
LITE: Efficiently Estimating Gaussian Probability of Maximality

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Abstract

We consider the problem of computing the *probability of maximality* (PoM) of a Gaussian random vector, i.e., the probability for each dimension to be maximal. This is a key challenge in applications ranging from Bayesian optimization to reinforcement learning, where the PoM not only helps with finding an optimal action, but yields a fine-grained analysis of the action domain, crucial in tasks such as drug discovery. Existing techniques are costly, scaling polynomially in computation and memory with the vector size. We introduce LITE, the first approach for estimating Gaussian PoM with *almost-linear time and memory* complexity. LITE achieves SOTA accuracy on a number of tasks, while being in practice several orders of magnitude faster than the baselines. This also translates to a better performance on downstream tasks such as entropy estimation and optimal control of bandits. Theoretically, we cast LITE as entropy-regularized UCB and connect it to prior PoM estimators.

1 INTRODUCTION

Bayesian optimization (Garnett 2023) has emerged as a cornerstone for large-scale experimental design and automated discovery. Similarly, contextual bandits (Lattimore and Szepesvári 2020) have been established as the leading model for personalized recommender systems (Li et al. 2010) and have proven essential in the alignment of large language models (Christiano et al. 2017; Rafailov et al. 2024). Finally, reinforcement learning (Sutton and Barto 2018) has become indispensable in control systems

and robotics (Kober et al. 2013). In spite of the vastly different application domains, these fields of study are highly related: they all adopt a Bayesian perspective on an unknown *reward vector* F over actions \mathcal{X} , whose posterior $p(F|\mathcal{D})$ is used for informed decision-making, where \mathcal{D} denotes the evidential data. Viewed as an interactive game between an agent and the world, these applications differ in the input context, the number of turns of the game (optimal trajectories vs. single-step optimal actions) and the definition of the reward. However, the key notion of *probability of maximality* (PoM) naturally occurs in all these scenarios, by assisting the agent in solving the decision-making problem. PoM is the probability measure that *Thompson sampling*-like algorithms (Thompson 1933; Russo and Van Roy 2016; Russo et al. 2018; Chapelle and Li 2011) choose actions from. Moreover, the entropy of this distribution, is the objective that information-theoretic Bayesian optimization seeks to minimize (Hennig and Schuler 2012; Hernández-Lobato et al. 2014; Wang and Jegelka 2017; Hvarfner et al. 2022). Lastly, under a suitable framing, PoM describes the data likelihood in inverse reinforcement learning (Thurstone 1927; Guo et al. 2010; Benavoli et al. 2021).

As a concrete example, let us devise a recall-optimal bandit strategy for virtual screening in molecular design (Gao et al. 2022; Wang-Henderson et al. 2023). The goal of this task is to suggest a small set E from a large domain of molecules \mathcal{X} , so that the probability of E containing the optimal molecule, a.k.a. the recall, is maximized. Figure 1 compares three solutions to this problem, and plots the recall as $|E|$ grows. Two baselines (Komiyama et al. 2015) are provided by the naive methods of selecting E via Thompson sampling (TS) or by choosing the top- $|E|$ molecules with the largest expected rewards (MEANS). We propose to instead first estimate PoM using LITE, and then choose its $|E|$ largest entries. The PoM-based method markedly outperforms the alternatives, and is in fact the provably optimal solution, under mild assumptions.

Despite the key role of Gaussian probability of maximality in Bayesian optimization (Garnett 2023), contextual bandits (Krause and Ong 2011), and

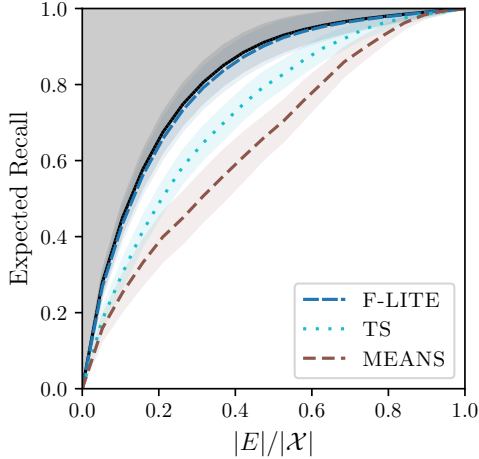


Figure 1: Selection of $E \subseteq \mathcal{X}$ according to the PoM estimates using LITE is near optimal (the gray shaded area is unachievable in expectation) and outperforms standard heuristics such as TS or selection based on the expected rewards (cf. Appendix D.1 for details).

reinforcement learning (Strens 2000), there has been limited investigation into its efficient estimation. In practice, often Thompson sampling is used to calculate a Monte Carlo estimate of PoM (Hennig and Schuler 2012). We refer to this technique as TS-MC¹, and demonstrate in Figure 2 that it becomes infeasible on sizable domains $|\mathcal{X}| \gg 1$, preventing large-scale real-world applications. A handful of works, which we cover next, provide explicit methods for estimation of PoM given a Gaussian distribution over the reward. Figure 2 compares our solution, LITE, with these works with respect to their computational complexity.

