

---

# Convergence Rates of Constrained Expected Improvement

---

**Haowei Wang**

National University of Singapore  
Singapore  
haowei\_wang@u.nus.edu

**Jingyi Wang**

Lawrence Livermore National Laboratory  
Livermore, CA 94550  
wang125@llnl.gov

**Nai-Yuan Chiang**

Lawrence Livermore National Laboratory  
Livermore, CA 94550  
chiang7@llnl.gov

**Zhongxiang Dai**

The Chinese University of Hong Kong, Shenzhen  
China  
daizhongxiang@cuhk.edu.cn

**Szu Hui Ng**

National University of Singapore  
Singapore  
isensh@nus.edu.sg

**Cosmin G. Petra**

Lawrence Livermore National Laboratory  
Livermore, CA 94550  
petra1@llnl.gov

## Abstract

Constrained Bayesian optimization (CBO) methods have seen significant success in black-box optimization with constraints. One of the most commonly used CBO methods is the constrained expected improvement (CEI) [Gardner et al., 2014] algorithm. CEI is a natural extension of expected improvement (EI) [Jones et al., 1998] when constraints are incorporated. However, the theoretical convergence rate of CEI has not been established. In this work, we study the convergence rate of CEI by analyzing its simple regret upper bound. First, we show that when the objective function  $f$  and constraint function  $c$  are assumed to each lie in a reproducing kernel Hilbert space (RKHS), CEI achieves the convergence rates of  $\mathcal{O}\left(t^{-\frac{1}{2}} \log^{\frac{d+1}{2}}(t)\right)$  and  $\mathcal{O}\left(t^{\frac{\nu}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t)\right)$  for the commonly used squared exponential and Matérn kernels, respectively. Second, we show that when  $f$  and  $c$  are assumed to be sampled from Gaussian processes (GPs), CEI achieves the same convergence rates with a high probability. Numerical experiments are performed to validate the theoretical analysis.

## 1 Introduction

Bayesian optimization (BO) is an efficient method for optimizing expensive black-box functions without derivatives. It leverages probabilistic surrogate models, most commonly Gaussian processes (GPs), to balance exploration and exploitation in the search for optimal solutions [Frazier, 2018]. BO has found widespread success in diverse fields such as structural design [Mathern et al., 2021], machine learning hyperparameter tuning [Wu et al., 2019], robotics [Calandra et al., 2016], fusion design [Wang et al., 2024], etc.

While traditional BO is typically applied to unconstrained settings, many real-world problems involve black-box constraints that must be satisfied. This has motivated growing interest in constrained

Bayesian optimization (CBO), where surrogate models are also constructed for constraint functions [Bernardo et al., 2011] that are complex and expensive to evaluate, making CBO especially valuable in applications like engineering design [Song et al., 2024] and automated machine learning [Ungredda and Branke, 2024]. One of the very key difference between unconstrained and constrained optimization is that the feasible region for constrained optimization problem consists of the search space where all constraints must be satisfied. A general form of the constrained BO problem is:

$$\underset{\mathbf{x} \in C}{\text{minimize}} \quad f(\mathbf{x}), \quad \text{subject to} \quad c(\mathbf{x}) \leq 0, \quad (1)$$

where  $f : \mathbb{R}^d \rightarrow \mathbb{R}$  is the objective function, and  $c : \mathbb{R}^d \rightarrow \mathbb{R}^m$  are the constraint functions. Both are defined on a compact input space  $C \subset \mathbb{R}^d$ . The objective and the constraint functions are both expensive black-box functions, that can only be evaluated through expensive physical or computer experiments. Throughout this paper, we consider the noise-free setting for both the objective and the constraints, *i.e.*, the function evaluations are deterministic and the true function values can be observed (see Remark 3.14 for discussion on the noisy case). In addition, a single constraint is considered, *i.e.*,  $m = 1$ , for simplicity of presentation. We note that our analysis can be easily extended to multiple constraints (see Remark 3.13 for details).

Broadly, CBO methods can be categorized into implicit and explicit approaches [Amini et al., 2025]. Implicit methods modify standard acquisition functions to incorporate constraints via merit functions or feasibility weights. Explicit methods estimate the feasible region directly and restrict search to this region. Among these, the constrained expected improvement (CEI) [Schonlau et al., 1998, Gelbart et al., 2014, Gardner et al., 2014] stands out as one of the most basic and widely adopted methods. CEI is a natural extension of the well-known expected improvement (EI) function [Jones et al., 1998], where the acquisition function is computed as the product of EI and the probability of feasibility. Thanks to this simple and interpretable formulation, CEI has been successfully applied across domains, and it remains one of the default choices in many constrained BO software packages [Balandat et al., 2020].

Despite its empirical popularity, the theoretical understanding of CEI lags behind. In contrast, unconstrained EI has been more extensively studied. Under a frequentist assumption where the objective  $f$  lies in a reproducing kernel Hilbert space (RKHS), Bull [2011] established the convergence rate of EI by deriving the simple regret upper bound. Other works explored the density of sampled sequences [Vazquez and Bect, 2010] or connections between EI and optimal computing budget allocation [Ryzhov, 2016]. However, convergence rates (*i.e.*, simple regret upper bound) for CEI have not been rigorously established—neither under frequentist nor under Bayesian settings. Here, Bayesian setting means the objective  $f$  is a function sampled from a GP.

Introducing constraints into EI significantly complicates the theoretical analysis. Unlike in the unconstrained case, the algorithm may need to explore infeasible regions to gain information on the constraint boundary. Furthermore, CEI’s acquisition function is inherently more complex and non-convex, posing challenges for analysis. On the other hand, the presence of constraints in CEI leads to changes in the sampling procedure. As a result, the key challenge to study the convergence rate of CEI lies in analyzing the exploration (searching for feasible regions) and exploitation (optimizing within feasible areas) since the feasibility threshold is unknown in the input space.

In this paper, we provide the first theoretical convergence rates for CEI, focusing on simple regret upper bounds under both the frequentist and Bayesian settings. Our convergence rates provide practitioners theoretical assurance for the practical deployment of CEI. Further, we would like to highlight that the obtained bounds under both settings are not direct extensions from current unconstrained results. We explain the technical challenges and how we address them in Section 3. Our contributions are summarized as follows:

- Under the frequentist setting, we derive simple regret upper bounds of  $\mathcal{O}\left(t^{-\frac{1}{2}} \log^{\frac{d+1}{2}}(t)\right)$  for the squared exponential (SE) kernel and  $\mathcal{O}\left(t^{\frac{-\nu}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t)\right)$  for Matérn kernels. These bounds are improved upon the direct extension of Bull [2011] to the constrained case for SE kernel with  $d \geq 3$  and Matérn kernels with  $d \geq 3, \nu \geq \frac{d}{d-2}$ . (see Theorem 3.7).
- Under the Bayesian setting, we achieve the same simple regret upper bounds with high probabilities. These bounds are established based on the newly derived bounds (see Theorem 3.11) on the difference between the improvement function and its corresponding EI in the Bayesian setting.

This paper is organized as follows. In Section 2, we describe the basics and preliminaries of BO, including the CEI algorithm. In Section 3, the simple regret upper bounds of CEI are established in both settings. Numerical experiments to validate the theoretical results are given in Section 4. Conclusions are made in Section 5. All proof details are presented in the appendix.

## 2 Background

CBO mainly consists of two components: the GP surrogates for the black-box objective function  $f$  and constraint function  $c$ , and the constrained acquisition function as the sequential sampling rule guiding for the global optimum.

### 2.1 Gaussian process models for $f$ and $c$

Without losing generality, let the mean function for the objective GP model prior be 0 and the covariance function (kernel) be  $k_f(\mathbf{x}, \mathbf{x}') : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ . At sample point  $\mathbf{x}_t \in C$ , we denote the objective function value as  $f(\mathbf{x}_t)$  and the observed constraint function value is  $c(\mathbf{x}_t)$ . Given  $t$  sample points, denote  $\mathbf{x}_{1:t} = [\mathbf{x}_1, \dots, \mathbf{x}_t]$  and  $\mathbf{f}_{1:t} = [f(\mathbf{x}_1), \dots, f(\mathbf{x}_t)]$ . Moreover, denote the  $t \times t$  covariance matrix  $\mathbf{K}_t^f = [k_f(\mathbf{x}_1, \mathbf{x}_1), \dots, k_f(\mathbf{x}_1, \mathbf{x}_t); \dots; k_f(\mathbf{x}_t, \mathbf{x}_1), \dots, k_f(\mathbf{x}_t, \mathbf{x}_t)]$ . The posterior distribution of  $f(\mathbf{x}) | \mathbf{x}_{1:t}, \mathbf{f}_{1:t} \sim \mathcal{N}(\mu_t^f(\mathbf{x}), (\sigma_t^f(\mathbf{x}))^2)$  can then be inferred using Bayes' rule as follows

$$\begin{aligned}\mu_t^f(\mathbf{x}) &= (\mathbf{k}_t^f(\mathbf{x}))^T (\mathbf{K}_t^f)^{-1} \mathbf{f}_{1:t}, \\ (\sigma_t^f)^2(\mathbf{x}) &= k_f(\mathbf{x}, \mathbf{x}) - (\mathbf{k}_t^f(\mathbf{x}))^T (\mathbf{K}_t^f)^{-1} \mathbf{k}_t^f(\mathbf{x}),\end{aligned}\tag{2}$$

where  $\mathbf{k}_t^f(\mathbf{x}) = [k_f(\mathbf{x}_1, \mathbf{x}), \dots, k_f(\mathbf{x}_t, \mathbf{x})]^T$ . Similarly, denote the kernel for  $c$  as  $k_c : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$  and the covariance matrix  $\mathbf{K}_t^c = [k_c(\mathbf{x}_1, \mathbf{x}_1), \dots, k_c(\mathbf{x}_1, \mathbf{x}_t); \dots; k_c(\mathbf{x}_t, \mathbf{x}_1), \dots, k_c(\mathbf{x}_t, \mathbf{x}_t)]$ . The posterior distribution for  $c$  is

$$\begin{aligned}\mu_t^c(\mathbf{x}) &= (\mathbf{k}_t^c(\mathbf{x}))^T (\mathbf{K}_t^c)^{-1} \mathbf{c}_{1:t}, \\ (\sigma_t^c)^2(\mathbf{x}) &= k_c(\mathbf{x}, \mathbf{x}) - (\mathbf{k}_t^c(\mathbf{x}))^T (\mathbf{K}_t^c)^{-1} \mathbf{k}_t^c(\mathbf{x}),\end{aligned}$$

where  $\mathbf{k}_t^c(\mathbf{x}) = [k_c(\mathbf{x}_1, \mathbf{x}), \dots, k_c(\mathbf{x}_t, \mathbf{x})]^T$ , and  $\mu_t^c(\mathbf{x})$  and  $(\sigma_t^c)^2(\mathbf{x})$  are the posterior mean and variance for  $c$ , respectively. Here we use the subscripts  $f, c$  and superscripts  $f, c$  to distinguish between GPs for  $f$  and  $c$ . Choices of the kernels  $k_f$  and  $k_c$  include the SE and Matérn kernels, which are among the most popular kernels for GP and BO. Their definitions are as follows.

$$k_{SE}(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{r^2}{2l^2}\right), \quad k_{Matérn}(\mathbf{x}, \mathbf{x}') = \frac{1}{\Gamma(\nu)2^{\nu-1}} \left(\frac{\sqrt{2\nu}r}{l}\right)^\nu B_\nu\left(\frac{\sqrt{2\nu}r}{l}\right),$$

where  $l > 0$  is the length hyper-parameters,  $r = \|\mathbf{x} - \mathbf{x}'\|_2$ ,  $\nu > 0$  is the smoothness parameter of the Matérn kernel, and  $B_\nu$  is the modified Bessel function of the second kind.

### 2.2 Constrained Expected Improvement

Acquisition functions are critical to the performances of BO algorithms. In the unconstrained setting, one of the most widely adopted acquisition functions is EI [Jones et al., 1998]. Given  $t$  samples, the improvement function of  $f$  used in EI is defined as

$$I_t^f(\mathbf{x}) = \max\{f_t^+ - f(\mathbf{x}), 0\},\tag{3}$$

where  $f_t^+ = \min_{i=1, \dots, t} f(\mathbf{x}_i)$ . The expectation of (3) conditioned on existing samples is EI, which has a closed form Brochu et al. [2010]:

$$EI_t^f(\mathbf{x}) = (f_t^+ - \mu_t^f(\mathbf{x}))\Phi(z_t^f(\mathbf{x})) + \sigma_t^f(\mathbf{x})\phi(z_t^f(\mathbf{x})),\tag{4}$$

where  $z_t^f(\mathbf{x}) = \frac{f_t^+ - \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}$ . The functions  $\phi$  and  $\Phi$  are the probability density function (PDF) and the cumulative distribution function (CDF) of the standard normal distribution, respectively. The  $t + 1$ th sample using EI is chosen by

$$\mathbf{x}_{t+1} = \operatorname{argmax}_{\mathbf{x} \in C} EI_t^f(\mathbf{x}).\tag{5}$$

Taking into account the constraint, the constrained improvement function in CEI [Gardner et al., 2014] is defined as

$$I_t^C = \Delta_t^c(\mathbf{x}) \max\{f_t^+ - f(\mathbf{x}), 0\}, \quad (6)$$

where  $\Delta_t^c \in \{0, 1\}$  is the feasibility indicator function where  $\Delta_t^c(\mathbf{x}) = 1$  if  $c(\mathbf{x}) \leq 0$  and  $\Delta_t^c(\mathbf{x}) = 0$  otherwise. The incumbent  $f_t^+$  in CEI is augmented to be the best feasible observation. CEI assumes that  $f$  and  $c$  are conditionally independent [Gardner et al., 2014]. Taking the conditional expectation of (6), the CEI function is

$$EI_t^C(\mathbf{x}) = P_t(\mathbf{x})EI_t^f(\mathbf{x}) = \Phi\left(-\frac{\mu_t^c(\mathbf{x})}{\sigma_t^c(\mathbf{x})}\right)EI_t^f(\mathbf{x}), \quad (7)$$

where  $P_t(\cdot)$  is the probability of feasibility (POF) function for  $c(\mathbf{x}) \leq 0$ . CEI chooses the next sample via

$$\mathbf{x}_{t+1} = \operatorname{argmax}_{\mathbf{x} \in C} P_t(\mathbf{x})EI_t^f(\mathbf{x}). \quad (8)$$

The CEI algorithm is given in Algorithm 1.

