Supplementary Material for the Paper entitled "Objective Bound Conditional Gaussian Process for Bayesian Optimization"

A Notations

In this supplementary material, we use the following notations:

$D_n = (\boldsymbol{X}_n, (f(X_n))) = (\boldsymbol{X}_n, \boldsymbol{f}_n)$

$\mu_{GP}(x; D_n) = k(x, \boldsymbol{X}_n)\boldsymbol{K(X_n, X_n)^{-1}} \boldsymbol{f}_n$

$\hat{\mu}(x; D_n, Z_M) = E[f(x)|D_n, x_M, Z_M] = \mu_{GP}(x; D_n, x_M, f(x_M))$

$\tilde{\mu}(x; D_n) = E[\hat{\mu}(x; D_n, Z_M)|D_n]$

$\sigma^2_{GP}(x; D_n) = \sigma^2_{GP}(x; \boldsymbol{X}_n) = k(x, x) - k(x, \boldsymbol{X}_n)\boldsymbol{K(X_n, X_n)^{-1}} k(\boldsymbol{X}_n, x)$

$\sigma^2_{GP,\sigma^2}(x; D_n) = \sigma^2_{GP,\sigma^2}(x; \boldsymbol{X}_n) = k(x, x) - k(x, \boldsymbol{X}_n)(\boldsymbol{K(X_n, X_n)} + \sigma^2 I_n)^{-1} k(\boldsymbol{X}_n, x)$

$\hat{\sigma}^2(x; D_n, Z_M) = Var[f(x)|D_n, x_M, Z_M] = \sigma^2_{GP}(x; \boldsymbol{X}_n, x_M) < \sigma^2_{GP}(x; \boldsymbol{X}_n)$

$\tilde{\sigma}^2(x; D_n) = E(\hat{\sigma}^2(x; D_n, Z_M)|D_n) + Var(\hat{\mu}(x; D_n, Z_M)|D_n)$ (Law of total variance)

$\Sigma_{n\times n} = K(\boldsymbol{X}_n, \boldsymbol{X}_n) - k(\boldsymbol{X}_n, x_M)k^{-1}(x_M, x_M)k(x_M, \boldsymbol{X}_n)$

B Inference for Case 2

We describe the inference procedure for Case 2 in Section 3.2 in more detail. As mentioned in Section 3, we use variational inference to estimate the parameters of OBCGP. The variational lower bound is expressed as

$$L(\theta, \phi; D_n) = E_{q_\phi(Z_M)}[\log p_\theta(\mathbf{f}_n|Z_M)] - KL(q_\phi(Z_M)||p(Z_M)).$$

In Case 2, we take beta(α, β) as a variational distribution over Z_M. A beta distribution provides various shapes of a density function, depending on the parameters. Therefore, it can approximate $p(Z_M|\mathbf{f}_n)$ flexibly. First of all, KL divergence has the following analytical formula:

$$KL(q_\phi(Z_M)||p(Z_M)) = \log \frac{B(1,\lambda)}{B(\alpha,\beta)} + (\alpha-1)\gamma(\alpha) + (\beta-\lambda)\gamma(\beta) + (1+\lambda-\alpha-\beta)\gamma(\alpha+\beta),$$

where $B(\alpha, \beta)$ is a beta function. The first term of $L(\theta, \phi; D_n)$ can also be computed using a closed-form expression as follows:

$$\begin{aligned}
&E_{q_\phi(Z_M)}[\log p_\theta(\mathbf{f}_n|Z_M)] \\
&\propto -\frac{1}{2}\log|\Sigma_{n\times n}| - \frac{1}{2}(\mathbf{f}_n - l_p\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)})^T\Sigma_{n\times n}^{-1}(\mathbf{f}_n - l_p\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)}) \\
&+ E_1^q(u_p - l_p)\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)}^T\Sigma_{n\times n}^{-1}(\mathbf{f}_n - l_p\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)}) - \frac{1}{2}E_2^q(u_p-l_p)^2\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)}^T\Sigma_{n\times n}^{-1}\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)},
\end{aligned} \quad (1)$$

where E_1^q and E_2^q are the first and second moments of $q_\phi(Z_M)$, respectively. Then, using Eq.(1), we can obtain the posterior mean and variance of $f(x^*)$, given D_n, as in Section 3.2.

C Derivation of Eq.(7)

In the inference procedure, when the parameters of (ψ, ϕ) are fixed, x_M should maximize $E_{q_\phi(Z_M)}[\log p_\theta(\boldsymbol{f}_n|Z_M)]$, because the KL divergence term does not contain x_M. Let $f^q(x_M)$ denote the the random variable following the posterior distribution of $f(x_M)$ in both Case 1 and Case 2 (see Section 6.1 in the paper). Then, $E_{q_\phi(Z_M)}[\log p_\theta(\boldsymbol{f}_n|Z_M)]$ can be written as follows:

$$\begin{aligned}
&E_{q_\phi(Z_M)}[\log p_\theta(\boldsymbol{f}_n|Z_M)] = E_{f^q(x_M)}[\log p_\theta(\boldsymbol{f}_n|f^q(x_M))] \\
&\propto E_{f^q(x_M)}[-\frac{1}{2}\log|\Sigma_{n\times n}| - \frac{1}{2}(\mathbf{f}_n - f^q(x_M)\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)})^T\Sigma_{n\times n}^{-1}(\mathbf{f}_n - f^q(x_M)\frac{k(\boldsymbol{X}_n, x_M)}{k(x_M,x_M)})].
\end{aligned}$$

To express this formula in terms of the GP posterior moments (i.e., $\mu_{GP}(x; D_n)$ and $\sigma^2_{GP}(x; D_n)$), we use the following two properties: For $n \times n$ matrix A and $n \times 1$ vectors b and c,

Property 1. $(A + bc^T)^{-1} = A^{-1} - \frac{A^{-1}bc^T A^{-1}}{1+c^T A^{-1}b}$

Property 2. $det(I + bc^T) = 1 + b^T c$

Using the property 1, we obtain $\Sigma_{n\times n}^{-1} = K^{-1} + \frac{K^{-1}k(X_n,x_M)k(x_m,X_n)K^{-1}}{\sigma_{GP}^2(x_M;D_n)}$. Also, using the property 2, we obtain $\log|\Sigma_{n\times n}| = \log(\sigma_{GP}^2(x;D_n)) + \log|K|$. Applying these results to $E_{q_\phi(Z_M)}[\log p_\theta(\boldsymbol{f}_n|Z_M)]$, Eq.(7) is derived.

