A. Proof of Lemma 2

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

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

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

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

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

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

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

$$f(x, z) \leq \omega \Rightarrow l_{t-1}(x, z) \leq \omega$$

$$P(f(x, Z) \leq \omega) \geq P(l_{t-1}(x, Z) \leq \omega).$$

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

$$P(f(x, Z) \leq \omega) \geq \alpha \Rightarrow P(l_{t-1}(x, Z) \leq \omega) \geq \alpha.$$

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

B. Proof of (4)

We prove that

$$r(x_t) \leq V_\alpha(u_{t-1}(x_t, Z)) - V_\alpha(l_{t-1}(x_t, Z)) \forall t \geq 1$$

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

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

$$V_\alpha(f(x, Z)) \leq V_\alpha(u_{t-1}(x, Z))$$

$$V_\alpha(f(x, Z)) \geq V_\alpha(l_{t-1}(x, Z)).$$

Hence,

$$r(x_t) \triangleq V_\alpha(f(x_t, Z)) - V_\alpha(f(x_{t-1}, Z))$$

$$\leq V_\alpha(u_{t-1}(x_t, Z)) - V_\alpha(l_{t-1}(x_{t-1}, Z)).$$

Since $x_t$ is selected as $\arg\max_{x \in \mathcal{D}_x} V_\alpha(u_{t-1}(x, Z))$,

$$V_\alpha(u_{t-1}(x_t, Z)) \leq V_\alpha(u_{t-1}(x_{t-1}, Z)),$$

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

\hfill \Box

C. Proof of Theorem 1

Theorem 1. For $\alpha \in (0,1), \forall x \in \mathcal{D}_x, \forall t \geq 1$, there exists a lacing value in $\mathcal{D}_z$ with respect to $x$ and $t$.

Proof. Recall that

$$\mathcal{Z}_1^\leq \triangleq \{ z \in \mathcal{D}_z : l_{t-1}(x, z) \leq V_\alpha(l_{t-1}(x, Z)) \}.$$ 

From the definition of $\mathcal{Z}_1^\leq$ and $V_\alpha(l_{t-1}(x, Z))$, we have

$$P(Z \in \mathcal{Z}_1^\leq) \geq \alpha.$$ 

Since $\alpha \in (0,1), \mathcal{Z}_1^\leq \neq \emptyset$. We prove the existence of LV by contradiction: (a) assuming that $\exists x \in \mathcal{D}_x, \exists t \geq 1, \forall z \in \mathcal{Z}_1^\leq, u_{t-1}(x, z) < V_\alpha(u_{t-1}(x, Z))$ and then, (b) proving that $V_\alpha(u_{t-1}(x, Z))$ is not a lower bound of $\{ \omega : P(u_{t-1}(x, Z) \leq \omega) \geq \alpha \}$ which is a contradiction.

Since the GP posterior mean $\mu_{t-1}$ and posterior standard deviation $\sigma_{t-1}$ are continuous functions in $\mathcal{D}_x \times \mathcal{D}_z, l_{t-1}$ and $u_{t-1}$ are continuous functions in the closed $\mathcal{D}_z \subset \mathbb{R}^{d_z}$ ($x$ and $t$ are given and remain fixed in this proof). We will prove that $\mathcal{Z}_1^\leq$ is closed in $\mathbb{R}^{d_z}$ by contradiction.

If $\mathcal{Z}_1^\leq$ is not closed in $\mathbb{R}^{d_z}$, there exists a limit point $z_p$ of $\mathcal{Z}_1^\leq$ such that $z_p \notin \mathcal{Z}_1^\leq$. Since $\mathcal{Z}_1^\leq \subset \mathcal{D}_z$ and $\mathcal{D}_z$ is closed in $\mathbb{R}^{d_z}, z_p \in \mathcal{D}_z$. Thus, for $z_p \notin \mathcal{Z}_1^\leq, l_{t-1}(x, z_p) > V_\alpha(l_{t-1}(x, Z))$ (from the definition of $\mathcal{Z}_1^\leq$). Then, there exists $\epsilon_0 > 0$ such that $l_{t-1}(x, z_p) > V_\alpha(l_{t-1}(x, Z)) + \epsilon_0$. The pre-image of the open interval $I_0 = (l_{t-1}(x, z_p) - \epsilon_0/2, l_{t-1}(x, z_p) + \epsilon_0/2)$ under $l_{t-1}$ is also an open set $\mathcal{Z}_1^\leq$ containing $z_p$ (because $l_{t-1}$ is a continuous function). Since $z_p$ is a limit point of $\mathcal{Z}_1^\leq$, there exists an $z' \in \mathcal{Z}_1^\leq \cap \mathcal{V}$. Then, $l_{t-1}(x, z') \in I_0$, so $l_{t-1}(x, z') \geq l_{t-1}(x, z_p) - \epsilon_0/2 \geq V_\alpha(l_{t-1}(x, Z)) + \epsilon_0/2 = V_\alpha(l_{t-1}(x, Z)) + \epsilon_0/2$. It contradicts $z' \in \mathcal{Z}_1^\leq$.