---

**Algorithm 1** CEI algorithm

---

- 1: Choose  $k_f(\cdot, \cdot)$ ,  $k_c(\cdot, \cdot)$ , and  $T_0$  initial samples  $\mathbf{x}_i, i = 1, \dots, T_0$ . Observe  $\mathbf{f}_{1:T_0}$  and  $\mathbf{c}_{1:T_0}$ .
  - 2: Train the GP surrogate models for  $f$  and  $c$  respectively conditioned on the initial observations.
  - 3: **for**  $t = T_0 + 1, T_0 + 2, \dots$  **do**
  - 4:     Find  $\mathbf{x}_{t+1}$  based on (8) (CEI).
  - 5:     Observe  $f(\mathbf{x}_{t+1})$  and  $c(\mathbf{x}_{t+1})$ .
  - 6:     Update the GP model with the addition of  $\mathbf{x}_{t+1}$ ,  $f(\mathbf{x}_{t+1})$ , and  $c(\mathbf{x}_{t+1})$ .
  - 7:     **if** Evaluation budget exhausted **then**
  - 8:         Exit
- 

CEI can be extended to multiple constraints assuming conditional independence among the constraints [Gardner et al., 2014]. Our derived convergence rates can also be readily extended to multiple constraints, as we explain in Remark 3.13.

### 3 Convergence rates of CEI

We present our main results of convergence rates for CEI by establishing the simple regret upper bounds. Denote the optimal solution to the constrained optimization problem (1) as  $\mathbf{x}^*$ . In the unconstrained case, the simple regret of EI is defined as  $f_t^+ - f(\mathbf{x}^*)$  [Bull, 2011]. In the constrained case, we require the current best observation to be feasible when compared to the optimal solution  $f(\mathbf{x}^*)$ , since one could have an infeasible sample point with smaller objective than  $f(\mathbf{x}^*)$ . Given that  $f_t^+$  is already defined as the best feasible observation till iteration  $t$  in CEI, we continue to use

$$r_t = f_t^+ - f(\mathbf{x}^*), \quad (9)$$

as the simple regret for CEI. In our analysis, we make the same underlying assumption as CEI that  $f_t^+$  exists. In the following, we first establish the convergence rate under the frequentist assumptions in Section 3.1, including an improved version of the rate under frequentist assumptions in Section 3.1.1. Then, we establish the convergence rate under Bayesian assumptions in Section 3.2.

#### 3.1 Simple regret upper bound under frequentist assumptions

In this section, we present the simple regret upper bound for CEI under the frequentist setting. Moreover, by adopting the information theory-based bounds and techniques in the noise-free cumulative regret bound of upper confidence bound (UCB) [Lyu et al., 2019], we derive an improved upper bound compared to Bull [2011]. The definition of RKHS is given below.

**Definition 3.1.** Let  $k$  be a positive definite kernel  $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$  with respect to a finite Borel measure supported on  $\mathcal{X}$ . A Hilbert space  $H_k$  of functions on  $\mathcal{X}$  with an inner product  $\langle \cdot, \cdot \rangle_{H_k}$  is

called a RKHS with kernel  $k$  if  $k(\cdot, \mathbf{x}) \in H_k$  for all  $\mathbf{x} \in \mathcal{X}$ , and  $\langle f, k(\cdot, \mathbf{x}) \rangle_{H_k} = f(\mathbf{x})$  for all  $\mathbf{x} \in \mathcal{X}, f \in H_k$ . The induced RKHS norm  $\|f\|_{H_k} = \sqrt{\langle f, f \rangle_{H_k}}$  measures the smoothness of  $f$  with respect to  $k$ .

In this section, we assume the following assumptions on the functions  $f$  and  $c$ .

**Assumption 3.2.** The functions  $f$  and  $c$  lie in the RKHS, denoted as  $\mathcal{H}_k^f(C)$  and  $\mathcal{H}_k^c(C)$  associated with their respective bounded kernel  $k_f$  and  $k_c$ , with the norm  $\|\cdot\|_{H_k^f}$  and  $\|\cdot\|_{H_k^c}$ . The kernels satisfy  $k_f(\mathbf{x}, \mathbf{x}') \leq 1, k_c(\mathbf{x}, \mathbf{x}') \leq 1, k_f(\mathbf{x}, \mathbf{x}) = 1$ , and  $k_c(\mathbf{x}, \mathbf{x}) = 1$ , for  $\forall \mathbf{x}, \mathbf{x}' \in C$ . The RKHS norms are bounded above by constants  $B_f$  and  $B_c$ , respectively, i.e.,  $\|f\|_{H_k^f} \leq B_f, \|c\|_{H_k^c} \leq B_c$ . Moreover, the bound constraints set  $C$  is compact.

**Technical Challenges under Frequentist Assumptions.** The main challenge in establishing a simple regret upper bound for CEI is how to incorporate the constraint  $c(\mathbf{x}) \leq 0$  and the probability of feasibility function  $P_t(\mathbf{x})$  into the analysis. Existing regret bounds analysis on CBO methods often focus on UCB-type methods [Lu and Paulson, 2022, Zhou and Ji, 2022], for which the acquisition functions do not have the multiplicative structure between the objective and the constraint.

Under Assumption 3.2, both  $f$  and  $c$  are bounded on  $C$  by their RKHS norm bound, as stated in Lemma B.1. The simple regret upper bound is given in the following theorem.

**Theorem 3.3.** Under Assumption 3.2, the CEI algorithm leads to the simple regret upper bound of

$$r_t \leq c_{\tau B} \frac{c_{\tau B}}{\Phi(-B_c)} \left[ B_f \frac{4}{t-2} + (0.4 + B_f) \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right], \quad (10)$$

for some  $t_k \in [\frac{t}{2} - 1, t]$ , and  $c_{\tau B} = \frac{\tau(B_f)}{\tau(-B_f)}$ .

**Sketch of Proof for Theorem 3.3.** We start by noticing that the sum of the difference between consecutive best feasible observations is bounded, i.e.,  $\sum_{t=1}^T f_{t-1}^+ - f_t^+ \leq 2B_f$ . Then, we adopt a technique in Bull [2011] to find  $t_k$  such that  $f_{t_k}^+ - f_{t_k+1}^+ \leq \frac{2B_f}{k}$ , where  $k \leq t_k \leq 2k$  and  $2k \leq t \leq 2(k+1)$ . Next, using the monotonicity of  $f_t^+$ ,  $r_t$  is bounded by  $r_{t_k}$ . Using the inequality between  $I_t^f$  and  $EI_t^f$  in Lemma B.4, we can bound  $r_{t_k}$  by the EI on objective:  $EI_{t_k}^f(\mathbf{x}^*)$ . Then, we transform  $EI_{t_k}^f(\mathbf{x}^*)$  into  $EI_{t_k}^f(\mathbf{x}_{t_k+1})$  by inserting the term  $P_{t_k}(\mathbf{x}^*)$ , taking advantage of the multiplicative structure of CEI. The upper bound of  $r_t$  then consists of the term  $\frac{1}{P_{t_k}(\mathbf{x}^*)} EI_{t_k}^f(\mathbf{x}_{t_k+1})$ . From the confidence interval  $|f(\mathbf{x}) - \mu_t^f(\mathbf{x})|$  (Lemma B.2) and the fact that  $f_{t_k}^+ - f_{t_k+1}^+ \leq \frac{2B_f}{k}$ , we can bound  $EI_{t_k}^f(\mathbf{x}_{t_k+1})$ . The constraint term  $\frac{1}{P_{t_k}(\mathbf{x}^*)}$  remains to be bounded. We use the confidence interval on  $|c(\mathbf{x}) - \mu_t^c(\mathbf{x})|$  in Lemma B.2 at  $\mathbf{x}^*$  and the fact that  $\mathbf{x}^*$  is a feasible solution to obtain a lower bound for  $P_{t_k}(\mathbf{x}^*)$ . This concludes the proof.

**Remark 3.4** (Constraint in the simple regret upper bound). The terms derived from the constraint function in (10) is  $\frac{1}{\Phi(-B_c)}$ , which emerges from the probability of feasibility function and  $\mu_t^c(\mathbf{x})$  and  $\sigma_t^c(\mathbf{x})$  of the GP model of  $c(\mathbf{x})$ . Thanks to the multiplicative structure between the objective and constraint in  $I_t^C$  (6) and  $EI_t^C$  (7), the simple regret upper bound maintains a similar form.

It is clear from (10) that the convergence of  $r_t$  relies on the posterior standard deviation  $\sigma_t^f(\mathbf{x}_{t+1})$ . Since  $t_k$  increases with  $t$ , as  $\sigma_t^f(\mathbf{x}_{t+1}) \rightarrow 0$ , so does  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1})$ . In the noise-free setting, the posterior variance can be bounded via the maximum distance between sample points and a given point. To obtain the rate of simple regret bound, we use Assumptions (1)-(4) in Bull [2011] and focus on squared exponential (SE) and Matérn kernels. Recall that the smoothness parameter of the Matérn kernel is  $\nu > 0$ . Both the SE and Matérn kernels satisfy Assumptions (1)-(4) in Bull [2011], with SE kernel obtained as  $\nu \rightarrow \infty$ . Further, define

$$\eta = \begin{cases} \alpha, & \nu \leq 1 \\ 0, & \nu > 1, \end{cases} \quad (11)$$

where  $\alpha = \frac{1}{2}$  if  $\nu \in \mathbb{N}$ , and  $\alpha = 0$  otherwise. Then, for SE and Matérn kernels,  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1})$  can be bounded with the following lemma.

**Lemma 3.5** (Bull [2011]). *For the SE kernel, there exists constant  $C' > 0$  so that given  $\forall t \in \mathbb{N}$ ,*

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq C' k^{-\frac{1}{d}} \quad (12)$$

*holds for at most  $k$  times, for  $\forall k \in \mathbb{N}$ ,  $k \leq t$  and  $i = 1, \dots, t-1$ . For Matérn kernels,*

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq C' k^{-\frac{\min\{\nu, 1\}}{d}} \log^\eta(k) \quad (13)$$

*holds at most  $k$  times.*

In the constrained setting, we are able to obtain the same rates as those in the unconstrained case [Bull, 2011] using Lemma 3.5.

**Corollary 3.6.** *Under Assumption 3.2, the CEI algorithm leads to the convergence rates of*

$$\mathcal{O}\left(t^{-\frac{1}{d}}\right) \text{ and } \mathcal{O}\left(t^{-\frac{\min\{\nu, 1\}}{d}} \log^\eta(t)\right), \quad (14)$$

*for SE and Matérn kernels, respectively, where  $\eta$  is from (11).*

Corollary 3.6 shows that the CEI algorithm is guaranteed to find the best feasible point asymptotically with the rates elaborated in (14). Also, we point out that the choice of kernels and their parameters affect the convergence rates. Since the SE kernel can be viewed as a Matérn kernel with  $\nu \rightarrow \infty$ , its convergence rate is better than Matérn kernels with  $\nu \leq 1$ . However, due to the limitations of the kernel analysis in Bull [2011] (see Remark 3.8), for  $\nu \geq 1$ , SE and Matérn kernels have similar convergence rates in Corollary 3.6. As we present in the following section, improved rates for both kernels can be obtained.

### 3.1.1 Improved simple regret upper bound under frequentist assumptions

Next, we apply maximum information gain and the corresponding information theory to obtain improved simple regret upper bounds.

**Theorem 3.7.** *Under Assumption 3.2, the CEI algorithm leads to the improved convergence rates of*

$$\mathcal{O}\left(t^{-\frac{1}{2}} \log^{\frac{d+1}{2}}(t)\right) \text{ and } \mathcal{O}\left(t^{-\frac{\nu}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t)\right), \quad (15)$$

*for SE and Matérn kernels, respectively.*

**Sketch of Proof for Theorem 3.7.** The proof follows similar steps to that of Theorem 3.3 but further bounds  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1})$  using  $\gamma_t^f$ . To do so, we first recognize that the bound using  $\gamma_t^f$  (Lemma A.3) is established in the noisy case where the posterior standard deviation has a different form as in (18). Using Lemma A.4, we can establish that the noise-free posterior standard deviation also satisfies  $\sum_{i=0}^{t-1} \sigma_i^f(\mathbf{x}_{i+1}) \leq \sqrt{C_\gamma t \gamma_t^f}$ . Then, from Lemma A.5, we can find a small enough  $\sigma_i^f(\mathbf{x}_{i+1})$ . Specifically, choose  $k = \lfloor t/3 \rfloor$ , where  $\lfloor x \rfloor$  denotes the largest integer smaller than  $x$ . Thus, we have  $3k \leq t \leq 3(k+1)$ . Then, there exists  $k \leq t_k \leq 3k$  such that  $f_{t_k}^+ - f_{t_k+1}^+ \leq \frac{2B_f}{k}$  and  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \leq \frac{\sqrt{t \gamma_t^f}}{k}$ . The rest of the proof follows from that of Theorem 3.7.

