No-Regret Bayesian Optimization with Stochastic Observation Failures

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Abstract

We study Bayesian optimization problems where observation of the objective function fails stochastically, e.g., synthesis failures in materials development. For this problem, although several heuristic methods have been proposed, they do not have theoretical guarantees and sometimes deteriorate in practice. We propose two algorithms that have a trade-off relation between regret bounds and practical performance. The first one is the first no-regret algorithm for this problem. The second one shows superior practical performance; however, we need some modification of the algorithm to obtain a no-regret guarantee, which is slightly worse than the first one. We demonstrate the effectiveness of our methods in numerical experiments, including the simulation function motivated by quasi-crystal synthesis.

1 INTRODUCTION

Bayesian optimization (BO) is a powerful framework for efficient black-box optimization. Applications of BO vary in a lot of fields, including robotics [Lizotte et al., 2007, Martinez-Cantin et al., 2007], experimental design [González et al., 2015], or hyperparameter tuning of machine learning models [Bergstra et al., 2011, Snoek et al., 2012]. Furthermore, several studies considered extensive settings, such as constrained [Gardner et al., 2014], parallel [Desautels et al., 2014], and robust optimization [Bogunovic et al., 2018].

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The studies for the BO problem where the observation can fail stochastically are also important for real-world applications. For example, in materials development, experiments sometimes fail due to uncontrollable experimental errors [Wakabayashi et al., 2022]. Another example is a robotics task in which failures occur due to the control error or uncertainty of the environment [Marco et al., 2021]. Thus, this paper focuses on the BO problems with stochastic observation failures, depending on an unknown failure probability function.

Several existing studies have proposed heuristic methods for this problem, such as considering the imputation of the failure observations [Forrester et al., 2006] or incorporating the surrogate model of failure probability into the expected improvement (EI) criterion [Lindberg and Lee, 2015]. However, these methods can show low optimization performance due to pessimistic heuristics or some approximations. In addition, a no-regret algorithm for this problem has not been proposed.

Contributions Our contributions are fourfold, as described below. Firstly, in Sec. 3, we propose a stochastic failure-aware Gaussian process upper confidence bound (SF-GP-UCB) algorithm. To our knowledge, SF-GP-UCB is the first algorithm whose regret upper bound is given under the BO problems with stochastic failures. Secondly, in Sec. 4, we further propose a stochastic failure-aware confidence bound-based improvement (SF-CBI) algorithm, which is motivated to compensate for the drawback of the practical behavior of SF-GP-UCB. Thirdly, in Sec. 5, we provide a variant of SF-GP-UCB, that is specific to Matérn kernels. We show this variant of SF-GP-UCB has no-regret guarantees under the smoothness assumptions of Matérn kernel, while the original SF-GP-UCB does not provide such guarantees. Lastly, in Sec. 6, we confirm that our algorithms have the same or better performance through several benchmarks, including the simulation function motivated by quasi-crystal synthesis.

Related Works Many works propose strategies to solve BO problems, including EI [Močkus, 1975], Gaussian process upper confidence bound (GP-UCB) [Srinivas et al., 2010], Thompson sampling [Russo and Van Roy, 2014], and entropy search methods [Hennig and Schuler, 2012]. We mainly focus on the GP-UCB-based method in this paper.

One setting closely related to ours is safe BO [Sui et al., 2015]. Safe BO assumes that an observation failure has catastrophic consequences, e.g., the destruction of equipment. Meanwhile, our setup allows multiple observation failures. Thus, safe BO for our problem is too conservative.

As discussed above, two methods have been proposed in our problem setup. Forrester et al. [2006] proposed to impute pessimistic predictions of the Gaussian process (GP) into the missing training output of the objective function when observation fails. Although this imputation strategy avoids querying inputs around past failure inputs, the performance can deteriorate if the input, whose output is imputed, is close to the optimum. Lindberg and Lee [2015] consider modeling the function of failure probability with a GP classifier (GPC) and incorporating GPC prediction into the EI criterion. However, GPC computations require approximations, which can degenerate the modeling accuracy of failure probability and optimization performance.

Finally, some recent works consider the BO problem with *deterministic* failures [Bachoc et al., 2020, Iwazaki et al., 2023]. In particular, Iwazaki et al. [2023] showed regret upper bound for this problem. Our algorithm is designed based on a similar concept to Iwazaki et al. [2023]; however, substantial differences exist in our work. Specifically, if the underlying failure is deterministic, the learner can completely eliminate past failed inputs from the search space. On the other hand, in our stochastic failure settings, since past failed inputs can succeed in the observation, the learner may need to query past failed inputs again.

2 PRELIMINARIES

Problem Settings Let $f : \mathcal{X} \to \mathbb{R}$ be a black-box objective function whose input domain $\mathcal{X} \subset \mathbb{R}^d$ is compact. Furthermore, let $g : \mathcal{X} \to [0, 1]$ be a black-box success function such that $g(\boldsymbol{x})$ represents a success probability of observation at input $\boldsymbol{x} \in \mathcal{X}$. At each step t, the learner chooses input $\boldsymbol{x}_t \in \mathcal{X}$; then, a success label $c_t \sim \mathrm{Bernoulli}(g(\boldsymbol{x}_t))$ is revealed to the learner. If $c_t = 1$, the learner obtains an observation $y_t = f(\boldsymbol{x}_t) + \epsilon_t$, where ϵ_t is a zero-mean noise. Otherwise, the learner obtains no information about f.

The Learner's Goal and Regret As a performance metric, we define the *regret* r_T at step T as $r_T = f(\boldsymbol{x}^*) - \max_{t \le T; c_t = 1} f(\boldsymbol{x}_t)$ if there exist some $t \le T$ such that $c_t = 1$ holds; otherwise, $r_T = \infty$. Here, $\boldsymbol{x}^* \coloneqq \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{X}; g(\boldsymbol{x}) > 0} f(\boldsymbol{x})$ is the unique maximizer on which the learner can make successful observations with strictly positive probability. We emphasize that our goal is minimizing the regret, not finding the optimal input $\boldsymbol{x}^*$. Our regret expresses the learner's motivation to obtain the highest successful output, which arises in various applications. For example, in material synthesis experiments, the researcher aims to successfully synthesize materials with the higher value of some physical property $f(\cdot)$ on a limited budget. In Appendix G, we discuss further potential applications of our settings.

Regularity Assumptions We make the following Assumptions 2.1–2.2, which are the standard set of assumptions for the regret analysis of BO Chowdhury and Gopalan [2017], Srinivas et al. [2010]. Hereafter, $\mathcal{F}_k$ denotes reproducing kernel Hilbert space (RKHS) [Aronszajn, 1950] corresponding to the kernel k. Furthermore, $\| \cdot \|_k$ denotes RKHS norm over $\mathcal{F}_k$.

Assumption 2.1 (Subgaussianity of ϵ_t.)**.** For any $t \in \mathbb{N}_+$, the noise ϵ_t is a conditionally σ-sub-Gaussian random variable. Namely, there exists $\sigma > 0$ such that $\mathbb{E}[e^{\lambda \epsilon_t} \mid H_{t-1} \cup \{\boldsymbol{x}_t\}] \le \exp(\lambda^2 \sigma^2 / 2)$ holds for any $t \in \mathbb{N}_+$ and $\lambda \in \mathbb{R}$, where $H_t \coloneqq \{\boldsymbol{x}_1, c_1, \tilde{y}_1, \ldots, \boldsymbol{x}_t, c_t, \tilde{y}_t\}$ is the history up to step t. Here, for notational convenience, we define $\tilde{y}_i$ as $\tilde{y}_i = c_i y_i$.

Assumption 2.2 (Smoothness of f)**.** There exists a known constant $B_f > 0$ such that $f \in \mathcal{F}_{k_f}$ with $\|f\|_{k_f} \le B_f$, where k_f is a known positive definite kernel which satisfies $k_f(\boldsymbol{x}, \boldsymbol{x}) \le 1$ for all $\boldsymbol{x} \in \mathcal{X}$.

One commonly used kernel in BO is the squared exponential (SE) kernel $k_f^{\mathrm{SE}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \coloneqq \exp[-w^2/(2\ell^2)]$, where $w = \|\boldsymbol{x} - \tilde{\boldsymbol{x}}\|_2$. Here, $l > 0$ is a lengthscale parameter. Another example is the Matérn kernel $k_f^{\mathrm{Matérn}}(\boldsymbol{x}, \tilde{\boldsymbol{x}}) \coloneqq 2^{1-\nu}\Gamma^{-1}(\nu) \left(w\sqrt{2\nu}/\ell\right)^{\nu} B_\nu \left(w\sqrt{2\nu}/\ell\right)$, where $\nu > 0$ and $B_\nu(\cdot)$ are the smoothness parameter and the Bessel function, respectively [Rasmussen et al., 2006].

To design an algorithm that efficiently leverages the success labels c_t, we further assume that the success function g also lies on the RKHS of another kernel.

Assumption 2.3 (Smoothness of g)**.** There exists a known constant $B_{\tilde{g}} > 0$ such that $\tilde{g} \in \mathcal{F}_{k_{\tilde{g}}}$ with $\|\tilde{g}\|_{k_{\tilde{g}}} \le B_{\tilde{g}}$, where the function $\tilde{g} : \mathcal{X} \to [-0.5, 0.5]$ is defined as $\tilde{g}(\boldsymbol{x}) = g(\boldsymbol{x}) - 0.5$. Moreover, $k_{\tilde{g}}$ is a known positive definite kernel which satisfies $\forall \boldsymbol{x} \in \mathcal{X},\ k_{\tilde{g}}(\boldsymbol{x}, \boldsymbol{x}) \le 1$.

Least-square Estimator on RKHS Our algorithm leverages the estimators of f and $\tilde{g}$ based on kernel ridge regression, and then construct confidence bounds under Assumptions 2.1–2.3. Let $\mathcal{I}_t^{(s)} \coloneqq \{i \in \mathbb{N}_+ \mid c_i = 1 \text{ and } i \le t\}$ and $n_t \coloneqq |\mathcal{I}_t^{(s)}|$ be a successful index set and the number of successful observations at step t, respectively. Based on the history up to step t, the least square estimators $\mu_{f,t}$ and $\mu_{\tilde{g},t}$ of f and $\tilde{g}$ on RKHS are respectively defined as

$$\mu_{f,t} = \underset{\hat{f} \in \mathcal{F}_{k_f}}{\arg\min} \Big\{ \sum_{i \in \mathcal{I}_t^{(s)}} [\hat{f}(\boldsymbol{x}_i) - y_i]^2 + \lambda_{f,t} \|\hat{f}\|_{\mathcal{F}_{k_f}} \Big\},$$

$$\mu_{\tilde{g},t} = \underset{\hat{g} \in \mathcal{F}_{k_{\tilde{g}}}}{\arg\min} \Big\{ \sum_{i=1}^{t} [\hat{g}(\boldsymbol{x}_i) - \tilde{c}_i]^2 + \lambda_{\tilde{g},t} \|\hat{g}\|_{\mathcal{F}_{k_{\tilde{g}}}} \Big\},$$

where $\lambda_{f,t} > 0$ and $\lambda_{\tilde{g},t} > 0$ are regularization parameters. Moreover, $\tilde{c}_i \coloneqq c_i - 0.5$ are training labels to estimate $\tilde{g}(\cdot)$. The representer theorem gives closed-form solutions of $\mu_{f,t}$ and $\mu_{\tilde{g},t}$ [Rasmussen et al., 2006], which are respectively defined as

$$\mu_{f,t}(\boldsymbol{x}) = \boldsymbol{k}_f \left(\boldsymbol{x}, D_t^{(f)}\right)^\top \left[\boldsymbol{K}_f(D_t^{(f)}) + \lambda_{f,t} \boldsymbol{I}_{n_t}\right]^{-1} \boldsymbol{y}_t^{(s)},$$

$$\mu_{\tilde{g},t}(\boldsymbol{x}) = \boldsymbol{k}_{\tilde{g}} \left(\boldsymbol{x}, D_t^{(\tilde{g})}\right)^\top \left[\boldsymbol{K}_{\tilde{g}}(D_t^{(\tilde{g})}) + \lambda_{\tilde{g},t} \boldsymbol{I}_t\right]^{-1} \tilde{\boldsymbol{c}}_t,$$

where $D_t^{(f)} \coloneqq (\boldsymbol{x}_i)_{i \in \mathcal{I}_t^{(s)}}$, $D_t^{(\tilde{g})} \coloneqq (\boldsymbol{x}_i)_{i \le t}$, $\boldsymbol{y}_t^{(s)} \coloneqq (y_i)_{i \in \mathcal{I}_t^{(s)}}$, and $\tilde{\boldsymbol{c}}_t \coloneqq (\tilde{c}_i)_{i \le t}$ are training inputs of f and $\tilde{g}$, training outputs of f, and training outputs of $\tilde{g}$, respectively. Furthermore, $\boldsymbol{k}_f(\boldsymbol{x}, D_t^{(f)}) \coloneqq [k_f(\boldsymbol{x}, \tilde{\boldsymbol{x}})]_{\tilde{\boldsymbol{x}} \in D_t^{(f)}} \in \mathbb{R}^{n_t}$, $\boldsymbol{K}_f(D_t^{(f)}) \coloneqq [k_f(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)})]_{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)} \in D_t^{(f)}} \in \mathbb{R}^{n_t \times n_t}$, and $\boldsymbol{I}_{n_t} \in \mathbb{R}^{n_t \times n_t}$ are kernel vector, kernel matrix defined based on $D_t^{(f)}$, and $n_t \times n_t$ identity matrix, respectively. We also define $\boldsymbol{k}_{\tilde{g}}(\boldsymbol{x}, D_t^{(\tilde{g})})$ and $\boldsymbol{K}_{\tilde{g}}(D_t^{(\tilde{g})})$ by replacing $(k_f, D_t^{(f)})$ in the definition of $\boldsymbol{k}_f(\boldsymbol{x}, D_t^{(f)})$ and $\boldsymbol{K}_f(D_t^{(f)})$ with $(k_{\tilde{g}}, D_t^{(\tilde{g})})$, respectively.

Confidence Bounds The above definitions of $\mu_{f,t}(\cdot)$ and $\mu_{\tilde{g},t}(\cdot)$ are the same as the posterior means of the GP regression. Under the Bayesian modeling assumptions of GP, $f(\boldsymbol{x})$ and $\tilde{g}(\boldsymbol{x})$ follow the Gaussian distribution; therefore, confidence bounds of $f(\boldsymbol{x})$ and $\tilde{g}(\boldsymbol{x})$ are obtained in the form of $[\mu_{f,t-1}(\boldsymbol{x}) \pm \beta_{f,t}^{1/2} \sigma_{f,t-1}(\boldsymbol{x})]$ and $[\mu_{\tilde{g},t-1}(\boldsymbol{x}) \pm \beta_{\tilde{g},t}^{1/2} \sigma_{\tilde{g},t-1}(\boldsymbol{x})]$, where $\sigma_{f,t}^2(\boldsymbol{x})$ and $\sigma_{\tilde{g},t}^2(\boldsymbol{x})$ are posterior variances defined as follows:

$$\sigma_{f,t}^2(\boldsymbol{x}) = k_f(\boldsymbol{x}, \boldsymbol{x}) - \boldsymbol{k}_f \left(\boldsymbol{x}, D_t^{(f)}\right)^\top \left[\boldsymbol{K}_f(D_t^{(f)}) + \lambda_{f,t} \boldsymbol{I}_{n_t}\right]^{-1} \boldsymbol{k}_f \left(\boldsymbol{x}, D_t^{(f)}\right),$$

$$\sigma_{\tilde{g},t}^2(\boldsymbol{x}) = k_{\tilde{g}}(\boldsymbol{x}, \boldsymbol{x}) - \boldsymbol{k}_{\tilde{g}} \left(\boldsymbol{x}, D_t^{(\tilde{g})}\right)^\top \left[\boldsymbol{K}_{\tilde{g}}(D_t^{(\tilde{g})}) + \lambda_{\tilde{g},t} \boldsymbol{I}_t\right]^{-1} \boldsymbol{k}_{\tilde{g}} \left(\boldsymbol{x}, D_t^{(\tilde{g})}\right).$$

The following lemma shows that valid frequentist confidence bounds are also obtained in a similar fashion to those that rely on Bayesian modeling assumptions.