Avoiding a direct estimation of PoM, EST² calculates a lower bound to Gaussian PoM (Wang et al. 2016) and provides a faster alternative to TS-MC. However, as our results demonstrate, this comes at the cost of a lower accuracy (cf. Table 1). LITE not only outperforms EST, but also scales computationally better to large domains.

Our approach is most closely related to a recent result on probabilistic inference in reinforcement learning (Tarbouriech et al. 2024) which proposed VAPOR³, a method for estimating sub-Gaussian PoM. Its authors suggest numerically solving a variational objective to obtain an approximation to PoM. In this work, we point out an interpretable closed-form solution to VAPOR. Furthermore, we

demonstrate that LITE achieves a significantly more accurate estimation of Gaussian PoM.

Our work adds to the literature on Gaussian PoM estimation through the following contributions:

- We introduce LITE (*Linear-Time Independence-based Estimators*), a novel family of efficient estimators for computing Gaussian PoM with two variants: **A**-LITE and **F**-LITE, which are designed for higher accuracy or faster runtime.
- LITE scales almost-linearly in complexity as the domain size grows. This is enabled by our key idea of adopting an INDEPENDENCE ASSUMPTION, reducing the complexity by a factor of at least $|\mathcal{X}|$.
- We empirically analyze the statistical accuracy, time, and memory scaling of PoM estimation using LITE and existing baselines. LITE achieves the pareto-optimal performance for these criteria.

2 PRELIMINARIES

We study random reward functions over large but finite action domains \mathcal{X} , concisely expressed as random vectors F of length $|\mathcal{X}|$. These reward vectors are assumed to follow a multivariate Gaussian, i.e.,

$$F \sim \mathcal{N}(\mu_F, \Sigma_F)$$

with mean μ_F and covariance matrix Σ_F .⁴ We let $F^* := \max_x F_x$ and $X^* := \arg \max_x F_x$ be its maximum and maximizer, respectively. We assume the maximizer to be unique almost surely, which is satisfied automatically as long as F does not contain same-mean, perfectly-correlated entries:

Assumption 1. X^* is almost surely unique, which is equivalently expressed as $\sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^*] = 1$.

Under this model, we are interested in calculating the *probability of maximality* (PoM), the probability of any coordinate being the maximizer:

$$p_x := \mathbb{P}[x \in X^*] = \mathbb{P}[F_x = F^*] = \mathbb{P}[F_x \geq F_z \ \forall z \neq x].$$

To see how p_x can be used, consider the recall-optimal bandit problem, in which the goal is to find a set of k arms $E \subseteq \mathcal{X}$ that maximizes the expected recall (true positives of maximizers). In other words, we solve

$$\arg \max_{E \subseteq \mathcal{X}: |E|=k} \mathbb{P}[X^* \in E] = \arg \max_{E \subseteq \mathcal{X}: |E|=k} \sum_{x \in E} p_x,$$

¹Appendix A presents a primer on TS and TS-MC.

²EST is short for “optimization as estimation with Gaussian processes in bandit settings”.

³VAPOR is short for “variational approximation of the posterior probability of optimality in RL”

⁴As we suggest in Section 6, the Gaussian assumption may be relaxed to all Lévy alpha-stable distributions.

Method	Operations
TS-MC	$\Theta(\mathcal{X} ^3 + \mathcal{X} ^2/\epsilon^2)$
INDEP. ASSUM.	$\Theta(\mathcal{X} \sqrt{\log(1/\epsilon)}/\epsilon)$
LITE (ours)	$\Theta(\mathcal{X} \log(\log(\mathcal{X})/\epsilon))$
F-VAPOR (ours)	$\Theta(\mathcal{X} \log(\log(\mathcal{X})/\epsilon))$
Memory	
TS-MC	$\Theta(\mathcal{X} ^2)$
INDEP. ASSUM.	$\Theta(\mathcal{X} + \sqrt{\log(1/\epsilon)}/\epsilon)$
LITE (ours)	$\Theta(\mathcal{X})$
F-VAPOR (ours)	$\Theta(\mathcal{X})$

