Efficient Gaussian Process Bandits
by Believing only Informative Actions

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Abstract
Bayesian optimization is a framework for global search via maximum a posteriori updates rather than simulated annealing, and has gained prominence for decision-making under uncertainty. In this work, we cast Bayesian optimization as a multi-armed bandit problem, where the payoff function is sampled from a Gaussian process (GP). Further, we focus on action selections via upper confidence bound (UCB) or expected improvement (EI) due to their prevalent use in practice. Prior works using GPs for bandits cannot allow the iteration horizon $T$ to be large, as the complexity of computing the posterior parameters scales cubically with the number of past observations. To circumvent this computational burden, we propose a simple statistical test: only incorporate an action into the GP posterior when its conditional entropy exceeds an $\epsilon$ threshold. Doing so permits us to derive sublinear regret bounds of GP bandit algorithms up to factors depending on the compression parameter $\epsilon$ for both discrete and continuous action sets. Moreover, the complexity of the GP posterior remains provably finite. Experimentally, we observe state of the art accuracy and complexity tradeoffs for GP bandit algorithms applied to global optimization, suggesting the merits of compressed GPs in bandit settings.

1. Introduction
Bayesian optimization is a framework for global optimization of a black box function via noisy evaluations (Frazier, 2018), and provides an alternative to simulated annealing (Kirkpatrick et al., 1983; Bertsimas & Tsitsiklis, 1993) or exhaustive search (Davis, 1991). These methods have proven adept at hyper-parameter tuning of machine learning models (Snoek et al., 2012; Li et al., 2017), nonlinear system identification (Srivastava et al., 2013), experimental design (Chaloner & Verdinelli, 1995; Press, 2009), and semantic mapping (Shotton et al., 2008).

More specifically, denote the function $f : \mathcal{X} \to \mathbb{R}$ we seek to optimize through noisy samples, i.e., for a given choice $x_t \in \mathcal{X}$, we observe $y_t = f(x_t) + \epsilon_t$ sequentially. We make no assumptions for now
on the convexity, smoothness, or other properties of \( f \), other than each function evaluation must be selected judiciously. Our goal is to select a sequence of actions \( \{x_t\} \) that eventuates in competitive performance with respect to the optimal selection \( x^* = \text{argmax}_{x \in X} f(x) \). For sequential decision making, a canonical performance metric is \textit{regret}, which quantifies the performance of a sequence of decisions \( \{x_t\} \) as compared with the optimal \( x^* \):

\[
\text{Reg}_T := \sum_{t=1}^{T} f(x^*) - f(x_t).
\] (1.1)

Regret in (1.1) is natural because at each time we quantify how far decision \( x_t \) was from optimal through the difference \( r_t := f(x^*) - f(x_t) \). An algorithm eventually learns the optimal strategy if it is no-regret: \( \text{Reg}_T / T \to 0 \) as \( T \to \infty \).

In this work, we focus on Bayesian optimization, which hypothesizes a likelihood on the relationship between the unknown function \( f(x) \) and action selection \( x \in X \). Then upon selecting an action \( x \), one tracks a posterior distribution, or \textit{belief model} [Powell & Ryzhov (2012)], over possible outcomes \( y = f(x) + \epsilon \) which informs how the next action is selected. In classical Bayesian inference, posterior distributions do not influence which samples \( (x, y) \) are observed next [Ghosal et al. (2000)]. In contrast, in multi-armed bandits, action selection \( x \) determines which observations form the posterior, which is why it is also referred to as \textit{active learning} [Jamieson et al. (2015)].

Two key questions in this setting are how to specify a (i) likelihood and (ii) action selection strategy. These specifications come with their own merits and drawbacks in terms of optimality and computational efficiency. Regarding (i) the likelihood model, when the action space \( X \) is discrete and of moderate size \( X = |X| \), one may track a probability for each element of \( X \), as in Thompson (posterior) sampling [Russo et al. (2018)], Gittins indices [Gittins et al. (2011)], and the Upper Confidence Bound (UCB) [Auer et al. (2002)]. These methods differ in their manner of action selection, but not distributional representation.

However, when the range of possibilities \( X \) is large, computational challenges arise. This is because the number of parameters one needs to define a posterior distribution over \( X \) is proportional to \( |X| \), an instance of the curse of dimensionality in nonparametric statistics. One way to circumvent this issue for continuous spaces is to discretize the action space according to a pre-defined time-horizon that determines the total number of selected actions [Bubeck et al. (2011); Magureanu et al. (2014)], and carefully tune the discretization to the time-horizon \( T \). The drawback of these approaches is that as \( T \to \infty \), the number of parameters in the posterior grows intractably large.

An alternative is to define a history-dependent distribution directly over the large (possibly continuous) space using, e.g., Gaussian Processes (GPs) [Rasmussen (2004)] or Monte Carlo (MC) methods [Smith (2013)]. Bandit action selection strategies based on such distributional representations have been shown to be no-regret in recent years – see [Srinivas et al. (2012); Gopalan et al. (2014)]. While MC methods permit the most general priors on the unknown function \( f \), computational and technical challenges arise when the prior/posterior no longer possess conjugacy properties [Gopalan et al. (2014)]. By contrast, GPs, stochastic processes with any finite collection of realizations of which are jointly Gaussian [Krigel (1951)], have a conjugate prior and posterior, and thus their parametric updates admit a closed form – see [Rasmussen (2004)] (Ch. 2).

The conjugacy of GPs has driven their use in bandit action selection. In particular, by connecting regret to maximum information-gain based exploration, which may be quantified by variance [Srinivas et al. (2012); De Freitas et al. (2012)], no-regret algorithms may be derived through variance maximization. Doing so yields actions which over-prioritize exploration, which may be balanced through, e.g., upper-confidence bound (UCB) based action selection. GP-UCB algorithms, and variants such as expected improvement (EI) [Wang & de Freitas (2014); Nguyen et al. (2017)], and step-wise uncertainty reduction (SUR) [Villemonteix et al. (2009)], including knowledge gradient [Frazier et al. (2008)], have been shown to be no-regret or statistically consistent [Bect et al. (2019)] in recent years.
However, these convergence results hinge upon requiring use of the dense GP whose posterior distribution [cf. (2.7)], has complexity cubic in $T$ due to the inversion of a Gram (kernel) matrix formed from the entire training set. Numerous efforts to reduce the complexity of GPs exist in the literature – see Csató & Opper (2002); Bauer et al. (2016); Bui et al. (2017). These methods all fix the complexity of the posterior and “project” all additional points onto a fixed likelihood “subspace.” Doing so, however, may cause uncontrollable statistical bias and divergence. In this work, we seek to explicitly design GPs to ensure both small regret and complexity which remains under control.

**Contributions.** In this context, we propose a statistical test for the GP that explicitly trades off memory and regret (1.1), motivated by compression routines that permit flexible representational complexity of nonparametric models Koppel (2019); Elvira et al. (2016). Specifically, we:

- propose a statistical test that operates inside GP UCB or EI which incorporates actions into the posterior only when conditional entropy exceeds an $\epsilon$ threshold (Sec. 2). We call these methods Compressed GP-UCB or Compressed GP-EI (Algorithm 1).
- derive sublinear regret bounds of GP bandit algorithms up to factors depending on the compression parameter $\epsilon$ for both discrete and continuous action sets (Sec. 3).
- establish that the complexity of the GP posterior remains provably finite (Sec. 3).
- experimentally employ these approaches for optimizing non-convex functions and tuning the regularizer and step-size of a logistic regressor, which obtains a state of the art trade off in regret versus computational efficiency relative to a few baselines. (Sec. 4).

## 2. Gaussian Process Bandits

### Information Gain and Upper-Confidence Bound:
To find $\mathbf{x}^* = \arg\max_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$ when $f$ is unknown, one may first globally approximate $f$ well, and then evaluate it at the maximizer. In order to formalize this approach, we propose to quantify how informative a collection of points $\{\mathbf{x}_u\} \subset \mathcal{X}$ is through information gain (Cover & Thomas, 2012), a standard quantity that tracks the mutual information between $f$ and observations $y_u = f(\mathbf{x}_u) + \epsilon_u$ all indices $u$ in some sampling set, defined as

$$I(\{y_u\}; f) = H(\{y_u\}) - H(\{y_u\} \mid f)$$

where $H(\{y_u\})$ denotes the entropy of observations $\{y_u\}$ and $H(\{y_u\} \mid f)$ denotes the entropy conditional on $f$. For a Gaussian $\mathcal{N}(\mu, \Sigma)$ with mean $\mu$ and covariance $\Sigma$, the entropy is given as

$$H(\mathcal{N}(\mu, \Sigma)) = \frac{1}{2} \log |2\pi e\Sigma|$$

which allows us to evaluate the information gain in closed form as

$$I(\{y_u\}; f) = \frac{1}{2} \log |2 + \sigma^{-2} \mathbf{K}_u|.$$  

Suppose we are tasked with finding a subset of $K$ points $\{\mathbf{x}_u\}_{u \leq T}$ that maximize the information gain. This amounts to a challenging subset selection problem whose exact solution cannot be found in polynomial time (Ko et al. 1995). However, near-optimal solutions may be obtained via greedy maximization, as information gain is submodular (Krause et al. 2008). Maximizing information gain, i.e., selecting $\mathbf{x}_t = \arg\max_{\mathbf{x} \in \mathcal{X}} I(\{y_u\}; f)$, is equivalent to (Srinivas et al. 2012)

$$\mathbf{x}_t = \arg\max_{\mathbf{x} \in \mathcal{X}} \sigma \mathbf{x}_{t-1} \cdot (\mathbf{x})$$
where \( \sigma_{X_{t-1}}(x) \) is the empirical standard deviation associated with a matrix \( X_{t-1} := [x_1 \cdots x_{t-1}] \in \mathbb{R}^{d \times (t-1)} \). We note that [2.4] may be shown to obtain the near-optimal selection of points in the sense that after \( T \) rounds, executing [2.4] guarantees

\[
I(\{y_u\}_{u=1}^T; f) \geq (1 - 1/e)I(\{y_u\}_{u=1}^K; f)
\]

for some \( K \leq T \) points via the theory of submodular functions \([\text{Nemhauser et al.}, 1978]\). Indeed, selecting points based upon [2.4] permits one to efficiently explore \( f \) globally. However, it dictates that action selection does not move towards the actual maximizer \( x^* \) of \( f \). For this, \( x_t \) should be chosen according to prior knowledge about the function \( f \), exploiting information about where \( f \) is large. To balance between these two extremes, a number of different acquisition functions \( \alpha(x) \) are possible based on the GP posterior – see \([\text{Powell & Ryzhov}, 2012]\). Here, for simplicity, we propose to do so either based upon the upper-confidence bound (UCB):

\[
x_t = \arg \max_{x \in X} \mu_{X_{t-1}}(x) + \sqrt{\beta_t \sigma_{X_{t-1}}(x)} \tag{2.5}
\]

with \( \beta_t \) as an exploration parameter \( \beta_t \), or the expected improvement (EI) \([\text{Nguyen et al.}, 2017]\), defined as

\[
x_t = \arg \max_{x \in X} \sigma_{t-1} \phi(z) + [\mu_{t-1}(x) - y_{t-1}^{\max}] \Phi(z), \tag{2.6}
\]

where \( y_{t-1}^{\max} = \max\{y_u\}_{u \leq t} \) is the maximum observation value of past data, \( z = z_{t-1}(x) = (\mu_{t-1}(x) - y_{t-1}^{\max})/\sigma_{t-1}(x) \) is the z-score of \( y_{t-1}^{\max} \), and \( \phi(z) \) and \( \Phi(z) \) denote the density and distribution function of a standard Gaussian distribution. Moreover, the aforementioned mean \( \mu_{t-1}(x) \) and standard deviation \( \sigma_{t-1}(x) \) in the preceding expressions are computed via a GP, to be defined next.

