)w & \text{if } w < 0 \end{cases}$$

where $w \in \mathbb{R}$. In particular, to estimate $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ as $\nu \in \mathbb{R}$, we find ν that minimizes:

$$\mathbb{E}_{\mathbf{z}\sim p(\mathbf{Z})}[\rho_{\alpha}(u_{t-1}(\mathbf{x},\mathbf{z})-\nu)].$$
(6)

A well-known example is when $\alpha = 0.5$ and ρ_{α} is the absolute value function, then the optimal ν is the median. The loss in (6) can be optimized using stochastic gradient descent with a random batch of samples of **Z** at each optimization iteration.

Maximization of $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ **.** Unfortunately, to maximize $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ over $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$, there is no gradient of $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ with respect to \mathbf{x} under the above approach. This situation resembles BO where there is no gradient information, but only noisy observations at input queries. Unlike BO, the observation (samples of $u_{t-1}(\mathbf{x}, \mathbf{Z})$ at \mathbf{x}) is not costly. Therefore, we propose the local neural surrogate optimization (LNSO) algorithm to find $\operatorname{argmax}_{\mathbf{x}\in\mathcal{D}_{\mathbf{x}}} V_{\alpha}(u_{t-1}(\mathbf{x},\mathbf{Z}))$ which is visualized in Fig. 2. Suppose the optimization is initialized at $\mathbf{x} = \mathbf{x}^{(0)}$, instead of maximizing $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ (whose gradient w.r.t. x is unknown), we maximize a surrogate function $q(\mathbf{x}, \boldsymbol{\theta}^{(0)})$ (modeled by a neural network) that approximates $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ well in a local region of $\mathbf{x}^{(0)}$, e.g., a ball $\mathcal{B}(\mathbf{x}^{(0)}, r)$ of radius r in Fig. 2. We obtain such parameters $\theta^{(0)}$ by minimizing the following loss function:

$$\mathcal{L}_{g}(\boldsymbol{\theta}, \mathbf{x}^{(0)}) \\ \triangleq \mathbb{E}_{\mathbf{x} \in \mathcal{B}(\mathbf{x}^{(0)}, r)} \mathbb{E}_{\mathbf{Z} \sim p(\mathbf{Z})} \left[\rho_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{z}) - g(\mathbf{x}; \boldsymbol{\theta})) \right]$$
(7)

where the expectation $\mathbb{E}_{\mathbf{x}\in\mathcal{B}(\mathbf{x}^{(0)},r)}$ is taken over a uniformly distributed **X** in $\mathcal{B}(\mathbf{x}^{(0)},r)$. Minimizing (7) can be performed with stochastic gradient descent. If maximizing $g(\mathbf{x}, \boldsymbol{\theta}^{(0)})$ leads to a value $\mathbf{x}^{(i)} \notin \mathcal{B}(\mathbf{x}^{(0)},r)$ (Fig. 2), we update the local region to be centered at $\mathbf{x}^{(i)}$ ($\mathcal{B}(\mathbf{x}^{(i)},r)$) and find $\boldsymbol{\theta}^{(i)} = \operatorname{argmin}_{\boldsymbol{\theta}} \mathcal{L}_g(\boldsymbol{\theta}, \mathbf{x}^{(i)})$ such that $g(\mathbf{x}, \boldsymbol{\theta}^{(i)})$ approximates $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ well $\forall \mathbf{x} \in \mathcal{B}(\mathbf{x}^{(i)}, r)$. Then, $\mathbf{x}^{(i)}$ is updated by maximizing $g(\mathbf{x}, \boldsymbol{\theta}^{(i)})$ for $\mathbf{x} \in \mathcal{B}(\mathbf{x}^{(i)}, r)$. The complete algorithm is described in Appendix H.



Figure 2. Plot of a hypothetical optimization path (as arrows) of LNSO initialized at $\mathbf{x}^{(0)}$. Input \mathbf{x} is 2-dimensional. The boundary of a ball \mathcal{B} of radius r is plotted as a dotted circle. When the updated \mathbf{x} moves out of \mathcal{B} , the center of \mathcal{B} and $\boldsymbol{\theta}$ are updated.

We prefer a small value of r so that the ball \mathcal{B} is small. In such case, $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ for $\mathbf{x} \in \mathcal{B}$ can be estimated well with a small neural network $g(\mathbf{x}, \boldsymbol{\theta})$ whose training requires a small number of iterations.

Search of Lacing Values. Given a continuous random variable Z, to find an LV w.r.t \mathbf{x}_t in line 4 of Algorithm 1, i.e., to find a z satisfying $d_u(\mathbf{z}) \triangleq u_{t-1}(\mathbf{x}_t, \mathbf{z}) - V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z})) \ge 0$ and $d_l(\mathbf{z}) \triangleq V_{\alpha}(l_t(\mathbf{x}_t, \mathbf{Z})) - l_{t-1}(\mathbf{x}_t, \mathbf{z}) \ge 0$, we choose a z that minimizes

$$\mathcal{L}_{\text{LV}}(\mathbf{z}) \triangleq \text{ReLU}(-d_u(\mathbf{z})) + \text{ReLU}(-d_l(\mathbf{z}))$$
(8)

where $\text{ReLU}(\omega) = \max(\omega, 0)$ is the rectified linear unit function ($\omega \in \mathbb{R}$). To include the heuristic in Section 3.3 which selects the LV with the highest probability density, we find z that minimizes

$$\mathcal{L}_{\text{LV-P}}(\mathbf{z}) \triangleq \mathcal{L}_{\text{LV}}(\mathbf{z}) - \mathbb{I}_{d_u(\mathbf{z}) \ge 0} \mathbb{I}_{d_l(\mathbf{z}) \ge 0} p(\mathbf{z})$$

where $\mathcal{L}_{LV}(\mathbf{z})$ is defined in (8); $p(\mathbf{z})$ is the probability density; $\mathbb{I}_{d_t(\mathbf{z})>0}$ and $\mathbb{I}_{d_t(\mathbf{z})>0}$ are indicator functions.