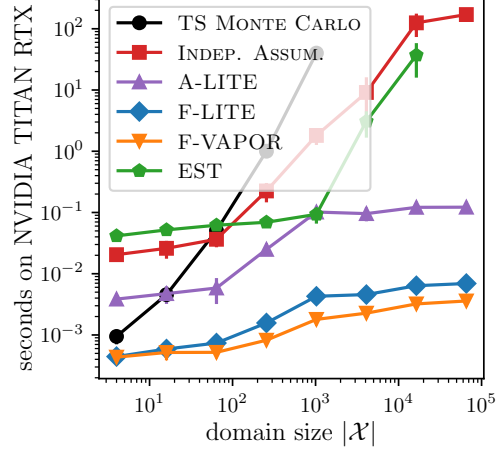


Figure 2: Asymptotic and empirical scaling of PoM estimators. Only LITE and F-VAPOR remain computationally feasible on large domains $|\mathcal{X}| \gg 1$ for the convergence threshold $\epsilon \in \Theta(1/|\mathcal{X}|)$. The minimal gap between F-LITE and F-VAPOR stems from evaluation of the slightly more expensive standard Gaussian cumulative distribution function as opposed to the exponential function. Appendix D.4 details the experimental setup.

where equality holds under Assumption 1. This objective is maximized precisely by setting E to the indices of the k largest entries of PoM, motivating our study.

The PoM is an elusive quantity: direct numerical integration over the probability density function of F must cover $|\mathcal{X}|$ -dimensional space, and Monte Carlo integration based on n i.i.d. Thompson samples (which we call TS-MC) converges very slowly at rate $1/\sqrt{n}$ (Morokoff and Caflisch 1995). To make matters worse, PoM is usually rather small, scaling inversely with $|\mathcal{X}|$.⁵ Therefore, to yield useful approximations, estimators of PoM need to be “ ϵ -accurate” with $\epsilon \in \Theta(1/|\mathcal{X}|)$, that is, they need to run until ϵ -convergence to their analytical limit.

Figures 2 and 4 demonstrate that TS-MC, the standard estimator for Gaussian PoM (Hennig and Schuler 2012), unfortunately does not scale to real-world domains (where $|\mathcal{X}|$ is often very large). Addressing these scalability issues, in this work we develop efficient estimators of Gaussian PoM that rely on the following key assumption:

Assumption 2. F is such that PoM can be reasonably approximated assuming independent entries in F , i.e.,

$$p_x = \mathbb{P}[F_x \geq F_z \forall z \neq x] \approx \tilde{p}_x = \mathbb{P}[\tilde{F}_x \geq \tilde{F}_z \forall z \neq x]$$

where $F \sim \mathcal{N}(\mu_F, \Sigma_F)$ and $\tilde{F} \sim \mathcal{N}(\mu_F, \text{diag}(\Sigma_F))$.

This mean-field approximation may hold by design, for instance in large-scale inverse reinforcement learning

⁵To see this, consider $F : \mathcal{X} \rightarrow \mathbb{R}$ as a discretization on a regular grid of a continuous Gaussian process on $[0, 1]^d$. Then the existence of the PDF of X^* mandates that PoM scale inversely to $|\mathcal{X}|$ as $|\mathcal{X}| \rightarrow \infty$. See also Appendix A.2.

such as RLHF (Christiano et al. 2017), or under a sufficiently coarse discretization of a continuous Gaussian process (Wang et al. 2016; Wang and Jegelka 2017). As we show experimentally in Section 5, LITE effectively estimates PoM in presence of dependence structure. For further discussion on the bias introduced by Assumption 2, we refer the reader to Appendix B.

3 ALMOST-LINEAR TIME POM ESTIMATION WITH LITE

We obtain the almost-linear-time estimator of PoM, LITE, in two steps. In the remainder of this paper we denote by ϕ the PDF and by Φ the CDF of the standard Gaussian, and defer all proofs to Appendix F.

First step. Under the independence assumption, we consider $\tilde{F} \sim \mathcal{N}(\mu_F, \text{diag}(\sigma_{F_1}^2, \dots, \sigma_{F_{|\mathcal{X}|}}^2))$ instead of F , and obtain its PoM via

$$\tilde{p}_x = \mathbb{P}[\tilde{F}_z \leq \tilde{F}_x \forall z \neq x] = \mathbb{E} \prod_{z \neq x} \mathbb{P}[\tilde{F}_z \leq \tilde{F}_x | \tilde{F}_x]. \quad (1)$$