**Gaussian Processes:** A Gaussian Process (GP) is a stochastic process for which every finite collection of realizations is jointly Gaussian. We hypothesize a Gaussian Process prior for \( f(x) \), which is specified by a mean function

\[
\mu(x) = \mathbb{E}[f(x)]
\]

and covariance kernel defined as

\[
\kappa(x, x') = \mathbb{E}[(f(x) - \mu(x)) (f(x') - \mu(x'))].
\]

Subsequently, we assume the prior is zero-mean \( \mu(x) = 0 \). GPs play multiple roles in this work: as a way of specifying smoothness and a prior for unknown function \( f \), as well as characterizing regret when \( f \) is a sample from a known GP \( GP(0; \kappa(x, x')) \). GPs admit a closed form for their conditional a posteriori mean and covariance given training set \( S_t = \{x_u, y_u\}_{u \leq t} \) as \([\text{Rasmussen}, 2004]\) Ch. 2.

\[
\begin{align*}
\mu_{X_t}(x) &= k_t(x)^T (K_t + \sigma^2 I)^{-1} y_t \\
\sigma^2_{X_t}(x) &= \kappa(x, x') - k_t(x)^T (K_t + \sigma^2 I)^{-1} k_t(x')
\end{align*} \tag{2.7}
\]

where \( k_t(x) = [\kappa(x_1, x), \cdots, \kappa(x_t, x)] \) denotes the empirical kernel map and \( K_t \) denotes the gram matrix of kernel evaluations whose entries are \( \kappa(x, x') \) for \( x \), \( x' \in \{x_u\}_{u \leq t} \). The \( X_t \) subscript underscores its role in parameterizing the mean and covariance. Further, note that [2.7] depends upon a linear observation model \( y_t = f(x_t) + \epsilon_t \) with Gaussian noise prior \( \epsilon_t \sim \mathcal{N}(0, \sigma^2) \). The parametric updates [2.7] depend on past actions \( \{x_u\}_{u \leq t} \), which causes the kernel dictionary \( X_t \) to grow by one at each iteration, i.e.,

\[
X_{t+1} = [X_t ; x_{t+1}] \in \mathbb{R}^{d \times t},
\]

and the posterior at time \( t+1 \) uses all past observations \( \{x_u\}_{u \leq t} \). Henceforth, the number of columns in the dictionary is called the *model order*. The GP posterior at time \( t+1 \) has model order \( t \)
Algorithm 1: Compressed GP-Bandits (COB)

\begin{verbatim}
for t = 1, 2, \ldots do
    Select action \( x_t \) via UCB (2.5) or EI (2.6):
    \[ x_t = \arg \max_{x \in \mathcal{X}} \alpha(x) \]
    Sample: \( y_t = f(x_t) + \epsilon_t \)
    If conditional entropy exceeds \( \epsilon \) threshold \( H(y_t | y_{t-1}) = \frac{1}{2} \log (2\pi e (\sigma^2 + \sigma_D^2(x_t))) > \epsilon \):
        Augment dictionary \( D_t = |D_{t-1}; x_t| \)
        Append \( y_t \) to target vector \( y_{D_t} = [y_{D_{t-1}}; y_t] \)
        Update posterior mean \( \mu_{D_t}(x) \) & variance \( \sigma_{D_t}(x) \)
        \[ \mu_{D_t}(x) = k_{D_t}(x)^T(K_{D_t} + \sigma^2 I)^{-1}y_{D_t} \]
        \[ \sigma_{D_t}^2(x) = \kappa(x, x') - k_{D_t}(x)^T(K_{D_t, D_t} + \sigma^2 I)^{-1}k_{D_t}(x') \]
    else
        Fix dict. \( D_t = D_{t-1} \), target \( y_{D_t} = y_{D_{t-1}} \), & GP.
        \( (\mu_{D_{t-1}}(x), \sigma_{D_{t-1}}(x), D_{t-1}) = (\mu_D(x), \sigma_D(x), D) \)
end for
\end{verbatim}

The resulting action selection strategy using the GP (2.7) is called GP-UCB, and its regret is established in (Srinivas et al., 2012) [Theorem 1 and 2] as sublinear with high probability up to factors depending on the maximum information gain \( \gamma_T \) over \( T \) points, which is defined as

\[ \gamma_T := \max_{\{x_u\}} I(\{y_u\}_{u=1}^T; f) \quad \text{such that} \quad |\{x_u\}| = T. \quad (2.8) \]

Compression Statistic: The fundamental role of information gain in the regret of GP, using either UCB or EI, provides a conceptual basis for finding a parsimonious GP posterior that nearly preserves no-regret properties of (2.5) - (2.7). To define our compression rule, first we define some key quantities related to approximate GPs. Suppose we select some other kernel dictionary \( D \in \mathbb{R}^{d \times M} \) rather than \( X_t \) at time \( t \), where \( M \) is the model order of the Gaussian Process. Then, the only difference is that the kernel matrix \( K_t \) in (2.7) and the empirical kernel map \( k_t(\cdot) \) are substituted by \( K_{DD} \) and \( k_D(\cdot) \), respectively, where the entries of \( [K_{DD}]_{mn} = \kappa(d_m, d_n) \) and \( \{d_u\}_{u=1}^M \subset \{x_u\}_{u \leq t} \). Further, \( y_D \) denotes the sub-vector of \( y_t \) associated with only the indices of training points in matrix \( D \). We denote the training subset associated with these indices as \( S_D := \{x_u, y_u\}_{u=1}^M \). By rewriting (2.7) with \( D \) as the dictionary rather than \( X_{t+1} \), we obtain

\[ \mu_D(x) = k_D(x_{t+1})[K_{D,D} + \sigma^2 I]^{-1}y_D \]
\[ \sigma_D^2(x) = \kappa(x, x') - k_D(x)^T(K_{D,D} + \sigma^2 I)^{-1}k_D(x') \quad (2.9) \]

The question, then, is how to select a sequence of dictionaries \( D_t \in \mathbb{R}^{t \times M_t} \) whose \( M_t \) columns comprise a subset of those of \( X_t \) in such a way to approximately preserve the regret bounds of (Srinivas et al., 2012) [Theorem 1 and 2] while ensuring the model order is moderate \( M_t \ll t \).

We propose using conditional entropy as a statistic to compress against, i.e., a new data point should be appended to the Gaussian process posterior only when its conditional entropy is at least \( \epsilon \),
which results in the following update rule for the dictionary $D_t \in \mathbb{R}^{p \times M_t}$:

$$\text{If } \mathbf{H}(y_t|\hat{y}_{t-1}) = \frac{1}{2} \log \left(2\pi e (\sigma_y^2 + \sigma^2_{D_{t-1}}(x_t))\right) > \epsilon \text{ then update } D_t = [D_{t-1} ; x_t]$$

else

$$\text{update } D_t = D_{t-1}, \quad (2.10)$$

where we define $\epsilon$ as the compression budget. This amounts to a statistical test of whether the action $x_t$ yielded an informative sample $y_t$ in the sense that its conditional entropy exceeds an $\epsilon$ threshold. Therefore, uninformative past decisions are dropped from belief formation about the present. The modification of GP-UCB, called Compressed GP-UCB, or CUB for short, uses (2.5) with the lazy GP belief model (2.9) defined by dictionary updates (2.10). Similarly, the compression version of EI is called Compressed EI or CEI for short. We present them together for simplicity as Algorithm 1 with the understanding that in practice, one must specify UCB (2.5) or EI (2.6). Next, we rigorously establish how Algorithm 1 trades off regret and memory through the $\epsilon$ threshold on conditional entropy for whether a point $(x_t, y_t)$ should be included in the GP.

3. Balancing Regret and Complexity

In this section, we establish that Algorithm 1 attains comparable regret (1.1) to the standard GP approach to bandit optimization under the canonical settings of the action space $X$ being a discrete finite set and a continuous compact Euclidean subset, when actions follow the upper-confidence bound (2.5). We further establish sublinear regret of the expected improvement (2.6) when the action section $X$ is discrete. We build upon techniques pioneered in (Srinivas et al., 2012; Nguyen et al., 2017). The points of departure in our analysis are: (i) the characterization of statistical bias induced by the compression rule (2.10) in the regret bounds, and (ii) the relating of properties of the posterior (2.10) and action selections (2.5)-(2.6) to topological properties of the action space $X$ to ensure the model order of the GP defined by (2.9) is at-worst finite for all $t$. Next we present the regret performance of Algorithm 1 when actions are selected according to the UCB (2.5).

**Theorem 3.1. (Regret of Compressed GP-UCB)** Fix $\delta \in (0,1)$ and suppose the Gaussian Process prior for $f$ has zero mean with covariance kernel $\kappa(x, x')$. Define constant $C := \frac{8}{\log(1 + \sigma^{-2})}$ Then under the following parameter selections and conditions on the data domain $X$, we have:

i. **(Finite decision set)** For finite cardinality $|X| = X$, with exploration parameter $\beta_t$ selected as

$$\beta_t = 2 \log \left(\frac{Xt^2 \pi^2}{6 \delta}\right),$$

the accumulated regret is sublinear regret with probability $1 - \delta$.

$$\mathbb{P} \left\{ \text{Reg}_T \leq \sqrt{C_1 T \beta_T \gamma_T} + \sqrt{\epsilon T} \right\} \geq 1 - \delta \quad (3.1)$$

where $\epsilon$ is the compression budget.

ii. **(General decision set)** For continuous set $X \subset [0, r]^d$, assume the derivative of the GP sample paths are bounded with high probability, i.e., for constants $a, b$,

$$\mathbb{P} \left\{ \sup_{x \in X} |\partial f / \partial x_j| > L \right\} \leq ae^{-(L/b)^2} \text{ for } j = 1, \ldots, d. \quad (3.2)$$

Then, under exploration parameter

$$\beta_t = 2 \log (Xt^2 \pi^2 / 3 \delta) + 2d \log \left(\frac{t^2 dr \sqrt{\log(4da/\delta)}}{\sqrt{\log(4da/\delta)}} \right),$$
the accumulated regret is
\[
P\left\{ \text{Reg}_T \leq \sqrt{C_1 T \beta_T \gamma_T} + \sqrt{T + \frac{\pi^2}{6}} \right\} \geq 1 - \delta. \quad (3.3)
\]

Theorem 3.1, whose proof is the supplementary material attached to the submission, establishes that Algorithm 1 with action selected according to (2.5) attains sublinear regret with high probability when the action space \( X \) is discrete and finite, as well as when it is a continuous compact subset of Euclidean space, up to factors depending on the maximum information gain (2.8) and the compression budget \( \epsilon \) in (2.10). The sublinear dependence of the information gain on \( T \) in terms of the parameter dimension \( d \) is derived in (Srinivas et al., 2012)[Sec. V-B] for common kernels such as the linear, Gaussian, and Matérn.

The proof follows a path charted in (Srinivas et al., 2012)[Appendix I], except that we must contend with the compression-induced error. Specifically, we begin by computing the confidence interval for each action \( x_t \) taken by the proposed algorithm at time \( t \). Then, we bound the instantaneous regret \( r_t := f(x^*) - f(\hat{x}_t) \) in terms of the problem parameters such as \( \beta_t, \delta, C, \epsilon, \) and information gain \( \gamma_T \) using the fact that the upper-confidence bound overshoots the maximizer. By summing over time with Cauchy-Schwartz, we build an upper-estimate of cumulative regret based on instantaneous regret \( r_t \). Unsurprisingly, an additional term appears due to our compression budget \( \epsilon \) in the final regret bounds, which for \( \epsilon = 0 \) reduces to (Srinivas et al., 2012)[Theorem 1 and 2]. However, rather than permitting the complexity of the GP to grow unbounded with \( T \), instead it grows only when informative actions are taken, and preserves the sublinear growth of regret for any \( \epsilon \) such that \( \sqrt{\epsilon T} = o(T) \) such as \( \epsilon = T^{2(p-1)} \) for any \( p < 1 \).