D Acquisition functions with GP

Given the observed data D_{n-1}, BOs (with GP) select the next query point by optimizing an acquisition function $\alpha(x; D_{n-1})$, which is computed based on the GP posterior. We discuss the detailed formula of acquisition functions with the GP.

GP-UCB. GP-UCB is an acquisition function motivated from the confidence bound on the GP posterior. Using the posterior distribution $f(x)|D_n \sim N(\mu_{GP}(x; D_{n-1}), \sigma_{GP}^2(x; D_{n-1}))$, GP-UCB sets $\alpha(x; D_n) = \mu_{GP}(x; D_n) + \lambda\sigma_{GP}(x; D_n)$, where λ is a positive hyperparameter. The next query point is selected so as to maximize $\alpha(x)$.

GP-EI. GP-EI is also based on the GP posterior. It sets $\alpha(x; D_n) = E_{f(x)|D_n}[(f(x) - \theta)^+]$, which can be expressed in a closed-form analytically. In detail, $\alpha(x; D_n) = [\phi(\gamma(x)) - \gamma(x)\Phi(\gamma(x))]\sigma_{GP}(x; D_n)$, where $\gamma(x) = \frac{\theta - \mu_{GP}(x;D_n)}{\sigma_{GP}(x;D_n)}$, and $\phi(\cdot)$ and $\Phi(\cdot)$ are the standard normal pdf and cdf, respectively. A popular choice of θ is the maximum observed function value.

GP-MES. Max-value entropy search (MES) acquisition function is an information-theoretic approach, which quantifies the information gain about the maximum function value. The acquisition function of GP-MES is $\alpha(x; D_n) = I(f_{opt}, \mathbf{f_n}|D_n, x)$, where $I(\cdot, \cdot)$ is the mutual information, and f_{opt} is the true optimal function value. GP-MES can be approximately computed based on the samples of f_{opt}, whose distribution is inferred through the Gumbel or GP posterior distribution (Wang and Jegelka, 2017).

E Acquisition functions with OBCGP

As discussed in Section 4, we can approximate the posterior distribution of the OBCGP as a Gaussian using moment matching. Then, we can readily evaluate acquisition functions mentioned in Section D for OBCGP, just by replacing $\mu_{GP}(x; D_n)$ and $\sigma^2_{GP}(x; D_n)$ with $\tilde{\mu}(x; D_n)$ and $\tilde{\sigma}^2(x; D_n)$ (see Section 3), respectively. For example, OBCGP-EI and OBCGP-UCB can be written as follows:

OBCGP-EI.

$$x_n = \text{argmax}_{x\in\Omega} \ [\phi(\tilde{\gamma}(x)) - \tilde{\gamma}(x)\Phi(\tilde{\gamma}(x))]\tilde{\sigma}(x; D_{n-1}), \qquad \tilde{\gamma}(x) = \frac{f_{best} - \tilde{\mu}(x; D_{n-1})}{\tilde{\sigma}(x; D_{n-1})}.$$

OBCGP-UCB.

$$x_n = \text{argmax}_{x\in\Omega} \ \tilde{\mu}(x; D_{n-1}) + \beta_n^{1/2}\hat{\sigma}(x; D_{n-1}, Z_M).$$

Alternatively, we can evaluate the acquisition functions using Monte Carlo samples from the OBCGP posterior, without the normal approximation, as discussed in Section 4. For example, the EI can be rewritten as $EI(x) = \alpha(x; D_n) = E[E[(f(x) - f_{best})^+|D_n, f(x_M)]|D_n]$. Then, the inner expectation term can be derived in a closed-form similar to the GP-EI, using the fact that given D_n and $f(x_M)$, $f(x)$ follows a normal distribution by definition of the OBCGP (Note that when we use the moment matching approximation, it is assumed that given D_n, $f(x)$ follows a normal distribution.) The outer expectation term can be approximated using Monte Carlo samples from $p(f(x_M)|D_n)$. We denote this sampling-based calculation of the EI by EIs, to differentiate the calculation of the EI based on the moment-matching approximation. We provide the experiments results of OBCGP-EIs in Section H.1. The inner expectation of the EI for the OBCGP have different closed-form expressions for Case 1 and Case 2 as follows:

OBCGP-EIs (Case 1)

$$\begin{aligned} x_n &= \text{argmax}_{x\in\Omega} \ E[E[(f(x) - f_{best})^+|D_{n-1}, f(x_M)]|D_{n-1}] \\ &\approx \text{argmax}_{x\in\Omega} \ \frac{1}{N}\sum_{i=1}^{N}[\phi(\gamma_1(x, Z_M^i)) - \gamma_1(x, Z_M^i)\Phi(\gamma_1(x, Z_M^i))]\hat{\sigma}(x; D_{n-1}, Z_M), \end{aligned}$$

where $\phi(\cdot)$ is the standard normal pdf, Z_M^i are the samples from $p(Z_M|D_{n-1}) \approx q_\phi(Z_M)$ for Case 1 (i.e., $Z_M^i \sim gamma(\alpha, \beta)$), $\gamma_1(x, Z_M^i) = [f_{best} - \mu_{GP}(x; D_{n-1}) - \frac{\Lambda(x,x_M)-k(x,x_M)}{\sigma^2_{GP}(x_M;D_{n-1})}(\mu_{GP}(x_M; D_{n-1}) - l_p - Z_M^i)]/\hat{\sigma}(x; D_{n-1}, Z_M)$, and $\Lambda(x, x_M) = k(x, \boldsymbol{X}_n)\boldsymbol{K(X_n, X_n)^{-1}}k(\boldsymbol{X}_n, x_M)$.