4. Experiments

In this section, we empirically evaluate the performance of V-UCB. The work of Cakmak et al. (2020) has motivated the use of the approximated variant of their algorithm ρKG^{apx} over its original version ρKG by showing that ρKG^{apx} achieves comparable empirical performances to ρKG while incurring much less computational cost. Furthermore, ρKG^{apx} has been shown to significantly outperform other competing algorithms (Cakmak et al., 2020). Therefore, we choose ρKG^{apx} as the main baseline to empirically compare with V-UCB. The experiments using ρKG^{apx} is performed by adding new objective functions to the existing implementation of Cakmak et al. (2020) at https://github.com/saitcakmak/BoRisk.

Regarding V-UCB, when D_z is finite and the distribution of **Z** is not uniform, we perform V-UCB by selecting z_t as an LV at random, labeled as *V-UCB Unif*, and by selecting z_t as the LV with the maximum probability mass, labeled as *V-UCB Prob*.

The performance metric is defined as $V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) - V_{\alpha}(f(\tilde{\mathbf{x}}, \mathbf{Z}))$ where $\tilde{\mathbf{x}}$ is the recommended input. The evaluation of VAR is described in Section 3.5. The recommended input is $\operatorname{argmax}_{\mathbf{x}\in\mathcal{D}_T} V_{\alpha}(\mu_{t-1}(\mathbf{x}, \mathbf{Z}))$ for V-UCB, and $\operatorname{argmin}_{\mathbf{x}\in\mathcal{D}_{\mathbf{x}}} \mathbb{E}_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))]$ for $\rho \mathrm{KG}^{apx}$ (Cakmak et al., 2020), where \mathbb{E}_{t-1} is the conditional expectation over the unknown f given the observations \mathcal{D}_{t-1} (approximated by a finite set of functions sampled from the GP posterior belief).³ We repeat each experiment 10 times with different random initial observations $\mathbf{y}_{\mathcal{D}_0}$ and plot both the mean (as lines) and the 70% confidence interval (as shaded areas) of the log 10 of the performance metric. The detailed descriptions of experiments are deferred to Appendix I.

4.1. Synthetic Benchmark Functions

We use 3 synthetic benchmark functions: Branin-Hoo, Goldstein-Price, and Hartmann-3D functions to construct 4 optimization problems: Branin-Hoo-(1, 1), Goldstein-Price-(1, 1), Hartmann-(1, 2), and Hartmann-(2, 1). The tuples represent (d_x, d_z) corresponding to the dimensions of x and z. The noise variance σ_n^2 is set to 0.01. The risk level α is 0.1. There are 2 different settings: finite \mathcal{D}_z ($|\mathcal{D}_z| = 64$ for Hartmann-(1, 2) and $|\mathcal{D}_z| = 100$ for the others) and continuous \mathcal{D}_z . In the latter setting, r = 0.1 and the surrogate function is a neural network of 2 hidden layers with 30 hidden neurons each, and sigmoid activation functions.

The results are shown in Fig. 3 and Fig. 4 for the settings of discrete $\mathcal{D}_{\mathbf{z}}$ and continuous $\mathcal{D}_{\mathbf{z}}$, respectively. When $\mathcal{D}_{\mathbf{z}}$ is discrete (Fig. 3), V-UCB Unif is on par with ρKG^{apx} in optimizing Branin-Hoo-(1, 1) and Goldstein-Price-(1, 1), and outperforms ρKG^{apx} in optimizing Hartmann-(1, 2) and Hartmann-(2, 1). V-UCB Prob is also able to exploit the probability distribution of \mathbf{Z} to outperform V-UCB Unif. When $\mathcal{D}_{\mathbf{z}}$ is continuous (Fig. 4), V-UCB Prob outperforms ρKG^{apx} . The unsatisfactory performance of ρKG^{apx} in some experiments may be attributed to its approximation of the inner optimization problem in the acquisition function (Cakmak et al., 2020), and the approximation of VAR using samples of \mathbf{Z} and the GP posterior belief.

4.2. Simulated Optimization Problems

The first problem is portfolio optimization adopted by (Cakmak et al., 2020). There are $d_x = 3$ optimization variables (risk and trade aversion parameters, and the holding cost multiplier) and $d_z = 2$ environmental random variables (bid-ask spread and borrow cost). The variable **Z** follows a discrete uniform distribution with $|\mathcal{D}_z| = 100$. Hence,

³While the work of Cakmak et al. (2020) considers a minimization problem of VAR, our work considers a maximization problem of VAR. Therefore, the objective functions for ρKG^{apx} are the negation of those for V-UCB. For V-UCB at risk level α , the risk level for ρKG^{apx} is $1 - \alpha$.



Figure 3. Synthetic benchmark functions with finite $\mathcal{D}_{\mathbf{z}}$.

there is no difference between V-UCB Unif and V-UCB Prob. Thus, we only report the results of the latter. The objective function is the posterior mean of a trained GP on the dataset in Cakmak et al. (2020) of size 3000 generated from CVXPortfolio. The noise variance σ_n^2 is set to 0.01. The risk level α is set to 0.2.

The second problem is a simulated robot pushing task for which we use the implementation from the work of Wang & Jegelka (2017). The simulation is viewed as a 3-dimensional function $\mathbf{h}(r_x, r_y, t_p)$ returning the 2-D location of the pushed object, where $r_x, r_y \in [-5, 5]$ are the robot location and $t_p \in [1, 30]$ is the pushing duration. The objective is to minimize the distance to a fixed goal location $\mathbf{g} = (g_x, g_y)^{\top}$, i.e., the objective function of the maximization problem is $f_0(r_x, r_y, t_p) = -\|\mathbf{h}(r_x, r_y, t_p) - \mathbf{g}\|$. We assume that there are perturbations in specifying the robot location W_x, W_y whose support \mathcal{D}_z includes 64 equi-distant points in $[-1,1]^2$ and whose probability mass is proportional to $\exp(-(W_x^2 + W_y^2)/0.4^2)$. It leads to a random objective function $f(r_x, r_y, t_p, W_x, W_y) \triangleq f_0(r_x + W_x, r_y +$ W_y, t_p). We aim to maximize the VAR of f which is more difficult than maximizing that of f_0 . Moreover, a random noise following $\mathcal{N}(0, 0.01)$ is added to the evaluation of f. The risk level α is set to 0.1.

