Bayesian Optimization under Heavy-tailed Payoffs

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Abstract

We consider black box optimization of an unknown function in the nonparametric Gaussian process setting when the noise in the observed function values can be heavy tailed. This is in contrast to existing literature that typically assumes sub-Gaussian noise distributions for queries. Under the assumption that the unknown function belongs to the Reproducing Kernel Hilbert Space (RKHS) induced by a kernel, we first show that an adaptation of the well-known GP-UCB algorithm with reward truncation enjoys sublinear $\tilde{O}\left(T^{\frac{2+\alpha}{2(1+\alpha)}}\right)$ regret even with only the $(1+\alpha)$-th moments, $\alpha \in (0,1]$, of the reward distribution being bounded ($\tilde{O}$ hides logarithmic factors). However, for the common squared exponential (SE) and Matérn kernels, this is seen to be significantly larger than a fundamental $\Omega(T^{\frac{1}{1+\alpha}})$ lower bound on regret. We resolve this gap by developing novel Bayesian optimization algorithms, based on kernel approximation techniques, with regret bounds matching the lower bound in order for the SE kernel. We numerically benchmark the algorithms on environments based on both synthetic models and real-world data sets.

1 Introduction

Black-box optimization of an unknown function $f : \mathbb{R}^d \to \mathbb{R}$ with expensive, noisy queries is a generic problem arising in domains such as hyper-parameter tuning for complex machine learning models [3], sensor selection [14], synthetic gene design [15], experimental design etc. The popular Bayesian optimization (BO) approach, towards solving this problem, starts with a prior distribution, typically a nonparametric Gaussian process (GP), over a function class, uses function evaluations to compute the posterior distribution over functions, and chooses the next function evaluation adaptively – using a sampling strategy – towards reaching the optimum. Popular sampling strategies include expected improvement [25], probability of improvement [40], upper confidence bounds [35], Thompson sampling [11], predictive-entropy search [17], etc.

The design and analysis of adaptive sampling strategies for BO typically involves the assumption of bounded, or at worst sub-Gaussian, distributions for rewards (or losses) observed by the learner, which is quite light-tailed. Yet, many real-world environments are known to exhibit heavy-tailed behavior, e.g., the distribution of delays in data networks is inherently heavy-tailed especially with highly variable or bursty traffic flow distributions that are well-modeled with heavy tails [20], heavy-tailed price fluctuations are common in finance and insurance data [29], properties of complex networks often exhibit heavy tails such as degree distribution [37], etc. This motivates studying methods for Bayesian optimization when observations are significantly heavy tailed compared to Gaussian.

A simple version of black box optimization – in the form of online learning in finite multi-armed bandits (MABs) – with heavy-tailed payoffs, was first studied rigorously by Bubeck et al. [8], where the payoffs are assumed to have bounded $(1+\alpha)$-th moment for $\alpha \in (0,1]$. They showed that for

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MABs with only finite variances (i.e., $\alpha = 1$), by using statistical estimators that are more robust than the empirical mean, one can still recover the optimal regret rate for MAB under the sub-Gaussian assumption. Moving further, Medina and Yang [24] consider these estimators for the problem of linear (parametric) stochastic bandits under heavy-tailed rewards and Shao et al. [34] show that almost optimal algorithms can be designed by using an optimistic, data-adaptive truncation of rewards. Some other important works include pure exploration under heavy-tailed noise [43], payoffs with bounded kurtosis [23], extreme bandits [10], heavy tailed payoffs with $\alpha \in (0, \infty)$ [38].

Against this backdrop, we consider regret minimization with heavy-tailed reward distributions in bandits with a potentially continuous arm set, and whose (unknown) expected reward function is nonparametric and assumed to have smoothness compatible with a kernel on the arm set. Here, it is unclear if existing BO techniques relying on statistical confidence sets based on sub-Gaussian observations can be made to work to attain nontrivial regret, since it is unlikely that these confidence sets will at all be correct. It is worth mentioning that in the finite dimensional setting, Shao et al. [34] solve the problem almost optimally, but their results do not carry over to the general nonparametric kernelized setup since their algorithms and regret bounds depend crucially on the finite feature dimension. We answer this affirmatively in this work, and formalize and solve BO under heavy tailed noise almost optimally. Specifically, this paper makes the following contributions.

- We adapt the GP-UCB algorithm to heavy-tailed payoffs by a truncation step, and show that it enjoys a regret bound of $\tilde{O}(\gamma_T T^{\frac{2+\alpha}{2(1+\alpha)}})$ where γ_T depends on the kernel associated with the RKHS and is generally sub-linear in T. This regret rate, however, is potentially sub-optimal due to a $\Omega(T^{\frac{1}{1+\alpha}})$ fundamental lower bound on regret that we show for two specific kernels, namely the squared exponential (SE) kernel and the Matérn kernel.
- We develop a new Bayesian optimization algorithm by truncating rewards in each direction of an approximate, finite-dimensional feature space. We show that the feature approximation can be carried out by two popular kernel approximation techniques: Quadrature Fourier features [26] and Nyström approximation [9]. The new algorithm under either approximation scheme gets regret $\tilde{O}(\gamma_T T^{\frac{1}{1+\alpha}})$, which is optimal upto log factors for the SE kernel.
- Finally, we report numerical results based on experiments on synthetic as well as real-world based datasets, for which the algorithms we develop are seen to perform favorably in the harsher heavy-tailed environments.

Related work. An alternative line of work uses approaches for black box optimization based on Lipschitz-type smoothness structure [22, 7, 2, 33], which is qualitatively different from RKHS smoothness type assumptions. Recently, Bogunovic et al. [5] consider GP optimization under an adversarial perturbation of the query points. But, the observation noise is assumed to be Gaussian unlike our heavy-tailed environments. Kernel approximation schemes in the context of BO usually focuses on reducing the cubic cost of gram matrix inversion [39, 41, 26, 9]. However, we crucially use these approximations to achieve optimal regret for BO under heavy tailed noise, which, we believe, might not be possible without resorting to the kernel approximations.

2 Problem formulation

Let $f : \mathcal{X} \rightarrow \mathbb{R}$ be a fixed but unknown function over a domain $\mathcal{X} \subset \mathbb{R}^d$ for some $d \in \mathbb{N}$. At every round, a learner queries f at a single point $x_t \in \mathcal{X}$, and observes a noisy payoff $y_t = f(x_t) + \eta_t$. Here the noise sequence $\eta_t, t \geq 1$ are assumed to be zero mean i.i.d. random variables such that the payoffs satisfy $\mathbb{E}\left[|y_t|^{1+\alpha} |\mathcal{F}_{t-1}\right] \leq v$ for some $\alpha \in (0, 1]$ and $v \in (0, \infty)$, where $\mathcal{F}_{t-1} = \sigma(\{x_\tau, y_\tau)\}_{\tau=1}^{t-1}, x_t)$ denotes the σ-algebra generated by the events so far[1]. Observe that this bound on the $(1 + \alpha)$-th moment at best yields bounded variance for y_t, and does not necessarily mean that y_t (or η_t) is sub-Gaussian as is assumed typically. The query point x_t at round t is chosen causally depending upon the history $\{(x_s, y_s)\}_{s=1}^{t-1}$ of query and payoff sequences available up to round $t - 1$. The learner's goal is to maximize its (expected) cumulative reward $\sum_{t=1}^{T} f(x_t)$ over a time horizon T or equivalently minimize its cumulative *regret* $R_T = \sum_{t=1}^{T} (f(x^\star) - f(x_t))$, where

[1]If instead the moment bound holds for each η_t then this can be translated to a moment bound for each y_t using, say, a bound on $f(x)$.

$x^\star \in \operatorname{argmax}_{x\in\mathcal{X}} f(x)$ is a maximum point of f (assuming the maximum is attained; not necessarily unique). A sublinear growth of R_T with T implies the time-average regret $R_T/T \to 0$ as $T \to \infty$.

Regularity assumptions: Attaining sub-linear regret is impossible in general for arbitrary reward functions f, and thus some regularity assumptions are needed. In this paper, we assume smoothness for f induced by the structure of a kernel on $\mathcal{X}$. Specifically, we make the standard assumption of a p.s.d. kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that $k(x,x) \le 1$ for all $x \in \mathcal{X}$, and f being an element of the reproducing kernel Hilbert space (RKHS) $\mathcal{H}_k(\mathcal{X})$ of smooth real valued functions on $\mathcal{X}$. Moreover, the RKHS norm of f is assumed to be bounded, i.e., $\|f\|_{\mathcal{H}} \le B$ for some $B < \infty$. Boundedness of k along the diagonal holds for any stationary kernel, i.e., where $k(x,x') = k(x-x')$, e.g., the *Squared Exponential* kernel k_{SE} and the *Matérn* kernel $k_{\text{Matérn}}$:

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

where $l > 0$ and $\nu > 0$ are hyperparameters of the kernels, $r = \|x - x'\|_2$ is the distance between x and x', and B_ν is the modified Bessel function.

3 Warm-up: the first algorithm

Towards designing a BO algorithm for heavy tailed observations, we briefly recall the standard GP-UCB algorithm for the sub-Gaussian setting. GP-UCB at time t chooses the point $x_t = \operatorname{argmax}_{x\in\mathcal{X}} \mu_{t-1}(x) + \beta_t\sigma_{t-1}(x)$ where $\mu_t(x) = k_t(x)^T(K_t + \lambda I_t)^{-1}Y_t$ and $\sigma_t^2(x) = k(x,x) - k_t(x)^T(K_t + \lambda I_t)^{-1}k_t(x)$ are the posterior mean and variance functions after t observations from a function drawn from the GP prior $GP_{\mathcal{X}}(0,k)$, with additive i.i.d. Gaussian noise $\mathcal{N}(0,\lambda)$. Here $Y_t = [y_1,\ldots,y_t]^T$ is the vector formed by observations, $K_t = [k(u,v)]_{u,v\in\mathcal{X}_t}$ is the kernel matrix computed at the set $\mathcal{X}_t = \{x_1,\ldots,x_t\}$, $k_t(x) = [k(x_1,x),\ldots,k(x_t,x)]^T$ and I_t is the identity matrix of order t. If the noise η_t is assumed conditionally R-sub-Gaussian, i.e., $\mathbb{E}\left[e^{\gamma\eta_t} \mid \mathcal{F}_{t-1}\right] \le \exp\left(\frac{\gamma^2R^2}{2}\right)$ for all $\gamma\in\mathbb{R}$, then using $\beta_{t+1} = O\left(R\sqrt{\ln|I_t + \lambda^{-1}K_t|}\right)$ ensures $\tilde{O}(\sqrt{T})$ regret [11], as the posterior GP concentrates rapidly on the true function f. However, when the sub-Gaussian assumption does not hold, we cannot expect the posterior GP to have such nice concentration property. In fact, it is known that the ridge regression estimator $\mu_t \in \mathcal{H}_k(\mathcal{X})$ of f is not robust when the noise exhibits heavy fluctuations [19]. So, in order to tackle heavy tailed noise, one needs more robust estimates $\widehat{\mu}_t$ of f along with suitable confidence sets. A natural idea to curb the effects of heavy fluctuations is to truncate high rewards [8]. Our first algorithm Truncated GP-UCB (Algorithm 1) is based on this idea.

Truncated GP-UCB (TGP-UCB) algorithm: At each time t, we truncate the reward y_t to zero if it is larger than a suitably chosen truncation level b_t, i.e., we set the truncated reward $\widehat{y}_t = y_t\mathbb{1}_{|y_t|\le b_t}$. Then, we construct the truncated version of the posterior mean as $\widehat{\mu}_t(x) = k_t(x)^T(K_t+\lambda I_t)^{-1}\widehat{Y}_t$ where $\widehat{Y}_t = [\widehat{y}_1,\ldots,\widehat{y}_t]^T$ and simply run GP-UCB with $\widehat{\mu}_t$ instead of μ_t. The truncation level b_t can be adapted with time t. We choose an increasing sequence of b_t's, i.e., as time progresses and confidence interval shrinks, we truncate less and less aggressively. Finally, in order to account for the bias introduced by truncation, we blow up the confidence width β_t of GP-UCB by a multiplicative factor of b_t so that $f(x)$ is contained in the interval $\widehat{\mu}_{t-1}(x) \pm \beta_t\sigma_{t-1}(x)$ with high probability. This helps us to obtain a sub-linear regret bound for TGP-UCB given in the Theorem 1, with a full proof deferred to appendix B.

Algorithm 1 Truncated GP-UCB (TGP-UCB)

Input: Parameters $\lambda > 0$, $\{b_t\}_{t\ge1}$, $\{\beta_t\}_{t\ge1}$
Set $\widehat{\mu}_0(x) = 0$ and $\sigma_0^2(x) = k(x,x) \forall x \in \mathcal{X}$
for $t = 1,2,3\ldots$ **do**
  Play $x_t = \operatorname{argmax}_{x\in\mathcal{X}} \widehat{\mu}_{t-1}(x) + \beta_t\sigma_{t-1}(x)$ and observe payoff y_t
  Set $\widehat{y}_t = y_t\mathbb{1}_{|y_t|\le b_t}$ and $\widehat{Y}_t = [\widehat{y}_1,\ldots,\widehat{y}_t]^T$
  Compute $\widehat{\mu}_t(x) = k_t(x)^T(K_t + \lambda I_t)^{-1}\widehat{Y}_t$ and $\sigma_t^2(x) = k_t(x)^T(K_t + \lambda I_t)^{-1}k_t(x)$
end for

Theorem 1 (Regret bound for TGP-UCB) *Let $f \in \mathcal{H}_k(\mathcal{X})$, $\|f\|_{\mathcal{H}} \le B$ and $k(x,x) \le 1$ for all $x \in \mathcal{X}$. Let $\mathbb{E}\left[|y_t|^{1+\alpha}|\mathcal{F}_{t-1}\right] \le v < \infty$ for some $\alpha \in (0,1]$ and for all $t \ge 1$. Then, for any $\delta \in (0,1]$, TGP-UCB, with $b_t = v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}}$ and $\beta_{t+1} = B + \frac{3}{\sqrt{\lambda}}\, b_t\sqrt{\ln|I_t + \lambda^{-1}K_t| + 2\ln(1/\delta)}$,* *enjoys, with probability at least* $1-\delta$*, the regret bound*

$$R_T = O\left(B\sqrt{T\gamma_T} + v^{\frac{1}{1+\alpha}}\sqrt{\gamma_T\left(\gamma_T + \ln(1/\delta)\right)}T^{\frac{2+\alpha}{2(1+\alpha)}}\right),$$

where $\gamma_T \equiv \gamma_T(k,\mathcal{X}) = \max_{A\subset\mathcal{X}:|A|=T}\frac{1}{2}\ln\left|I_t + \lambda^{-1}K_A\right|$.

Here, γ_T denotes the *maximum information gain* about any $f \sim GP_{\mathcal{X}}(0,k)$ after T noisy observations obtained by passing f through an i.i.d. Gaussian channel $\mathcal{N}(0,\lambda)$, and measures the reduction in the uncertainty of f after T noisy observations. It is a property of the kernel k and domain $\mathcal{X}$, e.g., if $\mathcal{X}$ is compact and convex, then $\gamma_T = O\left((\ln T)^{d+1}\right)$ for k_{SE} and $O\left(T^{\frac{d(d+1)}{2\nu+d(d+1)}}\ln T\right)$ for $k_{\text{Matérn}}$ [35].

Remark 1. An R-sub-Gaussian environment satisfies the moment condition with $\alpha = 1$ and $v = R^2$, so the result implies a sub-linear $\tilde{O}(T^{3/4})$ regret bound for TGP-UCB in sub-Gaussian environments.

4 Regret lower bound

Establishing lower bounds under general kernel smoothness structure is an open problem even when the payoffs are Gaussian. Similar to Scarlett et al. [31], we only focus on the SE and Matérn kernels.

Theorem 2 (Lower bound on cumulative regret) *Let* $\mathcal{X} = [0,1]^d$ *for some* $d \in \mathbb{N}$*. Fix a kernel* $k \in \{k_{SE}, k_{Matérn}\}$*,* $B > 0$*,* $T \in \mathbb{N}$*,* $\alpha \in (0,1]$ *and* $v > 0$*. Given any algorithm, there exists a function* $f \in \mathcal{H}_k(\mathcal{X})$ *with* $\|f\|_{\mathcal{H}} \le B$*, and a reward distribution satisfying* $\mathbb{E}\left[|y_t|^{1+\alpha}|\mathcal{F}_{t-1}\right] \le v$ *for all* $t \in [T] := \{1,2,\ldots,T\}$*, such that when the algorithm is run with this* f *and reward distribution, its regret satisfies*

1. $\mathbb{E}[R_T] = \Omega\left(v^{\frac{1}{1+\alpha}}\left(\ln\left(v^{-\frac{1}{\alpha}}B^{\frac{1+\alpha}{\alpha}}T\right)\right)^{\frac{d\alpha}{1+\alpha}}T^{\frac{1}{1+\alpha}}\right)$ *if* $k = k_{SE}$*,*
2. $\mathbb{E}[R_T] = \Omega\left(v^{\frac{\nu}{\nu(1+\alpha)+d\alpha}}B^{\frac{d\alpha}{\nu(1+\alpha)+d\alpha}}T^{\frac{\nu+d\alpha}{\nu(1+\alpha)+d\alpha}}\right)$ *if* $k = k_{Matérn}$*.*

The proof argument is inspired by that of Scarlett et al. [31], which provides the lower bound of BO under i.i.d. Gaussian noise, but with nontrivial changes to account for heavy tailed observations. The proof is based on constructing a finite subset of "difficult" functions in $\mathcal{H}_k(\mathcal{X})$. Specifically, we choose f as a uniformly sampled function from a finite set $\{f_1,\ldots,f_M\}$, where each f_j is obtained by shifting a common function $g \in \mathcal{H}_k(\mathbb{R}^d)$ by a different amount such that each of these has a unique maximum, and then cropping to $\mathcal{X} = [0,1]^d$. g takes values in $[-2\Delta, 2\Delta]$ with the maximum attained at $x = 0$. The function g is constructed properly, and the parameters Δ, M are chosen appropriately based on the kernel k, fixed constants B, T, α, v such that any Δ-optimal point for f_j fails to be Δ-optimal point for any other $f_{j'}$ and that $\|f_j\|_{\mathcal{H}} \le B$ for all $j \in [M]$. The reward function takes values in $\{sgn\left(f(x)\right)\left(\frac{v}{2\Delta}\right)^{\frac{1}{\alpha}}, 0\}$, with the former occurring with probability $\left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}}|f(x)|$, such that, for every $x \in \mathcal{X}$, the expected reward is $f(x)$ and $(1+\alpha)$-th raw moment is upper bounded by v. Now, if we can lower bound the regret averaged over $j \in [M]$, then there must exist some f_j for which the bound holds. The formal proof is deferred to Appendix C.

Remark 2. Theorem 2 suggests that (a) TGP-UCB may be suboptimal, and (b) for the SE kernel, it may be possible to design algorithms recovering $\tilde{O}(\sqrt{T})$ regret bound under finite variances ($\alpha = 1$).

5 An optimal algorithm under heavy tailed rewards

In view of the gap between the regret bound for TGP-UCB and the fundamental lower bound, it is possible that TGP-UCB (Algorithm 1) does not completely mitigate the effect of heavy-tailed fluctuations, and perhaps that truncation in a different domain may work better. In fact, for parametric linear bandits (i.e., BO with finite dimensional linear kernels), it has been shown that appropriate truncation in feature space improves regret performance as opposed to truncating raw observations [34], and in this case the feature dimension explicitly appears in the regret bound. However, the main challenge in the more general nonparametric setting is that the feature space is infinite dimensional, which would yield a trivial regret upper bound. If we can find an approximate feature map $\tilde{\varphi} : \mathcal{X} \to \mathbb{R}^m$ in a low-dimensional Euclidean inner product space $\mathbb{R}^m$ such that $k(x, y) \approx \tilde{\varphi}(x)^T \tilde{\varphi}(y)$, then we can perform the above feature adaptive truncation effectively as well as keep the error introduced due to approximation in control. Such a kernel approximation can be done efficiently either in a data independent way (Fourier features approximation [28]) or in a data dependent way (Nyström approximation [12]) and has been used in the context of BO to reduce the time complexity of GP-UCB [26, 9]. But in this work, the approximations are crucial to obtain optimal theoretical guarantees. We now describe our algorithm Adaptively Truncated Approximate GP-UCB (Algorithm 2).