OBCGP-EIs (Case 2)

$$\begin{aligned} x_n &= \operatorname{argmax}_{x\in\Omega}\ E[E[(f(x) - f_{best})^+|D_{n-1}, f(x_M)]|D_{n-1}] \\ &\approx \operatorname{argmax}_{x\in\Omega}\ \frac{1}{N}\sum_{i=1}^{N}[\phi(\gamma_2(x, Z_M^i)) - \gamma_2(x, Z_M^i)\Phi(\gamma_2(x, Z_M^i))]\hat{\sigma}(x; D_{n-1}, Z_M), \end{aligned}$$

where Z_M^i are the samples from $p(Z_M|D_{n-1}) \approx q_\phi(Z_M)$ for Case 2 (i.e., $Z_M^i \sim beta(\alpha, \beta)$) and $\gamma_2(x, Z_M^i) = [f_{best} - \mu_{GP}(x; D_{n-1}) - \frac{\Lambda(x,x_M)-k(x,x_M)}{\sigma^2_{GP}(x_M;D_{n-1})}(\mu_{GP}(x_M; D_{n-1}) - l_p - (u_p - l_p)Z_M^i)]/\hat{\sigma}(x; D_{n-1}, Z_M)$. For both cases, $\hat{\sigma}(x; D_{n-1}, Z_M) = \sqrt{\sigma^2_{GP}(x; D_{n-1}) - \frac{(\Lambda(x,x_M)-k(x,x_M))^2}{\sigma^2_{GP}(x_M;D_{n-1})}}$.

F Proof of Theorem 1

Suppose that we have observed up to the ith data point. Then, using the conditional GP model, $f(x)|D_i, x_M, Z_M \sim N(\hat{\mu}(x; D_i, Z_M), \hat{\sigma}^2(x; D_i, Z_M))$. In Theorem 1, we derive the bounded cumulative regret of OBCGP-UCB, which is the sum of instantaneous regrets. The first step to prove Theorem 1 is to find an appropriate β_i in OBCGP-UCB that makes instantaneous regret to be bounded. We can find such β_i from the results of Lemmas 1, 2 and 3.

Lemma 1 (Doob's Conditional independence property (Doob, 1953))**.** *If X, Y are conditional independent given Z, then*

$$P(X \in A|Y, Z) = P(X \in A|Z).$$

Lemma 2. *Pick $\delta \in (0, 1)$ and set $\beta_i = 2\log(\frac{|\Omega|\pi_i}{\delta(1-\gamma_i)})$, where $\sum_{i\geq 1}\pi_i^{-1} = 1, \pi_i > 0$ and $\gamma_i = \max(P(Z_M < E[Z_M|D_{i-1}]|D_{i-1}), P(Z_M > E[Z_M|D_{i-1}]|D_{i-1}))$. Then*

$$|f(x) - \tilde{\mu}(x; D_{i-1})| \leq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M) \quad \forall x \in \Omega \quad \forall i \geq 1$$

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

Proof. Note that if $r \sim N(0,1)$, then for $c > 0$,

$$P(r > c) = e^{-c^2/2}(2\pi)^{-1/2} \int e^{-(r-c)^2/2 - c(r-c)} \leq e^{-c^2/2} P(r > 0) = (1/2)e^{-c^2/2},$$

because $e^{-c(r-c)} \leq 1$ for $r \geq c$. Therefore, $P(\Big[|f(x) - \hat{\mu}(x; D_{i-1}, Z_M)| > \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M, Z_M) \leq e^{-\beta_i/2}$. Note that $f(x) - \hat{\mu}(x; D_{i-1}, Z_M)|D_{i-1}, x_M, Z_M \sim N(0, \hat{\sigma}^2(x; D_{i-1}, Z_M))$. Therefore, $f(x) - \hat{\mu}(x; D_{i-1}, Z_M)$ and Z_M are conditionally independent given D_{i-1}. Applying Lemma 1, we have

$$P(\Big[|f(x) - \hat{\mu}(x; D_{i-1}, Z_M)| > \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M) \leq e^{-\beta_i/2}. \tag{2}$$

Now, we consider the bound of $P(\Big[|f(x) - \tilde{\mu}(x; D_{i-1})| \geq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M)$. With the result in Eq.(2), we obtain the following bound:

$$\begin{aligned}
&P(\Big[|f(x) - \tilde{\mu}(x; D_{i-1})| \geq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M) \\
&= P(\Big[f(x) - \tilde{\mu}(x; D_{i-1}) \geq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M), \hat{\mu}(x; D_{i-1}, Z_M) > \tilde{\mu}(x; D_{i-1})\Big] \,|D_{i-1}, x_M) \\
&+ P(\Big[f(x) - \tilde{\mu}(x; D_{i-1}) \geq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M), \hat{\mu}(x; D_{i-1}, Z_M) \leq \tilde{\mu}(x; D_{i-1})\Big] \,|D_{i-1}, x_M) \\
&+ P(\Big[f(x) - \tilde{\mu}(x; D_{i-1}) \leq -\beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M), \hat{\mu}(x; D_{i-1}, Z_M) \geq \tilde{\mu}(x; D_{i-1})\Big] \,|D_{i-1}, x_M) \\
&+ P(\Big[f(x) - \tilde{\mu}(x; D_{i-1}) \leq -\beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M), \hat{\mu}(x; D_{i-1}, Z_M) < \tilde{\mu}(x; D_{i-1})\Big] \,|D_{i-1}, x_M) \\
&\leq P(\Big[|f(x) - \hat{\mu}(x; D_{i-1}, Z_M)| > \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M) \\
&+ \gamma_i P(\Big[|f(x) - \tilde{\mu}(x; D_{i-1})| \geq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M).
\end{aligned}$$