This formulation enables us to evaluate a tractable one-dimensional integral instead of the intractable $|\mathcal{X}|$ -dimensional integral under dependency structure. We denote the integrand of Equation (1) by

$$g^x(f) := \prod_{z \neq x} \mathbb{P}[\tilde{F}_z \leq f] = g(f)/\mathbb{P}[\tilde{F}_x \leq f]$$

with $g(f) := \prod_z \mathbb{P}[\tilde{F}_z \leq f]$. Through reuse of evaluations of $g(f)$, it costs as much to compute $(g^x(f_i))_{i=1}^n$ for one x as it does for all $x \in \mathcal{X}$. A good choice of $n+1 \in \Theta(\sqrt{\log(1/\epsilon)}/\epsilon)$ shared integration points then guarantees uniformly ϵ -convergent predictions:

Informal Proposition 1 (Formalized in Proposition 1). *Let $\epsilon \in (0, 1/4]$. With $n+1 \in \Theta(\sqrt{\log(1/\epsilon)}/\epsilon)$ appropriately set integration points $f_0, \dots, f_n \in \mathbb{R} \cup \{\pm\infty\}$, we estimate Gaussian PoM $\forall x \in \mathcal{X}$ by*

$$\tilde{q}_x := \sum_{i=0}^{n-1} \frac{g^x(f_{i+1}) + g^x(f_i)}{2} \mathbb{P}[\tilde{F}_x \in (f_i, f_{i+1}]].$$

It then holds for all $x \in \mathcal{X}$ that $|\tilde{p}_x - \tilde{q}_x| \leq \epsilon$.

The shared integrand $g(f)$ is computed in $\Theta(|\mathcal{X}|)$ for a single integration point. So, under the independence assumption, consistent estimation of PoM can be performed in just $\Theta(|\mathcal{X}|\sqrt{\log(1/\epsilon)}/\epsilon)$, our first significant runtime improvement over TS-MC.

Second step. To remove the linear scaling in $1/\epsilon$ that stems from numerical integration, we propose to approximate $g^x(f)$ with the CDF of a Gaussian:

$$g^x(f) = \prod_{z \neq x} \Phi\left(\frac{f - \mu_{F_z}}{\sigma_{F_z}}\right) \approx \Phi\left(\frac{f - m_x}{s_x}\right).$$

Under this variational approximation, we can solve the integral of Equation (1) in closed-form:

$$\tilde{p}_x = \mathbb{E}[g^x(\tilde{F}_x)] \approx \mathbb{E}\Phi\left(\frac{\tilde{F}_x - m_x}{s_x}\right) = \Phi\left(\frac{\mu_{F_x} - m_x}{\sqrt{\sigma_{F_x}^2 + s_x^2}}\right). \quad (2)$$

Both variants of LITE rely on Equation (2), but differ in how they approximate g^x , i.e., in how they determine the free variables m_x and s_x :

- A-LITE uses nested binary search to match the quartiles of $\Phi((\cdot - m_x)/s_x)$ to those of g^x .
- F-LITE sets $s_x = 0$ and leverages Assumption 1 to find a shared normalizing threshold $m_x = \kappa^*$.

In the following, we focus our exposition on the “fast” (and simpler) variant F-LITE, even though we find in our experiments that the “accurate” variant A-LITE tends to be the more faithful estimator. We include a detailed discussion of A-LITE in Appendix C.

3.1 Fast LITE

F-LITE approximates the Gaussian PoM in Equation (2) with $s_x = 0$, which is suggested by concentration of measure of the maximum,⁶ and leverages Assumption 1 to find a shared normalizing threshold κ^* :

$$\tilde{p}_x \approx q_x := \Phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \text{ with } \kappa^* \text{ s.t. } \sum_x q_x = 1.$$

⁶Proposition 9 in Appendix F shows that the distribution of the maximum concentrates as $|\mathcal{X}| \rightarrow \infty$.

Algorithm 1 F-LITE

Require: $\mu_F, \sigma_F, \epsilon$
 $\kappa_{low} \leftarrow \mu_F^{min} + \sigma_F^{min} \cdot -\Phi^{-1}(1/|\mathcal{X}|)$
 $\kappa_{up} \leftarrow \mu_F^{max} + \sigma_F^{max} \cdot -\Phi^{-1}(1/|\mathcal{X}|)$
 $\text{max-error} \leftarrow \epsilon$
while $\text{max-error} \geq \epsilon$ **do**
 $\kappa \leftarrow \frac{1}{2}\kappa_{up} + \frac{1}{2}\kappa_{low}$
 $s \leftarrow \sum_{x \in \mathcal{X}} \Phi\left(\frac{\mu_{F_x} - \kappa}{\sigma_{F_x}}\right)$
if $s > 1$ **then** $\kappa_{low} \leftarrow \kappa$ **else** $\kappa_{up} \leftarrow \kappa$
 $\text{max-error} \leftarrow \max_{x \in \mathcal{X}} \Phi\left(\frac{\mu_{F_x} - \kappa_{low}}{\sigma_{F_x}}\right) - \Phi\left(\frac{\mu_{F_x} - \kappa_{up}}{\sigma_{F_x}}\right)$
end while
 $q_x \leftarrow \frac{1}{2} \Phi\left(\frac{\mu_{F_x} - \kappa_{low}}{\sigma_{F_x}}\right) + \frac{1}{2} \Phi\left(\frac{\mu_{F_x} - \kappa_{up}}{\sigma_{F_x}}\right) \quad \forall x \in \mathcal{X}$
return $(q_x / \sum_{z \in \mathcal{X}} q_z)_{x \in \mathcal{X}}$

