Optimal Order Simple Regret for Gaussian Process Bandits

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Abstract

Consider the sequential optimization of a continuous, possibly non-convex, and expensive to evaluate objective function \( f \). The problem can be cast as a Gaussian Process (GP) bandit where \( f \) lives in a reproducing kernel Hilbert space (RKHS). The state of the art analysis of several learning algorithms shows a significant gap between the lower and upper bounds on the simple regret performance. When \( N \) is the number of exploration trials and \( \gamma_N \) is the maximal information gain, we prove an \( \tilde{O}(\sqrt{\gamma_N/N}) \) bound on the simple regret performance of a pure exploration algorithm that is significantly tighter than the existing bounds. We show that this bound is order optimal up to logarithmic factors for the cases where a lower bound on regret is known. To establish these results, we prove novel and sharp confidence intervals for GP models applicable to RKHS elements which may be of broader interest.

1 Introduction

Sequential optimization has evolved into one of the fastest developing areas of machine learning [Mazumdar et al., 2020]. We consider sequential optimization of an unknown objective function from noisy and expensive to evaluate zeroth-order\(^\dagger\) observations. That is a ubiquitous problem in academic research and industrial production. Examples of applications include exploration in reinforcement learning, recommendation systems, medical analysis tools and speech recognizers [Shahriari et al., 2016]. A notable application in the field of machine learning is automatic hyper-parameter tuning. Prevalent methods such as grid search can be prohibitively expensive [Bergstra et al., 2011, McGibbon et al., 2016]. Sequential optimization methods, on the other hand, are shown to efficiently find good hyper-parameters by an adaptive exploration of the hyper-parameter space [Falkner et al., 2018].

Our sequential optimization setting is as follows. Consider an objective function \( f \) defined over a domain \( \mathcal{X} \subset \mathbb{R}^d \), where \( d \in \mathbb{N} \) is the dimension of the input. A learning algorithm is allowed to perform an adaptive exploration to sequentially observe the potentially corrupted values of the objective function \( \{f(x_n) + \epsilon_n\}_{n=1}^N \), where \( \epsilon_n \) are random noises. At the end of \( N \) exploration trials, the learning algorithm returns a candidate maximizer \( \hat{x}_N^* \in \mathcal{X} \) of \( f \). Let \( x^* \in \text{argmax}_{x \in \mathcal{X}} f(x) \) be a true optimal solution. We may measure the performance of the learning algorithm in terms of simple regret; that is, the difference between the performance under the true optimal, \( f(x^*) \), and that under the learnt value, \( f(\hat{x}_N^*) \).

\(^\dagger\)Zeroth-order feedback signifies observations from \( f \) in contrast to first-order feedback which refers to observations from gradient of \( f \) as e.g. in stochastic gradient descent [see, e.g., Agarwal et al., 2011, Vakili and Zhao, 2019].
Our formulation falls under the general framework of continuum armed bandits that signifies receiving feedback only for the selected observation point \( x_n \) at each time \( n \) [Agrawal, 1995, Kleinberg, 2004, Bubeck et al., 2011a,b]. Bandit problems have been extensively studied under numerous settings and various performance measures including simple regret [see, e.g., Bubeck et al., 2011a, Carpentier and Valko, 2015, Deshmukh et al., 2018], cumulative regret [see, e.g., Auer et al., 2002, Slivkins, 2019, Zhao, 2019], and best arm identification [see, e.g., Audibert et al., 2010, Grover et al., 2018]. The choice of performance measure strongly depends on the application. Simple regret is suitable for situations with a preliminary exploration phase (for instance hyper-parameter tuning) in which costs are not measured in terms of rewards but rather in terms of resources expended [Bubeck et al., 2011a].

Due to infinite cardinality of the domain, approaching \( f(x^*) \) is feasible only when appropriate regularity assumptions on \( f \) and noise are satisfied. Following a growing literature [Srinivas et al., 2010, Chowdhury and Gopalan, 2017, Janz et al., 2020, Bakhtiari et al., 2020a], we focus on a variation of the problem where \( f \) is assumed to belong to a reproducing kernel Hilbert space (RKHS) that is a very general assumption. Almost all continuous functions can be approximated with the RKHS elements of practically relevant kernels such as Matérn family of kernels [Srinivas et al., 2010]. We consider two classes of noise: sub-Gaussian and light-tailed.

Our regularity assumption on \( f \) allows us to utilize Gaussian processes (GPs) which provide powerful Bayesian (surrogate) models for \( f \) [Rasmussen and Williams, 2006]. Sequential optimization based on GP models is often referred to as Bayesian optimization in the literature [Shahriari et al., 2016, Snoek et al., 2012, Frazier, 2018]. We build on prediction and uncertainty estimates provided by GP models to study an efficient adaptive exploration algorithm referred to as Maximum Variance Reduction (MVR). Under simple regret measure, MVR embodies the simple principle of exploring the points with the highest variance first. Intuitively, the variance in the GP model is considered as a measure of uncertainty about the unknown objective function and the exploration steps are designed to maximally reduce the uncertainty. At the end of exploration trials, MVR returns a candidate maximizer based on the prediction provided by the learnt GP model. With its simple structure, MVR is amenable to a tight analysis that significantly improves the best known bounds on simple regret. To this end, we derive novel and sharp confidence intervals for GP models applicable to RKHS elements. In addition, we provide numerical experiments on the simple regret performance of MVR comparing it to GP-UCB [Srinivas et al., 2010, Chowdhury and Gopalan, 2017], GP-PI [Hoffman et al., 2011] and GP-EI [Hoffman et al., 2011].

1.1 Main Results

Our main contributions are as follows.

We first derive novel confidence intervals for GP models applicable to RKHS elements (Theorems 1 and 2). As part of our analysis, we formulate the posterior variance of a GP model as the sum of two terms: the maximum prediction error from noise-free observations, and the effect of noise and 2). As part of our analysis, we formulate the posterior variance of a GP model as the sum of two terms: the maximum prediction error from noise-free observations, and the effect of noise and 2). As part of our analysis, we formulate the posterior variance of a GP model as the sum of two terms: the maximum prediction error from noise-free observations, and the effect of noise.

We then build on the confidence intervals for GP models to provide a tight analysis of the simple regret of the MVR algorithm (Theorem 3). In particular, we prove a high probability \( \tilde{O}(\sqrt{\frac{\gamma_N}{N}})^2 \) simple regret, where \( \gamma_N \) is the maximal information gain (see § 2.4). In comparison to the existing \( \tilde{O}(\frac{\gamma_N}{\sqrt{N}}) \) bounds on simple regret [see, e.g., Srinivas et al., 2010, Chowdhury and Gopalan, 2017, Scarlett et al., 2017], we show an \( O(\sqrt{\gamma_N}) \) improvement. It is noteworthy that our bound guarantees convergence to the optimum value of \( f \), while previous \( \tilde{O}(\frac{\gamma_N}{\sqrt{N}}) \) bounds do not, since although \( \gamma_N \) grows sublinearly with \( N \), it can grow faster than \( \sqrt{N} \).

We then specialize our results for the particular cases of practically relevant Matérn and Squared Exponential (SE) kernels. We show that our regret bounds match the lower bounds and close the gap reported in Scarlett et al. [2017], Cai and Scarlett [2020], who showed that an average simple regret of \( \epsilon \) requires \( N = \Omega \left( \frac{1}{\epsilon^2} \left( \log \left( \frac{1}{\epsilon} \right) \right)^{\frac{d}{2}} \right) \) exploration trials in the case of SE kernel. For the Matérn-\( \nu \) kernel

\[ \gamma_N = \Omega \left( \frac{1}{\epsilon^2} \left( \log \left( \frac{1}{\epsilon} \right) \right)^{\frac{d}{2}} \right) \]
\(\nu\) is the smoothness parameter, see § 2.1) they gave the analogous bound of \(N = \Omega \left( \left( \frac{1}{\epsilon} \right)^{d + \nu} \right)\).

They also reported a significant gap between these lower bounds and the upper bounds achieved by GP-UCB algorithm. In Corollary 1, we show that our analysis of MVR closes this gap in the performance and establishes upper bounds matching the lower bounds up to logarithmic factors.

In contrast to the existing results which mainly focus on Gaussian and sub-Gaussian distributions for noise, we extend our analysis to the more general class of light-tailed distributions, thus broadening the applicability of the results. This extension increases both the confidence interval width and the simple regret by only a multiplicative logarithmic factor. These results apply to e.g. the privacy preserving setting where often a light-tailed noise is employed [Basu et al., 2019, Ren et al., 2020, Zheng et al., 2020].

1.2 Literature Review

The celebrated work of Srinivas et al. Srinivas et al. [2010] pioneered the analysis of GP bandits by proving an \(\tilde{O}(\gamma N \sqrt{N})\) upper bound on the cumulative regret of GP-UCB, an optimistic optimization algorithm which sequentially selects \(x_n\) that maximize an upper confidence bound score over the search space. That implies an \(\tilde{O}\left( \frac{\gamma}{\epsilon^2} \right)\) simple regret [Scarlett et al., 2017]. Their analysis relied on deriving confidence intervals for GP models applicable to RKHS elements. They also considered a fully Bayesian setting where \(f\) is assumed to be a sample from a GP and noise is assumed to be Gaussian. Chowdhury and Gopalan [2017] built on feature space representation of GP models and self-normalized martingale inequalities, first developed in Abbasi-Yadkori et al. [2011] for linear bandits, to improve the confidence intervals of Srinivas et al. [2010] by a multiplicative \(\log(N)\) factor. That led to an improvement in the regret bounds by the same multiplicative \(\log(N)\) factor. A discussion on the comparison between these results and the confidence intervals derived in this paper is provided in § 3.3. A technical comparison with some recent advances in regret bounds requires introducing new notations and is deferred to Appendix A.