Therefore,

$$\begin{aligned}
&P(\Big[|f(x) - \tilde{\mu}(x; D_{i-1})| \geq \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M) \\
&\leq P(\Big[|f(x) - \hat{\mu}(x; D_{i-1}, Z_M)| > \beta_i^{1/2}\hat{\sigma}(x; D_{i-1}, Z_M)\Big] \,|D_{i-1}, x_M) \frac{1}{1-\gamma_i} \\
&\leq e^{-\beta_i/2} \frac{1}{1-\gamma_i},
\end{aligned}$$

where $\gamma_i = \max(P(Z_M < E[Z_M|D_{i-1}]|D_{i-1}), P(Z_M > E[Z_M|D_{i-1}]|D_{i-1}))$. Finally, applying the union bound,

$$f(x) - \tilde{\mu}(x; D_{i-1})| \leq \beta_i^{1/2} \hat{\sigma}(x; D_{i-1}, Z_M) \quad \forall x \in \Omega$$

holds with probability $\geq 1 - \frac{|\Omega| e^{-\beta_i/2}}{1-\gamma_i}$. Choosing $\beta_i = 2\log(\frac{|\Omega|\pi_i}{\delta(1-\gamma_i)})$, the statement holds. $\pi_i = \pi^2 n^2/6$ could be an example for this lemma. □

Lemma 3. *Define the instantaneous regret* $r_i = f(x_{opt}) - f(x_i)$*. If* $|f(x) - \tilde{\mu}(x; D_{i-1})| \leq \beta_i^{1/2} \hat{\sigma}(x; D_{i-1}, Z_M)$*, then* $r_i \leq 2\beta_i^{1/2} \hat{\sigma}(x_i; D_{i-1})$*.*

Proof. By the selection rule of the conditional GP-UCB, $\tilde{\mu}(x_i; D_{i-1}) + \beta_i^{1/2} \hat{\sigma}(x_i; D_{i-1}) \geq \tilde{\mu}(x_{opt}; D_{i-1}) + \beta_i^{1/2} \hat{\sigma}(x_{opt}; D_{i-1}, Z_M) \geq f(x_{opt})$. Thus,

$$r_i = f(x_{opt} - f(x_i)) \leq \beta_i^{1/2} \hat{\sigma}(x_i; D_{i-1}, Z_M) + \tilde{\mu}(x_i; D_{i-1}) - f(x_{opt}) \leq 2\beta_i^{1/2} \hat{\sigma}(x_i; D_{i-1}, Z_M).$$

□

Lemmas 4 and 5 show the relationship between the mutual information and the sum of posterior variances. From the result of Lemma 3, cumulative regret is bonded by the sum of $\beta_i^{1/2} \hat{\sigma}(x; D_{i-1}, Z_M)$. By using the result of Lemma 5, we will express the bound of cumulative regret in terms of mutual information.

Lemma 4 (Srinivas et al. (2009))**.** *Suppose* $y_i = f(x_i) + \epsilon_i$*, where* $\epsilon \sim N(0, \sigma^2)$ *and* $f \sim GP(0, K)$*. The mutual information between* f *and observation* $\boldsymbol{y}_n = \boldsymbol{f}_n + \epsilon_n$ *can be expressed in terms of* σ^2_{GP,σ^2}*:*

$$I(\boldsymbol{y}_n; \boldsymbol{f}_n, \sigma^2) = \frac{1}{2} \sum_{i=1}^{n} \log(1 + \sigma^{-2} \sigma^2_{GP,\sigma^2}(x_i; D_{i-1})).$$

Lemma 5. $I(\boldsymbol{y}_n; \boldsymbol{f}_n, \sigma^2) \geq \frac{1}{2} \sum_{i=1}^{n} \log(1 + \sigma^{-2} \sigma^2_{GP}(x_i; D_{i-1}))$*.*

Proof. Using the Woodbury identity or Kailath variant,

$$(\boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1}) + \sigma^2 I)^{-1} = \boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1})^{-1} - \sigma^2 \boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1})^{-1} (\boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1}) + \sigma^2 I)^{-1}.$$

Because $\sigma^2_{GP,\sigma^2}(x_i; D_{i-1}) = k(x_i, x_i) - k(x_i, \boldsymbol{X}_{i-1})(\boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1}) + \sigma^2 I)^{-1} k(\boldsymbol{X}_{i-1}, x_i)$, we have

$$\sigma^2_{GP,\sigma^2}(x_i; D_{i-1}) = \sigma^2_{GP}(x_i; D_{i-1}) + \sigma^2 k(x_i, \boldsymbol{X}_{i-1}) \tilde{K} k(\boldsymbol{X}_{i-1}, x_i),$$

where $\tilde{K} = \boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1})^{-1}(\boldsymbol{K}(\boldsymbol{X}_{i-1}, \boldsymbol{X}_{i-1}) + \sigma^2 I)^{-1}$. Because $\tilde{K}$ is positive-definite, we have $\sigma^2_{GP,\sigma^2}(x_i; D_{i-1}) \geq \sigma^2_{GP}(x_i; D_{i-1})$.