The results are shown in Fig. 5. We observe that V-UCB outperforms ρKG^{apx} in both problems. Furthermore, in comparison to our synthetic experiments, the difference between V-UCB Unif and V-UCB Prob is not significant in the robot pushing experiment. This is because the chance that a uniform sample of LV has a large probability mass



Figure 4. Synthetic benchmark functions with continuous $\mathcal{D}_{\mathbf{z}}$.

is higher in the robot pushing experiment due to a larger region of \mathcal{D}_{z} having high probabilities.



Figure 5. Simulated experiments.

5. Conclusion

To tackle the BO of VAR problem, we construct a no-regret algorithm, namely VAR *upper confidence bound* (V-UCB), through the design of a confidence bound of VAR and a set of *lacing values* (LV) that is guaranteed to exist. Besides, we introduce a heuristic to select an LV that improves the emprical performance of V-UCB over random selection of LV. We also draw an elegant connection between BO of VAR and adversarially robust BO in terms of both problem formulation and solutions. Lastly, we provide practical techniques for implementing VAR with continuous **Z**. While V-UCB is more computationally efficient than the the state-of-the-art ρKG^{apx} algorithm for BO of VAR, it also demonstrates competitive empirical performances in our experiments.

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A. Proof of Lemma 2

Lemma 2. Similar to the definition of $f(\mathbf{x}, \mathbf{Z})$, let $l_{t-1}(\mathbf{x}, \mathbf{Z})$ and $u_{t-1}(\mathbf{x}, \mathbf{Z})$ denote the random function over \mathbf{x} where the randomness comes from the random variable \mathbf{Z} ; l_{t-1} and u_{t-1} are defined in (3). Then, $\forall \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, t \geq 1$, $\alpha \in (0, 1)$,

$$V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \in I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \\ \triangleq [V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})), V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))]$$

holds with probability $\geq 1 - \delta$ for δ in Lemma 1, where $V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z}))$ and $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ are defined as (1).

Proof. Conditioned on the event $f(\mathbf{x}, \mathbf{z}) \in I_{t-1}[f(\mathbf{x}, \mathbf{z})] \triangleq [l_{t-1}(\mathbf{x}, \mathbf{z}), u_{t-1}(\mathbf{x}, \mathbf{z})]$ for all $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \geq 1$ which occurs with probability $\geq 1 - \delta$ for δ in Lemma 1, we will prove that $V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) \leq V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$. The proof of $V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ can be done in a similar manner.

From $f(\mathbf{x}, \mathbf{z}) \in I_{t-1}[f(\mathbf{x}, \mathbf{z})] \triangleq [l_{t-1}(\mathbf{x}, \mathbf{z}), u_{t-1}(\mathbf{x}, \mathbf{z})]$ for all $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \ge 1$ we have $\forall \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \ge 1$,

 $f(\mathbf{x}, \mathbf{z}) \ge l_{t-1}(\mathbf{x}, \mathbf{z}) \ .$

Therefore, for all $\omega \in \mathbb{R}$, $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$, $\mathbf{z} \in \mathcal{D}_{\mathbf{z}}$, $t \geq 1$,

$$f(\mathbf{x}, \mathbf{z}) \le \omega \Rightarrow l_{t-1}(\mathbf{x}, \mathbf{z}) \le \omega$$
$$P(f(\mathbf{x}, \mathbf{Z}) \le \omega) \le P(l_{t-1}(\mathbf{x}, \mathbf{Z}) \le \omega) .$$

So, for all $\omega \in \mathbb{R}$, $\alpha \in (0, 1)$, $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$, $t \ge 1$,

$$P(f(\mathbf{x}, \mathbf{Z}) \le \omega) \ge \alpha \Rightarrow P(l_{t-1}(\mathbf{x}, \mathbf{Z}) \le \omega) \ge \alpha$$
.

Hence, the set $\{\omega : P(f(\mathbf{x}, \mathbf{Z}) \leq \omega) \geq \alpha\}$ is a subset of $\{\omega : P(l_{t-1}(\mathbf{x}, \mathbf{Z}) \leq \omega) \geq \alpha\}$ for all $\alpha \in (0, 1), \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, t \geq 1$, which implies that $\inf\{\omega : P(f(\mathbf{x}, \mathbf{Z}) \leq \omega) \geq \alpha\} \geq \inf\{\omega : P(l_{t-1}(\mathbf{x}, \mathbf{Z}) \leq \omega) \geq \alpha\}$, i.e., $V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) \leq V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))$ for all $\alpha \in (0, 1), \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, t \geq 1$. \Box

B. Proof of (4)

We prove that

$$r(\mathbf{x}_t) \le V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \ \forall t \ge 1$$

which holds with probability $\geq 1 - \delta$ for δ in Lemma 1.

Proof. Conditioned on the event $V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \in I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \triangleq [V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})), V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))]$ for all $\alpha \in (0, 1)$, $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}, t \geq 1$, which occurs with probability $\geq 1 - \delta$ in Lemma 2,

$$V_{\alpha}(f(\mathbf{x}_{*}, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}_{*}, \mathbf{Z}))$$
$$V_{\alpha}(f(\mathbf{x}_{t}, \mathbf{Z})) \geq V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z}))$$

Hence,

$$r(\mathbf{x}_{t}) \triangleq V_{\alpha}(f(\mathbf{x}_{*}, \mathbf{Z})) - V_{\alpha}(f(\mathbf{x}_{t}, \mathbf{Z}))$$

$$\leq V_{\alpha}(u_{t-1}(\mathbf{x}_{*}, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z})) . \quad (9)$$

Since \mathbf{x}_t is selected as $\operatorname{argmax}_{\mathbf{x}\in\mathcal{D}_{\mathbf{x}}} V_{\alpha}(u_{t-1}(\mathbf{x},\mathbf{Z}))$,

$$V_{\alpha}(u_{t-1}(\mathbf{x}_*, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z}))$$

equivalently, $V_{\alpha}(u_{t-1}(\mathbf{x}_{*}, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}_{t}, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z}))$. Hence, from (9), $r(\mathbf{x}_{t}) \leq V_{\alpha}(u_{t-1}(\mathbf{x}_{t}, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z}))$ for all $\alpha \in (0, 1)$ and $t \geq 1$.

C. Proof of Theorem 1

Theorem 1. $\forall \alpha \in (0, 1), \forall \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \forall t \ge 1$, there exists a lacing value in $\mathcal{D}_{\mathbf{z}}$ with respect to \mathbf{x} and t.