5.1 Adaptively Truncated Approximate GP-UCB (ATA-GP-UCB) algorithm

At each round t, we select an arm x_t which maximizes the approximate (under kernel approximation) GP-UCB score $\tilde{\mu}_{t-1}(x) + \beta_t \tilde{\sigma}_{t-1}(x)$, where $\tilde{\mu}_{t-1}(x)$ and $\tilde{\sigma}^2_{t-1}(x)$ denote approximate posterior mean and variance from the previous round, respectively and β_t is an appropriately chosen confidence width. Then, we update $\tilde{\mu}_t(x)$ and $\tilde{\sigma}^2_t(x)$ as follows. First, we find a feature embedding $\tilde{\varphi}_t \in \mathbb{R}^{m_t}$, of some appropriate dimension m_t, which approximates the kernel efficiently. Then, we find the rows $u_1^T, \ldots, u_{m_t}^T$ of the matrix $\tilde{V}_t^{-1/2} \tilde{\Phi}_t^T$, where $\tilde{\Phi}_t = [\tilde{\varphi}_t(x_1), \ldots, \tilde{\varphi}_t(x_t)]^T$ and $\tilde{V}_t = \tilde{\Phi}_t^T \tilde{\Phi}_t + \lambda I_{m_t}$, and use those as the weight vectors for truncating the rewards in each of m_t directions by setting $\widehat{r}_i = \sum_{\tau=1}^{t} u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \le b_t}$ for all $i \in [m_t]$, where b_t specifies the truncation level. Then, we find our estimate of f as $\tilde{\theta}_t = \tilde{V}_t^{-1/2} [\widehat{r}_1, \ldots, \widehat{r}_{m_t}]^T$. Finally, we approximate the posterior mean as $\tilde{\mu}_t(x) = \tilde{\varphi}_t(x)^T \tilde{\theta}_t$ and the posterior variance as (i) $\tilde{\sigma}^2_t(x) = \lambda \tilde{\varphi}_t(x)^T \tilde{V}_t^{-1} \tilde{\varphi}_t(x)$ for the Fourier features approximation, or as (ii) $\tilde{\sigma}^2_t(x) = k(x, x) - \tilde{\varphi}_t(x)^T \tilde{\varphi}_t(x) + \lambda \tilde{\varphi}_t(x)^T \tilde{V}_t^{-1} \tilde{\varphi}_t(x)$ for the Nyström approximation. Now it only remains to describe how to find the feature embeddings $\tilde{\varphi}_t$.

(a) Quadrature Fourier features (QFF) approximation: If k is a bounded, continuous, positive definite, stationary kernel satisfying $k(x, x) = 1$, then by Bochner's theorem [4], k is the Fourier transform of a probability measure p, i.e., $k(x, y) = \int_{\mathbb{R}^d} p(\omega) \cos(\omega^T (x - y)) d\omega$. For the SE kernel, this measure has density $p(\omega) = \left(\frac{l}{\sqrt{2\pi}}\right)^d e^{-\frac{l^2 \|\omega\|_2^2}{2}}$ (abusing notation for measure and density). Mutny and Krause [26] show that for any stationary kernel k on $\mathbb{R}^d$ whose inverse Fourier transform decomposes product wise, i.e., $p(\omega) = \prod_{j=1}^{d} p_j(\omega_j)$, we can use Gauss-Hermite quadrature [18] to approximate it. If $\mathcal{X} = [0, 1]^d$, the SE kernel is approximated as follows. Choose $\bar{m} \in \mathbb{N}$ and $m = \bar{m}^d$, and construct the $2m$-dimensional feature map

$$\tilde{\varphi}(x)_i = \begin{cases} \sqrt{\nu(\omega_i)} \cos\left(\frac{\sqrt{2}}{l} \omega_i^T x\right) & \text{if } 1 \le i \le m, \\ \sqrt{\nu(\omega_{i-m})} \sin\left(\frac{\sqrt{2}}{l} \omega_{i-m}^T x\right) & \text{if } m + 1 \le i \le 2m. \end{cases} \tag{1}$$

Here the set $\{\omega_1, \ldots, \omega_m\} = \overbrace{A_{\bar{m}} \times \cdots \times A_{\bar{m}}}^{d \text{ times}}$, where $A_{\bar{m}}$ is the set of $\bar{m}$ (real) roots of the $\bar{m}$-th Hermite polynomial $H_{\bar{m}}$, and $\nu(z) = \prod_{j=1}^{d} \frac{2^{\bar{m}-1} \bar{m}!}{\bar{m}^2 H_{\bar{m}-1}(z_j)^2}$ for all $z \in \mathbb{R}^d$. For our purposes, we will have ATA-GP-UCB work with the embedding $\tilde{\varphi}_t(x) = \tilde{\varphi}(x)$ of dimension $m_t = 2m$ for all $t \ge 1$.

Remark 3. The seminal work of Rahimi and Recht [28] that develops random Fourier feature (RFF) approximation of any stationary kernel is based on the feature map $\tilde{\varphi}(x) = \frac{1}{\sqrt{m}} [\cos(\omega_1^T x), \ldots, \cos(\omega_m^T x), \sin(\omega_1^T x), \ldots, \sin(\omega_m^T x)]^T$, where each ω_i is sampled independently from $p(\omega)$. However, RFF embeddings do not appear to be useful for our purpose of achieving sublinear regret (see discussion after Lemma 1), so we work with the QFF embedding.

(b) Nyström approximation: Unlike the QFF approximation where the basis functions (cosine and sine) do not depend on the data, the basis functions used by the Nyström method are data dependent. For a set of points $\mathcal{X}_t = \{x_1, \ldots, x_t\}$, the Nyström method [42] approximates the kernel matrix K_t as follows: First sample a random number m_t of points from $\mathcal{X}_t$ to construct a dictionary $\mathcal{D}_t = \{x_{i_1}, \ldots, x_{i_{m_t}}\}; i_j \in [t]$, according to the following distribution. For each $i \in [t]$, include x_i in $\mathcal{D}_t$ independently with probability $p_{t,i} = \min\{q \tilde{\sigma}^2_{t-1}(x_i), 1\}$ for a suitably chosen parameter q (which trades off between the quality and the size of the embedding). Then, compute the (approximate) finite-dimensional feature embedding $\tilde{\varphi}_t(x) = \left(K_{\mathcal{D}_t}^{1/2}\right)^{\dagger} k_{\mathcal{D}_t}(x)$, where

$K_{\mathcal{D}_t} = [k(u,v)]_{u,v\in\mathcal{D}_t}$, $k_{\mathcal{D}_t}(x) = [k(x_{i_1},x),\ldots,k(x_{i_{m_t}},x)]^T$ and $A^\dagger$ denotes the pseudo inverse of any matrix A. We call the entire procedure NyströmEmbedding (pseudocode in appendix).

Algorithm 2 Adaptively Truncated Approximate GP-UCB (ATA-GP-UCB)

Input: Parameters $\lambda > 0$, $\{b_t\}_{t\geq 1}$, $\{\beta_t\}_{t\geq 1}$, q, a kernel approximation (QFF or Nyström)
Set: $\tilde{\mu}_0(x) = 0$ and $\tilde{\sigma}_0^2(x) = k(x,x)$ for all $x \in \mathcal{X}$
for $t = 1, 2, 3\ldots$ **do**
  Play $x_t = \mathrm{argmax}_{x\in\mathcal{X}}\, \tilde{\mu}_{t-1}(x) + \beta_t\tilde{\sigma}_{t-1}(x)$ and observe payoff y_t
  Set $\tilde{\varphi}_t(x) = \begin{cases}\tilde{\varphi}(x) & \textit{if QFF approximation}\\ \text{NyströmEmbedding}\big(\{(x_i,\tilde{\sigma}_{t-1}(x_i))\}_{i=1}^t, q\big) & \textit{if Nyström approximation}\end{cases}$
  Set $\tilde{\Phi}_t^T = [\tilde{\varphi}_t(x_1),\ldots,\tilde{\varphi}_t(x_t)]$ and $\tilde{V}_t = \tilde{\Phi}_t^T\tilde{\Phi}_t + \lambda I_{m_t}$, where m_t is the dimension of $\tilde{\varphi}_t$
  Find the rows $u_1^T,\ldots,u_{m_t}^T$ of $\tilde{V}_t^{-1/2}\tilde{\Phi}_t^T$ and set $\widehat{r}_i = \sum_{\tau=1}^t u_{i,\tau}y_\tau \mathbb{1}_{|u_{i,\tau}y_\tau|\leq b_t}$ for all $i\in[m_t]$
  Set $\tilde{\theta}_t = \tilde{V}_t^{-1/2}[\widehat{r}_1,\ldots,\widehat{r}_{m_t}]^T$ and compute $\tilde{\mu}_t(x) = \tilde{\varphi}_t(x)^T\tilde{\theta}_t$
  Set $\tilde{\sigma}_t^2(x) = \begin{cases}(i)\ \lambda\tilde{\varphi}_t(x)^T\tilde{V}_t^{-1}\tilde{\varphi}_t(x) & \textit{if QFF approximation}\\ (ii)\ k(x,x) - \tilde{\varphi}_t(x)^T\tilde{\varphi}_t(x) + \lambda\tilde{\varphi}_t(x)^T\tilde{V}_t^{-1}\tilde{\varphi}_t(x) & \textit{if Nyström approximation}\end{cases}$
end for

Remark 4. It is well known (λ-ridge leverage score sampling [1]) that, by sampling points proportional to their posterior variances $\sigma_t^2(x)$, one can obtain an accurate embedding $\tilde{\varphi}_t(x)$, which in turn gives an accurate approximation $\tilde{\sigma}_t^2(x)$. But, computation of $\sigma_t^2(x)$ in turn requires inverting K_t, which takes at most $O(t^3)$ time. So, we make use of the already computed approximations $\tilde{\sigma}_{t-1}^2(x)$ to sample points at round t, without significantly compromising on the accuracy of the embeddings [9].

Remark 5. The choice (i) of $\tilde{\sigma}_t^2(x)$ in Algorithm 2 ensures accurate estimation of the variance of x under the QFF approximation [26]. But, the same choice leads to severe underestimation of the variance under the Nyström approximation, specially when x is far away from $\mathcal{D}_t$. The choice (ii) of $\tilde{\sigma}_t^2(x)$ in Algorithm 2 is known as *deterministic training conditional* in the GP literature [27] and provably prevents the phenomenon of variance starvation under Nyström approximation [9].

5.2 Cumulative regret of ATA-GP-UCB with QFF embeddings

The following lemma shows that the data adaptive truncation of all the historical rewards and a good approximation of the kernel help us obtain a tighter confidence interval than TGP-UCB.

Lemma 1 (Tighter confidence sets with QFF truncation) *For any $\delta \in (0,1]$, ATA-GP-UCB with QFF approximation and parameters $b_t = (v/\ln(2mT/\delta))^{\frac{1}{1+\alpha}}\, t^{\frac{1-\alpha}{2(1+\alpha)}}$ and $\beta_{t+1} = B + 4\sqrt{m/\lambda}\ v^{\frac{1}{1+\alpha}}\,(\ln(2mT/\delta))^{\frac{\alpha}{1+\alpha}}\, t^{\frac{1-\alpha}{2(1+\alpha)}}$, ensures that with probability at least $1-\delta$, uniformly over all $t\in[T]$ and $x\in\mathcal{X}$,*

$$|f(x) - \tilde{\mu}_{t-1}(x)| \leq \beta_t\tilde{\sigma}_{t-1}(x) + O(B\varepsilon_m^{1/2}t^2), \tag{2}$$

where the QFF dimension m is such that $\sup_{x,y\in\mathcal{X}}\left|k(x,y) - \tilde{\varphi}(x)^T\tilde{\varphi}(y)\right| =: \varepsilon_m < 1$.

Here, the scaling $t^{\frac{1-\alpha}{2(1+\alpha)}}$ of the confidence width β_t is much less than the scaling $t^{\frac{1}{2(1+\alpha)}}$ of TGP-UCB, which eventually leads to a tighter confidence interval. However, in order to achive sublinear cumulative regret, we need to ensure that the approximation error ε_m decays at least as fast as $O(1/T^6)$ and feature dimension m grows no faster than polylog(T). This will ensure that the regret accumulated due to the second term in the RHS of 2 is $O(1)$, as well as the contribution from the first term is $\tilde{O}(T^{\frac{1}{1+\alpha}})$, since sum of the approximate posterior standard deviations grows only as $\tilde{O}(\sqrt{mT})$. Now, the QFF embedding (1) of k_{SE} can be shown to achieve $\varepsilon_m \leq d2^{d-1}\frac{1}{\sqrt{2}\bar{m}^{\bar{m}}}\left(\frac{e}{4l^2}\right)^{\bar{m}} = O\left(\frac{d2^{d-1}}{(\bar{m}l^2)^{\bar{m}}}\right)$ [26]. The decay is exponential when $\bar{m} > 1/l^2$ and $d = O(1)$[2]. Now, setting $\bar{m} = \Theta\left(\log_{4/e}\left(T^6\right)\right)$, we can ensure that $\varepsilon_m^{1/2}T^3 = O(1)$ and $m = O\left((\ln T)^d\right)$, and thus, in turn, a sublinear regret bound [3]. The following theorem states this formally, with a full proof deferred to Appendix D.2.

[2] For most BO applications, the effective dimensionality of the problem is low, e.g., additive models [21, 30].
[3] Under RFF approximation $\varepsilon_m = \tilde{O}(\sqrt{1/m})$ [36]. Hence, ATA-GP-UCB does not achieve sublinear regret.

Theorem 3 (Regret bound for ATA-GP-UCB with QFF embedding) *Fix any $\delta \in (0,1]$. Then, under the same hypothesis of Theorem 1, for $\mathcal{X} = [0,1]^d$ and $k = k_{SE}$, ATA-GP-UCB under QFF approximation, with parameters b_t and β_t set as in Lemma 1, and with the embedding $\tilde{\varphi}$ from 1 such that $\bar{m} > 1/l^2$ and $\bar{m} = \Theta\left(\log_{4/e}\left(T^6\right)\right)$, enjoys, with probability at least $1-\delta$, the regret bound*

$$R_T = O\left(B\sqrt{T(\ln T)^{d+1}} + v^{\frac{1}{1+\alpha}}\left(\ln\left(\frac{T(\ln T)^d}{\delta}\right)\right)^{\frac{\alpha}{1+\alpha}}\sqrt{\ln T}\,(\ln T)^d\,T^{\frac{1}{1+\alpha}}\right).$$

Remark 6. When the variance of the rewards is finite (i.e., $\alpha = 1$), the cumulative regret for ATA-GP-UCB under QFF approximation of the SE kernel is $O((\ln T)^{d+1}\sqrt{T})$, which now recovers the state-of-the-art regret bound of GP-UCB under sub-Gaussian rewards [26, Corollary 2] unlike the earlier TGP-UCB. It is worth pointing out that the bound in Theorem 3 is only for the SE kernel defined on $\mathcal{X} = [0,1]^d$, and designing a no-regret BO strategy under the QFF approximation of any other stationary kernel still remains a open question even when the rewards are sub-Gaussian [26].

5.3 Cumulative regret of ATA-GP-UCB with Nyström embeddings

Now, we will show that ATA-GP-UCB under Nyström approximation achives optimal regret for any stationary kernel defined on $\mathcal{X} \subset \mathbb{R}^d$ without any restriction on d. Similar to Lemma 1, ATA-GP-UCB under Nyström approximation also maintains tighter confidence sets than TGP-UCB. As before, the confidence sets are useful only if the dimension of the embeddings m_t grows no faster than polylog(t). Not only that, we also need to ensure that the approximate posterior variances are only a constant factor away from the exact ones. Then, since sum of the posterior standard deviations grows only as $O(\sqrt{T\gamma_T})$, we can achieve the optimal $\tilde{O}(T^{\frac{1}{1+\alpha}})$ regret scaling. Now for any $\varepsilon \in (0,1)$, setting $q = 6\frac{1+\varepsilon}{1-\varepsilon}\ln(2T/\delta)/\varepsilon^2$, the Nyström embeddings $\tilde{\varphi}_t$ can be shown to achieve $m_t \le 6\frac{1+\varepsilon}{1-\varepsilon}\left(1+\frac{1}{\lambda}\right) q\gamma_t$ and $\frac{1-\varepsilon}{1+\varepsilon}\sigma_t^2(x) \le \tilde{\sigma}_t^2(x) \le \frac{1+\varepsilon}{1-\varepsilon}\sigma_t^2(x)$ with probability at least $1-\delta$ [9], which helps us to achieve an optimal regret bound. The following theorem states this formally, with a full proof deferred to Appendix D.3.

Theorem 4 (Regret bound for ATA-GP-UCB with Nyström embedding) *Fix any $\delta \in (0,1]$, $\varepsilon \in (0,1)$ and set $\rho = \frac{1+\varepsilon}{1-\varepsilon}$. Then, under the same hypothesis of Theorem 1, ATA-GP-UCB under Nyström approximation, and with parameters $q = 6\rho\ln(4T/\delta)/\varepsilon^2$, $b_t = (v/\ln(4m_tT/\delta))^{\frac{1}{1+\alpha}}\, t^{\frac{1-\alpha}{2(1+\alpha)}}$ and $\beta_{t+1} = B(1+\frac{1}{\sqrt{1-\varepsilon}}) + 4\sqrt{m_t/\lambda}\, v^{\frac{1}{1+\alpha}}\,(\ln(4m_tT/\delta))^{\frac{\alpha}{1+\alpha}}\, t^{\frac{1-\alpha}{2(1+\alpha)}}$, enjoys, with probability at least $1-\delta$, the regret bound*

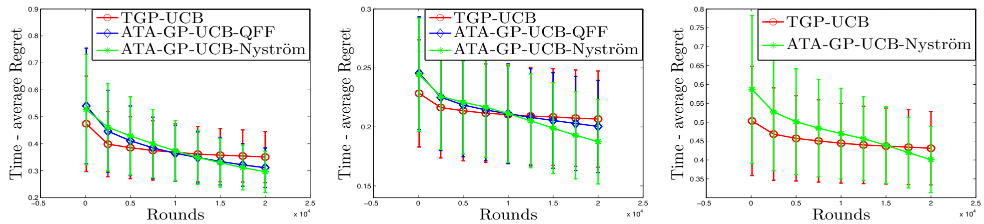
$$R_T = O\left(\rho B\left(1+\frac{1}{\sqrt{1-\varepsilon}}\right)\sqrt{T\gamma_T} + \frac{\rho^2}{\varepsilon}\,v^{\frac{1}{1+\alpha}}\left(\ln\left(\frac{\gamma_T\ln(T/\delta)T}{\delta}\right)\right)^{\frac{\alpha}{1+\alpha}}\sqrt{\ln(T/\delta)}\gamma_T T^{\frac{1}{1+\alpha}}\right).$$

Remark 7. Theorems 3 and 4 imply that ATA-GP-UCB achieves $\tilde{O}\big(v^{\frac{1}{1+\alpha}}(\ln T)^d T^{\frac{1}{1+\alpha}}\big)$ regret bound for k_{SE}, which matches the lower bound (Theorem 2) upto a factor of $\frac{\alpha}{1+\alpha}$ in the exponent of $\ln T$, as well as a few extra $\ln T$ factors hidden in the notation $\tilde{O}$. For the Matérn kernel, the bound is $\tilde{O}\big(T^{\frac{1}{1+\alpha}\frac{2\nu+(2+\alpha)d(d+1)}{2\nu+d(d+1)}}\big)$, which is sublinear only when $\frac{d(d+1)}{2\nu} < \alpha$[4], and the gap from the lower bound is more significant in this case. It is worth mentioning that a similar gap is present even for the (easier) setting of sub-Gaussian rewards [31] and there might exist better algorithms which can bridge this gap. When the variance of the rewards is finite (i.e., $\alpha = 1$), the cumulative regret for ATA-GP-UCB under Nyström approximation is $\tilde{O}(\gamma_T\sqrt{T})$, which recovers the state-of-the-art regret bound under sub-Gaussian rewards [9, Thm. 2]. For the linear bandit setting, i.e. when the feature map $\tilde{\varphi}_t(x) = x$ itself, substituting $\gamma_T = O(d\ln T)$, we find that the regret upper bound in Theorem 4 recovers the (optimal) regret bound of [34, Thm. 3] up to a logarithmic factor.