**Remark 3.8** (Improved rate of convergence). As mentioned above, the rates in Corollary 3.6 are the same as those to the known convergence rates for EI in Bull [2011]. Meanwhile, the rates in Theorem 3.7 is an improvement over those of Bull [2011] for SE kernel with  $d \geq 3$  and Matérn kernels with  $d \geq 3, \nu \geq \frac{d}{d-2}$ . To achieve this, we applied techniques from regret bound analysis on noise-free UCB [Lyu et al., 2019] that allows us to use maximum information gain to bound the sum of  $\sigma_t^f(\mathbf{x}_{t+1})$ . Then, we use our techniques in the proof of Theorem 3.3 to bound an individual  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1})$ . In Bull [2011], the  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1})$  is bounded by the Taylor expansion of the kernel functions. Therefore, the rates of decrease are limited to quadratic terms for both SE and Matérn kernels, since their Taylor expansions around 0 for  $\|\mathbf{x} - \mathbf{x}'\|_2$  are quadratic at best. On the other hand, maximum information gain has been a focus of research for years, leading to tight bounds on  $\gamma_t^f$  that take advantages of the spectral properties of the kernels [Vakili et al., 2021]. Hence, using  $\gamma_t^f$  to bound  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1})$  can produce a faster rate. As the open question raised in Vakili [2022] gets answered, further improvement of the convergence rates is possible, e.g., using techniques from Iwazaki [2025].

### 3.2 Simple regret upper bound under Bayesian assumptions

In this section, we present the simple regret upper bound for CEI under the Bayesian assumptions. We again use the maximum information gain to derive the simple regret upper bound.

**Assumption 3.9.** The objective function  $f$  is sampled from  $GP(0, k_f(\mathbf{x}, \mathbf{x}'))$ . The constraint function  $c$  is sampled from  $GP(0, k_c(\mathbf{x}, \mathbf{x}'))$ . The kernels satisfy  $k_f(\mathbf{x}, \mathbf{x}') \leq 1$ ,  $k_f(\mathbf{x}, \mathbf{x}) = 1$ ,  $k_c(\mathbf{x}, \mathbf{x}') \leq 1$ , and  $k_c(\mathbf{x}, \mathbf{x}) = 1$ . Moreover, the bound constraint set  $C$  is compact. Further, the objective function  $f$  is assumed to be Lipschitz continuous (of 1-norm) under the Bayesian setting, similar to Srinivas et al. [2009]. In addition,  $c$  is also Lipschitz continuous on  $C$ .

In the remaining of this section we will work under Assumption 3.9.

**Technical Challenges under Bayesian Assumptions.** In addition to the challenges in the frequentist setting, the bounds on EI in the Bayesian setting are not available in current literature, to the best of our knowledge. Starting from the confidence interval on  $|f(\mathbf{x}) - \mu_t^f(\mathbf{x})|$ , we derive the bounds on  $|I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x})|$  with high probability, an important step towards the bound on  $r_t$ . Noticeably, under the Bayesian setting, the bounds are satisfied with a given probability  $1 - \delta$ , where  $\delta \in (0, 1)$ . Hence, the simple regret upper bounds are presented with a probability as well.

The simple regret upper bound is given in the following theorem.

**Theorem 3.10.** Let  $\beta = 2 \log(6c_\alpha/\delta)$ , where  $c_\alpha = \frac{1+2\pi}{2\pi}$ . Under Assumption 3.9, the CEI algorithm leads to the simple regret upper bound

$$r_t \leq c_\tau(\beta) \frac{1}{\Phi(-\sqrt{\beta})} \left[ \frac{4M_f}{t-2} + (0.4 + \beta^{1/2}) \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right], \quad (16)$$

for some  $t_k \in [\frac{t}{2} - 1, t]$ ,  $c_\tau(\beta) = \frac{\tau(\beta^{1/2})}{\tau(-\beta^{1/2})}$ , and constant  $M_f > 0$  with probability  $\geq 1 - \delta$ .

The constant  $M_f$  is from Lemma C.1. The convergence rate is given in the next theorem.

**Theorem 3.11.** Let  $\beta = 2 \log(6c_\alpha/\delta)$ , where  $c_\alpha = \frac{1+2\pi}{2\pi}$ . Under Assumption 3.9, the CEI algorithm leads to the convergence rates of

$$\mathcal{O}\left(t^{-\frac{1}{2}} \log^{\frac{d+1}{2}}(t)\right) \text{ and } \mathcal{O}\left(t^{\frac{-\nu}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t)\right), \quad (17)$$

for SE and Matérn kernels, respectively, with probability  $\geq 1 - \delta$ .

**Sketch of Proof for Theorem 3.10.** Recall that  $f$  and  $c$  are assumed conditionally independent in CEI. We start from the bound on the confidence interval for  $f$ :  $|f(\mathbf{x}) - \mu_t^f(\mathbf{x})| \leq \beta^{1/2} \sigma_t^f(\mathbf{x})$ , with probability  $\geq 1 - \delta$ , where  $\beta = 2 \log(1/\delta)$ , as in Lemma C.2. Similarly,  $|c(\mathbf{x}) - \mu_t^c(\mathbf{x})| \leq \beta^{1/2} \sigma_t^c(\mathbf{x})$  with probability  $\geq 1 - \delta$ . These are well-known results [Srinivas et al., 2009]. Then, we derive the subsequent bounds  $|I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x})| \leq \sqrt{\beta} \sigma_t^f(\mathbf{x})$ , where  $\beta = \max\{1.44, 2 \log(c_\alpha/\delta)\}$  and  $c_\alpha = \frac{1+2\pi}{2\pi}$  with probability  $\geq 1 - \delta$  (Lemma C.4). Then, we prove the relationship in Lemma C.5 that  $I_t^f(\mathbf{x}) \leq \frac{\tau(\sqrt{\beta})}{\tau(-\sqrt{\beta})} EI_t^f(\mathbf{x})$  with probability  $\geq 1 - \delta$ . We can now follow the general analysis framework in Section 3.1 and Theorem 3.3 to obtain the simple regret upper bound under Bayesian assumptions.

**Remark 3.12** (Comparison to the frequentist setting). Comparing Theorem 3.7 to Theorem 3.11, the convergence rates in the frequentist and Bayesian settings are the same. This is because simple regret focuses on the best feasible solution  $f_t^+$  and thus the parameters in Theorem 3.3 and 3.10 do not depend on  $t$ . That is,  $c_{\tau B}$ ,  $B_c$ ,  $B_f$ ,  $M_f$ , and  $\beta$  do not depend on  $t$ . However, we note that  $\beta$  depends on the desired probability  $\delta$ .

**Remark 3.13** (Multiple constraints). As mentioned in Section 1, our results can be readily applied to CEI with multiple constraints for both frequentist and Bayesian settings. Consider  $m$  constraints  $c_i(\mathbf{x}) \leq 0$ ,  $i = 1, \dots, m$ . Assuming conditional independence of the constraints, the CEI function is  $EI_t^C(\mathbf{x}) = \prod_{i=1}^m P_t^i(\mathbf{x}) EI_t^f(\mathbf{x}) = \prod_{i=1}^m \Phi\left(\frac{-\mu_t^{c_i}(\mathbf{x})}{\sigma_t^{c_i}(\mathbf{x})}\right) EI_t^f(\mathbf{x})$ , where  $P_t^i$  is the probability of feasibility function of constraint  $c_i(\mathbf{x}) \leq 0$ , and  $\mu_t^{c_i}(\mathbf{x})$  and  $\sigma_t^{c_i}(\mathbf{x})$  are the posterior mean and standard deviation for  $c_i$ , respectively. By making the assumption that each constraint function lies

in its corresponding RKHS of the kernel  $k_{c_i}$ , we have  $|c_i(\mathbf{x}) - \mu_t^{c_i}(\mathbf{x})| \leq B_{c_i} \sigma_t^{c_i}(\mathbf{x})$ , where  $B_{c_i}$  is the upper bound of RKHS norm associated with kernel  $k_{c_i}$  and function  $c_i$ . We can then apply the analysis framework in this paper to obtain an upper bound similar to that of Theorem 3.3, where the term  $\frac{1}{\Phi(-B_c)}$  is replaced with  $\prod_{i=1}^m \frac{1}{\Phi(-B_{c_i})}$ . We note that to ensure probability  $1 - \delta$ , the parameter  $\beta$  needs to increase with the number of constraints as well, e.g.,  $\beta = 2 \log((m + 5)c_\alpha/\delta)$ .

*Remark 3.14* (Extension to the noisy setting). Extending our analysis to the noisy setting is non-trivial, and we discuss the associated challenges for noisy objective and constraint functions separately. A noisy constraint function introduces additional complications in defining feasibility. If only noisy observations of the constraint values are available, the notion of a feasible sample and the definition of  $f_t^+$  becomes ambiguous. As a result, major modifications to the CEI algorithm are required to appropriately handle the uncertainty introduced by noise.

For the noisy objective function, CEI can be adapted similarly to the noisy EI formulation by treating the best feasible noisy observation as the incumbent. However, to the best of our knowledge, a theoretical guarantee on the simple regret bound for the noisy unconstrained setting remains unavailable. Recent work by Wang et al. [2025] provides a framework for deriving noisy simple regret bounds based on the best observed value,  $r_t^s = y_t^+ - f(\mathbf{x}_t)$ , which can be extended to CEI. Specifically, by defining  $r_t^s$  as the simple regret for CEI with  $y_t^+$  denoting the best feasible noisy observation, a similar proof strategy as in Theorem 3.10 yields an analogous upper bound. In the Bayesian setting with i.i.d. Gaussian noise on the objective and noise-free constraint observations, the upper bound on  $r_t^s$  converges at a rate of  $\mathcal{O}\left(t^{-1/2} \log^{(d+1)/2} t\right)$  for SE kernels and  $\mathcal{O}\left(t^{-\nu/(2\nu+d)} \log^{\nu/(2\nu+d)} t\right)$  for Matérn kernels.

*Remark 3.15* (Infeasible initial sample). It is well known that one potential issue with CEI is the requirement of the initial feasible sample [Gardner et al., 2014]. That is,  $f_t^+$  exists from the initial samples so that the CEI calculation can proceed. Methods proposed to address this issue typically employ separate strategies when no feasible samples are available and revert to the standard CEI formulation once feasibility is established, e.g., relying only on the constraint surrogate model [Lin et al., 2024, Letham et al., 2019]. In addition, introducing a tolerance parameter in the constraint can further mitigate this problem by allowing near-feasible points when the degree of violation is small.

*Remark 3.16* (Tolerance in constraints). In gradient-based optimization methods, a tolerance for constraint violation is often used to improve the performance and flexibility of algorithms Wächter and Biegler [2006], Nocedal and Wright [2006]. Motivated by this, we introduce a tolerance parameter  $\lambda \geq 0$ , where a point  $\mathbf{x}$  is considered feasible if  $c(\mathbf{x}) \leq \lambda$  and infeasible otherwise. The corresponding CEI with tolerance is defined as  $EI_t^C(\mathbf{x}, \lambda) = P_t(\mathbf{x}, \lambda) EI_t^f(\mathbf{x}) = \Phi\left(\frac{\lambda - \mu_t^c(\mathbf{x})}{\sigma_t^c(\mathbf{x})}\right) EI_t^f(\mathbf{x})$ . Clearly, the standard CEI formulation is recovered when  $\lambda = 0$ .

The simple regret bound is affected by  $\lambda$  and should lead to  $\frac{1}{\Phi(\lambda - B_c)}$  in place of  $\frac{1}{\Phi(-B_c)}$ . In fact, we can replace  $\frac{1}{\Phi(\lambda - B_c)}$  with  $1/\Phi\left(\frac{\lambda}{\sigma_{t_k}^c(\mathbf{x}^*)} - B_c\right)$ , which is time-varying. One can follow the proof of Theorem 3.3 to obtain this term, which emerges from the confidence interval of  $c$  at  $t_k$ ,  $\mathbf{x}^*$  and  $c(\mathbf{x}^*) \leq 0$ .

As the sample iteration increases, the inclusion of  $\sigma_{t_k}^c(\mathbf{x}^*)$  is important in balancing  $-B_c$  that can lead to a large simple regret upper bound. We explain the intuition below. As  $t \rightarrow \infty$ ,  $t_k \rightarrow \infty$  and  $k \rightarrow \infty$ . We know  $\sigma_t^f(\mathbf{x}_{t+1}) \rightarrow 0$ , and hence  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \rightarrow 0$  and  $r_t \rightarrow 0$ . That is, the simple regret upper bound of CEI with  $\lambda > 0$  converges. Thus,  $\mathbf{x}_t$  approaches at least one of the optimal solutions. Suppose without losing generality,  $\mathbf{x}_t \rightarrow \mathbf{x}^*$ . Then, by definition  $\sigma_{t_k}^c(\mathbf{x}^*) \rightarrow 0$ .

Consequently, we should have  $\frac{\lambda}{\sigma_{t_k}^c(\mathbf{x}^*)} \rightarrow \infty$  for  $\lambda > 0$ . Then, we have  $\Phi\left(\frac{\lambda}{\sigma_{t_k}^c(\mathbf{x}^*)}\right) \rightarrow 1$ . Therefore,  $1/\Phi\left(\frac{\lambda}{\sigma_{t_k}^c(\mathbf{x}^*)} - B_c\right) \rightarrow 1$  and  $B_c$  does not affect the simple regret upper bound asymptotically. We note that the convergence rate of CEI with tolerance remains similar since it is dominated by the maximum information gain of  $f$ .

## 4 Numerical experiments

Although this paper is primarily theoretical, we conduct numerical experiments to support the theoretical results. We apply the CEI algorithm to eight synthetic problems that are randomly



generated from RKHS of kernels and GP priors, and five benchmark problems commonly used in the CBO literature. These numerical experiments are not intended to demonstrate superior performance over the state-of-the-art CBO algorithms. Instead, they serve as empirical evidence for the theoretical analysis presented in this work. All experiments are conducted on M1 (16GB memory)<sup>1</sup>.