Proof. Recall that

$$\mathcal{Z}_l^{\leq} \triangleq \left\{ \mathbf{z} \in \mathcal{D}_{\mathbf{z}} : l_{t-1}(\mathbf{x}, \mathbf{z}) \leq V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) \right\}.$$

From to the definition of \mathcal{Z}_l^{\leq} and $V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z}))$, we have

$$P(\mathbf{Z} \in \mathcal{Z}_l^{\leq}) \ge \alpha . \tag{10}$$

Since $\alpha \in (0,1)$, $Z_l^{\leq} \neq \emptyset$. We prove the existence of LV by contradiction: (a) assuming that $\exists \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \exists t \geq 1, \forall \mathbf{z} \in Z_l^{\leq}, u_{t-1}(\mathbf{x}, \mathbf{z}) < V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ and then, (b) proving that $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ is not a lower bound of $\{\omega : P(u_{t-1}(\mathbf{x}, \mathbf{Z}) \leq \omega) \geq \alpha\}$ which is a contradiction.

Since the GP posterior mean μ_{t-1} and posterior standard deviation σ_{t-1} are continuous functions in $\mathcal{D}_{\mathbf{x}} \times \mathcal{D}_{\mathbf{z}}$, l_{t-1} and u_{t-1} are continuous functions in the closed $\mathcal{D}_{\mathbf{z}} \subset \mathbb{R}^{d_z}$ (x and t are given and remain fixed in this proof). We will prove that \mathcal{Z}_l^{\leq} is closed in \mathbb{R}^{d_z} by contradiction.

If \mathcal{Z}_l^{\leq} is not closed in \mathbb{R}^{d_z} , there exists a limit point \mathbf{z}_p of \mathcal{Z}_l^{\leq} such that $\mathbf{z}_p \notin \mathcal{Z}_l^{\leq}$. Since $\mathcal{Z}_l^{\leq} \subset \mathcal{D}_{\mathbf{z}}$ and $\mathcal{D}_{\mathbf{z}}$ is closed in \mathbb{R}^{d_z} , $\mathbf{z}_p \in \mathcal{D}_{\mathbf{z}}$. Thus, for $\mathbf{z}_p \notin \mathcal{Z}_l^{\leq}$, $l_{t-1}(\mathbf{x}, \mathbf{z}_p) > V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z}))$ (from the definition of \mathcal{Z}_l^{\leq}). Then, there exists $\epsilon_0 > 0$ such that $l_{t-1}(\mathbf{x}, \mathbf{z}_p) > V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) + \epsilon_0$. The pre-image of the open interval $I_0 = (l_{t-1}(\mathbf{x}, \mathbf{z}_p) - \epsilon_0/2, l_{t-1}(\mathbf{x}, \mathbf{z}_p) + \epsilon_0/2)$ under l_{t-1} is also an open set \mathcal{V} containing \mathbf{z}_p (because l_{t-1} is a continuous function). Since \mathbf{z}_p is a limit point of \mathcal{Z}_l^{\leq} , there exists an $\mathbf{z}' \in \mathcal{Z}_l^{\leq} \cap \mathcal{V}$. Then, $l_{t-1}(\mathbf{x}, \mathbf{z}') \in I_0$, so $l_{t-1}(\mathbf{x}, \mathbf{z}') \geq l_{t-1}(\mathbf{x}, \mathbf{z}_p) - \epsilon_0/2 \geq V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) + \epsilon_0 - \epsilon_0/2 = V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) + \epsilon_0/2$. It contradicts $\mathbf{z}' \in \mathcal{Z}_l^{\leq}$.

Therefore, Z_l^{\leq} is a closed set in \mathbb{R}^{d_z} . Besides, since $\{u_{t-1}(\mathbf{x}, \mathbf{z}) : \mathbf{z} \in Z_l^{\leq}\}$ is upper bounded by $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ (due to our assumption), so $\sup\{u_{t-1}(\mathbf{x}, \mathbf{z}) : \mathbf{z} \in \mathcal{Z}_l^{\leq}\} \text{ exists. Let } \mathbf{z}_l^+ \text{ be such }$ that $u_{t-1}(\mathbf{x}, \mathbf{z}_l^+) \triangleq \sup\{u_{t-1}(\mathbf{x}, \mathbf{z}) : \mathbf{z} \in \mathcal{Z}_l^{\leq}\}.$ Then, $\mathbf{z}_l^+ \in \mathcal{Z}_l^{\leq}$ because \mathcal{Z}_l^{\leq} is closed.

Moreover, from our assumption that $\forall \mathbf{z} \in \mathcal{Z}_l^{\leq}, u_{t-1}(\mathbf{x}, \mathbf{z}) < V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z})),$ we have $u_{t-1}(\mathbf{x}, \mathbf{z}_l^+) < V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z})).$ Furthermore,

$$P(u_{t-1}(\mathbf{x}, \mathbf{Z}) \le u_{t-1}(\mathbf{x}, \mathbf{z}_l^+)) \ge P(\mathbf{Z} \in \mathcal{Z}_l^{\le}) \ge \alpha$$
.

where the first inequality is because $u_{t-1}(\mathbf{x}, \mathbf{z}_l^+) = \sup\{u_{t-1}(\mathbf{x}, \mathbf{z}) : \mathbf{z} \in \mathcal{Z}_l^{\leq}\}$ and the last inequality is from (10). Hence, $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}) \text{ is not a lower bound}$ of $\{\omega : P(u_{t-1}(\mathbf{x}, \mathbf{Z}) \leq \omega) \geq \alpha\}$.

D. Proof of Lemma 3

Lemma 3. By selecting \mathbf{x}_t as a maximizer of $V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))$ and selecting \mathbf{z}_t as an LV w.r.t \mathbf{x}_t , the instantaneous regret is upper-bounded by:

$$r(\mathbf{x}_t) \le 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \ \forall t \ge 1$$

with probability $\geq 1 - \delta$ for δ in Lemma 1.