The performance of Bayesian optimization algorithms has been extensively studied under numerous settings including contextual information [Krause and Ong, 2011], high dimensional spaces [Djolonga et al., 2013, Mutny and Krause, 2018], safety constraints [Berkenkamp et al., 2016, Sui et al., 2018], parallelization [Kandasamy et al., 2018], meta-learning [Wang et al., 2018a], multi-fidelity evaluations [Kandasamy et al., 2019], ordinal models [Picheny et al., 2019], corruption tolerance [Bobu govic et al., 2020, Cai and Scarlett, 2020], and neural tangent kernels [Zhou et al., 2020, Zhang et al., 2020]. Javidi and Shekhar [2018] introduced an adaptive discretization of the search space improving the computational complexity of a GP-UCB based algorithm. Sparse approximation of GP posteriors are shown to preserve the regret orders while improving the computational complexity of Bayesian optimization algorithms [Mutny and Krause, 2018, Calandriello et al., 2019, Vakili et al., 2020b]. Under the RKHS setting with noisy observations, GP-TS [Chowdhury and Gopalan, 2017] and GP-EI [Nguyen et al., 2017, Wang and de Freitas, 2014] are also shown to achieve the same regret guarantees as GP-UCB (up to logarithmic factors). All these works report \(\tilde{O}(\frac{\gamma}{\sqrt{N}})\) regret bounds.

The regret bounds are also reported under other often simpler settings such as noise-free observations [Bull, 2011, Vakili et al., 2020c, \(\epsilon_n = 0, \forall n\)] or a Bayesian regret that is averaged over a known prior on \(f\) [Kandasamy et al., 2018, Wang et al., 2018b, Wang and Jegelka, 2017, Scarlett, 2018, Shekhar and Javidi, 2021, Grünewälder et al., 2010, de Freitas et al., 2012, Kawaguchi et al., 2015], rather than for a fixed and unknown \(f\) as in our setting.

Other lines of work on continuum armed bandits exist relying on other regularity assumptions such as Lipschitz continuity [Kleinberg, 2004, Bubeck et al., 2011b, Carpentier and Valko, 2015, Kleinberg et al., 2008], convexity [Agarwal et al., 2011] and unimodality [Combes et al., 2020], to name a few. A notable example is Bubeck et al. [2011b] who showed that hierarchical algorithms based on tree search yield \(O(N^{\frac{d+1}{d+2}})\) cumulative regret. We do not compare with these results due to the inherent difference in the regularity assumptions.

1.3 Organization

In § 2, the problem formulation, the regularity assumptions, and the preliminaries on RKHS and GP models are presented. The novel confidence intervals for GP models are proven in § 3. MVR
algorithm and its analysis are given in § 4. The experiments are presented in § 5. We conclude with a discussion in § 6.

2 Problem Formulation and Preliminaries

Consider an objective function \( f : \mathcal{X} \rightarrow \mathbb{R} \), where \( \mathcal{X} \subseteq \mathbb{R}^d \) is a convex and compact domain. Consider an optimal point \( x^* \in \text{argmax}_{x \in \mathcal{X}} f(x) \). A learning algorithm \( A \) sequentially selects observation points \( \{x_n \in \mathcal{X}\}_{n \in \mathbb{N}} \) and observes the corresponding noise disturbed objective values \( \{y_n = f(x_n) + \epsilon_n\}_{n \in \mathbb{N}} \), where \( \epsilon_n \) is the observation noise. We use the notations \( \mathcal{H}_n = \{X_n, Y_n\} \), \( X_n = [x_1, x_2, ..., x_n]^\top \), \( Y_n = [y_1, y_2, ..., y_n]^\top \), \( x_n \in \mathcal{X}, y_n \in \mathbb{R} \), for all \( n \geq 1 \). In a simple regret setting, the learning algorithm determines a sequence of mappings \( \{\mathcal{S}_n\}_{n \geq 1} \) where each mapping \( \mathcal{S}_n : \mathcal{H}_n \rightarrow \mathcal{X} \) predicts a candidate maximizer \( \hat{x}_n^* \). For algorithm \( A \), the simple regret under a budget of \( N \) tries is defined as

\[
\mathcal{R}^A_N = f(x^*) - f(\hat{x}_N^*).
\] (1)

The budget \( N \) may be unknown \textit{a priori}. Notationwise, we use \( F_n = [f(x_1), f(x_2), \ldots, f(x_n)]^\top \) and \( E_n = [\epsilon_1, \epsilon_2, \ldots, \epsilon_n]^\top \) to denote the noise free part of the observations and the noise history, respectively, similar to \( X_n \) and \( Y_n \).

2.1 Gaussian Processes

The Bayesian optimization algorithms build on GP (surrogate) models. A GP is a random process \( \{f(x)\}_{x \in \mathcal{X}} \), where each of its finite subsets follow a multivariate Gaussian distribution. The distribution of a GP is fully specified by its mean function \( \mu(x) = \mathbb{E}[f(x)] \) and a positive definite kernel (or covariance function) \( k(x, x') = \mathbb{E}[(f(x) - \mu(x))(f(x') - \mu(x'))] \). Without loss of generality, it is typically assumed that \( \forall x \in \mathcal{X}, \mu(x) = 0 \) for prior GP distributions.

Conditioning GPs on available observations provides us with powerful non-parametric Bayesian (surrogate) models over the space of functions. In particular, using the conjugate property, conditioned on \( \mathcal{H}_n \), the posterior of \( f \) is a GP with mean function \( \mu_n(x) = \mathbb{E}[f(x)|\mathcal{H}_n] \) and kernel function \( k_n(x, x') = \mathbb{E}((f(x) - \mu_n(x))(f(x') - \mu_n(x'))|\mathcal{H}_n) \) specified as follows:

\[
\mu_n(x) = k^\top(x, X_n)(k(X_n, X_n) + \lambda^2 I_n)^{-1} Y_n,
\]

\[
k_n(x, x') = k(x, x') - k^\top(x, X_n)(k(X_n, X_n) + \lambda^2 I_n)^{-1} k(x, X_n), \quad \sigma_n^2(x) = k_n(x, x), \quad \sigma_n^2 = \mathbb{E}(\epsilon^2|\mathcal{H}_n), \quad \lambda > 0 \text{ is a real number.}
\] (2)

In practice, Matérn and squared exponential (SE) are the most commonly used kernels for Bayesian optimization [see, e.g., Shahriari et al., 2016, Snoek et al., 2012],

\[
k_{\text{Matérn}}(x, x') = \frac{1}{\Gamma(\nu)2^{\nu-1}} \left( \frac{\sqrt{2\nu \rho}}{l} \right)^\nu B_\nu \left( \frac{\sqrt{2\nu \rho}}{l} \right), \quad k_{\text{SE}}(x, x') = \exp \left( -\frac{\rho^2}{2l^2} \right),
\]

where \( l > 0 \) is referred to as lengthscale, \( \rho = ||x - x'||_2 \) is the Euclidean distance between \( x \) and \( x' \), \( \nu > 0 \) is referred to as the smoothness parameter, \( \Gamma \) and \( B_\nu \) are, respectively, the Gamma function and the modified Bessel function of the second kind. Variation over parameter \( \nu \) creates a rich family of kernels. The SE kernel can also be interpreted as a special case of Matérn family when \( \nu \to \infty \).

2.2 RKHSs and Regularity Assumptions on \( f \)

Consider a positive definite kernel \( k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R} \) with respect to a finite Borel measure (e.g., the Lebesgue measure) supported on \( \mathcal{X} \). A Hilbert space \( H_k \) of functions on \( \mathcal{X} \) equipped with an inner product \( \langle \cdot, \cdot \rangle_{H_k} \) is called an RKHS with reproducing kernel \( k \) if the following is satisfied. For all \( x \in \mathcal{X}, k(\cdot, x) \in H_k \), and for all \( x \in \mathcal{X} \) and \( f \in H_k \), \( f(\cdot, x)_{H_k} = f(x) \) (reproducing property). A constructive definition of RKHS requires the use of Mercer theorem which provides an
alternative representation for kernels as an inner product of infinite dimensional feature maps [e.g., Kanagawa et al., 2018, Theorem 4.1], and is deferred to Appendix B. We have the following regularity assumption on the objective function $f$.

**Assumption 1** The objective function $f$ is assumed to live in the RKHS corresponding to a positive definite kernel $k$. In particular, $\|f\|_{H_k} \leq B$, for some $B > 0$, where $\|f\|_{H_k} = \langle f, f \rangle_{H_k}$.

For common kernels, such as Matérn family of kernels, members of $H_k$ can uniformly approximate any continuous function on any compact subset of the domain $\mathcal{X}$ [Srinivas et al., 2010]. This is a very general class of functions; more general than e.g. convex or Lipschitz. It has thus gained increasing interest in recent years.

### 2.3 Regularity Assumptions on Noise

We consider two different cases regarding the regularity assumption on noise. Let us first revisit the definition of sub-Gaussian distributions.