#### 4.1 Synthetic problems

In this section, we study objective and constraint functions drawn from reproducing kernel Hilbert spaces (RKHSs) as well as from Gaussian process priors with Matérn ( $\nu = 2.5$ ) and squared exponential (SE) kernels, across input dimensions  $d \in 2, 4$ . The domain is the hypercube  $[0, 1]^d$ . For RKHS cases (the frequentist setting), the functions are generated with a similar approach to Chowdhury and Gopalan [2017]. Specifically, both objective  $f(x)$  and constraint functions  $c(x)$  are generated by sampling from the RKHS associated with a chosen kernel (Matérn/SE kernels with a length scale of 0.2). Each function is constructed as a weighted sum of kernel evaluations at 100 randomly selected basis points, with weights drawn from a standard normal distribution. Formally, the function takes the form  $f(x) = \sum_{i=1}^n \alpha_i k(x, X_i)$ , where  $k$  is the kernel,  $X_i$  are basis points, and  $\alpha_i$  are random coefficients;  $c(x)$  is generated similarly. For the GP cases (the Bayesian setting), the functions are generated with an approach similar to Srinivas et al. [2009]. Specifically, we uniformly choose 1000 points in the design space and sample randomly from a multivariate Gaussian distribution defined by the GP prior with the chosen kernel.

For each synthetic problem, we conducted 100 independent trials. The number of initial design is set to  $10d$ , and 50 optimization iterations were performed for all cases. We plotted the log-log curve of simple regret against the number of iterations in Figure 1. In all cases, we consistently observed sublinear convergence patterns, which align well with our theoretical guarantees.

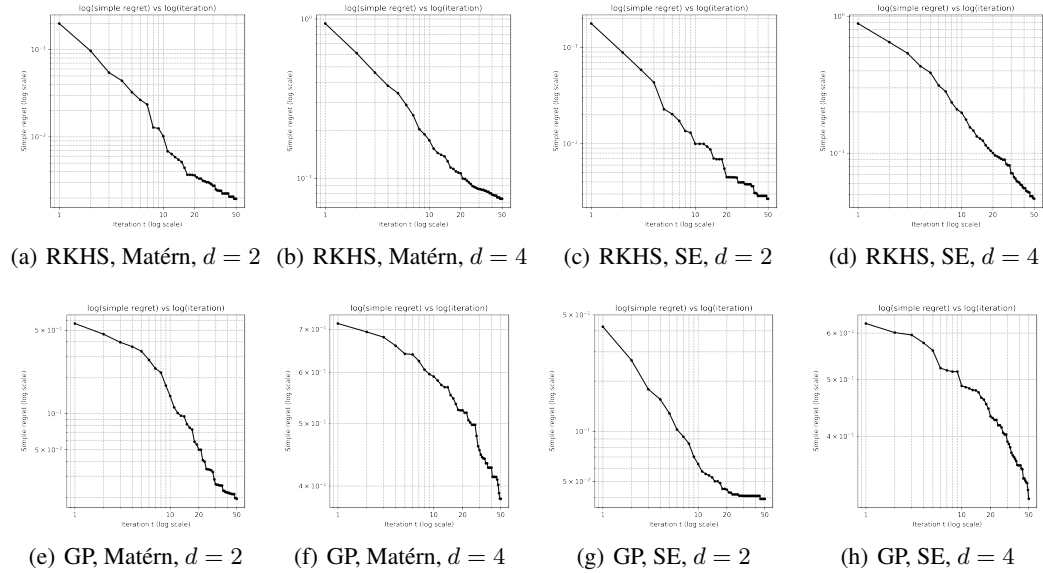


Figure 1: The log-log plots for simple regret vs optimization iterations of CEI for the synthetic problems.

#### 4.2 Test problems

Next, we evaluate simple regret of CEI on five commonly used test problems in the literature of CBO. Specifically, Problem 1 tests performance in a small feasible region, which was previously studied in Gardner et al. [2014], Ariafar et al. [2019]. Problem 2 includes multiple constraints and local minimums, which has been used in Gramacy et al. [2016], Hernández-Lobato et al. [2015]. Problem

<sup>1</sup>Codes are available in <https://github.com/Haowei-Wang/Convergence-Rates-of-Constrained-Expected-Improvement>.

3 is a four-dimensional problem, previously studied in Picheny et al. [2016], Ariaifar et al. [2019]. Problem 4 is the six-dimensional Hartmann problem, previously tested in Letham et al. [2019]. Problem 5 is the Rosenbrock function, where the global minimum lies in a narrow region. The mathematical formulations of the five functions are presented in Appendix D. For two-dimensional problems, we also include the contour plots of the objective and constraint functions in Appendix D. The SE kernel is used for the GP modeling (similar performance is observed for the Matérn kernel) and the hyper-parameters are estimated by a standard maximum likelihood method.

For each test problem, we conducted 100 independent trials with different random initial designs. When CEI fails to identify a feasible sample, we adopt the same heuristic strategy as in Letham et al. [2019]. The numerical results are summarized in Figure 2. The solid line represents the median of the simple regret, and the dotted lines represent the 25th percentile and 75th percentile of the simple regret, respectively. From the figures, we observe that CEI consistently reduces simple regret, aligning with the asymptotic convergence theories established in this paper. Accross all problems, the simple regret converges to 0 quickly. The 25th percentile and 75th percentile results demonstrate the good statistical properties of CEI.

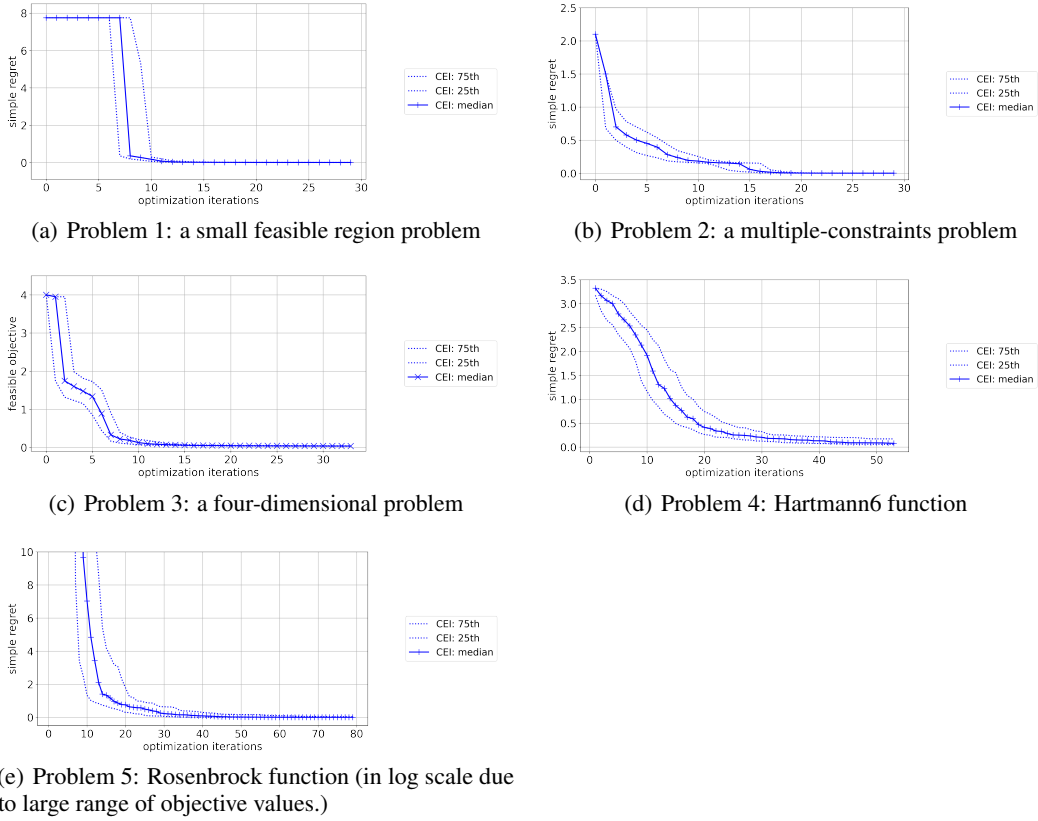


Figure 2: Simple regret of CEI for five test problems.

## 5 Conclusions

In this paper, we studied the simple regret upper bounds of the CEI algorithm, one of the most widely adopted CBO methods. Under both frequentist and Bayesian assumptions on the objective and constraint functions, we establish for the first time the convergence rates for CEI. Our results provide theoretical support and validation for the empirical success of CEI.

## References

- [1] S. Amini, I. Vannieuwenhuyse, and A. Morales-Hernández. Constrained bayesian optimization: A review. *IEEE Access*, 13:1581–1593, 2025. doi: 10.1109/ACCESS.2024.3522876.
- [2] S. Ariafar, J. Coll-Font, D. Brooks, and J. Dy. ADMMBO: Bayesian optimization with unknown constraints using ADMM. *Journal of Machine Learning Research*, 20(123):1–26, 2019.
- [3] M. Balandat, B. Karrer, D. R. Jiang, S. Daulton, B. Letham, A. G. Wilson, and E. Bakshy. BoTorch: A Framework for Efficient Monte-Carlo Bayesian Optimization. In *Advances in Neural Information Processing Systems* 33, 2020. URL <http://arxiv.org/abs/1910.06403>.
- [4] J. Bernardo, M. J. Bayarri, J. O. Berger, A. P. Dawid, D. Heckerman, A. F. Smith, and M. West. Optimization under unknown constraints. *Bayesian Statistics*, 9:229, October 2011.
- [5] E. Brochu, V. M. Cora, and N. De Freitas. A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning. *arXiv preprint arXiv:1012.2599*, December 2010.
- [6] A. D Bull. Convergence rates of efficient global optimization algorithms. *Journal of Machine Learning Research*, 12(10), 2011.
- [7] R. Calandra, A. Seyfarth, J. Peters, and M. P. Deisenroth. Bayesian optimization for learning gaits under uncertainty. *Annals of Mathematics and Artificial Intelligence*, 76:5–23, February 2016.
- [8] S. R. Chowdhury and A. Gopalan. On kernelized multi-armed bandits. In *International Conference on Machine Learning*, pages 844–853. PMLR, 2017.
- [9] P. I. Frazier. Bayesian optimization. In *Recent advances in optimization and modeling of contemporary problems*, pages 255–278, October 2018.
- [10] J. R. Gardner, M. J. Kusner, Z. Xu, K. Q. Weinberger, and J. P. Cunningham. Bayesian optimization with inequality constraints. In *Proceedings of the 31st International Conference on International Conference on Machine Learning - Volume 32, ICML’14*, pages II–937–II–945. JMLR.org, 2014.
- [11] M. A. Gelbart, J. Snoek, and R. P. Adams. Bayesian optimization with unknown constraints. *arXiv preprint arXiv:1403.5607*, 2014.
- [12] R. B. Gramacy, G. A. Gray, S. L. Digabel, H. K. lee, P. R. Ranjan, G. Wells, and S. M. Wild. Modeling an augmented lagrangian for blackbox constrained optimization. *technometrics*, 58(1):1–11, 2016.
- [13] J. M. Hernández-Lobato, M. Gelbart, M. Hoffman, R. Adams, and Z. Ghahramani. Predictive entropy search for Bayesian optimization with unknown constraints. In *International conference on machine learning*, pages 1699–1707. PMLR, 2015.
- [14] S. Iwazaki. Gaussian process upper confidence bound achieves nearly-optimal regret in noise-free gaussian process bandits. *arXiv preprint arXiv:2502.19006*, 2025.
- [15] D. R. Jones, M. Schonlau, and W. J. Welch. Efficient global optimization of expensive black-box functions. *Journal of Global optimization*, 13:455–492, 1998.
- [16] B. Letham, B. Karrer, G. Ottoni, and E. Bakshy. Constrained Bayesian optimization with noisy experiments. *Bayesian Anal.*, 14(2), 2019.
- [17] Q. Lin, J. Hu, Q. Zhou, L. Shu, and A. Zhang. A multi-fidelity bayesian optimization approach for constrained multi-objective optimization problems. *Journal of Mechanical Design*, 146(7): 071702, 2024.
- [18] C. Lu and J. A Paulson. No-regret bayesian optimization with unknown equality and inequality constraints using exact penalty functions. *IFAC-PapersOnLine*, 55(7):895–902, 2022.