Lemma 2.4. *Suppose Assumption 2.3 holds. Let $\delta \in (0,1)$ and $\lambda^{(\tilde{g})} > 0$ such that $\lambda_{\tilde{g},t} = \lambda^{(\tilde{g})}$ holds for all $t \in \mathbb{N}_+$. Furthermore, let $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda^{(\tilde{g})-1/2} \sqrt{0.5[\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) + \ln(1/\delta)]}$ with $\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) = 0.5 \sup_{D \in \mathcal{X}^t} \ln\det\left[\boldsymbol{I}_t + \lambda^{(\tilde{g})-1} \boldsymbol{K}_{\tilde{g}}(D)\right]$. Then, with probability at least $1-\delta$, $\mathrm{lcb}_t^{(\tilde{g})}(\boldsymbol{x}) \le \tilde{g}(\boldsymbol{x}) \le \mathrm{ucb}_t^{(\tilde{g})}(\boldsymbol{x})$ holds for any $t \in \mathbb{N}_+$ and $\boldsymbol{x} \in \mathcal{X}$, where $\mathrm{lcb}_t^{(\tilde{g})}(\boldsymbol{x}) = \mu_{\tilde{g},t-1}(\boldsymbol{x}) - \beta_{\tilde{g},t}^{1/2} \sigma_{\tilde{g},t-1}(\boldsymbol{x})$ and $\mathrm{ucb}_t^{(\tilde{g})}(\boldsymbol{x}) = \mu_{\tilde{g},t-1}(\boldsymbol{x}) + \beta_{\tilde{g},t}^{1/2} \sigma_{\tilde{g},t-1}(\boldsymbol{x})$.*

Lemma 2.4 directly follows from Lemma 3.11 in Abbasi-Yadkori [2013] and the fact that the error term $\tilde{g}(\boldsymbol{x}_i) - \tilde{c}_i$ is conditionally 1/2-sub-Gaussian. Similarly, Lemma A.1 in Appendix A gives the confidence bounds $[\mathrm{lcb}_t^{(f)}(\boldsymbol{x}), \mathrm{ucb}_t^{(f)}(\boldsymbol{x})]$ of $f(\boldsymbol{x})$. Note that $\beta_{f,t}$ depends on n_t, while $\beta_{\tilde{g},t}$ depends on t instead of n_t.

In the above lemma, the quantity $\gamma_t^{(\tilde{g})}$ is called *maximum information gain* (MIG) [Srinivas et al., 2010]. MIGs are used to characterize the regret upper bounds of BO. Furthermore, the sub-linear upper bounds of MIGs are known for several commonly used kernels, including SE and Matérn kernels [Vakili et al., 2021].

Finally, from Lemma 2.4, we also construct valid confidence bounds $[\mathrm{lcb}_t^{(g)}(\boldsymbol{x}), \mathrm{ucb}_t^{(g)}(\boldsymbol{x})]$ of $g(\boldsymbol{x})$ by setting $\mathrm{lcb}_t^{(g)}(\boldsymbol{x}) = 0.5 + \mathrm{lcb}_t^{(\tilde{g})}(\boldsymbol{x})$ and $\mathrm{ucb}_t^{(g)}(\boldsymbol{x}) = 0.5 + \mathrm{ucb}_t^{(\tilde{g})}(\boldsymbol{x})$.

3 UCB STRATEGY UNDER STOCHASTIC FAILURES

Drawback of Standard GP-UCB We first start by considering standard GP-UCB that simply ignores failure events. Namely, consider the algorithm whose $\boldsymbol{x}_t$ is defined as $\boldsymbol{x}_t \in \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(f)}(\boldsymbol{x})$. One clear drawback of standard GP-UCB is that the query points $\boldsymbol{x}_t$ may get stuck on the same point since $\mathrm{ucb}_t^{(f)}(\boldsymbol{x})$ is not updated while $c_t = 0$. Specifically, when $\min_{\boldsymbol{x} \in \mathcal{X}} g(\boldsymbol{x})$ is zero (or sufficiently small), the number of successful observations could cease to grow; therefore, the regret of standard GP-UCB does not converge to zero in the worst-case sense.

Warmup: Algorithm with a Fixed Threshold Before explaining our SF-GP-UCB algorithm, we first introduce a simplified version of SF-GP-UCB to clarify the core ideas of our algorithm construction and theory. To construct a no-regret algorithm (i.e., the algorithm that achieves $r_T \to 0$ as $T \to \infty$), the algorithm must collect enough number of successful observations by avoiding the region whose success probability is almost zero. One simple idea to achieve this goal is to eliminate *unpromising inputs*, whose success probability is less than the pre-specified threshold $h > 0$ with high probability, from the search space.

Here, let $\mathcal{H}_t(h)$ and $\mathcal{L}_t(h)$ be the estimated super- and sub-level sets, which are respectively defined as $\mathcal{H}_t(h) = \{\boldsymbol{x} \in \mathcal{X} \mid \mathrm{lcb}_t^{(g)}(\boldsymbol{x}) \geq h\}$ and $\mathcal{L}_t(h) = \{\boldsymbol{x} \in \mathcal{X} \mid \mathrm{ucb}_t^{(g)}(\boldsymbol{x}) < h\}$. We also define an unclassified set $\mathcal{U}_t(h) \coloneqq \mathcal{X} \setminus (\mathcal{H}_t(h) \cup \mathcal{L}_t(h))$. Then, we consider the following variant of GP-UCB:

$$\boldsymbol{x}_t \in \underset{\boldsymbol{x} \in \mathcal{H}_t(h) \cup \mathcal{U}_t(h)}{\arg\max} \; \mathrm{ucb}_t^{(f)}(\boldsymbol{x}). \tag{1}$$

Hereafter, we call this algorithm SF-GP-UCB-fixed. Intuitively, the search space $\mathcal{H}_t(h) \cup \mathcal{U}_t(h)$ in Eq. (1) gradually adjusts to super-level set $\mathcal{H}(h) \coloneqq \{\boldsymbol{x} \in \mathcal{X} \mid g(\boldsymbol{x}) \geq h\}$ as the estimation of g becomes accurate. Therefore, the number of successful observations n_t is anticipated to grow in $\Omega(ht)$ since $g(\boldsymbol{x}_t) \geq h$ for sufficiently large t. We formally prove this intuition in Lemma 3.1.

Lemma 3.1 (Lower bound of n_t for SF-GP-UCB–fixed)**.** *Suppose Assumption 2.3 and $\lambda_{\tilde{g},t} = \lambda^{(\tilde{g})} > 0$ hold for any $t \in \mathbb{N}_+$. Let $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda^{(\tilde{g})-1/2}\sqrt{0.5[\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) + \ln(2/\delta)]}$ with any $\delta \in (0,1)$. Then, for any algorithm that satisfies $\boldsymbol{x}_t \in \mathcal{H}_t(h) \cup \mathcal{U}_t(h)$ with some $h \geq 0$, with probability at least $1-\delta$, the following lower bound for the number of successful observations holds for any $t \in \mathbb{N}_+$:*

$$n_t \geq (3-e)\left[ht - \sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}\left(\lambda^{(\tilde{g})}\right)}\right] - \ln\frac{\pi^2 t^2}{3\delta}, \tag{2}$$

where $C = \sqrt{8/\ln(1+\lambda^{(\tilde{g})-1})}$.

The proof of Lemma 3.1 is in Appendix B. From Lemma 3.1, SF-GP-UCB-fixed is guaranteed to attain linear number of successful observations $n_t \coloneqq \Omega(ht)$ if the term $\sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})}$ is sub-linear. For example, if $k_{\tilde{g}}$ is SE kernel, $\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) = \mathcal{O}((\ln t)^{d+1})$; therefore, $\sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})} = \mathcal{O}(t^{1/2}(\ln t)^{(d+1)/3})$, which is sub-linear.

By leveraging Lemma 3.1, the regret upper bounds of SF-GP-UCB-fixed are obtained as the following Theorem 3.2, whose proof is given in Appendix B.

Theorem 3.2 (Regret upper bound for SF-GP-UCB–fixed)**.** *Suppose Assumptions 2.1–2.3, $\lambda_{f,t} = \lambda^{(f)}$, and $\lambda_{\tilde{g},t} = \lambda^{(\tilde{g})} > 0$ hold for any $t \in \mathbb{N}_+$. Let $\beta_{f,t}^{1/2} = B_f + \sigma\lambda^{(f)-1/2}\sqrt{2[\gamma_t^{(f)}(\lambda^{(f)}) + \ln(2/\delta)]}$ and $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda^{(\tilde{g})-1/2}\sqrt{0.5[\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) + \ln(4/\delta)]}$ with any $\delta \in (0,1)$. Furthermore, suppose $\sqrt{\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})/t} = o(1)$. Moreover, assume the super-level set $\mathcal{H}(h) \coloneqq \{\boldsymbol{x} \in \mathcal{X} \mid g(\boldsymbol{x}) \geq h\}$ is not an empty set. Then, with probability at least $1-\delta$, the following two statements simultaneously hold. i) By at most step $\overline{T}_1$, $n_t \geq 1$ holds, where $\overline{T}_1$ is the smallest natural number t that satisfies the following inequality with $C = \sqrt{8/\ln(1+\lambda^{(\tilde{g})-1})}$:*

$$(3-e)\left[ht - \sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}\left(\lambda^{(\tilde{g})}\right)}\right] - \ln\frac{2\pi^2 t^2}{3\delta} \geq 1. \tag{3}$$

ii) Define $\boldsymbol{x}_h^*$ as $\boldsymbol{x}_h^* \in \arg\max_{\boldsymbol{x} \in \mathcal{H}(h)} f(\boldsymbol{x})$. Then, for any $T \geq \overline{T}_1$, the following regret upper bounds of SF-GP-UCB-fixed holds:

$$r_T \leq f(\boldsymbol{x}^*) - f(\boldsymbol{x}_h^*) + \mathcal{O}\left(\sqrt{\frac{\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})}{hT}}\right). \tag{4}$$

Our proof leverages the existing adaptive confidence bound in RKHS, which also leads to the same constructions of the confidence width $\beta_t^{(f)}$, $\beta_t^{(\tilde{g})}$ in our theorem as that of standard GP-UCB[1]. Furthermore, except for the additional dependence of $1/\sqrt{h}$, the second term of Eq. (4) has the same form as the simple regret bound of GP-UCB for the standard problem without failures. The drawback of SF-GP-UCB-fixed is the overestimation risk of $g(\boldsymbol{x}^*)$. From Theorem 3.2, if $h > g(\boldsymbol{x}^*)$, the regret is not guaranteed to become zero since the first term of $f(\boldsymbol{x}^*) - f(\boldsymbol{x}_h^*) > 0$; namely, the worst-case regret of SF-GP-UCB-fixed is not guaranteed to converge to zero. Moreover, if $\mathcal{H}(h) = \emptyset$, SF-GP-UCB-fixed may be ill-defined while running it since the search space $\mathcal{H}_t(h) \cup \mathcal{U}_t(h)$ can become an empty set.

Algorithm 1 The SF-GP-UCB algorithm

Require: Decreasing function $b : (0,\infty) \to (0,\infty)$, initial scale parameter $s_0 > 0$.
1: **for** $t = 1$ to T **do**
2: $s_t = \min\{s_{t-1}, b^{-1}(t)\max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\}$.
3: $h_t = s_t b(t)$.
4: $\boldsymbol{x}_t \in \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)} \mathrm{ucb}_t^{(f)}(\boldsymbol{x})$.
5: Obtain success label $c_t \sim \mathrm{Bernoulli}(g(\boldsymbol{x}_t))$.
6: If $c_t = 1$, Observe $y_t \coloneqq f(\boldsymbol{x}_t) + \epsilon_t$.
7: **end for**

Proposed Algorithm: SF-GP-UCB Our SF-GP-UCB algorithm is interpreted as the extended version of SF-GP-UCB-fixed, whose h is adaptively decreased by step t. Such adaptive decreasing strategy of parameters is also used in Iwazaki et al. [2023], by which we are inspired; however, their ideas are not directly applicable to the algorithm construction and the theoretical analysis of our settings. Algorithm 1 shows the

[1] Strictly speaking, the dependence of the confidence level δ is different due to the union bounds.

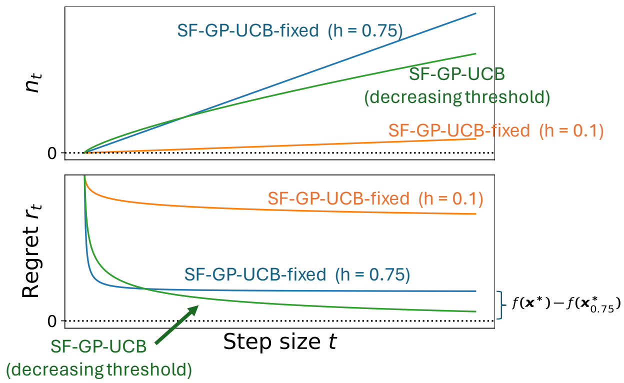

Figure 1: Illustrative image of the relation between the thresholds of our algorithms and resulting n_t (top) and regret (bottom). In SF-GP-UCB-fixed with a high threshold (blue), a large number of n_t is guaranteed. Therefore, resulting regret is diminishing rapidly at first; however, the gap $f(\boldsymbol{x}^*) - f(\boldsymbol{x}_h^*)$ due to overestimation of $g(\boldsymbol{x}^*)$ does not vanish. Meanwhile, in SF-GP-UCB-fixed with a low threshold (orange), the overestimation risk is low; however, the growing rate of n_t and diminishing rate of regret is too slow. Intuitively, SF-GP-UCB (green) takes the middle of such two algorithms by adaptively decreasing thresholds.

pseudo-code of SF-GP-UCB. Specifically, SF-GP-UCB controls the threshold h_t at step t as $h_t = s_t b(t)$, where s_t and $b(t)$ are scaling and decreasing factors at step t, respectively. Then, query points $\boldsymbol{x}_t$ are defined as line 4 in Algorithm 1, which replace the fixed threshold h of Eq. (1) with the adaptive threshold h_t.

Intuitively, the function b has the role that controls the decreasing rate of threshold h_t by balancing between the number of successful observations n_t and the overestimation risk of $g(\boldsymbol{x}^*)$. Fig. 1 shows an illustrative image. In Lemma B.3 of Appendix B, which is an adaptive threshold version of Lemma 3.1, we show that enough number of n_t is guaranteed by setting $b(t) = t^{-\tau}$ with $\tau \in (0, 1/2)$.

While the decreasing factor $b(t)$ is specified before running the algorithm, the scaling factor s_t is defined adaptively as line 2 in Algorithm 1. The scaling factor s_t has the role that avoids the search space $\mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$ becoming an empty set. More specifically, s_t is set as the value that the search space $\mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$ includes at least one input. This is easily checked by the fact that $\mathrm{argmax}_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x}) \subset \mathcal{U}_t(h_t)$ holds if s_t is less than $b^{-1}(t) \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})$, which is the second term on line 2 in Algorithm 1.

Here, the following Theorem 3.3 shows the regret upper bound of SF-GP-UCB.

Theorem 3.3 (Regret upper bound of SF-GP-UCB)**.** *Suppose Assumptions 2.1–2.3, $\lambda_{f,t} = \lambda^{(f)}$, and $\lambda_{\tilde{g},t} = \lambda^{(\tilde{g})}$ hold for any $t \in \mathbb{N}_+$. Let $\beta_{f,t}^{1/2} = B_f + \sigma \lambda^{(f)-1/2} \sqrt{2[\gamma_t^{(f)}(\lambda^{(f)}) + \ln(2/\delta)]}$, $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda^{(\tilde{g})-1/2} \sqrt{0.5[\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) + \ln(4/\delta)]}$ with any $\delta \in (0,1)$, and $b(t) = t^{-\tau}$ for any $\tau \in (0, 1/2)$. Furthermore, suppose $\sqrt{\beta_{\tilde{g},t} \gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})/t^{1-2\tau}} = o(1)$. Then, with probability at least $1-\delta$, the following two statements simultaneously hold. i) By at most step $\overline{T}_2$, $n_t \geq 1$ holds, where $\overline{T}_2$ is the smallest natural number t that satisfies the following inequality with $C = \sqrt{8/\ln(1 + \lambda^{(\tilde{g})-1})}$ and $\overline{g} = \max_{\boldsymbol{x} \in \mathcal{X}} g(\boldsymbol{x})$:*

$$
\begin{aligned}
&(3-e)\frac{\min\{s_0, \overline{g}\}}{1-\tau}(t^{1-\tau} - 1) \\
&\quad - (3-e)\sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}\left(\lambda^{(\tilde{g})}\right)} - \ln\frac{2\pi^2 t^2}{3\delta} \geq 1.
\end{aligned}
\tag{5}
$$

ii) Define $\overline{T}_3$ as $\overline{T}_3 = (g^{-1}(\boldsymbol{x}^*)s_0)^{1/\tau}$. Then, for any $T \geq \overline{T}_2$, the following regret upper bound of SF-GP-UCB holds:

$$
r_T \leq \mathcal{O}\left(\frac{\overline{T}_3 B_f}{T^{1-\tau}} + \sqrt{\frac{\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})}{T^{1-\tau}}}\right). \tag{6}
$$

Compared with Theorem 3.2 of SF-GP-UCB-fixed, in Theorem 3.3, the first term $f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{h_t}^*)$ in Eq. (4) is replaced with $\mathcal{O}(\overline{T}_3 B_f / T^{1-\tau})$, which converges to zero as $T \to \infty$. Therefore, if $\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)}) = o(T^{1-\tau})$ and the assumptions of Theorem 3.3 hold, the regret of SF-GP-UCB is guaranteed to converge to zero. For example, if k_f and k_g are both SE kernels, SF-GP-UCB is a no-regret algorithm.

Limitations of Our Analysis Our analysis of SF-GP-UCB has the following two limitations. First, there are cases where the convergence is not guaranteed in Matérn kernels. To obtain no-regret guarantees of SF-GP-UCB, we require the condition that $\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)}) = o(T^{1-\tau})$ and $\sqrt{\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})/t^{1-2\tau}} = o(1)$ are both satisfied. Since the MIG of Matérn kernel increases polynomially, there exists a case in which we cannot set any $\tau \in (0, 1/2)$ to satisfy the above two conditions. Second, the requirement of $1/T^{1-\tau}$ dependence is unknown. Even in the existing work that considers deterministic failures, the successful numbers are guaranteed to grow linearly, resulting in the same rate of regret upper bound as GP-UCB without failures [Iwazaki et al., 2023]. The deterioration from linear order T to $T^{1-\tau}$ is a specific problem to stochastic failures. The analysis of whether this deterioration is a potentially unavoidable limitation of our problem settings is desired.