Therefore, $\mathcal{Z}_1^\leq$ is a closed set in $\mathbb{R}^{d_z}$. Besides, since $\{u_{t-1}(x, z) : z \in \mathcal{Z}_1^\leq\}$ is upper bounded by $V_\alpha(u_{t-1}(x, Z))$ (due to our assumption), so
sup{u_{t-1}(x, z) : z \in Z_l^\leq} exists. Let z_t^* be such that u_{t-1}(x, z_t^*) \equiv \sup\{u_{t-1}(x, z) : z \in Z_l^\leq\}. Then, z_t^* \in Z_l^\leq because Z_l^\leq is closed. Moreover, from our assumption that \forall z \in Z_l^\leq, u_{t-1}(x, z) < V_\alpha(u_{t-1}(x, Z)), we have u_{t-1}(x, z_t^*) < V_\alpha(u_{t-1}(x, Z)). Furthermore,
\[ P(u_{t-1}(x, Z) \leq u_{t-1}(x, z_t^*)) \geq P(Z \in Z_l^\leq) \geq \alpha. \]

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

\[ \square \]

D. Proof of Lemma 3

Lemma 3. By selecting x_t as a maximizer of V_\alpha(u_{t-1}(x, Z)) and selecting z_t as an LV w.r.t x_t, the instantaneous regret is upper-bounded by:
\[ r(x_t) \leq 2\beta_1^{1/2} \sigma_{t-1}(x_t, z_t) \forall t \geq 1 \]
with probability \geq 1 - \delta for \delta in Lemma 1.

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

From (4), by selecting z_t as an LV, for all t \geq 1,
\[ r(x_t) \leq V_\alpha(u_{t-1}(x, Z)) - V_\alpha(l_{t-1}(x_t, Z)) \leq u_{t-1}(x_t, z_t) - l_{t-1}(x_t, z_t) \]
(since z_t is an LV)
\[ \leq \mu_{t-1}(x_t, z_t) + \beta_1^{1/2} \sigma_{t-1}(x_t, z_t) \]
\[ - \mu_{t-1}(x_t, z_t) + \beta_1^{1/2} \sigma_{t-1}(x_t, z_t) \]
\[ = 2\beta_1^{1/2} \sigma_{t-1}(x_t, z_t). \]

\[ \square \]

E. Bound on the Average Cumulative Regret

Conditioned on the event f(x, z) \in I_{t-1}[f(x, z)] \triangleq [l_{t-1}(x, z), u_{t-1}(x, z)] for all x \in D_x, z \in D_z, t \geq 1 which occurs with probability \geq 1 - \delta in Lemma 1, it follows that r(x_t) \leq 2\beta_1^{1/2} \sigma_{t-1}(x_t, z_t) \forall t \geq 1 in Lemma 3. Therefore,
\[ R_T \triangleq \sum_{t=1}^T r(x_t) \leq \sum_{t=1}^T 2\beta_1^{1/2} \sigma_{t-1}(x_t, z_t) \leq 2\beta_T^{1/2} \sum_{t=1}^T \sigma_{t-1}(x_t, z_t) \]

since \beta_t is a non-decreasing sequence.

From Lemma 5.4 and the Cauchy-Schwarz inequality in (Srinivas et al., 2010), we have
\[ 2 \sum_{t=1}^T \sigma_{t-1}(x_t, z_t) \leq \sqrt{C_1 T \gamma_T} \]

where \(C_1 = 8/\log(1 + \sigma_n^2)\). Hence,
\[ R_T \leq \sqrt{C_1 T \beta_T \gamma_T}. \]

Equivalently, \(R_T / T \leq \sqrt{C_1 \beta_T \gamma_T / T}\). Since \(\gamma_T\) 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 \(r(x_{t_*(T)})\)

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

At T-th iteration, by recommending x_{t_*(T)} as an estimate of x_t where \(t_*(T) \triangleq \arg\max_{t \in \{1, \ldots, T\}} V_\alpha(l_{t-1}(x_t, Z))\), we have
\[ V_\alpha(l_{t_*(T)}(x_{t_*(T)}, Z)) = \max_{t \in \{1, \ldots, T\}} V_\alpha(l_{t-1}(x_t, Z)) \geq \frac{1}{T} \sum_{t=1}^T V_\alpha(l_{t-1}(x_t, Z)). \]