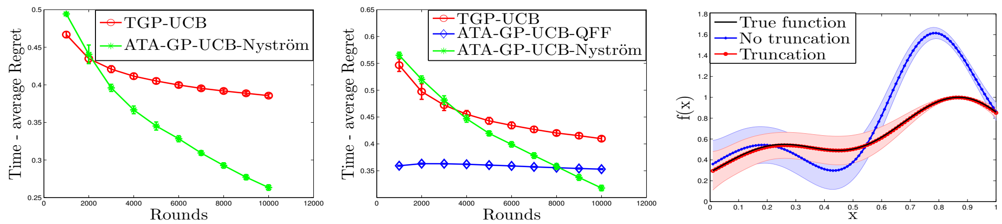
5.4 Computational complexity of ATA-GP-UCB

(a) Time complexity: Under the (data-dependent) Nyström approximation, constructing the dictionary D_t takes $O(t)$ time at each step t. Then, we compute the embeddings $\tilde{\varphi}_t(x)$ for all arms in

[4] This holds, for example, Matérn kernel on $\mathbb{R}^2$ with $\nu = 3.5$ when variance of the rewards is finite ($\alpha = 1$).



(a) k_{SE}, $f \in$ RKHS, Student's-t (b) k_{SE}, $f \in$ RKHS, Pareto (c) $k_{\text{Matérn}}$, $f \in$ RKHS, Student's-t



(d) Stock market data (e) Light sensor data (f) Effect of truncation on GP-UCB

Figure 1: (a)-(e) Time-average regret (R_T/T) for TGP-UCB, ATA-GP-UCB with QFF approximation (ATA-GP-UCB-QFF) and Nyström approximation (ATA-GP-UCB-Nyström) on heavy-tailed data. (f) Confidence sets ($\mu_t \pm \sigma_t$) formed by GP-UCB with and without truncation under heavy fluctuations.

$O(m_t^3 + m_t^2 \left|\mathcal{X}\right|)$ time, where $\left|\mathcal{X}\right|$ is the cardinality of $\mathcal{X}$. Now, construction of $\tilde{V}_t$ takes $O(m_t^2 t)$ time, since we need to rebuild it from the scratch. Then, $\tilde{V}_t^{-1/2}$ is computed in $O(m_t^3)$ time. We can now compute $\tilde{\mu}_t(x)$ and $\tilde{\sigma}_t^2(x)$ for all arms in $O(m_t^2 t + m_t \left|\mathcal{X}\right|)$ and $O(m_t^2 \left|\mathcal{X}\right|)$ time, respectively, using already computed $\tilde{\varphi}_t(x)$ and $\tilde{V}_t^{-1/2}$. Thus per-step time complexity is $O\left(m_t^2(t + \left|\mathcal{X}\right|)\right)$, since $m_t \leq t$. For continuous $\mathcal{X}$, one can approximately maximize the GP-UCB score by grid search / Branch and Bound methods such as DIRECT [6]. In fact it can be maximized within $O(\varepsilon)$ accuracy by making $O(\varepsilon^{-d})$ calls to it, yielding a per-step time complexity of $O(m_t^2(t + \varepsilon^{-d}))$. Since $m_t = \tilde{O}(\gamma_t)$ and γ_t is poly-logarithmic in t for SE kernel, per step time complexity is $\tilde{O}(t + \varepsilon^{-d})$. For Matérn kernel, the complexity is $\tilde{O}(t^p(t + \varepsilon^{-d})), 1 < p < 2$. Similarly, under (data-independent) QFF approximation, the per-step time complexity is $O(m^3 + m^2(t + \varepsilon^{-d})) = \tilde{O}(t + \varepsilon^{-d})$ since $m = O((\ln T)^d)$ for the SE kernel.

(b) Space complexity: Note that under Nyström approximation, at each round t we need to store all previously chosen arms, the matrix $\tilde{V}_t^{-1/2}$ and the vectors $\tilde{\varphi}_t(x)$. Hence, the per-step space complexity of ATA-GP-UCB is $O(t + m_t(m_t + \varepsilon^{-d})) = O(m_t(m_t + \varepsilon^{-d}))$ for small enough ε. Under QFF approximation, the complexity is $O(m(m + \varepsilon^{-d}))$.

6 Experiments

We numerically compare the performance of TGP-UCB (Algorithm 1), ATA-GP-UCB with QFF (ATA-GP-UCB-QFF) and Nyström (ATA-GP-UCB-Nyström) approximations (Algorithm 2) on both synthetic and real-world heavy-tailed environments. (Our codes are available here.) The confidence width β_t and truncation level b_t of our algorithms, and the trade-off parameter q used in Nyström approximation are set order-wise similar to those recommended by theory (Theorems 1, 3 and 4). We use $\lambda = 1$ in all algorithms and $\varepsilon = 0.1$ in ATA-GP-UCB-Nyström. We plot the mean and standard deviation (under independent trials) of the time-average regret R_T/T in Figure 1. We use the following datasets.

1. Synthetic data: We generate the objective function $f \in \mathcal{H}_k(\mathcal{X})$ with $\mathcal{X}$ set to be a discretization of $[0, 1]$ into 100 evenly spaced points. Each $f = \sum_{i=1}^{p} a_i k(\cdot, x_i)$ was generated using an SE kernel with $l = 0.2$ and by uniformly sampling $a_i \in [-1, 1]$ and support points $x_i \in \mathcal{X}$ with $p = 100$. We set $B = \max_{x \in \mathcal{X}} \left|f(x)\right|$. To generate the rewards, first we consider $y(x) = f(x) + \eta$, where the noise η are samples from the Student's t-distribution with 3 degrees of freedom (Figure 1 a). Here, the variance is bounded ($\alpha = 1$) and hence $v = B^2 + 3$. Next, we generate the rewards as samples from the Pareto distribution with shape parameter 2 and scale parameter $f(x)/2$. f is generated similarly, except that here we sample a_i's uniformly from $[0, 1]$. Then, we set B as before leading to the bound of $(1 + \alpha)$-th raw moments $v = \frac{B^{1+\alpha}}{2^\alpha(1-\alpha)}$. We plot the results for $\alpha = 0.9$ (Figure 1 b). We use $m = 32$ features (in consistence with Theorem 3) for ATA-GP-UCB-QFF in these experiments. Next, we generate f using the Matérn kernel with $l = 0.2$ and $\nu = 2.5$, and consider the same Student's-t distribution as earlier to generate rewards. As we do not have the theory of ATA-GP-UCB-QFF for the Matérn kernel yet, we exclude evaluating it here (Figure 1 c). We perform 20 trials for 2×10^4 rounds and for each trial we evaluate on a different f (which explains the high error bars).

2. Stock market data: We consider a representative application of identifying the most profitable stock in a given pool of stocks. This is motivated by the practical scenario that an investor would like to invest a fixed budget of money in a stock and get as much return as possible. We took the adjusted closing price of 29 stocks from January 4th, 2016 to April 10th, 2019. We conduct Kolmogrov-Smirnov (KS) test to find out that the null hypothesis of stock prices following a Gaussian distribution is rejected against the favor of a heavy-tailed distribution. We take the empirical mean of stock prices as our objective function f and empirical covariance of the normalized stock prices as our kernel function k (since stock behaviors are mostly correlated with one another). We consider $\alpha = 1$ and set v as the empirical average of the squared prices. Since the kernel is data dependent, we cannot run ATA-GP-UCB-QFF here. We average over 10 independent trials of the algorithms (Figure 1 d).

3. Light sensor data: We take light sensor data collected in the CMU Intelligent Workplace in Nov 2005 containing locations of 41 sensors, 601 train samples and 192 test samples in the context of learning the maximum average reading of the sensors. For each sensor, we find that the KS test on its readings rejects the Gaussian against the favor of a heavy-tailed distribution. We take the empirical average of the test samples as our objective f and empirical covariance of the normalized train samples as our kernel k. We consider $\alpha = 1$, set v as the empirical mean of the squared readings and B as the maximum of the average readings. For ATA-GP-UCB-QFF, we fit a SE kernel with $l^2 = 0.1$ on the given sensor locations and approximate it with $m = 16^2 = 256$ features (Figure 1 e).

Observations: We find that ATA-GP-UCB outperforms TGP-UCB uniformly over all experiments, which is consistent with our theoretical results. We also see that the performance of ATA-GP-UCB under the Nyström approximation is no worse than that under the QFF approximation. Not only that, the scope of the latter is limited due to its dependence on the analytical form of the kernel, whereas the former is data-adaptive and hence, well suited for practical purposes.

Effect of truncation: For heavy-tailed rewards, the sub-Gaussian constant $R = \infty$. Hence, we exclude evaluating GP-UCB in the above experiments. Now, we demonstrate the effect of truncation on GP-UCB in the following experiment. First, we generate a function $f \in \mathcal{H}_k(\mathcal{X})$ and normalize it between $[0, 1]$. Then, we simulate rewards as $y(x) = f(x) + \eta$, where η takes values in $\{-10, 10\}$, uniformly, for any single random point in $\mathcal{X}$, and is zero everywhere else. We run GP-UCB with $\beta_t = \ln t$ and see that the posterior mean after $T = 10^4$ rounds is not a good estimate of f. However, by truncating reward samples which exceeds $t^{1/4}$ (truncation threshold in TGP-UCB when $\alpha = 1$) at round t, we get an (almost) accurate estimator of f. Not only that, the confidence interval around this estimator contains f at every point in $\mathcal{X}$, which in turn ensures good performance. We plot the respective confidence sets averaged over 50 such randomizations of noise (Figure 1 f).

7 Conclusion

To the best of our knowledge, this is the first work to formulate and solve BO under heavy-tailed observations. We have demonstrated the failure of existing BO methods and developed (almost) optimal algorithms using kernel approximation techniques, which are easy to implement and perform well in practice, with rigorous theoretical guarantees. It is worth noting that using a Bernstein type concentration bound in each direction of the approximate feature space, we are able to obtain the near optimal regret scaling for ATA-GP-UCB (Algorithm 2). Instead, if one can derive a Bernstein type bound for self-normalized processes which depends on the $(1 + \alpha)$-th moments of rewards, then one may not have to resort to feature approximation to get optimal regret. Further, instead of truncating the payoffs, one can also consider building and studying a median of means-style estimator [8] in the (approximate) feature space and hope to develop an optimal algorithm.

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Appendix

A Preliminaries

First, we review some useful matrix identities.

Lemma 2 *[16, Lemma 12] Let $A \succeq B \succ 0$ be positive definite matrices. Then $A^{-1} \bullet (A - B) = \ln \frac{|A|}{|B|}$, where $X \bullet Y := \sum_{i=1}^{n} \sum_{j=1}^{n} X_{i,j} Y_{i,j}$ for any two matrices $X, Y \in \mathbb{R}^{n \times n}$.*

Lemma 3 *For any linear operator $A : \mathcal{H}_k(\mathcal{X}) \to \mathbb{R}^t$ and its adjoint $A^T : \mathbb{R}^t \to \mathcal{H}_k(\mathcal{X})$, and for any $\lambda > 0$,*

$$(A^T A + \lambda I_{\mathcal{H}})^{-1} A^T = A^T (A A^T + \lambda I_t)^{-1}, \tag{3}$$

and

$$I_{\mathcal{H}} - A^T (A A^T + \lambda I_t) A = \lambda (A^T A + \lambda I_{\mathcal{H}})^{-1}. \tag{4}$$

Proof The proofs follow from the fact that $(A^T A + \lambda I_{\mathcal{H}}) A^T = A^T (A A^T + \lambda I_t)$ for any $\lambda > 0$. ■

Next, we review some relevant definitions and results, which will be useful in the analysis of our algorithms. We first begin with the definition of *Maximum Information Gain*, first appeared in [35], which basically measures the reduction in uncertainty about the unknown function after some noisy observations (rewards).

For a function $f : \mathcal{X} \to \mathbb{R}$ and any subset $A \subset \mathcal{X}$ of its domain, we use $f_A := [f(x)]_{x \in A}$ to denote its restriction to A, i.e., a vector containing f's evaluations at each point in A (under an implicitly understood bijection from coordinates of the vector to points in A). In case f is a random function, f_A will be understood to be a random vector. For jointly distributed random variables X and Y, $I(X; Y)$ denotes the Shannon mutual information between them.

Definition 1 (Maximum Information Gain (MIG)) *Let $f : \mathcal{X} \to \mathbb{R}$ be a (possibly random) real-valued function defined on a domain $\mathcal{X}$, and t a positive integer. For each subset $\mathcal{X} \subset D$, let Y_A denote a noisy version of f_A obtained by passing f_A through a channel $\mathbb{P}[Y_A | f_A]$. The Maximum Information Gain (MIG) about f after t noisy observations is defined as*

$$\gamma_t := \max_{A \subset \mathcal{X} : |A| = t} I(f_A; Y_A).$$

(We omit mentioning explicitly the dependence on the channels for ease of notation.)

Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be a symmetric positive semi-definite kernel and for any $A \subset \mathcal{X}$, let K_A denotes the induced kernel matrix.

Lemma 4 (MIG under GP prior and additive Gaussian noise [35]) *Let $f \sim GP_{\mathcal{X}}(0, k)$ be a sample from a Gaussian process over $\mathcal{X}$ and Y_A denote a noisy version of f_A obtained by passing f_A through a channel that adds iid $\mathcal{N}(0, \lambda)$ noise to each element of f_A. Then,*

$$\gamma_t \equiv \gamma_t(k, \mathcal{X}) = \max_{A \subset \mathcal{X} : |A| = t} \frac{1}{2} \ln \left| I + \lambda^{-1} K_A \right|.$$

Srinivas et al. [35] proved upper bounds over γ_t for commonly used kernels. The bounds are given in Lemma 5.

Lemma 5 (MIG for common kernels [35]) *Let $\mathcal{X}$ be a compact and convex subset of $\mathbb{R}^d$ and the kernel k satisfies $k(x, x') \leq 1$ for all $x, x' \in \mathcal{X}$. Then for*

- *Linear kernel:* $\gamma_t = O(d \ln t)$.
- *Squared Exponential kernel:* $\gamma_t = O\left((\ln t)^{d+1}\right)$.
- *Matérn kernel:* $\gamma_t = O\left(t^{\frac{d(d+1)}{2\nu + d(d+1)}} \ln t\right)$.

Note that, MIG depends only *sublinearly* on the number of observations t for all these kernels and it will serve as a key instrument to obtain our regret bounds by virtue of Lemma 4 and 6.

Now, observe that any kernel function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}, \mathcal{X} \subset \mathbb{R}^d$ is associated with a non-linear feature map $\varphi : \mathcal{X} \to \mathcal{H}_k(\mathcal{X})$ such that $k(x, y) = \langle \varphi(x), \varphi(y) \rangle_{\mathcal{H}}$, where $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ denotes the inner product in the RKHS $\mathcal{H}_k(\mathcal{X})$ and $\|\cdot\|_{\mathcal{H}}$ denotes the corresponding norm. Observe that for any $h \in \mathcal{H}_k(\mathcal{X})$, $h(x) = \langle h, \varphi(x) \rangle_{\mathcal{H}}$ by the reproducing property. For a set $\{x_1, \ldots, x_t\} \subset \mathcal{X}$ define the operator $\Phi_t : \mathcal{H}_k(\mathcal{X}) \to \mathbb{R}^t$ such that for any $h \in \mathcal{H}_k(\mathcal{X})$, $\Phi_t h = [\langle \varphi(x_1), h \rangle_{\mathcal{H}}, \ldots, \langle \varphi(x_t), h \rangle_{\mathcal{H}}]^T$, and denote its adjoint by $\Phi_t^T : \mathbb{R}^t \to \mathcal{H}_k(\mathcal{X})$. By reproducing property $\varphi_t h = [h(x_1), \ldots, h(x_t)]^T$. For any $\lambda > 0$, define $V_t = \Phi_t^T \Phi_t + \lambda I_{\mathcal{H}}$, where $I_{\mathcal{H}} : \mathcal{H}_k(\mathcal{X}) \to \mathcal{H}_k(\mathcal{X})$ denotes the identity operator. For a positive definite operator $V : \mathcal{H}_k(\mathcal{X}) \to \mathcal{H}_k(\mathcal{X})$, define the inner product $\langle \cdot, \cdot \rangle_V := \langle \cdot, V \cdot \rangle_{\mathcal{H}}$ with corresponding norm $\|\cdot\|_V$. Observe that, under this definition, the posterior variance $\sigma_t^2(x) = \lambda \|\varphi(x)\|^2_{V_t^{-1}}$.

Lemma 6 (Sum of predictive variances and MIG) *If $k(x, x) \leq 1$ for all $x \in \mathcal{X}$, then*

$$\sum_{s=1}^{t} \sigma_{s-1}^2(x_s) \leq 2\,(1 + \lambda)\,\gamma_t.$$

Proof Observe that $V_t = V_{t-1} + \varphi(x_t)\varphi(x_t)^T$. Therefore, by Sherman–Morrison-Woodbury matrix identity, we have $V_t^{-1} = V_{t-1}^{-1} - \frac{V_{t-1}^{-1}\varphi(x_t)\varphi(x_t)^T V_{t-1}^{-1}}{1+\varphi(x_t)^T V_{t-1}^{-1}\varphi(x_t)}$. This, in turn, implies that

$$\|\varphi(x)\|^2_{V_t^{-1}} = \|\varphi(x)\|^2_{V_{t-1}^{-1}} - \frac{\langle \varphi(x), \varphi(x_t) \rangle^2_{V_{t-1}^{-1}}}{1 + \|\varphi(x_t)\|^2_{V_{t-1}^{-1}}} \overset{(a)}{\geq} \|\varphi(x)\|^2_{V_{t-1}^{-1}} \left(1 - \frac{\|\varphi(x_t)\|^2_{V_{t-1}^{-1}}}{1 + \|\varphi(x_t)\|^2_{V_{t-1}^{-1}}}\right) = \frac{\|\varphi(x)\|^2_{V_{t-1}^{-1}}}{1 + \|\varphi(x_t)\|^2_{V_{t-1}^{-1}}}$$

where (a) follows from Cauchy-Schwartz inequality. Since $V_{t-1} \succeq \lambda I_{\mathcal{H}}$, we have $\|\varphi(x_t)\|^2_{V_{t-1}^{-1}} \leq \frac{1}{\lambda}\|\varphi(x_t)\|^2_{\mathcal{H}} = \frac{1}{\lambda} k(x_t, x_t) \leq \frac{1}{\lambda}$. This implies that $\|\varphi(x)\|^2_{V_{t-1}^{-1}} \leq (1 + \frac{1}{\lambda})\,\|\varphi(x)\|^2_{V_t^{-1}}$ and therefore

$$\sigma_{t-1}^2(x) \leq \left(1 + \frac{1}{\lambda}\right) \sigma_t^2(x) \text{ for all } x \in \mathcal{X}. \tag{5}$$

Observe that $\varphi(x_t)^T V_t^{-1} \varphi(x_t) = V_t^{-1} \bullet \varphi(x_t)\varphi(x_t)^T = V_t^{-1} \bullet (V_t - V_{t-1})$ since for any $a \in \mathbb{R}^n$ and $B \in \mathbb{R}^{n \times n}$, $a^T B a = B \bullet aa^T$. Then from Lemma 2, we have $\frac{1}{\lambda}\sigma_t^2(x_t) = \ln \frac{|V_t|}{|V_{t-1}|}$ and thus, in turn,

$$\frac{1}{\lambda}\sum_{s=1}^{t} \sigma_s^2(x_s) \leq \ln \frac{|V_t|}{|V_0|} = \ln \left|\lambda^{-1}\Phi_t^T\Phi_t + I_{\mathcal{H}}\right| = \ln \left|\lambda^{-1}\Phi_t\Phi_t^T + I_t\right| = \ln \left|\lambda^{-1}K_t + I_t\right|. \tag{6}$$

Combining 5 and 6, we get

$$\sum_{s=1}^{t} \sigma_{s-1}^2(x_s) \leq \left(1 + \frac{1}{\lambda}\right) \sum_{s=1}^{t} \sigma_s^2(x_s) \leq (1 + \lambda) \ln \left|\lambda^{-1}K_t + I_t\right|.$$

Now the result follows from Lemma 4. ■

B Analysis of TGP-UCB

The following lemma states a self-normalized concentration inequality for RKHS-valued martingales.