Next, we analyze the performance of Algorithm 1 when actions are selected according to the expected improvement (2.6).

**Theorem 3.2. (Regret of Compressed GP-EI)** Suppose we select actions based upon Expected Improvement (2.6) together with the conditional entropy-based rule (2.10) for retaining past points into the GP posterior, as detailed in Algorithm 1. Then, under the same conditions and parameter selection \( \beta_t \) as in Theorem 3.1, when \( X \) is a finite discrete set, the regret \( \text{Reg}_T \) is sublinear with probability \( 1 - \delta \), i.e.,
\[
P\left\{ \text{Reg}_T \leq \sqrt{\frac{2T (\gamma_T + \epsilon T)}{\log (1 + \sigma^{-2})} \left[ \sqrt{3(\beta_T + 1 + R^2)} + \sqrt{\beta_T} \right]} \right\} \geq 1 - \delta, \quad (3.4)
\]
where
\[
R := \sup_{t \geq 0} \sup_{x \in X} \frac{|\mu_{t-1}(x) - y_{\text{max}}|}{\sigma_{t-1}(x)}
\]
is the maximum value of the z score, is as defined in Lemma 9.7.

The proof is proved in Appendix 9. In Theorem 3.2, we have characterized how the regret of Algorithm 1 depends on the compression budget \( \epsilon \) for when the actions are selected according to the EI rule. We note (3.4) holds for the discrete action space \( X \). The result for the continuous action space \( X \) follows from the proof of statement ii of Theorem 3.1, and the proof of Theorem 3.2. The proof of Theorem 3.2 follows a similar path presented in the Nguyen et al. (2017). We start by upper bounding the instantaneous improvements achieved by the proposed compressed EI algorithm in terms of the acquisitions function in Lemma 9.3. Further, the sum of the predictive variances for the compressed version over \( T \) instances is upper bounded in terms of the maximum information gain \( \gamma_T \) in Lemma 9.5. Then we upper bound the cumulative sum of the instantaneous regret \( r_t = f(x^*) - f(\hat{x}_t) \) in terms of the model parameters such as \( \gamma_T, \sigma, \beta_T, R, \) and \( \epsilon \). Similar to the analysis that gives rise to Theorem 3.1, an additional term arises due to compression-induced
error, which explicitly trades off regret and complexity. Moreover, note that $\epsilon = 0$ reduces to the result of [Nguyen et al.] (2017).

Next, we establish the main merit of doing this statistical test inside a bandit algorithm is that it controls the complexity of the belief model that decides action selections. In particular, Theorem 3.3 formalizes that the dictionary $D_T$ defined by (2.10) in Algorithm 1 will always have finite number of elements $M_T(\epsilon)$ even if $T \to \infty$, which is stated next.

**Theorem 3.3.** Suppose that the conditional entropy $H(\{y_t\} \mid f)$ is bounded for all $T$. Then, the number of elements in the dictionary $D_T$ denoted by $M_T(\epsilon)$ in the GP posterior of Algorithm 1 is finite as $T \to \infty$ for fixed compression threshold $\epsilon$.

The implications of Theorem 3.3 are that Algorithm 1 only retains significant actions in belief formation and drops extraneous points. Interestingly, this result states that despite infinitely many actions being taken in the limit, only finite many of them are $\epsilon$-informative. In principle, one could make $\epsilon$ adaptive with $t$ to improve performance, but analyzing such a choice becomes complicated as relating the worst-case model complexity to the covering number of the space $X$ would then depend on variable sets whose conditional entropy is at least $\epsilon_t$. In the next section, we evaluate the merit of these conceptual results on experimental settings involving black box non-convex optimization and hyper-parameter tuning of linear logistic regressors.

### 4. Experiments

In this section, we evaluate the performance of the statistical compression method under a few different action selections (acquisition functions). Specifically, Algorithm 1 employs the Upper Confidence Bound (UCB) or Expected Improvement (EI) ([Nguyen et al.] 2017) acquisition function, but the key insight here is a modification of the GP posterior, not the action selection. Thus, we validate its use for Most Probable Improvement (MPI) ([Wang & de Freitas] 2014) as well, defined as

$$\alpha^{MPI}(x) = \sigma_{t-1} \phi(z) + [\mu_{t-1}(x) - \xi] \Phi(z),$$

$$\xi = \arg \max_x [\mu_{t-1}(x) - \xi]$$

where $\phi(z)$ and $\Phi(z)$ denote the standard Gaussian density and distribution functions, and $z = (\mu_{t-1}(x) - \xi)/\sigma_{t-1}(x)$ is the centered $z$-score. We further compare the compression scheme against Budgeted Kernel Bandits (BKB) proposed by ([Calandriello et al.] 2019) which proposes to randomly add or drop points according to a distribution that is inversely proportional to the posterior variance, also on the aforementioned acquisition functions.

Unless otherwise specified, the squared exponential kernel is used to represent the correlation between the input, the lengthscale is set to $\theta = 1.0$, the noise prior is set to $\sigma^2 = 0.001$, the compression budget $\epsilon = 10^{-4}$ and the confidence bounds hold with probability of at least $\delta = 0.9$. As a common practice across all three problems, we initialize the Gaussian priors with $d$ training data randomly collected from the input domain, where $d$ is the input dimension. We quantify the performance using Mean Average Regret over the iterations and the clock time. In addition, the model order, or number of points defining the GP posterior, is visualized over time to characterize the compression of the training dictionary. To ensure fair evaluations, all the listed simulations were performed on a PC with 1.8 GHz Intel Core i7 CPU and 16 GB memory. Same initial priors and parameters are used to assess computational efficiency in terms of the compression.

#### 4.1 Example function

Firstly, we evaluate our proposed method on an example function given by Equation 4.1

$$f(x) = \sin(x) + \cos(x) + 0.1 \times x$$  \hspace{1cm} (4.1)
Figure 1: We display mean average regret vs iteration (top row) and clock time (middle row) for the proposed algorithm with uncompressed and BKB variants on the example function for various acquisition functions. Observe that our proposed compression scheme attains comparable regret to the dense GP. Moreover, the associated model complexity of the GP settles to an intrinsic constant discerned by the learning process (bottom row), as compared with alternatives which either randomly vary, or grow unbounded.

| Acquisition | Uncompressed | Compressed BKB |
|-------------|--------------|----------------|
| UCB         | 6.756        | 5.335          |
| EI          | 7.594        | 4.133          |
| MPI         | 5.199        | 3.864          |

Table 1: Clock Times (in seconds) with example function

A random Gaussian noise is induced at every observation of f, to emulate the practical applications of Bayesian Optimization where the black box functions are often corrupted by noise.

The results of this experiment are shown in Figure 1 and the associated wall clock times are demonstrated in Table 1. Observe that the compression rule (2.10) yields regret that is typically comparable to the dense GP, with orders of magnitude reduction in model complexity. This complexity reduction, in turn, permits a state of the art tradeoff in regret versus wall clock time for certain acquisition functions, i.e., the UCB and EI, but not MPI. Interestingly, the model complexity of Algorithm 1 settles to a constant discerned by the covering number (metric entropy) of the action space, validating the conceptual result of Theorem 3.3.
Table 2: Clock Times (in seconds) on the Rosenbrock

| Acquisition | Uncompressed | Compressed | BKB  |
|-------------|--------------|------------|------|
| UCB         | 2.412        | **1.905**  | 3.143|
| EI          | 2.604        | **2.246**  | 3.801|
| MPI         | 2.533        | **2.186**  | 3.237|

Table 3: Clock Times (in seconds) with Hyperparameter Tuning

| Acquisition | Uncompressed | Compressed | BKB  |
|-------------|--------------|------------|------|
| UCB         | 5.18         | **5.288**  | 4.836|
| EI          | 5.948        | **5.611**  | 4.82 |
| MPI         | 5.642        | **4.99**   | 4.867|

4.2 Rosenbrock Function

For the second experiment, we compare the compressed variants with their baseline algorithm on a two-dimensional non-convex function popularly known as the Rosenbrock Function, given by:

\[ f(x, y) = (a - x)^2 + b(y - x^2)^2 \]

The Rosenbrock function is a common benchmark non-convex function used to validate the performance of global optimization methods. Here we set its parameters as \( a = 1 \) and \( b = 10 \) for simplicity throughout. Again, we run various (dense and reduced-order) Gaussian Process bandit algorithms with different acquisition functions.

The results of this experiment are displayed in Figure 2 with associated wall clock times collected in Table 2. Again, we observe that compression with respect to conditional entropy yields a minimal reduction in performance in terms of regret while translating to a significant reduction of complexity. Specifically, rather than growing linearly with the number of past actions, as is standard in nonparametric statistics, the model order settles down to an intrinsic constant determined by the metric entropy of the action space. This means that we obtain a state of the art tradeoff in model complexity versus regret, as compared with the dense GP or probabilistic dropping inversely proportional to the variance, as in [Calandriello et al., 2019].

4.3 Hyper-parameter Tuning in Logistic Regression

In this subsection, we propose using bandit algorithms to automate the hyper-parameter tuning of machine learning algorithms. More specifically, we propose using Algorithm 1 and variants with different acquisition functions to tune the following hyper-parameters of a supervised learning scheme, whose concatenation forms the action space: the learning rate, batch size, dropout of the inputs, and the \( \ell_2 \) regularization constant. The specific supervised learning problem we focus on is the training of a multi-class logistic regressor over the MNIST training set [LeCun & Cortes, 2010] for classifying handwritten digits. The instantaneous reward here is the statistical accuracy on a hold-out validation set. Considering the high-dimensional input domain and the number of training examples, GP dictionary may explode to a large size. In large-scale settings, the input space could be much larger with many more hyper-parameters to tune, in which case GPs may be computationally intractable. The statistical compression proposed here ameliorates this issue by keeping the size of training dictionary in check, which makes it feasible for hyper-parameter tuning as the number of training examples becomes large.
Figure 2: We display mean average regret vs iteration (top row) and clock time (middle row) for the proposed algorithm with uncompressed and BKB variants on the Rosenbrock function for various acquisition functions. The compression based on conditional entropy yields regret to comparable to the dense GP, with an associated model order that settles to a constant extracted by the optimization process (bottom row), as compared with alternatives which either randomly vary, or grow unbounded.

The results of this implementation are given in Figure 3 with associated compute times in Table 3. Observe that the trend identified in the previous two examples translates into practice here: the compression technique (2.10) yields algorithms whose regret is comparable to the dense GP, with a significant reduction in model complexity that eventually settles to a constant. This constant is a fundamental measure of the complexity of the action space required for finding a no-regret policy. Overall, then, one can run Algorithm 1 on the back-end of any training scheme for supervised learning in order to automate the selection of hyper-parameters in perpetuity without worrying about eventual slowdown.

5. Conclusions

We considered bandit problems whose action spaces are discrete but have large cardinality, or are continuous. The canonical performance metric, regret, quantifies how well bandit action selection is against a best comparator in hindsight. By connecting regret to maximum information-gain based exploration which may be quantified by variance, one may find no-regret algorithms through variance maximization. Doing so yields actions which over-prioritize exploration. To balance between
exploration and exploitation, that is, moving towards the optimum in finite time, we focused on upper-confidence bound based action selection. Following a number of previous works for bandits with large action spaces, we parameterized the action distribution as a Gaussian Process in order to have a closed form expression for the a posteriori variance.