Here, κ^* can be found efficiently using binary search. We summarize F-LITE in Algorithm 1. The boundaries of the binary search window and the implied complexity is derived in the following proposition:

Informal Proposition 2 (Formalized in Proposition 2). *Observe that $\sum_{x \in \mathcal{X}} \Phi((\mu_{F_x} - \kappa)/\sigma_{F_x})$ is continuous and monotonically decreasing in κ . We determine bounds $\kappa_{low}, \kappa_{up}$ on κ^* such that $\kappa_{up} - \kappa_{low} \in \Theta(\sqrt{\log |\mathcal{X}|})$. Therefore, with κ^k the k -th iterate of binary search and $k \in \Theta(\log(\log(|\mathcal{X}|)/\epsilon))$ it holds for all $x \in \mathcal{X}$ that $|\mathbb{P}[F_x \geq \kappa^*] - \mathbb{P}[F_x \geq \kappa^k]| \leq \epsilon$.*

Each iteration of binary search requires summing the entries q_x , and therefore the compute cost of F-LITE is almost-linear at $\Theta(|\mathcal{X}| \log(\log(|\mathcal{X}|)/\epsilon))$ operations. This provides us with an efficient PoM estimator that can be applied to real-world tasks with large domains.

3.2 Properties of F-LITE

Differentiability. F-LITE admits a closed-form expression for the derivatives of the estimated PoMs w.r.t. the parameters μ_F and σ_F of the Gaussian reward vector. Such derivatives are essential for the use of PoM estimates as data likelihoods in machine learning. For example, the likelihood of k -option preference feedback (a case of inverse RL) is measured by PoM (Christiano et al. 2017; Bradley and Terry 1952; Thurstone 1927), and derivatives are key to end-to-end learning of such preferences.

Proposition 3. *Let $h_x := \phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \frac{1}{\sigma_{F_x}}$. Then*

$$\frac{dq_x}{d\mu_{F_z}} = h_x \cdot \left(\mathbb{1}_{x=z} - \frac{h_z}{\sum_{w \in \mathcal{X}} h_w} \right) \quad (3)$$

$$\frac{dq_x}{d\sigma_{F_z}} = h_x \cdot \left(\mathbb{1}_{x=z} - \frac{h_z}{\sum_{w \in \mathcal{X}} h_w} \right) \cdot \frac{\kappa^* - \mu_{F_z}}{\sigma_{F_z}}. \quad (4)$$

Here, h_x is a sensitivity factor. Equations (3) and (4) are remarkably interpretable: increasing μ_{F_z} renders z a more likely and $x \neq z$ a less likely maximizer. Moreover, increasing σ_{F_z} renders z a more likely and $x \neq z$ a less likely maximizer if $q_z < 0.5$ (here uncertainty helps), otherwise z becomes a less likely and $x \neq z$ a more likely maximizer.

Balancing two sources of exploration. Efficient exploration is a key challenge in many domains of machine learning, including Bayesian optimization and reinforcement learning. The necessity for exploration in optimization arises when we are uncertain about the rewards of actions. In estimation of PoM, we face the same challenge: a faithful estimate of PoM needs to account for what we do not know, and assign a larger PoM to points with low mean and large variance than to points with low mean and low variance. Remarkably, we show in the following that F-LITE can be seen as a combination of two common exploration-inducing approaches: optimism in the form of an upper-confidence bound (Kushner 1962; Garnett 2023; Jones 2001; Srinivas et al. 2010; Vanchinathan et al. 2015; Chen et al. 2017), short UCB, and entropy regularization (Ziebart 2010; Neu et al. 2017; Geist et al. 2019; Mnih et al. 2016; Haarnoja et al. 2018).