- [19] Y. Lyu, Y. Yuan, and I. W. Tsang. Efficient batch black-box optimization with deterministic regret bounds. *arXiv preprint arXiv:1905.10041*, 2019.
- [20] A. Mathern, O. S. Steinholtz, A. Sjöberg, et al. Multi-objective constrained Bayesian optimization for structural design. *Structural and Multidisciplinary Optimization*, 63:689–701, February 2021.
- [21] J. Nocedal and S. Wright. *Numerical Optimization*. Springer-Verlag, New York, 2006.
- [22] V. Picheny, R. B. Gramacy, S. Wild, and S. Le Digabel. Bayesian optimization under mixed constraints with a slack-variable augmented lagrangian. *Advances in neural information processing systems*, 29, 2016.
- [23] I. O. Ryzhov. On the convergence rates of expected improvement methods. *Operations Research*, 64(6):1515–1528, 2016.
- [24] M. Schonlau, W. J. Welch, and D. R. Jones. Global versus local search in constrained optimization of computer models. *Lecture notes-monograph series*, pages 11–25, 1998.
- [25] J. Song, Y. Cui, P. Wei, M. A. Valdebenito, and W. Zhang. Constrained bayesian optimization algorithms for estimating design points in structural reliability analysis. *Reliability Engineering System Safety*, 241:109613, 2024.
- [26] N. Srinivas, A. Krause, S. M. Kakade, and M. Seeger. Gaussian process optimization in the bandit setting: No regret and experimental design. *arXiv preprint arXiv:0912.3995*, 2009.
- [27] J. Ungredda and J. Branke. Bayesian optimisation for constrained problems. *ACM Trans. Model. Comput. Simul.*, 34(2), April 2024.
- [28] S. Vakili. Open problem: Regret bounds for noise-free kernel-based bandits. In *Conference on Learning Theory*, pages 5624–5629. PMLR, 2022.
- [29] S. Vakili, K. Khezeli, and V. Picheny. On information gain and regret bounds in gaussian process bandits. In *International Conference on Artificial Intelligence and Statistics*, pages 82–90. PMLR, 2021.
- [30] E. Vazquez and J. Bect. Convergence properties of the expected improvement algorithm with fixed mean and covariance functions. *Journal of Statistical Planning and inference*, 140(11): 3088–3095, 2010.
- [31] J. Wang, N. Chiang, A. Gillette, and J. L. Peterson. A multifidelity bayesian optimization method for inertial confinement fusion design. *Physics of Plasmas*, 31(3), 2024.
- [32] J. Wang, H. Wang, C. G. Petra, and N. Y. Chiang. On the convergence of noisy bayesian optimization with expected improvement. *arXiv preprint arXiv:2501.09262*, 2025.
- [33] J. Wu, X. Chen, H. Zhang, L. Xiong, H. Lei, and S. Deng. Hyperparameter optimization for machine learning models based on bayesian optimization. *Journal of Electronic Science and Technology*, 17(1):26–40, 2019.
- [34] A. Wächter and L. Biegler. On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Math. Program.*, 106(1):25–27, 2006.
- [35] X. Zhou and B. Ji. On kernelized multi-armed bandits with constraints. *Advances in neural information processing systems*, 35:14–26, 2022.

## NeurIPS Paper Checklist

### 1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope?

Answer: [\[Yes\]](#)

Justification: NA

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

### 2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [\[Yes\]](#)

Justification: The assumptions for our theoretical analysis are clearly stated.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

### 3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [\[Yes\]](#)

Justification: NA

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

#### 4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [\[Yes\]](#)

Justification: We provide all the details and supplemental codes.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
  - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
  - (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
  - (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
  - (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

#### 5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

#### 6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

#### 7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.

- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

#### 8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

#### 9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

#### 10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [NA]

Justification: This is a theoretical paper focused on existing algorithms.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to



generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.

- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

#### 11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [NA]

Justification: We do not have such data.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

#### 12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.
- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, [paperswithcode.com/datasets](https://paperswithcode.com/datasets) has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.
- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

#### 13. New assets

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [Yes]

Justification: NA

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

#### 14. Crowdsourcing and research with human subjects

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: NA

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

#### 15. Institutional review board (IRB) approvals or equivalent for research with human subjects

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: NA

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

#### 16. Declaration of LLM usage

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

Answer: [NA]

Justification: NA

Guidelines:

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.

## A Background information and preliminary results

### A.1 Information gain

To obtain state-of-the-art simple regret upper bound, we utilize the information theory results that are well-established in previous literature [26, 8, 29]. Using  $f$  as the example, let  $A \subset C$  denote a set of sampling points. Assume that the observations are noisy at sample points with  $y_A = f(x_A) + \epsilon_A$  at  $x \in A$ , where  $\epsilon_A \sim \mathcal{N}(0, \sigma^2)$  denotes the independent and identically distributed Gaussian noises. The maximum information gain is defined as follows.

**Definition A.1.** Given  $x_A$  and  $y_A$ , the mutual information between  $f$  and  $y_A$  is  $I(y_A; f_A) = H(y_A) - H(y_A|f_A)$ , where  $H$  denotes the entropy. The maximum information gain  $\gamma_T^f$  after  $T$  samples is  $\gamma_T^f = \max_{A \subset C, |A|=T} I(y_A; f_A)$ .

The rate of increase for  $\gamma_t^f$  depends on the property of the kernel. For common kernels such as the SE kernel and the Matérn kernel,  $\gamma_t^f$  has been widely studied in literature and the state-of-the-art rates of  $\gamma_t^f$  are summarized in Lemma A.2 [29].

**Lemma A.2.** For GP with  $t$  samples, the SE kernel has  $\gamma_t = \mathcal{O}(\log^{d+1}(t))$ , and the Matérn kernel with smoothness parameter  $\nu > 0.5$  has  $\gamma_t = \mathcal{O}(t^{\frac{d}{2\nu+d}} (\log^{\frac{2\nu}{2\nu+d}}(t)))$ .

The maximum information gain  $\gamma_t^c$  for the constraint function can be defined similarly.

While  $\gamma_t^f$  is defined in the noisy case, we can readily apply it to the noise-free case and bound  $\sigma_t^f(x_{t+1})$  using techniques similar to that in [19]. To do so, we note that given the Gaussian observation noise  $\epsilon_t \sim \mathcal{N}(0, \sigma^2)$  in the GP model, the posterior prediction for  $f$  becomes

$$\begin{aligned}\tilde{\mu}_t^f(x) &= \mathbf{k}_t^f(x)(\mathbf{K}_t^f + \sigma^2 \mathbf{I})^{-1} \mathbf{f}_{1:t}, \\ (\tilde{\sigma}_t^f)^2(x) &= k^f(x, x) - (\mathbf{k}_t^f)^T(x)(\mathbf{K}_t^f + \sigma^2 \mathbf{I})^{-1} \mathbf{k}_t^f(x),\end{aligned}\tag{18}$$

Similarly, we can define the posterior predictions for  $c$  with noise in the GP model as  $\tilde{\mu}_t^c(x)$  and  $\tilde{\sigma}_t^c(x)$ . The sum of posterior variance for GP generated by (2) satisfy the next lemma, based on information theory [26].

**Lemma A.3.** The sum of GP posterior variances given  $t$  samples satisfy

$$\sum_{t=1}^T \tilde{\sigma}_{t-1}^c(x_t) \leq \sqrt{C_\gamma T \gamma_T^c}, \quad \sum_{t=1}^T \tilde{\sigma}_{t-1}^f(x_t) \leq \sqrt{C_\gamma T \gamma_T^f},\tag{19}$$

where  $C_\gamma = \frac{2}{\log(1+\sigma^{-2})}$  and  $\gamma_t^f$  and  $\gamma_t^c$  are the maximum information gains for  $f$  and  $c$ , respectively.

We have the following lemma for  $\tilde{\sigma}_t^f(x)$  and  $\sigma_t^f(x)$ .

**Lemma A.4.** The noise-free (GP) posterior standard deviation satisfies  $\sigma_t^f(x) < \tilde{\sigma}_t^f(x)$  for  $\forall \sigma > 0$ .

*Proof.* We first note that all the eigenvalues of  $\mathbf{K}_t^f$  is smaller than those of  $\mathbf{K}_t^f + \sigma^2 \mathbf{I}$ , since  $\mathbf{K}_t^f$  is symmetric and positive definite. Thus,

$$(\mathbf{k}_t^f)^T(x)(\mathbf{K}_t^f + \sigma^2 \mathbf{I})^{-1} \mathbf{k}_t^f(x) < (\mathbf{k}_t^f)^T(x)(\mathbf{K}_t^f)^{-1} \mathbf{k}_t^f(x),\tag{20}$$

for  $\forall \sigma > 0$  and  $\mathbf{k}_t^f(x)$ . Therefore, by their definitions (2) and (18), the proof is complete.  $\square$

The posterior standard deviation under assumptions (1)-(4) in [6] in the frequentist and noise-free setting is given in Lemma 3.5, whose proof is given below.

*Proof.* By Lemma 7 in [6], there exists  $C' > 0$  so that

$$\sigma_i^f(x_{i+1}) \geq C' k^{-\frac{\min\{\nu, 1\}}{d}} \log^\eta(k),\tag{21}$$

at most  $k$  times, for  $\forall k \in \mathbb{N}$ ,  $k \leq t$ , and  $i = 1, \dots, t-1$ . Therefore, for the SE kernel,

$$\sigma_i^f(x_{i+1}) \geq C' k^{-\frac{1}{d}},\tag{22}$$

at most  $k$  times. For Matérn kernels, we have (21) at most  $k$  times.  $\square$

Using maximum information gain, a tighter bound on the posterior standard deviation can be obtained in the next lemma.

**Lemma A.5.** *Given  $\forall t \in \mathbb{N}$  and  $i = 1, 2, \dots, t-1$ , for SE kernel, there exists constant  $C' > 0$  so that*

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq C' \frac{t^{\frac{1}{2}} \log^{\frac{d+1}{2}}(t)}{k}, \quad (23)$$

*holds for at most  $k$  times, for  $\forall k \leq t$ . Similarly, for Matérn kernels with  $\nu > 0.5$ ,*

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq C' \frac{t^{\frac{\nu+d}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t)}{k}, \quad (24)$$

*holds at most  $k$  times.*

*Proof.* From Lemma A.4 and Lemma A.3, we can write that

$$\sum_{i=1}^t \sigma_{i-1}^f(\mathbf{x}_i) \leq \sqrt{t\gamma_t^f}, \quad (25)$$

where we use without losing generality  $C_\gamma \leq 1$ . Therefore, for any  $k \in \mathbb{N}$  and  $k \leq t$ ,

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq \frac{\sqrt{t\gamma_t^f}}{k}, \quad (26)$$

at most  $k$  times. Therefore, for SE kernel, by Lemma A.2, there exists  $C' > 0$  such that

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq C' \frac{t^{\frac{1}{2}} \log^{\frac{d+1}{2}}(t)}{k}, \quad (27)$$

at most  $k$  times. For Matérn kernels with  $\nu > 0.5$ ,

$$\sigma_i^f(\mathbf{x}_{i+1}) \geq C' \frac{t^{\frac{\nu+d}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t)}{k}, \quad (28)$$

at most  $k$  times. □

Next, we state some basic properties of  $\phi$ ,  $\Phi$  and  $\tau$  as a lemma.

**Lemma A.6.** *The PDF and CDF of standard normal distribution satisfy  $0 < \phi(x) \leq \phi(0) < 0.4$ ,  $\Phi(x) \in (0, 1)$ , for any  $x \in \mathbb{R}$ . Given a random variable  $\xi$  sampled from the standard normal distribution:  $\xi \sim \mathcal{N}(0, 1)$ , we have  $\mathbb{P}\{\xi > c | c > 0\} \leq \frac{1}{2}e^{-c^2/2}$ . Similarly, for  $c < 0$ ,  $\mathbb{P}\{\xi < c | c < 0\} \leq \frac{1}{2}e^{-c^2/2}$ . The function  $\tau(\cdot)$  is monotonically increasing.*

The last statement in Lemma A.6 is a well-known result (e.g., see proof of Lemma 5.1 in [26]).

The next lemma proves basic properties for  $EI_t^f$ .

**Lemma A.7.** *For  $\forall \mathbf{x} \in C$ ,  $EI_t^f(\mathbf{x}) \geq 0$  and  $EI_t^f(\mathbf{x}) \geq f_t^+ - \mu_t^f(\mathbf{x})$ . Moreover,*

$$z_t^f(\mathbf{x}) \leq \frac{EI_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} < \begin{cases} \phi(z_t^f(\mathbf{x})), & z_t^f(\mathbf{x}) < 0, \\ z_t^f(\mathbf{x}) + \phi(z_t^f(\mathbf{x})), & z_t^f(\mathbf{x}) \geq 0. \end{cases} \quad (29)$$

*Proof.* From the definition of  $I_t^f$  and  $EI_t^f$ ,  $EI_t^f(\mathbf{x}) \geq 0$  and  $EI_t^f(\mathbf{x}) \geq y_t^+ - \mu_t^f(\mathbf{x})$  follow immediately. By (4),

$$\frac{EI_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} = z_t^f(\mathbf{x})\Phi(z_t^f(\mathbf{x})) + \phi(z_t^f(\mathbf{x})). \quad (30)$$

If  $z_t^f(\mathbf{x}) < 0$ , or equivalently  $f_t^+ - \mu_t^f(\mathbf{x}) < 0$ , (30) leads to  $\frac{EI_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} < \phi(z_t^f(\mathbf{x}))$ . If  $z_t^f(\mathbf{x}) \geq 0$ , we can write  $\frac{EI_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} < z_t^f(\mathbf{x}) + \phi(z_t^f(\mathbf{x}))$ . The left inequality in (29) is an immediate result of  $EI_t^f(\mathbf{x}) \geq f_t^+ - \mu_t^f(\mathbf{x})$ . □

## B Proofs for simple regret upper bound under frequentist assumptions

We state the boundedness result as a Lemma for easy reference.

**Lemma B.1.** *Under Assumption 3.2,  $|f(\mathbf{x})| \leq B_f$  and  $|c(\mathbf{x})| \leq B_c$  for all  $\mathbf{x} \in C$ .*

*Proof.* By Assumption 3.2, we can write

$$|f(\mathbf{x})| \leq \|f\|_{H_k^f} k_f(\mathbf{x}, \mathbf{x}) \leq B_f. \quad (31)$$

Similarly,

$$|c(\mathbf{x})| \leq \|c\|_{H_k^c} k_c(\mathbf{x}, \mathbf{x}) \leq B_c. \quad (32)$$

□

The following Lemma is a well-established result [8].

**Lemma B.2.** *At any given  $\mathbf{x} \in C$  and  $t \in \mathbb{N}$ , the confidence intervals satisfy*

$$|f(\mathbf{x}) - \mu_t^f(\mathbf{x})| \leq B_f \sigma_t^f(\mathbf{x}), |c(\mathbf{x}) - \mu_t^c(\mathbf{x})| \leq B_c \sigma_t^c(\mathbf{x}). \quad (33)$$

Next, we present a lemma on the relationship between  $I_t^f$  and  $EI_t^f$ , previously seen in [6].