Lemma 7 (RKHS-valued martingale control [13]) *Let $\{z_t\}_{t \geq 1}$ be an $\mathbb{R}^d$-valued discrete time stochastic processes such that z_t is predictable with respect to a filtration $\{\mathcal{G}_t\}_{t \geq 0}$, i.e., z_t is $\mathcal{G}_{t-1}$-measurable for all $t \geq 1$. Let $\{w_t\}_{t \geq 1}$ be a real-valued stochastic process such that for all $t \geq 1$, w_t*

is (a) $\mathcal{G}_t$-measurable, and (b) R-sub-Gaussian conditionally on $\mathcal{G}_{t-1}$ for some $R > 0$. Then, for any $\delta \in (0, 1]$, with probability at least $1 - \delta$, uniformly over all $t \geq 1$,

$$\left\| \sum_{\tau=1}^{t} w_\tau \varphi(z_\tau) \right\|_{Z_t^{-1}} \leq R \sqrt{2 \left(\frac{1}{2} \ln \frac{|Z_t|}{|Z|} + \ln(1/\delta) \right)}.$$

where $Z_t = Z + \sum_{\tau=1}^{t} \varphi(z_\tau)\varphi(z_\tau)^T$ and $Z : \mathcal{H}_k(\mathbb{R}^d) \to \mathcal{H}_k(\mathbb{R}^d)$ is a positive definite operator.

Observe that $\sum_{\tau=1}^{t} w_\tau \varphi(z_\tau)$ is $\mathcal{G}_t$-measurable and $\mathbb{E}\left[\sum_{\tau=1}^{t} w_\tau \varphi(z_\tau) | \mathcal{G}_{t-1}\right] = \sum_{\tau=1}^{t-1} w_\tau \varphi(z_\tau)$. The process $\left(\sum_{\tau=1}^{t} w_\tau \varphi(z_\tau)\right)_{t \geq 1}$ is thus a martingale with respect to the filtration $(\mathcal{G}_t)_{t \geq 0}$ with values in the RKHS $\mathcal{H}_k(\mathcal{X})$, whose deviation is measured by the norm weighted by Z_t^{-1}, which is derived from the process itself. Hence, the name self-normalized concentration inequality. Now, we will show that f lies in the confidence sets constructed by TGP-UCB with high probability.

Lemma 8 (Confidence sets of TGP-UCB contains f) *Let $f \in \mathcal{H}_k(\mathcal{X})$, $\|f\|_{\mathcal{H}} \leq B$ and $k(x, x) \leq 1$ for all $x \in \mathcal{X}$. Let $\mathbb{E}\left[|y_t|^{1+\alpha} | \mathcal{F}_{t-1}\right] \leq v < \infty$ for some $\alpha \in (0, 1]$ and for all $t \geq 1$. Then, for any $\delta \in (0, 1]$, TGP-UCB, with $b_t = v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}}$ and $\beta_{t+1} = B + \frac{3}{\sqrt{\lambda}} v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}} \sqrt{\ln|I_t + \lambda^{-1} K_t| + 2\ln(1/\delta)}$, ensures, with probability at least $1 - \delta$, uniformly over all $x \in \mathcal{X}$ and $t \geq 1$, that*

$$|f(x) - \widehat{\mu}_{t-1}(x)| \leq \beta_t \sigma_{t-1}(x).$$

Proof First, we define $\alpha_t(x) = k_t(x)^T (K_t + \lambda I_t)^{-1} f_t$, where $f_t = [f(x_1), \ldots, f(x_t)]^T$ is a vector containing f's evaluations up to round t. By reproducing property, $\alpha_t(x) = \langle \varphi(x), \Phi_t^T (\Phi_t \Phi_t^T + \lambda I_t)^{-1} \Phi_t f \rangle_{\mathcal{H}}$. Then, we have

$$f(x) - \alpha_t(x) = \langle \varphi(x), \left(I_{\mathcal{H}} - \Phi_t^T (\Phi_t \Phi_t^T + \lambda I_t)^{-1} \Phi_t\right) f \rangle_{\mathcal{H}} \overset{(a)}{=} \lambda \langle \varphi(x), f \rangle_{V_t^{-1}} = \lambda \langle V_t^{-1/2} \varphi(x), V_t^{-1/2} f \rangle_{\mathcal{H}},$$

where (a) follows from 4. By Cauchy-Schwartz inequality, we have for any $x \in \mathcal{X}$

$$\begin{aligned} |f(x) - \alpha_t(x)| &\leq \lambda \left\| V_t^{-1/2} \varphi(x) \right\|_{\mathcal{H}} \left\| V_t^{-1/2} f \right\|_{\mathcal{H}} \\ &\overset{(a)}{\leq} \lambda^{1/2} \|\varphi(x)\|_{V_t^{-1}} \|f\|_{\mathcal{H}} \overset{(b)}{\leq} B \, \sigma_t(x). \end{aligned} \tag{7}$$

Here in (a) we have used the fact that $V_t^{-1} \preceq \lambda^{-1} I_{\mathcal{H}}$, and hence, $\left\| V_t^{-1/2} f \right\|_{\mathcal{H}} \leq \lambda^{-1/2} \|f\|_{\mathcal{H}}$. (b) follows from $\|f\|_{\mathcal{H}} \leq B$. Now, let $\widehat{\eta}_t = \widehat{y}_t - f(x_t), t = 1, 2, \ldots$ denotes the truncated noise and $\widehat{N}_t = [\widehat{\eta}_1, \ldots, \widehat{\eta}_t]^T$ denotes the vector formed by the first t of those. This implies $\widehat{\mu}_t(x) = \alpha_t(x) + k_t(x)^T (K_t + \lambda I_t)^{-1} \widehat{N}_t$. Thus

$$k_t(x)^T (K_t + \lambda I_t)^{-1} \widehat{N}_t = \langle \varphi(x), \Phi_t^T (\Phi_t \Phi_t^T + \lambda I_t)^{-1} \widehat{N}_t \rangle_{\mathcal{H}} \overset{(a)}{=} \langle \varphi(x), \Phi_t^T \widehat{N}_t \rangle_{V_t^{-1}},$$

where (a) uses equation 3. By Cauchy-Schwartz inequality, we have for any $x \in \mathcal{X}$

$$\left| k_t(x)^T (K_t + \lambda I_t)^{-1} \widehat{N}_t \right| \leq \|\varphi(x)\|_{V_t^{-1}} \left\| \Phi_t^T \widehat{N}_t \right\|_{V_t^{-1}} = \lambda^{-1/2} \left\| \Phi_t^T \widehat{N}_t \right\|_{V_t^{-1}} \sigma_t(x). \tag{8}$$

Now, by triangle inequality, we have

$$|f(x) - \widehat{\mu}_t(x)| \leq |f(x) - \alpha_t(x)| + \left| k_t(x)^T (K_t + \lambda I_t)^{-1} \widehat{N}_t \right|.$$

Hence from equation 7 and 8, we get

$$|f(x) - \widehat{\mu}_t(x)| \leq \left(B + \lambda^{-1/2} \left\| \Phi_t^T \widehat{N}_t \right\|_{V_t^{-1}} \right) \sigma_t(x). \tag{9}$$

Now, we define $\xi_t = \widehat{\eta}_t - \mathbb{E}\left[\widehat{\eta}_t | \mathcal{F}_{t-1}\right]$. Then, we have

$$\Phi_t^T \widehat{N}_t = \sum_{\tau=1}^{t} \widehat{\eta}_\tau \varphi(x_\tau) = \sum_{\tau=1}^{t} \xi_\tau \varphi(x_\tau) + \sum_{\tau=1}^{t} \mathbb{E}\left[\widehat{\eta}_\tau | \mathcal{F}_{\tau-1}\right] \varphi(x_\tau). \tag{10}$$

Observe that $\xi_t = \widehat{y}_t - \mathbb{E}\left[\widehat{y}_t | \mathcal{F}_{t-1}\right]$, and hence $|\xi_t| \leq 2b_t$. This implies that ξ_t is zero-mean $2b_t$-sub-Gaussian random variable conditioned on $\mathcal{F}_{t-1}$. Further, observe that ξ_t is $\mathcal{F}_t$- measurable and x_t is $\mathcal{F}_{t-1}$- measurable. Hence, Lemma 7 implies that for any $\delta \in (0,1]$, with probability at least $1-\delta$, for all $t \in \mathbb{N}$:

$$\begin{aligned} \left\| \sum_{\tau=1}^{t} \xi_\tau \varphi(x_\tau) \right\|_{V_t^{-1}} &\leq 2b_t \sqrt{2\left(\frac{1}{2}\ln\left|I_{\mathcal{H}} + \lambda^{-1}\Phi_t^T\Phi_t\right| + \ln(1/\delta)\right)} \\ &= 2b_t \sqrt{2\left(\frac{1}{2}\ln\left|I_t + \lambda^{-1}K_t\right| + \ln(1/\delta)\right)} \end{aligned} \tag{11}$$

Now for any $a \in \mathbb{R}^t$,

$$\left\| \sum_{\tau=1}^{t} a_\tau \varphi(x_\tau) \right\|_{V_t^{-1}}^2 = \left\|\Phi_t^T a\right\|_{V_t^{-1}}^2 = a^T\Phi_t(\Phi_t^T\Phi_t + \lambda I_{\mathcal{H}})^{-1}\Phi_t^T a \stackrel{(a)}{=} a^T\Phi_t\Phi_t^T(\Phi_t\Phi_t^T + \lambda I_t)^{-1} a \stackrel{(b)}{\leq} \|a\|_2^2,$$

where (a) follows from 3 and (b) follows from the fact that $\Phi_t\Phi_t^T(\Phi_t\Phi_t^T + \lambda I_t)^{-1} \preceq I_t$. Therefore $\left\|\sum_{\tau=1}^t \mathbb{E}\left[\widehat{\eta}_\tau|\mathcal{F}_{\tau-1}\right]\varphi(x_\tau)\right\|_{V_t^{-1}}^2 \leq \sum_{\tau=1}^t \mathbb{E}\left[\widehat{\eta}_\tau|\mathcal{F}_{\tau-1}\right]^2$. Further, observe that $\mathbb{E}\left[\widehat{\eta}_t|\mathcal{F}_{t-1}\right] = \mathbb{E}\left[y_t \mathbb{1}_{|y_t|\leq b_t}|\mathcal{F}_{t-1}\right] - f(x_t) = -\mathbb{E}\left[y_t\mathbb{1}_{|y_t|>b_t}|\mathcal{F}_{t-1}\right]$. This implies

$$\left\| \sum_{\tau=1}^{t} \mathbb{E}\left[\widehat{\eta}_\tau | \mathcal{F}_{\tau-1}\right] \varphi(x_\tau) \right\|_{V_t^{-1}}^2 \leq \sum_{\tau=1}^{t} \mathbb{E}\left[y_\tau \mathbb{1}_{|y_\tau|>b_\tau}|\mathcal{F}_{\tau-1}\right]^2 \leq \sum_{\tau=1}^{t} \frac{1}{b_\tau^{2\alpha}} \mathbb{E}\left[\left|y_\tau\right|^{1+\alpha}|\mathcal{F}_{\tau-1}\right]^2 \leq v^2 \sum_{\tau=1}^{t} \frac{1}{b_\tau^{2\alpha}}.$$

Now setting $b_t = v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}}$, we get

$$\left\| \sum_{\tau=1}^{t} \mathbb{E}\left[\widehat{\eta}_\tau | \mathcal{F}_{\tau-1}\right] \varphi(x_\tau) \right\|_{V_t^{-1}} \leq v^{\frac{1}{1+\alpha}} \sqrt{\sum_{\tau=1}^{t} \tau^{-\frac{\alpha}{1+\alpha}}} \leq v^{\frac{1}{1+\alpha}} \sqrt{\int_0^t \tau^{-\frac{\alpha}{1+\alpha}} d\tau} \leq \sqrt{2} v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}}. \tag{12}$$

Combining 9,10, 11 and 12, we have that for any $\delta \in (0,1]$, with probability at least $1-\delta$, uniformly over all $t \geq 1$ and $x \in \mathcal{X}$:

$$\begin{aligned} |f(x) - \widehat{\mu}_t(x)| &\leq \left(B + \sqrt{2/\lambda}\, v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}} \left(1 + 2\sqrt{\frac{1}{2}\ln|I_t + \lambda^{-1}K_t| + \ln(1/\delta)}\right)\right) \sigma_t(x) \\ &\leq \left(B + 3\sqrt{2/\lambda}\, v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}} \sqrt{\frac{1}{2}\ln|I_t + \lambda^{-1}K_t| + \ln(1/\delta)}\right) \sigma_t(x). \end{aligned} \tag{13}$$

Further observe that $|f(x) - \widehat{\mu}_0(x)| = |f(x)| = |\langle f, k(x,\cdot)\rangle_{\mathcal{H}}| \leq \|f\|_{\mathcal{H}} k^{1/2}(x,x) \leq B\sigma_0(x)$. Now the result follows by setting $\beta_{t+1} = B + \frac{3}{\sqrt{\lambda}} v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}} \sqrt{\ln|I_t + \lambda^{-1}K_t| + 2\ln(1/\delta)}$, for all $t \geq 0$. ■

Now, we will prove Theorem 1. For for any $\delta \in (0,1]$, we have, with probability at least $1-\delta$, uniformly over all $t \geq 1$, the instantaneous regret of TGP-UCB (Algorithm 1) is

$$\begin{aligned} r_t &= f(x^\star) - f(x_t) \\ &\stackrel{(a)}{\leq} \widehat{\mu}_{t-1}(x^\star) + \beta_t\sigma_{t-1}(x^\star) - f(x_t) \\ &\stackrel{(b)}{\leq} \widehat{\mu}_{t-1}(x_t) + \beta_t\sigma_{t-1}(x_t) - f(x_t) \\ &\stackrel{(c)}{\leq} 2\beta_t\sigma_{t-1}(x_t). \end{aligned}$$

Here (a) and (c) follow from 13, and (b) is due to the choice of TGP-UCB(Algorithm 1). Since from Lemma 4, $\ln\left|I_t + \lambda^{-1}K_t\right| \le \gamma_t$, we have $\beta_t \le B + 3\sqrt{2/\lambda}\; v^{\frac{1}{1+\alpha}} t^{\frac{1}{2(1+\alpha)}} \sqrt{\gamma_t + \ln(1/\delta)}$, which is an increasing sequence t. Further, see that $\sum_{t=1}^{T} \sigma_{t-1}(x_t) \overset{(a)}{\le} \sqrt{T \sum_{t=1}^{T} \sigma_{t-1}^2(x_t)} \overset{(b)}{\le} \sqrt{2(1+\lambda)\gamma_T T}$, where (a) is due to Cauchy-Schwartz inequality and (b) is due to Lemma 6. Hence, for any $\delta \in (0,1]$, with probability at least $1-\delta$, the cumulative regret of TGP-UCB after T rounds is

$$R_T = O\left(B\sqrt{T\gamma_T} + v^{\frac{1}{1+\alpha}} \sqrt{\gamma_T(\gamma_T + \ln(1/\delta))} T^{\frac{2+\alpha}{2(1+\alpha)}}\right).$$

C Regret lower bound: proof of Theorem 2

Our analysis builds heavily on that of the optimization setting with $f \in \mathcal{H}_k(\mathcal{X})$ and with Gaussian noise studied in [31], but with important differences. Roughly speaking, we use the same construction of f as in [31], but we construct the rewards differently to capture the heavy-tailed scenario. We now proceed with the formal proof.

C.1 Construction of the ground-truth function

- Let $g(x)$ be a function on $\mathbb{R}^d$ with the following properties:
  1. The RKHS norm of g is bounded: $\|g\|_{\mathcal{H}} \le B$.
  2. $|g(x)| \le 2\Delta$ with a maximum value of 2Δ at $x = 0$ and $g(x) < \Delta$ when $\|x\|_\infty > w$ for some $w > 0$ and $\Delta > 0$, to be chosen later.
- Letting $g(x)$ be such a function, we construct M functions $f_1, \ldots, f_M$ first by shifting g such that each f_j has its maximum at a unique point in a uniform grid, and then by restricting them to the domain $\mathcal{X} = [0,1]^d$. Using a step size w in each dimension, one can construct a grid of size $M = \lfloor (\frac{1}{w})^d \rfloor$ of the domain $\mathcal{X}$, and hence M such functions f_j. In this process we ensure that any Δ-optimal point for f_j fails to be Δ-optimal point for any other $f_{j'}$.
- Finally, we choose f as a uniformly sampled function from the set $\{f_1, \ldots, f_M\}$.

It remains to choose g, w, and Δ so that the above properties are satisfied.

- For some absolute constant $\zeta > 0$ we choose $g(x) = \frac{2\Delta}{h(0)} h(\frac{x\zeta}{w})$, where h is the inverse Fourier transform of the *multi-dimensional bump function*: $H(\omega) = e^{-\frac{1}{1-\|\omega\|_2^2}} \mathbb{1}_{\{\|\omega\|_2^2 \le 1\}}$. Note that since H is real and symmetric, the maximum of h is attained at $x = 0$, and hence the maximum of g is $g(0) = 2\Delta$, as desired. Further, since H has finite energy, $h(x) \to 0$ as $\|x\|_2 \to \infty$. Hence, there exists an absolute constant ζ such that $h(x) < \frac{1}{2}h(0)$ when $\|x\|_\infty > \zeta$, and thus $g(x) < \Delta$ for $\|x\|_\infty > w$, as desired.
- It now remains to choose w and Δ to ensure that $\|g\|_{\mathcal{H}} \le B$, for a given B. Note that, while a smaller Δ ensures a low RKHS norm, a smaller w increases it. Hence, as long as Δ is very small, we can afford to take $w << 1$, so that there is no risk of having $M = 0$. For $\frac{\Delta}{B} << 1$, it is shown in [31] that the condition $\|g\|_{\mathcal{H}} \le B$ can be achieved with $w = \frac{\zeta\pi l}{\sqrt{\ln \frac{B(2\pi l^2)^{d/4} h(0)}{2\Delta}}}$ for the SE kernel, and with $w = \zeta\left(\frac{2\Delta(8\pi^2)^{(\nu+d/2)/2}}{Bc^{-1/2}h(0)}\right)^{1/\nu}$ for the Matérn kernel for some $c > 0$. We consider Δ as arbitrary for now, but later this will be chosen to ensure that $\frac{\Delta}{B}$ is sufficiently small.
- From the choice of w, we see that $M = \Theta\left((\ln \frac{B}{\Delta})^d\right)$ for the SE kernel, and $M = \Theta\left((\frac{B}{\Delta})^{\frac{d}{\nu}}\right)$ for the Matérn kernel. Note that the assumption of sufficiently small $\frac{\Delta}{B}$ in ensures that $M >> 1$, i.e. there are enough number of functions to sample from.

C.2 Construction of the reward distribution

For any given $\alpha \in (0, 1]$, $v > 0$ and $x \in [0, 1]^d$, we define the reward distribution as

$$y(x) = \begin{cases} sgn\left(f(x)\right) \left(\frac{v}{2\Delta}\right)^{\frac{1}{\alpha}} & \text{with probability } \left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}} |f(x)|, \\ 0 & \text{otherwise.} \end{cases} \tag{14}$$

Note that 14 is a valid probability distribution as long as $\Delta \leq \frac{1}{2} v^{\frac{1}{1+\alpha}}$. Then, $\mathbb{E}\left[y(x)\right] = |f(x)|\, sgn((f(x)) = f(x)$ and $\mathbb{E}\left[|y(x)|^{1+\alpha}\right] = \left(\frac{v}{2\Delta}\right)^{\frac{1+\alpha}{\alpha}} \left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}} |f(x)| = \frac{v|f(x)|}{2\Delta} \leq v$ for any $\alpha \in (0, 1]$. Thus, we ensure that the $(1 + \alpha)$-th absolute moment of the rewards are upper bounded by v.