□

Combining the results of Lemmas 3 and 5, we can prove Theorem 1. First of all, we have $\sum_{i=1}^n r_i^2 \leq \sum_{i=1}^n 4\beta_i \hat{\sigma}^2(x_i; D_{i-1}, Z_M)$ from Lemma 3. By the definition of $\tilde{\beta}_i = \beta_i + 2\log(1-\gamma_i)$, $\tilde{\beta}_i$ is non-decreasing, thus $\beta_i \leq \tilde{\beta}_i - 2\log(1-\gamma)$ for all $i \leq n$. Then we have the following inequality:

$$\begin{aligned}
\sum_{i=1}^n r_i^2 &\leq \sum_{i=1}^n 4(\tilde{\beta}_i - 2\log(1-\gamma))\hat{\sigma}^2(x_i; D_{i-1}, Z_M) \leq \sum_{i=1}^n 4(\tilde{\beta}_i - 2\log(1-\gamma))\sigma^2_{GP}(x_i; D_{i-1}) \\
&\leq \sum_{i=1}^n 4(\tilde{\beta}_i - 2\log(1-\gamma)) k_0^3 (k_0^{-2} \frac{\sigma^2_{GP}(x_i; D_{i-1})}{k_0}) \\
&\leq \sum_{i=1}^n 4(\tilde{\beta}_i - 2\log(1-\gamma)) k_0^3 C_2 \log(1 + k_0^{-2} \frac{\sigma^2_{GP}(x_i; D_{i-1})}{k_0}).
\end{aligned}$$

With $C_2 = k_0^{-2}/\log(1+k_0^{-2}) \geq 1$, $s \leq C_2 \log(1+s)$ holds for $s \in [0, k_0^{-2}]$. Since $k_0^{-2}\frac{\sigma^2_{GP}(x_i;D_{i-1})}{k_0} \leq k_0^{-2}$, the inequality $k_0^{-2}\frac{\sigma^2_{GP}(x_i;D_{i-1})}{k_0} \leq C_2 \log(1+k_0^{-2}\frac{\sigma^2_{GP}(x_i;D_{i-1})}{k_0}+)$ holds. From the result of Lemma 5, we can show $\sum_{i=1}^n r_i^2 \leq \sum_{i=1}^n 8(\tilde{\beta}_i - 2\log(1-\gamma)) C_2 k_0^3 I(\boldsymbol{y}_i; \boldsymbol{f}_i, k_0^3)$. By setting $C_1 = 8C_2k_0^3$, the statement of Theorem 1 holds.

G Regret bound: general decision set case

Theorem 1 assumes the finite decision set, $|\Omega| < \infty$. We generalize the results in Theorem 1 to any compact and convex $\Omega \subset R^d$. The following assumption is needed.

Assumption: for some constants $a, b > 0$

$$P(\sup_{x \in \Omega \subset R^d} |\partial f / \partial x_j| > L) \leq a e^{-(L/b)^2}, \quad j = 1, \ldots, d.$$

The above implies that $P(\forall j, \forall x \in \Omega |\partial f/\partial x_j| < L) \geq 1 - dae^{-L^2/b^2}$. Therefore, with probability greater than $1 - dae^{-L^2/b^2}$, we have

$$\forall x \in \Omega, |f(x) - f(x')| \leq L \parallel x - x' \parallel_1 . \tag{3}$$

Now, let us choose a discretization of Ω_i of size $(\kappa_i)^d$ such that for all $x \in \Omega_i$,

$$\parallel x - [x]_i \parallel_1 \leq rd/\kappa_i,$$

where $[x]_i$ is the closest point to x in Ω_i. Then, we establish the following theorem for the cumulative regret bound of OBCGP-UCB on general decision set Ω.

Theorem 2. *Pick $\delta \in (0,1)$ and set $\tilde{\beta}_i = 2\log(\frac{4\pi_i}{\delta}) + 4d\log(dnbr\sqrt{\log 4da/\delta})$, where $\sum_{i\geq 1}\pi_i^{-1} = 1, \pi_i > 0$ and $\gamma_i = \max(P(Z_M < E[Z_M|D_{i-1}]|D_{i-1}), P(Z_M > E[Z_M|D_{i-1}]|D_{i-1}))$. With the assumption that $\gamma_i < \gamma \in [0,1)$ for all $i \geq 1$, the following holds with probability $\geq 1-\delta$:*

$$\sum_{i=1}^{n} r_i \leq \sqrt{(\tilde{\beta}_i - 2\log(1-\gamma))C_1 n\eta_n} + \frac{\pi^2}{6},$$

where $k_0 = k(x,x)$ is constant for all $x \in \Omega$, and $\eta_n = Max_{A\subset\Omega,|A|=n} I(\boldsymbol{y}_n; \boldsymbol{f}_n, k_0^3)$.

Similar to the proof of Theorem 1, we begin with finding an appropriate β_i that makes instantaneous regret to be bounded. $\tilde{\mu}([x_{opt}]_i; D_{i-1})$ and $\hat{\sigma}([x_{opt}]_i; D_{i-1}, Z_M)$ considered in Lemma 6 allow us to use Lemma 3 because $[x_{opt}]_i \in \Omega_i$, $|\Omega_i| \leq \infty$.

Lemma 6. *Pick $\delta \in (0,1)$ and set $\beta_i = 2\log(\frac{2\pi_i}{\delta(1-\gamma_i)}) + 4d\log(dtbr\sqrt{\log 2da/\delta})$, where $\sum_{i\geq 1}\pi_i^{-1} = 1, \pi_i > 0$ and $\gamma_i = \max(P(Z_M < E[Z_M|D_{i-1}]|D_{i-1}), P(Z_M > E[Z_M|D_{i-1}]|D_{i-1}))$. Let $\kappa_i = dt^2 dr\sqrt{\log(2da/\delta)}$, and $[x_{opt}]_i$ denote the closest point to x_{opt} in Ω_i. Then*

$$|f(x_{opt}) - \tilde{\mu}([x_{opt}]_i; D_{i-1})| \leq \beta_i^{1/2}\hat{\sigma}([x_{opt}]_i; D_{i-1}, Z_M) + \frac{1}{i^2} \qquad \forall i \geq 1$$

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

Proof. Using Eq.(3), we have that with probability $\geq 1 - \delta/2$,

$$\forall x \in \Omega, |f(x) - f(x')| \leq b\sqrt{\log(2da/\delta)} \parallel x - x' \parallel_1 .$$

Thus

$$\forall x \in \Omega_i, |f(x) - f([x]_i)| \leq rdb\sqrt{\log(2da/\delta)}/\kappa_i.$$