Unfortunately, Gaussian Processes exhibit complexity challenges when operating ad infinitum: the complexity of computing posterior parameters grows cubically with the time index. While numerous previous memory-reduction methods exist for GPs, designing compression for bandit optimization is relatively unexplored. Within this gap, we proposed a compression rule for the GP posterior explicitly derived by information-theoretic regret bounds, where the conditional entropy encapsulates the per-step progress of the bandit algorithm. This compression only includes past actions whose conditional entropy exceeds an $\epsilon$-threshold to enter into the posterior.
As a result, we derived explicit tradeoffs between model complexity and information-theoretic regret. Moreover, the complexity of the resulting GP posterior is at worst finite and depends on the covering number (metric entropy) of the action space, a fundamental constant that determines the bandit problem’s difficulty. In experiments, we observed a favorable tradeoff between regret, model complexity, and iteration index/clock time for a couple toy non-convex optimization problems as well as the actual problem of how to tune hyper-parameters of a supervised machine learning model.

Future directions include extensions to non-stationary bandit problems, generalizations to history-dependent action selection strategies such as step-wise uncertainty reduction methods (Villemonteix et al., 2009), and information-theoretic compression of deep neural networks based on bandit algorithms.

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Supplementary Material for
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6. Preliminaries

Before proceeding with the proofs in detail, we define some notation to clarify the exposition. For instance, in the analysis, it is important to differentiate the actions taken by the standard (uncompressed) GP-UCB algorithm defined by (2.5) - (2.7) from that of Algorithm 1 which employs information gain-based compression. Therefore, we proposed the following notations.

i. We denote the parameters of the posterior defined by (2.7) without compression as \( \mu_t : \mu_X_t \) for the mean, and \( \sigma_t : \sigma_X_t \) for the covariance, and the resulting action sequence (2.5) as \( x_t \).

ii. For the proposed Algorithm 1, we denote \( \hat{x}_t \) for actions, \( \hat{\mu}_t : \mu_D_t \) for the means, and \( \hat{\sigma}_t : \sigma_D_t \) for the covariance functions to emphasize that they are approximations of the scheme in (Srinivas et al., 2012).

We further re-write the proposed Algorithm 1 here in Algorithm 2 utilizing this notation.

**Algorithm 2** Compressed GP-UCB Algorithm (CUB)

for \( t = 1, 2, \ldots \) do

Find \( \hat{x}_t \) by solving an optimization problem:

\[
\hat{x}_t = \text{arg max}_{x \in X} \hat{\mu}_t - \frac{1}{\sqrt{2 \beta_t \hat{\sigma}_t}}(x)
\]

Sample: \( \hat{y}_t = f(\hat{x}_t) + \epsilon_t \)

If conditional entropy exceeds \( \epsilon \) threshold

\[
H(\hat{y}_t|\hat{y}_{t-1}) = \frac{1}{2} \log (2\pi e (\sigma^2 + \hat{\sigma}_t^{-2}(\hat{x}_t))) > \epsilon
\]

Augment dictionary \( D_t = [D_{t-1}; \hat{x}_t] \) and target vector \( \hat{y}_{D_t} = [\hat{y}_{D_{t-1}}; \hat{y}_t] \)

Update posterior mean \( \hat{\mu}_t(x) \) and variance \( \hat{\sigma}_t(x) \)

\[
\hat{\mu}_t(x) = k_{D_t}(x)^T(K_{D_t} + \sigma^2 I)^{-1}\hat{y}_{D_t}
\]

\[
\hat{\sigma}_t^2(x) = k(x, x') - k_{D_t}(x)^T(K_{D_t} + \sigma^2 I)^{-1}k_{D_t}(x')
\]

Else

Dictionary \( D_t = D_{t-1} \) and GP remain unchanged

\[
(\hat{\mu}_t(x), \hat{\sigma}_t(x), D_t) = (\hat{\mu}_{t-1}(x), \hat{\sigma}_{t-1}(x), D_{t-1})
\]

end for

Subsequently, we pursue proofs in terms of the aforementioned definitions.

7. Proof of Theorem 3.1

The statement of Theorem 3.1 is divided into two parts for finite decision set (statement (i)) and compact convex action space (statement (ii)). Next, we present the proof for both the statements separately.

7.1 Proof of Theorem 3.1 statement (i)

The proof of Theorem 3.1(i) is based on upper bounding the difference \( |f(x) - \hat{\mu}_{t-1}(x)| \) in terms of a scaled version of the standard deviation \( \beta_t^{1/2} \hat{\sigma}_{t-1}(x) \), which we state next.
Lemma 7.1. Choose \( \delta \in (0, 1) \) and let \( \beta_t = 2 \log(|\mathcal{X}|/\pi_t/\delta) \), for some \( \pi_t \) such that \( \sum_{t \geq 1} \pi_t^{-1} = 1, \pi_t > 0 \). Then, the parameters of the approximate GP posterior in Algorithm 1 satisfies

\[
|f(x) - \mu_{t-1}(x)| \leq \beta_t^{1/2} \sigma_{t-1}(x) \quad \forall x \in \mathcal{X}, \forall t \geq 1
\]  

(7.1)

holds with probability at least \( 1 - \delta \).

Proof. At each \( t \), we have dictionary \( \mathbf{D}_{t-1} \) which contains the data points (actions taken so far) for the function \( f(x) \). For a given \( \mathbf{D}_{t-1} \) and \( \mathbf{y}_{\mathbf{D}_t} \), \( f(x) \sim N(\mu_{t-1}, \sigma_{t-1}) \). In Algorithm 2, we take actions \( \{\mathbf{x}_u\}_{u \leq t} \) and observe \( \{\mathbf{y}_u\}_{u \leq t} \) which are different from \( \{\mathbf{x}_u\}_{u \leq t} \) and \( \{\mathbf{y}_u\}_{u \leq t} \) of the uncompressed bandit algorithm [cf. (2.5) - (2.7)].

Hence, \( (\hat{\mu}_{t-1}, \hat{\sigma}_{t-1}) \) are the parameters of a Gaussian whose entropy is given by \( H(\hat{\mu}_{t-1}) = \frac{1}{2} \log[2\pi e \hat{\sigma}_{t-1}] \). This Gaussian is parametrized by the collection of data points \( (\hat{x}, \hat{y}) \in \mathcal{S}_{\mathbf{D}_{t-1}} \). At \( t \), we take an action \( \hat{x}_t \) after which we observe \( \hat{y}_t \). Then, we check for the conditional entropy \( H(\hat{y}_t | \hat{x}_t) \). If the conditional entropy is higher than \( \epsilon \) then we update the GP distribution, otherwise not (2.10).

Hence, there is a fundamental difference between the posterior distributions and action selections.

We seek to analyze the performance of the proposed algorithm in terms the regret defined against the optimal \( f(x^*) \). To do so, we exploit some properties of the Gaussian, specifically, for random variable \( r \sim N(0, 1) \), the cumulative density function can be expressed

\[
P(r > c) = \frac{1}{\sqrt{2\pi}} \int_c^{\infty} e^{-\frac{r^2}{2}} dr
\]  

(7.2)

\[
= e^{-\frac{c^2}{2}} \frac{1}{\sqrt{2\pi}} \int_c^{\infty} e^{-\frac{(r-c)^2}{2}} dr
\]

\[
= e^{-\frac{c^2}{2}} \frac{1}{\sqrt{2\pi}} \int_c^{\infty} e^{-\frac{(r-c)^2}{2}} e^{-c(r-c)} dr.
\]

For \( c > 0 \) and \( r \geq c \), we have that \( e^{-c(r-c)} \leq 1 \). Furthermore, the integral term scaled by \( \frac{1}{\sqrt{2\pi}} \) resembles the Gaussian density integrated from \( c \) to \( \infty \) for a random variable \( r \) with mean \( c \) and unit standard deviation, integrated to \( 1/2 \). Therefore, we get

\[
P(r > c) \leq e^{-c^2/2} P(r > 0) = \frac{1}{2} e^{-c^2/2}.
\]  

(7.3)

Using the expression \( r = (f(x) - \hat{\mu}_{t-1}(x))/\hat{\sigma}_{t-1}(x) \) and \( c = \beta_t^{1/2} \) for some sequence of nonnegative scalars \( \{\beta_t\}_{t \geq 0} \). Substituting this expression into the left-hand side of (7.2) using the left-hand side of (7.3), we obtain

\[
P\left\{ |f(x) - \hat{\mu}_{t-1}(x)| > \beta_t^{1/2} \hat{\sigma}_{t-1}(x) \right\} \leq e^{-\beta_t/2}.
\]  

(7.4)

Now apply Boole’s inequality to the preceding expression to write

\[
P\left\{ \bigcup_{x \in \mathcal{X}} |f(x) - \hat{\mu}_{t-1}(x)| > \beta_t^{1/2} \hat{\sigma}_{t-1}(x) \right\}
\]

\[
\leq \sum_{x \in \mathcal{X}} P\left\{ |f(x) - \hat{\mu}_{t-1}(x)| > \beta_t^{1/2} \hat{\sigma}_{t-1}(x) \right\}
\]

\[
\leq |\mathcal{X}| e^{-\beta_t/2}.
\]  

(7.5)

To obtain the result in the statement of Lemma 7.1, select the constant sequence \( \beta_t \) such that \( |\mathcal{X}| e^{\beta_t/2} = \frac{4}{\pi_t} \), with scalar parameter sequence \( \pi_t := \pi^2 t^2 / 6 \). Applying Boole’s inequality again over
all time points $t \in \mathbb{N}$, we get

$$P\left\{ \bigcup_{t=1}^{\infty} |f(x) - \hat{\mu}_{t-1}(x)| > \beta_t^{1/2} \hat{\sigma}_{t-1}(x) \right\}$$

$$\leq \sum_{t=1}^{\infty} P\left\{ \bigcup_{t=1}^{\infty} |f(x) - \hat{\mu}_{t-1}(x)| > \beta_t^{1/2} \hat{\sigma}_{t-1}(x) \right\}$$

$$\leq \sum_{t=1}^{\infty} \frac{\delta}{\pi_t}$$

$$= \delta. \quad (7.6)$$

The last equality $\sum_{t=1}^{\infty} \frac{\delta}{\pi_t} = \delta$ is true since $\sum_{t=1}^{\infty} 1/t^2 = \pi^2/6$. We reverse the inequality to obtain an upper bound on the absolute difference between the true function and the estimated mean function for all $x \in \mathcal{X}$ and $t \geq 1$ such that

$$|f(x) - \hat{\mu}_{t-1}(x)| \leq \beta_t^{1/2} \hat{\sigma}_{t-1}(x), \quad \forall x \in \mathcal{X}, \forall t \geq 1 \quad (7.7)$$

holds with probability $1 - \delta$, as stated in Lemma 7.1.

**Lemma 7.2.** Fix $t \geq 1$. If $|f(x) - \hat{\mu}_{t-1}(x)| \leq \beta_t^{1/2} \hat{\sigma}_{t-1}(x)$ for all $x \in \mathcal{X}$, the instantaneous regret is bounded as

$$r_t \leq 2\beta_t^{1/2} \hat{\sigma}_{t-1}(x_t). \quad (7.8)$$

**Proof.** Since Algorithm 2 chooses the next sampling point $\hat{x}_t = \arg\max \hat{\mu}_{t-1}(x) + \sqrt{\hat{\sigma}_t} \hat{\sigma}_{t-1}(x)$ at each step, we have

$$\hat{\mu}_{t-1}(\hat{x}_t) + \sqrt{\hat{\sigma}_t} \hat{\sigma}_{t-1}(\hat{x}_t) \geq \hat{\mu}_{t-1}(x^*) + \sqrt{\hat{\sigma}_t} \hat{\sigma}_{t-1}(x^*)$$

$$\geq f(x^*), \quad (7.9)$$

by the definition of the maximum, where $x^*$ is the optimal point. The instantaneous regret is then bounded as

$$r_t = f(x^*) - f(\hat{x}_t)$$

$$\leq \hat{\mu}_{t-1}(\hat{x}) + \beta_t^{1/2} \hat{\sigma}_{t-1}(\hat{x}_t) - f(\hat{x}_t). \quad (7.10)$$

But from Lemma 7.1 we have that $|f(x) - \hat{\mu}_{t-1}(x)| \leq \beta_t^{1/2} \hat{\sigma}_{t-1}(x)$ holds with probability $1 - \delta$. This implies that

$$r_t = f(x^*) - f(\hat{x}_t) \leq 2\sqrt{\hat{\sigma}_t} \hat{\sigma}_{t-1}(\hat{x}_t). \quad (7.11)$$

Then, (7.11) quantifies the instantaneous regret of action $\hat{x}_t$ taken by Algorithm 2 as stated in Lemma 7.2.