Proposition 4. *Define the variational objective*

$$\mathcal{W}(p) := \sum_{x \in \mathcal{X}} p_x \cdot \left(\mu_{F_x} + \underbrace{\sqrt{2\tilde{I}(p_x) \cdot \sigma_{F_x}}}_{\text{exploration bonus}} \right), \quad (5)$$

with the quasi-surprisal $\tilde{I}(u) := (\phi(\Phi^{-1}(u))/u)^2/2$. Then the maximizer of \mathcal{W} among elements of the probability simplex is given by F-LITE, i.e., by q with

$$q_x := \Phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \text{ with } \kappa^* \text{ s.t. } \sum_x q_x = 1.$$

The quasi-surprisal $\tilde{I}(\cdot)$ behaves similarly to the surprisal $-\ln(\cdot)$, a key quantity in information theory (Cover 1999). In fact, their asymptotics coincide:

$$\tilde{I}(1) = 0 = -\ln(1) \text{ and } \tilde{I}(u) \sim -\ln u \text{ as } u \rightarrow 0^+.$$

The objective from Equation (5) is maximized for those probability distributions p that are concentrated around points with large mean μ_{F_x} and points with large exploration bonus. The uncertainty σ_{F_x} about F_x is the standard exploration bonus of UCB algorithms. In Equation (5), σ_{F_x} is weighted by the quasi-surprisal, which acts as entropy regularization: it increases the entropy of p by uniformly pushing p_x away from zero. The variational objective suggests that Thompson sampling (Thompson 1933; Russo and Van Roy 2016; Russo et al. 2018; Chapelle and Li 2011), i.e., sampling from PoM, achieves exploration through two means:

1. **Optimism:** by preferring points with large uncertainty σ_{F_x} about the reward value F_x .
2. **Decision uncertainty:** by assigning some probability mass to all x , that is, by remaining uncertain about which x is the maximizer.

Interestingly, the recall task from Figure 1 is solved by choosing actions with highest PoM. Contrary to initial intuition, the good performance of LITE in the recall task indicates that optimism and decision uncertainty, normally associated with exploration, are also useful for pure exploitation.

4 LANDSCAPE OF POM ESTIMATION

Motivated by the intimate relation between PoM estimation in the form of F-LITE and decision-making, we next connect PoM to several methods developed for Bayesian optimization and reinforcement learning.

Probability of improvement. F-LITE measures the probability of improvement over the normalizing threshold κ^* : $q_x := \Phi((\mu_{F_x} - \kappa^*)/\sigma_{F_x}) = \mathbb{P}[F_x \geq \kappa^*]$. Similarly, the true PoM can be seen as measuring a probability of improvement: $p_x = \mathbb{P}[F_x \geq F^*]$. By comparing the two expressions, the normalizing threshold in F-LITE can be understood as a deterministic surrogate for the maximum. Probability of improvement is widely known as an acquisition function in Bayesian optimization (Kushner 1964; Garnett 2023; Jones 2001; Žilinskas 1992), with the threshold κ^* typically set to the best observation.

Estimating the maximum reward value. The EST(-imate) algorithm (Wang et al. 2016) proposes to approximate Gaussian PoM with its lower bound

$$\tilde{p}_x \approx \frac{\mathbb{P}[\tilde{F}_x \geq \tilde{\kappa}]}{1 - \mathbb{P}[\tilde{F}_x \geq \tilde{\kappa}]} \prod_{z \in \mathcal{X}} \mathbb{P}[\tilde{F}_z \leq \tilde{\kappa}],$$

where $\tilde{\kappa} = \mathbb{E}[\tilde{F}^*]$ with $\tilde{F} \sim \mathcal{N}(\mu_F, \text{diag}(\Sigma_F))$. It then directly uses this lower bound as an acquisition function for Bayesian optimization. With the denominator being usually close to 1, EST corresponds to a globally rescaled F-LITE, but using the expectation of \tilde{F}^* instead of the normalizing threshold κ^* as a surrogate for the maximum. In our experiments, we linearly normalize the PoM predicted by EST to sum to 1, creating a stronger baseline for us to beat.

UCB + entropy regularization. In analogy to our variational formulation of F-LITE, VAPOR (Tarbouriech et al. 2024) proposes to maximize

	Synthetic Distributions	1-dim GP	2-dim GP (E.2)	DropWave (E.3)	Quadcopter
EST	11.54 ± 0.20	45.6 ± 2.7	15.1 ± 1.2	5.17 ± 0.64	14.3 ± 2.0
VAPOR	9.89 ± 0.11	37.0 ± 2.0	15.7 ± 1.0	5.70 ± 0.72	17.2 ± 2.5
F-LITE (ours)	4.65 ± 0.08	13.7 ± 1.0	10.9 ± 0.7	4.87 ± 0.60	11.1 ± 1.4
A-LITE (ours)	3.76 ± 0.06	14.1 ± 1.0	7.5 ± 0.5	4.32 ± 0.53	8.7 ± 0.9
INDEP. ASSUM.	0.00 ± 0.00	6.7 ± 0.4	6.6 ± 0.2	3.85 ± 0.54	9.0 ± 1.0