As for the first limitation described above, we show that the convergence of SF-GP-UCB with carefully chosen regularization parameters is guaranteed for Matérn kernels in Sec. 5. We leave the solution of the second limitation as future work.

4 MORE PRACTICAL VARIANTS OF SF-GP-UCB

Practical Behavior of SF-GP-UCB and its Drawback Although the regret of SF-GP-UCB is guaranteed to become arbitrarily small for sufficiently large step sizes, we confirmed some undesirable behavior of SF-GP-UCB for practitioners, especially in early iterations. From the definition of SF-GP-UCB, the query point $\boldsymbol{x}_t$ does not change until one of the following two events occurs: 1) the learner succeeds at $\boldsymbol{x}_t$, or 2) the queried point is classified as a sub-level set at the next step, namely, $\boldsymbol{x}_t \in \mathcal{L}_{t+1}(h_{t+1})$. Therefore, even if SF-GP-UCB queries the point whose failure probability is excessively lower than h_t, the same point is successively chosen until one of the above two events occurs, regardless of other inputs in the search space $\mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$ are promising to have a higher success probability. An example in a one-dimensional problem is shown in the top of Fig. 2. Note that such behavior is not problematic in large step size regimes since, for sufficiently large t, the search space $\mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$ does not contain the inputs whose success probabilities are excessively lower than h_t.

Confidence Bound-Based Improvement Algorithm From a high-level point of view, we can interpret SF-GP-UCB as the algorithm that repeatedly solves constraint optimization problems whose thresholds are adaptively determined so as to obtain enough successful observations. Motivated by this interpretation, we propose the stochastic failure-aware confidence bound-based improvement (SF-CBI) algorithm, which alleviates the aforementioned problematic behavior of SF-GP-UCB.

The pseudo-code of SF-CBI is shown in Algorithm 2 in Appendix C. The construction of SF-CBI is inspired by confidence-bound based improvement algorithm [Inatsu et al., 2022], which mimics the expected constrained improvement (ECI) criteria [Gardner et al., 2014] of constrained BO problems. In SF-CBI, the query point $\boldsymbol{x}_t$ is chosen as $\boldsymbol{x}_t \in \arg\max_{\boldsymbol{x}\in\mathcal{X}} \alpha_t(\boldsymbol{x})$ with $\alpha_t(\boldsymbol{x}) \coloneqq \alpha_t^{(\mathrm{CI})}(\boldsymbol{x}) \times \alpha_t^{(\mathrm{CP})}(\boldsymbol{x})$, where $\alpha_t^{(\mathrm{CI})}(\boldsymbol{x})$ and $\alpha_t^{(\mathrm{CP})}(\boldsymbol{x})$ are the quantities that mimic improvement from the current best value and constraint satisfaction probability, respectively. These are defined as

$$\alpha_t^{(\mathrm{CI})}(\boldsymbol{x}) = \max\{0, \mathrm{ucb}_t^{(f)}(\boldsymbol{x}) - \hat{f}_t^*\},$$

$$\alpha_t^{(\mathrm{CP})}(\boldsymbol{x}) = \begin{cases} 1 & \boldsymbol{x} \in \mathcal{H}_t(h_t), \\ 0 & \boldsymbol{x} \in \mathcal{L}_t(h_t), \\ \max\left\{ \frac{\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) - h_t}{\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) - \widetilde{\mathrm{lcb}}_t^{(g)}(\boldsymbol{x})}, \zeta \right\} & \boldsymbol{x} \in \mathcal{U}_t(h_t). \end{cases}$$

Here, $\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) = \min\{1, \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\}$, $\widetilde{\mathrm{lcb}}_t^{(g)}(\boldsymbol{x}) = \max\{0, \mathrm{lcb}_t^{(g)}(\boldsymbol{x})\}$, and $\hat{f}_t^*$ is a constrained current best value, which is defined as $\hat{f}_t^* = \max_{i \in \mathcal{I}_t^{(\mathrm{SF})}} \mu_{t-1}^{(f)}(\boldsymbol{x}_i)$ if $\mathcal{I}_t^{(\mathrm{SF})} \neq \emptyset$; otherwise, $\hat{f}_t^* = \min_{\boldsymbol{x}\in\mathcal{X}} \mu_{t-1}^{(f)}(\boldsymbol{x})$, where $\mathcal{I}_t^{(\mathrm{SF})} = \{i \in \mathbb{N}_+ \mid i \leq t-1, c_i = 1, \boldsymbol{x}_i \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)\}$. Furthermore, $\zeta \in (0, 1]$ is a *barrier* parameter, which prevents $\alpha_t^{(\mathrm{CP})}(\boldsymbol{x})$ to become unstable if $\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x})$ and $\widetilde{\mathrm{lcb}}_t^{(g)}(\boldsymbol{x})$ are concentrated around the threshold h_t. Note that existing works of constrained (or safe) BO also introduce a hyperparameter similar to ζ, which is motivated to simplify the theoretical treatment of the case that underlying functions are close to the threshold [Inatsu et al., 2022, Sui et al., 2015, 2018].

Comparison between SF-GP-UCB and SF-CBI Intuitively, SF-CBI is a version of SF-GP-UCB that takes into account the more fine-grained information of success function g. We can see this by confirming that SF-CBI coincides with SF-GP-UCB if we set $\zeta = 1$. By decreasing ζ from 1 to 0, SF-CBI chooses $\boldsymbol{x}_t$ by further taking into account the difference of $\alpha_t^{(\mathrm{CP})}(\boldsymbol{x})$, which alleviates the aforementioned drawback of SF-GP-UCB. We depict an example at the bottom of Fig. 2. Furthermore, we can see that SF-CBI tends to show better practical performance than SF-GP-UCB in Sec. 6.

Meanwhile, the weakness of SF-CBI is the degradation of the worst-case performance that is guaranteed by theory. Furthermore, to obtain such a worst-case regret guarantee, we require slight modifications in the original SF-CBI. In fact, Theorem D.1 in Appendix D.2 shows that the regret upper bound of SF-CBI is worse than that of SF-GP-UCB by the factor η/ζ, where $\eta \geq 1$ is a constant. We give detailed discussions about the theory of SF-CBI in Appendix D.2.

5 NO-REGRET ALGORITHM FOR MATÉRN RKHS

In the following theorem, by adaptively scaling regularization parameters, we show that SF-GP-UCB attains no-regret guarantees even for the case that both k_f and $k_{\tilde{g}}$ are Matérn kernels.

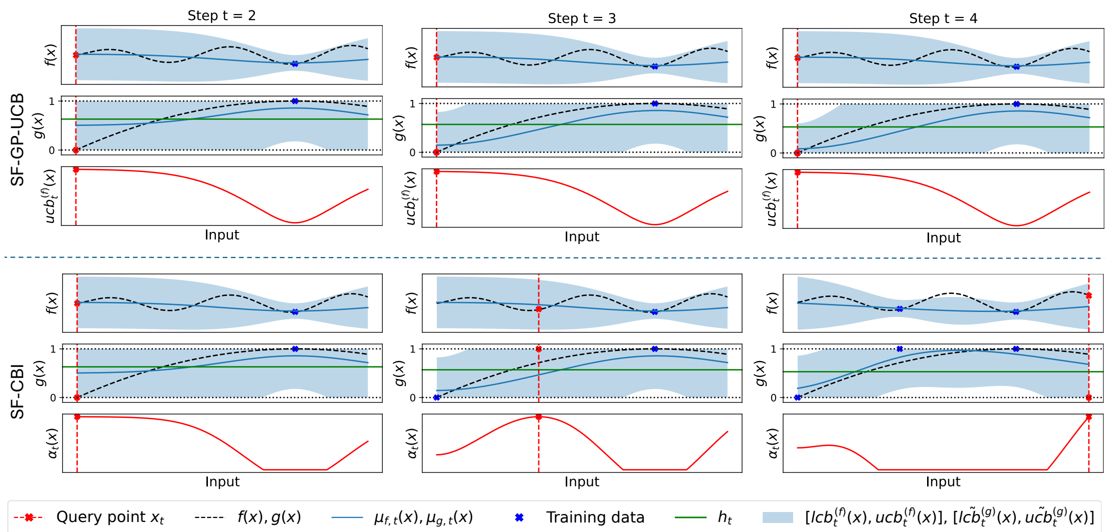

Figure 2: Example behaviors of our algorithms during the first three steps. In SF-GP-UCB (top), since query point $\boldsymbol{x}_t$ does not change until $\boldsymbol{x}_t \notin \mathcal{H}_t(\boldsymbol{x}_t) \cup \mathcal{U}_t(\boldsymbol{x}_t)$ holds, the same points whose success probability is almost zero are successively chosen. Intuitively, SF-CBI (bottom) avoids such behavior by incorporating more fine-grained information of $\mu_{g,t}$ and $\sigma_{g,t}$ into the querying strategy.

Theorem 5.1. *Let k_f and $k_{\tilde{g}}$ be Matérn kernels, whose smoothness parameters are $\nu_f > 1/2$ and $\nu_{\tilde{g}} > 1/2$, respectively. Suppose Assumptions 2.1–2.3 hold. Furthermore, let $\delta \in (0,1)$, $s_0 > 0$, and $\tau \in (0, \min\{\nu_f/(\nu_f + d), \nu_{\tilde{g}}/(2\nu_{\tilde{g}} + 2d)\})$. Moreover, let us respectively define $\lambda_{f,t}$, $\lambda_{\tilde{g},t}$, $\beta_{f,t}$, and $\beta_{\tilde{g},t}$ as $\lambda_{f,t} = t^{1/(1+\psi_f)}$, $\lambda_{\tilde{g},t} = t^{1/(1+\psi_{\tilde{g}})}$, $\beta_{f,t}^{1/2} = B_f + \sigma\lambda_{f,t}^{-1/2}\sqrt{2[\gamma_t^{(f)}(\lambda_{f,t}) + \ln((t^2\pi^2)/(3\delta))]}$, and $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda_{\tilde{g},t}^{-1/2}\sqrt{0.5[\gamma_t^{(\tilde{g})}(\lambda_{\tilde{g},t}) + \ln((2t^2\pi^2)/(3\delta))]}$, where $\psi_f = (2\nu_f + d)/d$ and $\psi_{\tilde{g}} = (2\nu_{\tilde{g}} + d)/d$. Then, when running Algorithm 1, the following holds with probability at least $1 - \delta$:*

$$r_T = \mathcal{O}^*\left(T^{\frac{d}{2\nu_f + 2d} - \frac{1-\tau}{2}}\right) \to 0 \quad (\text{as} \quad T \to \infty), \tag{7}$$

where the $\mathcal{O}^*(\cdot)$ notation ignores logarithmic factors.

The proof of Theorem 5.1 is in Appendix E. Particularly, Theorem E.1 in Appendix E is a detailed version of Theorem 5.1, which includes the dependence of g.

The high-level ideas of the proof strategy of Theorem 5.1 rely on those of Whitehouse et al. [2023]. However, we would like to note that some non-trivial theoretical treatments, which are described below, are required in our proof. First, to guarantee convergence of SF-GP-UCB, a careful choice of τ is required in addition to the adaptive choice of regularization parameters $\lambda_{f,T}$ and $\lambda_{\tilde{g},T}$. Second, Whitehouse et al. [2023] consider the setting that the total step size T is known. Therefore, their algorithm sets a regularization parameter $\lambda_{f,t}$ that depends on T before running the algorithm. On the other hand, we adaptively choose regularization parameters at each step t. This modification makes our theoretical analysis more complex than that of Whitehouse et al. [2023].

6 NUMERICAL EXPERIMENTS

In this section, we confirm the performance of SF-GP-UCB and SF-CBI through numerical experiments. As baseline methods of existing works, we adopt GP-UCB [Srinivas et al., 2010], expected feasible improvement with GPC (EFIGPC) [Bachoc et al., 2020, Lindberg and Lee, 2015], and PenalizedEI Forrester et al. [2006]. GP-UCB is an algorithm that simply ignores the failure observations in GP-UCB. EFIGPC is the algorithm whose acquisition function is defined as the product of EI and the posterior successful probability of GPC. PenalizedEI is the algorithm whose failed observations are imputed by the lower confidence bound of the GP. In SF-GP-UCB and SF-CBI, we set $s_0 = 0.75$, $\zeta = 0.20$. Furthermore, we set τ as $\tau = 1/4$ in the experiments with SE kernels. If we use Matérn 5/2, we set τ as $\tau = 1/6$. These settings of τ are chosen as the middle values of the intervals on which Theorem 3.3 and Theorem 5.1 are valid. Similar setting strategies are also used in Iwazaki et al. [2023]. In Appendix F, further details of experiments are described, including each hyperparameter setting of kernels and algorithms.

1D-Synthetic Function We first start with two pairs of simple 1D-synthetic functions depicted in Fig. 6

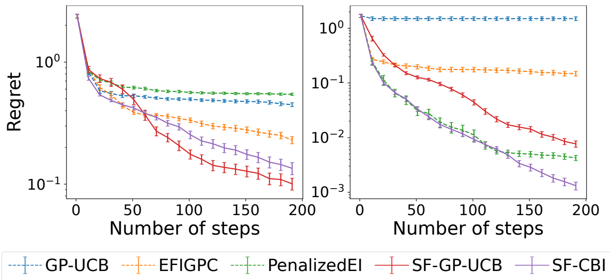

Figure 3: The results of an experiment with synthetic functions depicted in Fig. 6. The plot shows an average and one standard error of regret with 100 different seeds. The left and right figures show the results with functions depicted in the top and bottom figures of Fig. 6 in Appendix F, respectively.

of Appendix F. Each function is designed to confirm the performance when the optimum has a high (low) failure probability. Fig. 3 shows the results. We can confirm that SF-CBI achieves better performance than other methods. In SF-GP-UCB, the poor performances are confirmed during steps 10 to 50 in the first plot of Fig. 3. The source of this behavior comes from the drawback of SF-GP-UCB, as discussed in Sec. 4. In the second plot of Fig. 3, PenalizedEI achieves better performance. It is reasonable since, in this setting, the values of f on the region whose failure probability is high are low; therefore, by avoiding such an unpromising region with pessimistically imputed observations, PenalizedEI tends to focus on searching regions where the optimum lies.

2D-RKHS Test Functions and Sensitivity Analysis We further run experiments with 2D-RKHS test functions generated from the sample path of GP. We generate 10 test functions and run experiments with 20 different seeds in each function. Namely, we ran a total of 200 experiments and reported average regret. The results are in Fig. 4. We can confirm that SF-GP-UCB and SF-CBI perform the same or better than other baselines. Furthermore, we study the performance sensitivity of our algorithms in 2D-RKHS test functions and leave the results in Appendix F.4, indicating that SF-GP-UCB and SF-CBI achieve good performance with various parameter settings.

Benchmark Function for Constrained BO We also confirm the performance by recasting the benchmark problems of constrained BO to our settings. In this problem, we assume that success labels c_t are obtained as $c_t = \mathbb{1}\{\tilde{g}(\boldsymbol{x}_t) + \upsilon_t \geq 0\}$, where $\upsilon_t \sim \mathcal{N}(0, 1/4)$ and $\tilde{g}$ is a constraint function of the original problem. Namely, we consider the setting that a failure

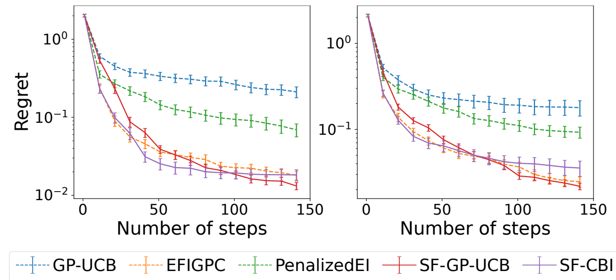

Figure 4: The results of experiments with 2D-RKHS test functions. The left and right figures show the results of the RKHS test functions which are constructed from SE and Matérn 5/2 kernels.

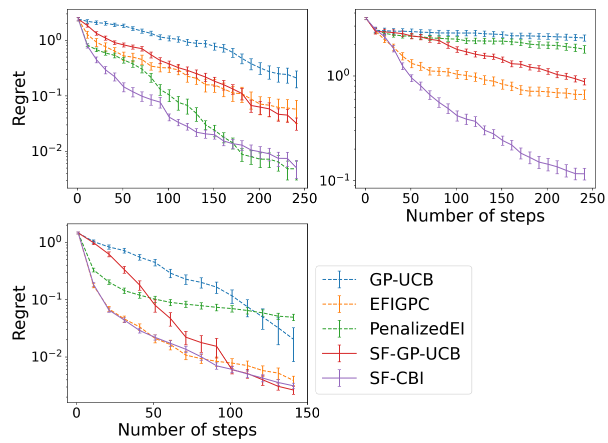

Figure 5: The results of experiments with Gardner (top-left), Hartmann (top-right), and simulation function of quasi-crystal (bottom-left). The plot shows the average regret with 100 different seeds.

event will occur by constraint unsatisfaction, which occurs stochastically by uncontrollable Gaussian noise. We leverage Gardner [Gardner et al., 2014] and Hartmann [Letham et al., 2019] test problems, whose input domains are 2D and 3D, respectively. The top plots of Fig. 5 show the results. In both experiments, SF-CBI shows better performance.