**Lemma B.3.** *At  $\mathbf{x} \in C, t \in \mathbb{N}$ ,*

$$I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x}) \leq B_f \sigma_t^f(\mathbf{x}). \quad (34)$$

**Lemma B.4.** *The improvement function  $I_t^f(\mathbf{x})$  and  $EI_t^f(\mathbf{x})$  satisfy*

$$I_t^f(\mathbf{x}) \leq \frac{\tau(B_f)}{\tau(-B_f)} EI_t^f(\mathbf{x}), \quad (35)$$

for  $\forall \mathbf{x} \in C$  and  $t \geq 1$ .

*Proof.* If  $f_t^+ - f(\mathbf{x}) \leq 0$ , then  $I_t^f(\mathbf{x}) = 0$ . Since  $EI_t^f(\mathbf{x}) \geq 0$ , (35) is trivial. If  $f_t^+ - f(\mathbf{x}) > 0$ , by Lemma B.2,

$$f_t^+ - \mu_t^f(\mathbf{x}) = f_t^+ - f(\mathbf{x}) + f(\mathbf{x}) - \mu_t^f(\mathbf{x}) > f(\mathbf{x}) - \mu_t^f(\mathbf{x}) > -B_f \sigma_t^f(\mathbf{x}). \quad (36)$$

From the monotonicity of  $\tau$ , we have

$$\tau\left(\frac{f_t^+ - \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right) > \tau(-B_f), \quad (37)$$

and therefore,

$$EI_t^f(\mathbf{x}) = \sigma_t^f(\mathbf{x}) \tau\left(\frac{f_t^+ - \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right) > \tau(-B_f) \sigma_t^f(\mathbf{x}). \quad (38)$$

From Lemma B.3,

$$I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x}) \leq B_f \sigma_t^f(\mathbf{x}). \quad (39)$$

Applying (39) to (38) leads to

$$EI_t^f(\mathbf{x}) > \frac{\tau(-B_f)}{B_f + \tau(-B_f)} I_t^f(\mathbf{x}) = \frac{\tau(-B_f)}{\tau(B_f)} I_t^f(\mathbf{x}). \quad (40)$$

□

Proof of Theorem 3.3 is given next.

*Proof.* From Lemma B.1,

$$\sum_{i=0}^{t-1} f_i^+ - f_{i+1}^+ = f_0^+ - f_t^+ \leq 2B_f. \quad (41)$$

Since  $f_i^+ - f_{i+1}^+ \geq 0$ ,  $f_i^+ - f_{i+1}^+ \geq \frac{2B_f}{k}$  at most  $k$  times for any  $k \in \mathbb{N}$ . Further,  $f(\mathbf{x}_t) \geq f_t^+$  for  $\forall t \in \mathbb{N}$ . Choose  $k = \lfloor t/2 \rfloor$ , where  $\lfloor x \rfloor$  is the largest integer smaller than  $x$  so that  $2k \leq t \leq 2(k+1)$ . Then, there exists  $k \leq t_k \leq 2k$  so that  $f_{t_k}^+ - f_{t_k+1}^+ < \frac{2B_f}{k}$  and  $f_{t_k+1}^+ - f(\mathbf{x}_{t_k+1}) \leq 0$ .

From Lemma B.4,

$$\begin{aligned} r_t &= f_t^+ - f(\mathbf{x}^*) \leq f_{t_k}^+ - f(\mathbf{x}^*) \leq I_{t_k}^f(\mathbf{x}^*) \\ &\leq \frac{\tau(B_f)}{\tau(-B_f)} EI_{t_k}^f(\mathbf{x}^*) = c_{\tau B} \frac{P_{t_k}(\mathbf{x}^*)}{P_{t_k}(\mathbf{x}^*)} EI_{t_k}^f(\mathbf{x}^*) \\ &\leq c_{\tau B} \frac{P_{t_k}(\mathbf{x}_{t_k+1})}{P_{t_k}(\mathbf{x}^*)} EI_{t_k}^f(\mathbf{x}_{t_k+1}), \end{aligned} \quad (42)$$

where  $c_{\tau B} = \frac{\tau(B_f)}{\tau(-B_f)}$ . Using  $P_t(\mathbf{x}) \leq 1$ , (42) implies

$$\begin{aligned} r_t &\leq \frac{c_{\tau B}}{P_{t_k}(\mathbf{x}^*)} \left[ (f_{t_k}^+ - \mu_{t_k}^f(\mathbf{x}_{t_k+1})) \Phi(z_{t_k}^f(\mathbf{x}_{t_k+1})) + \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \phi(z_{t_k}^f(\mathbf{x}_{t_k+1})) \right] \\ &\leq \frac{c_{\tau B}}{P_{t_k}(\mathbf{x}^*)} \left[ (f_{t_k}^+ - \mu_{t_k}^f(\mathbf{x}_{t_k+1})) \Phi(z_{t_k}^f(\mathbf{x}_{t_k+1})) + 0.4 \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right], \end{aligned} \quad (43)$$

where the last inequality uses  $\phi(\cdot) < 0.4$ . From Lemma B.2,

$$\begin{aligned} f_{t_k}^+ - \mu_{t_k}^f(\mathbf{x}_{t_k+1}) &= f_{t_k}^+ - f_{t_k+1}^+ + f_{t_k+1}^+ - f(\mathbf{x}_{t_k+1}) + f(\mathbf{x}_{t_k+1}) - \mu_{t_k}^f(\mathbf{x}_{t_k+1}) \\ &\leq f_{t_k}^+ - f_{t_k+1}^+ + B_f \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \leq \frac{2B_f}{k} + B_f \sigma_{t_k}^f(\mathbf{x}_{t_k+1}). \end{aligned} \quad (44)$$

Using (44) in (43), we have

$$r_t \leq \frac{c_{\tau B}}{P_{t_k}(\mathbf{x}^*)} \left[ \frac{2B_f}{k} + (B_f + 0.4) \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right]. \quad (45)$$

Next, we consider the function  $P_{t_k}$  at  $\mathbf{x}^*$ . Using the fact that  $c(\mathbf{x}^*) \leq 0$ , we have by Lemma B.2,

$$\mu_{t_k}^c(\mathbf{x}^*) \leq B_c \sigma_{t_k}^c(\mathbf{x}^*) + c(\mathbf{x}^*) \leq B_c \sigma_{t_k}^c(\mathbf{x}^*). \quad (46)$$

Thus,

$$\frac{-\mu_{t_k}^c(\mathbf{x}^*)}{\sigma_{t_k}^c(\mathbf{x}^*)} \geq -B_c. \quad (47)$$

From the monotonicity of  $\Phi$ , we have

$$P_{t_k}(\mathbf{x}^*) = \Phi \left( \frac{-\mu_{t_k}^c(\mathbf{x}^*)}{\sigma_{t_k}^c(\mathbf{x}^*)} \right) \geq \Phi(-B_c). \quad (48)$$

Applying (48) to (43), we have

$$r_t \leq \frac{c_{\tau B}}{\Phi(-B_c)} \left[ \frac{2B_f}{k} + (B_f + 0.4) \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right]. \quad (49)$$

As  $t \rightarrow \infty$ ,  $t_k \rightarrow \infty$  and  $k \rightarrow \infty$ . Further, if  $\sigma_t^f(\mathbf{x}_{t+1}) \rightarrow 0$ ,  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \rightarrow 0$  and  $r_t \rightarrow 0$ .  $\square$

Proof of Corollary 3.6 is presented next.

*Proof.* We consider the convergence rate for  $r_t$  under additional assumptions for the kernel. From Lemma 3.5, for both SE and Matérn kernels,  $\sigma_i^f(\mathbf{x}_{i+1}) \geq C' k^{-\frac{\min\{\nu, 1\}}{d}} \log^\eta(k)$  at most  $k$  times for any  $k \in \mathbb{N}$  and  $i = 1, \dots, t$ .

Choose  $k = \lfloor t/3 \rfloor$  so that  $3k \leq t \leq 3(k+1)$ . Following the proof of Theorem 3.3, there exists  $k \leq t_k \leq 3k$  where  $f_{t_k}^+ - f_{t_k+1}^+ < \frac{2B_f}{k}$ ,  $f(\mathbf{x}_{t_k+1}) \geq f_{t_k+1}^+$ , and  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1}) < C' k^{-\frac{\min\{\nu, 1\}}{d}} \log^\eta(k)$ . Similar to (49), we can obtain

$$r_t \leq \frac{c_{\tau B}}{\Phi(-B_c)} \left[ \frac{2B_f}{k} + (B_f + 0.4) C' k^{-\frac{\min\{\nu, 1\}}{d}} \log^\eta(k) \right]. \quad (50)$$

The convergence rates follow.  $\square$

### B.1 Proofs for improved simple regret upper bound under frequentist assumptions

Proof of Theorem 3.7 is given below.

*Proof.* From the proof of Lemma A.5, we know  $\sigma_i^f(\mathbf{x}_{i+1}) \geq \frac{\sqrt{t\gamma_t^f}}{k}$  at most  $k$  times for any  $k \leq t$  and  $i = 1, \dots, t$ .

Choose  $k = \lceil t/3 \rceil$  so that  $3k \leq t \leq 3(k+1)$ . Following the proof of Theorem 3.3, there exists  $k \leq t_k \leq 3k$  where  $f_{t_k}^+ - f_{t_k+1}^+ < \frac{2B_f}{k}$ ,  $f(\mathbf{x}_{t_k+1}) \geq f_{t_k+1}^+$ , and  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1}) < 3\frac{\sqrt{t\gamma_t^f}}{t-3}$ . Similar to (50), we can obtain

$$r_t \leq \frac{c_{B_f}}{\Phi(-B_c)} \left[ 3\frac{2B_f}{t-3} + 3(B_f + 0.4)\frac{\sqrt{t\gamma_t^f}}{t-3} \right]. \quad (51)$$

The convergence rates of the simple regret upper bound follow from Lemma A.5.  $\square$

We provide the sample complexity of Theorem 3.7 below.

**Corollary B.5.** *Under Assumption 3.2, the CEI algorithm achieves a  $\epsilon$  sample complexity of*

$$\mathcal{O}\left(\frac{1}{\epsilon^2}[\log(1/\epsilon)]^{d+1}\right) \text{ and } \mathcal{O}\left(\epsilon^{-\frac{2\nu+d}{\nu}} \log(1/\epsilon)\right), \quad (52)$$

for SE and Matérn kernels, respectively.

*Proof.* Using Theorem 3.7, to achieve simple regret of most  $\epsilon$  for SE kernel, set

$$t^{-\frac{1}{2}} \log^{\frac{d+1}{2}}(t) = \epsilon.$$

Solving asymptotically for  $t$  gives the sample complexity

$$t(\epsilon) = \mathcal{O}\left(\frac{1}{\epsilon^2}[\log(1/\epsilon)]^{d+1}\right).$$

Similarly, for Matérn kernels, we have

$$\epsilon = t^{\frac{-\nu}{2\nu+d}} \log^{\frac{\nu}{2\nu+d}}(t), \quad (53)$$

which completes the proof.  $\square$

### C Proofs for simple upper bound regret under Bayesian assumptions

We state the boundedness of  $f$  and  $c$  as a Lemma for easy reference.

**Lemma C.1.** *Under Assumption 3.9, there exists  $M_f > 0$  such that  $|f(\mathbf{x})| \leq M_f$ . Similarly, there exists  $M_c > 0$  such that  $|c(\mathbf{x})| \leq M_c$ .*

We recall a well-known result on confidence interval of  $|f(\mathbf{x}) - \mu_t^f(\mathbf{x})|$  under Assumption 3.9 [26].

**Lemma C.2.** *Given  $\delta \in (0, 1)$ , let  $\beta = 2\log(1/\delta)$ . For any given  $\mathbf{x} \in C$  and  $t \in \mathbb{N}$ ,*

$$|f(\mathbf{x}) - \mu_t^f(\mathbf{x})| \leq \sqrt{\beta\sigma_t^f(\mathbf{x})}, \quad (54)$$

holds with probability  $\geq 1 - \delta$ . Similarly, with  $\delta \in (0, 1)$  and  $\beta = 2\log(1/\delta)$ .

$$|c(\mathbf{x}) - \mu_t^c(\mathbf{x})| \leq \sqrt{\beta\sigma_t^c(\mathbf{x})}, \quad (55)$$

with probability  $\geq 1 - \delta$ .



*Proof.* We prove the inequalities for  $f$ . Under Assumption 3.9,  $f(\mathbf{x}) \sim \mathcal{N}(\mu_t(\mathbf{x}), \sigma_t^2(\mathbf{x}))$ . By Lemma A.6,

$$\mathbb{P}\left\{f(\mathbf{x}) - \mu_t^f(\mathbf{x}) > \sqrt{\beta}\sigma_t^f(\mathbf{x})\right\} = 1 - \Phi\left(\sqrt{\beta}\right) \leq \frac{1}{2}e^{-\frac{\beta}{2}}. \quad (56)$$

Similarly,

$$\mathbb{P}\left\{f(\mathbf{x}) - \mu_t^f(\mathbf{x}) < -\sqrt{\beta}\sigma_t^f(\mathbf{x})\right\} \leq \frac{1}{2}e^{-\frac{\beta}{2}}. \quad (57)$$

Thus,

$$\mathbb{P}\left\{|f(\mathbf{x}) - \mu_t^f(\mathbf{x})| < \sqrt{\beta}\sigma_t^f(\mathbf{x})\right\} \geq 1 - e^{-\frac{\beta}{2}}. \quad (58)$$

Let  $e^{-\frac{\beta}{2}} = \delta$  and (54) is proven. Similarly, (55) can be proven.  $\square$

The next lemma address  $I_t^f$  under the Bayesian assumption.