By choosing $\kappa_i = dt^2 br\sqrt{\log(2da/\delta)}$, we obtain

$$\forall x \in \Omega_i, |f(x) - f([x]_i)| \leq \frac{1}{i^2}.$$

By definition of Ω_i, we have $|\Omega_i| = (dt^2 br\sqrt{\log(2da/\delta)})^d$. Applying Lemma 2 with the replacement of δ and $|\Omega|$ with $\delta/2$ and $|\Omega_i|$, respectively, we show that the statement holds. □

Lemma 7. *Pick* $\delta \in (0, 1)$ *and set* $\beta_i = 2\log(\frac{\pi_i}{\delta(1-\gamma_i)})$, *where* $\sum_{i\geq 1} \pi_i^{-1} = 1, \pi_i > 0$ *and* $\gamma_i = \max(P(Z_M < E[Z_M|D_{i-1}]|D_{i-1}), P(Z_M > E[Z_M|D_{i-1}]|D_{i-1}))$. *Then*

$$|f(x_i) - \tilde{\mu}(x_i; D_{i-1})| \leq \beta_i^{1/2}\hat{\sigma}(x_i; D_{i-1}, Z_M) \quad \forall i \geq 1$$

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

Combining Lemmas 6 and 7, we obtain the bound of instantaneous regret as in Lemma 8, which is similar to Lemma 3.

Lemma 8. *Pick* $\delta \in (0, 1)$ *and set* $\beta_i = 2\log(\frac{4\pi_i}{\delta(1-\gamma_i)}) + 4d\log(dtbr\sqrt{\log 4da/\delta})$, *where* $\sum_{i\geq 1} \pi_i^{-1} = 1, \pi_i > 0$ *and* $\gamma_i = \max(P(Z_M < E[Z_M|D_{i-1}]|D_{i-1}), P(Z_M > E[Z_M|D_{i-1}]|D_{i-1}))$. *Then for all* $i \geq 1$

$$r_i \leq 2\beta_i^{1/2}\hat{\sigma}(x_i; D_{i-1}, Z_M) + \frac{1}{i^2}$$

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

Proof. To prove Lemma 8, we use $\delta/2$ in Lemmas 6 and 7, so that both lemmas hold with probability greater than $1 - \delta$. Because β_i specified in Lemma 6 is greater than β_i specified in Lemma 7 for all $\delta \in (0, 1)$ with β_i in Lemma 6 chosen as $\delta/2$ (this β_i is the same as that in Lemma 8), the statements of Lemmas 6 and 7 hold with probability greater than $1 - \delta$. First note that $\tilde{\mu}(x_i; D_{i-1}) + \beta^{1/2}\hat{\sigma}(x_i; D_{i-1}, Z_M) \geq \tilde{\mu}([x_{opt}]_i; D_{i-1}) + \beta^{1/2}\hat{\sigma}([x_{opt}]_i; D_{i-1}, Z_M)$. Combining this with Lemma 6, we have

$$\begin{aligned} r_i &= f(x_{opt}) - f(x_i) \\ &\leq \beta_i^{1/2}\hat{\sigma}(x_i; D_{i-1}, Z_M) + 1/i^2 + \tilde{\mu}(x_i; D_{i-1}) - f(x_i) \\ &\leq 2\beta_i^{1/2}\hat{\sigma}(x_i; D_{i-1}, Z_M) + 1/i^2. \end{aligned}$$

□

Combining Lemmas 8 and 5, we can finally prove Theorem 2. Note that β_i in Lemma 8 is the same as $\tilde{\beta}_i - 2\log(1 - \gamma_i)$. Combining the fact that $\tilde{\beta}_i$ is non-decreasing, as shown in Theorem 1, and the result of Lemma 8, we can show that the following inequality holds with probability $\geq 1 - \delta$:

$$\sum_{i=1}^{n} 4\beta_i\hat{\sigma}^2(x_i; D_{i-1}, Z_M) \leq (\tilde{\beta}_i - 2\log(1 - \gamma))C_1\eta_n.$$

Applying the Cauchy-Schwartz inequality, we have

$$\sum_{i=1}^{n} 2\beta_i^{1/2}\hat{\sigma}(x_i; D_{i-1}, Z_M) \leq \sqrt{(\tilde{\beta}_i - 2\log(1 - \gamma))C_1 n\eta_n}.$$

Thus,

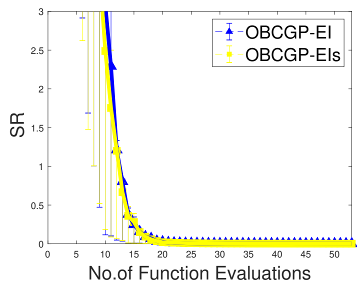
$$\sum_{i=1}^{n} r_i \leq \sqrt{(\tilde{\beta}_i - 2\log(1 - \gamma))C_1 n\eta_n} + \frac{\pi^2}{6}.$$

H Further experiments

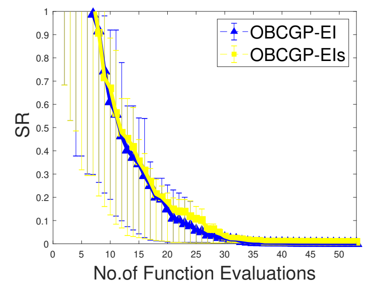
H.1 Comparison between OBCGP-EI and OBCGP-EIs

We compare the BO results for the simulated functions using OBCGP-EI and OBCGP-EIs. Under the same experimental settings in Section 6.2, we run the BO experiments for each function using OBCGP-EI and OBCGP-EIs. Figure A presents the results, and we can see that OBCGP-EI and

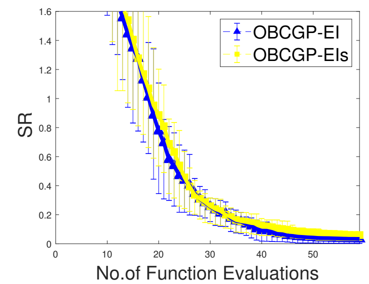
OBCGP-EIs show a slight difference in the speed to reach the optimum, but equally found the true optimum after sufficient iterations.