Simulation Function of Quasi-Crystal Synthesis We perform experiments using a simulation function created by real data for quasi-crystal synthesis in the Al-Cu-Mn alloy [Grushko and Mi, 2016, Liu et al., 2021]. As used in the experiments of Iwazaki et al. [2023], the quasi-crystal synthesis succeeds in certain deterministic domains of input composition; however, in practice, the input composition can fluctuate due to uncontrollable experimental errors. In this experiment, we let the user-specified input composition have normally distributed errors; thus, the quasi-crystal synthesis succeeds stochastically. We simultaneously optimize for maximum phonon thermal conductivity of the formed quasi-crystal. Fig. 5 (bottom-left) shows the result, which confirms the good performance of our algorithms.

7 CONCLUSIONS

We consider BO problems whose observations can fail stochastically. We propose a novel SF-GP-UCB algorithm in which the first regret upper bound is given. We further discuss the drawback of SF-GP-UCB and propose SF-CBI, which is a practical variant of SF-GP-UCB. The numerical experiments show the effectiveness of our algorithms.

Acknowledgements

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Checklist

1. For all models and algorithms presented, check if you include:
   (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model. [Yes. We describe the mathematical setting, assumptions, and algorithm in Sec. 2, Sec. 3, and Sec. 4.]
   (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm. [No. The time and space complexity of our algorithm is clearly almost the same as the standard algorithm such as GP-UCB.]
   (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries. [No]
2. For any theoretical claim, check if you include:
   (a) Statements of the full set of assumptions of all theoretical results. [Yes]
   (b) Complete proofs of all theoretical results. [Yes]
   (c) Clear explanations of any assumptions. [Yes]
3. For all figures and tables that present empirical results, check if you include:
   (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL). [Yes. See Sec. 6 and Appendix F.]
   (b) All the training details (e.g., data splits, hyperparameters, how they were chosen). [Yes. See Appendix F.]
   (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). [Yes]
   (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). [No]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
   (a) Citations of the creator If your work uses existing assets. [Not Applicable]

   (b) The license information of the assets, if applicable. [Not Applicable]
   (c) New assets either in the supplemental material or as a URL, if applicable. [Not Applicable]
   (d) Information about consent from data providers/curators. [Not Applicable]
   (e) Discussion of sensible content if applicable, e.g., personally identifiable information or offensive content. [Not Applicable]

5. If you used crowdsourcing or conducted research with human subjects, check if you include:
   (a) The full text of instructions given to participants and screenshots. [Not Applicable]
   (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. [Not Applicable]
   (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. [Not Applicable]

Supplementary Materials for the Submission: "No-Regret Bayesian Optimization with Stochastic Observation Failures"

A PRELIMINARIES FOR PROOFS

In this section, for completeness of our paper, we describe the existing theoretical tools, which are leveraged in our theoretical analysis.

Lemma A.1. *Suppose Assumptions 2.1–2.2 hold. Let $\delta \in (0,1)$ and $\lambda^{(f)} > 0$ such that $\lambda_{f,t} = \lambda^{(f)}$ holds for all $t \in \mathbb{N}_+$. Furthermore, let $\beta_{f,t}^{1/2} = B_f + \sigma \lambda^{(f)-1/2}\sqrt{2[\gamma_{n_t}^{(f)}(\lambda^{(f)}) + \ln(1/\delta)]}$ with*

$$\gamma_{n_t}^{(f)}(\lambda^{(f)}) = \frac{1}{2}\sup_{D \in \mathcal{X}^{n_t}} \ln\det\left[\boldsymbol{I}_{n_t} + \lambda^{(f)-1}\boldsymbol{K}_f(D)\right].$$

Then, the following holds with probability at least $1-\delta$:

$$\forall t \in \mathbb{N}_+, \forall \boldsymbol{x} \in \mathcal{X}, \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \le f(\boldsymbol{x}) \le \mathrm{ucb}_t^{(f)}(\boldsymbol{x}), \tag{8}$$

where $\mathrm{lcb}_t^{(f)}(\boldsymbol{x}) = \mu_{f,t-1}(\boldsymbol{x}) - \beta_{f,t}^{1/2}\sigma_{f,t-1}(\boldsymbol{x})$ and $\mathrm{ucb}_t^{(f)}(\boldsymbol{x}) = \mu_{f,t-1}(\boldsymbol{x}) + \beta_{f,t}^{1/2}\sigma_{f,t-1}(\boldsymbol{x})$.

Lemma A.2. *Fix any algorithm and $t \in \mathbb{N}_+$. Suppose $\lambda_{\tilde{g},i} = \lambda^{(\tilde{g})} > 0$ holds for any $i \in \mathbb{N}_+$. Then, the following inequality holds:*

$$\sum_{i=1}^{t} \sigma_{\tilde{g},i-1}(\boldsymbol{x}_i) \le \sqrt{\frac{2t\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})}{\ln(1+\lambda^{(\tilde{g})-1})}}. \tag{9}$$

Lemma A.3. *Fix any algorithm and $t \in \mathbb{N}_+$. Suppose $\lambda_{f,i} = \lambda^{(f)} > 0$ holds for any $i \in \mathbb{N}_+$. Then, if $n_t \ge 1$, the following inequality holds:*

$$\sum_{i \in \mathcal{I}_t^{(s)}} \sigma_{f,i-1}(\boldsymbol{x}_i) \le \sqrt{\frac{2n_t\gamma_{n_t}^{(f)}(\lambda^{(f)})}{\ln(1+\lambda^{(f)-1})}}. \tag{10}$$

Lemmas A.2–A.3 follows from Lemmas 5.3–5.4 in Srinivas et al. [2010].

Lemma A.4 (Thereom 1 in Beygelzimer et al. [2011] or Lemma 11 in Bogunovic et al. [2020])**.** *Let $M_1, \dots, M_t$ be an sequence of real-valued random variables adapted to filtration $\mathcal{G}_i$. Furthermore, suppose the following statements hold:*

- $\mathbb{E}[M_i \mid \mathcal{G}_{i-1}] = 0$ *for any $i \le t$.*
- *There exists $R \ge 0$ such that $M_i \le R$ for any $i \le t$.*

Then, the following inequality holds for any $\delta \in (0,1)$:

$$\mathbb{P}\left(\sum_{i=1}^{t} M_i \le \frac{V}{R}(e-2) + R\ln\frac{1}{\delta}\right) \ge 1-\delta, \tag{11}$$

where $V = \sum_{i=1}^{t}\mathbb{E}[M_i^2 \mid \mathcal{G}_{i-1}]$.

Lemma A.5 (Corollary 1 in Vakili et al. [2021])**.** *Let k_f be a Matérn kernel with smoothness parameter $\nu_f > 1/2$. Then, the following holds for any $\lambda > 0$:*

$$\gamma_t^{(f)}(\lambda) \le \left[\left(\frac{C_f t}{\lambda}\right)^{1/\psi_f} \ln^{-1/\psi_f}\left(1+\frac{t}{\lambda}\right) + 1\right]\ln\left(1+\frac{t}{\lambda}\right), \tag{12}$$

where C_f is a constant that only depends on hyperparameter ℓ of k_f. Furthermore, we set $\psi_f = (2\nu_f + d)/d$.

B PROOFS OF SECTION 3

B.1 Proof of Lemma 3.1

We first give the following general lower bounds of n_t, which is applicable for any algorithm.

Lemma B.1 (General lower bound of n_t)**.** *Fix any algorithm and $\delta \in (0, 1)$. Then, the following statement holds with probability at least $1 - \delta$:*

$$\forall t \in \mathbb{N}_+,\ n_t \geq (3 - e) \sum_{i=1}^{t} g(\boldsymbol{x}_i) - \ln \frac{\pi^2 t^2}{6\delta}. \tag{13}$$

Proof. Define M_i and $\mathcal{G}_{t-1}$ as $M_i = g(\boldsymbol{x}_i) - c_i$ and $\mathcal{G}_i = H_i$, respectively. Then, $M_i \leq 1$ and $\mathbb{E}[M_i \mid \mathcal{G}_{i-1}] = 0$ hold for any $i \in \mathbb{N}_+$. Furthermore, $\sum_{i=1}^{t} \mathbb{E}[M_i^2 \mid \mathcal{G}_{i-1}] = \sum_{i=1}^{t} g(\boldsymbol{x}_i)[1 - g(\boldsymbol{x}_i)]$ holds for any $t \in \mathbb{N}_+$ since the conditional distribution of c_i is Bernoulli$(g(\boldsymbol{x}_i))$. Therefore, by applying Lemma A.4, the following inequality holds with probability at least $1 - \delta$:

$$\sum_{i=1}^{t} [g(\boldsymbol{x}_i) - c_i] \leq (e - 2) \sum_{i=1}^{t} g(\boldsymbol{x}_i)[1 - g(\boldsymbol{x}_i)] + \ln \frac{1}{\delta}. \tag{14}$$

Moreover,

$$\begin{aligned}
&\sum_{i=1}^{t} [g(\boldsymbol{x}_i) - c_i] \leq (e - 2) \sum_{i=1}^{t} g(\boldsymbol{x}_i)[1 - g(\boldsymbol{x}_i)] + \ln \frac{1}{\delta} \\
&\Rightarrow \sum_{i=1}^{t} [g(\boldsymbol{x}_i) - c_i] \leq (e - 2) \sum_{i=1}^{t} g(\boldsymbol{x}_i) + \ln \frac{1}{\delta} \\
&\Leftrightarrow n_t \geq (3 - e) \sum_{i=1}^{t} g(\boldsymbol{x}_i) - \ln \frac{1}{\delta}.
\end{aligned} \tag{15}$$

By replacing δ with $6\delta/(t^2\pi^2)$ and taking union bound for all $t \in \mathbb{N}_+$, we obtain the desired statement (13). $\square$

We give the proof of Lemma 3.1 below.

Proof of Lemma 3.1. By taking union bound in Lemma 2.4 and Lemma B.1, the following two events simultaneously hold with probability at least $1 - \delta$:

- $n_t \geq (3 - e) \sum_{i=1}^{t} g(\boldsymbol{x}_i) - \ln((\pi^2 t^2)/(3\delta))$ holds for any $t \in \mathbb{N}_+$.
- $\mathrm{lcb}_t^{(g)}(\boldsymbol{x}) \leq g(\boldsymbol{x}) \leq \mathrm{ucb}_t^{(g)}(\boldsymbol{x})$ holds for any $t \in \mathbb{N}_+$ and $\boldsymbol{x} \in \mathcal{X}$.

It is enough to show Eq. (2) holds for any $t \in \mathbb{N}_+$ under the above two events. Hereafter, we suppose the above two events hold; then,

$$
\begin{aligned}
& n_t \geq (3-e) \sum_{i=1}^{t} g(\boldsymbol{x}_i) - \ln \frac{\pi^2 t^2}{3\delta} && (16)\\
& \Rightarrow n_t \geq (3-e) \sum_{i=1}^{t} \mathrm{lcb}_i^{(g)}(\boldsymbol{x}_i) - \ln \frac{\pi^2 t^2}{3\delta} && (17)\\
& \Leftrightarrow n_t \geq (3-e) \sum_{i=1}^{t} \left[\mathrm{ucb}_i^{(g)}(\boldsymbol{x}_i) - 2\beta_{\tilde{g},i}^{1/2} \sigma_{\tilde{g}}(\boldsymbol{x}_i)\right] - \ln \frac{\pi^2 t^2}{3\delta} && (18)\\
& \Rightarrow n_t \geq (3-e) \sum_{i=1}^{t} \left[h - 2\beta_{\tilde{g},i}^{1/2} \sigma_{\tilde{g}}(\boldsymbol{x}_i)\right] - \ln \frac{\pi^2 t^2}{3\delta} && (19)\\
& \Leftrightarrow n_t \geq (3-e) \left[ht - 2\beta_{\tilde{g},t}^{1/2} \sum_{i=1}^{t} \sigma_{\tilde{g}}(\boldsymbol{x}_i)\right] - \ln \frac{\pi^2 t^2}{3\delta} && (20)\\
& \Rightarrow n_t \geq (3-e) \left[ht - \sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})}\right] - \ln \frac{\pi^2 t^2}{3\delta}, && (21)
\end{aligned}
$$

where:

- Eq. (19) follows from $h \geq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}_t)$ since $\boldsymbol{x}_t \in \mathcal{H}_t(h) \cup \mathcal{U}_t(h)$.
- Eq. (20) follows from the fact that $\beta_{\tilde{g},i}^{1/2}$ are monotonically increasing.
- Eq. (21) follows by applying Lemma A.2.

The proof is completed since Eq. (21) is the desired inequality. □

B.2 Proof of Theorem 3.2

Proof of Theorem 3.2. From Lemma 2.4, Lemma 3.1, and Lemma A.1, the following three events simultaneously hold with probability at least $1-\delta$ by applying union bound:

$$
\begin{aligned}
& \forall \boldsymbol{x} \in \mathcal{X},\ \forall t \in \mathbb{N}_+,\ \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \leq f(\boldsymbol{x}) \leq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}), && (22)\\
& \forall \boldsymbol{x} \in \mathcal{X},\ \forall t \in \mathbb{N}_+,\ \mathrm{lcb}_t^{(g)}(\boldsymbol{x}) \leq g(\boldsymbol{x}) \leq \mathrm{ucb}_t^{(g)}(\boldsymbol{x}), && (23)\\
& \forall t \in \mathbb{N}_+,\ n_t \geq (3-e)\left(ht - \sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})}\right) - \ln \frac{2\pi^2 t^2}{3\delta}. && (24)
\end{aligned}
$$

Therefore, it is enough to show that the statement 1 and statement 2 of Theorem 3.2 holds under the events (22)–(24). Since the statement 1 of Theorem 3.2 clearly holds from Eq. (24) and the definition of $\tilde{T}_1$, we focus on showing the statement 2. Here, from the events (22)–(23) and the definition of $\boldsymbol{x}_h^*$, $\boldsymbol{x}_h^* \in \mathcal{H}_t(h) \cup \mathcal{U}_t(h)$ holds for all $t \in \mathbb{N}_+$. Therefore,

$$
\begin{aligned}
\sum_{t \in \mathcal{I}_T^{(s)}} [f(\boldsymbol{x}_h^*) - f(\boldsymbol{x}_t)] &\leq \sum_{t \in \mathcal{I}_T^{(s)}} \left[\mathrm{ucb}_t^{(f)}(\boldsymbol{x}_t) - \mathrm{lcb}_t^{(f)}(\boldsymbol{x}_t)\right] && (25)\\
&\leq 2\beta_{f,T}^{1/2} \sum_{t \in \mathcal{I}_T^{(s)}} \sigma_{t-1}^{(f)}(\boldsymbol{x}_t) && (26)\\
&= \sqrt{\frac{8}{\ln(1+\lambda^{(f)-1})} n_T \beta_{f,T} \gamma_T^{(f)}(\lambda^{(f)})}, && (27)
\end{aligned}
$$

where Eq. (25) follows from the definition of $\boldsymbol{x}_t$. Furthermore, Eq. (27) holds by applying Lemma A.3. Since $f(\boldsymbol{x}_h^*) - \max_{t \in \mathcal{I}_T^{(s)}} f(\boldsymbol{x}_t) \le \sum_{t \in \mathcal{I}_T^{(s)}} [f(\boldsymbol{x}_h^*) - f(\boldsymbol{x}_t)] / n_t$,

$$r_T = f(\boldsymbol{x}^*) - f(\boldsymbol{x}_h^*) + f(\boldsymbol{x}_h^*) - \max_{t \in \mathcal{I}_T^{(s)}} f(\boldsymbol{x}_t) \tag{28}$$

$$\le f(\boldsymbol{x}^*) - f(\boldsymbol{x}_h^*) + \frac{1}{n_T} \sum_{t \in \mathcal{I}_T^{(s)}} [f(\boldsymbol{x}_h^*) - f(\boldsymbol{x}_t)]. \tag{29}$$

The proof is completed by combining the above inequality with Eq. (27) and $n_T = \Omega(hT)$. □

B.3 Proof of Theorem 3.3

Lemma B.2. *Fix any algorithm. Suppose the following event holds:*

$$\forall t \in \mathbb{N}_+,\ \forall \boldsymbol{x} \in \mathcal{X},\ g(\boldsymbol{x}) \le \mathrm{ucb}_t^{(g)}(\boldsymbol{x}). \tag{30}$$

Assume the function b is a decreasing function such that $b(1) = 1$. Furthermore, define $(s_t)_{t \in \mathbb{N}_+}$ and $(h_t)_{t \in \mathbb{N}_+}$ as

$$s_t = \min\{s_{t-1}, b^{-1}(t) \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\}, \tag{31}$$

$$h_t = s_t b(t), \tag{32}$$

where $s_0 > 0$. Then, $s_t \ge \min\{s_0, \overline{g}\}$ holds for any $t \in \mathbb{N}_+$, where $\overline{g} = \max_{\boldsymbol{x} \in \mathcal{X}} g(\boldsymbol{x})$.