Table 1: Mean and standard error of TV distance (averaged across $|\mathcal{X}|$ and BO-steps) in percentage %. A-LITE and F-LITE consistently outperform competing efficient PoM estimators from the literature. The INDEPENDENCE ASSUMPTION is provided as an expensive baseline, since all considered efficient estimators build on it.

the variational objective

$$\mathcal{V}(p) = \sum_{x \in \mathcal{X}} p_x \cdot \left(\mu_{F_x} + \sqrt{2 \ln(1/p_x)} \cdot \sigma_{F_x} \right) \quad (6)$$

on the probability simplex to estimate PoM. To solve Equation (6), they use Frank-Wolfe (Jaggi 2013; Lacoste-Julien and Jaggi 2015) with $k \in \Theta(\epsilon^{-5} |\mathcal{X}|^4)$ steps to ensure $\mathcal{V}(p^*) - \mathcal{V}(p) \leq \epsilon$ with no bounds on $\|p^* - p\|_\infty$ (Bolte et al. 2023). Instead, we derive a previously unknown near closed-form solution to VAPOR whose iterates converge exponentially at a linear rate:

Proposition 5 (Fast VAPOR). *The maximizer to Equation (6) on the probability simplex admits the closed-form expression*

$$v_x := v \left(\frac{\mu_{F_x} - \nu^*}{\sigma_{F_x}} \right) \text{ with } \nu^* \text{ s.t. } \sum_x v_x = 1,$$

where $v(c) := \exp(-(\sqrt{c^2 + 4} - c)^2/8)$.

Moreover, to find ν^* we can use binary search with $k \in \Theta(\log(\sqrt{\log |\mathcal{X}|}/\epsilon))$ iterations, ensuring that the k -th iterate v^k satisfies $\|v^* - v^k\|_\infty < \epsilon$.

Note the similarity to F-LITE: we have only replaced Φ by the sigmoidal v . As such, Algorithm 1 is easily adapted to obtain a novel almost-linear-time implementation of VAPOR, which we call F-VAPOR.

5 EXPERIMENTS

Next, we compare the PoMs estimated by A-LITE and F-LITE against the efficient baselines EST and VAPOR. We measure the total variation distance to the “ground truth” PoM obtained via expensive TS-MC as well as the root mean squared relative error on the down-stream task of entropy estimation. The INDEPENDENCE ASSUMPTION is computing an asymptotically exact estimate under Assumption 2, which we report as a (up to significance) error lower bound for independence-based PoM estimators. The code is available at <https://github.com/lasgroup/LITE>.

5.1 PoM Estimation

To compare PoM estimators in various settings (for various (μ_F, Σ_F)), we rely on synthetic distributions as well as posteriors produced during Bayesian optimization. Table 1 provides a summary of our results.

Synthetic distributions. We obtain a set of synthetic (μ_F, σ_F) by independently sampling $\mu_{F_x} \sim \mathcal{U}([0, 5])$ and $\sigma_{F_x} \sim \mathcal{U}([1/2, 10])$ for all x . We employ Proposition 1 for the ground-truth PoM, i.e., estimation under the INDEPENDENCE ASSUMPTION. Figure 3a shows how A-LITE and F-LITE significantly outperform VAPOR and EST. We remark that estimation of PoM seems to become easier on large domains. We suspect that more repetition in μ_F and σ_F leads to a more uniform PoM that is easier to estimate. Similar results on alternative distributions over μ_F, σ_F are provided in Appendix E.1.

Samples from a Gaussian process. Figure 3b shows the total variation distance between a ground-truth estimate using TS-MC and the PoM of the various estimators. The posteriors are derived from calibrated Bayesian optimization with f_{true} sampled from a squared exponential prior on a one-dimensional domain. A-LITE and F-LITE outperform VAPOR and EST by a large margin. F-LITE becomes most accurate at late stages of optimization, once F^* becomes quite concentrated. The details of the experimental setup are in Appendix D.5.