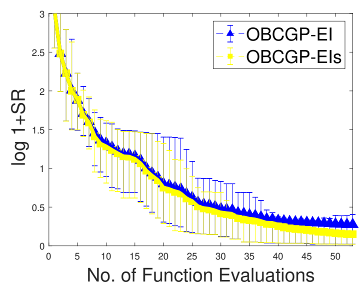
(a) Branin (f_b)



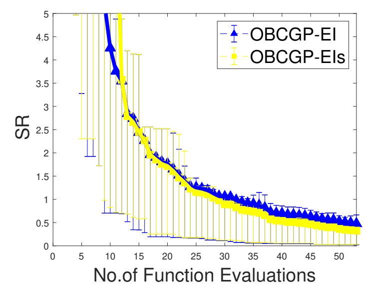
(b) Camel (f_c)



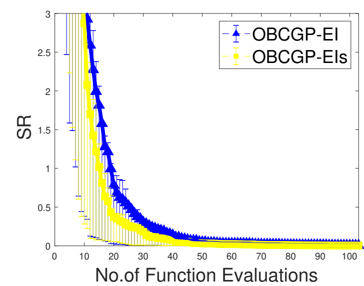
(c) Hartmann (f_h)



(d) Goldstein (f_g)



(e) Rosenbrock (f_r)



(f) Branin-20D (f_r)

Figure A: Comparison between OBCGP-EI and OBCGP-EIs.

H.2 Experiments with prior bound information for the simulated functions

Recall that OBCGP can inherently incorporate a new type of prior knowledge, i.e., the bounds on the optimal objective values, if it is available. To show this advantage, we conducted further experiments by assuming certain upper and lower bounds for each test function. We assumed that upper and lower bounds for each function were available from expert knowledge. To assume reasonable upper bounds, for each function, we evaluated ten randomly selected data points using Latin hypercube sampling 200 times, and recorded the minimum objective value of the ten evaluated points each time. The average of the 200 minimum values was assumed as the upper bound for each function. Lower bound values cannot be assumed in the same way; thus, lower bounds were chosen arbitrarily for each function. In addition, we set some upper bound to be chosen arbitrarily tight (denote as UB*), so that we can compare the performance of OBCGP in comparison with GP according to whether the upper bound is tight or loose.

The assumed values of the upper and lower bounds are presented in Table A, along with the simple regret of the proposed BO at the 55th iteration, with and without incorporating the bound information. By incorporating prior knowledge, OBCGP achieved even better performances. The results show the benefits of incorporating prior knowledge if it is available and that OBCGP is an effective tool to incorporate prior knowledge of the bound on the optimal objective value into BO for effective black-box optimization. Note that such prior knowledge cannot be readily incorporated using traditional BOs.

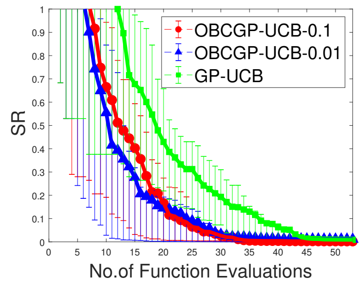
Table A: SR at final iterations

f	min value	type	GP -EI	GP -UCB	GP -MES	OBCGP -UCB no prior	OBCGP -EI no prior	OBCGP -UCB	OBCGP -EI
f_b	0.3978	UB:5.56	0.0380 (0.2156)	0.0018 (0.0045)	0.0335 (0.2160)	0.0010 (0.0021)	0.0015 (0.0022)	0.0007 (0.0011)	0.0012 (0.0008)
		LB:-1.0						0.0007 (0.0010)	0.0009 (0.0001)
f_c	-1.0316	UB:5.09	0.0241 (0.0425)	0.0082 (0.0099)	0.0179 (0.0348)	0.0020 (0.0018)	0.0014 (0.0016)	0.0018 (0.0021)	0.0011 (0.0021)
		LB:-5.0						0.0017 (0.0019)	0.0013 (0.0009)
f_h	-3.3223	UB:-1.098	0.1139 (0.0607)	0.5214 (0.1574)	0.3092 (0.0970)	0.0633 (0.0579)	0.0636 (0.0580)	0.0527 (0.0339)	0.0611 (0.0571)
		LB:-5.0						0.0589 (0.0211)	0.0629 (0.0512)
f_g	3.0	UB:226.1	9.1987 (17.2445)	9.6020 (17.0215)	11.9401 (15.2202)	6.2325 (19.9017)	7.9661 (20.3988)	6.1128 (17.3328)	7.6512 (21.0019)
		UB*:10.0						0.3116 (0.5531)	0.1830 (0.4113)
		LB:0.0						4.2931 (19.2389)	6.9938 (18.1127)
f_r	0.0	UB:33.5	0.9513 (1.2916)	1.1745 (1.4594)	1.3216 (1.5368)	0.2864 (0.7355)	0.4121 (1.1022)	0.2177 (0.5512)	0.2247 (0.6624)
		UB*:3.0						0.0791 (0.0925)	0.0705 (0.1018)
		LB:-1.0						0.2799 (0.7712)	0.3988 (1.1144)

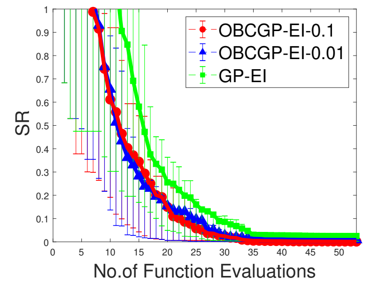
Furthermore, the comparison of the results of OBCGP with UB and UB* for f_g and f_r shows that the tighter upper bound (UB*) induced a significant improvement of performance. Note that these functions (f_g and f_r) are highly volatile and thus it is difficult to find the optimum because of several local minima. However, if some helpful bound knowledge is available, OBCGP can use it to find the global optimum more effectively.