Proof. Uner the event (30), $s_1 = \min\{s_0, b^{-1}(1) \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\} \ge \min\{s_0, \overline{g}\}$. For $t = 2$, $s_2 = \min\{s_1, b(2)^{-1} \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\} \ge \min\{s_1, b^{-1}(1)\overline{g}\} \ge \min\{s_0, \overline{g}\}$. By repeating similar arguments, $s_t \ge \min\{s_0, \overline{g}\}$ also holds for $t \ge 3$. □

Lemma B.3 (Lower bound of n_t with adaptive threshold h_t)**.** *Suppose Assumption 2.3 and $\lambda_{\tilde{g},t} = \lambda^{(\tilde{g})} > 0$ hold for any $t \in \mathbb{N}_+$. Let $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda^{(\tilde{g})-1/2} \sqrt{4[\gamma_t^{(g)}(\lambda^{(\tilde{g})}) + \ln(2/\delta)]}$ with any $\delta \in (0,1)$ and $b(t) = t^{-\tau}$ with any $\tau \in (0, 1/2)$. Furthermore, define $(s_t)_{t \in \mathbb{N}_+}$ and $(h_t)_{t \in \mathbb{N}_+}$ as*

$$s_t = \min\{s_{t-1}, b^{-1}(t) \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\}, \tag{33}$$

$$h_t = s_t b(t), \tag{34}$$

where $s_0 \in (0, 1)$. Then, when running an algorithm whose query points $\boldsymbol{x}_t$ satisfy $\boldsymbol{x}_t \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$, with probability at least $1 - \delta$, the following lower bound for the number of successful observations holds for any $t \in \mathbb{N}_+$:

$$n_t \ge (3 - e) \left[\frac{\min\{s_0, \overline{g}\}}{1 - \tau} (t^{1-\tau} - 1) - \sqrt{C t \beta_{\tilde{g},t} \gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})} \right] - \ln \frac{\pi^2 t^2}{3\delta}, \tag{35}$$

where $C = \sqrt{8 / \ln(1 + \lambda^{(\tilde{g})-1})}$.

Proof. Since $\boldsymbol{x}_i \in \mathcal{H}_i(h_i) \cup \mathcal{U}_i(h_i)$ holds, $\mathrm{ucb}_i^{(g)}(\boldsymbol{x}_i) \ge h_i$ holds for all $i \in \mathbb{N}_+$. By combining this fact with Lemma 2.4 and Lemma B.1, the following inequality holds with probability at least $1 - \delta$:

$$n_t \ge (3 - e) \sum_{i=1}^{t} g(\boldsymbol{x}_i) - \ln \frac{\pi^2 t^2}{3\delta} \tag{36}$$

$$\ge (3 - e) \sum_{i=1}^{t} \left[\mathrm{ucb}_i^{(g)}(\boldsymbol{x}_i) - 2\beta_{\tilde{g},i}^{1/2} \sigma_{\tilde{g},i-1}(\boldsymbol{x}_i) \right] - \ln \frac{\pi^2 t^2}{3\delta} \tag{37}$$

$$\ge (3 - e) \left[\sum_{i=1}^{t} h_t - 2\beta_{\tilde{g},t}^{1/2} \sum_{i=1}^{t} \sigma_{\tilde{g},i-1}(\boldsymbol{x}_i) \right] - \ln \frac{\pi^2 t^2}{3\delta}. \tag{38}$$

In Eq. (38), the term $\sum_{i=1}^{t} h_i$ is further bounded from below as follows:

$$
\begin{aligned}
\sum_{i=1}^{t} h_i &\geq \min\{s_0, \overline{g}\} \sum_{i=1}^{t} i^{-\tau} \\
&\geq \min\{s_0, \overline{g}\} \int_{1}^{t} i^{-\tau} \mathrm{d}i \\
&\geq \min\{s_0, \overline{g}\} \frac{t^{1-\tau} - 1}{1 - \tau},
\end{aligned}
\tag{39}
$$

where the first inequality of Eq. (39) holds by applying Lemma B.2. Finally, by combining Eq. (38) with Eq. (39) and Lemma A.2, the desired statement is obtained. □

Proof of Theorem 3.3. From the definition of $\boldsymbol{x}_t$ of SF-GP-UCB, $\boldsymbol{x}_t \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$, which is the conditions of Lemma B.3, holds. By taking union bound, the following three events simultaneously hold with probability at least $1 - \delta$:

$$
\forall \boldsymbol{x} \in \mathcal{X},\ \forall t \in \mathbb{N}_+,\ \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \leq f(\boldsymbol{x}) \leq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}), \tag{40}
$$

$$
\forall \boldsymbol{x} \in \mathcal{X},\ \forall t \in \mathbb{N}_+,\ \mathrm{lcb}_t^{(g)}(\boldsymbol{x}) \leq g(\boldsymbol{x}) \leq \mathrm{ucb}_t^{(g)}(\boldsymbol{x}), \tag{41}
$$

$$
\forall t \in \mathbb{N}_+,\ n_t \geq (3 - e) \left(\frac{\min\{s_0, \overline{g}\}}{1 - \tau} (t^{1-\tau} - 1) - \sqrt{C t \beta_{\tilde{g},t} \gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})} \right) - \ln \frac{\pi^2 t^2}{3\delta}. \tag{42}
$$

Therefore, it is enough to show that the statement 1 and statement 2 of Theorem 3.3 hold under the events (40)–(42). The statement 1 of Theorem 3.3 is easily follows by combining the event (42) with the definition of $\overline{T}_2$. As for the proof of the statement 2, we repeat the similar argument of the proof of Theorem 3.3 by replacing fixed threshold h with h_t. Here, let us define $\boldsymbol{x}_{h_t}^*$ as $\boldsymbol{x}_{h_t}^* = \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{H}(h_t)}$, where $\mathcal{H}(h_t) \coloneqq \{\boldsymbol{x} \in \mathcal{X} \mid g(\boldsymbol{x}) \geq h_t\}$ is the super-level set defined with h_t. Note that $f(\boldsymbol{x}_{h_t}^*) \leq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}_t)$ follows from $\boldsymbol{x}_t \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$ and the events (40)–(41). Therefore, by resorting the similar arguments around Eq. (25)–(27) in the proof of Theorem 3.3, the following inequality holds:

$$
\sum_{t \in \mathcal{I}_T^{(s)}} \left[f(\boldsymbol{x}_{h_t}^*) - f(\boldsymbol{x}_t) \right] \leq \sqrt{\frac{8}{\ln(1 + \lambda^{(f)-1})} n_T \beta_{f,T} \gamma_T^{(f)}(\lambda^{(f)})}. \tag{43}
$$

Moreover, from the definition of $\overline{T}_3$, $h_{\overline{T}_3} \leq s_0 \overline{T}_3^{-\tau} = g(\boldsymbol{x}^*)$ holds, which implies $f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{h_t}^*) = 0$ for any $t \geq \overline{T}_3$. Hence, the following inequality holds:

$$
\begin{aligned}
r_T &= f(\boldsymbol{x}^*) - \max\nolimits_{t \in \mathcal{I}_T^{(s)}} f(\boldsymbol{x}_t) \\
&\leq \frac{1}{n_T} \sum_{t \in \mathcal{I}_T^{(s)}} [f(\boldsymbol{x}^*) - f(\boldsymbol{x}_t)] \\
&\leq \frac{1}{n_T} \sum_{t \in \mathcal{I}_T^{(s)}} \left[f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{h_t}^*) \right] + \frac{1}{n_T} \sum_{t \in \mathcal{I}_T^{(s)}} \left[f(\boldsymbol{x}_{h_t}^*) - f(\boldsymbol{x}_t) \right] \\
&\leq \frac{2\overline{T}_3 B_f}{n_T} + \sqrt{\frac{8 \beta_{f,T} \gamma_T^{(f)}(\lambda^{(f)})}{n_T \ln(1 + \lambda^{(f)-1})}},
\end{aligned}
\tag{44}
$$

where the second term in the last line of Eq. (44) follows from Eq. (43). Furthermore, the first term follows from the fact that $\sum_{t \in \mathcal{I}_T^{(s)}} \left[f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{h_t}^*) \right] \leq 2\overline{T}_3 B_f$ holds since $\|f\|_\infty \leq B_f$. Finally, from Lemma B.3 and the assumption $\sqrt{\beta_{\tilde{g},t} \gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})}) / t^{1-2\tau}} = o(1)$, the order of n_T is $n_T = \Omega(T^{1-\tau})$. The proof is completed by combining this fact with Eq. (44). □

C PSEUDO-CODE OF SF-CBI

We give the pseudo-code of SF-CBI in Algorithm 2.

Algorithm 2 The SF-CBI algorithm

Require: Kernel k_f, k_g, decreasing function $b : (0, \infty) \to (0, \infty)$, initial scale parameter $s_0 \in (0, 1)$, width parameters of confidence bounds $\beta_{f,t}$, $\beta_{g,t}$, barrier parameter $\zeta \in (0, 1]$.

for $t = 1$ to T **do**

$s_t = \min\{s_{t-1}, b^{-1}(t) \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\}$.

$h_t = s_t b(t)$.

Calculate the estimated current best $\hat{f}_t^*$ as

$$\hat{f}_t^* = \begin{cases} \max_{i \in \mathcal{I}_t^{(\mathrm{SF})}} \mu_{t-1}^{(f)}(\boldsymbol{x}_i) & \text{if } \mathcal{I}_t^{(\mathrm{SF})} \neq \emptyset, \\ \min_{\boldsymbol{x} \in \mathcal{X}} \mu_{t-1}^{(f)}(\boldsymbol{x}) & \text{otherwise} \end{cases}. \tag{45}$$

Calculate $\alpha_t^{(\mathrm{CI})}(\boldsymbol{x})$ and $\alpha_t^{(\mathrm{CP})}(\boldsymbol{x})$ as

$$\alpha_t^{(\mathrm{CI})}(\boldsymbol{x}) = \max\left\{0, \mathrm{ucb}_t^{(f)}(\boldsymbol{x}) - \hat{f}_t^*\right\}, \tag{46}$$

$$\alpha_t^{(\mathrm{CP})}(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \mathcal{H}_t(h_t), \\ 0 & \text{if } \boldsymbol{x} \in \mathcal{L}_t(h_t), \\ \max\left\{\frac{\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) - h_t}{\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) - \widetilde{\mathrm{lcb}}_t^{(g)}(\boldsymbol{x})}, \zeta\right\} & \text{if } \boldsymbol{x} \in \mathcal{U}_t(h_t) \end{cases}. \tag{47}$$

Choose $\boldsymbol{x}_t$ as $\boldsymbol{x}_t \in \arg\max_{\boldsymbol{x} \in \mathcal{X}} [\alpha_t^{(\mathrm{CI})}(\boldsymbol{x}) \times \alpha_t^{(\mathrm{CP})}(\boldsymbol{x})]$.

Obtain success label $c_t \sim \mathrm{Bernoulli}(g(\boldsymbol{x}_t))$.

if $c_t = 1$ **then**

Observe $y_t = f(\boldsymbol{x}_t) + \epsilon_t$.

end if

end for

D DETAILS OF THE THEORY OF SF-CBI

D.1 Modification of SF-CBI for the Theory

Instead of giving a theory for the original SF-CBI, we give a theory for a modified version whose pseudo-code is shown in Algorithm 3. The differences between the original SF-CBI and the modified one are the following:

1. The definition of the estimated current best (Eq. (48)). Specifically, we replace $\mu_{f,t-1}$ in the original definition with pessimistic estimate $\mathrm{lcb}_t^{(f)}$. We would like to note that such a pessimistic estimation of the current best value is commonly used in theoretical analysis of GP-UCB-based algorithm [Bogunovic et al., 2018], while existing works report that GP-UCB-based algorithm with $\mu_{t,f}^{(f)}$-based estimation of current best value tends to have higher practical performance [Nguyen et al., 2021].

2. The combination of SF-GP-UCB querying strategy based on the confidence width (line 7–10 in Algorithm 3). Specifically, we leverage the SF-GP-UCB query strategy when the ratio of confidence width at the vanilla SF-CBI querying point and its confidence bound-based improvement becomes below the prespecified η. Intuitively, we require this modification to guarantee that the algorithm does not get stuck on the vanilla SF-CBI query points by ignoring other promising input candidates.

The following Theorem D.1 give the convergence guarantees of the modified version of SF-CBI.

Theorem D.1. *Suppose Assumptions 2.1–2.3, $\lambda_{f,t} = \lambda^{(f)}$, and $\lambda_{\tilde{g},t} = \lambda^{(\tilde{g})} > 0$ hold for any $t \in \mathbb{N}_+$. Let $\beta_{f,t}^{1/2} = B_f + \sigma \lambda^{(f)-1/2} \sqrt{2[\gamma_t^{(f)}(\lambda^{(f)}) + \ln(2/\delta)]}$, $\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda^{(\tilde{g})-1/2} \sqrt{0.5[\gamma_t^{(g)}(\lambda^{(\tilde{g})}) + \ln(4/\delta)]}$ with any $\delta \in (0, 1)$, $\zeta \in (0, 1]$, and $b(t) = t^{-\tau}$ for any $\tau \in (0, 1/2)$. Furthermore, suppose $\sqrt{\beta_{\tilde{g},t} \gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})/t^{1-2\tau}} = o(1)$. Then, when running Algorithm 3, with probability at least $1 - \delta$, the following two statements simultaneously hold:*

Algorithm 3 The modified version of SF-CBI algorithm

Require: Kernel k_f, k_g, decreasing function $b : (0, \infty) \to (0, \infty)$, initial scale parameter $s_0 \in (0, 1)$, width parameters of confidence bounds $\beta_{f,t}$, $\beta_{g,t}$, barrier parameter $\zeta \in (0, 1]$, width threshold $\eta \geq 1$.

for $t = 1$ to T **do**

  $s_t = \min\{s_{t-1}, b^{-1}(t) \max_{\boldsymbol{x} \in \mathcal{X}} \mathrm{ucb}_t^{(g)}(\boldsymbol{x})\}$.

  $h_t = s_t b(t)$.

  Calculate the modified version of current best $\hat{f}^*_{t,\mathrm{mod}}$ as

$$\hat{f}^*_{t,\mathrm{mod}} = \begin{cases} \max_{i \in \mathcal{I}_t^{(\mathrm{SF})}} \mathrm{lcb}_t^{(f)}(\boldsymbol{x}_i) & \text{if } \mathcal{I}_t^{(\mathrm{SF})} \neq \emptyset, \\ \min_{\boldsymbol{x} \in \mathcal{X}} \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) & \text{otherwise} \end{cases}. \tag{48}$$

  Calculate $\alpha^{(\mathrm{CI})}_{t,\mathrm{mod}}(\boldsymbol{x})$ and $\alpha_t^{(\mathrm{CP})}(\boldsymbol{x})$ as

$$\alpha^{(\mathrm{CI})}_{t,\mathrm{mod}}(\boldsymbol{x}) = \max\left\{0, \mathrm{ucb}_t^{(f)}(\boldsymbol{x}) - \hat{f}^*_{t,\mathrm{mod}}\right\}, \tag{49}$$

$$\alpha_t^{(\mathrm{CP})}(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{x} \in \mathcal{H}_t(h_t), \\ 0 & \text{if } \boldsymbol{x} \in \mathcal{L}_t(h_t), \\ \max\left\{ \frac{\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) - h_t}{\widetilde{\mathrm{ucb}}_t^{(g)}(\boldsymbol{x}) - \widetilde{\mathrm{lcb}}_t^{(g)}(\boldsymbol{x})}, \zeta \right\} & \text{if } \boldsymbol{x} \in \mathcal{U}_t(h_t) \end{cases}. \tag{50}$$

  Choose $\tilde{\boldsymbol{x}}_t = \underset{\boldsymbol{x} \in \mathcal{X}}{\arg\max} \left[\alpha_t^{(\mathrm{CP})}(\boldsymbol{x}) \times \alpha^{(\mathrm{CI})}_{t,\mathrm{mod}}(\boldsymbol{x})\right]$

  if $\alpha_t^{(\mathrm{CP})}(\tilde{\boldsymbol{x}}_t) \times \alpha^{(\mathrm{CI})}_{t,\mathrm{mod}}(\tilde{\boldsymbol{x}}_t) \leq \eta \left[\mathrm{ucb}_t^{(f)}(\tilde{\boldsymbol{x}}_t) - \mathrm{lcb}_t^{(f)}(\tilde{\boldsymbol{x}}_t)\right]$ **then**

    Choose $\boldsymbol{x}_t$ as $\boldsymbol{x}_t = \tilde{\boldsymbol{x}}_t$.

  else

    Choose $\boldsymbol{x}_t$ as $\boldsymbol{x}_t \in \underset{\boldsymbol{x} \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)}{\arg\max} \mathrm{ucb}_t^{(f)}(\boldsymbol{x})$.

  end if

  Obtain success label $c_t \sim \mathrm{Bernoulli}(g(\boldsymbol{x}_t))$.

  if $c_t = 1$ **then**

    Observe $y_t = f(\boldsymbol{x}_t) + \epsilon_t$.

  end if

end for

1. *For at most step $\overline{T}_2$, $n_t \geq 1$ holds, where $\overline{T}_2$ is the smallest natural number t that satisfies*

$$(3 - e)\left[\frac{\min\{s_0, \overline{g}\}}{1 - \tau}(t^{1-\tau} - 1) - \sqrt{Ct\beta_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda^{(\tilde{g})})}\right] - \ln\frac{2\pi^2 t^2}{3\delta} \geq 1. \tag{51}$$

Here, $C = \sqrt{8/\ln(1 + \lambda^{(\tilde{g})-1})}$ and $\overline{g} = \max_{\boldsymbol{x} \in \mathcal{X}} g(\boldsymbol{x})$.