Proof. Conditioned on the event $f(\mathbf{x}, \mathbf{z}) \in I_{t-1}[f(\mathbf{x}, \mathbf{z})] \triangleq [l_{t-1}(\mathbf{x}, \mathbf{z}), u_{t-1}(\mathbf{x}, \mathbf{z})]$ for all $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \geq 1$ which occurs with probability $\geq 1 - \delta$ in Lemma 1, it follows that $V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \in I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \triangleq [V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})), V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))]$ for all $\alpha \in (0, 1), \mathbf{x} \in \mathcal{D}_{\mathbf{x}}$, and $t \geq 1$ in Lemma 2.

From (4), by selecting \mathbf{z}_t as an LV, for all $t \ge 1$,

$$\begin{aligned} r(\mathbf{x}_t) &\leq V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \\ &\leq u_{t-1}(\mathbf{x}_t, \mathbf{z}_t) - l_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \text{ (since } \mathbf{z}_t \text{ is an LV)} \\ &\leq \mu_{t-1}(\mathbf{x}_t, \mathbf{z}_t) + \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \\ &- \mu_{t-1}(\mathbf{x}_t, \mathbf{z}_t) + \beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \\ &= 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \text{ .} \end{aligned}$$

E. Bound on the Average Cumulative Regret

Conditioned on the event $f(\mathbf{x}, \mathbf{z}) \in I_{t-1}[f(\mathbf{x}, \mathbf{z})] \triangleq [l_{t-1}(\mathbf{x}, \mathbf{z}), u_{t-1}(\mathbf{x}, \mathbf{z})]$ for all $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \geq 1$ which occurs with probability $\geq 1 - \delta$ in Lemma 1, it follows that $r(\mathbf{x}_t) \leq 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \ \forall t \geq 1$ in Lemma 3. Therefore,

$$R_T \triangleq \sum_{t=1}^T r(\mathbf{x}_t) \le \sum_{t=1}^T 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t)$$
$$\le 2\beta_T^{1/2} \sum_{t=1}^T \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t)$$

since β_t is a non-decreasing sequence.

From Lemma 5.4 and the Cauchy-Schwarz inequality in (Srinivas et al., 2010), we have

$$2\sum_{t=1}^{T} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \le \sqrt{C_1 T \gamma_T}$$
(11)

where $C_1 = 8/\log(1 + \sigma_n^{-2})$. Hence,

$$R_T \le \sqrt{C_1 T \beta_T \gamma_T} \,.$$

Equivalently, $R_T/T \leq \sqrt{C_1 \beta_T \gamma_T/T}$. Since γ_T is shown to be bounded for several common kernels in (Srinivas et al., 2010), the above implies that $\lim_{T\to\infty} R_T/T = 0$, i.e., the algorithm is no-regret.

F. Bound on $r(\mathbf{x}_{t_*(T)})$

Conditioned on the event $f(\mathbf{x}, \mathbf{z}) \in I_{t-1}[f(\mathbf{x}, \mathbf{z})] \triangleq [l_{t-1}(\mathbf{x}, \mathbf{z}), u_{t-1}(\mathbf{x}, \mathbf{z})]$ for all $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}, \mathbf{z} \in \mathcal{D}_{\mathbf{z}}, t \geq 1$, which occurs with probability $\geq 1 - \delta$ in Lemma 1, it follows that $V_{\alpha}(f(\mathbf{x}, \mathbf{Z})) \in I_{t-1}[V_{\alpha}(f(\mathbf{x}, \mathbf{Z}))] \triangleq [V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})), V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z}))]$ for all $\alpha \in (0, 1), \mathbf{x} \in \mathcal{D}_{\mathbf{x}}, t \geq 1$ in Lemma 2. Furthermore, we select \mathbf{z}_t as an LV, so $l_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \leq V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}_t, \mathbf{Z})) \leq u_{t-1}(\mathbf{x}_t, \mathbf{z}_t)$ according to the Definition 1.

At *T*-th iteration, by recommending $\mathbf{x}_{t_*(T)}$ as an estimate of \mathbf{x}_* where $t_*(T) \triangleq \operatorname{argmax}_{t \in \{1, \dots, T\}} V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z}))$, we have

$$V_{\alpha}(l_{t_{*}(T)-1}(\mathbf{x}_{t_{*}(T)}, \mathbf{Z})) = \max_{t \in \{1, \dots, T\}} V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z}))$$
$$\geq \frac{1}{T} \sum_{t=1}^{T} V_{\alpha}(l_{t-1}(\mathbf{x}_{t}, \mathbf{Z})).$$

Therefore,

$$r(\mathbf{x}_{t_*(T)}) = V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) - V_{\alpha}(f(\mathbf{x}_{t_*(T)}, \mathbf{Z}))$$

$$\leq V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) - V_{\alpha}(l_{t_*(T)-1}(\mathbf{x}_{t_*(T)}, \mathbf{Z}))$$

$$\leq \frac{1}{T} \sum_{t=1}^T \left(V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) - V_{\alpha}(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \right) .$$

Furthermore, $V_{\alpha}(f(\mathbf{x}_*, \mathbf{Z})) \leq V_{\alpha}(u_{t-1}(\mathbf{x}_*, \mathbf{Z}))$ from our

condition, so

$$\begin{aligned} r(\mathbf{x}_{t_*(T)}) &\leq \frac{1}{T} \sum_{t=1}^T \left(V_\alpha(f(\mathbf{x}_*, \mathbf{Z})) - V_\alpha(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \right) \\ &\leq \frac{1}{T} \sum_{t=1}^T \left(V_\alpha(u_{t-1}(\mathbf{x}_*, \mathbf{Z})) - V_\alpha(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \right) \\ &\leq \frac{1}{T} \sum_{t=1}^T \left(V_\alpha(u_{t-1}(\mathbf{x}_t, \mathbf{Z})) - V_\alpha(l_{t-1}(\mathbf{x}_t, \mathbf{Z})) \right) \\ &\leq \frac{1}{T} \sum_{t=1}^T \left(u_{t-1}(\mathbf{x}_t, \mathbf{z}_t) - l_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \right) \text{ (since } \mathbf{z}_t \text{ is an LV)} \\ &\leq \frac{1}{T} \sum_{t=1}^T 2\beta_t^{1/2} \sigma_{t-1}(\mathbf{x}_t, \mathbf{z}_t) \\ &\leq \sqrt{\frac{C_1\beta_T\gamma_T}{T}} \text{ (from Appendix E) .} \end{aligned}$$