**Lemma C.3.** *Under Assumption 3.9, the probability distribution of  $I_t^f$  satisfies*

$$\mathbb{P}\{I_t^f(\mathbf{x}) \leq a\} = \begin{cases} 0, & a < 0, \\ \Phi\left(\frac{a}{\sigma_t^f(\mathbf{x})} - z_t^f(\mathbf{x})\right), & a \geq 0. \end{cases} \quad (59)$$

*Proof.* Under Assumption 3.9, at a given  $t$ ,  $f(\mathbf{x}) \sim \mathcal{N}(\mu_t^f(\mathbf{x}), \sigma_t^f(\mathbf{x}))$ . Since  $I_t^f(\mathbf{x}) \geq 0$  for all  $\mathbf{x}$ , (59) follows immediately if  $a < 0$ . For  $a \geq 0$ ,

$$\mathbb{P}\{I_t^f(\mathbf{x}) \leq a\} = \mathbb{P}\{f_t^+ - f(\mathbf{x}) \leq a\} = 1 - \mathbb{P}\{f(\mathbf{x}) \leq f_t^+ - a\}.$$

Using basic properties of the standard normal CDF,

$$1 - \mathbb{P}\{f(\mathbf{x}) \leq f_t^+ - a\} = 1 - \Phi\left(\frac{f_t^+ - a - \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right) = \Phi\left(\frac{a - f_t^+ + \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right). \quad \square$$

Next, we present the relationship between  $I_t^f(\mathbf{x})$  and  $EI_t^f(\mathbf{x})$ .

**Lemma C.4.** *Given  $\delta \in (0, 1)$ , let  $\beta = \max\{1.44, 2\log(c_\alpha/\delta)\}$ , where constant  $c_\alpha = \frac{1+2\pi}{2\pi}$ . Under Assumption 3.9, at given  $\mathbf{x} \in C$  and  $t \in \mathbb{N}$ ,*

$$\mathbb{P}\left\{|I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x})| \leq \sqrt{\beta}\sigma_t^f(\mathbf{x})\right\} \geq 1 - \delta. \quad (60)$$

*Proof.* Given a scalar  $w > 1$ , we consider the probabilities

$$\mathbb{P}\left\{I_t^f(\mathbf{x}) > \sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x})\right\} \quad \text{and} \quad \mathbb{P}\left\{I_t^f(\mathbf{x}) < -\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x})\right\}. \quad (61)$$

Consider the first probability in (61). From Lemma A.7,  $EI_t^f(\mathbf{x}) \geq 0$  for  $\forall \mathbf{x}$  and  $t$ . Therefore,  $\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x}) > 0$ . From Lemma A.7, Lemma C.3, and the monotonicity of  $\Phi$ , we have

$$\begin{aligned} \mathbb{P}\left\{I_t^f(\mathbf{x}) > \sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x})\right\} &= 1 - \Phi\left(\frac{\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x}) - f_t^+ + \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right) \\ &\leq 1 - \Phi(w) \leq \frac{1}{2}e^{-\frac{w^2}{2}}, \end{aligned} \quad (62)$$

where the last inequality is from Lemma A.6.

For the second probability in (61), we further distinguish between two cases. First, consider  $-\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x}) < 0$ . From Lemma C.3,

$$\mathbb{P}\left\{I_t^f(\mathbf{x}) < -\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x})\right\} = 0. \quad (63)$$

Second, consider the premise  $-\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x}) \geq 0$ . By Lemma C.3, we have

$$\mathbb{P}\left\{I_t^f(\mathbf{x}) < -\sigma_t^f(\mathbf{x})w + EI_t^f(\mathbf{x})\right\} = \Phi\left(-w + \frac{EI_t^f(\mathbf{x}) - f_t^+ + \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right). \quad (64)$$

To proceed, we show that  $f_t^+ - \mu_t^f(\mathbf{x}) \geq 0$ . Suppose on the contrary,  $f_t^+ - \mu_t^f(\mathbf{x}) < 0$  and thus  $z_t^f(\mathbf{x}) < 0$ . From Lemma A.7,

$$\frac{EI_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} < \phi(z_t^f(\mathbf{x})) \leq \phi(0) < 1 \leq w, \quad (65)$$

which contradicts the premise of this case. Thus, we have  $f_t^+ - \mu_t^f(\mathbf{x}) \geq 0$  (and  $z_t^f(\mathbf{x}) \geq 0$ ). From the definition (4), since  $\Phi \in (0, 1)$ ,

$$\frac{EI_t^f(\mathbf{x}) - f_t^+ + \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} = \left[ z_t^f(\mathbf{x}) \left( \Phi(z_t^f(\mathbf{x})) - 1 \right) + \phi(z_t^f(\mathbf{x})) \right] < \phi(z_t^f(\mathbf{x})). \quad (66)$$

In addition, by the premise of this case and Lemma A.7,

$$w \leq \frac{EI_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})} \leq z_t^f(\mathbf{x}) + \phi(z_t^f(\mathbf{x})). \quad (67)$$

Given that  $w > 1$  and  $\phi(0) \geq \phi(z_t^f(\mathbf{x}))$ , we have

$$z_t^f(\mathbf{x}) + \phi(0) > z_t^f(\mathbf{x}) + \phi(z_t^f(\mathbf{x})) > w, \quad z_t^f(\mathbf{x}) > w - \phi(0) > 0. \quad (68)$$

As  $z_t(\mathbf{x}) \geq 0$  increases,  $\phi(z_t(\mathbf{x})) > 0$  decreases. Thus, we have

$$\frac{z_t^f(\mathbf{x})}{\phi(z_t^f(\mathbf{x}))} > \frac{w - \phi(0)}{\phi(w - \phi(0))}, \quad \phi(z_t^f(\mathbf{x})) < \frac{\phi(w - \phi(0))}{w - \phi(0)} z_t^f(\mathbf{x}). \quad (69)$$

Denote  $c_1(w) = \frac{w - \phi(0)}{w - \phi(0) + \phi(w - \phi(0))}$ . Applying (69) to (67), we obtain

$$c_1(w)w < z_t^f(\mathbf{x}), \quad \phi(z_t^f(\mathbf{x})) < \phi(c_1(w)w). \quad (70)$$

Applying (70) and (66) to (64), we obtain

$$\begin{aligned} \mathbb{P} \left\{ I_t^f(\mathbf{x}) < -w\sigma_t^f(\mathbf{x}) + EI_t^f(\mathbf{x}) \right\} &< \Phi \left( -w + \phi(z_t^f(\mathbf{x})) \right) \\ &< \Phi \left( -w + \phi(c_1(w)w) \right). \end{aligned} \quad (71)$$

Notice that  $\phi(c_1(w)w) < \phi(c_1(w)) < \phi(c_1(w))w$  due to  $w > 1$ . By the definition of  $\Phi$  and mean value theorem,

$$\begin{aligned} \Phi(-w + \phi(c_1(w)w)) &= \Phi(-w) + \int_{-w}^{-w + \phi(c_1(w)w)} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2} dx \leq \Phi(-w) + \\ &\frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}(w - \phi(c_1(w)w))^2} \phi(c_1(w)w) \leq \Phi(-w) + \frac{1}{2\pi} e^{-\frac{1}{2}((1 - \phi(c_1(w)))w)^2} e^{-\frac{1}{2}(c_1(w)w)^2} \\ &\leq \Phi(-w) + \frac{1}{2\pi} e^{-\frac{1}{2}c_2(w)w^2} \leq \frac{1}{2} e^{-\frac{1}{2}w^2} + \frac{1}{2\pi} e^{-\frac{1}{2}c_2(w)w^2}, \end{aligned} \quad (72)$$

where  $c_2(w) = [1 - \phi(c_1(w))]^2 + [c_1(w)]^2$ . The last inequality in (72) again uses Lemma A.6. Notice that  $c_2(w)$  increases with  $w$  and for  $w \geq 1.2$ ,  $c_2(w) > 1$ . Thus,  $e^{-\frac{1}{2}w^2} > e^{-\frac{1}{2}c_2(w)w^2}$  for  $w \geq 1.2$ , which simplifies (72) to

$$\Phi(-w + \phi(c_1(w)w)) < c_{\pi 1} e^{-\frac{1}{2}w^2}. \quad (73)$$

where  $c_{\pi 1} = \frac{1+\pi}{2\pi}$ . Therefore, by (71) and (73), if  $w \geq 1.2$ ,

$$\mathbb{P} \{ I_t(\mathbf{x}) < -\sigma_t(\mathbf{x})w + EI_t(\mathbf{x}) \} < c_{\pi 1} e^{-\frac{1}{2}w^2}. \quad (74)$$

Combining (74) with (62) and (63), we have

$$\mathbb{P} \left\{ \left| I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x}) \right| > w\sigma_t^f(\mathbf{x}) \right\} < c_\alpha e^{-\frac{1}{2}w^2}, \quad (75)$$

where  $c_\alpha = \frac{1+2\pi}{2\pi}$  for  $w \geq 1.2$ . The probability in (75) monotonically decreases with  $w$ . Let  $\delta = c_\alpha e^{-\frac{1}{2}w^2}$ . Then, taking the logarithm of  $\delta$  leads to  $\log(\frac{1+2\pi}{2\pi\delta}) = \frac{1}{2}w^2$ . Let  $\beta = \max\{w^2, 1.2^2\}$ , and the proof is complete.  $\square$

The relationship between  $I_t^f(\mathbf{x})$  and  $EI_t^f(\mathbf{x})$  under the GP prior assumption is given in the following lemma.

**Lemma C.5.** Given  $\delta \in (0, 1)$ , let  $\beta = 2 \log(2c_\alpha/\delta)$ , where  $c_\alpha = \frac{1+2\pi}{2\pi}$ . At given  $\mathbf{x} \in C$  and  $t \in \mathbb{N}$ ,

$$\frac{\tau(-\sqrt{\beta})}{\tau(\sqrt{\beta})} I_t^f(\mathbf{x}) \leq EI_t^f(\mathbf{x}), \quad (76)$$

holds with probability  $\geq 1 - \delta$

*Proof.* From Lemma C.2, with probability  $\geq 1 - \delta$ , (54) stands. If  $f_t^+ - f(\mathbf{x}) \leq 0$ , then  $I_t(\mathbf{x}) = 0$ . Since  $EI_t(\mathbf{x}) \geq 0$ , (76) is trivial. If  $f_t^+ - f(\mathbf{x}) > 0$ , by Lemma C.2,

$$\begin{aligned} f_t^+ - \mu_t^f(\mathbf{x}) &= f_t^+ - f(\mathbf{x}) + f(\mathbf{x}) - \mu_t^f(\mathbf{x}) > f(\mathbf{x}) - \mu_t^f(\mathbf{x}) \\ &> -\sqrt{\beta} \sigma_t^f(\mathbf{x}), \end{aligned} \quad (77)$$

with probability greater than  $\geq 1 - \delta/2$ . From the monotonicity of  $\tau$ , we have

$$\tau\left(\frac{f_t^+ - \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right) > \tau(-\sqrt{\beta}), \quad (78)$$

and therefore,

$$EI_t^f(\mathbf{x}) = \sigma_t^f(\mathbf{x}) \tau\left(\frac{f_t^+ - \mu_t^f(\mathbf{x})}{\sigma_t^f(\mathbf{x})}\right) > \tau(-\sqrt{\beta}) \sigma_t^f(\mathbf{x}), \quad (79)$$

with probability greater than  $1 - \delta/2$ . Using  $\delta/2$  in Lemma C.4,

$$I_t^f(\mathbf{x}) - EI_t^f(\mathbf{x}) \leq \sqrt{\beta} \sigma_t^f(\mathbf{x}), \quad (80)$$

with probability  $\geq 1 - \delta/2$ . Applying (80) to (79) with union bound leads to

$$EI_t^f(\mathbf{x}) > \frac{\tau(-\sqrt{\beta})}{\sqrt{\beta} + \tau(-\sqrt{\beta})} I_t^f(\mathbf{x}) = \frac{\tau(-\sqrt{\beta})}{\tau(\sqrt{\beta})} I_t^f(\mathbf{x}), \quad (81)$$

with probability greater than  $1 - \delta$ .  $\square$

We can now prove Theorem 3.10.

*Proof.* From Lemma C.1,

$$\sum_{i=0}^{t-1} f_i^+ - f_{i+1}^+ = f_0^+ - f_t^+ \leq 2M_f. \quad (82)$$

Given that  $f_i^+ - f_{i+1}^+ \geq 0$ ,  $f_i^+ - f_{i+1}^+ \geq \frac{2M_f}{k}$  at most  $k$  times for any  $k \in \mathbb{N}$ . Choose  $k = \lceil t/2 \rceil$ , where  $\lceil x \rceil$  is the largest integer smaller than  $x$  so that  $2k \leq t \leq 2(k+1)$ . Then, there exists  $k \leq t_k \leq 2k$  so that  $f_{t_k}^+ - f_{t_k+1}^+ < \frac{2M_f}{k}$  and  $f(\mathbf{x}_{t_k+1}) \geq f_{t_k+1}^+$ .