2. *The following holds:*

$$r_T = \mathcal{O}\left(\frac{\overline{T}_3 B_f}{T^{1-\tau}} + \frac{\eta}{\zeta}\sqrt{\frac{\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})}{T^{1-\tau}}}\right), \tag{52}$$

where $\overline{T}_3 = (g^{-1}(\boldsymbol{x}^*)s_0)^{1/\tau}$.

The above theorem shows $\mathcal{O}\left(\eta\zeta^{-1}\sqrt{\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})/T^{1-\tau}}\right)$ of the regret, which worsen $\mathcal{O}\left(\sqrt{\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})/T^{1-\tau}}\right)$ of SF-GP-UCB by factor $\eta\zeta^{-1} \geq 1$. This theoretical result contradicts the results of our numerical experiments that the practical performance of SF-CBI tends to outperform that of SF-GP-UCB. Filling this gap between theory and practice is an important direction of future research. However, we believe it is also useful to show some extent of convergence of SF-CBI.

D.2 Proof of Theorem D.1

Proof of Theorem D.1. By the definition of $\alpha_t^{(\mathrm{CP})}$ and $\alpha_{t,\mathrm{mod}}^{(\mathrm{CI})}$, the query points $\boldsymbol{x}_t$ of Algorithm 3 satisfy $\boldsymbol{x}_t \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)$ for any t. By taking union bound, the events (40)–(42) simultaneously holds with probability at least $1-\delta$. Hereafter, we consider to show that the statement 1 and statement 2 of Theorem D.1 hold under the events (40)–(42). The statement 1 of Theorem D.1 clearly holds from the definition of $\overline{T}_2$ and the event (42). Next, we show the statement 2. Let us define $\boldsymbol{x}_{h_t}^*$ as $\boldsymbol{x}_{h_t}^* = \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{H}(h_t)} f(\boldsymbol{x})$, where $\mathcal{H}(h_t) = \{\boldsymbol{x} \in \mathcal{X} \mid g(\boldsymbol{x}) \geq h_t\}$. Furthermore, let us fix any index $t \leq T$ that satisfies $c_t = 1$. Then, if $\boldsymbol{x}_t = \tilde{\boldsymbol{x}}_t$,

$$
\begin{aligned}
f(\boldsymbol{x}_{h_t}^*) - \max_{i \leq T; c_i = 1} f(\boldsymbol{x}_i) &\leq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}_{h_t}^*) - \hat{f}_{t,\mathrm{mod}}^* && (53)\\
&\leq \max\left\{\mathrm{ucb}_t^{(f)}(\boldsymbol{x}_{h_t}^*) - \hat{f}_{t,\mathrm{mod}}^*, 0\right\} && (54)\\
&= \alpha_{t,\mathrm{mod}}^{(\mathrm{CI})}(\boldsymbol{x}_{h_t}^*) && (55)\\
&\leq \zeta^{-1}\alpha_{t,\mathrm{mod}}^{(\mathrm{CI})}(\boldsymbol{x}_{h_t}^*) \times \alpha_t^{(\mathrm{CP})}(\boldsymbol{x}_{h_t}^*) && (56)\\
&\leq \zeta^{-1}\alpha_{t,\mathrm{mod}}^{(\mathrm{CI})}(\boldsymbol{x}_t) \times \alpha_t^{(\mathrm{CP})}(\boldsymbol{x}_t) && (57)\\
&\leq \zeta^{-1}\eta\left[\mathrm{ucb}_t^{(f)}(\boldsymbol{x}_t) - \mathrm{lcb}_t^{(f)}(\boldsymbol{x}_t)\right] && (58)\\
&\leq 2\zeta^{-1}\eta\beta_{f,t}^{1/2}\sigma_{t-1}^{(f)}(\boldsymbol{x}_t). && (59)
\end{aligned}
$$

where Eq. (56) follows since $\alpha_t^{(\mathrm{CP})}(\boldsymbol{x}) \geq \zeta$ holds from the definition of $\alpha_t^{(\mathrm{CP})}$. If $\boldsymbol{x}_t \in \mathrm{argmax}_{\boldsymbol{x} \in \mathcal{H}_t(h_t) \cup \mathcal{U}_t(h_t)} \mathrm{ucb}_t^{(f)}(\boldsymbol{x})$,

$$
\begin{aligned}
f(\boldsymbol{x}_{h_t}^*) - \max_{i \leq T; c_i = 1} f(\boldsymbol{x}_i) &\leq f(\boldsymbol{x}_{h_t}^*) - f(\boldsymbol{x}_t) && (60)\\
&\leq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}_t) - \mathrm{lcb}_t^{(f)}(\boldsymbol{x}_t) && (61)\\
&\leq 2\zeta^{-1}\eta\beta_{f,t}^{1/2}\sigma_{t-1}^{(f)}(\boldsymbol{x}_t). && (62)
\end{aligned}
$$

Therefore, we have $f(\boldsymbol{x}_{h_t}^*) - \max_{i \leq T; c_i = 1} f(\boldsymbol{x}_i) \leq 2\zeta^{-1}\eta\beta_{f,t}^{1/2}\sigma_{t-1}^{(f)}(\boldsymbol{x}_t)$. By taking the arithmetic mean, we have

$$
\frac{1}{n_T}\sum_{t \in \mathcal{I}_T^{(s)}}\left[f(\boldsymbol{x}_{h_t}^*) - \max_{i \leq T; c_i = 1} f(\boldsymbol{x}_i)\right] \leq \frac{2\eta\beta_{f,T}^{1/2}}{\zeta n_t}\sum_{t \in \mathcal{I}_T^{(s)}}\sigma_{t-1}^{(f)}(\boldsymbol{x}_t) \leq \frac{\eta}{\zeta}\sqrt{\frac{8\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})}{n_T \ln(1+\lambda^{(f)-1})}}, \tag{63}
$$

where the last inequality follows by applying Lemma A.3. Finally, by using Eq. (39), (42), and (63), we obtain

$$
\begin{aligned}
f(\boldsymbol{x}^*) - \max_{i \leq T; c_i = 1} f(\boldsymbol{x}_i) &= \frac{1}{n_T}\sum_{t \in \mathcal{I}_T^{(s)}}\left[f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{h_t}^*)\right] + \frac{1}{n_T}\sum_{t \in \mathcal{I}_T^{(s)}}\left[f(\boldsymbol{x}_{h_t}^*) - \max_{i \leq T; c_i = 1} f(\boldsymbol{x}_i)\right] && (64)\\
&\leq \frac{2\overline{T}_3 B_f}{n_T} + \frac{\eta}{\zeta}\sqrt{\frac{8\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})}{n_T \ln(1+\lambda^{(f)-1})}} && (65)\\
&= \mathcal{O}\left(\frac{\overline{T}_3 B_f}{T^{1-\tau}} + \frac{\eta}{\zeta}\sqrt{\frac{\beta_{f,T}\gamma_T^{(f)}(\lambda^{(f)})}{T^{1-\tau}}}\right). && (66)
\end{aligned}
$$

□

E PROOF OF THEOREM 5.1

Instead of Theorem 5.1, we describe the proof of the following detailed version of Theorem 5.1.

Theorem E.1 (Detailed version of Theorem 5.1)**.** *Let k_f and $k_{\tilde{g}}$ be Matérn kernels, whose smoothness parameters are $\nu_f > 1/2$ and $\nu_{\tilde{g}} > 1/2$, respectively. Suppose Assumptions 2.1–2.3 holds. Furthermore, let $\delta \in (0,1)$, $s_0 > 0$,* *and* $\tau \in (0, \min\{\nu_f/(\nu_f + d), \nu_{\tilde{g}}/(2\nu_{\tilde{g}} + 2d)\})$*. Moreover, let us respectively define* $\lambda_{f,t}$*,* $\lambda_{\tilde{g},t}$*,* $\beta_{f,t}$*, and* $\beta_{\tilde{g},t}$ *as*

$$\lambda_{f,t} = t^{1/(1+\psi_f)}, \lambda_{\tilde{g},t} = t^{1/(1+\psi_{\tilde{g}})}, \tag{67}$$

$$\beta_{f,t}^{1/2} = B_f + \sigma\lambda_{f,t}^{-1/2}\sqrt{2(\gamma_t^{(f)}(\lambda_{f,t}) + \ln((t^2\pi^2)/(3\delta)))}, \tag{68}$$

$$\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \lambda_{\tilde{g},t}^{-1/2}\sqrt{0.5[\gamma_t^{(\tilde{g})}(\lambda_{\tilde{g},t}) + \ln((2t^2\pi^2)/(3\delta))]}, \tag{69}$$

where $\psi_f = (2\nu_f + d)/d$ *and* $\psi_{\tilde{g}} = (2\nu_{\tilde{g}} + d)/d$*. Then, when running Algorithm 1, the following two statements simultaneously hold with probability at least* $1 - \delta$*:*

- *For at most step* $\overline{T}_4$*,* $n_t \geq 1$ *holds, where* $\overline{T}_4$ *is the smallest natural number* t *that satisfies*

$$(3 - e)\left[\frac{\min\{s_0, \overline{g}\}}{1 - \tau}(t^{1-\tau} - 1) - 4\sqrt{\tilde{\beta}_{\tilde{g},t}\lambda_{\tilde{g},t}\gamma_t^{(\tilde{g})}(\lambda_{\tilde{g},t})}\right] - \ln\frac{2\pi^2 t^2}{3\delta} \geq 1. \tag{70}$$

  Here, $\overline{g} = \max_{\boldsymbol{x}\in\mathcal{X}} g(\boldsymbol{x})$*.*

- *For any* $T \geq \overline{T}_4$*, the following regret upper bounds of SF-CBI holds:*

$$r_T \leq \mathcal{O}\left(\frac{B\overline{T}_3}{T^{1-\tau}} + \sqrt{\frac{\tilde{\beta}_{f,T}\lambda_{f,T}\gamma_T^{(f)}(\lambda_{f,T})}{T^{1-\tau}}}\right) = \mathcal{O}^*\left(\frac{B\overline{T}_3}{T^{1-\tau}} + T^{\frac{d}{2\nu_f+2d} - \frac{1-\tau}{2}}\right), \tag{71}$$

  where $\overline{T}_3 = [g^{-1}(\boldsymbol{x}^*)s_0]^{1/\tau}$*.*

Here, $\beta_{\tilde{g},t}$ *and* $\beta_{f,t}$ *are respectively defined as*

$$\tilde{\beta}_{\tilde{g},t}^{1/2} = B_g + \frac{1}{\sqrt{2}}\sqrt{C_g^{1/\psi_{\tilde{g}}}\ln\left(1 + T^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)}\right)\ln^{-1/\psi_{\tilde{g}}} 2 + \left[\ln\left(1 + T^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)}\right) + \ln\frac{2\pi^2T^2}{3\delta}\right]}, \tag{72}$$

$$\tilde{\beta}_{f,t}^{1/2} = B_f + \frac{\sigma}{\sqrt{2}}\sqrt{C_f^{1/\psi_f}\ln\left(1 + T^{\psi_f/(\psi_f+1)}\right)\ln^{-1/\psi_f} 2 + \left[\ln\left(1 + T^{\psi_f/(\psi_f+1)}\right) + \ln\frac{2\pi^2T^2}{3\delta}\right]}. \tag{73}$$

Furthermore, $C_g > 0$ *and* $C_f > 0$ *are constants that depend on* ℓ *of* $k_{\tilde{g}}$ *and* k_f*, respectively.*

We first start by giving the versions of Lemma A.2 and Lemma A.3 when the regularization parameters are adaptively chosen.

Lemma E.2. *Suppose* $1 \leq \lambda_{\tilde{g},t} \leq \lambda_{\tilde{g},t+1}$ *holds for any* $t \in \mathbb{N}_+$*. Then, for any* $T \in \mathbb{N}_+$*,*

$$\sum_{t=1}^{T}\sigma_{\tilde{g},t-1}(\boldsymbol{x}_t) \leq \sqrt{4\lambda_{\tilde{g},T}T\gamma_T^{(\tilde{g})}(\lambda_{\tilde{g},T})}. \tag{74}$$

Lemma E.3. *Suppose* $1 \leq \lambda_{f,t} \leq \lambda_{f,t+1}$ *holds for any* $t \in \mathbb{N}_+$*. Then, for any* $T \in \mathbb{N}_+$*,*

$$\sum_{t\in\mathcal{I}_T^{(s)}}\sigma_{f,t-1}(\boldsymbol{x}_t) \leq \sqrt{4\lambda_{f,T}n_T\gamma_{n_T}^{(f)}(\lambda_{f,T})}. \tag{75}$$

The above lemmas directly follow from Lemma 4 in Chowdhury and Gopalan [2017] and the fact that $\sigma_{\tilde{g},t-1}(\boldsymbol{x}_t)$ is monotonically increasing as a function of $\lambda_{\tilde{g},t}$. We also give the following Lemma E.4, which gives the confidence bounds of f with adaptive $\lambda_{f,t}$.

Lemma E.4 (Confidence bounds of f for adaptive $\lambda_{f,t}$)**.** *Suppose Assumptions 2.1–2.2 hold. Furthermore, let us define* $\beta_{f,t}$ *as*

$$\beta_{f,t}^{1/2} = B_f + \frac{\sigma}{\lambda_{f,t}^{1/2}}\sqrt{2\left[\gamma_t^{(f)}(\lambda_{f,t}) + \ln\frac{\pi^2t^2}{6\delta}\right]} \tag{76}$$

with any $\delta \in (0, 1)$*. Then, the following holds with probability at least* $1 - \delta$*:*

$$\forall t \in \mathbb{N}_+,\ \forall\boldsymbol{x} \in \mathcal{X},\ \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \leq f(\boldsymbol{x}) \leq \mathrm{ucb}_t^{(f)}(\boldsymbol{x}). \tag{77}$$

Proof. From Lemma A.1, for any $t \in \mathbb{N}_+$, the following holds with probability at least $1 - 6\delta/(\pi^2 t^2)$:

$$\forall \boldsymbol{x} \in \mathcal{X},\ \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \le f(\boldsymbol{x}) \le \mathrm{ucb}_t^{(f)}(\boldsymbol{x}). \tag{78}$$

By taking union bounds, with probability at least $1 - \sum_{t \in \mathbb{N}_+} 6\delta/(\pi^2 t^2) := 1 - \delta$:

$$\forall t \in \mathbb{N}_+,\ \forall \boldsymbol{x} \in \mathcal{X},\ \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \le f(\boldsymbol{x}) \le \mathrm{ucb}_t^{(f)}(\boldsymbol{x}). \tag{79}$$

□

Similarly, the following Lemma E.5 are obtained by resorting to the same arguments in proof of Lemma E.4.