**Definition 1** A random variable $X$ is called sub-Gaussian if its moment generating function $M(h) \triangleq \mathbb{E}[\exp(hX)]$ is upper bounded by that of a Gaussian random variable.

The sub-Gaussian assumption implies that $\mathbb{E}[X] = 0$. It also allows us to use Chernoff-Hoeffding concentration inequality [Antonini et al., 2008] in our analysis.

We next recall the definition of light-tailed distributions.

**Definition 2** A random variable $X$ is called light-tailed if its moment-generating function exists, i.e., there exists $h_0 > 0$ such that for all $|h| \leq h_0$, $M(h) < \infty$.

For a zero mean light-tailed random variable $X$, we have [Chareka et al., 2006]

$$M(h) \leq \exp(\xi_0 h^2/2), \forall |h| \leq h_0, \xi_0 = \sup \{M^{(2)}(h), |h| \leq h_0\},$$

(3)

where $M^{(2)}(\cdot)$ denotes the second derivative of $M(\cdot)$ and $h_0$ is the parameter specified in Definition 2. We observe that the upper bound in (3) is the moment generating function of a zero mean Gaussian random variable with variance $\xi_0$. Thus, light-tailed distributions are also called locally sub-Gaussian distributions [Vakili et al., 2013].

We provide confidence intervals for GP models and regret bounds for MVR under each of the following assumptions on the noise terms.

**Assumption 2 (Sub-Gaussian Noise)** The noise terms $\epsilon_n$ are i.i.d. over $n$. In addition, $\forall h \in \mathbb{R}, \forall n \in \mathbb{N}, \mathbb{E}[e^{h\epsilon_n}] \leq \exp(h^2 R^2/2)$, for some $R > 0$.

**Assumption 3 (Light-Tailed Noise)** The noise terms $\epsilon_n$ are i.i.d. zero mean random variables over $n$. In addition, $\forall h \leq h_0, \forall n \in \mathbb{N}, \mathbb{E}[e^{h\epsilon_n}] \leq \exp(h^2 \xi_0), for some \xi_0 > 0$.

Bayesian optimization uses GP priors for the objective function $f$ and assumes a Gaussian distribution for noise (for its conjugate property). It is noteworthy that the use of GP models is merely for the purpose of algorithm design and does not affect our regularity assumptions on $f$ and noise. We use the notation $\hat{f}$ to distinguish the GP model from the fixed $f$.

### 2.4 Maximal Information Gain

The regret bounds derived in this work are given in terms of the maximal information gain, defined as $\gamma_N = \sup_{X_N, f} \mathcal{I}(Y_N; f)$, where $\mathcal{I}(Y_N; f)$ denotes the mutual information between $Y_n$ and $\hat{f}$ [see, e.g., Cover, 1999, Chapter 2]. In the case of a GP model, the mutual information can be given as $\mathcal{I}(Y_n; \hat{f}) = \frac{1}{2} \log \det \left( I_n + \frac{1}{\nu^2} k(X_n, X_n) \right)$, where $\det$ denotes the determinant of a square matrix. Note that the maximal information gain is kernel-specific and $X_N$-independent. Upper bounds on $\gamma_N$ are derived in Srinivas et al. [2010], Janz et al. [2020], Vakili et al. [2020a] which are commonly used to provide explicit regret bounds. In the case of Matérn and SE, $\gamma_N = \mathcal{O} \left( N \pi^{d+1} (\log(N))^{d+1} \right)$ and $\gamma_N = \mathcal{O} \left( (\log(N))^{d+1} \right)$, respectively [Vakili et al., 2020a].
3 Confidence Intervals for Gaussian Process Models

The analysis of bandit problems classically builds on confidence intervals applicable to the values of the objective function [see, e.g., Auer, 2002, Bubeck et al., 2012]. The GP modelling allows us to create confidence intervals for complex functions over continuous domains. In particular, we utilize the prediction \( \mu_n \) and the uncertainty estimate \( \sigma_n \) provided by GP models in building the confidence intervals which become an important building block of our analysis in the next section. To this end, we first prove the following proposition which formulates the posterior variance of a GP model as the sum of two terms: the maximum prediction error for an RKHS element from noise free observations and the effect of noise.

**Proposition 1** Let \( \sigma_n^2 \) be the posterior variance of the surrogate GP model as defined in (2). Let \( Z_n^T(x) = k^T(x, X_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1} \). We have

\[
\sigma_n^2(x) = \sup_{f : \|f\|_{\mu_n} \leq 1} (f(x) - Z_n^T(x) F_n)^2 + \lambda^2 \|Z_n(x)\|^2_{F_n}.
\]

Notice that the first term \( f(x) - Z_n^T(x) F_n \) captures the maximum prediction error from noise free observations \( F_n \). The second term captures the effect of noise in the surrogate GP model (and is independent of \( F_n \)). A detailed proof for Proposition 1 is provided in Appendix C.

Proposition 1 elicits new connections between GP models and kernel ridge regression. While the equivalence of the posterior mean in GP models and the regressor in kernel ridge regression is well known, the interpretation of posterior variance of GP models as the maximum prediction error for an RKHS element is less studied [see Kanagawa et al., 2018, Section 3, for a detailed discussion on the connections between GP models and kernel ridge regression].

3.1 Confidence Intervals under Sub-Gaussian Noise

The following theorem provides a confidence interval for GP models applicable to RKHS elements under the assumption that the noise terms are sub-Gaussian.

**Theorem 1** Assume Assumptions 1 and 2 hold. Provided \( n \) noisy observations \( \mathcal{H}_n = \{X_n, Y_n\} \) from \( f \), let \( \mu_n \) and \( \sigma_n \) be as defined in (2). Assume \( X_n \) are independent of \( E_n \). For a fixed \( x \in \mathcal{X} \), define the upper and lower confidence bounds, respectively,

\[
U^\delta_n(x) \triangleq \mu_n(x) + (B + \beta(\delta))\sigma_n(x), \quad \text{and} \quad L^\delta_n(x) \triangleq \mu_n(x) - (B + \beta(\delta))\sigma_n(x),
\]

with \( \beta(\delta) = \frac{B}{\sqrt{2 \log(\frac{1}{\delta})}} \), where \( \delta \in (0, 1) \), and \( B \) and \( R \) are the parameters specified in Assumptions 1 and 2.

We have

\[
 f(x) \leq U^\delta_n(x) \quad \text{w.p. at least } 1 - \delta, \quad \text{and} \quad f(x) \geq L^\delta_n(x) \quad \text{w.p. at least } 1 - \delta.
\]

We can write the difference in the objective function and the posterior mean as follows.

\[
f(x) - \mu_n(x) = f(x) - Z_n^T(x) Y_n = f(x) - Z_n^T(x) F_n - Z_n^T(x) E_n.
\]

The first term can be bounded directly following Proposition 1. The second term is bounded as a result of Proposition 1 and Chernoff-Hoeffding inequality. A detailed proof of Theorem 1 is provided in Appendix D.

3.2 Confidence Intervals under Light-Tailed Noise

We now extend the confidence intervals to the case of light-tailed noise. The main difference with sub-Gaussian noise is that Chernoff-Hoeffding inequality is no more applicable. We derive new bounds accounting for light-tailed noise in the analysis of Theorem 2.

**Theorem 2** Assume Assumptions 1 and 3 hold. For a fixed \( x \in \mathcal{X} \), define the upper and lower confidence bounds \( U^\delta_n(x) \) and \( L^\delta_n(x) \) similar to Theorem 1 with \( \beta(\delta) = \frac{1}{2} \sqrt{2 \left( \xi_0 \vee \frac{2 \log(1 + \frac{1}{\delta})}{h_0^2} \right) \log(\frac{1}{\delta})} \).

3The notation \( \vee \) is used to denote the maximum of two real numbers, \( \forall a, b \in \mathbb{R}, (a \vee b) \triangleq \max(a, b) \).
where $\delta \in (0, 1)$, and $B, h_0$ and $\xi_0$ are specified in Assumptions 1 and 3. Assume $X_n$ are independent
of $E_n$. We have

$$f(x) \leq U^\delta_n(x) \quad \text{w.p. at least } 1 - \delta, \text{ and } f(x) \geq L^\delta_n(x) \quad \text{w.p. at least } 1 - \delta.$$ 

In comparison to Theorem 1, under the light-tailed assumption, the confidence interval width increases
with a multiplicative $O(\sqrt{\log(\frac{1}{\delta})})$ factor. A detailed proof of Theorem 2 is provided in Appendix D.

**Remark 1** Theorems 1 and 2 rely on the assumption that $X_n$ are independent of $E_n$. As we shall see in § 4, this assumption is satisfied when the confidence intervals are applied to the analysis of MVR.

### 3.3 Comparison with the Existing Confidence Intervals

The most relevant work to our Theorems 1 and 2 is [Chowdhury and Gopalan, 2017, Theorem 2] which itself was an improvement over [Srinivas et al., 2010, Theorem 6]. Chowdhury and Gopalan [2017] built on feature space representation of GP kernels and self-normalized martingale
inequalities [Abbasi-Yadkori et al., 2011, Peña et al., 2008] to establish a $1 - \delta$ confidence interval
in the same form as in Theorem 1, under Assumptions 1 and 2, with confidence interval width

$$B + R \sqrt{2(\gamma_n + 1 + \log(\frac{1}{\delta}))}$$

(instead of $B + \beta(\delta)$). There is a stark contrast between this confidence interval and the one given in Theorem 1 in its dependence on $\gamma_n$ which has a relatively large and possibly polynomial in $n$ value. That contributes an extra $O(\sqrt{\gamma_n})$ multiplicative factor to regret.