C.3 Preliminary notations and lemmas

Now, we introduce the following notations, also used in [31]:

- y_m denote the reward function when the underlying ground truth is f_m for $m = 1, \ldots, M$. f_0 denotes the function which is zero everywhere, and y_0 the corresponding reward function. $P_m(Y_T)$ (resp. $P_0(Y_T)$) denotes the probability density function of the reward sequence $Y_T = \{y_1, \ldots, y_T\}$ when the underlying function is f_m (resp. f_0). $P_m(y|x)$ (resp. $P_0(y|x)$) denotes the conditional density of the reward y given the selected point x when the underlying function is f_m (resp. f_0).
- $\mathbb{E}_m$ (resp. $\mathbb{E}_0$) and $\mathbb{P}_m$ (resp. $\mathbb{P}_0$) denote expectations and probabilities (with respect to the noisy rewards) when the underlying function is f_m (resp. f_0). $\mathbb{E}[\cdot] = \frac{1}{M}\sum_{m=1}^{M} \mathbb{E}_m[\cdot]$ (resp. $\mathbb{P}_m[\cdot]$) denote the expectation (resp. probability) with respect to the noisy rewards and f drawn uniformly from $\{f_1, \ldots, f_M\}$.
- $\{\mathcal{R}_m\}_{m=1}^{M}$ denote a partition of $\mathcal{X}$ into M regions such that each $f_m, m = 1, \ldots, M$ has its maximum at the center of $\mathcal{R}_m$. $v_m^j = \max_{x\in\mathcal{R}_j} |f_m(x)|$ denotes the maximum absolute value of f_m in the region $\mathcal{R}_j$ and $D_m^j = \max_{x\in\mathcal{R}_j} D_{\mathrm{KL}}\left(P_0(\cdot|x)||P_m(\cdot|x)\right)$ denotes the maximum KL divergence between $P_0(\cdot|x)$ and $P_m(\cdot|x)$ within $\mathcal{R}_j$. $N_j = \sum_{t=1}^{T} \mathbb{1}_{\{x_t\in\mathcal{R}_j\}}$ denotes the number of points within $\mathcal{R}_j$ that are selected up to time T.

Next, we present some useful lemmas from [31].

Lemma 9 *[31, Lemma 3] Under the preceding definitions, we have* $\mathbb{E}_m[N_j] \leq \mathbb{E}_0[N_j] + T\sqrt{D_{KL}(P_0||P_m)}$ *for all* $m = 1, \ldots, M$ *and* $j = 1, \ldots, M$.

Lemma 10 *[31, Lemma 4] Under the preceding definitions, we have* $D_{KL}(P_0||P_m) \leq \sum_{j=1}^{M} \mathbb{E}_0[N_j] D_m^j$ *for all* $m = 1, \ldots, M$.

Lemma 11 *[31, Lemma 5] The functions* f_m *constructed in Section C.1 are such that the quantities* v_m^j *satisfy:*
(a) $\sum_{m=1}^{M} v_m^j = O(\Delta)$ *for all* $j = 1, \ldots, M$ *and (b)* $\sum_{j=1}^{M} v_m^j = O(\Delta)$ *for all* $m = 1, \ldots, M$.

C.4 Analysis of expected cumulative regret

Observe that $\mathbb{E}_m[f(x_t)] \leq \sum_{j=1}^{M} \mathbb{P}_m[x_t \in \mathcal{R}_j] v_m^j$. This implies

$$\mathbb{E}_m\left[\sum_{t=1}^{T} f(x_t)\right] \leq \sum_{j=1}^{M} v_m^j \mathbb{E}_m[N_j] \leq \sum_{j=1}^{M} v_m^j \left(\mathbb{E}_0[N_j] + T\sqrt{\sum_{j'=1}^{M} \mathbb{E}_0[N_{j'}] D_m^{j'}}\right),$$

where the last inequality follows from Lemma 9. Now averaging over $m = 1, \ldots, M$ we obtain the following:

$$\mathbb{E}\left[\sum_{t=1}^{T} f(x_t)\right] \leq \frac{1}{M}\sum_{m=1}^{M}\sum_{j=1}^{M} v_m^j \left(\mathbb{E}_0[N_j] + T\sqrt{\sum_{j'=1}^{m} \mathbb{E}_0[N_{j'}] D_m^{j'}}\right). \tag{15}$$

We can bound the first term as follows:

$$\frac{1}{M}\sum_{m=1}^{M}\sum_{j=1}^{M} v_m^j \mathbb{E}_0[N_j] = \frac{1}{M}\sum_{j=1}^{M}\sum_{m=1}^{M} v_m^j \mathbb{E}_0[N_j] \overset{(a)}{=} O\left(\frac{\Delta}{M}\right)\sum_{j=1}^{M}\mathbb{E}_0[N_j] \overset{(b)}{=} O\left(\frac{T\Delta}{M}\right), \quad (16)$$

where (a) follows from part (a) of Lemma 11, and (b) follows from $\sum_{j=1}^{M} N_j = T$. In order to bound the second term, first we note that $y_0(x) = 0$ for all $x \in \mathcal{X}$. Therefore, we have

$$\begin{aligned} D_{\mathrm{KL}}\left(P_0(\cdot|x)||P_m(\cdot|x)\right) = \ln \frac{1}{1-\left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}}|f_m(x)|} &\overset{(a)}{\leq} \frac{\left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}}|f_m(x)|}{1-\left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}}|f_m(x)|} \\ &\overset{(b)}{\leq} \frac{\left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}}|f_m(x)|}{1-(2\Delta)^{\frac{1+\alpha}{\alpha}}v^{-\frac{1}{\alpha}}} \\ &\overset{(c)}{\leq} 2\left(\frac{2\Delta}{v}\right)^{\frac{1}{\alpha}}|f_m(x)|. \end{aligned}$$

Here (a) holds because $\ln(x) \leq x-1$ for all $x \geq 1$, (b) holds as $|f(x)| \leq 2\Delta$ and (c) holds for $\Delta \leq \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}$. Observe that this choice of Δ is compatible with 14. This implies that for all $j = 1, \ldots, M$,

$$D_m^j \leq 2^{\frac{1+\alpha}{\alpha}}\left(\frac{\Delta}{v}\right)^{\frac{1}{\alpha}} v_m^j \text{ if } \Delta \leq \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}. \quad (17)$$

Now, we can bound the second term as follows:

$$\begin{aligned} \frac{1}{M}\sum_{m=1}^{M}\sum_{j=1}^{M} v_m^j\sqrt{\sum_{j'=1}^{m}\mathbb{E}_0[N_{j'}]D_m^{j'}} &\overset{(a)}{=} O(\Delta)\frac{1}{M}\sum_{m=1}^{M}\sqrt{\sum_{j'=1}^{M}\mathbb{E}_0[N_{j'}]D_m^{j'}} \\ &\overset{(b)}{\leq} O(\Delta)\sqrt{\frac{1}{M}\sum_{m=1}^{M}\sum_{j'=1}^{M}\mathbb{E}_0[N_{j'}]D_m^{j'}} \\ &\overset{(c)}{\leq} O(\Delta)2^{\frac{1+\alpha}{2\alpha}}\left(\frac{\Delta}{v}\right)^{\frac{1}{2\alpha}}\sqrt{\frac{1}{M}\sum_{m=1}^{M}\sum_{j'=1}^{M}\mathbb{E}_0[N_{j'}]v_m^{j'}} \\ &\overset{(d)}{=} O(\Delta)2^{\frac{1+\alpha}{2\alpha}}\left(\frac{\Delta}{v}\right)^{\frac{1}{2\alpha}}\sqrt{O\left(\frac{\Delta}{M}\right)\sum_{j'=1}^{M}\mathbb{E}_0[N_{j'}]} \\ &\overset{(e)}{=} O\left(\Delta\frac{(2\Delta)^{\frac{1+\alpha}{2\alpha}}}{v^{\frac{1}{2\alpha}}}\sqrt{\frac{T}{M}}\right). \quad (18) \end{aligned}$$

Here (a) follows from part (b) of Lemma 11, (b) follows from Jensen's inequality, (c) follows from 17 if $\Delta \leq \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}$, (d) follows from part (a) of Lemma 11, and (e) follows from $\sum_{j=1}^{M} N_j = T$. Substituting 16 and 18 in 15 gives

$$\mathbb{E}\left[\sum_{t=1}^{T} f(x_t)\right] \leq CT\Delta\left(\frac{1}{M} + \frac{(2\Delta)^{\frac{1+\alpha}{2\alpha}}}{v^{\frac{1}{2\alpha}}}\sqrt{\frac{T}{M}}\right) \text{ for } \Delta \leq \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}. \quad (19)$$

Since $f(x^\star) = 2\Delta$, the expected cumulative regret

$$\mathbb{E}\left[R_T\right] = Tf(x^\star) - \mathbb{E}\left[\sum_{t=1}^{T} f(x_t)\right] \geq T\Delta\left(2 - \frac{C}{M} - \frac{C\,(2\Delta)^{\frac{1+\alpha}{2\alpha}}}{v^{\frac{1}{2\alpha}}}\sqrt{\frac{T}{M}}\right) \text{ for } \Delta \leq \frac{1}{2}\left(\frac{1}{2}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}.$$

Since $M \to \infty$ as $\frac{\Delta}{B} \to 0$, we have $\frac{C}{M} \leq \frac{1}{2}$ for sufficiently small $\frac{\Delta}{B}$. Hence, we have

$$\begin{aligned} \mathbb{E}\left[R_T\right] &\geq T\Delta\left(\frac{3}{2} - C\frac{(2\Delta)^{\frac{1+\alpha}{2\alpha}}}{v^{\frac{1}{2\alpha}}}\sqrt{\frac{T}{M}}\right) \\ &\geq T\Delta \quad \text{for } \Delta \leq \frac{1}{2}\left(\min\left\{\frac{1}{2}, \frac{M}{4C^2T}\right\}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}. \quad (20) \end{aligned}$$

Now, if $M \leq 2C^2T$, then

$$\mathbb{E}\left[R_T\right] = \Omega\left(v^{\frac{1}{1+\alpha}} M^{\frac{\alpha}{1+\alpha}} T^{\frac{1}{1+\alpha}}\right) \text{ for } \frac{1}{4}\left(\frac{M}{4C^2T}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}} \leq \Delta \leq \frac{1}{2}\left(\frac{M}{4C^2T}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}. \quad (21)$$

C.4.1 Application to the squared exponential kernel

For the SE kernel, we have from the choice $M = \Theta\left((\ln \frac{B}{\Delta})^d\right)$, along with the upper and lower bounds on Δ in 21, that $\Delta = \Theta\left(\left(\frac{1}{T}(\ln \frac{B}{\Delta})^d\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}\right)$. This, in turn, implies that $\ln \frac{B}{\Delta} = \ln \frac{BT^{\frac{\alpha}{1+\alpha}}}{v^{\frac{1}{1+\alpha}}} - \ln\left(\Theta(1)\left(\ln \frac{B}{\Delta}\right)^{\frac{d\alpha}{1+\alpha}}\right)$. Since $d = O(1)$ and $\frac{\alpha}{1+\alpha} \in (0, \frac{1}{2}]$, the second term behaves as $\Theta(\ln\ln \frac{B}{\Delta})$, which is $\Theta\left(\frac{1}{2}\ln \frac{B}{\Delta}\right)$ for sufficiently small $\frac{\Delta}{B}$. This, implies that $\ln \frac{B}{\Delta} = \Theta\left(\ln \frac{BT^{\frac{\alpha}{1+\alpha}}}{v^{\frac{1}{1+\alpha}}}\right)$, and thus, in turn, $M = \Theta\left(\left(\ln \frac{BT^{\frac{\alpha}{1+\alpha}}}{v^{\frac{1}{1+\alpha}}}\right)^d\right)$ and $\Delta = \Theta\left(v^{\frac{1}{1+\alpha}}\left(\ln \frac{BT^{\frac{\alpha}{1+\alpha}}}{v^{\frac{1}{1+\alpha}}}\right)^{\frac{d\alpha}{1+\alpha}} T^{-\frac{\alpha}{1+\alpha}}\right)$. Note that the choice of M ensures that $M \leq 2C^2T$ and the choice of Δ ensures that $\frac{\Delta}{B}$ is indeed sufficiently small as long as $v^{\frac{1}{1+\alpha}} \leq C'BT^{\frac{\alpha}{1+\alpha}}$ for some sufficiently small constant C' [5]. Now, substituting M in 21, we obtain $\mathbb{E}\left[R_T\right] = \Omega\left(v^{\frac{1}{1+\alpha}}\left(\ln \frac{BT^{\frac{\alpha}{1+\alpha}}}{v^{\frac{1}{1+\alpha}}}\right)^{\frac{d\alpha}{1+\alpha}} T^{\frac{1}{1+\alpha}}\right) = \Omega\left(v^{\frac{1}{1+\alpha}}\left(\ln \frac{B^{\frac{1+\alpha}{\alpha}}T}{v^{\frac{1}{\alpha}}}\right)^{\frac{d\alpha}{1+\alpha}} T^{\frac{1}{1+\alpha}}\right)$, since, generally, $d = O(1)$ and $\frac{\alpha}{1+\alpha} \in (0, \frac{1}{2}]$.

C.4.2 Application to the Matérn kernel

For the Matérn kernel, we have from the choice $M = \Theta\left((\frac{B}{\Delta})^{\frac{d}{\nu}}\right)$, along with the upper and lower bounds on Δ in 21, that $\Delta = \Theta\left(\left(\frac{1}{T}\left(\frac{B}{\Delta}\right)^{\frac{d}{\nu}}\right)^{\frac{\alpha}{1+\alpha}} v^{\frac{1}{1+\alpha}}\right)$. This, in turn, implies that $\Delta = \Theta\left(v^{\frac{\nu/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}} B^{\frac{d\alpha/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}} T^{-\frac{\nu\alpha/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}}\right)$ and $M = \Theta\left(v^{-\frac{d/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}} B^{\frac{d}{\nu+d\alpha/(1+\alpha)}} T^{\frac{d\alpha/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}}\right)$. Once again, we see that the choice of M ensures that $M \leq 2C^2T$ and the choice of Δ ensures that $\frac{\Delta}{B}$ is indeed sufficiently small as long as $v^{\frac{1}{1+\alpha}} \leq C'BT^{\frac{\alpha}{1+\alpha}}$ for some sufficiently small constant C'. Now, substituting M in 21, we obtain $\mathbb{E}\left[R_T\right] = \Omega\left(v^{\frac{\nu/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}} B^{\frac{d\alpha/(1+\alpha)}{\nu+d\alpha/(1+\alpha)}} T^{\frac{1}{1+\alpha}\frac{\nu+d\alpha}{\nu+d\alpha/(1+\alpha)}}\right) = \Omega\left(v^{\frac{\nu}{\nu(1+\alpha)+d\alpha}} B^{\frac{d\alpha}{\nu(1+\alpha)+d\alpha}} T^{\frac{\nu+d\alpha}{\nu(1+\alpha)+d\alpha}}\right)$.

D Analysis of ATA-GP-UCB

D.1 Construction of tighter confidence set using data adaptive truncation

The following lemma helps us to show that $(1+\alpha)$-th norm of $u_i \in \mathbb{R}^t$ is $t^{\frac{1-\alpha}{2(1+\alpha)}}$, where $u_i^T, i \in [m_t]$ are the rows of $\tilde{V}_t^{-1/2}\tilde{\Phi}_t^T$.

Lemma 12 *Let $A \in \mathbb{R}^{p\times q}$. Let $c_i \in \mathbb{R}^p, i = 1, \ldots, q$ be the i-th column of $A(A^TA + \lambda I_q)^{-1/2}$. Then for any $\beta \in [1, \infty)$, we have $\left\|c_i\right\|_\beta \leq p^{\frac{2-\beta}{2\beta}}$ for all $i \in [q]$.*

Proof Let the singular value decomposition of A be $U\Sigma V^T$, where U and V are unitary matrices. This implies $A(A^TA + \lambda I_q)^{-1/2} = U\Sigma(\Sigma^T\Sigma + \lambda I_q)^{-1/2}V^T$. Now, the i-th column of $A(A^TA + \lambda I_q)^{-1/2}$ is given by $c_i = U\Sigma(\Sigma^T\Sigma + \lambda I)^{-1/2}V^Te_i$. Therefore,

$$\begin{aligned}
\left\|c_i\right\|_2 = \left\|U\Sigma(\Sigma^T\Sigma + \lambda I)^{-1/2}V^Te_i\right\|_2 &= \left\|\Sigma(\Sigma^T\Sigma + \lambda I)^{-1/2}V^Te_i\right\|_2 \\
&\leq \left\|\Sigma(\Sigma^T\Sigma + \lambda I)^{-1/2}\right\|_2 \left\|V^Te_i\right\|_2 \leq 1.
\end{aligned}$$

[5] In our setting, B and v are constants that do not scale with T and the condition is trivially satisfied.

Now the result follows from the fact that for any $a \in \mathbb{R}^p$, $\|a\|_2 \leq 1$ the maximum value of $\|a\|_\beta$ for any $\beta \in [1, \infty)$ is $p^{\frac{2-\beta}{2\beta}}$ with the maximum attained at $[\frac{1}{\sqrt{p}}, \ldots, \frac{1}{\sqrt{p}}]^T$. ■

Now, we will show that the data adaptive truncation of ATA-GP-UCB helps us to achieve tighter confidence sets than TGP-UCB.

Lemma 13 (Effect of data adaptive truncation) *For any $\delta \in (0, 1]$, ATA-GP-UCB with $b_t = (v/\ln(2m_t T/\delta))^{\frac{1}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}$, ensures, with probability at least $1 - \delta$, that uniformly over all $t \in [T]$,*

$$\left\| \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t - \tilde{\theta}_t \right\|_{\tilde{V}_t} \leq 4\sqrt{m_t}\, v^{\frac{1}{1+\alpha}} \left(\ln(2m_t T/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}},$$

where $f_t = [f(x_1), \ldots, f(x_t)]^T$ is a vector containing f's evaluations up to round t.