Therefore,
\[ r(x_{t_*(T)}) = V_\alpha(f(x_{t_*(T)}, Z)) - V_\alpha(f(x_{t_*(T)}, Z)) \leq V_\alpha(f(x_{t_*(T)}, Z)) - V_\alpha(l_{t_*(T)}(x_{t_*(T)}, Z)) \]
\[ \leq \frac{1}{T} \sum_{t=1}^T (V_\alpha(f(x, Z)) - V_\alpha(l_{t-1}(x_t, Z))). \]

Furthermore, \(V_\alpha(f(x, Z)) \leq V_\alpha(u_{t-1}(x_t, Z))\) from our
condition, so
\[
\begin{align*}
r(x_{t*}(T)) & \leq \frac{1}{T} \sum_{t=1}^{T} (V_0(f(x_t, Z)) - V_0(l_{t-1}(x_t, Z))) \\
& \leq \frac{1}{T} \sum_{t=1}^{T} (V_0(u_{t-1}(x_t, Z)) - V_0(l_{t-1}(x_t, Z))) \\
& \leq \frac{1}{T} \sum_{t=1}^{T} (V_0(u_{t-1}(x_t, Z)) - V_0(l_{t-1}(x_t, Z))) \\
& \leq \frac{1}{T} \sum_{t=1}^{T} (u_{t-1}(x_t, z_t) - l_{t-1}(x_t, z_t)) \text{ (since } z_t \text{ is an LV)}
\end{align*}
\]

\[
\leq \frac{1}{T} \sum_{t=1}^{T} 2\beta_t^{1/2} \sigma_t^{-1}(x_t, z_t)
\leq \sqrt{\frac{C_1 \beta_T \gamma_T}{T}} \text{ (from Appendix E)}.
\]

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

G. Proof of Theorem 2 and Its Corollaries

G.1. Proof of Theorem 2

**Theorem 2.** Let $W$ be a random variable with the support $D_W \subset \mathbb{R}^{d_w}$ and dimension $d_w$. Let $h$ be a continuous function mapping from $w \in D_w$ to $\mathbb{R}$. Then, $h(W)$ denotes the random variable whose realization is the function $h$ evaluated at a realization $w$ of $W$. Suppose $h(w)$ has a minimizer $w_{\text{min}} \in D_w$, then $\lim_{\alpha \to \alpha^+} V_0(h(W)) = h(w_{\text{min}})$.

Recall that the support $D_w$ of $W$ is defined as the smallest closed subset of $\mathbb{R}^{d_w}$ such that $P(W \in D_w) = 1$, and $w_{\text{min}} \in D_w$ minimizes $h(w)$.

**Lemma 4.** For all $\alpha \in (0, 1)$, $V_0(h(W))$ is a nondecreasing function, i.e.,

$$\forall 1 > \alpha > \alpha' > 0, V_0(h(W)) \geq V_{\alpha'}(h(W)).$$

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

$$P(h(W) \leq \omega) \geq \alpha \Rightarrow P(h(W) \leq \omega) \geq \alpha'.$$

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

$$\inf\{\omega : P(h(W) \leq \omega) \geq \alpha\} \geq \inf\{\omega : P(h(W) \leq \omega) \geq \alpha'\}$$

i.e., $V_0(h(W)) \geq V_{\alpha'}(h(W))$. \hfill \qed

Let

$$\omega_0^+ \triangleq \lim_{\alpha \to 0^+} V_0(h(W)). \tag{12}$$

Then, from Lemma 4, the following lemma follows.

**Lemma 5.** For all $\alpha \in (0, 1)$, and $\omega_{\alpha^+}$ defined in (12)

$$\omega_0^+ \leq V_0(h(W)).$$

We use Lemma 5 to prove the following lemma.

**Lemma 6.** For all $w \in D_w$, and $\omega_{\alpha^+}$ defined in (12)

$$\omega_0^+ \leq h(w)$$

which implies that

$$\omega_0^+ \leq h(w_{\text{min}}).$$

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

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

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

$$P(h(W) \leq \omega_0^+) \geq P(h(W) \leq h(w') + \epsilon_1/2) \geq P(h(W) \in I_h) > 0.$$