Neither of these two results (our Theorem 1 and [Chowdhury and Gopalan, 2017, Theorem 2]) imply
the other. Although our confidence interval is much tighter, there are two important differences in the
settings of these theorems. One difference is in the probabilistic dependencies between the observation
points $x_n$ and the noise terms $\{\epsilon_j\}_{j<n}$. While Theorem 1 assumes that $X_n$ are independents of $E_n$, [Chowdhury and Gopalan, 2017, Theorem 2] allows for the dependence of $x_n$ on the previous noise terms $\{\epsilon_j\}_{j<n}$. This is a reflection of the difference in the analytical requirements of MVR
and GP-UCB. The other difference is that [Chowdhury and Gopalan, 2017, Theorem 2] holds for all $x \in \mathcal{X}$. While, Theorem 1 holds for a single $x \in \mathcal{X}$. As we will see in § 4.2, a probability union
bound can be used to obtain confidence intervals applicable to all $x$ in a discretization of $\mathcal{X}$, which
contributes only logarithmic terms to regret in contrast to $O(\sqrt{\gamma_n})$. Roughly speaking, we are trading
off the extra $O(\sqrt{\gamma_n})$ term for restricting the confidence interval to hold for a single $x$. It remains an
open problem whether the same can be done when $x_n$ are allowed to depend on $\{\epsilon_j\}_{j<n}$.

### 4 Maximum Variance Reduction and Simple Regret

In this section, we first formally present an exploration policy based on GP models referred to as Maximum Variance Reduction (MVR). We then utilize the confidence intervals for GP models derived in § 3 to prove bounds on the simple regret of MVR.

#### 4.1 Maximum Variance Reduction Algorithm

MVR relies on the principle of reducing the maximum uncertainty where the uncertainty is measured
by the posterior variance of the GP model. After $N$ exploration trials, MVR returns a candidate
maximizer according to the prediction provided by the learnt GP model. A pseudo-code is given in Algorithm 1.

#### 4.2 Regret Analysis

For the analysis of MVR, we assume there exists a fine discretization of the domain for RKHS elements, which is a standard assumption in the literature [see, e.g., Srinivas et al., 2010, Chowdhury and Gopalan, 2017, Vakili et al., 2020b].

**Assumption 4** For each given $n \in \mathbb{N}$ and $f \in H_\delta$ with $\|f\|_{H_\delta} \leq B$, there exists a discretization $D_n$ of $\mathcal{X}$ such that $f(x) - f([x]_n) \leq \frac{1}{\sqrt{n}}$, where $[x]_n = \text{argmin}_{x' \in D_n} \|x' - x\|_2$ is the closest point in $D_n$ to $x$, and $|D_n| \leq C B^4 n^{d/2}$, where $C$ is a constant independent of $n$ and $B$.

\[\text{The effect of } \lambda \text{ is absorbed in } \gamma_n.\]
For instance, in the case of Matérn-

Algorithm 1 Maximum Variance Reduction (MVR)

1: Initialization: \( k, X, f, \sigma^2_0(x) = k(x, x) \).
2: for \( n = 1, 2, \ldots, N \) do
3: \( x_n = \arg\max_{x \in X} \sigma^2_{n-1}(x) \), where a tie is broken arbitrarily.
4: Update \( \sigma^2_n(.) \) according to (2).
5: end for
6: return \( x^*_N = \arg\max_{x \in X} \mu_N(x) \), where a tie is broken arbitrarily.

Assumption 4 is a mild assumption that holds for typical kernels such as SE and Matérn [Srinivas et al., 2010, Chowdhury and Gopalan, 2017]. The following theorem provides a high probability bound on the regret performance of MVR when the noise terms satisfy either Assumption 2 or 3.

**Theorem 3** Consider the Gaussian process bandit problem. Under Assumptions 1, 4, and (2 or 3), for \( \delta \in (0, 1) \), with probability at least \( 1 - \delta \), MVR satisfies

\[
R^{MVR}_N \leq \sqrt{\frac{2\gamma_N}{\log(1 + \frac{1}{N})} N \left( 2B + \beta(\frac{\delta}{3}) + \beta \left( \frac{1}{3C} \left( B + \sqrt{N} \beta(2\delta/3N) \right)^d \right) \log(N^{d/2}) \right)} + \frac{2}{\sqrt{N}},
\]

where under Assumption 2, \( \beta(\delta) = \frac{R}{4\sqrt{2\log(\frac{1}{\delta})}} \), and under Assumption 3, \( \beta(\delta) = \frac{1}{\sqrt{2}} \left( \xi_0 \sqrt{\frac{2\log(\frac{1}{\delta})}{h_0^2}} \right) \log(\frac{1}{\delta}) \), and \( B, R, h_0, \xi_0, \) and \( C \) are the constants specified in Assumptions 1, 2, 3 and 4.

A detailed proof of the theorem is provided in Appendix E.

**Remark 2** Under Assumptions 2 and 3, respectively, the regret bounds can be simplified as

\[
R^{MVR}_N = O \left( \sqrt{\frac{\gamma_N \log(N^{d/\delta})}{N}} \right), \quad \text{and} \quad R^{MVR}_N = O \left( \sqrt{\frac{\gamma_N}{N^{d/\delta}}} \right).
\]

For instance, in the case of Matérn-\( \nu \) kernel, under Assumption 2 and 3, respectively,

\[
r^{MVR}_N = O \left( N^{\frac{\nu}{\nu+\pi}} (\log(N))^{\frac{\pi}{\nu+\pi}} \sqrt{\log(N^{d/\delta})} \right), \quad \text{and} \quad r^{MVR}_N = O \left( N^{\frac{\nu}{\nu+\pi}} (\log(N))^{\frac{\pi}{\nu+\pi}} \log(N^{d/\delta}) \right),
\]

which always converge to zero as \( N \) grows (unlike the existing regret bounds).

**Remark 3** In the analysis of Theorem 3, we apply Assumption 4 to \( \mu_N \) as well as \( f \). For this purpose, we derive a high probability \( B + \sqrt{N} \beta(2\delta/3N) \) upper bound on \( \| \mu_N \|_{H_k} \) (see Lemma 4 in Appendix E), which appears in the regret bound expression.

### 4.3 Optimal Order Simple Regret with SE and Matérn Kernels

To enable a direct comparison with the lower bounds on simple regret proven in Scarlett et al. [2017], Cai and Scarlett [2020], in the following corollary, we state a dual form of Theorem 3 for the Matérn and SE kernels. Specifically we formalize the number of exploration trials required to achieve an average \( \epsilon \) regret.

**Corollary 1** Consider the GP bandit problem with an SE or a Matérn kernel. For \( \epsilon \in (0, 1) \), define \( N_\epsilon = \min \{ N \in \mathbb{N} : \mathbb{E}[r^{MVR}_N] \leq \epsilon, \forall n \geq N \} \). Under Assumptions 1, 4, and (2 or 3), upper bounds on \( N_\epsilon \) are reported in Table 1.

| Kernel     | Under Assumption 2 | Under Assumption 3 |
|------------|--------------------|--------------------|
| SE         | \( O \left( \left( \frac{1}{\delta} \right)^2 \log(\frac{1}{\delta})^{d+2} \right) \) | \( O \left( \left( \frac{1}{\delta} \right)^2 \log(\frac{1}{\delta})^{d+3} \right) \) |
| Matérn-\( \nu \) | \( O \left( \left( \frac{1}{\delta} \right)^{3+\#} (\log(\frac{1}{\delta}))^{4+d} \right) \) | \( O \left( \left( \frac{1}{\delta} \right)^{2+\#} (\log(\frac{1}{\delta}))^{6+d} \right) \) |

Table 1: The upper bounds on \( N_\epsilon \) defined in Corollary 1 with SE or Matérn kernel.
A proof is provided in Appendix F. Scarlett et al. [2017], Cai and Scarlett [2020] showed that for the SE kernel, an average simple regret of \( \epsilon \) requires 
\[ N \epsilon = \Omega \left( \frac{1}{\epsilon^2} \log \left( \frac{1}{\epsilon} \right)^{\frac{1}{2}} \right) \].

For the Matérn-\( \nu \) kernel they gave the analogous bound of 
\[ N \epsilon = \Omega \left( \left( \frac{1}{\epsilon} \right)^{2+\frac{\nu}{2}} \right) \].

They also reported significant gaps between these lower bounds and the existing results [see, e.g., Scarlett et al., 2017, Table I]. Comparing with Corollary 1, our bounds are tight in all cases up to \( \log(1/\epsilon) \) factors.

5 Experiments

In this section, we provide numerical experiments on the simple regret performance of MVR, Improved GP-UCB (IGP-UCB) as presented in Chowdhury and Gopalan [2017], and GP-PI and GP-EI as presented in Hoffman et al. [2011].