**Lemma 7.3.** The information gain of actions selected by Algorithm 1, denoted as $\hat{f}_T = (f(\hat{x}_t)) \in \mathbb{R}^T$, admits a closed from in terms of the posterior variance of the compressed GP and the variance of the noise prior as

$$I(\hat{y}_T; \hat{f}_T) = \frac{1}{2} \sum_{t \in M_T(\epsilon)} \log(1 + \sigma^{-2} \hat{\sigma}^2_{t-1}(x_t)) \quad (7.12)$$

where $M_T(\epsilon)$ denotes the number of elements in dictionary $D_T$.
Proof. The standard GP (2.7) incorporates all past actions \(X_t = [x_1, x_2, \ldots, x_t]\) and observations \(y_t = [y_1, y_2, \ldots, y_t]^T\) into its representation. In contrast, in Algorithm 2, due to conditional entropy-based compression, we retain only a subset of the elements \(S_{D_t}\) with \(M_t(\epsilon)\) points such that \(|D_t| = M_t(\epsilon)\leq t\) for all \(t\). Next, we note that for a dense GP with covariance matrix \(\sigma^2 I\), the information gain is given as \((\mbox{Cover & Thomas, 2012})\)

\[
I(y_t; f_t) = H(y_t) - \frac{1}{2} \log |2\pi e \sigma^2 I|, \tag{7.13}
\]

where it holds that

\[
\frac{1}{2} \log |2\pi e \sigma^2 I| = \frac{1}{2} \sum_{t=1}^T \log(2\pi e \sigma^2) \tag{7.14}
\]

since \(y_t \in \mathbb{R}^t\). In contrast, for Algorithm 2, we have \(\hat{y}_t \in \mathbb{R}^{M_t(\epsilon)}\). Next, expand the entropy term \(H(\hat{y}_t)\) where \(\hat{y}_t = [\hat{y}_{t-1}; \hat{y}_t]\) before compression to write

\[
H(\hat{y}_t) = H(\hat{y}_{t-1}) + H(\hat{y}_t|\hat{y}_{t-1})
\]

\[
= H(\hat{y}_{t-1}) + \frac{1}{2} \log (2\pi e (\sigma^2 + \hat{\sigma}^2_{t-1}(\hat{x}_t))). \tag{7.15}
\]

We add the current point \((\hat{x}_t, y_t)\) only if its conditional entropy \(H(\hat{y}_t|\hat{y}_{t-1})\) only is more than \(\epsilon\). Otherwise, the GP is unchanged, and we drop the update. That is, the GP parameters remain constant for \(|H(\hat{y}_t) - H(\hat{y}_{t-1})| \leq \epsilon\). The above expression holds for each \(t\), now take summation over \(t = 1\) to \(T\), since \(H(\hat{y}_0) = 0\), we get

\[
H(\hat{y}_T) = \frac{1}{2} \sum_{t=1}^{M_T(\epsilon)} \log(2\pi e \sigma^2) + \frac{1}{2} \sum_{t=1}^{M_T(\epsilon)} \log(1 + \sigma^2 \hat{\sigma}^2_{t-1}(\hat{x}_t)). \tag{7.16}
\]

From the expression for information gain (7.13), we have that

\[
I(\hat{y}_T; \hat{f}_T) = \frac{1}{2} \sum_{t=1}^{M_T(\epsilon)} \log(1 + \sigma^2 \hat{\sigma}^2_{t-1}(\hat{x}_t)) \tag{7.17}
\]

which is as stated in Lemma 7.3 \(\square\)

Lemma 7.4. Let us define \(\beta_t\) as in Lemma 7.1 and choose \(\delta \in (0, 1)\), then for Algorithm 2 with probability at least \(\geq 1 - \delta\) we have

\[
\sum_{t=1}^{T} r_t^2 \leq \beta_T C \left[ I(\hat{y}_T; \hat{f}_T) + \epsilon T \right] \tag{7.18}
\]

where \(C = \frac{8}{\log(1 + e^{-\epsilon})}\).

Proof. By Lemma 7.1 and 7.2 we have

\[
r_t^2 \leq 4\beta_t \hat{\sigma}^2_{t-1}(\hat{x}_t) \tag{7.19}
\]

for all \(t\) with probability \(1 - \delta\). Since \(\beta_t\) is non-decreasing, we obtain

\[
4\beta_t \hat{\sigma}^2_{t-1}(\hat{x}_t) \leq 4\beta_T \sigma^2 (\sigma^2 \hat{\sigma}^2_{t-1}(\hat{x}_t)). \tag{7.20}
\]
In addition, note that, by definition, we restrict $\kappa(x, x') \leq 1$. Thus, $\hat{\delta}_{t-1}^2(\hat{x}_t) = \kappa(\hat{x}_t, x_t) \leq 1$ for all $t$. Furthermore, using the fact that $\frac{1}{\log(1+s)}$ is monotonically increasing for positive $s$, we get

$$\frac{\sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t)}{\log(1 + \sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t))} \leq \frac{\sigma^{-2}}{\log(1 + \sigma^{-2})}. \quad (7.21)$$

This implies that

$$\sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t) \leq \frac{\sigma^{-2}}{\log(1 + \sigma^{-2})}\log(1 + \sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t)). \quad (7.22)$$

Multiplying both sides by $4\beta_T\sigma^2$, we obtain

$$4\beta_T\hat{\delta}_{t-1}^2(\hat{x}_t) \leq 4\beta_T C_2 \log(1 + \sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t)) \quad (7.23)$$

where $C_2 = \frac{\sigma^{-2}}{\log(1 + \sigma^{-2})}$. Next, substitute the upper bound in (7.23) on the right hand side of (7.19), we get

$$\sum_{t=1}^{T} r_t^2 \leq 4\beta_T\sigma^2 C_2 \sum_{t=1}^{T} \log(1 + \sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t)) \quad (7.24)$$

This is the key step. Now we decompose the summand in right-hand side of (7.24) into terms whose conditional entropy is less than $\epsilon$ and those which are greater

$$\sum_{t=1}^{T} \log(1 + \sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t)) = \sum_{t \in M_T(\epsilon)} \log(1 + \sigma^{-2}\hat{\delta}_{t-1}^2(\hat{x}_t)) + \epsilon(T - M_T(\epsilon)) \quad (7.25)$$

where we exploit the fact that at time $T$ there are at most $T - M_T(\epsilon)$ removed points whose conditional entropy is less than $\epsilon$. Then, apply Lemma 7.3 to the first term on the right-hand side of the preceding expression, define, $C = \frac{8}{\log(1 + \sigma^{-2})}$, and substitute the result into the right-hand side of (7.24) to write

$$\sum_{t=1}^{T} r_t^2 \leq \beta_T C \left[ I(\hat{y}_T; \hat{f}_T) + \epsilon(T - M_T(\epsilon)) \right] \leq \beta_T C \left[ I(\hat{y}_T; \hat{f}_T) + cT \right]. \quad (7.26)$$

Now, it is straightforward to establish the result of Theorem 3.1 statement (i). Note that by the Cauchy Schwartz inequality, we can write

$$\text{Reg}_T \leq \sqrt{T \sum_{t=1}^{T} r_t^2} \leq \sqrt{T \beta_T C_1 \left[ I(\hat{y}_T; \hat{f}_T) + cT \right]} = \sqrt{C_1 T \beta_T \gamma_T} + cT \quad (7.27)$$

which is as stated in Theorem 3.1(i).
7.2 Proof of Theorem 3.1 statement (ii)

Now, we present the regret analysis for the general settings where \( X \subset \mathbb{R}^d \) is a compact set. It is nontrivial to extend Theorem 3.1(i) to the general compact action spaces. For instance, the result in Lemma 7.1 does not hold for infinite action space \( X \) since it involves the use of \(|X|\) which is infinite for the general compact space \( X \), which causes the bound in Lemma 7.1 to be infinite. We proceed with a different approach based on exploiting smoothness hypotheses we impose on the underlying ground truth function \( f \).

We begin by stating an analogue of Lemma 7.1 that holds for continuous spaces which quantifies the confidence of the decisions taken using Algorithm 2.

**Lemma 7.5.** Select exploration parameter \( \beta_t = 2 \log(\pi_t/\delta) \) and choose likelihood threshold \( \delta \in (0, 1) \) with \( \sum_{t \geq \tau_i} \frac{1}{\pi_t} = 1, \pi_t > 0 \). Then for the Algorithm 2 we have that

\[
|f(\hat{x}_t) - \hat{\mu}_{t-1}(\hat{x}_t)| \leq \beta_t^{1/2} \hat{\sigma}_{t-1}(\hat{x}_t), \quad \forall t \geq 1
\]  

(7.28)

holds with probability at least \( 1 - \delta \).

**Proof.** For a given \( t \) and \( x \in X \), the dictionary \( D_{t-1} \) elements are deterministic conditioned on the observations \( \hat{y}_{t-1} \), which implies that \( f(x) \sim \mathcal{N}(\hat{\mu}_{t-1}(x), \hat{\sigma}_{t-1}^2(x)) \). Following the similar steps to the proof of Lemma 7.1 it holds that

\[
P\left\{|f(\hat{x}_t) - \hat{\mu}_{t-1}(\hat{x}_t)| > \beta_t^{1/2} \hat{\sigma}_{t-1}(\hat{x}_t)\right\} \leq e^{-\beta_t/2}.
\]  

(7.29)

Since we have \( \beta_t = 2 \log(\pi_t/\delta) \), apply Boole’s inequality (union bound) for \( t \in \mathbb{N} \) to conclude Lemma 7.5. \( \Box \)

Note that the result in Lemma 7.5 is for a particular action \( \hat{x}_t \) of Algorithm 2 rather than for any action \( x \) as given by Lemma 7.1. To derive the regret of the Algorithm 2 we need to characterize the confidence bound stated in Lemma 7.5 for the optimal action \( x^* \). To do so, we discretize the action space \( X \) into different sets \( X_t \subset X \) and we use \( X_t \) at instance \( t \). This discretization is purely for the purpose of analysis and has not been used in the algorithm implementation. We provide the confidence for these subsets \( X_t \) in the next Lemma 7.6.

**Lemma 7.6.** Select exploration parameter \( \beta_t = 2 \log(\|X_t|\pi_t/\delta) \) and likelihood tolerance \( \delta \in (0, 1) \) with \( \sum_{t \geq \tau_i} \frac{1}{\pi_t} = 1, \pi_t > 0 \). Then Algorithm 2 satisfies

\[
|f(x) - \hat{\mu}_{t-1}(x)| \leq \beta_t^{1/2} \hat{\sigma}_{t-1}(x), \quad \forall x \in X_t, \quad \forall t \geq 1
\]  

(7.30)

with probability at least \( 1 - \delta \).