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

$$V_{\alpha_0}(h(W)) \triangleq \inf\{\omega : P(h(W) \leq \omega) \geq \alpha_0\} \leq h(w') + \epsilon_1/2 < \omega_0^+$$

which is a contradiction to Lemma 5. \hfill \qed

**Lemma 7.** For $\omega_{\alpha^+}$ defined in (12)

$$\omega_0^+ \geq h(w_{\text{min}}). \tag{13}$$

**Proof.** By contradiction, we assume that $\omega_{\alpha^+} < h(w_{\text{min}})$. Then there exists $\epsilon_2 > 0$ that $\omega_{\alpha^+} + \epsilon_2 < h(w_{\text{min}})$. Since $\omega_{\alpha^+} \triangleq \lim_{\alpha \to 0^+} V_0(h(W))$ so there exists $\alpha_0 > 0$ such that $V_{\alpha_0}(h(W)) \in (\omega_{\alpha^+}, \omega_{\alpha^+} + \epsilon_2)$. However,

$$P(h(W) \leq V_0(h(W))) \leq P(h(W) \leq \omega_{\alpha^+} + \epsilon_2 < h(w_{\text{min}})) = 0$$
which contradicts the fact that $\alpha_0 > 0$. Therefore, $\omega_0^+ \geq h(\omega_{\text{min}})$.

From (12), Lemma 6 and Lemma 7,

$$\lim_{\alpha \to 0^+} V_\alpha(h(W)) = h(\omega_{\text{min}})$$

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

G.2. Corollary 2.2

From Theorem 2, $D_z$ is a closed subset of $\mathbb{R}^d_z$, and $u_l - 1(x, z)$, $l_l - 1(x, z)$ are continuous functions over $z \in D_z$, it follows that the selected $x_t$ by both STABLEOPT (in (5)) and V-UCB are the same. Furthermore,

$$Z_l^\leq \Delta \left\{ z \in D_z : l_{l - 1}(x, z) \leq V_\alpha(l_{l - 1}(x, Z)) \right\}$$

$$= \left\{ z \in D_z : l_{l - 1}(x, z) \leq \min_{x \in D_z} l_{l - 1}(x, z') \right\}$$

$$= D_z \cap \{ z \in D_z : l_{l - 1}(x, z) = \min_{x \in D_z} l_{l - 1}(x, z') \}$$

Therefore, the set of lacing values is $Z_l^\leq \cap Z_u^\geq = Z_l^\leq = \left\{ z \in D_z : l_{l - 1}(x, z) = \min_{x \in D_z} l_{l - 1}(x, z') \right\}$ any of which is also the selected $z_l$ in (5) by STABLEOPT. Thus, the selected $z_l$ by both STABLEOPT and V-UCB are the same.

H. Local Neural Surrogate Optimization

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

- Whenever the current updated $x^{(i)}$ is not in $B(x_c, r)$ (line 4), the center $x_c$ of the ball $B$ is updated to be $x^{(i)}$ (line 6) and the surrogate function $g(x, \theta)$ is re-trained (lines 7-12).

- The surrogate function $g(x, \theta)$ is (re-)trained to estimate $V_\alpha(h(x, Z))$ well for all $x \in B(x_c, r)$ (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 $x \in B(x_c, r)$ (line 9):

$$\mathcal{L}_g(\mathcal{X}, \mathcal{Z}) \Delta \frac{1}{|\mathcal{X}||\mathcal{Z}|} \sum_{x \in \mathcal{X}, z \in \mathcal{Z}} [\rho_\alpha(h(x, z) - g(x, \theta))]$$

(14)

where $\rho_\alpha$ is the pinball function in Sec. 3.5.

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

I. Experimental Details

Regarding the construction of $D_z$ in optimizing the synthetic benchmark functions, the discrete $D_z$ is selected as equi-distance points (e.g., by dividing $[0, 1]^{d_z}$ into a grid). The probability mass of $Z$ is defined as $P(Z = z) \propto \exp(-(z - 0.5)^2/0.1^2)$ (the subtraction $z - 0.5$ is element-wise). 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 $D_z$ is discrete, there is a large region of $Z$ with low probability $P(Z)$ in experiments with synthetic benchmark functions.

This is to highlight the advantage of V-UCB Prob in exploiting $P(Z)$ 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 experiment (Fig. 5b) than that in the experiment with Hartmann-3D-$(1, 2)$ (Fig. 3c).

When the closed-form expression of the objective func-
To show the advantage of LNSO, we set the number of iterations of BO. We set $\beta_i$ to be small enough so 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 $\beta_i$ is often considered as excessively conservative (Bogunovic et al., 2016; Srinivas et al., 2010; Bogunovic et al., 2018). We set $\beta_i = 2 \log(t^2 \pi^2 / 0.6)$ in our experiments while $\beta_i$ can be tuned to achieved better exploration-exploitation trade-off (Srinivas et al., 2010) or multiple values of $\beta_i$ can be used in a batch mode (Torossian et al., 2020).

Fig. 7 shows the performance advantage of our V-UCB method over a baseline that selects the input query as a random $(\mathbf{x}, \mathbf{z}) \in D_X \times D_Z$, labeled as Random in the figure.