Proof The proof is inspired from Shao et al. [34], with some changes. Fix any $t \in \mathbb{N}$. Let $u_i^T \in \mathbb{R}^{1\times t}$, $i = 1, \ldots, m_t$ denotes the i-th row of $\tilde{V}_t^{-1/2} \tilde{\Phi}_t^T$ where $\tilde{V}_t = \tilde{\Phi}_t^T \tilde{\Phi}_t + \lambda I_{m_t}$. Let $r_i = u_i^T Y_t = \sum_{\tau=1}^t u_{i,\tau} y_\tau$ denotes the sum of weighted historical rewards in the i-th dimension of the feature space with the weight vector u_i and $\widehat{r}_i = \sum_{\tau=1}^t u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t}$ denotes the corresponding truncation. Let $\mathcal{F}'_{t,\tau} = \sigma(\{x_1, \ldots, x_t\} \cup \{y_1, \ldots, y_\tau\}), \tau = 0, 1, 2, \ldots, t$ denotes the σ-algebra generated by the arms played up to time t and rewards obtained up to time τ. Observe that $\mathcal{F}'_{t,0} \subseteq \mathcal{F}'_{t,1} \subseteq \mathcal{F}'_{t,2} \subseteq \ldots$ and define $\mathcal{F}'_t = \mathcal{F}'_{t,0}$. Then, $\mathbb{E}[Y_t|\mathcal{F}'_t] = f_t$ and $u_i, i = 1, \ldots, m_t$ are $\mathcal{F}'_t$-measurable. Therefore, we have $\mathbb{E}[r_i|\mathcal{F}'_t] = u_i^T f_t = \sum_{\tau=1}^t u_{i,\tau} f(x_\tau) = \sum_{\tau=1}^t \mathbb{E}\left[u_{i,\tau} y_\tau | \mathcal{F}'_{t,\tau-1}\right]$ for all $i \in [m_t]$. This implies

$$\begin{aligned}
& \left|\widehat{r}_i - \mathbb{E}[r_i|\mathcal{F}'_t]\right| \\
= & \left| \sum_{\tau=1}^t u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} - \sum_{\tau=1}^t \mathbb{E}\left[u_{i,\tau} y_\tau | \mathcal{F}'_{t,\tau-1}\right] \right| \\
= & \left| \sum_{\tau=1}^t u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} - \sum_{\tau=1}^t \mathbb{E}\left[u_{i,\tau} y_\tau \left(\mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} + \mathbb{1}_{|u_{i,\tau} y_\tau| > b_t}\right) | \mathcal{F}'_{t,\tau-1}\right] \right| \\
\leq & \left| \sum_{\tau=1}^t \left(u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} - \mathbb{E}\left[u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} | \mathcal{F}'_{t,\tau-1}\right]\right) \right| + \sum_{\tau=1}^t \mathbb{E}\left[|u_{i,\tau} y_\tau| \, \mathbb{1}_{|u_{i,\tau} y_\tau| > b_t} | \mathcal{F}'_{t,\tau-1}\right].
\end{aligned}$$

Now, we will bound the second term first. Observe that $\mathbb{E}\left[|u_{i,\tau} y_\tau| \, \mathbb{1}_{|u_{i,\tau} y_\tau| > b_t} | \mathcal{F}'_{t,\tau-1}\right] \leq b_t^{-\alpha} \mathbb{E}\left[|u_{i,\tau} y_\tau|^{1+\alpha} \mathbb{1}_{|u_{i,\tau} y_\tau| > b_t} | \mathcal{F}'_{t,\tau-1}\right] \leq b_t^{-\alpha} |u_{i,\tau}|^{1+\alpha} \mathbb{E}\left[|y_\tau|^{1+\alpha} | \mathcal{F}'_{t,\tau-1}\right]$. Now since the noise variables are sampled independent of the arms played, it holds that $\mathbb{E}\left[|y_\tau|^{1+\alpha} | \mathcal{F}'_{t,\tau-1}\right] = \mathbb{E}\left[|y_\tau|^{1+\alpha} | \mathcal{F}_{\tau-1}\right]$ and therefore

$$\sum_{\tau=1}^t \mathbb{E}\left[|u_{i,\tau} y_\tau| \, \mathbb{1}_{|u_{i,\tau} y_\tau| > b_t} | \mathcal{F}'_{t,\tau-1}\right] \leq v b_t^{-\alpha} \sum_{\tau=1}^t |u_{i,\tau}|^{1+\alpha}.$$

Now, we will bound the first term. For that, we define $M_{t,\tau} := u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} - \mathbb{E}\left[u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} \;\middle|\; \mathcal{F}'_{t,\tau-1}\right], \tau = 1, 2, \ldots, t$. It is easy to see that $(M_{t,\tau})_{\tau \geq 1}$ is a martingale difference sequence with respect to the filtration $(\mathcal{F}'_{t,\tau})_{\tau \geq 0}$ and $|M_{t,\tau}| \leq 2b_t$ almost surely. Further, $\mathbb{V}[M_\tau \mid \mathcal{F}'_{t,\tau-1}] = \mathbb{V}[u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} \mid \mathcal{F}'_{t,\tau-1}] \leq \mathbb{E}\left[u_{i,\tau}^2 y_\tau^2 \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} \;\middle|\; \mathcal{F}'_{t,\tau-1}\right] \leq b_t^{1-\alpha} |u_{i,\tau}|^{1+\alpha} \mathbb{E}\left[|y_\tau|^{1+\alpha} \;\middle|\; \mathcal{F}'_{t,\tau-1}\right] \leq v b_t^{1-\alpha} |u_{i,\tau}|^{1+\alpha}$. Then by Bernstein's inequality [32], we have that for any $\gamma \in [0, 1/2b_t]$ and $\delta \in (0, 1]$, with probability at least $1 - \delta$,

$$\left| \sum_{\tau=1}^t \left(u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t} - \mathbb{E}\left[u_{i,\tau} y_\tau \mathbb{1}_{|u_{i,\tau} y_\tau| \leq b_t}\right]\right) \right| \leq \frac{1}{\gamma} \ln(2/\delta) + \gamma(e-2) \sum_{\tau=1}^t v b_t^{1-\alpha} |u_{i,\tau}|^{1+\alpha}.$$

Now setting $\gamma = 1/2b_t$, we obtain that for any $i \in [m_t]$ and $\delta \in (0,1]$, with probability at least $1-\delta$,

$$\begin{aligned}
\left|\widehat{r}_i - \mathbb{E}\left[r_i|\mathcal{F}'_t\right]\right| &\leq 2b_t \ln(2/\delta) + 2vb_t^{-\alpha} \sum_{\tau=1}^{t} \left|u_{i,\tau}\right|^{1+\alpha} \\
&= 2b_t \ln(2/\delta) + 2vb_t^{-\alpha} \left\|u_i\right\|_{1+\alpha}^{1+\alpha} \\
&\overset{(a)}{\leq} 2b_t \ln(2/\delta) + 2vb_t^{-\alpha} t^{\frac{1-\alpha}{2}} \\
&\overset{(b)}{\leq} 4v^{\frac{1}{1+\alpha}} \left(\ln(2/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}. \qquad (22)
\end{aligned}$$

Here (a) follows from Lemma 12 and (b) holds for $b_t = (v/\ln(2/\delta))^{\frac{1}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}$. Now observe that $\tilde{V}_t^{1/2}\tilde{\theta}_t = [\widehat{r}_1, \ldots, \widehat{r}_{m_t}]^T$ and $\tilde{V}_t^{-1/2}\tilde{\Phi}_t^T f_t = [u_1^T f_t, \ldots, u_{m_t}^T f_t]^T = [\mathbb{E}\left[r_1|\mathcal{F}'_t\right], \ldots, \mathbb{E}\left[r_{m_t}|\mathcal{F}'_t\right]]^T$. This implies

$$\left\|\tilde{V}_t^{-1}\tilde{\Phi}_t^T f_t - \tilde{\theta}_t\right\|_{\tilde{V}_t} = \left\|\tilde{V}_t^{-1/2}\tilde{\Phi}_t^T f_t - \tilde{V}_t^{1/2}\tilde{\theta}_t\right\|_2 = \sqrt{\sum_{i=1}^{m_t}\left(\widehat{r}_i - \mathbb{E}\left[r_i|\mathcal{F}'_{t-1}\right]\right)^2}.$$

Therefore, by taking an union bound over all $i \in [m_t]$ and setting $\delta = \delta/m_t$ in 22, we obtain that for any $t \in \mathbb{N}$ and $\delta \in (0,1]$, with probability at least $1-\delta$,

$$\left\|\tilde{V}_t^{-1}\tilde{\Phi}_t^T f_t - \tilde{\theta}_t\right\|_{\tilde{V}_t} \leq 4\sqrt{m_t}\, v^{\frac{1}{1+\alpha}} \left(\ln(2m_t/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}.$$

Now the result follows by taking another union bound over all $t \in [T]$ and setting $\delta = \delta/T$. ■

D.2 Analysis of ATA-GP-UCB under quadrature Fourier features (QFF) approximation

D.2.1 Error due to Fourier feature approximation

Definition 2 (Uniform Approximation [26]) *Let $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}, \mathcal{X} \subset \mathbb{R}^d$ be a kernel, then a feature map $\tilde{\varphi} : \mathcal{X} \to \mathbb{R}^m$ uniformly approximates k within an accuracy ε_m if and only if,*

$$\sup_{x,y\in\mathcal{X}} \left|k(x,y) - \tilde{\varphi}(x)^T\tilde{\varphi}(y)\right| \leq \varepsilon_m. \qquad (23)$$

Lemma 14 (QFF error) *[26, Theorem 1] Let $\mathcal{X} = [0,1]^d$, $k = k_{SE}$ and $\tilde{\varphi}$ be as in 1. Then,*

$$\varepsilon_m \leq d2^{d-1}\frac{1}{\sqrt{2}\bar{m}^{\bar{m}}}\left(\frac{e}{4l^2}\right)^{\bar{m}}.$$

Lemma 14 implies that QFF embedding (1) of k_{SE} satisfies $\varepsilon_m = O\left(\frac{d2^{d-1}}{(\bar{m}l^2)^{\bar{m}}}\right)$ where $m = \bar{m}^d$. We can achieve exponential decay only when $\bar{m} > 1/l^2$, and in that case $O\left((d + \ln(d/\varepsilon_m))^d\right)$ features are required to obtain an ε_m-accurate approximation of the SE kernel. In contrast, Sriperumbudur and Szabó [36] show that for any compact $\mathcal{X} \subset \mathbb{R}^d$, the uniform approximation error using RFF is $\varepsilon_m = O_p(\sqrt{d\ln|\mathcal{X}|/m})$, i.e. at least $O(d\ln|\mathcal{X}|/\varepsilon_m^2)$ features are required to obtain an ε_m-accurate approximation of k. In most of the BO applications either $d = O(1)$, or there are enough structure (e.g. generalized additive models) such that effective dimensionality of the problem is low. In that case $O(1/\varepsilon_m^2)$ and $O((\ln(1/\varepsilon_m)^d)$ features are needed to obtain ε_m-accuracy with RFF and QFF approximations, respectively.

Now, recall that the posterior mean and variance of a GP prior $GP_{\mathcal{X}}(0,k)$ with iid Gaussian noise $\mathcal{N}(0,\lambda)$ are given by $\mu_t(x) = k_t(x)^T(K_t + \lambda I_t)^{-1}Y_t$ and $\sigma_t^2(x) = k(x,x) - k_t(x)^T(K_t + \lambda I_t)^{-1}k_t(x)$, respectively. Let $\alpha_t(x) = k_t(x)^T(K_t + \lambda I_t)^{-1}f_t$ denotes the expected posterior mean and $\tilde{\alpha}_t(x) = \tilde{k}_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1}f_t$ denotes the approximation of $\alpha_t(x)$, where $\tilde{k}_t(x) = \tilde{\Phi}_t\tilde{\varphi}(x)$ and $\tilde{K}_t = \tilde{\Phi}_t\tilde{\Phi}_t^T$. Define $\tilde{k}(x,y) = \tilde{\varphi}(x)^T\tilde{\varphi}(y)$. Then, the approximate posterior variance under QFF approximation is $\tilde{\sigma}_t^2(x) = \lambda\tilde{\varphi}_t(x)^T\tilde{V}_t^{-1}\tilde{\varphi}_t(x) = \tilde{k}(x,x) - \tilde{k}_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1}\tilde{k}_t(x)$. Now, we will show that the error introduced by uniform approximation reflects in the approximation of the posterior variance and the expected posterior mean.

Lemma 15 (Error in posterior mean and variance approximations) *Let $f \in \mathcal{H}_k(\mathcal{X})$, $\|f\|_{\mathcal{H}} \leq B$ and $k(x,x) \leq 1$ for all $x \in \mathcal{X}$. Let $\tilde{\varphi} : \mathcal{X} \to \mathbb{R}^m$ be a feature map such that 23 holds for some $\varepsilon_m < 1$, and $\tilde{\varphi}(x)^T\tilde{\varphi}(y) \leq 1$ for all $x, y \in \mathcal{X}$. Then for all $x \in \mathcal{X}$ and $t \geq 1$, we have*

$$(i) \quad |\alpha_t(x) - \tilde{\alpha}_t(x)| = O(B\varepsilon_m t^2/\lambda) \quad \textit{and} \quad (ii) \quad |\sigma_t(x) - \tilde{\sigma}_t(x)| = O(\varepsilon_m^{1/2} t/\lambda).$$

Proof This proof is inspired from [26], with some notable changes. First, observe that

$$\begin{aligned}
& \left|k_t(x)^T(K_t + \lambda I_t)^{-1} f_t - \tilde{k}_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1} f_t\right| \\
\overset{(a)}{\leq} & \left|\left(k_t(x) - \tilde{k}_t(x)\right)^T (K_t + \lambda I_t)^{-1} f_t\right| + \left|\tilde{k}_t(x)^T \left((K_t + \lambda I_t)^{-1} - (\tilde{K}_t + \lambda I_t)^{-1}\right) f_t\right| \\
\overset{(b)}{\leq} & \left\|k_t(x) - \tilde{k}_t(x)\right\|_2 \left\|(K_t + \lambda I_t)^{-1} f_t\right\|_2 + \left\|\tilde{k}_t(x)\right\|_2 \left\|\left((K_t + \lambda I_t)^{-1} - (\tilde{K}_t + \lambda I_t)^{-1}\right) f_t\right\|_2 \\
\overset{(c)}{\leq} & \left\|k_t(x) - \tilde{k}_t(x)\right\|_2 \left\|(K_t + \lambda I_t)^{-1}\right\|_2 \|f_t\|_2 + \left\|\tilde{k}_t(x)\right\|_2 \left\|(K_t + \lambda I_t)^{-1} - (\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \|f_t\|_2,
\end{aligned}$$

where (a) uses triangle inequality, (b) uses Cauchy-Schwartz inequality and (c) uses the definition of operator norm. By our hypothesis, $\|f_t\|_2 \leq Bt^{1/2}$, $\left\|\tilde{k}_t(x)\right\|_2 \leq t^{1/2}$ and $\left\|k_t(x) - \tilde{k}_t(x)\right\|_2 \leq \varepsilon_m t^{1/2}$. Now

$$\begin{aligned}
\left\|(K_t + \lambda I_t)^{-1} - (\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 &= \left\|(K_t + \lambda I_t)^{-1}\left((\tilde{K}_t + \lambda I_t) - (K_t + \lambda I_t)\right)(\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \\
&= \left\|(K_t + \lambda I_t)^{-1}(\tilde{K}_t - K_t)(\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \\
&\overset{(a)}{\leq} \left\|(K_t + \lambda I_t)^{-1}\right\|_2 \left\|\tilde{K}_t - K_t\right\|_2 \left\|(\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \\
&\overset{(b)}{\leq} \varepsilon_m t/\lambda^2,
\end{aligned}$$

where (a) follows from the sub-multiplicative property of operator norm and (b) follows from the facts that $\left\|K_t - \tilde{K}_t\right\|_2 \leq \sqrt{\sum_{1 \leq i,j \leq t}(k(x_i, x_j) - \tilde{k}(x_i, x_j))^2} \leq \varepsilon_m t$, and that for any p.s.d. matrix $A \in \mathbb{R}^{t \times t}$, $\left\|(A + \lambda I_t)^{-1}\right\|_2 = \lambda_{\max}\{(A + \lambda I_t)^{-1}\} = 1/\lambda_{\min}\{A + \lambda I_t\} \leq 1/\lambda$. Therefore, for all $x \in \mathcal{X}$ and $t \geq 1$, we have

$$|\alpha_t(x) - \tilde{\alpha}_t(x)| \leq \left(\varepsilon_m t^{1/2}/\lambda + \varepsilon_m t^{3/2}/\lambda^2\right) Bt^{1/2} = O(B\varepsilon_m t^2/\lambda).$$

Now, since $\left|k(x,y) - \tilde{k}(x,y)\right| \leq \varepsilon_m$ for all $x, y \in \mathcal{X}$, we have $\tilde{k}_t(x) = k_t(x) + a_t(x)$ where $\|a_t(x)\|_\infty \leq \varepsilon_m$. This implies

$$\begin{aligned}
& \left|\sigma_t^2(x) - \tilde{\sigma}_t^2(x)\right| \\
= \;& \left|k(x,y) - \tilde{k}(x,y)\right| + \left|\tilde{k}_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1}\tilde{k}_t(x) - k_t(x)^T(K_t + \lambda I_t)^{-1}k_t(x)\right| \\
\leq \;& \varepsilon_m + \left|k_t(x)^T\left((\tilde{K}_t + \lambda I_t)^{-1} - (K_t + \lambda I_t)^{-1}\right)k_t(x)\right| + 2\left|a_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1}k_t(x)\right| \\
& \qquad + \left|a_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1}a_t(x)\right| \\
\overset{(a)}{\leq} \;& \varepsilon_m + \left\|(\tilde{K}_t + \lambda I_t)^{-1} - (K_t + \lambda I_t)^{-1}\right\|_2 \|k_t(x)\|_2^2 + 2\|a_t(x)\|_2 \left\|(\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \|k_t(x)\|_2 \\
& \qquad + \left\|(\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \|a_t(x)\|_2^2 \\
\overset{(b)}{\leq} \;& \varepsilon_m + \varepsilon_m t^2/\lambda^2 + 2\varepsilon_m t/\lambda + \varepsilon_m^2 t/\lambda = O(\varepsilon_m t^2/\lambda^2) \text{ for } \varepsilon_m < 1.
\end{aligned}$$

Here (a) is due to Cauchy-Schwartz inequality and definition of operator norm. (b) uses $\|k_t(x)\|_2 \leq t^{1/2}$, $\|a_t(x)\|_2 \leq \varepsilon_m t^{1/2}$, $\left\|(\tilde{K}_t + \lambda I_t)^{-1} - (K_t + \lambda I_t)^{-1}\right\|_2 \leq \varepsilon_m t/\lambda^2$ and $\left\|(\tilde{K}_t + \lambda I_t)^{-1}\right\|_2 \leq 1/\lambda$. Now, the result follows from the fact that for any $a, b \geq 0$, $(a+b)^{1/2} \leq a^{1/2} + b^{1/2}$. ■

Now, we are ready to prove Lemma 1.

D.2.2 Proof of Lemma 1

Under the QFF approximation, we have $\tilde{\varphi}_t = \tilde{\varphi}$ and $m_t = m$ for all $t \geq 1$. Hence, we have $\tilde{\mu}_t(x) = \tilde{\varphi}(x)^T \tilde{\theta}_t$ and $\tilde{\alpha}_t(x) = \tilde{\varphi}(x)^T \tilde{\Phi}_t^T (\tilde{\Phi}_t \tilde{\Phi}_t^T + \lambda I_t)^{-1} f_t = \tilde{\varphi}(x)^T \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t$, where the last equality follows from 3. Now, by Cauchy-Schwartz inequality,

$$|\tilde{\alpha}_t(x) - \tilde{\mu}_t(x)| \leq \left\| \tilde{V}_t^{-1} \tilde{\Phi}^T f_t - \tilde{\theta}_t \right\|_{\tilde{V}_t} \|\tilde{\varphi}(x)\|_{\tilde{V}_t^{-1}} = \lambda^{-1/2} \left\| \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t - \tilde{\theta}_t \right\|_{\tilde{V}_t} \tilde{\sigma}_t(x).$$

Hence, from Lemma 13, we have, for any $\delta \in (0,1]$, with probability at least $1-\delta$, uniformly over all $x \in \mathcal{X}$ and $t \in [T]$, that

$$|\tilde{\alpha}_t(x) - \tilde{\mu}_t(x)| \leq 4\sqrt{m/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(2mT/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}} \tilde{\sigma}_t(x). \tag{24}$$

By triangle inequality,

$$|f(x) - \tilde{\mu}_t(x)| \leq |f(x) - \alpha_t(x)| + |\alpha_t(x) - \tilde{\alpha}_t(x)| + |\tilde{\alpha}_t(x) - \tilde{\mu}_t(x)|.$$

Now, from 7, $|f(x) - \alpha_t(x)| \leq B\sigma_t(x)$ and thus, in turn, from Lemma 15, $|f(x) - \alpha_t(x)| = B\tilde{\sigma}_t(x) + O(B\varepsilon_m^{1/2} t/\lambda)$. Also, from Lemma 15, $|\alpha_t(x) - \tilde{\alpha}_t(x)| = O(B\varepsilon_m t^2/\lambda)$. Now combining these with 24, we obtain, for any $\delta \in (0,1]$, with probability at least $1-\delta$, uniformly over all $x \in \mathcal{X}$ and $t \in [T]$, that

$$\begin{aligned} |f(x) - \tilde{\mu}_t(x)| &\leq \left(B + 4\sqrt{m/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(2mT/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}\right) \tilde{\sigma}_t(x) + O(B\varepsilon_m^{1/2} t/\lambda) + O(B\varepsilon_m t^2/\lambda) \\ &= \left(B + 4\sqrt{m/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(2mT/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}\right) \tilde{\sigma}_t(x) + O(B\varepsilon_m^{1/2} t^2/\lambda) \end{aligned}$$

for $\varepsilon_m < 1$. Further observe that $|f(x) - \tilde{\mu}_0(x)| = |f(x)| \leq Bk^{1/2}(x,x) = B\sigma_0(x) \leq B\tilde{\sigma}_0(x) + B\varepsilon_m^{1/2}$. Now the result follows by setting $\beta_{t+1} = B + 4\sqrt{m/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(2mT/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}$ for all $t \geq 0$.