We follow the experiment set up in Chowdhury and Gopalan [2017] to generate test functions from the RKHS. First, 100 points are uniformly sampled from interval \([0, 1]\). A GP sample with kernel \( k \) is drawn over these points. Given this sample, the mean of posterior distribution is used as the test function \( f \). Parameter \( \lambda^2 \) is set to 1% of the function range. For IGP-UCB we set the parameters exactly as described in Chowdhury and Gopalan [2017]. The GP model is equipped with SE or Matérn-2.5 kernel with \( l = 0.2 \). We use 2 different models for the noise: a zero mean Gaussian with variance equal to \( \lambda^2 \) (a sub-Gaussian distribution) and a zero mean Laplace with scale parameter equal to \( \lambda \) (a light-tailed distribution). We run each experiment over 25 independent trials and plot the average simple regret in Figure 1. More experiments on two commonly used benchmark functions for Bayesian optimization (Rosenbrock and Hartman3) are reported in Appendix G. Further details on the experiments are provided in the supplementary material.

![Figure 1: Comparison of the simple regret performance of Bayesian optimization algorithms on samples from RKHS.](image)

6 Discussion

In this paper, we proved novel and sharp confidence intervals for GP models applicable to RKHS elements. We then built on these results to prove \( \tilde{O}(\sqrt{\gamma_N/N}) \) bounds for the simple regret of an adaptive exploration algorithm under the framework of GP bandits. In addition, for the practically relevant SE and Matérn kernels, where a lower bound on regret is known Scarlett et al. [2017], Cai and Scarlett [2020], we showed the order optimality of our results up to logarithmic factors. That closes a significant gap in the literature of analysis of Bayesian optimization algorithms under the performance measure of simple regret.

The limitation of our work adhering to simple regret is that neither our theoretical nor experimental result proves that MVR is a better algorithm in practice. Overall, exploration-exploitation oriented
algorithms such as GP-UCB may perform worse than MVR in terms of simple regret due to two reasons. One is over-exploitation of local maxima when $f$ is multi-modal, and the other is dependence on an exploration-exploitation balancing hyper-parameter that is often set too conservatively, to guarantee low regret bounds. Furthermore, their existing analytical regret bounds are suboptimal and possibly vacuous (non-diminishing; when $\gamma_N$ grows faster than $\sqrt{N}$, as discussed). On the other hand, when compared in terms of cumulative regret ($\sum_{n=1}^{N} f(x^*) - f(x_n)$), MVR suffers from a linear regret.

The main value of our work is in proving tight bounds on the simple regret of a GP based exploration algorithm, when other Bayesian optimization algorithms such as GP-UCB lack a proof for an always diminishing and non-vacuous regret under the same setting as ours. It remains an open question whether the possibly vacuous regret bounds of GP-UCB (as well as GP-TS and GP-EI whose analysis is inspired by that of GP-UCB) is a fundamental limitation or an artifact of its proof.

It is worth reiterating that simple regret is favorable in situations with a preliminary exploration phase (for instance hyper-parameter tuning) [Bubeck et al., 2011a]. It has been explicitly studied under numerous settings, e.g., [Bubeck et al., 2011a, Carpentier and Valko, 2015, Deshmukh et al., 2018, Lipschitz continuous $f$], [Bull, 2011, $f$ in RKHS, noise-free observations], [Grünewälder et al., 2010, de Freitas et al., 2012, Kawaguchi et al., 2015, a known prior distribution on $f$, noise-free observations], [Contal et al., 2013, a known prior distribution on $f$, noisy observations], [Scarlett et al., 2017, Cai and Scarlett, 2020, Shekhar and Javidi, 2020, Bogunovic et al., 2016, $f$ in RKHS, noisy observations]. See also § 1.2 and Appendix A for comparison with existing results including Shekhar and Javidi [2020], Bogunovic et al. [2016].
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A Further Comparison with the Existing Regret Bounds

There are several Bayesian optimization algorithms namely GP-UCB [Srinivas et al., 2010], IGPG-UCB, GP-TS [Chowdhury and Gopalan, 2017], TruVar [Bogunovic et al., 2016], GP-EI [Wang and de Freitas, 2014, Nguyen et al., 2017] and KernelUCB [Valko et al., 2013] which enjoy theoretical upper bounds on regret (under Assumptions 1, 2 and 4), which grow at least as fast as \( \mathcal{O}(\frac{1}{\sqrt{N}}) \). These bounds do not necessarily converge to zero, since \( \gamma_N \) can grow faster than \( \sqrt{N} \) resulting in vacuous regret bounds. For example, in the case of a Matérn-\( \nu \) kernel, replacing \( \gamma_N = \mathcal{O}(N^{\frac{d+1}{2d}}) \) [Vakili et al., 2020a] results in an \( \tilde{O}(N^{\frac{d+1}{2d}}) \) regret which does not converge to zero for \( d > 2\nu \), meaning the algorithm does not necessarily approach \( f(x^*) \). Janz et al. [2020] developed a GP-UCB based algorithm, specific to Matérn family of kernels, that constructs a cover for the search space, as many hypercubes, and fits an independent GP to each cover element. This algorithm, referred to as \( \pi \)-GP-UCB, was proven to achieve diminishing regret for all \( \nu > 1 \) and \( d \geq 1 \). Recently, Shekhar and Javidi [2020] introduced LP-GP-UCB where the GP model is augmented with local polynomial estimators to construct a multi-scale upper confidence bound guiding the sequential optimization. They further improved the regret bounds of Janz et al. [2020] and showed that LP-GP-UCB matches the lower bounds for some configuration of parameters \( \nu \) and \( d \) in the case of a Matérn kernel.

Defining \( I_0 = (0, 1), I_1 = (1, \frac{d(d+1)}{2}), I_2 = (\frac{d(d+1)}{2}, \frac{d^2+5d+12}{4}) \) and \( I_3 = (0, \infty) \setminus (I_0 \cup I_1 \cup I_2), \) their bounds on simple regret are as follows. For \( \nu \in I_0 \cup I_1, r_N^{\text{GP-UCB}} = \tilde{O}(N^{\frac{1}{2d}}). \) For \( \nu \in I_2, r_N^{\text{GP-UCB}} = \tilde{O}(N^{\frac{d+1}{2d}}). \) For \( \nu \in I_3, r_N^{\text{GP-UCB}} = \tilde{O}(N^{\frac{d+1}{2d}}) \) [see, Shekhar and Javidi, 2020, Sec. 3.2, for a detailed discussion on the bounds on the simple regret of LP-GP-UCB]. In comparison, our bounds on simple regret match the \( \Omega(N^{\frac{1}{2d}}) \) lower bound, up to logarithmic factors, with all parameters \( \nu \) and \( d \). In addition, LP-GP-UCB is impractical due to large constant factors, though a practical heuristic was also given. While, MVR enjoys a simple implementation and works efficiently in practice. Of important theoretical value, SupKernelUCB Valko et al. [2013], which builds on episodic independent batches of observations was proven to achieve \( \tilde{O}(\sqrt{\frac{d}{N}}) \) regret on a finite set \( \{|x| < \infty\}. \) SupKernelUCB is also reported to perform poorly in practice [Janz et al., 2020, Calandra et al., 2019, Cai and Scarlett, 2020].

It is noteworthy that our techniques do not directly apply to the analysis ofcumulative regret of algorithms such as GP-UCB. The key difference is that in MVR the observation points \( x_n \) are independent of the noise terms \( \epsilon_n \) (although \( x_n \) are allowed to depend on \( \{x_j\}_{j<n} \) and \( \tilde{x}_N \) is allowed to depend on \( \{x_n, \epsilon_n\}_{n\leq N} \), while in GP-UCB \( x_n \) are allowed to depend on \( \{\epsilon_j\}_{j<n} \) (see also Sec. 3.3). It remains an interesting open question whether the state of the art upper bound on the regret performance of GP-UCB [Chowdhury and Gopalan, 2017] is tight or the gap with the lower bound [Scarlett et al., 2017] is an artifact of its proof.

B Constructive Definition of RKHS

A constructive definition of RKHS requires the use of Mercer theorem which provides an alternative representation for kernels as an inner product of infinite dimensional feature maps [see, e.g., Kanagawa et al., 2018, Theorem 4.1].

**Mercer Theorem:** Let \( k \) be a continuous kernel with respect to a finite Borel measure. There exists \( \{(\lambda_m, \phi_m)\}_{m=1}^{\infty} \) such that \( \lambda_m \in \mathbb{R}^+, \phi_m \in H_k \), for \( m \geq 1 \), and

\[
k(x, x') = \sum_{m=1}^{\infty} \lambda_m \phi_m(x) \phi_m(x').
\]

The RKHS can consequently be represented in terms of \( \{(\lambda_m, \phi_m)\}_{m=1}^{\infty} \) using Mercer’s representation theorem [see, e.g., Kanagawa et al., 2018, Theorem 4.2].
Mercer’s Representation Theorem: Let \( \{ (\lambda_m, \phi_m) \}_{m=1}^{\infty} \) be the same as in Mercer Theorem. Then, the RKHS of \( k \) is given by
\[
H_k = \left\{ f(\cdot) = \sum_{m=1}^{\infty} w_m \lambda_m \phi_m(\cdot) : \| f \|^2_{H_k} = \sum_{m=1}^{\infty} w_m^2 < \infty \right\}.
\]

Mercer’s representation theorem indicates that \( \{ \lambda_m \phi_m \}_{m=1}^{\infty} \) form an orthonormal basis for \( H_k \). It also provides a constructive definition for the RKHS as the span of this orthonormal basis, and a definition for the norm of a member \( f \) as the \( L_2 \) norm of the weights \( w_m \).