The proof for the statement of Lemma 7.6 is analogous to Lemma 7.1. The distinguishing feature is that we replace \( X \) with \( X_t \). Next, to obtain the regret bound for Algorithm 2 we need to characterize the confidence bound for optimal action \( x^* \). Doing so first requires bounding the error due to the discretization. From the hypothesis stated in Theorem 3.1(ii), we may write

\[
P\left\{\forall j, \forall x, \quad |\partial f/\partial x_j| < L \right\} \geq 1 - ade^{-(L/b)^2}
\]  

(7.31)

which states that the function \( f \) is Lipschitz with probability greater than \( 1 - ade^{-(L/b)^2} \), hence it holds that

\[
|f(x) - f(x')| \leq L\|x - x'\|_1
\]  

(7.32)
for all $x \in X$. To obtain the confidence at $x^*$, choose the discretization such that the size of each set $X_i$ is $(\tau_i)^d$ so that for each $x \in X$, it holds that

$$\|x - [x]\|_1 \leq \frac{rd}{\tau_i}$$  \hspace{1cm} (7.33)

where $[x]\_i$ is the closest point in $X_i$ to the original point $x$. Next, we present the result which provides the confidence for $x^*$ in Lemma 7.7.

**Lemma 7.7.** Suppose that exploration parameter is selected as $\beta_t = 2 \log(2\pi t/\delta) + 4d \log(dt b \sqrt{\log(2da/\delta)})$ and fix likelihood tolerance $\delta \in (0, 1)$ such that $\sum_{i \geq 1} \frac{1}{\pi_t} = 1$, $\pi_t > 0$ and $\tau_t = t^2 rda \sqrt{\log(2da/\delta)}$. Then Algorithm 2 satisfies

$$|f(x^*) - \tilde{\mu}_{t-1}([x^*]_i)| \leq \frac{1}{\tau_t^2} + \beta_t^{1/2} \tilde{\sigma}_{t-1}([x^*]_i), \quad \forall x \in X_i, \quad \forall t \geq 1$$  \hspace{1cm} (7.34)

with probability at least $1 - \delta$.

**Proof.** Let us denote $\delta = dae \frac{r db}{\tau_t^2}$, then from the Lipschitz property in (7.32), we can write that

$$|f(x) - f(x^*)| \leq b \sqrt{\log(2da/\delta)} \|x - x^*\|_1$$  \hspace{1cm} (7.35)

for all $x \in X$ with probability greater than $1 - \frac{\delta}{2}$. Since the expression holds for any $x^*$, let us choose $x^* = [x]_i$, we get

$$|f(x) - f([x]_i)| \leq b \sqrt{\log(2da/\delta)} \|x - [x]_i\|_1.$$

From the bound in (7.33), we get

$$|f(x) - f([x]_i)| \leq rda \sqrt{\log(2da/\delta)} / \tau_t.$$  \hspace{1cm} (7.37)

By selecting the discretization $\tau_t = t^2 rdb \sqrt{\log(2da/\delta)}$, we can write

$$|f(x) - f([x]_i)| \leq \frac{1}{\tau_t^2}.$$  \hspace{1cm} (7.38)

for all $x \in X$. Next, we add and subtract the optimal discretized point $f([x^*]_i)$ as

$$|f(x^*) - \tilde{\mu}_{t-1}([x^*]_i)| = |f(x^*) - f([x^*]_i) - (f([x^*]_i) - \tilde{\mu}_{t-1}([x^*]_i))|$$

$$\leq |f(x^*) - f([x^*]_i)| + |f([x^*]_i) - \tilde{\mu}_{t-1}([x^*]_i)|.$$  \hspace{1cm} (7.39)

From Lemma 7.6 and the upper bound in (7.38), we can rewrite the inequality in (7.39) as follows

$$|f(x^*) - \tilde{\mu}_{t-1}([x^*]_i)| \leq \frac{1}{\tau_t^2} + \beta_t^{1/2} \tilde{\sigma}_{t-1}([x^*]_i).$$  \hspace{1cm} (7.40)

which is stated in Lemma 7.7. \hspace{1cm} $\square$

Next, we provide a Lemma which characterizes the regret $r_t$ at each instant $t$ for the general compact action spaces. The result is stated in Lemma 7.8.

**Lemma 7.8.** Suppose the exploration parameter is selected as $\beta_t = 2 \log(4\pi t/\delta) + 4d \log(dt b r \sqrt{\log(4da/\delta)})$ and with likelihood tolerance $\delta \in (0, 1)$ chosen such that $\sum_{i \geq 1} \frac{1}{\pi_t} = 1$, $\pi_t > 0$ and discretization parameter satisfying $\tau_t = t^2 rdb \sqrt{\log(2da/\delta)}$. Then Algorithm 2 satisfies

$$r_t \leq 2\beta_t^{1/2} \tilde{\sigma}_{t-1}(\hat{x}_t) + \frac{1}{\tau_t^2},$$  \hspace{1cm} (7.41)

with probability at least $1 - \delta$.  

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Proof. In Lemma 7.5 and Lemma 7.7, $\delta/2$ is used to make the probability of the events more than $1 - \delta$. Next, note that for a general compact set $X$, from the definition of the action $\hat{x}_t$ in Algorithm 2, it holds that
\begin{equation}
\hat{\mu}_{t-1}(\hat{x}_t) + \beta_t^{1/2}\hat{\sigma}_{t-1}(\hat{x}_t) \geq \hat{\mu}_{t-1}([x^*]_t) + \beta_t^{1/2}\hat{\sigma}_{t-1}([x^*]_t).
\end{equation}
(7.42)
From the statement of Lemma 7.7, it holds that
\begin{equation}
\hat{\mu}_{t-1}([x^*]_t) + \beta_t^{1/2}\hat{\sigma}_{t-1}([x^*]_t) + \frac{1}{t^2} \geq f(x^*).
\end{equation}
(7.43)
Consider the regret at $t$, which may be related to the over-approximation by the upper-confidence bound as
\begin{equation}
rt = f(x^*) - f(\hat{x}_t) \leq \hat{\mu}_{t-1}([x^*]_t) + \beta_t^{1/2}\hat{\sigma}_{t-1}([x^*]_t) + \frac{1}{t^2} - f(\hat{x}_t)
\end{equation}
(7.44)
\begin{equation}
\leq \hat{\mu}_{t-1}(\hat{x}_t) + \beta_t^{1/2}\hat{\sigma}_{t-1}(\hat{x}_t) + \frac{1}{t^2} - f(\hat{x}_t)
\end{equation}
(7.45)
\begin{equation}
= \beta_t^{1/2}\hat{\sigma}_{t-1}(\hat{x}_t) + \frac{1}{t^2} + \hat{\mu}_{t-1}(\hat{x}_t) - f(\hat{x}_t).
\end{equation}
(7.46)
Using the result in Lemma 7.6, we can write
\begin{equation}
rt \leq 2\beta_t^{1/2}\hat{\sigma}_{t-1}(\hat{x}_t) + \frac{1}{t^2}
\end{equation}
(7.47)
which completes the proof. \qed

We are ready to present the proof of statement (ii) in Theorem 3.1. Begin by noting that the first term on the right-hand side of Lemma 7.8 coincides with the left-hand side of (7.23), and therefore may be upper-estimated by (7.27), which permits us to write
\begin{equation}
\sum_{t=1}^{T} 4\beta_t\hat{\sigma}_{t-1}^2(\hat{x}_t) \leq C_1\beta_T(\hat{\gamma}_T + \epsilon T).
\end{equation}
(7.48)
Apply the Cauchy-Schwartz inequality to the preceding expression to obtain
\begin{equation}
\sum_{t=1}^{T} 2\beta_t^{1/2}\hat{\sigma}_{t-1}(\hat{x}_t) \leq \sqrt{C_1T}\beta_T(\hat{\gamma}_T + \epsilon T).
\end{equation}
(7.49)
Substitute the upper bound in (7.49) into the right hand side of (7.47) which yields
\begin{equation}
\sum_{t=1}^{T} rt \leq \sqrt{C_1T}\beta_T(\hat{\gamma}_T + \epsilon T) + \frac{\pi^2}{6}
\end{equation}
(7.50)
which is as stated in the Theorem 3.1(ii). We have also used Euler’s formula to the upper bound the summation of the second term on the right-hand side of Lemma 7.8 across time $\sum_{t=1}^{T} \frac{1}{t^2} \leq \frac{\pi^2}{6}$ to conclude (7.50).
8. Proof of Theorem 3.3

Proof. For brevity, we denote the model order by $M_t := M_t(\epsilon)$ in this subsection. Consider the model order of the dictionary $D_{t-1}$ and $D_t$ generated by Algorithm 2 denoted by $M_{t-1}$ and $M_t$, respectively, at two arbitrary subsequent times $t - 1$ and $t$. The number of elements in $D_{t-1}$ are $M_{t-1}$. After performing the algorithm update at $t$, we either add a new sample $(x_t, y_t)$ to the dictionary and increase the model order by one, i.e., $M_t = M_{t-1} + 1$, or we do not, in which case $M_t = M_{t-1}$. The evolution of the conditional entropy of the algorithm, from the update in (7.15), allows us to write

$$H(\hat{y}_t) = H(\hat{y}_{t-1}) + H(y_t | \hat{y}_{t-1}).$$

(8.1)

Suppose the model order $M_t$ is equal to that of $M_{t-1}$, i.e. $M_t = M_{t-1}$. We skip the posterior update if $H(y_t | \hat{y}_{t-1}) \leq \epsilon$. In other words, we drop the update if $|H(\hat{y}_t) - H(\hat{y}_{t-1})| \leq \epsilon$. Thus, the negation holds for this case, stated as

$$H(y_t | \hat{y}_{t-1}) \leq \epsilon.$$  

(8.2)

Consequently, if $H(y_t | \hat{y}_{t-1}) \leq \epsilon$, then (8.2) holds and the model order does not grow. Thus it suffices to consider $H(y_t | \hat{y}_{t-1})$.

Therefore, each time a new point is added to the model, if the corresponding conditional entropy is guaranteed to be at least $\epsilon$ with respect to the information provided by the current dictionary. With the assumption that the conditional entropy is bounded almost surely, we can show that the model order will remain finite as long as we have $\epsilon > 0$. Next, we follow a similar argument to that of the proof of Theorem 3.1 in [Engel et al., 2004]. Since the range of conditional entropy is compact, any infinite cover of the space contains a finite sub-cover. Therefore, there are finitely many points that cover the space whose conditional entropy is greater than $\epsilon$. \qed

9. Proofs for Expected Improvement Acquisition Function

9.1 Definitions and Technical Lemmas

We expand upon the details of the expected improvement acquisition function. First we review a few key quantities. Define the improvement $I_t(x) = \max \{0, f(x) - \xi\}$ over incumbent $\xi = \hat{y}_{t-1}^{\max} = \max \{y_u : u \leq t\}$, which is the maximum over past observations. Denote by $z = z_{t-1} = (\mu_{t-1}(x) - \hat{y}_{t-1}^{\max})/\sigma_{t-1}(x)$ as the z-score of $\hat{y}_{t-1}^{\max}$. Then, the expected improvement computes the expectation over improvement $I_t(x)$ which may be evaluated using the Gaussian density $\phi(z)$ and distribution functions $\Phi(z)$ as:

$$\alpha_t(\hat{y}_t) = \sigma_t \phi(z) + [\mu_t(x) - \xi] \Phi(z), \quad \xi = \hat{y}_{t-1}^{\max} = \max \{y_u : u \leq t\}$$

(9.1)

As the convention in [Nguyen et al., 2017], when the variance $\sigma_t(x) = 0$, we set $\alpha_t(x) = 0$. Define the function $\tau(z) = 2\Phi(z) + \phi(z)$ to alleviate the notation henceforth.