D.2.3 Proof of Theorem 3

For any $\delta \in (0,1]$, we have, with probability at least $1-\delta$, uniformly over all $t \in [T]$, the instantaneous regret

$$\begin{aligned} r_t &= f(x^\star) - f(x_t) \\ &\overset{(a)}{\leq} \tilde{\mu}_{t-1}(x^\star) + \beta_t \tilde{\sigma}_{t-1}(x^\star) + O(B\varepsilon_m^{1/2} t^2/\lambda) - f(x_t) \\ &\overset{(b)}{\leq} \tilde{\mu}_{t-1}(x_t) + \beta_t \tilde{\sigma}_{t-1}(x_t) - f(x_t) + O(B\varepsilon_m^{1/2} t^2/\lambda) \\ &\overset{(c)}{\leq} 2\beta_t \tilde{\sigma}_{t-1}(x_t) + O(B\varepsilon_m^{1/2} t^2/\lambda)). \end{aligned}$$

Here (a) and (c) follow from Lemma 1 and (b) is due to the choice of ATA-GP-UCB (Algorithm 2). Now Observe that $(\beta_t)_{t \geq 1}$ is an increasing sequence in t. Further,

$$\sum_{t=1}^{T} \tilde{\sigma}_{t-1}(x_t) \overset{(a)}{\leq} \sqrt{T \sum_{t=1}^{T} \tilde{\sigma}_{t-1}^2(x_t)} \overset{(b)}{\leq} \sqrt{2(1+\lambda) T \tilde{\gamma}_T} = O(\sqrt{mT \ln T}).$$

Here (a) follows from Cauchy-Schwartz inequality, (b) from Lemma 6, and (c) from Lemma 5 noting that $\tilde{k}$ is a linear kernel defined on $\mathbb{R}^{2m}$. Hence for any $\delta \in (0,1]$, with probability at least $1-\delta$, the cumulative regret of ATA-GP-UCB after T rounds is

$$\begin{aligned} R_T &= O\left(\beta_T \sqrt{Tm \ln T}\right) + \sum_{t=1}^{T} O(B\varepsilon_m^{1/2} t^2/\lambda) \\ &= O\left(B\sqrt{Tm \ln T} + m v^{\frac{1}{1+\alpha}} \left(\ln(mT/\delta)\right)^{\frac{\alpha}{1+\alpha}} (\ln T)^{1/2} T^{\frac{1}{1+\alpha}} + B\varepsilon_m^{1/2} T^3\right). \end{aligned}$$

From Lemma 14 if $\bar{m} \geq 1/l^2$ and $d = O(1)$, we have $\varepsilon_m = O((e/4)^{\bar{m}})$. Further if $\bar{m} \geq \log_{4/e}(T^6)$, then $\varepsilon_m^{1/2} T^3 = O(1)$. Now choosing $\bar{m} = \Theta\left(\log_{4/e}(T^6)\right)$, we can ensure that $m = O((\ln T)^d)$ [6].

[6] For the RFF approximation, we have $\varepsilon_m = O_p(1/\sqrt{m})$ if $d = O(1)$. Now in order to make the last term $\varepsilon_m^{1/2} T^3$ behave as $O(1)$, we have to take $m = O(T^{12})$ features which will eventually blow up the first two terms by the same order. Hence, we will never achieve sub-linear regret bound using RFF approximation.

Therefore for any $\delta \in (0,1]$, with probability at least $1-\delta$, the cumulative regret of ATA-GP-UCB under QFF approximation after T rounds is

$$R_T = O\left(B\sqrt{T(\ln T)^{d+1}} + v^{\frac{1}{1+\alpha}} \left(\ln \left(T(\ln T)^d/\delta\right)\right)^{\frac{\alpha}{1+\alpha}} \sqrt{\ln T}(\ln T)^d T^{\frac{1}{1+\alpha}} \right).$$

D.3 Analysis of ATA-GP-UCB under Nyström approximation

D.3.1 Construction of dictionary and its properties

Given the kernel matrix K_t, we define an accurate dictionary as follows.

Definition 3 (ε-accurate dictionary [9]) *For any $\varepsilon \in (0,1)$, a dictionary $\mathcal{D}_t \subseteq \{x_1, \ldots, x_t\}$ is said to be ε-accurate with respect to the kernel matrix K_t if*

$$\left\|(K_t + \lambda I)^{-1/2} K_t^{1/2} (I_t - S_t^2) K_t^{1/2} (K_t + \lambda I)^{-1/2}\right\|_2 \leq \varepsilon,$$

where S_t is the selection matrix associated with the dictionary $\mathcal{D}_t$ such that $[S_t]_{i,i} = 1/\sqrt{p_{t,i}}$ if $x_i \in \mathcal{D}_t$, and 0, elsewhere.

The following lemma states two more equivalent condition for a dictionary to be accurate.

Lemma 16 *Let $V_{\mathcal{D}_t} = \Phi_t^T S_t^2 \Phi_t + \lambda I_{\mathcal{H}}$. Then, the following are equivalent:*

1. $\left\|(K_t + \lambda I)^{-1/2} K_t^{1/2} (I_t - S_t^2) K_t^{1/2} (K_t + \lambda I)^{-1/2}\right\|_2 \leq \varepsilon$,
2. $\left\|(\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} \Phi_t^T (I_t - S_t^2) \Phi_t (\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2}\right\|_{\mathcal{H}} \leq \varepsilon$,
3. $(1-\varepsilon) V_t \preceq V_{\mathcal{D}_t} \preceq (1+\varepsilon) V_t$.

Proof Let $\Phi_t = U \Sigma V^T$ be the singular value decomposition of Φ_t. Then $\Phi_t(\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} = U\Sigma(\Sigma^T\Sigma + \lambda I_{\mathcal{H}})^{-1} V^T$, $(\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} \Phi_t^T = V(\Sigma^T \Sigma + \lambda I_{\mathcal{H}})^{-1} \Sigma^T U^T$ and $K_t = U \Sigma \Sigma^T U^T$. Therefore

$$\begin{aligned}
& \left\|(\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} \Phi_t^T (I_t - S_t^2) \Phi_t (\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2}\right\|_{\mathcal{H}} \\
= & \left\|V(\Sigma^T\Sigma + \lambda I_{\mathcal{H}})^{-1/2} \Sigma^T U^T (I_t - S_t^2) U \Sigma (\Sigma^T \Sigma + \lambda I_{\mathcal{H}})^{-1/2} V^T\right\|_{\mathcal{H}} \\
= & \left\|(\Sigma^T\Sigma + \lambda I_{\mathcal{H}})^{-1/2} \Sigma^T U^T (I_t - S_t^2) U \Sigma (\Sigma^T \Sigma + \lambda I_{\mathcal{H}})^{-1/2}\right\|_{\mathcal{H}} \\
= & \left\|(\Sigma\Sigma^T + \lambda I_t)^{-1/2} (\Sigma\Sigma^T)^{1/2} U^T (I_t - S_t^2) U (\Sigma\Sigma^T)^{1/2} (\Sigma\Sigma^T + \lambda I_t)^{-1/2}\right\|_2 \\
= & \left\|U(\Sigma\Sigma^T + \lambda I_t)^{-1/2} (\Sigma\Sigma^T)^{1/2} U^T (I_t - S_t^2) U (\Sigma\Sigma^T)^{1/2} (\Sigma\Sigma^T + \lambda I_t)^{-1/2} U^T\right\|_2 \\
= & \left\|(K_t + \lambda I)^{-1/2} K_t^{1/2} (I_t - S_t^2) K_t^{1/2} (K_t + \lambda I)^{-1/2}\right\|_2,
\end{aligned}$$

which proves that $1 \iff 2$. Now, Observe that

$$\begin{aligned}
& \left\|(\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} \Phi_t^T (I_t - S_t^2) \Phi_t (\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2}\right\|_{\mathcal{H}} \leq \varepsilon \\
\iff & -\varepsilon I_{\mathcal{H}} \preceq (\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} (\Phi_t^T \Phi_t - \Phi_t^T S_t^2 \Phi_t)(\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1/2} \preceq \varepsilon I_{\mathcal{H}} \\
\iff & -\varepsilon I_{\mathcal{H}} \preceq V_t^{-1/2} (V_t - V_{\mathcal{D}_t}) V_t^{-1/2} \preceq \varepsilon I_{\mathcal{H}} \\
\iff & -\varepsilon V_t \preceq V_t - V_{\mathcal{D}_t} \preceq \varepsilon V_t \\
\iff & (1-\varepsilon) V_t \preceq V_{\mathcal{D}_t} \preceq (1+\varepsilon) V_t,
\end{aligned}$$

which proves $2 \iff 3$. ■

An ε-accurate dictionary can be obtained by including points proportional to their λ-ridge leverage scores defined as follows.

Definition 4 (Ridge leverage score [1]) *For a set of points $\{x_1, \ldots, x_t\}$ and a constant $\lambda > 0$, the λ- ridge leverage score of the point $x_i, i \in [t]$ is defined as*

$$l_{t,i} = e_i^T K_t (K_t + \lambda I_t)^{-1} e_i,$$

where $e_i \in \mathbb{R}^t$ is the i-th standard basis vector.

Ridge leverage score (RLS) can be interpreted in many ways and it is well studied in the literature. Here we observe that

$$e_i^T K_t(K_t+\lambda I_t)^{-1} e_i = e_i^T \Phi_t \Phi_t^T (\Phi_t \Phi_t^T + \lambda I_t)^{-1} e_i = e_i^T \Phi_t (\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1} \Phi_t^T e_i = \|\varphi(x_i)\|^2_{V_t^{-1}}.$$

Therefore $l_{t,i} = \frac{1}{\lambda}\sigma_t^2(x_i)$, i.e., the RLS of x_i is proportional its posterior variance $\sigma_t^2(x_i)$ under the GP prior $GP_{\mathcal{X}}(0,k)$. However, the exact computation of λ-ridge leverage scores in turn requires inverting the kernel matrix K_t which requires $O(t^3)$ time. This motivates the need for a fast approximation of RLS such that it can be used to construct an ε-accurate dictionary. Calandriello et al. [9] show that, instead of using the exact ridge leverage scores (or, equivalently, posterior variances) if we use the approximate variances from the previous round to sample points in the current round, then we will be able to obtain an accurate dictionary. Not only that, the dictionary size will grow no faster than the maximum information gain of the underlying kernel. Now, we present the NyströmEmbedding procedure which is used in Algorithm 2.

Algorithm 3 NyströmEmbedding

Input: $\{(x_i, \tilde{\sigma}_{t-1}(x_i))\}_{i=1}^t, q$
Set: $\mathcal{D}_t = \emptyset$
for $i = 1, 2, 3 \ldots, t$ **do**
  Sample $z_{t,i} \sim \mathcal{B}\left(\min\{q\tilde{\sigma}^2_{t-1}(x_i), 1\}\right)$
  If $z_{t,i} = 1$, set $\mathcal{D}_t = \mathcal{D}_t \cup \{x_i\}$
end for
Return $\tilde{\varphi}_t(x) = \left(K_{\mathcal{D}_t}^{1/2}\right)^+ k_{\mathcal{D}_t}(x)$

The following lemma states the properties of the dictionaries $\mathcal{D}_t$ constructed using Algorithm 3.

Lemma 17 (Properties of the dictionary) *For any $\varepsilon \in (0,1)$ and $\delta \in (0,1]$, set $\rho = \frac{1+\varepsilon}{1-\varepsilon}$ and $q = \frac{6\rho \ln(2T/\delta)}{\varepsilon^2}$. Then, with probability at least $1-\delta$, uniformly over all $t \in [T]$,*

$$(1-\varepsilon)V_t \preceq V_{\mathcal{D}_t} \preceq (1+\varepsilon)V_t \quad \textit{and} \quad m_t \leq 6\rho\left(1+\frac{1}{\lambda}\right) q\gamma_t.$$

Lemma 17 is a restatement of [9, Theorem 1] and it is presented in this form for the sake of brevity and completeness. Now, we will show that using the Nyström embeddings $\tilde{\varphi}_t(x)$, we can prevent the variance starvation which generally arises due to approximation.

D.3.2 Preventing variance starvation with Nyström embeddings

Recall that the posterior mean and variance of a GP prior $GP_{\mathcal{X}}(0,k)$ with iid Gaussian noise $\mathcal{N}(0,\lambda)$ are given by $\mu_t(x) = k_t(x)^T(K_t + \lambda I_t)^{-1} Y_t$ and $\sigma_t^2(x) = k(x,x) - k_t(x)^T(K_t + \lambda I_t)^{-1} k_t(x)$, respectively. Let $\alpha_t(x) = k_t(x)^T(K_t + \lambda I_t)^{-1} f_t$ denotes the expected posterior mean and $\tilde{\alpha}_t(x) = \tilde{k}_t(x)^T(\tilde{K}_t + \lambda I_t)^{-1} f_t$ denotes the approximation of $\alpha_t(x)$, where $\tilde{k}_t(x) = \tilde{\Phi}_t \tilde{\varphi}(x)$ and $\tilde{K}_t = \tilde{\Phi}_t \tilde{\Phi}_t^T$. Then, we have $\alpha_t(x) = \langle \varphi(x), V_t^{-1}\Phi_t^T f_t\rangle_{\mathcal{H}}$ and $\tilde{\alpha}_t(x) = \tilde{\varphi}_t(x)^T \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t$. Now, we can rewrite the posterior variance as $\sigma_t^2(x) = \lambda \|\varphi(x)\|^2_{V_t^{-1}}$, whereas the approximate posterior variance under Nyström approximation is given by $\tilde{\sigma}_t^2(x) = k(x,x) - \tilde{\varphi}_t(x)^T\tilde{\varphi}_t(x) + \lambda \tilde{\varphi}_t(x)^T \tilde{V}_t^{-1} \tilde{\varphi}_t(x)$. This choice of $\tilde{\sigma}_t^2(x)$ helps us to negate the variance starvation which arises due to feature approximation. Now, we will justify this choice of $\tilde{\sigma}_t^2(x)$ by showing that it can be derived by projecting $\varphi(x)$ to a smaller RKHS. The idea is inspired from Calandriello et al. [9].

Projection to a smaller RKHS: For any dictionary $\mathcal{D}_t = \{x_{i_1}, \ldots, x_{i_{m_t}}\}, i_j \in [t]$, define the operator $\Phi_{\mathcal{D}_t} : \mathcal{H}_k(\mathcal{X}) \to \mathbb{R}^{m_t}$ such that for any $h \in \mathcal{H}_k(\mathcal{X})$, $\Phi_{\mathcal{D}_t} h =$

$\left[\langle\varphi(x_{i_1}), h\rangle_{\mathcal{H}}, \ldots, \langle\varphi(x_{i_{m_t}}), h\rangle_{\mathcal{H}}\right]^T$ and denote its adjoint by $\Phi_{\mathcal{D}_t}^T : \mathbb{R}^{m_t} \to \mathcal{H}_k(\mathcal{X})$. Let $\widehat{\varphi}_t(x) = P_t\varphi(x)$ be the projection of $\varphi(x)$ to the subspace spanned by the columns of the operator $\Phi_{\mathcal{D}_t}^T$, where the projection operator $P_t : \mathcal{H}_k(\mathcal{X}) \to \mathrm{Col}(\Phi_{\mathcal{D}_t}^T)$ is given by $P_t = \Phi_{\mathcal{D}_t}^T(\Phi_{\mathcal{D}_t}\Phi_{\mathcal{D}_t}^T)^+\Phi_{\mathcal{D}_t}$. It is easy to see that $P_t^T = P_t$ and $P_t^2 = P_t$. Now, for any set $\{x_1, \ldots, x_t\} \subset \mathcal{X}$ define the operator $\widehat{\Phi}_t : \mathcal{H}_k(\mathcal{X}) \to \mathbb{R}^t$ such that for any $h \in \mathcal{H}_k(\mathcal{X})$, $\widehat{\Phi}_t h = [\langle\widehat{\varphi}_t(x_1), h\rangle_{\mathcal{H}}, \ldots, \langle\widehat{\varphi}_t(x_t), h\rangle_{\mathcal{H}}]^T$, and denote its adjoint by $\widehat{\Phi}_t^T : \mathbb{R}^t \to \mathcal{H}_k(\mathcal{X})$.

Lemma 18 (Approximate posterior variance and mean under projection) *Let $\widehat{V}_t = \widehat{\Phi}_t^T\widehat{\Phi}_t + \lambda I_{\mathcal{H}}$ for any $\lambda > 0$. Then, we have*

$$\tilde{\sigma}_t^2(x) = \lambda \left\|\varphi(x)\right\|_{\widehat{V}_t^{-1}}^2 \quad \textit{and} \quad \tilde{\alpha}_t(x) = \langle\varphi(x), \widehat{V}_t^{-1}\widehat{\Phi}_t^T f_t\rangle_{\mathcal{H}}.$$

Proof Since $K_{\mathcal{D}_t} = \Phi_{\mathcal{D}_t}\Phi_{\mathcal{D}_t}^T$, we have the projection $P_t = \Phi_{\mathcal{D}_t}^T(K_{\mathcal{D}_t})^+\Phi_{\mathcal{D}_t}$. Now, observe that $\langle\varphi(x), \varphi(y)\rangle_{P_t} = \left((K_{\mathcal{D}_t}^{1/2})^\dagger\Phi_{\mathcal{D}_t}\varphi(x)\right)^T\left((K_{\mathcal{D}_t}^{1/2})^\dagger\Phi_{\mathcal{D}_t}\varphi(y)\right) = \left((K_{\mathcal{D}_t}^{1/2})^\dagger k_{\mathcal{D}_t}(x)\right)^T\left((K_{\mathcal{D}_t}^{1/2})^\dagger k_{\mathcal{D}_t}(y)\right) = \tilde{\varphi}_t(x)^T\tilde{\varphi}_t(y)$. Also, note that $\widehat{\Phi}_t^T = P_t\Phi_t^T$. This implies $\widehat{\Phi}_t\varphi(x) = \Phi_t P_t\varphi(x) = [\langle\varphi(x_1), \varphi(x)\rangle_{P_t}, \ldots, \langle\varphi(x_t), \varphi(x)\rangle_{P_t}]^T = [\tilde{\varphi}_t(x_1)^T\tilde{\varphi}_t(x), \ldots, \tilde{\varphi}_t(x_t)^T\tilde{\varphi}_t(x)]^T = \tilde{\Phi}_t\tilde{\varphi}_t(x)$. Further, the (i,j)-th entry of $\widehat{\Phi}_t\widehat{\Phi}_t^T$ is given by $[\widehat{\Phi}_t\widehat{\Phi}_t^T]_{i,j} = \langle P_t\varphi(x_i), P_t\varphi(x_j)\rangle_{\mathcal{H}} = \langle\varphi(x_i), \varphi(x_j)\rangle_{P_t} = \tilde{\varphi}_t(x_i)^T\tilde{\varphi}_t(x_j)$ and hence, $\widehat{\Phi}_t\widehat{\Phi}_t^T = \tilde{\Phi}_t\tilde{\Phi}_t^T$. Then, we have

$$\begin{aligned}
\lambda \left\|\varphi(x)\right\|_{\widehat{V}_t^{-1}}^2 &= \lambda\langle\varphi(x), (\widehat{\Phi}_t^T\widehat{\Phi}_t + \lambda I_{\mathcal{H}})^{-1}\varphi(x)\rangle_{\mathcal{H}} \\
&\overset{(a)}{=} \langle\varphi(x), \left(I_{\mathcal{H}} - \widehat{\Phi}_t^T(\widehat{\Phi}_t\widehat{\Phi}_t^T + \lambda I_t)^{-1}\widehat{\Phi}_t\right)\varphi(x)\rangle_{\mathcal{H}} \\
&\overset{(b)}{=} k(x,x) - \tilde{\varphi}_t(x)^T\tilde{\Phi}_t^T(\tilde{\Phi}_t\tilde{\Phi}_t^T + \lambda I_t)^{-1}\tilde{\Phi}_t\tilde{\varphi}_t(x) \\
&\overset{(c)}{=} k(x,x) - \tilde{\varphi}_t(x)^T\tilde{\Phi}_t^T\tilde{\Phi}_t(\tilde{\Phi}_t^T\tilde{\Phi}_t + \lambda I_{m_t})^{-1}\tilde{\varphi}_t(x) \\
&= k(x,x) - \tilde{\varphi}_t(x)^T\tilde{\varphi}_t(x) + \lambda\tilde{\varphi}_t(x)^T\tilde{V}_t^{-1}\tilde{\varphi}_t(x) = \tilde{\sigma}_t^2(x).
\end{aligned}$$