Lemma E.5 (Confidence bounds of $\tilde{g}$ for adaptive $\lambda_{\tilde{g},t}$)**.** *Suppose Assumption 2.3 holds. Furthermore, let us define $\beta_{\tilde{g},t}$ as*

$$\beta_{\tilde{g},t}^{1/2} = B_{\tilde{g}} + \frac{1}{\lambda_{\tilde{g},t}^{1/2}} \sqrt{0.5 \left[\gamma_t^{(\tilde{g})}(\lambda_{\tilde{g},t}) + \ln \frac{\pi^2 t^2}{6\delta} \right]} \tag{80}$$

with any $\delta \in (0,1)$. Then, the following holds with probability at least $1-\delta$:

$$\forall t \in \mathbb{N}_+,\ \forall \boldsymbol{x} \in \mathcal{X},\ \mathrm{lcb}_t^{(g)}(\boldsymbol{x}) \le g(\boldsymbol{x}) \le \mathrm{ucb}_t^{(g)}(\boldsymbol{x}). \tag{81}$$

Proof of Theorem 5.1. Suppose the following three events simultaneously hold:

$$\begin{aligned}
&\forall T \in \mathbb{N}_+,\ n_T \ge (3-e) \sum_{t=1}^{T} g(\boldsymbol{x}_t) - \ln \frac{2\pi^2 T^2}{3\delta}, \\
&\forall t \in \mathbb{N}_+,\ \forall \boldsymbol{x} \in \mathcal{X},\ \mathrm{lcb}_t^{(f)}(\boldsymbol{x}) \le f(\boldsymbol{x}) \le \mathrm{ucb}_t^{(f)}(\boldsymbol{x}), \\
&\forall t \in \mathbb{N}_+,\ \forall \boldsymbol{x} \in \mathcal{X},\ \mathrm{lcb}_t^{(g)}(\boldsymbol{x}) \le g(\boldsymbol{x}) \le \mathrm{ucb}_t^{(g)}(\boldsymbol{x}).
\end{aligned} \tag{82}$$

Then, by resorting to the same arguments of Lemma B.3, we have

$$n_T \ge (3-e) \left[\min\{s_0, \overline{g}\} \frac{T^{1-\tau} - 1}{1-\tau} - 2 \sum_{t=1}^{T} \beta_{\tilde{g},t}^{1/2} \sigma_{\tilde{g},t-1}(\boldsymbol{x}_t) \right] - \ln \frac{2\pi^2 T^2}{3\delta}. \tag{83}$$

Here, note that $\beta_{\tilde{g},t}$ are not monotonically increasing since the regularization parameters $\lambda_{\tilde{g},t}$ are chosen adaptively depending on t. For any natural number $t \le T$, we further derive the upper bounds of $\beta_{\tilde{g},t}$ as

$$\beta_{\tilde{g},t}^{1/2} \tag{84}$$

$$= B_{\tilde{g}} + \frac{1}{\lambda_{\tilde{g},t}^{1/2}} \sqrt{0.5 \left(\gamma_t^{(\tilde{g})}(\lambda_{\tilde{g},t}) + \ln \frac{2t^2\pi^2}{3\delta} \right)} \tag{85}$$

$$\le B_{\tilde{g}} + \sqrt{\frac{1}{2t^{1/(\psi_{\tilde{g}}+1)}} \left(\left(\frac{C_g t}{\lambda_{\tilde{g},t}} \right)^{1/\psi_{\tilde{g}}} \ln^{-1/\psi_{\tilde{g}}} \left(1 + \frac{t}{\lambda_{\tilde{g},t}} \right) + 1 \right) \ln \left(1 + \frac{t}{\lambda_{\tilde{g},t}} \right) + \frac{1}{2t^{1/(\psi_{\tilde{g}}+1)}} \ln \frac{2\pi^2 t^2}{3\delta}} \tag{86}$$

$$= B_{\tilde{g}} + \sqrt{\frac{1}{2t^{1/(\psi_{\tilde{g}}+1)}} \left(C_g^{1/\psi_{\tilde{g}}} t^{1/(\psi_{\tilde{g}}+1)} \ln^{-1/\psi_{\tilde{g}}} \left(1 + t^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) + 1 \right) \ln \left(1 + t^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) + \frac{1}{2t^{1/(\psi_{\tilde{g}}+1)}} \ln \frac{2\pi^2 t^2}{3\delta}} \tag{87}$$

$$= B_{\tilde{g}} + \sqrt{\frac{1}{2} C_g^{1/\psi_{\tilde{g}}} \ln^{-1/\psi_{\tilde{g}}} \left(1 + t^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) \ln \left(1 + t^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) + \frac{1}{2t^{1/(\psi_{\tilde{g}}+1)}} \left(\ln \left(1 + t^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) + \ln \frac{2\pi^2 t^2}{3\delta} \right)} \tag{88}$$

$$\le B_g + \frac{1}{\sqrt{2}} \sqrt{C_g^{1/\psi_{\tilde{g}}} \ln \left(1 + T^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) \ln^{-1/\psi_{\tilde{g}}} 2 + \left(\ln \left(1 + T^{\psi_{\tilde{g}}/(\psi_{\tilde{g}}+1)} \right) + \ln \frac{2\pi^2 T^2}{3\delta} \right)} \tag{89}$$

$$:= \tilde{\beta}_{\tilde{g},t}^{1/2}. \tag{90}$$

Similarly, $\beta_{f,t}^{1/2} \leq \tilde{\beta}_{f,t}^{1/2}$ also holds. From the definition of $\tilde{\beta}_{\tilde{g},t}^{1/2}$, $\tilde{\beta}_{\tilde{g},t}^{1/2}$ are monotonically increasing. Therefore, from Eq. (83), we have

$$n_T \geq (3-e)\left[\min\{s_0, \overline{g}\}\frac{T^{1-\tau}-1}{1-\tau} - 2\tilde{\beta}_{\tilde{g},T}^{1/2}\sum_{t=1}^{T}\sigma_{\tilde{g},t-1}(\boldsymbol{x}_t)\right] - \ln\frac{2\pi^2T^2}{3\delta} \tag{91}$$

$$\Rightarrow n_T \geq (3-e)\left[\min\{s_0, \overline{g}\}\frac{T^{1-\tau}-1}{1-\tau} - 4\sqrt{\tilde{\beta}_{\tilde{g},T}\lambda_{\tilde{g},T}T\gamma_T^{(g)}(\lambda_{\tilde{g},T})}\right] - \ln\frac{2\pi^2T^2}{3\delta} \tag{92}$$

$$\Rightarrow n_T \geq (3-e)\left[\min\{s_0, \overline{g}\}\frac{T^{1-\tau}-1}{1-\tau} - 4\sqrt{\tilde{\beta}_{\tilde{g},T}T^{(2+\psi_{\tilde{g}})/(1+\psi_{\tilde{g}})}\gamma_T^{(\tilde{g})}(\lambda_{\tilde{g},T})}\right] - \ln\frac{2\pi^2T^2}{3\delta}. \tag{93}$$

Here, $\sqrt{\tilde{\beta}_{\tilde{g},T}T^{(2+\psi_{\tilde{g}})/(1+\psi_{\tilde{g}})}\gamma_T^{(\tilde{g})}(\lambda_{\tilde{g},T})} = \mathcal{O}^*(T^{(3+\psi_{\tilde{g}})/(2+2\psi_{\tilde{g}})}) = \mathcal{O}^*(T^{(\nu_{\tilde{g}}+2d)/(2\nu_{\tilde{g}}+2d)})$ holds since $\gamma_T^{(\tilde{g})}(\lambda_{\tilde{g},T}) = \mathcal{O}^*(T^{1/(\psi_{\tilde{g}}+1)})$. Therefore, if we set τ as $\tau < 1-(\nu_{\tilde{g}}+2d)/(2\nu_{\tilde{g}}+2d) = \nu_{\tilde{g}}/(2\nu_{\tilde{g}}+2d)$, $n_T = \Omega(T^{1-\tau})$. This implies that the natural number $\overline{T}_4$ exists.

Then, for any $T \geq \overline{T}_4$,

$$r_T = \frac{1}{n_T}\sum_{t\in\mathcal{I}_T^{(s)}}\left[f(\boldsymbol{x}^*) - f(\boldsymbol{x}_{h_t}^*)\right] + \frac{1}{n_T}\sum_{t\in\mathcal{I}_T^{(s)}}\left[f(\boldsymbol{x}_{h_t}^*) - \max_{t\leq T; c_t=1} f(\boldsymbol{x}_t)\right] \tag{94}$$

$$\leq \frac{2B\overline{T}_3}{n_T} + \frac{2}{n_T}\sum_{t\in\mathcal{I}_T^{(s)}}\beta_{f,t}^{1/2}\sigma_{f,t-1}(\boldsymbol{x}_t) \tag{95}$$

$$\leq \frac{2B\overline{T}_3}{n_T} + \frac{2\tilde{\beta}_{f,T}^{1/2}}{n_T}\sum_{t\in\mathcal{I}_T^{(s)}}\sigma_{f,t-1}(\boldsymbol{x}_t) \tag{96}$$

$$\leq \frac{2B\overline{T}_3}{n_T} + 4\sqrt{\frac{\tilde{\beta}_{f,T}\lambda_{f,T}\gamma_T^{(f)}(\lambda_{f,T})}{n_T}}. \tag{97}$$

Since $n_T = \Omega(T^{1-\tau})$,

$$r_T = \mathcal{O}\left(\frac{B\overline{T}_3}{T^{1-\tau}} + \sqrt{\frac{\tilde{\beta}_{f,T}\lambda_{f,T}\gamma_T^{(f)}(\lambda_{f,T})}{T^{1-\tau}}}\right) \tag{98}$$

$$= \mathcal{O}^*\left(\frac{B\overline{T}_3}{T^{1-\tau}} + T^{\frac{d}{2\nu_f+2d} - \frac{1-\tau}{2}}\right). \tag{99}$$

Finally, by noting that the events (82) simultaneously hold with probability at least $1-\delta$, we complete the proof. □

F DETAILS OF SECTION 6

F.1 Details of Test Functions

In this subsection, we describe the details of test functions we use in Sec. 6.

1D-synthetic Functions The objective function $f_{1\mathrm{D}} : [0,1] \to \mathbb{R}$, which is depicted as blue line in Fig. 6, is defined as follows:

$$f_{1\mathrm{D}}(x) = \frac{3}{2}\left[x^{1/4}\sin(15x) - \frac{1}{10}\right]. \tag{100}$$

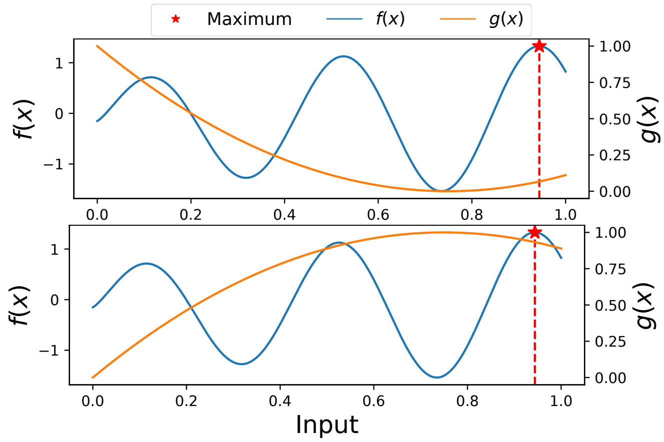

Figure 6: The 1D synthetic functions of experiments.

Furthermore, let $g_{\mathrm{1D-low}} : [0, 1] \to [0, 1]$ and $g_{\mathrm{1D-high}} : [0, 1] \to [0, 1]$ be the success functions depicted in the top and bottom of Fig. 6, respectively. The functions $g_{\mathrm{1D-low}}$ and $g_{\mathrm{1D-high}}$ are respectively defined as

$$g_{\mathrm{1D-low}}(x) = \frac{16}{9}\left(\frac{3}{4} - x\right)^2, \tag{101}$$

$$g_{\mathrm{1D-high}}(x) = 1 - \frac{16}{9}\left(\frac{3}{4} - x\right)^2. \tag{102}$$

2D-RKHS Test Functions As described in Sec. 6, we make 10 test functions generated from the GP sample path. To generate the test function, we use SE kernel and Matérn5/2 kernel, whose kernel hyperparameter ℓ is set as 0.3. When we generate success function g from the GP sample path, to prevent the output range from violating $[0, 1]$, we rescale the originally generated function g_{org} as

$$g(\boldsymbol{x}) = \frac{g_{\mathrm{org}}(\boldsymbol{x}) - \min_{\boldsymbol{x} \in \mathcal{X}} g_{\mathrm{org}}(\boldsymbol{x})}{\max_{\boldsymbol{x} \in \mathcal{X}} g_{\mathrm{org}}(\boldsymbol{x}) - \min_{\boldsymbol{x} \in \mathcal{X}} g_{\mathrm{org}}(\boldsymbol{x})}. \tag{103}$$

Hartmann The objective function $f_{\mathrm{Hartmann}} : [0, 1]^3 \to \mathbb{R}$ is given as follows:

$$f_{\mathrm{Hartmann}}(\mathbf{x}) = \sum_{i=1}^{4} \alpha_i \exp\left(-\sum_{j=1}^{3} A_{ij}\left(x_j - P_{ij}\right)^2\right), \quad \text{where} \tag{104}$$

$$\alpha = (1.0, 1.2, 3.0, 3.2)^\top, \tag{105}$$

$$\boldsymbol{A} = \begin{pmatrix} 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \\ 3.0 & 10 & 30 \\ 0.1 & 10 & 35 \end{pmatrix}, \tag{106}$$

$$\boldsymbol{P} = 10^{-4}\begin{pmatrix} 3689 & 1170 & 2673 \\ 4699 & 4387 & 7470 \\ 1091 & 8732 & 5547 \\ 381 & 5743 & 8828 \end{pmatrix}. \tag{107}$$

The success function $g_{\mathrm{Hartmann}} : [0, 1]^3 \to [0, 1]$ is defined as follows:

$$g_{\mathrm{Hartmann}}(\boldsymbol{x}) = \Phi\left(-\frac{\tilde{g}_{\mathrm{Hartmann}}(\boldsymbol{x})}{0.25}\right), \tag{108}$$

where $\Phi(\cdot)$ is the cumulative distribution function of standard normal distribution. Furthermore, $\tilde{g}_{\mathrm{Hartmann}}$ is the original constraint function, which is defined as

$$\tilde{g}_{\mathrm{Hartmann}}(\boldsymbol{x}) = \|\boldsymbol{x}\|_2 - 1. \tag{109}$$

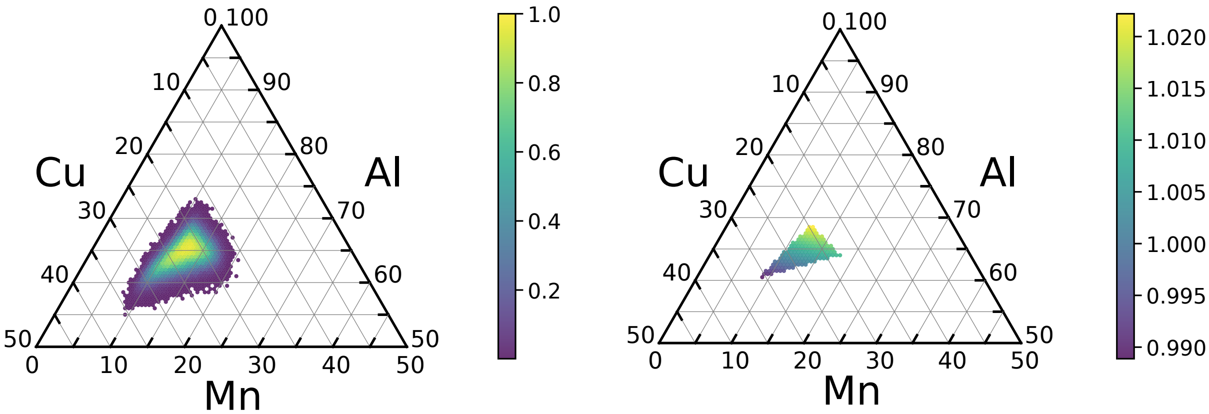

Figure 7: Simulation function for the quasi-crystal is shown. Left: probability of successful observation for the specified input composition for non-zero probability computed over 1,000 MC experiments at each point. Right: objective function to be maximized for the actual input composition. Note that the spread of the probability on the left-hand side can be understood in terms of the migration from the specified composition to the actual composition. If the actual composition falls inside the range of quasi-crystal synthesis, a successful observation can be made.

Gardner The objective function $f_{\text{Gardner}} : [0,1]^2 \to \mathbb{R}$ and the success function $g_{\text{Gardner}} : [0,1]^2 \to [0,1]$ are respectively defined as

$$f_{\text{Gardner}}(\boldsymbol{x}) = -\tilde{f}_{\text{Gardner}}(6\boldsymbol{x}),\ g(\boldsymbol{x}) = \Phi\left(-\frac{\tilde{g}_{\text{Gardner}}(6\boldsymbol{x})}{0.25}\right), \tag{110}$$

where $\tilde{f}_{\text{Gardner}}$ and $\tilde{g}_{\text{Gardner}}$ are original objective and constraint functions, which are given as follows:

$$\tilde{f}_{\text{Gardner}}(x_1, x_2) = \cos(2x_1)\cos(x_2) + \sin(x_1), \tag{111}$$

$$\tilde{g}_{\text{Gardner}}(x_1, x_2) = \cos(x_1)\cos(x_2) - \sin(x_1)\sin(x_2) - 0.5. \tag{112}$$

Simulation Function of Quasi-Crystal The quasi-crystal simulation function is defined following the work by Iwazaki et al. [2023]. We consider the formation quasi-crystal in the Al-Cu-Mn ternary system. The success function $g_{\text{qc}} : [0,1]^2 \to [0,1]$ has two input variables x_{Cu} and x_{Mn} corresponding to the composition percentage, whose range is normalized to $[0,1]^2$. Their original search ranges are defined as $20 < x_{\text{Cu,org}} < 25$, $10 < x_{\text{Mn,org}} < 15$, and the remaining Al percentage is fixed by $x_{\text{Al,org}} + x_{\text{Cu,org}} + x_{\text{Mn,org}} = 100$; then, we normalize $x_{\text{Cu,org}}$ and $x_{\text{Mn,org}}$ to $[0,1]$. We presume there exist experimental errors so that the actual composition deviates from the specified composition. We assign a normal distributed error with a standard deviation of 5% relative to the specified composition. The success of the experiment is defined as the successful formation of the quasi-crystal under the specified composition. The deterministic successful region is defined using real data [Grushko and Mi, 2016]. From this successful region and normally distributed error, the success function is defined and is illustrated on the left of Fig. 7. The objective function $f_{\text{ptc}} : [0,1]^2 \to \mathbb{R}$ to be maximized is defined as a heuristic function for the phonon thermal conductivity of quasi-crystals using data from Takagiwa et al. [2021]. The right plot of Fig. 7 depicts the objective function.

F.2 Details of Algorithms

We describe the details of the algorithms that are used in Sec. 6.

GP-UCB At each step t, GP-UCB choose the query point $\boldsymbol{x}_t$ as $\boldsymbol{x}_t \in \operatorname{argmax}_{\boldsymbol{x} \in \mathcal{X}} \text{ucb}_t^{(f)}(\boldsymbol{x})$. This is an application of standard GP-UCB to our setting by simply ignoring failures. We set the width parameter $\beta_{t,f}^{1/2}$ of confidence bound as $\beta_{t,f}^{1/2} = 2\ln 2(n_t + 1)$.

EFIGPC At each step t, EFIGPC choose the query point $\boldsymbol{x}_t$ as $\boldsymbol{x}_t \in \operatorname{argmax}_{\boldsymbol{x} \in \mathcal{X}} P_{t,\text{GPC}}(\boldsymbol{x}) \times \text{EI}(\boldsymbol{x})$, where $P_{t,\text{GPC}}(\boldsymbol{x})$ is a posterior probability of GPC at step t with expectation propagation-based approximation.