Recall the definitions of $\mu_t$ and $\sigma_t$ in Section 6. Further, define maximum observation $\hat{y}_{t-1}^{\max} = \max \{y_u : u \in M_t\}$ over $M_t$, the set of indices associated with past selected points [2.10], the compressed improvement $I_t(x) = \max \{0, f(x) - \hat{y}_{t-1}^{\max}\}$, and the associated z-scores as $\hat{z} = \hat{z}_{t-1}(x) := (\mu_t(x) - \hat{y}_{t-1}^{\max})/\hat{\sigma}_{t-1}(x)$. These definitions then allow us to define the compressed variant of the expected improvement acquisition function as

$$\hat{\alpha}_t(\hat{y}_t) = \hat{\sigma}_{t-1}(x) + [\hat{\mu}_{t-1}(x) - \xi] \Phi(z), \quad \xi = \hat{y}_{t-1}^{\max} = \max \{y_u : u \in M_t\}$$

(9.2)

Before proceeding with the proof, we first verify several properties and lemmas key to the regret bound in [Nguyen et al., 2017] to illuminate whether there is a dependence on the GP dictionary as $X_t$ or the subset $D_t$. 

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Lemma 9.1. The acquisition function $\alpha_{EI}^t(x)$ in (2.6) may be expressed in terms of the variance, and the density $\phi$ and distribution $\Phi$ functions of the Gaussian as $\alpha_{EI}^t(x) = \tau(z_{t-1}(x))$. Moreover, $\alpha_{EI}^t(x) \leq \tau(z_{t-1}(x))$ for $\sigma_{t-1}(x) \leq 1$.

**Proof.** Begin with (2.6):

$$\alpha_{EI}^t(x) = \sigma_{t-1}(x) \phi(z) + [\mu_{t-1}(x) - \xi] \Phi(z), \quad y_{t-1}^{\max} = \max\{y_u \in S_t\}.\]$$

Now substitute in the definition of the $z$-score: $z_{t-1}(x) = (\mu_{t-1}(x) - y_{t-1}^{\max})/\sigma_{t-1}(x)$ and $\tau(z) = z\Phi(z) + \phi(z)$ to write

$$\alpha_{EI}^t(x) = \sigma_{t-1}(x)[z\Phi(z) + \phi(z)]$$

$$= \sigma_{t-1}(x)\tau(z_{t-1}(x))$$

(9.3)

Using $\sigma_{t-1}(x) \leq 1$ allows us to conclude Lemma 9.1. \qed

We underscore that (9.3) exploits properties of $\tau$ independent of whether $y_{t-1}^{\max}$ is computed over points in $\{y_u\}_{u \leq t}$ or amongst only a subset. Therefore, as a corollary, we have that an identical property holds for the compressed expected improvement (9.2).

**Corollary 9.2.** The compressed expected improvement acquisition function $\hat{\alpha}_{EI}^t(x)$ in (9.2) satisfies the identity $\hat{\alpha}_{EI}^t(x) = \hat{\sigma}_{t-1}(x)\tau(\hat{z}_{t-1}(x))$. Moreover, $\hat{\alpha}_{EI}^t(x) \leq \tau(\hat{z}_{t-1}(x))$ for $\hat{\sigma}_{t-1}(x) \leq 1$.

In contrast to (Nguyen et al., 2017)[Lemma 5] and (Srinivas et al., 2012)[Theorem 6 hold], which require the target function $f^*$ to belong to an RKHS with finite RKHS norm, we focus on the case where the decision set $X$ has finite cardinality, whereby Lemma 7.1. We consider this case to keep the analysis simple and elegant for the EI algorithm. The analysis for the general compact decision set follows similar steps as those taken for Compressed GP-UCB, but would instead employ Lemma 7.5 together with accounting for discretization-induced error, leading to an additional constant factor on the right-hand side of the regret bound.

Next, we relate the instantaneous improvement minus the scaled standard deviation to the expected improvement (2.6).

**Lemma 9.3.** The expected improvement (2.6) upper-bounds the instantaneous improvement $I_t(x) = \max\{0, f(x) - y_{t-1}^{\max}\}$ minus a proper scaling of the standard deviation, i.e.

$$I_t(x) - \sqrt{\beta_t} \sigma_{t-1}(x) \leq \alpha_{EI}^t(x)$$

(9.4)

**Proof.** If $\sigma_{t-1}(x) = 0$, then $\alpha_{EI}^t(x) = I_t(x) = 0$, which makes the result hold with equality. Suppose $\sigma_{t-1}(x) > 0$. Then, define the following normalized quantities

$$q = \frac{f(x) - y_{t-1}^{\max}}{\sigma_{t-1}(x)}; \quad z = \frac{\mu_{t-1}(x) - y_{t-1}^{\max}}{\sigma_{t-1}(x)}$$

(9.5)

Now, consider the expression for the expected improvement (2.6), using the identity of Lemma 9.1

$$\alpha_{EI}^t(x) = \sigma_{t-1}(x)\tau(z_{t-1}(x))$$

(9.6)

Now apply the upper-confidence bound, which says that $|\mu_t(x) - f(x)| \leq \sqrt{\beta_t} \sigma_t(x)$ with probability $1 - \delta$, since the action space is discrete, as in 7.1. Doing so permits us to write

$$\sigma_{t-1}(x)\tau(z_{t-1}(x)) \geq \sigma_{t-1}(x)\tau(q - \sqrt{\beta_t}) \quad \text{with prob. } 1 - \delta$$

(9.7)

$$\geq \sigma_{t-1}(x)(q - \sqrt{\beta_t}) \quad \text{with prob. } 1 - \delta$$

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Subsequently, we suppress the with high probability qualifier with the understanding that it’s implicit and applies to all subsequent statements. If \( I_t(x) = 0 \), then (9.4) holds automatically. Therefore, suppose \( I_t(x) > 0 \). Then, substitute the definition of \( q \) into the right-hand side of (9.7) to obtain:

\[
\sigma_{t-1}(x) \left( \frac{f(x) - \hat{y}_{t}^{\text{max}}}{\sigma_{t-1}(x)} - \sqrt{\beta_t} \right) = f(x) - \hat{y}_{t}^{\text{max}} - \sigma_{t-1}(x) \sqrt{\beta_t} \\
= I_t(x) - \sigma_{t-1}(x) \sqrt{\beta_t}. \tag{9.8}
\]

Thus, when we combine (9.6) - (9.8), we obtain the result stated in (9.4).

Again, we note by substituting the identity (Lemma 9.3) that begins the proof of Lemma 9.3 by the statement of Corollary 9.2, and defining the \( z \)-score quantities (9.5) but with substitution of \( \hat{y}_{t}^{\text{max}} \), we may apply properties of the upper-confidence bound (Lemma 7.1), which continue to hold when we replace the posterior of the dense GP with that of the compressed GP. This logic permits us to obtain the following as a corollary.

**Corollary 9.4.** The compressed expected improvement (9.2) upper-bounds the compressed instantaneous improvement \( \hat{I}_t(x) = \max\{0, f(x) - \hat{y}_{t}^{\text{max}}\} \) minus a proper scaling of the standard deviation, i.e.

\[
\hat{I}_t(x) - \sqrt{\beta_t} \sigma_{t-1}(x) \leq \alpha EI_t(x). \tag{9.9}
\]

Next, we present a variant of [Nguyen et al., 2017][Lemma 7] which connects the accumulation of posterior variances to maximum information gain. This result is akin to previously stated Lemmas 7.1 and 7.2.

[Nguyen et al., 2017][Lemma 8] defines a constant \( C \) such that the two terms on the right-hand side of Lemma 7.8 can be merged through the appropriate definition of a stopping criterion and modified definition of \( \beta_t \). We obviate this additional detail through the following modified lemma.

**Lemma 9.5.** The sum of the predictive variances is bounded by the maximum information gain \( \gamma_T \) as

\[
\sum_{t=1}^{T} \sigma_{t-1}^2(x) \leq \frac{2}{\log(1 + \sigma^{-2})} \gamma_T \tag{9.10}
\]

**Proof.** Consider the sum of posterior variances as

\[
\sum_{t=1}^{T} \sigma_{t-1}^2(x) = \sum_{t=1}^{T} \sigma^2 \left( \frac{\sigma_{t-1}^2(x) \sigma^{-2}}{s^2} \right) \leq \sum_{t=1}^{T} \sigma^2 \left[ \frac{\log(1 + s^2)}{\sigma^2 \log(1 + \sigma^{-2})} \right] \tag{9.11}
\]

where we have used the fact that the logarithm satisfies the inequality \( \frac{x}{\log(1+x)} \geq 1 \) for \( x = \sigma^{-2} \) to write \( \frac{1}{\sigma^2 \log(1 + \sigma^{-2})} \geq 1 \) together with \( \frac{1}{\log(1 + \sigma^{-2})} \geq \frac{1}{\log(1 + s^2)} \) on the right-hand side of (9.11). Now, pull the denominator outside the sum in the preceding expression, and multiply and divide by 2 to obtain the information for a single point \( (x_t, y_t) \) as \( \frac{1}{2} \log(1 + \sigma^{-2}) \sigma_{t-1}^2(x) \) in the summand as:

\[
\sum_{t=1}^{T} \sigma^2 \left[ \frac{\log(1 + s^2)}{\sigma^2 \log(1 + \sigma^{-2})} \right] = \sigma^2 \frac{2}{\sigma^2 \log(1 + \sigma^{-2})} \frac{1}{2} \sum_{t=1}^{T} \log(1 + \sigma_{t-1}^2(x)) \sigma^{-2} \tag{9.12}
\]
which after canceling a factor of $\sigma^2$ and noting that the sum of information gains at points $y_t$ accumulates to that of the full set $\{y_t\}$ [cf. (2.3)], similarly to (7.13) - (7.14), we obtain

$$ \frac{2}{\log(1 + \sigma^{-2})} \frac{1}{2} \sum_{t=1}^{T} \log(1 + \sigma_t^2(x)\sigma^{-2}) = \frac{2}{\log(1 + \sigma^{-2})} I(\{y_t\}; f) \leq \frac{2}{\log(1 + \sigma^{-2})} \gamma_T $$

(9.13)

where $\gamma_T$ is the maximum information gain over $T$ points [cf. (2.8)].

Here is a key point of departure in the analysis of employing conditional entropy-based compression (2.10) relative to the dense GP. Lemma 9.5 necessitates summing over all $t = 1, \ldots, T$. By contrast, using (2.10) together with selecting $x_t = \text{argmax}_{x_t \in X} \hat{\sigma}_t^2(x)$, we may break the sum on the left-hand side of (9.14) into those points retained in indexing set $\mathcal{M}_T$ and those not. Thus, we obtain the following lemma which is unique to our analysis.