From Lemma C.5 and  $\beta = 2 \log(6c_\alpha/\delta)$ , with probability  $\geq 1 - \delta/3$ ,

$$\begin{aligned} r_t &= f_t^+ - f(\mathbf{x}^*) \leq f_{t_k}^+ - f(\mathbf{x}^*) \leq I_{t_k}^f(\mathbf{x}^*) \\ &\leq \frac{\tau(\beta^{1/2})}{\tau(-\beta^{1/2})} EI_{t_k}^f(\mathbf{x}^*) = c_\tau(\beta) \frac{P_{t_k}(\mathbf{x}^*)}{P_{t_k}(\mathbf{x}^*)} EI_{t_k}^f(\mathbf{x}^*) \leq c_\tau(\beta) \frac{P_{t_k}(\mathbf{x}_{t_k+1})}{P_{t_k}(\mathbf{x}^*)} EI_{t_k}^f(\mathbf{x}_{t_k+1}) \\ &= c_\tau(\beta) \frac{P_{t_k}(\mathbf{x}_{t_k+1})}{P_{t_k}(\mathbf{x}^*)} \left[ (f_{t_k}^+ - \mu_{t_k}^f(\mathbf{x}_{t_k+1})) \Phi(z_{t_k}^f(\mathbf{x}_{t_k+1})) + \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \phi(z_{t_k}^f(\mathbf{x}_{t_k+1})) \right] \\ &\leq c_\tau(\beta) \frac{P_{t_k}(\mathbf{x}_{t_k+1})}{P_{t_k}(\mathbf{x}^*)} \left[ (f_{t_k}^+ - \mu_{t_k}^f(\mathbf{x}_{t_k+1})) \Phi(z_{t_k}^f(\mathbf{x}_{t_k+1})) + 0.4 \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right], \end{aligned} \quad (83)$$

where the last inequality uses  $\phi(\cdot) < 0.4$ . From Lemma C.2, we have with probability  $\geq 1 - \delta/3$ ,

$$\begin{aligned} f_{t_k}^+ - \mu_{t_k}^f(\mathbf{x}_{t_k+1}) &= f_{t_k}^+ - f(\mathbf{x}_{t_k+1}) + f(\mathbf{x}_{t_k+1}) - \mu_{t_k}^f(\mathbf{x}_{t_k+1}) \\ &\leq f_{t_k}^+ - f_{t_k+1}^+ + \beta^{1/2} \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \leq \frac{2M_f}{k} + \beta^{1/2} \sigma_{t_k}^f(\mathbf{x}_{t_k+1}). \end{aligned} \quad (84)$$

Applying (84) to (83), we have with probability  $\geq 1 - 2\delta/3$ ,

$$r_t \leq c_\tau(\beta) \frac{P_{t_k}(\mathbf{x}_{t_k+1})}{P_{t_k}(\mathbf{x}^*)} \left[ \frac{2M_f}{k} + (0.4 + \beta^{1/2}) \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right]. \quad (85)$$

Next, we consider the probability function  $P_{t_k}$  at  $\mathbf{x}^*$  and  $\mathbf{x}_{t_k+1}$ . Using the fact that  $c(\mathbf{x}^*) \leq 0$ , we have by Lemma C.2 at  $\mathbf{x}^*$  and  $t_k$ ,

$$\mu_{t_k}^c(\mathbf{x}^*) \leq \sqrt{\beta} \sigma_{t_k}^c(\mathbf{x}^*) + c(\mathbf{x}^*) \leq \sqrt{\beta} \sigma_{t_k}^c(\mathbf{x}^*), \quad (86)$$

with probability  $\geq 1 - \delta/3$ . Thus, with probability  $\geq 1 - \delta/3$ ,

$$\frac{-\mu_{t_k}^c(\mathbf{x}^*)}{\sigma_{t_k}^c(\mathbf{x}^*)} \geq -\sqrt{\beta}. \quad (87)$$

From the monotonicity of  $\Phi$ , we have with probability  $\geq 1 - \delta/3$ ,

$$\Phi\left(\frac{-\mu_{t_k}^c(\mathbf{x}^*)}{\sigma_{t_k}^c(\mathbf{x}^*)}\right) \geq \Phi(-\sqrt{\beta}), \quad (88)$$

Using (88), the  $P_{t_k}$  functions have

$$\frac{P_{t_k}(\mathbf{x}_{t_k+1})}{P_{t_k}(\mathbf{x}^*)} \leq \frac{1}{\Phi(-\sqrt{\beta})}, \quad (89)$$

with probability  $\geq 1 - \delta/3$ . Applying (89) to (85), we have

$$r_t \leq c_\tau(\beta) \frac{1}{\Phi(-\sqrt{\beta})} \left[ \frac{2M_f}{k} + (0.4 + \beta^{1/2}) \sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \right], \quad (90)$$

with probability  $\geq 1 - \delta$ .

□

The proof of Theorem 3.11 is next.

*Proof.* From Lemma A.5,  $\sigma_i^f(\mathbf{x}_{i+1}) \geq \frac{\sqrt{\gamma_t^f t}}{k}$ , where  $i = 1, \dots, t-1$ , at most  $k$  times for any  $k \in \mathbb{N}$  and  $k \leq t$ . Choose  $k = \lceil t/3 \rceil$  which leads to  $3k \leq t \leq 3(k+1)$ . There exists  $t_k$  so that  $\sigma_{t_k}^f(\mathbf{x}_{t_k+1}) \leq \frac{\sqrt{t\gamma_t^f}}{k}$ . Following the proof for (90), we have

$$r_t \leq c_\tau(\beta) \frac{1}{\Phi(-\sqrt{\beta})} \left[ \frac{2M_f}{k} + (0.4 + \beta^{1/2}) \frac{\sqrt{t\gamma_t^f}}{k} \right], \quad (91)$$

with probability  $\geq 1 - \delta$ . Using Lemma A.2, the proof is complete.

□

The sample complexity is given in the next corollary, whose proof is similar to that of Corollary B.5 and omitted.

**Corollary C.6.** Let  $\beta = 2\log(6c_\alpha/\delta)$ , where  $c_\alpha = \frac{1+2\pi}{2\pi}$ . Under Assumption 3.9, the CEI algorithm has the sample complexity

$$\mathcal{O}\left(\frac{1}{\epsilon^2} [\log(1/\epsilon)]^{d+1}\right) \text{ and } \mathcal{O}\left(\epsilon^{-\frac{2\nu+d}{\nu}} \log(1/\epsilon)\right), \quad (92)$$

for SE and Matérn kernels, respectively, with probability  $\geq 1 - \delta$ .

## D Test problems

The mathematical formulations of the testing problems in Section 4.2 are given in this section. The objective, constraint functions and the optimal  $f$  of Problem 1 is given below.

$$\begin{aligned} f(\mathbf{x}) &= \sin(x_1) + x_2, \\ c(\mathbf{x}) &= \sin(x_1) \sin(x_2) + 0.95 \leq 0, \\ x_i &\in [0, 6], i = 1, 2, \\ f^* &= 0.25. \end{aligned} \tag{93}$$

The objective, constraint functions and the optimal  $f$  of Problem 2 is given below.

$$\begin{aligned} f(\mathbf{x}) &= x_1 + x_2 \\ c_1(\mathbf{x}) &= -0.5 \sin(2\pi(x_1^2 - 2x_2)) - x_1 - 2x_2 + 1.5 \leq 0 \\ c_2(\mathbf{x}) &= x_1^2 + x_2^2 - 1.5 \leq 0 \\ x_i &\in [0, 1], i = 1, 2 \\ f^* &= 0.6. \end{aligned} \tag{94}$$

The objective, constraint functions and the optimal  $f$  of Problem 3 is given below.

$$\begin{aligned} f(\mathbf{x}) &= x_1 + x_2 + x_3 + x_4 \\ c_1 &= 1.1 - \sum_{i=1}^4 E_i \exp \left( \sum_{j=1}^4 -A_{j,i} (x_j - P_{j,i})^2 \right) \\ x_i &\in [0, 1], i = 1, \dots, 4 \\ E &= [1, 1.2, 3, 3.2]^\top \\ P &= \begin{bmatrix} 0.131 & 0.232 & 0.234 & 0.404 \\ 0.169 & 0.413 & 0.145 & 0.882 \\ 0.556 & 0.830 & 0.352 & 0.873 \\ 0.012 & 0.373 & 0.288 & 0.574 \end{bmatrix} \\ A &= \begin{bmatrix} 10 & 0.05 & 3 & 17 \\ 3 & 10 & 3.5 & 8 \\ 17 & 17 & 1.7 & 0.05 \\ 3.5 & 0.1 & 10 & 10 \end{bmatrix} \\ f^* &= 0. \end{aligned} \tag{95}$$

The objective, constraint functions and the optimal  $f$  of Problem 4 is given below.

$$\begin{aligned} f(\mathbf{x}) &= - \sum_{i=1}^4 \alpha_i \exp \left( - \sum_{j=1}^6 A_{ij} (x_j - P_{ij})^2 \right) \\ c(\mathbf{x}) &= \sum_{j=1}^4 x_j - 3 \\ x_i &\in [0, 1], i = 1, \dots, 6 \\ \alpha &= [1.0, 1.2, 3.0, 3.2]^\top \\ A &= \begin{bmatrix} 10 & 3.0 & 17 & 3.5 & 1.7 & 8.0 \\ 0.05 & 10 & 17 & 0.1 & 8.0 & 14 \\ 3.0 & 3.5 & 1.7 & 10 & 17 & 8.0 \\ 17 & 8.0 & 0.05 & 10 & 0.1 & 14 \end{bmatrix} \\ P &= \begin{bmatrix} 0.131 & 0.170 & 0.557 & 0.012 & 0.828 & 0.587 \\ 0.233 & 0.414 & 0.831 & 0.374 & 0.100 & 0.999 \\ 0.235 & 0.145 & 0.352 & 0.288 & 0.305 & 0.665 \\ 0.405 & 0.883 & 0.873 & 0.574 & 0.109 & 0.038 \end{bmatrix} \\ f^* &= -3.32. \end{aligned} \tag{96}$$

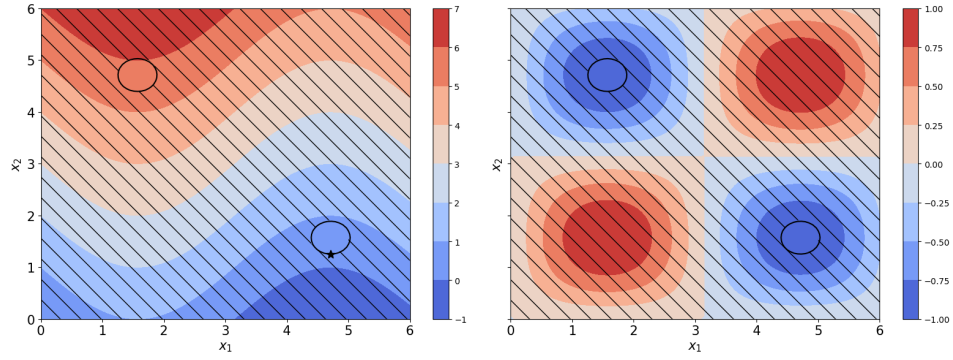


Figure 3: Contour plots for the objective function (left) and constraint function (right) for Problem 1. The infeasible region is marked on the plots. The global optimum is marked with a star sign.

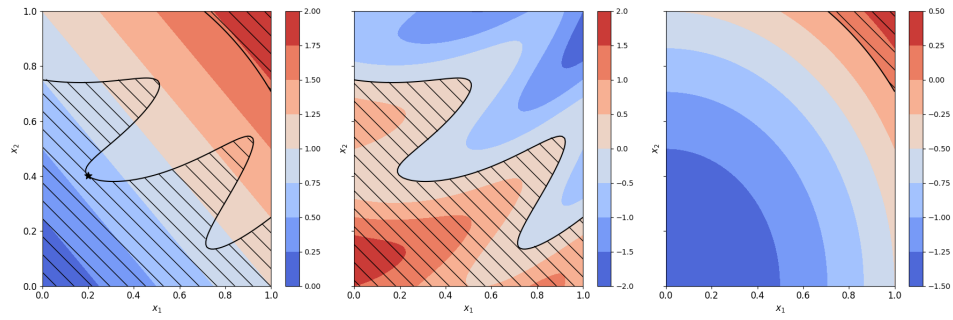


Figure 4: Contour plots for the objective function (left) and the two constraint functions (middle and right) for Problem 2. The infeasible region is marked with black line on the objective contour. The global optimum is marked with a star sign.

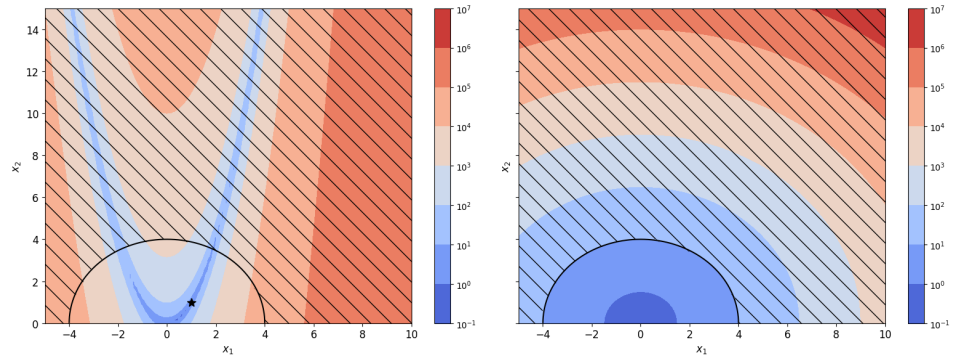


Figure 5: Contour plots for the objective function (left) and constraint function (right) for Problem 5. The infeasible region is marked on the plots. The global optimum is marked with a star sign.

The objective, constraint functions and the optimal  $f$  of Problem 5 is given below.

$$\begin{aligned}f(\mathbf{x}) &= 100(x_2 - x_1^2)^2 + (1 - x_1)^2 \\c_1(\mathbf{x}) &= \sqrt{x_1^2 + x_2^2} - 4 \\c_2(\mathbf{x}) &= x_1^2 + x_2^2 - 1.5, \\x_1 &\in [-5, 10], \ x_2 \in [0, 15] \\f^* &= 0.\end{aligned}\tag{97}$$

The contour plots of Problem 1, 2, and 5 are given in Figure 3, 4, and 5.