Since γ_T is shown to be bounded for several common kernels in (Srinivas et al., 2010), the above implies that $\lim_{T\to\infty} r(\mathbf{x}_{t_*(T)}) = 0.$

G. Proof of Theorem 2 and Its Corollaries

G.1. Proof of Theorem 2

Theorem 2. Let \mathbf{W} be a random variable with the support $\mathcal{D}_w \subset \mathbb{R}^{d_w}$ and dimension d_w . Let h be a continuous function mapping from $\mathbf{w} \in \mathcal{D}_w$ to \mathbb{R} . Then, $h(\mathbf{W})$ denotes the random variable whose realization is the function h evaluation at a realization \mathbf{w} of \mathbf{W} . Suppose $h(\mathbf{w})$ has a minimizer $\mathbf{w}_{\min} \in \mathcal{D}_w$, then $\lim_{\alpha \to 0^+} V_\alpha(h(\mathbf{W})) = h(\mathbf{w}_{\min})$.

Recall that the support \mathcal{D}_w of \mathbf{W} is defined as the smallest closed subset \mathcal{D}_w of \mathbb{R}^{d_z} such that $P(\mathbf{W} \in \mathcal{D}_w) = 1$, and $\mathbf{w}_{\min} \in \mathcal{D}_w$ minimizes $h(\mathbf{w})$.

Lemma 4. For all $\alpha \in (0, 1)$, $V_{\alpha}(h(\mathbf{W}))$ is a nondecreasing function, i.e.,

$$\forall 1 > \alpha > \alpha' > 0, V_{\alpha}(h(\mathbf{W})) \ge V_{\alpha'}(h(\mathbf{W}))$$

Proof. Since $\alpha > \alpha'$, for all $\omega \in \mathbb{R}$,

$$P(h(\mathbf{W}) \le \omega) \ge \alpha \Rightarrow P(h(\mathbf{W}) \le \omega) \ge \alpha'$$
.

Therefore, $\{\omega : P(h(\mathbf{W}) \le \omega) \ge \alpha\}$ is a subset of $\{\omega : P(h(\mathbf{W}) \le \omega) \ge \alpha'\}$. Thus,

$$\inf \{ \omega : P(h(\mathbf{W}) \le \omega) \ge \alpha \}$$
$$\ge \inf \{ \omega : P(h(\mathbf{W}) \le \omega) \ge \alpha' \}$$
i.e., $V_{\alpha}(h(\mathbf{W})) \ge V_{\alpha'}(h(\mathbf{W}))$.

Let

$$\omega_{0^+} \triangleq \lim_{\alpha \to 0^+} V_{\alpha}(h(\mathbf{W})) . \tag{12}$$

Then, from Lemma 4, the following lemma follows. Lemma 5. For all $\alpha \in (0, 1)$, and ω_{0^+} defined in (12)

$$\omega_{0^+} \le V_\alpha(h(\mathbf{W}))$$

We use Lemma 5 to prove the following lemma. Lemma 6. For all $\mathbf{w} \in \mathcal{D}_w$, and ω_{0^+} defined in (12)

$$\omega_{0^+} \le h(\mathbf{w})$$

which implies that

$$\omega_{0^+} \le h(\mathbf{w}_{\min})$$
.

Proof. By contradiction, we assume that there exists $\mathbf{w}' \in \mathcal{D}_w$ such that $\omega_{0^+} > h(\mathbf{w}')$. Then, there exists $\epsilon_1 > 0$ such that $\omega_{0^+} > h(\mathbf{w}') + \epsilon_1$. Consider the pre-image \mathcal{V} of the open interval $I_h = (h(\mathbf{w}') - \epsilon_1/2, h(\mathbf{w}') + \epsilon_1/2$. Since h is a continuous function, \mathcal{V} is an open set and it contains \mathbf{w}' (as I_h contains $h(\mathbf{w}')$). Then, consider the set $\mathcal{V} \cap \mathcal{D}_w \supset \{\mathbf{w}'\} \neq \emptyset$, we prove $P(\mathbf{W} \in \mathcal{V} \cap \mathcal{D}_z) > 0$ by contradiction as follows.

If $P(\mathbf{W} \in \mathcal{V} \cap \mathcal{D}_w) = 0$ then the closure of $\mathcal{D}_w \setminus \mathcal{V}$ is a closed set that is smaller than \mathcal{D}_w (since \mathcal{V} is an open set, \mathcal{D}_w is a closed set, and $\mathcal{V} \cap \mathcal{D}_w$ is not empty) and satisfies $P(\mathbf{W} \in \mathcal{D}_w \setminus \mathcal{V}) = 1$, which contradicts the definition of \mathcal{D}_w . Thus, $P(\mathbf{W} \in \mathcal{V} \cap \mathcal{D}_w) > 0$.

Therefore, $P(h(\mathbf{W}) \in I_h) > 0$. So,

$$P(h(\mathbf{W}) \le \omega_{0^+})$$

$$\ge P(h(\mathbf{W}) \le h(\mathbf{w}') + \epsilon_1/2)$$

$$\ge P(h(\mathbf{W}) \in I_h)$$

$$> 0.$$

Let us consider $\alpha_0 = P(h(\mathbf{W}) \le h(\mathbf{w}') + \epsilon_1/2) > 0$, the VAR at α_0 is

$$V_{\alpha_0}(h(\mathbf{W})) \triangleq \inf\{\omega : P(h(\mathbf{W}) \le \omega) \ge \alpha_0\}$$

$$\le h(\mathbf{w}') + \epsilon_1/2$$

$$< \omega_{0^+}$$

which is a contradiction to Lemma 5.