The RKHS of Matérn is equivalent to a Sobolev space with parameter \( \nu + \frac{d}{2} \) [Kanagawa et al., 2018, Teckentrup, 2018]. This observation provides an intuitive interpretation for the norm of Matérn RKHS as proportional to the cumulative \( L_2 \) norm of the weak derivatives of \( f \) up to \( \nu + \frac{d}{2} \) order. I.e., in the case of Matérn family, Assumption 1 on the norm of \( f \) translates to the existence of weak derivatives of \( f \) up to \( \nu + \frac{d}{2} \) order which can be understood as a versatile measure for the smoothness of \( f \) controlled by \( \nu \). In the case of SE kernel, the regularity assumption implies the existence of all weak derivatives of \( f \). For the details on the definition of weak derivatives and Sobolev spaces see Hunter and Nachtergaele [2011].

C Proof of Proposition

Recall the notations \( Y_n = [y_1, y_2, \ldots, y_n]^\top \), \( F_n = [f(x_1), f(x_2), \ldots, f(x_n)]^\top \), \( Z_n^\top(x) = k^\top(x, X_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1}. \) Let \( \zeta_i(x) = [Z_n(x)]_{i} \). From the closed form expression for the posterior mean of GP models, we have \( \mu_n(x) = \bar{Z}_n(x) Y_n \).

The proof of Proposition 1 uses the following lemma.

Lemma 1 For a positive definite kernel \( k \) and its corresponding RKHS, the following holds.
\[
\sup_{f : \|f\|_{H_k} \leq 1} \left( f(x) - \sum_{i=1}^{n} \zeta_i(x) f(x_i) \right)^2 = \left\| \bar{k}(\cdot, x) - \sum_{i=1}^{n} \zeta_i(x) \bar{k}(\cdot, x_i) \right\|^2_{H_k}. \tag{5}
\]

The lemma establishes the equivalence of the RKHS norm of a linear combination of feature vectors induced by \( k \) to the supremum of the linear combination of the corresponding function values, over the functions in the unit ball of the RKHS. For a proof, see [Kanagawa et al., 2018, Lemma 3.9].

Expanding the RKHS norm in the right hand side through an algebraic manipulation, we get
\[
\begin{align*}
\left\| \bar{k}(\cdot, x) - \sum_{i=1}^{n} \zeta_i(x) \bar{k}(\cdot, x_i) \right\|^2_{H_k}
&= k(x, x) - 2 \sum_{i=1}^{n} \zeta_i(x) k(x, x_i) + \sum_{i=1}^{n} \sum_{j=1}^{n} \zeta_i(x) \zeta_j(x) k(x_i, x_j) \\
&= k(x, x) - 2 \sum_{i=1}^{n} \zeta_i(x) k(x, x_i) + (Z_n(x))^\top k(X_n, X_n) Z_n(x) \\
&= k(x, x) - 2(k(x, X_n))^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(x, X_n) \\
&\quad + (k(x, X_n))^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(X_n, X_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(x, X_n) \\
&= k(x, x) - 2k(x, X_n)^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(x, X_n) \\
&\quad + (k(x, X_n))^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(X_n, X_n) + \lambda^2 I_n - \lambda^2 I_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(x, X_n) \\
&= k(x, x) - 2k(x, X_n)^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(X_n, X_n) \\
&\quad + (k(x, X_n))^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(x, X_n) - \lambda^2 k(x, X_n)^\top (k(X_n, X_n) + \lambda^2 I_n)^{-2} k(x, X_n) \\
&= k(x, x) - (k(X_n, X_n))^\top (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(X_n, X_n) - \lambda^2 k(x, X_n)^\top (k(X_n, X_n) + \lambda^2 I_n)^{-2} k(x, X_n) \\
&= \sigma_n^2(x) - \lambda^2 \left\| Z_n(x) \right\|^2.
\end{align*}
\]
We now proceed using Assumption 2 to prove Theorem 1. We utilize Proposition 1 to conclude that\[ \|\tilde{f}(x) - Z_n^\top(x) F_n\|^2 \leq \lambda^2 \|Z_n(x)\|^2. \]

Rearranging and combining with (5), we arrive at

\[ \sigma_n^2(x) = \sup_{f: |f|_{H_k} \leq 1} \left( f(x) - Z_n^\top(x) F_n \right)^2 + \lambda^2 \|Z_n(x)\|^2. \]

### D Proof of Theorems 1 and 2

Recall the closed form expression for the posterior mean of GP models \( \mu_n(x) = Z_n^\top(x) Y_n \). We can expand the prediction error in terms of prediction error due to noise-free observations and the effect of noise as follows

\[
\begin{align*}
    f(x) - \mu_n(x) &= f(x) - Z_n^\top(x) Y_n \\
    &= f(x) - Z_n^\top(x) F_n - Z_n^\top(x) E_n. \\
    &= f(x) - Z_n^\top(x) F_n - Z_n^\top(x) E_n.
\end{align*}
\]

(6)

We now use Proposition 1 to bound both terms.

**Prediction error due to noise free observations** can be simply bounded by \( B \sigma_n \) as a direct result of Proposition 1. Specifically let \( \tilde{f}(. \) = \( f(.) / B \) so that \( ||\tilde{f}||_{H_k} \leq 1 \). Also, let \( \tilde{F}_n = \left[ \tilde{f}(x_1), \tilde{f}(x_2), \ldots, \tilde{f}(x_n) \right]^\top \).\[
|f(x) - Z_n^\top(x) F_n| = B|\tilde{f}(x) - Z_n^\top(x) \tilde{F}_n| \\
\leq B \sigma_n(x),
\]

(7)

where the inequality follows from Proposition 1 and \( ||\tilde{f}||_{H_k} \leq 1 \).

We now proceed using Assumption 2 to prove Theorem 1.

**The effect of noise** is bounded using the sub-Gaussianity assumption. In particular, we show that \( Z_n^\top(x) E_n \) is a sub-Gaussian random variable whose moment generating function is bounded by that of a Gaussian random variable with variance \( \frac{R^2 \sigma_n^2(x)}{\lambda^2} \).

\[
\begin{align*}
    \mathbb{E} \left[ \exp(Z_n^\top(x) E_n) \right] &= \mathbb{E} \left[ \exp \left( \sum_{i=1}^n \zeta_i(x) \epsilon_i \right) \right] \\
    &= \prod_{i=1}^n \exp(\zeta_i(x) \epsilon_i) \\
    &\leq \prod_{i=1}^n \exp \left( \frac{R^2 \zeta_i(x)^2}{2} \right) \\
    &= \exp \left( \frac{R^2 \sum_{i=1}^n \zeta_i(x)^2}{2} \right) \\
    &= \exp \left( \frac{R^2 \|Z_n(x)\|^2}{2} \right) \\
    &\leq \exp \left( \frac{R^2 \sigma_n^2(x)}{2 \lambda^2} \right). \\
\end{align*}
\]

where the second equation is a result of independence of \( \zeta_i(x) \epsilon_i \) terms that follows from the assumptions of i.i.d. noise terms and \( X_n \) being independent of \( E_n \). The first inequality holds by Assumption 2. We utilize Proposition 1 to conclude that \( \|Z_n(x)\|^2 \leq \frac{\sigma_n^2(x)}{\lambda^2} \) which results in the
second inequality. Thus, using Chernoff-Hoeffding inequality [Antonini et al., 2008],

\[
Z_n(x)E_n \geq -\frac{\sigma_n(x)R}{\lambda} \sqrt{2 \log(\frac{1}{\delta})} \text{ w.p. at least } 1 - \delta,
\]

\[
Z_n(x)E_n \leq \frac{\sigma_n(x)R}{\lambda} \sqrt{2 \log(\frac{1}{\delta})} \text{ w.p. at least } 1 - \delta.
\] (8)

Putting together (6), (7) and (8), Theorem 1 is proven.

We now move to the proof of Theorem 2. For the simplicity of the notation let us use

\[
\tau = \|Z_n(x)\| \sqrt{2(\xi_0 \vee \frac{2 \log(1/\delta)}{h_0^2}) \log(\frac{1}{\delta})},
\] (9)

\[
\xi = \xi_0 \vee \frac{2 \log(1/\delta)}{h_0^2}.
\] (10)

We have, for \( \theta = \frac{\tau}{\xi \|Z_n(x)\|^2} \),

\[
\Pr[Z_n^T(x)E_n \geq \tau] = \Pr \left[ \exp(\theta Z_n^T(x)E_n) \geq \exp(\theta \tau) \right]
\]

\[
\leq \exp(-\theta \tau) \mathbb{E} \left[ \exp(\theta Z_n^T(x)E_n) \right]
\]

\[
= \exp(-\theta \tau) \mathbb{E} \left[ \exp \left( \sum_{i=1}^n \theta \zeta_i(x) \epsilon_i \right) \right]
\]

\[
= \exp(-\theta \tau) \prod_{i=1}^n \mathbb{E} \left[ \exp(\theta \zeta_i(x) \epsilon_i) \right]
\]

\[
\leq \exp(-\theta \tau) \prod_{i=1}^n \exp \left( \frac{1}{2} \xi_0 \theta^2 (\zeta_i(x))^2 \right)
\]

\[
= \exp \left( \frac{1}{2} \xi_0 \theta^2 \|Z_n(x)\|^2 - \theta \tau \right)
\]

\[
= \exp \left( \frac{\xi_0 \tau^2}{2\xi^2 \|Z_n(x)\|^2} - \frac{\tau^2}{\xi \|Z_n(x)\|^2} \right)
\]

\[
\leq \exp \left( \frac{-\tau^2}{2\|Z_n(x)\|^2} \right)
\]

\[
= \delta.
\] (11)

The first line is obtained since \( \exp(\theta z) \) is an increasing function in \( z \). The first inequality amounts for an application of Markov inequality. The fourth line is a result of independence of \( \zeta_i(x) \epsilon_i \) terms that follows from the assumptions of i.i.d. noise terms and \( X_n \) being independent of \( E_n \). The second inequality holds by definition of light-tailed distributions. Notice that the careful choice of \( \tau \) and \( \theta \) ensures \( \theta \zeta_i(x) \leq h_0 \), which will be validated next. The seventh line is obtained by replacing the value of \( \theta \). The last inequality is obtained by \( \xi_0 \leq \xi \). The last line is resulted from replacing the value of \( \tau \) from (9).