Furthermore, $\mathrm{EI}(\boldsymbol{x})$ represent an EI at input $\boldsymbol{x}$ whose current best value y_t^* at step t is defined as $y_t^* = \max_{i \in \mathcal{I}_{t-1}^{(s)}} y_i$.

PenalizedEI At each step t, PenalizedEI choose the query point $\boldsymbol{x}_t$ as the maximum point of EI. If the failure occurs at any step t, the algorithm compute imputed value $\overline{y}_t$ as $\overline{y}_t = \overline{\mathrm{lcb}}_t^{(f)}(\boldsymbol{x}_t)$, and update $\overline{\mu}_{f,t}$ and $\overline{\sigma}_{f,t}$. Here, we use overlined notation of $\mathrm{lcb}_t^{(f)}$, $\mu_{f,t}$ and $\sigma_{f,t}$ to distinguish original definition of $\mathrm{lcb}_t^{(f)}$, $\mu_{f,t}$ and $\sigma_{f,t}$ from those whose training outputs include imputed values. We set the width parameter of confidence bound, which is used to calculate $\overline{\mathrm{lcb}}_t^{(f)}$, as $2 \ln 2(t+1)$.

SF-GP-UCB, SF-CBI As described in Sec. 6, we set $s_0 = 0.75$ and $\zeta = 0.2$. Furthermore, we set $\tau = 1/4$ if we use SE kernel; otherwise, we set $\tau = 1/6$. Moreover, we use the width parameter of confidence bound as $\beta_{f,t}^{1/2} = 2 \ln 2(n_t + 1)$ and $\beta_{\tilde{g},t}^{1/2} = 2$, respectively.

F.3 Details of Parameter Settings

In all experiments except for the quasi-crystal simulation function, we set noise ϵ_t as $\epsilon_t \sim \mathcal{N}(0, 0.2)$. Furthermore, we set regularization parameters $\lambda_{f,t}$ and $\lambda_{\tilde{g},t}$ as $\lambda_{f,t} = \lambda_{\tilde{g},t} = 0.2$ for any $t \in \mathbb{N}_+$. We define input domain $\mathcal{X}$ as uniformly separated grid points. Table 1 shows the settings of $\mathcal{X}$, k_f, and $k_{\tilde{g}}$, which are used in each experiment.

Table 1: Parameter settings used in experiments. Note that we use the same $k_{\tilde{g}}$ for the kernel of GPC, which is leveraged in EFIGPC.

Test function name	d	Kernel type	Kernel parameters	Input domain $\mathcal{X}$
1D-synthetic	1	SE kernel	$l_f = 0.3$, $l_{\tilde{g}} = 0.3$	2000 uniform grids of $[0, 1]$
2D-RKHS (SE)	2	SE kernel	$l_f = 0.5$, $l_{\tilde{g}} = 0.5$	Products of 30 uniform grids of $[0, 1]$
2D-RKHS (Matérn 5/2)	2	Matérn 5/2	$l_f = 0.5$, $l_{\tilde{g}} = 0.5$	Products of 30 uniform grids of $[0, 1]$
Gardner	2	SE kernel	$l_f = 0.25$, $l_{\tilde{g}} = 0.5$	Products of 50 uniform grids of $[0, 1]$
Hartmann	3	SE kernel	$l_f = 0.5$, $l_{\tilde{g}} = 1.0$	Products of 20 uniform grids of $[0, 1]$
Quasi-crystal	2	SE kernel	$l_f = 0.3$, $l_{\tilde{g}} = 0.3$	Products of 50 uniform grids of $[0, 1]$

F.4 Additional Results of Sensitivity Analysis

In this subsection, we study the sensitivity against the parameter settings of SF-GP-UCB and SF-CBI through 2D-RKHS test functions.

Figures 8–10 show the results of experiments with various parameter settings of s_0, τ, and ζ, respectively. From these results, we can confirm the following:

1. The performance of our algorithms consistently has better performance than that of GP-UCB.
2. The best parameter setting in each experiment depends on the algorithm and the kernel we use; however, we cannot confirm a large performance difference between the best parameter choice and the parameter setting that we used in Sec. 6. These results show that the performances of our algorithms are not too sensitive to parameter settings, while small performance improvement is expected by parameter tuning.
3. In experiments with SE kernel, the performances of SF-GP-UCB with $s_0 = 0.5$ and $\tau = 0.40$ have a poorer performance compared to other parameter settings. From these results, the default choices of s_0 and τ, which satisfy $0.6 \leq s_0 \leq 1.0$ and $0.1 \leq \tau \leq 0.3$, are reasonable.

G DISCUSSION ABOUT PROBLEM SETTING OF OBSERVATION FAILURES

Further Potential Applications We describe further potential applications for our problem setting as follows:

- **The material discovery**: Besides the quasi-crystal problem of our numerical experiments, experiment failure is a common problem in the scientific discovery of new material. For example, Wakabayashi et al.

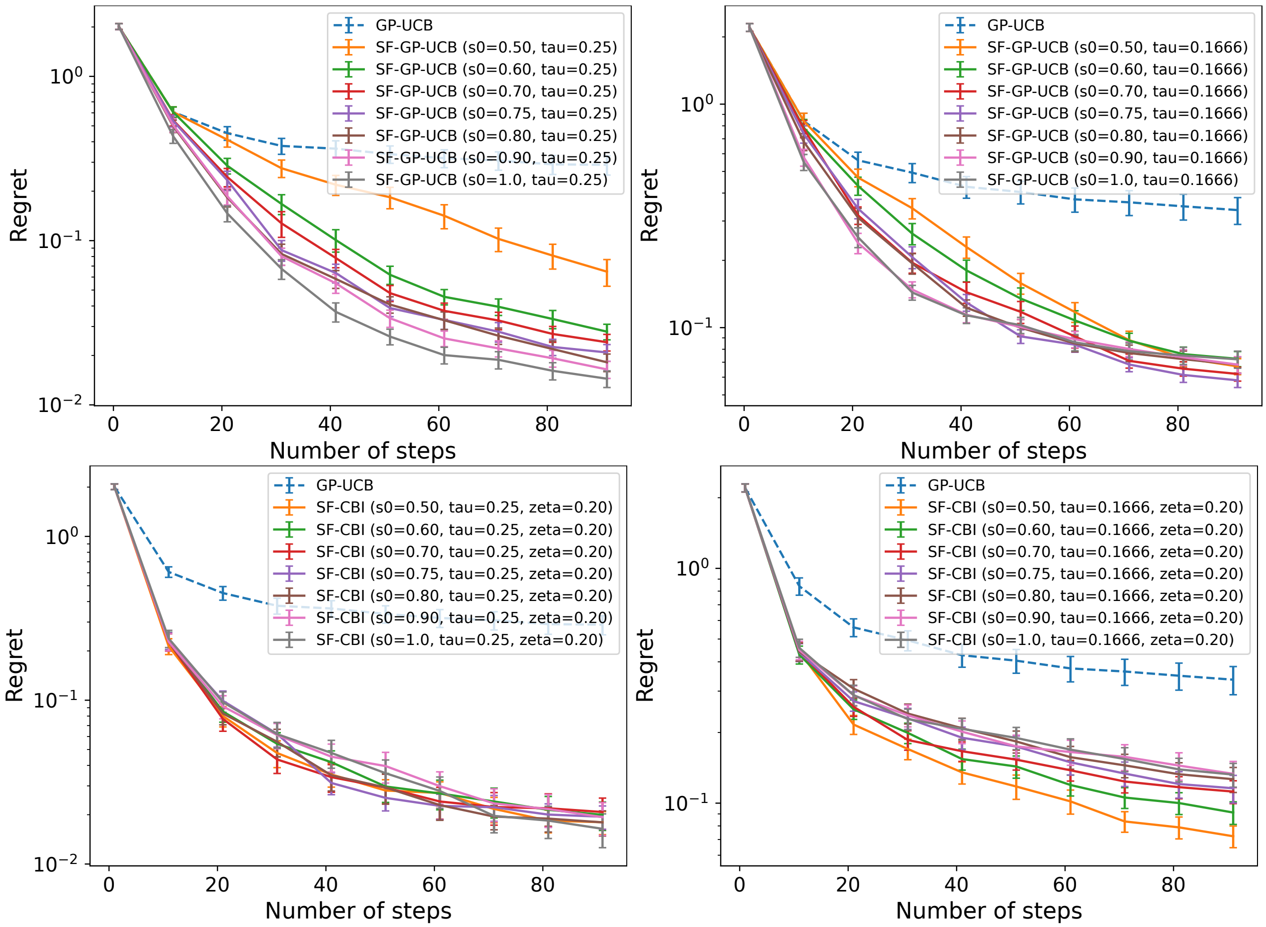

Figure 8: The results of experiments with various parameter settings of s_0. The top and bottom figures represent the results of SF-GP-UCB and SF-CBI, respectively. The left and right figures show the results with test functions, which are generated from SE and Matérn5/2 kernels, respectively.

[2022] considers the optimization problem with the same motivation as ours for the application of the material informatics field.

- **The hyperparameter tuning of complex and unstable models**: The hyperparameter tuning of the complex model may fail due to unstable behavior of learning (e.g., the divergence of the gradient, accumulation of the numerical error, etc.). If we adopt the stochastic learning algorithm for the model, the failure event occurs stochastically, and the problem setting becomes the same as ours. Here, hyperparameter tuning examples under observation failures are also discussed in Bachoc et al. [2020].
- **Robotics**: The control of the robot faces a lot of uncertainty (e.g., control error, environmental conditions, etc.); therefore, The desired results may not always be obtained by controlling the robot, but failures are bound to occur. Marco et al. [2021] considers the failure in robotics, although the problem settings are more application-specific than our formulations.

Another Formulation Motivated by the quasi-crystal synthesis problem, the formulation of this paper focuses on making the successful event for obtaining the highest output. On the other hand, some applications should focus on finding desired input whose expected corresponding output is as high as possible. For example, in the parameter tuning of the manufacturing system, the learner's goal is finding the desired parameter $\tilde{\boldsymbol{x}}^*$ so that both the resulting product quality $f(\tilde{\boldsymbol{x}}^*)$ and the success probability of $g(\tilde{\boldsymbol{x}}^*)$ of the production becomes high. To adapt such scenarios, one naive formulation is to consider the maximization of the new objective function $\tilde{f}(\boldsymbol{x}) := f(\boldsymbol{x})g(\boldsymbol{x})$ by assuming that the objective function is properly shifted as $f(\boldsymbol{x}) \geq 0$. In such formulation, we can solve the maximization problem of $\tilde{f}(\boldsymbol{x})$ within the standard GP-UCB framework under

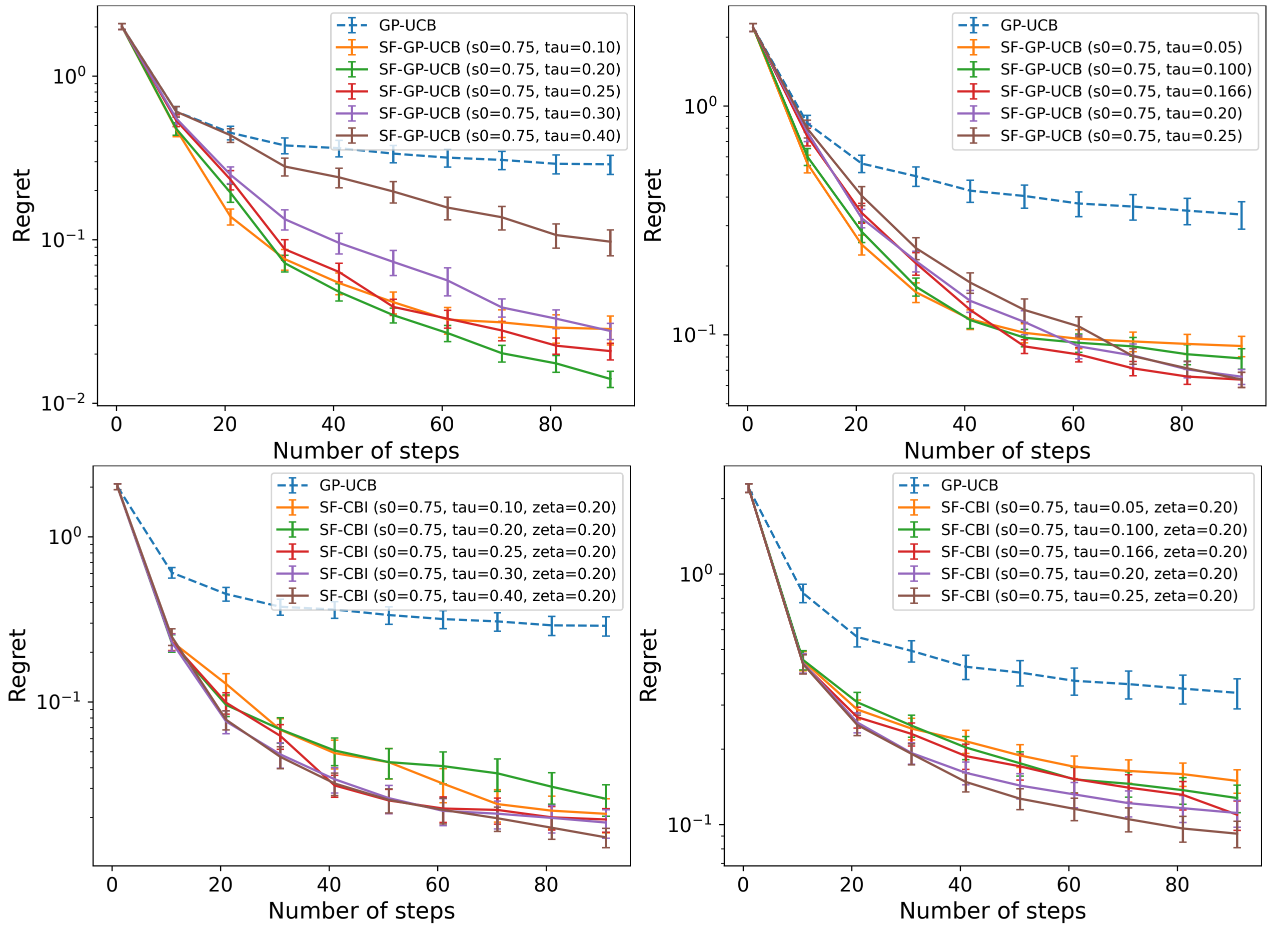

Figure 9: The results of experiments with various parameter settings of τ. The top and bottom figures represent the results of SF-GP-UCB and SF-CBI, respectively. The left and right figures show the results with test functions, which are generated from SE and Matérn5/2 kernels, respectively.

the same assumptions as our paper. Actually, since $y_t c_t$ is the unbiased estimator of $\tilde{f}(\boldsymbol{x})$, and the error term $y_t c_t - f(\boldsymbol{x})g(\boldsymbol{x})$ is σ-sub-Gaussian random variable, the valid confidence bound of $\tilde{f}(\boldsymbol{x})$ is constructed by using Lemma 3.11 in Abbasi-Yadkori [2013][2].

[2] Strictly speaking, the additional independence assumption between y_t and c_t is needed here in addition to the assumptions of our paper.

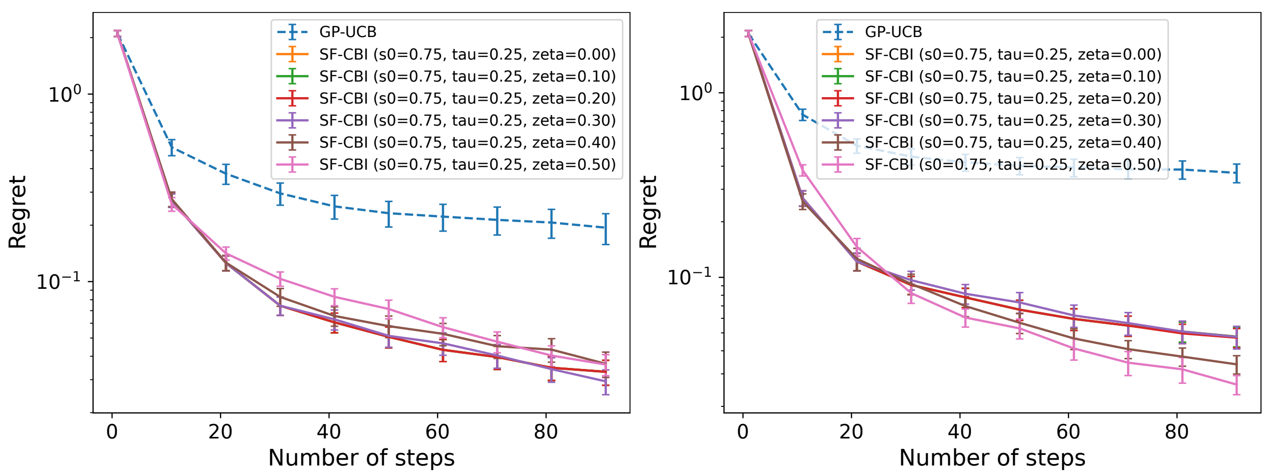

Figure 10: The results of experiments with various parameter settings of ζ. The left and right figures show the results with test functions, which are generated from SE and Matérn5/2 kernels, respectively.