H.3 Sensitivity Analysis of λ with more functions

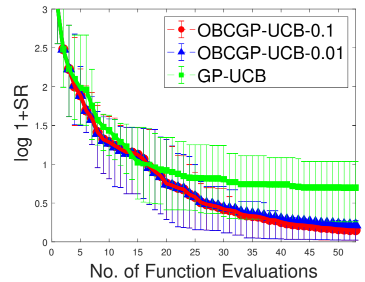
In Section 6.3, we discussed the results of sensitivity analysis of λ using Branin and Hartmann 6 functions. Here we present additional results on Camel, Goldstein, Rosen brock, and Branin-20D functions in Figure B, which were not reported in Section 6.3 because of page limit.



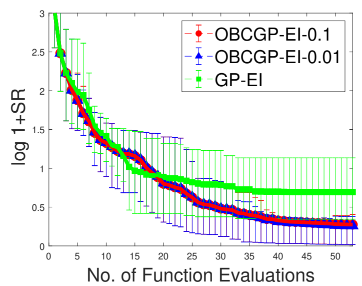
(a) OBCGP-UCB (Camel)



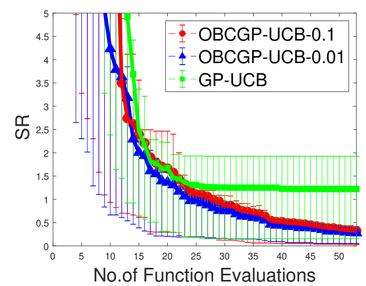
(b) OBCGP-EI (Camel)



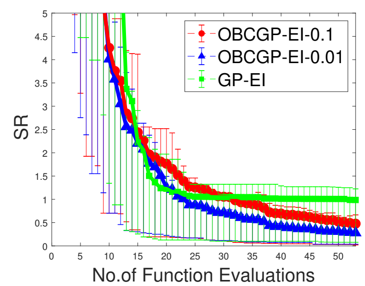
(c) OBCGP-UCB (Goldstein)



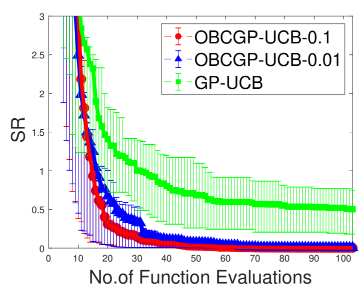
(d) OBCGP-EI (Goldstein)



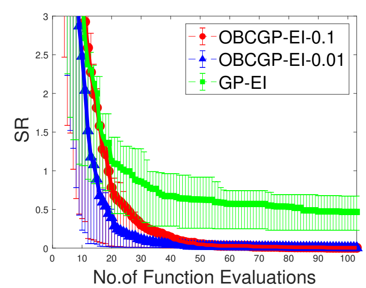
(e) OBCGP-UCB (Rosenbrock)



(f) OBCGP-EI (Rosenbrock)



(g) OBCGP-UCB (Branin-20D)



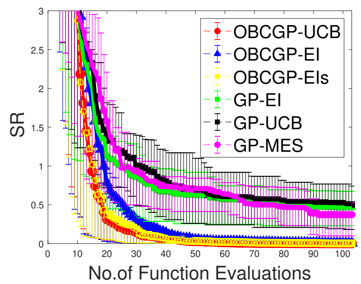
(h) OBCGP-EI (Branin-20D)

Figure B: Sensitivity analysis of λ for OBCGP (Case 1) on BO performance. Two values of λ (0.1 and 0.01) were considered.

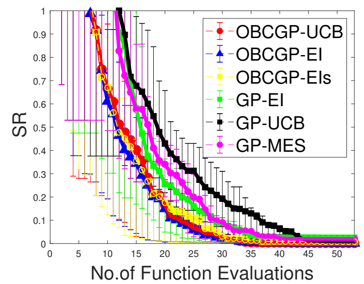
H.4 Experiments with GP-MES and OBCGP-EIs for the simulated functions

Figure C presents additional BO results for the simulated functions using GP-MES and OBCGP-EIs, compared to Figure 3 in the paper. Although GP-MES showed better performance than

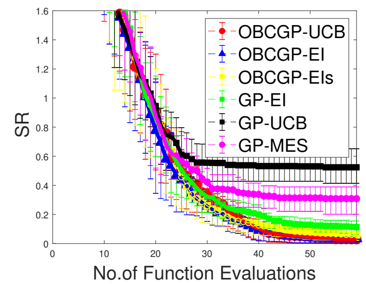
GP-UCB and GP-EI on some simulated functions, BO with OBCGP still outperformed any BO methods with GP on all the simulated functions.



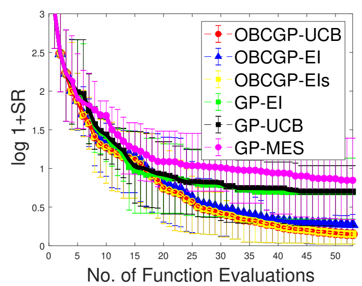
(a) Branin



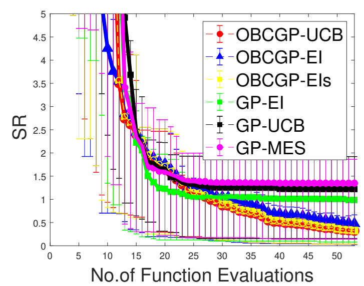
(b) Camel



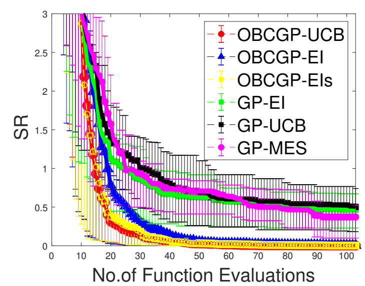
(c) Hartmann



(d) Goldstein



(e) Rosenbrock



(f) Branin-20D

Figure C: Comparison of the performances of BO with the OBCGP and BO with the GP

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