It remains to validate \( \theta \zeta_i(x) \leq h_0 \).

\[
\theta \zeta_i(x) = \frac{\tau}{\xi \|Z_n(x)\|^2} \zeta_i(x)
\]

\[
= \frac{\sqrt{2 \log(\frac{1}{\delta})} \zeta_i(x)}{\sqrt{\xi \|Z_n(x)\|^2}}
\]

\[
\leq h_0 \frac{\zeta_i(x)}{\|Z_n(x)\|^2}
\]

\[
\leq h_0,
\]
where we replace $\theta = \frac{\tau}{\xi ||Z_n||^2}$, and the values of $\tau$ and $\xi$ from (9) and (10), respectively. For the first inequality, notice that $\frac{2 \log(1/\delta)}{h_0^2} \leq \xi$ from the definition of $\xi$ (10). For the second inequality notice that $\zeta_i(x) \leq ||Z_n(x)||$.

We thus proved

$$Z_n(x)E_n \leq \tau, \text{ w.p. at least } 1 - \delta.$$ (12)

Similarly, we can prove

$$Z_n(x)E_n \geq -\tau, \text{ w.p. at least } 1 - \delta.$$ (13)

Replacing $||Z_n(z)|| \leq \frac{R}{\lambda} \sigma_n(x)$ from Proposition 1 in the value of $\tau$ (9), and combining (12) and (13) with (6) and (7), Theorem 2 is proven.

E Proof of Theorem 3

The MVR algorithm selects the points with the highest variance first. Thus, $\forall x \in \mathcal{X}$,

$$\sigma^2_{n-1}(x) \leq \sigma^2_{n-1}(x_n).$$ (14)

By definition of conditional variance of normal distributions and due to positive definiteness of covariance matrix, conditioning on a larger set of points reduces the variance. Specifically, we have, for all $x \in \mathcal{X}$ and $\forall n \leq N$,

$$\sigma^2_N(x) \leq \sigma^2_{n-1}(x).$$ (15)

Combining (14) and (15), we have, $\forall x \in \mathcal{X}$ and $\forall n \leq N$,

$$\sigma^2_N(x) \leq \sigma^2_{n-1}(x_n).$$

Averaging both sides over $n$ (from 1 to $N$), we have

$$\sigma^2_N(x) \leq \frac{1}{N} \sum_{n=1}^{N} \sigma^2_{n-1}(x_n).$$ (16)

We now use the following lemma to bound $\sigma^2_N(x)$.

**Lemma 2** Recall $I(Y_n; \hat{f}) = \frac{1}{2} \log \det(I_n + \frac{1}{\lambda^2} k(X_n, X_n))$. For the cumulative conditional variance of the GP model, we have

$$\sum_{n=1}^{N} \sigma^2_{n-1}(x_n) \leq \frac{2}{\log(1 + \frac{1}{\lambda^2})} I(Y_n; \hat{f}).$$

A proof can be found in Srinivas et al. [2010].

We thus have, for all $x \in \mathcal{X}$,

$$\sigma^2_N(x) \leq \frac{2 I(Y_n; \hat{f})}{\log(1 + \frac{1}{\lambda^2})N} \leq \frac{2 \gamma_N}{\log(1 + \frac{1}{\lambda^2})N},$$ (17)

where $\gamma_N$ is the maximal information gain defined in Sec. 2.4.

Let $B_0(\delta) = B + \sqrt{N} \beta(2\delta/N)$. At the end of this section, in Lemma 4, we prove that

$$\|\mu_N\|_{H_k} \leq B_0(\delta), \text{ w.p. at least } 1 - \delta.$$ (18)

Notice that $\mu_n$ is a random function due to the randomness in noise. Let us define the event $\mathcal{E} = \{\|\mu_N\|_{H_k} \leq B_0(\delta/3)\}$. We have $\Pr[\mathcal{E}] \geq 1 - \frac{\delta}{3}$. 

19
We now prove a high probability upper bound on

Thus, assuming that the inequality given in (19), the confidence interval for

Using (17) to bound

Using a probability union bound, we have,

We thus have, under event $E$

The first inequality comes from Assumption 4 on discretization $D_N(δ)$ and $f$. The second inequality comes from the definition of MVR which ensures $μ_N(\hat{x}_N^*) ≥ μ_N(x)$, for all $x ∈ X$. For the last inequality, we use Assumption 4 on the existence of a discretization $D_N(δ)$ and $μ_N$. Notice that under event $E$, the posterior mean of the GP model belongs to the same RKHS with its norm bounded by $B_0(δ/3)$.

Thus, assuming that the inequality given in (19), the confidence interval for $f(x^*)$ with $1 − δ/3$ confidence, and $E$, all three hold true (notice that each of these three events hold true with probability at least $1 − \frac{δ}{3}$), using a probability union bound, we have

Using (17) to bound $σ_N(x^*)$ and $σ_N(\hat{x}_N^*)$, and replacing $|D_N(δ)|$ with its upper bound, we get

which completes the proof.

We now prove a high probability upper bound on $\|μ_n\|_{H_k}$.

Let us first formally state the equivalence of the posterior mean in GP models and the regressor in kernel ridge regression.

Lemma 3 Conditioned on a set of noisy observation $H_n$ from $f$, recall the expression for the posterior mean of the GP model $μ_n(x) = Z_n^\top(x)Y_n$. We have the following equality

$$μ_n = \arg\min_{g ∈ H_k} \left( λ^2\|g\|^2_{H_k} + \sum_{i=1}^n (g(x_i) − y_i)^2 \right).$$
For a proof, see [Kanagawa et al., 2018, Theorem 3.4]. Lemma 3 establishes the equivalence of the posterior mean in GP models and the regressor in kernel ridge regression. It indicates that the posterior mean of GP models is a mean squared error estimator, regularized by the RKHS norm, where $\lambda^2$ is the regularization parameter. We use this lemma to show that the posterior mean of the GP model with high probability lives in the same RKHS as $f$.

**Lemma 4** Conditioned on a set of noisy observation $\mathcal{H}_n$ from $f$ with $\|f\|_{\mathcal{H}_k} \leq B$, the RKHS norm of the posterior mean of the GP model $\mu_n(x) = Z_n^T(x)Y_n$ satisfies the following

$$\|\mu_n\|_{\mathcal{H}_k} \leq B + \sqrt{n}\beta(2\delta/n), \text{ w.p. at least } 1 - \delta,$$

where $\beta(\delta) = \frac{B}{\sqrt{2}} \sqrt{2 \log \left(\frac{1}{\delta}\right)}$ under Assumption 2, and $\beta(\delta) = \frac{1}{\sqrt{2}} \sqrt{2 \log \left(\frac{1}{\delta}\right)} \log \left(\frac{1}{\delta}\right)$ under Assumption 3.

**Proof of Lemma 4:** We have

$$\|\mu_n\|_{\mathcal{H}_k} = \|Z_n^T(\cdot)F_n + Z_n^T(\cdot)\|_{\mathcal{H}_k} \leq \|Z_n^T(\cdot)\|_{\mathcal{H}_k} + \|Z_n^T(\cdot)\|_{\mathcal{H}_k}.$$  

From Lemma 3, we have

$$\lambda^2\|Z_n^T(\cdot)\|_{\mathcal{H}_k}^2 + \sum_{i=1}^{n}(Z_n^T(x_i)F_n - f(x_i))^2 \leq \lambda^2\|f\|_{\mathcal{H}_k}^2 + \sum_{i=1}^{n}(f(x_i) - f(x_i))^2$$

Thus,

$$\|Z_n^T(\cdot)\|_{\mathcal{H}_k} \leq \|f\|_{\mathcal{H}_k},$$

where $\|f\|_{\mathcal{H}_k} \leq B$. It thus remains to bound the second term on the right hand side of (24).

$$\|Z_n^T(\cdot)\|_{\mathcal{H}_k}^2 = \|k^T(x, X_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1} E_n\|_{\mathcal{H}_k}^2$$

$$= E_n^T (k(X_n, X_n) + \lambda^2 I_n)^{-1} k(X_n, X_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1} E_n$$

$$= E_n^T (k(X_n, X_n) + \lambda^2 I_n)^{-1} (k(X_n, X_n) + \lambda^2 I_n) (k(X_n, X_n) + \lambda^2 I_n)^{-1} E_n$$

$$- \lambda^2 E_n^T (k(X_n, X_n) + \lambda^2 I_n)^{-2} E_n$$

$$\leq E_n^T (k(X_n, X_n) + \lambda^2 I_n)^{-1} E_n$$

$$\leq \frac{1}{\lambda^2}\|E_n\|_{L_2}^2,$$

where for the second line we used the reproducing property of the RKHS, for the first inequality we used positive definiteness of $(k(X_n, X_n) + \lambda^2 I_n)^{-2}$ that is a result of positive definiteness of $k(X_n, X_n)$, and for the last inequality we used positive definiteness of $k(X_n, X_n)$.