**Lemma 9.6.** The sum of the predictive variances $\hat{\sigma}_{t-1}(x)$ of the compressed GP is bounded by the maximum information gain $\gamma_T$ [cf. (2.8)] as

$$ \sum_{t=1}^{T} \hat{\sigma}_{t-1}^2(x) \leq \frac{2}{\log(1 + \sigma^{-2})} (\gamma_T + \epsilon T) $$

(9.14)

*Proof.* Identical algebraic steps from (9.11) to (9.12) allow us to write (9.12) while substituting $\sigma_t$ by $\hat{\sigma}_t$:

$$ \frac{2}{\log(1 + \sigma^{-2})} \frac{1}{2} \sum_{t=1}^{T} \log(1 + \hat{\sigma}_{t-1}^2(x)\sigma^{-2}) $$

$$ = \frac{2}{\log(1 + \sigma^{-2})} \frac{1}{2} \left[ \sum_{t \in \mathcal{M}_T} \log(1 + \hat{\sigma}_{t-1}^2(x)\sigma^{-2}) + \sum_{t \notin \mathcal{M}_T} \log(1 + \sigma_{t-1}^2(x)\sigma^{-2}) \right] $$

$$ \leq \frac{2}{\log(1 + \sigma^{-2})} \frac{1}{2} \sum_{t \in \mathcal{M}_T} \log(1 + \hat{\sigma}_{t-1}^2(x)\sigma^{-2}) + \epsilon(T - M_T(\epsilon)) $$

(9.15)

where we have used the fact that $\log(1 + \hat{\sigma}_{t-1}^2(x)\sigma^{-2})$ defines the conditional entropy. Moreover, at time $T$, we have model complexity $M_T(\epsilon)$, which has had at most $T - M_T(\epsilon)$ points removed, each of which have conditional entropy less than or equal to $\epsilon$ on the right-hand side of the preceding expression. Then, using the definition of $I(\hat{y}_T; \hat{f}_T)$ in (7.17), and denoting $\gamma_T$ as the maximum information gain over $T$ points [cf. (2.8)], we may write

$$ \frac{2}{\log(1 + \sigma^{-2})} \frac{1}{2} \sum_{t \in \mathcal{M}_T} \log(1 + \hat{\sigma}_{t-1}^2(x)\sigma^{-2}) + \epsilon(T - M_T(\epsilon)) $$

$$ \leq \frac{2}{\log(1 + \sigma^{-2})} \left[ I(\hat{y}_T; \hat{f}_T) + \epsilon(T - M_T(\epsilon)) \right] $$

$$ \leq \frac{2}{\log(1 + \sigma^{-2})} \left[ \gamma_T + \epsilon(T - M_T(\epsilon)) \right] $$

(9.16)

where we have used the fact that maximum information gain monotonically increases as we add more points to upper-estimate $\gamma_{M_T}$ by $\gamma_T$, and upper-estimate $\epsilon(T - M_T(\epsilon))$ by $\epsilon T$ for ease of exposition to conclude Lemma 9.6.

Next we present a technical result regarding a property of the centered density $\tau(z) = \Phi(z) + \phi(z)$ at $z$-score $z_{t-1}(x) = (\mu_{t-1}(x) - \hat{y}_{t-1}^{\text{max}}) / \sigma_{t-1}(x)$.
Lemma 9.7. The negative $z$ score of the centered density function $\tau(z) = z\Phi(z) + \phi(z)$ at $z_{t-1}(x) = (\mu_{t-1}(x) - \hat{y}^{\text{max}}_{t-1})/\sigma_{t-1}(x)$ may be upper-bounded as

$$
\tau(-z_{t-1}(x_t)) \leq 1 + \frac{R}{\max_{\tau} \Phi(z)} \leq R
$$

Proof. The properties of $\tau(z)$ depend on the sign of $\mu_{t-1}(x) - y^{\text{max}}$. Thus, we break the proof into two parts. First, suppose $\mu_{t-1}(x) - y^{\text{max}} > 0$. Then, $\tau(z) \leq 1 + \frac{R}{\max_{\tau} \Phi(z)}$ for $z \geq 0$ to $\tau(-z_{t-1}(x_t))$ to write

$$
\tau(-z_{t-1}(x_t)) \leq 1 + \frac{y^{\text{max}} - \mu_{t-1}(x)}{\sigma_{t-1}(x)} \leq R
$$

On the other hand, for $\mu_{t-1}(x) - y^{\text{max}} \leq 0$, we may apply the property $\tau(z) \leq \phi(z)$ for $z \leq 0$ to write:

$$
\tau(-z_{t-1}(x_t)) \leq \frac{1}{\sqrt{2\pi}} \exp\{-\frac{1}{2} z^{2}_{t-1}(x_t)\} \leq 1
$$

The preceding expressions taken together permit us to conclude (9.17).

We underscore that Lemma 9.7 exploits properties of the shifted Gaussian density $\tau(z)$ which does not depend on whether the GP is dense or compressed, and therefore identical logic applies to $\tau$ in the context dense (2.6) or compressed expected improvement (9.2).

9.2 Proof of Theorem 3.2

With these lemmas, we are ready to shift focus to the proof of the main theorem. We follow the general strategy of [Nguyen et al., 2017] (Theorem 4) except that we must also address compression-induced errors. Begin then by considering the instantaneous regret $r_t = f(x^*) - f(x_t)$, to which we add and subtract $\hat{y}^{\text{max}}_{t-1}$:

$$
r_t = f(x^*) - f(x_t) = f(x^*) - \hat{y}^{\text{max}}_{t-1} + \hat{y}^{\text{max}}_{t-1} - f(x_t)
$$

We restrict focus to $A_t$, the first term on the right-hand side of the preceding expression, provided that $I_t(x^*) = f(x^*) - \hat{y}^{\text{max}}_{t-1} > 0$:

$$
A_t = f(x^*) - \hat{y}^{\text{max}}_{t-1} = I_t(x^*)
$$

where we apply the inequality that relates the expected improvement to the upper-confidence bound in Corollary 9.4. Next, use the optimality condition of the action selection $\hat{a}^{\text{EI}}_t(x^*) = \hat{a}^{\text{EI}}_t(x)$ with the identity $\hat{a}^{\text{EI}}_t(x) = \hat{\sigma}_{t-1}(x)\tau(\hat{z}_{t-1}(x))$ in Corollary 9.2 to write

$$
\hat{a}^{\text{EI}}_t(x^*) + \sqrt{\beta_t} \hat{\sigma}_{t-1}(x^*) \leq \hat{a}^{\text{EI}}_t(x) + \sqrt{\beta_t} \hat{\sigma}_{t-1}(x^*)
$$

$$
= \hat{\sigma}_{t-1}(x)\tau(\hat{z}_{t-1}(x)) + \sqrt{\beta_t} \hat{\sigma}_{t-1}(x^*)
$$

Now let’s shift gears to $B_t$, the second term on the right-hand side of (9.18). Add and subtract $\hat{\mu}_{t-1}(x_t)$

$$
B_t = \hat{y}^{\text{max}}_{t-1} - \hat{\mu}_{t-1}(x_t) + \hat{\mu}_{t-1}(x_t) - f(x_t)
$$

$$
\leq \hat{y}^{\text{max}}_{t-1} - \hat{\mu}_{t-1}(x_t) + \hat{\sigma}_{t-1}(x_t) \sqrt{\beta_t} \quad \text{with prob. } 1 - \delta
$$

$$
= \hat{\sigma}_{t-1}(x_t)(\hat{z}_{t-1}(x_t) + \hat{\sigma}_{t-1}(x_t) \sqrt{\beta_t} \quad \text{with prob. } 1 - \delta
$$

(9.21)
The first inequality comes from the property of the upper-confidence bound (Lemma \ref{lemma:ucb_property}) for finite discrete decision sets $\mathcal{X}$, which holds with probability $1 - \delta$. The second equality comes from the definition of $\hat{z}_{t-1}(\bar{x}_t) := (\mu_{t-1}(\bar{x}_t) - \hat{y}_{t-1}^{\text{max}})/\hat{\sigma}_{t-1}(\bar{x}_t)$ by multiplying through by $-\hat{\sigma}_{t-1}(\bar{x}_t)$. Subsequently, we suppress the high probability qualifier, with the understanding that it’s implicit.

We rewrite the preceding expression using the fact that $z = \tau(z) - \tau(-z)$

$$\hat{\sigma}_{t-1}(\bar{x}_t)(-\hat{z}_{t-1}(\bar{x}_t) + \hat{\sigma}_{t-1}(\bar{x}_t)\sqrt{\beta_t})$$

$$= \hat{\sigma}_{t-1}(\bar{x}_t)\left[\tau(-\hat{z}_{t-1}(\bar{x}_t)) + \sqrt{\beta_t} - \tau(\hat{z}_{t-1}(\bar{x}_t))\right]$$

(9.22)

Now, let’s return to (9.18), substituting in the right-hand sides of (9.20) and (9.22) for $A_t$ and $B_t$, respectively, to obtain:

$$r_t \leq \hat{\sigma}_{t-1}(\bar{x}_t)\left[\sqrt{\beta_t} + \tau(-\hat{z}_{t-1}(\bar{x}_t))\right] + \sqrt{\beta_t} \hat{\sigma}_{t-1}(x^*)$$

$$\leq \hat{\sigma}_{t-1}(\bar{x}_t)\left[\sqrt{\beta_t} + 1 + R_t\right] + \sqrt{\beta_t} \hat{\sigma}_{t-1}(x^*)$$

(9.23)

where we apply Lemma \ref{lemma:bound} to $\tau(-\hat{z}_{t-1}(\bar{x}_t))$ in the preceding expression. The definition of $R$ is in (9.17). First, we focus on the square of $L_t$ on the right-hand side of (9.23), which we sum from $t = 1, \ldots, T$:

$$\sum_{t=1}^{T} L_t^2 = \sum_{t=1}^{T} \hat{\sigma}_{t-1}^2(\bar{x}_t)\left[\sqrt{\beta_t} + 1 + R_t\right]^2$$

(9.24)

Apply the sum-of-squares inequality $(a + b + c) \leq 3(a^2 + b^2 + c^2)$ to obtain

$$\sum_{t=1}^{T} \hat{\sigma}_{t-1}^2(\bar{x}_t)\left[\sqrt{\beta_t} + 1 + R_t\right]^2 \leq \sum_{t=1}^{T} \hat{\sigma}_{t-1}^2(\bar{x}_t)3\left[\beta_t + 1 + R_t^2\right]$$

$$\leq 3\left[\beta_T + 1 + R_T^2\right] \sum_{t=1}^{T} \hat{\sigma}_{t-1}^2(\bar{x}_t)$$

(9.25)

where we use the fact that $\beta_t \leq \beta_T$. Now, apply Lemma \ref{lemma:bound} to the right-hand side of the preceding expression to obtain

$$3\left[\beta_T + 1 + R_T^2\right] \sum_{t=1}^{T} \hat{\sigma}_{t-1}^2(\bar{x}_t) \leq \frac{6(\beta_T + 1 + R_T^2)(\gamma_T + cT)}{\log(1 + \sigma^{-2})}$$

(9.26)

to which we further apply Cauchy-Schwarz to obtain

$$\sum_{t=1}^{T} L_t \leq \sqrt{T} \sum_{t=1}^{T} L_t^2 \leq \sqrt{6T(\beta_T + 1 + R_T^2)(\gamma_T + cT)} \log(1 + \sigma^{-2})$$

(9.27)
Now, we shift focus back to $U_t$ in (9.23) to which we apply $\beta_t \leq \beta_T$, Cauchy-Schwartz (in the form of the sum of squares inequality), and Lemma 9.6:

$$
\sum_{t=1}^{T} U_t = \sum_{t=1}^{T} \sqrt{\beta_t \sigma_t(x^*)} \leq \sqrt{\beta_T \sum_{t=1}^{T} \sigma_t(x^*)} \\
\leq \beta_T \sum_{t=1}^{T} \sigma_t(x^*) \\
\leq \beta_T \sqrt{T} \sqrt{\sum_{t=1}^{T} \sigma_t^2(x^*)} \\
\leq \sqrt{2T\beta_T (\gamma_T + \epsilon_T)} \log (1 + \sigma^{-2}) \quad (9.28)
$$

Now, we can aggregate the inequalities in (9.27) and (9.28), together with the fact that $R_T := f(x^*) - f(x_T)$ satisfies $R_T \leq \sum_i U_i + L_t$ to conclude:

$$
R_T \leq \sqrt{\frac{6T(\beta_T + R^2)(\gamma_T + \epsilon_T)}{\log(1 + \sigma^{-2})}} + \sqrt{\frac{2T\beta_T (\gamma_T + \epsilon_T)}{\log(1 + \sigma^{-2})}} \\
= \sqrt{\frac{2T(\gamma_T + \epsilon_T)}{\log(1 + \sigma^{-2})}} \left[ \sqrt{3(\beta_T + 1 + R^2)} + \sqrt{\beta_T} \right] \\
= \mathcal{O} (\sqrt{T}) \quad (9.29)
$$

which is sublinear for any $\epsilon$ chosen such that $\epsilon T > \mathcal{O}(1/T)$.