Lemma 7. For ω_{0^+} defined in (12)

$$\omega_{0^+} \ge h(\mathbf{w}_{\min}) \,. \tag{13}$$

Proof. By contradiction, we assume that $\omega_{0^+} < h(\mathbf{w}_{\min})$. Then there exists $\epsilon_2 > 0$ that $\omega_{0^+} + \epsilon_2 < h(\mathbf{w}_{\min})$. Since $\omega_{0^+} \triangleq \lim_{\alpha \to 0^+} V_\alpha(h(\mathbf{W}))$ so there exits $\alpha_0 > 0$ such that $V_{\alpha_0}(h(\mathbf{W})) \in (\omega_{0^+}, \omega_{0^+} + \epsilon_2)$. However,

$$P(h(\mathbf{W}) \le V_{\alpha_0}(h(\mathbf{W})))$$

$$\le P(h(\mathbf{W}) \le \omega_{0^+} + \epsilon_2 < h(\mathbf{w}_{\min}))$$

$$= 0$$

which contradicts the fact that $\alpha_0 > 0$. Therefore, $\omega_{0^+} \ge$ \square $h(\mathbf{w}_{\min}).$

From (12), Lemma 6 and Lemma 7,

$$\lim_{\alpha \to 0^+} V_{\alpha}(h(\mathbf{W})) = h(\mathbf{w}_{\min})$$

which directly leads to the result in Corollary 2.1 for a continuous function $f(\mathbf{x}, \mathbf{z})$ over $\mathbf{z} \in \mathcal{D}_{\mathbf{z}}$. While \mathbf{Z} can follow any probability distribution defined on the support $\mathcal{D}_{\mathbf{z}}$, we can choose the distribution of \mathbf{Z} as a uniform distribution over $\mathcal{D}_{\mathbf{z}}$.

G.2. Corollary 2.2

From Theorem 2, $\mathcal{D}_{\mathbf{z}}$ is a closed subset of \mathbb{R}^{d_z} , and $u_{t-1}(\mathbf{x}, \mathbf{z}), l_{t-1}(\mathbf{x}, \mathbf{z})$ are continuous functions over $\mathbf{z} \in$ $\mathcal{D}_{\mathbf{z}}$, it follows that the selected \mathbf{x}_t by both STABLEOPT (in (5)) and V-UCB are the same. Furthermore,

$$\begin{aligned} \mathcal{Z}_{l}^{\leq} &\triangleq \{ \mathbf{z} \in \mathcal{D}_{\mathbf{z}} : l_{t-1}(\mathbf{x}, \mathbf{z}) \leq V_{\alpha}(l_{t-1}(\mathbf{x}, \mathbf{Z})) \} \\ &= \{ \mathbf{z} \in \mathcal{D}_{\mathbf{z}} : l_{t-1}(\mathbf{x}, \mathbf{z}) \leq \min_{\mathbf{z}' \in \mathcal{D}_{\mathbf{z}}} l_{t-1}(\mathbf{x}, \mathbf{z}') \} \\ &= \{ \mathbf{z} \in \mathcal{D}_{\mathbf{z}} : l_{t-1}(\mathbf{x}, \mathbf{z}) = \min_{\mathbf{z}' \in \mathcal{D}_{\mathbf{z}}} l_{t-1}(\mathbf{x}, \mathbf{z}') \} , \\ \mathcal{Z}_{u}^{\geq} &\triangleq \{ \mathbf{z} \in \mathcal{D}_{\mathbf{z}} : u_{t-1}(\mathbf{x}, \mathbf{z}) \geq V_{\alpha}(u_{t-1}(\mathbf{x}, \mathbf{Z})) \} \\ &= \{ \mathbf{z} \in \mathcal{D}_{\mathbf{z}} : u_{t-1}(\mathbf{x}, \mathbf{z}) \geq \min_{\mathbf{z}' \in \mathcal{D}_{\mathbf{z}}} u_{t-1}(\mathbf{x}, \mathbf{z}') \} \\ &= \mathcal{D}_{\mathbf{z}} . \end{aligned}$$

Therefore, the set of lacing values is $\mathcal{Z}_l^{\leq} \cap \mathcal{Z}_u^{\geq} = \mathcal{Z}_l^{\leq} =$ $\{\mathbf{z} \in \mathcal{D}_{\mathbf{z}} : l_{t-1}(\mathbf{x}, \mathbf{z}) = \min_{\mathbf{z}' \in \mathcal{D}_{\mathbf{z}}} l_{t-1}(\mathbf{x}, \mathbf{z}')\}$ any of which is also the selected \mathbf{z}_t in (5) by STABLEOPT. Thus, the selected \mathbf{z}_t by both STABLEOPT and V-UCB are the same.

H. Local Neural Surrogate Optimization

The local neural surrogate optimization (LNSO) to maximize a VAR $V_{\alpha}(h(\mathbf{x}, \mathbf{Z}))$ is described in Algorithm 2. The algorithm can be summarized as follows:

- Whenever the current updated $\mathbf{x}^{(i)}$ is not in $\mathcal{B}(\mathbf{x}_c, r)$ (line 4), the center \mathbf{x}_c of the ball \mathcal{B} is updated to be $\mathbf{x}^{(i)}$ (line 6) and the surrogate function $q(\mathbf{x}, \boldsymbol{\theta})$ is re-trained (lines 7-12).
- The surrogate function $g(\mathbf{x}, \boldsymbol{\theta})$ is (re-)trained to estimate $V_{\alpha}(h(\mathbf{x}, \mathbf{Z}))$ well for all $\mathbf{x} \in \mathcal{B}(\mathbf{x}_c, r)$ (lines 7-12) with stochastic gradient descent by minimizing the following loss function given random mini-batches \mathcal{Z} of **Z** (line 8) and \mathcal{X} of $\mathbf{x} \in \mathcal{B}(\mathbf{x}_c, r)$ (line 9):

$$\mathcal{L}_{g}(\mathcal{X}, \mathcal{Z}) \triangleq \frac{1}{|\mathcal{X}||\mathcal{Z}|} \sum_{\mathbf{x} \in \mathcal{X}, \mathbf{z} \in \mathcal{Z}} [\rho_{\alpha}(h(\mathbf{x}, \mathbf{z}) - g(\mathbf{x}; \boldsymbol{\theta}))]$$
(14)