Under Assumption 2, as a result of Chernoff-Hoeffding inequality,

$$\epsilon_i^2 \leq 2R^2 \log \left(\frac{1}{2\delta^2}\right), \text{ w.p. at least } 1 - \delta'.$$

Using a probability union bound over $i = 1, 2, \ldots, n$, with $\delta' = \frac{\delta}{n}$,

$$\frac{1}{\lambda^2}\|E_n\|_{L_2}^2 \leq \frac{2nR^2}{\lambda^2} \log \left(\frac{n}{2\delta^2}\right), \text{ w.p. at least } 1 - \delta.$$  

Under Assumption 3, as a result of (11) (with $n = 1$, and $Z_n = 1$),

$$\epsilon_i^2 \leq 2(\xi_0 + \frac{2\log(1/2\delta^2)}{\delta^2}) \log \left(\frac{1}{2\delta^2}\right), \text{ w.p. at least } 1 - \delta'.$$

Using a probability union bound over $i = 1, 2, \ldots, n$, with $\delta' = \frac{\delta}{n}$,

$$\frac{1}{\lambda^2}\|E_n\|_{L_2}^2 \leq \frac{2nR^2}{\lambda^2} (\xi_0 + \frac{2\log(n/2\delta)^2}{\delta^2}) \log \left(\frac{n}{2\delta^2}\right), \text{ w.p. at least } 1 - \delta.$$  

(27)

Combining the bounds on the both terms on the right hand side of (24), the lemma is proven.
F  Proof of Corollary 1

We use Theorem 3 to derive a bound on the expected regret of MVR.

First, notice that $|f(x)| \leq k_0 B$ where $k_0 = \max_{x \in X} k(x, x)$, which can be proven using the reproducing property of the RKHS.

$$|f(x)| = \|f(x)\|_{H_k} \leq \|f\|_{H_k} \max_{x \in X} k(x, x) = \|f\|_{H_k} \sqrt{k(x, x)} \leq k_0 B.$$ 

So, we have $\max_{x \in X} f(x^*) - f(x) \leq 2k_0 B$. Let $E$ denote the event that $r_{N}^{\text{MVR}} \leq \bar{r}$, where

$$\bar{r} = \sqrt{\frac{2\gamma N}{\log(1 + \frac{1}{\pi})^N}} \left( 2B + \beta(1 + \frac{1}{3\sqrt{N}}) + \beta \left( \frac{1}{3C\sqrt{N}} \left( B + \sqrt{N}\beta(2/3N\sqrt{N})^d N^{d/2} \right) \right) \right) + \frac{2}{\sqrt{N}}$$

is the upper bound on regret given in Theorem 3 with $\delta = \frac{1}{\sqrt{N}}$. From Theorem 3, we have $\Pr\{E\} \geq 1 - \frac{1}{\sqrt{N}}$.

Using the law of total expectation, we have

$$E[r_{N}^{\text{MVR}}] = E[E[r_{N}^{\text{MVR}}|E] Pr[E] + E[r_{N}^{\text{MVR}}|\bar{E}] Pr[\bar{E}] \leq \bar{r} + \frac{2k_0 B}{\sqrt{N}} = O \left( \frac{\gamma N}{N} \beta(N^{d+\frac{1}{2}}) \right).$$

Under Assumption 2

$$E[r_{N}^{\text{MVR}}] = O \left( \frac{\gamma N}{N} \log(N^{d+\frac{1}{2}}) \right). \quad (28)$$

Under Assumption 3

$$E[r_{N}^{\text{MVR}}] = O \left( \frac{\gamma N}{N} \log(N^{d+\frac{1}{2}}) \right). \quad (29)$$

For SE kernel, $\gamma_N = O \left( \log^{d+1}(N) \right)$ [Srinivas et al., 2010]. Selecting $N \propto \left( \frac{1}{\epsilon} \right)^2 \log^{d+2}(\frac{1}{\epsilon})$ and $N \propto \left( \frac{1}{\epsilon} \right)^2 \log^d(\frac{1}{\epsilon})$, with proper constants, under Assumptions 2 and 3, respectively, results in $E[r_{N}^{\text{MVR}}] \leq \epsilon$. In the case of Matérn kernel, $\gamma_N = O \left( N^{\frac{d}{2\nu} \log(N)} \right)$ [Vakili et al., 2020a]. Selecting $N \propto \left( \frac{1}{\epsilon} \right)^{2+\frac{d}{2}} (\log(\frac{1}{\epsilon}))^{\frac{d}{2\nu}+2}$ and $N \propto \left( \frac{1}{\epsilon} \right)^{2+\frac{d}{2}} (\log(\frac{1}{\epsilon}))^{\frac{d}{2\nu}+2}$, with proper constants, under Assumptions 2 and 3, respectively, results in $E[r_{N}^{\text{MVR}}] \leq \epsilon$.

Finding the exact constants requires solving a non-linear equation involving log function which is a tedious task.

Noticing that $E[r_{n}^{\text{MVR}}]$ is a decreasing function in $n$ completes the proof.

G  Supplemental Material on the Experiments

In this section, we provide further details on the experiments. We also provide additional experiments on two commonly used benchmark functions for Bayesian optimization.
G.1 Additional Experiments

In Section 5, we provided experiments on the comparison of the simple regret performance of Bayesian optimization algorithms on synthetically generated functions in RKHS. In this section, we consider two commonly used benchmark functions for Bayesian optimization: Hartman3 and Rosenbrock as presented in Azimi et al. [2012], Picheny et al. [2013]. The parameters of the kernels, noise and $\lambda$ are set exactly as described in Section 5. We plot the average simple regret for all four learning algorithms considered in Section 5, over 50 independent experiments, with Hartman3 test function in Figure 2, and with Rosenbrock test function in Figure 3. The details on the source code is provided in the next section. The data used for generating the figures is provided in the supplementary material.

![Graphs showing comparison of simple regret performance for Bayesian optimization algorithms on Hartman3 test function](image)

(a) SE, Gaussian Noise  
(b) Matérn, Gaussian Noise  
(c) SE, Laplace Noise  
(d) Matérn, Laplace Noise

Figure 2: Comparison of the simple regret performance of Bayesian optimization algorithms on Hartman3 test function.

G.2 Additional Details on the Experiments

In the paper, we have provided a complete theoretical analysis of sample complexity. Here, we briefly mention the computational complexity of the algorithms. There are two computational bottlenecks in implementing Bayesian optimization algorithms. First bottleneck is the update of the GP model based on past observations which requires an $O(n^3)$ computation at time $n$, due to the matrix inversion, $(k(X_n, X_n) + \lambda^2 I_n)^{-1}$, step. Sparse approximations of matrix inversion Calandriello et al. [2019] or sparse variational models Titsias [2009], Hensman et al. [2013], Vakili et al. [2020b] can reduce the computational complexity from $O(n^3)$ to $O(n)$, however at the price of introducing an approximation error. Second bottleneck is the selection of the observation point based on the acquisition functions which are summarized next for each algorithm.

- **IGP-UCB**: $\mu_n(x) + \beta_n^\delta \sigma_n(x)$ where $\beta_n^\delta = \left( B + R \sqrt{2(\gamma_n + 1 + \log(\frac{1}{\delta}))} \right)$.

- **GP-PI**: $\Pr[f(x) \geq \mu^+ + \alpha] = \Phi \left( \frac{\mu_n(x) - \mu^+ - \alpha}{\sigma_n(x)} \right)$, where $\mu^+ = \max_{i<n} \mu_i(x_i)$, $\alpha > 0$ is a user selected hyper-parameter (set to 0.01 in our experiments as suggested in Hoffman et al. [2011]), and $\Phi$ is the cumulative density function of the standard normal distribution.

- **GP-EI**: $\kappa \Phi \left( \frac{\kappa}{\sigma_n(x)} + \sigma_n(x) \phi \frac{\kappa}{\sigma_n(x)} \right)$, where $\kappa = \mu_n(x) - \mu^+ - \alpha$, and $\phi$ and $\Phi$ denote the probability density function and cumulative density function of the standard normal distribution, respectively. The parameters $\mu^+$ and $\alpha$ are set similar to GP-PI, following Hoffman et al. [2011].
Figure 3: Comparison of the simple regret performance of Bayesian optimization algorithms on Rosenbrock test function.

The standard approach in finding the maximizer of the acquisition function is to evaluate it on a grid discretizing the search space [Chowdhury and Gopalan, 2017]. For a grid of size $M$, this requires $O(Mn)$ computations at time $n$. We have used the same discretization for all algorithms.

A practical idea to improve the computational cost in implementing Bayesian optimization algorithms is to use an off-the-shelf optimizer to solve the optimization of the acquisition function at each iteration (instead of using a grid). This method, although can lead to significant gains in computational complexity, invalidates the existing regret bounds, due to lack of guarantees for an accurate optimization of the acquisition function (that is often non-convex). We have thus used the discretization method following most related work with analytical regret guarantees [e.g., Srinivas et al., 2010, Chowdhury and Gopalan, 2017].