Here (a) follows from 4, (b) is due to $\widehat{\Phi}_t\varphi(x) = \tilde{\Phi}_t\tilde{\varphi}_t(x)$ and $\widehat{\Phi}_t\widehat{\Phi}_t^T = \tilde{\Phi}_t\tilde{\Phi}_t^T$, and (c) follows from 3. Now observe that

$$\begin{aligned}
\langle\varphi(x), \widehat{V}_t^{-1}\widehat{\Phi}_t^T f_t\rangle_{\mathcal{H}} &= \langle\varphi(x), (\widehat{\Phi}_t^T\widehat{\Phi}_t + \lambda I_{\mathcal{H}})^{-1}\widehat{\Phi}_t^T f_t\rangle_{\mathcal{H}} \\
&\overset{(a)}{=} \langle\varphi(x), \widehat{\Phi}_t^T(\widehat{\Phi}_t\widehat{\Phi}_t^T + \lambda I_t)^{-1}f_t\rangle_{\mathcal{H}} \\
&\overset{(b)}{=} \tilde{\varphi}_t(x)^T\tilde{\Phi}_t^T(\tilde{\Phi}_t\tilde{\Phi}_t^T + \lambda I_t)^{-1}f_t \\
&\overset{(c)}{=} \tilde{\varphi}_t(x)^T(\tilde{\Phi}_t^T\tilde{\Phi}_t + \lambda I_{m_t})^{-1}\tilde{\Phi}_t^T f_t \\
&= \tilde{\varphi}_t(x)^T\tilde{V}_t^{-1}\tilde{\Phi}_t^T f_t = \tilde{\alpha}_t(x).
\end{aligned}$$

Here (a) and (c) follow from 3, and (b) is due to $\widehat{\Phi}_t\varphi(x) = \tilde{\Phi}_t\tilde{\varphi}_t(x)$ and $\widehat{\Phi}_t\widehat{\Phi}_t^T = \tilde{\Phi}_t\tilde{\Phi}_t^T$. ■

Lemma 19 (Accuracy of approximate posterior variance) *For an ε-accurate dictionary (Definition 3), we have*

$$\frac{1-\varepsilon}{1+\varepsilon}\sigma_t^2(x) \le \tilde{\sigma}_t^2(x) \le \frac{1+\varepsilon}{1-\varepsilon}\sigma_t^2(x).$$

Proof From Lemma 18, we have $\tilde{\sigma}_t^2(x) = \lambda\langle\varphi(x), \widehat{V}_t^{-1}\varphi(x)\rangle_{\mathcal{H}}$. Now, observe that $\widehat{V}_t = P_t\Phi_t^T\Phi_t P_t + \lambda I_{\mathcal{H}} = P_t V_t P_t + \lambda(I_{\mathcal{H}} - P_t)$. From Lemma 16, we have $(1-\varepsilon)V_t \preceq V_{\mathcal{D}_t} \preceq (1+\varepsilon)V_t$

for any ε-accurate dictionary $\mathcal{D}_t$. This implies that

$$\begin{aligned}\widehat{V}_t &\preceq \frac{1}{1-\varepsilon} P_t V_{\mathcal{D}_t} P_t + \lambda(I_{\mathcal{H}} - P_t)\\ &= \frac{1}{1-\varepsilon} P_t \Phi_t^T S_t^2 \Phi_t P_t + \frac{\lambda\varepsilon}{1-\varepsilon} P_t + \lambda I_{\mathcal{H}}\\ &\overset{(a)}{\preceq} \frac{1}{1-\varepsilon}(\Phi_t^T S_t^2 \Phi_t + \lambda I_{\mathcal{H}})\\ &\preceq \frac{1+\varepsilon}{1-\varepsilon} V_t,\end{aligned}$$

where (a) follows from $P_t \Phi_t^T S_t = \Phi_t^T S_t$ and $P_t \preceq I_{\mathcal{H}}$. Therefore, we have

$$\tilde{\sigma}_t^2(x) \geq \frac{1-\varepsilon}{1+\varepsilon} \lambda \langle \varphi(x), V_t^{-1}\varphi(x)\rangle_{\mathcal{H}} = \frac{1-\varepsilon}{1+\varepsilon}\sigma_t^2(x).$$

Similarly, we can show that $\widehat{V}_t \succeq \frac{1-\varepsilon}{1+\varepsilon} V_t$ and thus, in turn, $\tilde{\sigma}_t^2(x) \leq \frac{1+\varepsilon}{1-\varepsilon}\sigma_t^2(x)$. ■

Now, we will show that the confidence sets formed by ATA-GP-UCB (Algorithm 2) under Nyström approximation is tighter compared to that of TGP-UCB.

D.3.3 Confidence sets of ATA-GP-UCB under Nyström approximation

First, we define the following two events. Fix any $\varepsilon \in (0, 1)$ and $\delta \in (0, 1]$. Let $E_{1,t}$ denotes the event that the dictionary $\mathcal{D}_t$ is ε-accurate, i.e,

$$(1-\varepsilon)V_t \preceq V_{\mathcal{D}_t} \preceq (1+\varepsilon)V_t,$$

and $E_{2,t}$ denotes the event that the size of the dictionary $\mathcal{D}_t$ is at most $6\rho(1+\frac{1}{\lambda})q\gamma_t$, i.e.,

$$m_t \leq 6\rho \left(1 + \frac{1}{\lambda}\right) q\gamma_t,$$

where $\rho = \frac{1+\varepsilon}{1-\varepsilon}$ and $q = \frac{6\rho\ln(2T/\delta)}{\varepsilon^2}$. Then from Lemma 17, we have $\mathbb{P}\left[\cap_{t=1}^T (E_{1,t} \cap E_{2,t})\right] \geq 1-\delta$. Let $\mathcal{G}_t = \sigma\left(\{x_i, (z_{i,j})_{j=1}^i\}_{i=1}^t\right), t \geq 1$ denotes the σ-algebra generated by the arms played and the outcomes of the NyströmEmbedding procedure(Algorithm 3) up to time t. See that $(\mathcal{G}_t)_{t\geq 1}$ defines a filtration, and both $E_{1,t}$ and $E_{2,t}$ are $\mathcal{G}_t$ measurable.

Lemma 20 (Tighter confidence sets with Nyström embedding) *Fix any $\delta \in (0, 1]$, $\varepsilon \in (0, 1)$ and set $\rho = \frac{1+\varepsilon}{1-\varepsilon}$. Then, ATA-GP-UCB under Nyström approximation, and with parameters $q = 6\rho\ln(4T/\delta)/\varepsilon^2$, $b_t = (v/\ln(4m_tT/\delta))^{\frac{1}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}$ and $\beta_{t+1} = B(1+\frac{1}{\sqrt{1-\varepsilon}}) + 4\sqrt{m_t/\lambda}\, v^{\frac{1}{1+\alpha}} (\ln(4m_tT/\delta))^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}$, ensures, with probability at least $1-\delta$, uniformly over all $t \in [T]$ and $x \in \mathcal{X}$, that*

$$|f(x) - \tilde{\mu}_{t-1}(x)| \leq \beta_t \tilde{\sigma}_{t-1}(x),$$

where m_t is the dimension of the Nyström embedding $\tilde{\varphi}_t$ constructed at round t.

Proof From Lemma 18, we have $\tilde{\alpha}_t(x) = \langle \varphi(x), \widehat{V}_t^{-1}\widehat{\Phi}_t^T f_t\rangle_{\mathcal{H}}$. Therefore,

$$\begin{aligned}|f(x) - \tilde{\alpha}_t(x)| &= \left|\langle \varphi(x), f - \widehat{V}_t^{-1}\widehat{\Phi}_t^T f_t\rangle_{\mathcal{H}}\right|\\ &\overset{(a)}{\leq} \|\varphi(x)\|_{\widehat{V}_t^{-1}} \left\|f - \widehat{V}_t^{-1}\widehat{\Phi}_t^T f_t\right\|_{\widehat{V}_t}\\ &= \lambda^{-1/2}\left\|(\widehat{\Phi}_t^T\widehat{\Phi}_t + \lambda I_{\mathcal{H}})f - \widehat{\Phi}_t^T \Phi_t f\right\|_{\widehat{V}_t^{-1}} \tilde{\sigma}_t(x)\\ &\overset{(b)}{=} \lambda^{-1/2}\left\|\lambda f - \widehat{\Phi}_t^T \Phi_t (I_{\mathcal{H}} - P_t) f\right\|_{\widehat{V}_t^{-1}} \tilde{\sigma}_t(x)\\ &\overset{(c)}{\leq} \left(\lambda^{1/2}\left\|\widehat{V}_t^{-1/2} f\right\|_{\mathcal{H}} + \lambda^{-1/2}\left\|\widehat{V}_t^{-1/2}\widehat{\Phi}_t^T\Phi_t(I_{\mathcal{H}} - P_t)f\right\|_{\mathcal{H}}\right)\tilde{\sigma}_t(x)\\ &\overset{(d)}{\leq} \left(\|f\|_{\mathcal{H}} + \lambda^{-1/2}\left\|\widehat{V}_t^{-1/2}\widehat{\Phi}_t^T\right\|_{\mathcal{H}} \|\Phi_t(I_{\mathcal{H}} - P_t)\|_{\mathcal{H}} \|f\|_{\mathcal{H}}\right)\tilde{\sigma}_t(x)\\ &\overset{(e)}{\leq} B\left(1 + \lambda^{-1/2}\|\Phi_t(I_{\mathcal{H}} - P_t)\|_{\mathcal{H}}\right)\tilde{\sigma}_t(x).\end{aligned}$$

Here (a) is by Cauchy-Schwartz inequality, (b) uses the fact that $\widehat{\Phi}_t = \Phi_t P_t$, (c) is by triangle inequality, (d) follows from $\left\| \widehat{V}_t^{-1/2} f \right\|_{\mathcal{H}} \leq \lambda^{-1/2} \|f\|_{\mathcal{H}}$, and (e) follows from the fact that $\left\| \widehat{V}_t^{-1/2} \widehat{\Phi}_t^T \right\|_{\mathcal{H}}^2 = \lambda_{\max}\left(\widehat{\Phi}_t (\widehat{\Phi}_t^T \widehat{\Phi}_t + \lambda I_{\mathcal{H}})^{-1} \widehat{\Phi}_t^T \right) = \lambda_{\max}\left(\widehat{\Phi}_t \widehat{\Phi}_t^T (\widehat{\Phi}_t \widehat{\Phi}_t^T + \lambda I_t)^{-1} \right) \leq 1$, and that $\|f\|_{\mathcal{H}} \leq B$. Now see that $\mathrm{Col}(\Phi_{\mathcal{D}_t}^T) = \mathrm{Col}(\Phi_t^T S_t)$, and hence $P_t = \Phi_t^T S_t (S_t \Phi_t \Phi_t^T S_t)^+ S_t \Phi_t$. Therefore

$$I_{\mathcal{H}} - P_t \preceq I_{\mathcal{H}} - \Phi_t^T S_t (S_t \Phi_t \Phi_t^T S_t + \lambda I_{\mathcal{H}})^{-1} S_t \Phi_t \overset{(a)}{=} \lambda (\Phi_t^T S_t^2 \Phi_t + \lambda I_{\mathcal{H}})^{-1} = \lambda V_{\mathcal{D}_t}^{-1},$$

where (a) follows from 4. Now given a filtration $\mathcal{G}_t$ such that $E_{1,t}$ is true, we have $I_{\mathcal{H}} - P_t \preceq \frac{\lambda}{1-\varepsilon} V_t^{-1}$, and hence $\|\Phi_t(I_{\mathcal{H}} - P_t)\|_{\mathcal{H}}^2 = \lambda_{\max}\left(\Phi_t (I_{\mathcal{H}} - P_t)\Phi_t^T\right) \leq \frac{\lambda}{1-\varepsilon} \lambda_{\max}\left(\Phi_t (\Phi_t^T \Phi_t + \lambda I_{\mathcal{H}})^{-1} \Phi_t^T\right) = \frac{\lambda}{1-\varepsilon} \lambda_{\max}\left(\Phi_t \Phi_t^T (\Phi_t \Phi_t^T + \lambda I_t)^{-1}\right) \leq \frac{\lambda}{1-\varepsilon}$. Therefore, given a filtration $\mathcal{G}_t$ such that $E_{1,t}$ is true,

$$|f(x) - \tilde{\alpha}_t(x)| \leq B\left(1 + \frac{1}{\sqrt{1-\varepsilon}}\right) \tilde{\sigma}_t(x). \tag{25}$$

Now, we have $\tilde{\mu}_t(x) = \tilde{\varphi}_t(x)^T \tilde{\theta}_t$ and $\tilde{\alpha}_t(x) = \tilde{\varphi}_t(x)^T \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t$. Also observe that $\lambda \|\tilde{\varphi}_t(x)\|_{\tilde{V}_t^{-1}}^2 = \tilde{\sigma}_t^2(x) + \tilde{\varphi}_t(x)^T \tilde{\varphi}_t(x) - k(x,x) = \tilde{\sigma}_t^2(x) - \langle \varphi(x), (I_{\mathcal{H}} - P_t)\varphi(x) \rangle_{\mathcal{H}} \leq \tilde{\sigma}_t^2(x)$, since by definition $P_t \preceq I_{\mathcal{H}}$. Then, by Cauchy-Schwartz inequality

$$|\tilde{\alpha}_t(x) - \tilde{\mu}_t(x)| \leq \left\| \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t - \tilde{\theta}_t \right\|_{\tilde{V}_t} \|\tilde{\varphi}(x)\|_{\tilde{V}_t^{-1}} \leq \lambda^{-1/2} \left\| \tilde{V}_t^{-1} \tilde{\Phi}_t^T f_t - \tilde{\theta}_t \right\|_{\tilde{V}_t} \tilde{\sigma}_t(x).$$

Now, Lemma 13 implies that for any $\delta \in (0, 1]$, with probability at least $1 - \delta$, uniformly over all $t \in [T]$ and $x \in \mathcal{X}$,

$$|\tilde{\alpha}_t(x) - \tilde{\mu}_t(x)| \leq 4\sqrt{m_t/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(2m_t T/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}} \tilde{\sigma}_t(x). \tag{26}$$

By triangle inequality,

$$|f(x) - \tilde{\mu}_t(x)| \leq |f(x) - \tilde{\alpha}_t(x)| + |\tilde{\alpha}_t(x) - \tilde{\mu}_t(x)|.$$

Now, combining 25 and 26, for any $\delta \in (0, 1]$ and given a filtration $(\mathcal{G}_t)_{t \geq 1}$ such that $E_{1,t}$ is true for all $t \in [T]$, we have, with probability at least $1 - \delta$, uniformly over all $t \in [T]$ and $x \in \mathcal{X}$,

$$|f(x) - \tilde{\mu}_t(x)| \leq \left(B\left(1 + \frac{1}{\sqrt{1-\varepsilon}}\right) + 4\sqrt{m_t/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(2m_t T/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}} \right) \tilde{\sigma}_t(x).$$

From Lemma 17, the event $E_{1,t}$ is true for all $t \in [T]$ with probability at least $1 - \delta$. Now taking an union bound, we obtain that for any $\delta \in (0, 1]$, with probability at least $1 - \delta$, uniformly over all $t \in [T]$ and $x \in \mathcal{X}$,

$$|f(x) - \tilde{\mu}_t(x)| \leq \left(B\left(1 + \frac{1}{\sqrt{1-\varepsilon}}\right) + 4\sqrt{m_t/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(4m_t T/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}} \right) \tilde{\sigma}_t(x).$$

Further observe that $|f(x) - \tilde{\mu}_0(x)| = |f(x)| \leq B k^{1/2}(x,x) \leq B(1 + 1/\sqrt{1-\varepsilon})\tilde{\sigma}_0(x)$. Now, the result follows by setting $\beta_{t+1} = B\left(1 + \frac{1}{\sqrt{1-\varepsilon}}\right) + 4\sqrt{m_t/\lambda}\, v^{\frac{1}{1+\alpha}} \left(\ln(4m_t T/\delta)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}$ for all $t \geq 0$. ■

Now we are ready to prove the regret bound of ATA-GP-UCB under Nyström approximation.

D.3.4 Proof of Theorem 4

For any $\delta \in (0, 1]$, we have, with probability at least $1 - \delta$, uniformly over all $t \in [T]$, the instantaneous regret

$$\begin{aligned} r_t &= f(x^\star) - f(x_t) \\ &\overset{(a)}{\leq} \tilde{\mu}_{t-1}(x^\star) + \beta_t \tilde{\sigma}_{t-1}(x^\star) - f(x_t) \\ &\overset{(b)}{\leq} \tilde{\mu}_{t-1}(x_t) + \beta_t \tilde{\sigma}_{t-1}(x_t) - f(x_t) \\ &\overset{(c)}{\leq} 2\beta_t \tilde{\sigma}_{t-1}(x_t) \end{aligned}$$

Here (a) and (c) follow from Lemma 20, and (b) is due to the choice of ATA-GP-UCB (Algorithm 2). From Lemma 17, given a filtration $(\mathcal{G}_t)_{t\geq 1}$ such that the event $E_{2,t}$ is true for all $t \in [T]$, we have $m_t = O\left(\frac{\rho^2}{\varepsilon^2}\gamma_t \ln(T/\delta)\right)$. This, in turn, implies that

$$\beta_t = O\left(B\left(1+\frac{1}{\sqrt{1-\varepsilon}}\right) + \frac{\rho}{\varepsilon}\sqrt{\gamma_t \ln(T/\delta)}\, v^{\frac{1}{1+\alpha}} \left(\ln\left(\frac{\gamma_t \ln(T/\delta)T}{\delta}\right)\right)^{\frac{\alpha}{1+\alpha}} t^{\frac{1-\alpha}{2(1+\alpha)}}\right).$$

Further, given a filtration $(\mathcal{G}_t)_{t\geq 1}$ such that the event $E_{1,t}$ is true for all $t \in [T]$, we have

$$\sum_{t=1}^{T} \tilde{\sigma}_{t-1}(x_t) \overset{(a)}{\leq} \rho \sum_{t=1}^{T} \sigma_{t-1}(x_t) \overset{(b)}{\leq} \rho \sqrt{T \sum_{t=1}^{T} \sigma^2_{t-1}(x_t)} \overset{(c)}{\leq} \rho\sqrt{2(1+\lambda)T\gamma_T} = O\left(\rho\sqrt{T\gamma_T}\right).$$

Here (a) follows from Lemma 16, (b) follows from Cauchy-Schwartz inequality, and (c) follows from Lemma 6. Now from Lemma 17, with probability at least $1-\delta$, both $E_{1,t}$ and $E_{2,t}$ are true for all $t \in [T]$. Hence, by virtue of an union bound, we obtain that for any $\delta \in (0,1]$, with probability at least $1-\delta$, the cumulative regret of ATA-GP-UCB under Nyström appproximation after T rounds is

$$R_T = O\left(\rho B\left(1+\frac{1}{\sqrt{1-\varepsilon}}\right)\sqrt{T\gamma_T} + \frac{\rho^2}{\varepsilon}\, v^{\frac{1}{1+\alpha}} \left(\ln\left(\frac{\gamma_T \ln(T/\delta)T}{\delta}\right)\right)^{\frac{\alpha}{1+\alpha}} \sqrt{\ln(T/\delta)}\gamma_T T^{\frac{1}{1+\alpha}}\right).$$

E Addendum to experiments

Compared to this paper's setting, Bubeck et al. [8] makes weaker assumptions (i.e., no regularity structure on arms' rewards) and shows a more general but weaker regret bound (especially if the number of arms is very large) which is not surprising – more structure allows for lower regret. Our results show how smoothness in the arms' rewards (which is common in practice) can be exploited to achieve better regret. Numerical comparisons of the Robust-UCB algorithm (with truncated mean estimator) of Bubeck et al. [8] with our algorithms on the lightsensor data indicate that ATA-GP-UCB-Nyström performs much better than Robust-UCB, suggesting that it is indeed able to capture the smoothness structure present in the data. Theoretically if there are only K arms, the cumulative regret of ATA-GP-UCB will be better than that of Robust-UCB as long as $\gamma_T \leq K^{\frac{\alpha}{1+\alpha}}$. This holds if $K^{\frac{\alpha}{1+\alpha}} \geq (\ln T)^d$ for SE kernel and if $K^{\frac{\alpha}{1+\alpha}} \geq T^{\frac{1}{1+\nu}}$ for Matérn kernel (on $\mathbb{R}$). This is typically true if K is large and in fact, for a continuous set of arms the analysis of Robust-UCB yields a trivial regret upper bound of infinity. This introduces additional challenges that require a different set of ideas and is quite representative of real world problems, e.g., hyperparameter tuning in ML.