Algorithm 2 LNSO of $V_{\alpha}(h(\mathbf{x}, \mathbf{Z}))$

- 1: Input: target function h; domain $\mathcal{D}_{\mathbf{x}}$; initializer $\mathbf{x}^{(0)}$; α ; a generator of Z samples gen_Z; radius r; no. of training iterations t_v, t_q ; optimization stepsizes γ_x, γ_q 2: Randomly initialize θ_s
- 3: for $i = 1, 2, ..., t_v$ do
- if i = 1 or $\|\mathbf{x}^{(i)} \mathbf{x}_c\| \ge \delta_x$ then Initialize $\boldsymbol{\theta}^{(0)} = \boldsymbol{\theta}_s$ 4:
- 5:
- Update the center of \mathcal{B} : $\mathbf{x}_c = \mathbf{x}^{(i)}$ 6:
- 7: for $j = 1, 2, ..., t_g$ do
- Draw n_z samples of **Z**: $\mathcal{Z} = \text{gen}_{\mathbb{Z}}(n_z)$. 8:
- 9: Draw a set \mathcal{X} of n_x uniformly distributed samples in $\mathcal{B}(\mathbf{x}_c, r)$. 12 (N C)

10: Update
$$\theta^{(j)} = \theta^{(j-1)} - \gamma_g \frac{d\mathcal{L}_g(\mathcal{X}, \mathcal{Z})}{d\theta} \Big|_{\theta = \theta^{(j-1)}}$$

where $\mathcal{L}_g(\mathcal{X}, \mathcal{Z})$ is defined in (14).

- 11: end for
- 12: $\boldsymbol{\theta}_s = \boldsymbol{\theta}_{t_a}$
- 13: end if
- Update $\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + \gamma_x \frac{dg(\mathbf{x}; \boldsymbol{\theta}_s)}{d\mathbf{x}} \Big|_{\mathbf{x} = \mathbf{x}^{(i-1)}}$. 14:
- Project $\mathbf{x}^{(i)}$ into $\mathcal{D}_{\mathbf{x}}$. 15:
- 16: end for
- 17: Return $\mathbf{x}^{(t_v)}$

where ρ_{α} is the pinball function in Sec. 3.5.

• Instead of directly maximizing $V_{\alpha}(h(\mathbf{x}, \mathbf{Z}))$ whose gradient w.r.t \mathbf{x} is unavailable, we find \mathbf{x} that maximizes the surrogate function $g(\mathbf{x}, \boldsymbol{\theta}_s)$ (line 14) where $\boldsymbol{\theta}_s$ is the parameters trained in lines 7-12.

I. Experimental Details

Regarding the construction of \mathcal{D}_{z} in optimizing the synthetic benchmark functions, the discrete $\mathcal{D}_{\mathbf{z}}$ is selected as equi-distanct points (e.g., by dividing $[0, 1]^{d_z}$ into a grid). The probability mass of Z is defined as $P(\mathbf{Z} = \mathbf{z}) \propto$ $\exp(-(\mathbf{z}-0.5)^2/0.1^2)$ (the subtraction $\mathbf{z}-0.5$ is elementwise). The continuous Z follows a 2-standard-deviation truncated independent Gaussian distribution with the mean of 0.5 and standard deviation 0.125. It is noted that when $\mathcal{D}_{\mathbf{z}}$ is discrete, there is a large region of Z with low probability $P(\mathbf{Z})$ in experiments with synthetic benchmark functions. This is to highlight the advantage of V-UCB Prob in exploiting $P(\mathbf{Z})$ compared with V-UCB Unif. In the robot pushing experiment, the region of Z with low probability is smaller than that in the experiments with synthetic benchmark functions (e.g., Hartmann-(1, 2)), which is illustrated in Fig. 6. Therefore, the gap in the performance between V-UCB Unif and V-UCB Prob is smaller in the robot pushing pushing experiment (Fig. 5b) than that in the experiment with Hartmann-(1, 2) (Fig. 3c).

When the closed-form expression of the objective func-



Figure 6. Plots of the log values of the un-normalized probabilities of the discrete \mathbf{Z} for the Hartmann-(1, 2) in the left plot and Robot pushing (3, 2) in the right plot. The orange dots show the realizations of the discrete \mathbf{Z} .

tion is known (e.g., synthetic benchmark functions) in the evaluation of the performance metric, the maximum value $\max_{\mathbf{x}\in\mathcal{D}_{\mathbf{x}}}V_{\alpha}(f(\mathbf{x},\mathbf{Z}))$ can be evaluated accurately. On the other hand, when the closed-form expression of the objective function is unknown even in the evaluation of the performance metric (e.g., the simulated robot pushing experiment), the maximum value $\max_{\mathbf{x}\in\mathcal{D}_{\mathbf{x}}}V_{\alpha}(f(\mathbf{x},\mathbf{Z}))$ is estimated by $\max_{\mathbf{x}\in\mathcal{D}_{T}}V_{\alpha}(f(\mathbf{x},\mathbf{Z})) + 0.01$ where \mathcal{D}_{T} are input queries in the experiments with both V-UCB and ρKG^{apx} . The addition of 0.01 is to avoid $-\infty$ value in plots of the log values of the performance metric.

The sizes of the initial observations \mathcal{D}_0 are 3 for the Branin-Hoo and Goldstein-Price functions; 10 for the Hartmann-3D function; 20 for the portfolio optimization problem; and 30 for the simulated robot pushing task. The initial observations are randomly sampled for different random repetitions of the experiments, but they are the same between the same iterations in V-UCB and ρKG^{apx} .

The hyperparameters of GP (i.e., the length-scales and signal variance of the SE kernel) and the noise variance σ_n^2 are estimated by maximum likelihood estimation (Rasmussen & Williams, 2006) every 3 iterations of BO. We set a lower bound of 0.0001 for the noise variance σ_n^2 to avoid numerical errors.

To show the advantage of LNSO, we set the number of samples of W to be 10 for both V-UCB and ρKG^{apx} . The number of samples of x, i.e., $|\mathcal{X}|$, in LNSO (line 9 of Algorithm 2) is 50. The radius r of the local region \mathcal{B} is set to be a small value of 0.1 such that a small neural network works well: 2 hidden layers with 30 hidden neurons at each layer; the activation functions of the hidden layers and the output layer are sigmoid and linear functions, respectively.

Since the theoretical value of β_t is often considered as excessively conservative (Bogunovic et al., 2016; Srinivas et al., 2010; Bogunovic et al., 2018). We set $\beta_t = 2\log(t^2\pi^2/0.6)$ in our experiments while β_t can be tuned to achieved better exploration-exploitation trade-off (Srinivas et al., 2010) or

multiple values of β_t can be used in a batch mode (Torossian et al., 2020).