DropWave function. In practice, Bayesian optimization is run on a single test function and calibrated through marginal likelihood maximization of the prior parameters. Figure 4 demonstrates the accuracy/runtime operating points according to the various considered PoM estimators under different choices of the convergence parameter $\epsilon = 1/(\alpha \cdot |\mathcal{X}|)$. Here, f_{true} is set to the drop-wave function, notorious for its difficulty in Bayesian optimization, quantized to 625 points. Given sufficient compute, consistent estimation through TS-MC is recommended. However, as

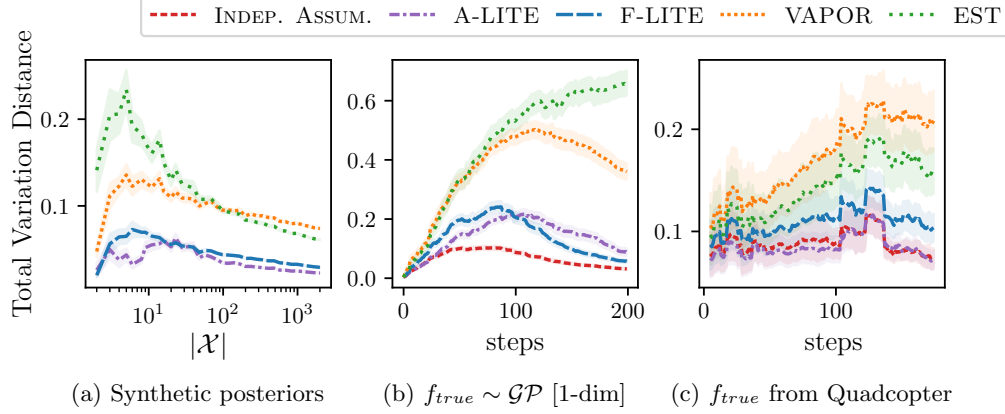


Figure 3: LITE universally outperforms VAPOR and EST in terms of TV-distance to the ground-truth, which is estimated using the INDEPENDENCE ASSUMPTION (Figure 3a) and TS-MC (Figures 3b, 3c).

shown in Figure 2, TS-MC scales worse than the INDEPENDENCE ASSUMPTION (and LITE) to large domains. Consequently, as the domain size $|\mathcal{X}|$ increases the point at which TS-MC starts to outperform them is shifted to the right into a computationally infeasible region. Experimental details can be found in Appendix D.7. For additional experiments on drop-wave (which feature in Table 1), see Appendix E.3.

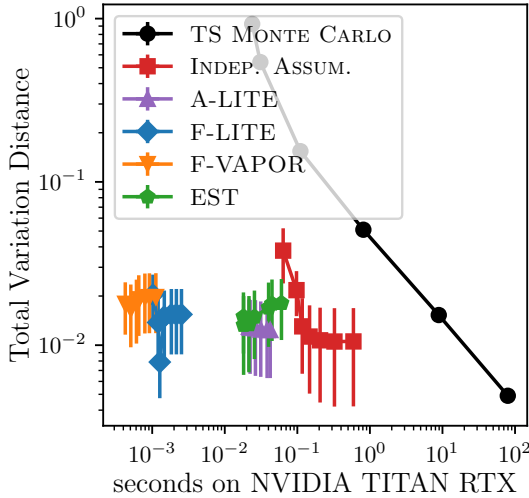


Figure 4: TS-MC is consistent, but only becomes competitive with high computational cost. Instead, the biased but efficient PoM estimators quickly converge to decent accuracy at low computational cost. Here, F is distributed according to the posteriors of Bayesian optimization with f_{true} set to drop-wave.

Quadcopter simulation. Finally, we consider the TV distance during Bayesian optimization of the parameters of a quadcopter controller (Hübötter et al. 2024), see Figure 3c. The ground-truth PoM is estimated using TS-MC. f_{true} , a function of the parameters, describes the degree to which a controller

manages to stabilize a quadcopter in a simulated environment under randomly sampled perturbations. The controller presents eight degrees of freedom, 4 of which are solved using a heuristic, resulting in Bayesian optimization in four-dimensional space. To ensure tractable computation of a ground-truth PoM, we uniformly at random subsample the domain to 400 discrete points. Details are in Appendix D.6. As in the other experiments, estimation under the INDEPENDENCE ASSUMPTION is most accurate, swiftly followed by A-LITE and F-LITE. VAPOR and EST are less performant in comparison.

5.2 PoM Entropy Estimation

Information theory (Gray 2011) proposes to measure uncertainty with the Shannon entropy $H[X^*] := \sum_x p_x \ln(1/p_x)$. Unfortunately, there is no known unbiased Monte Carlo estimator of entropy without access to p_x (Paninski 2003). Furthermore, the standard procedure of using TS-MC provably under-estimates the entropy unless many samples are used: let $q_x := \sum_{i=1}^n \mathbf{1}_{x \in \arg \max f_i} / n$ for i.i.d. $f_i \sim p(f|\mathcal{D})$. Then either $q_x \geq 1/n$ or $q_x = 0$, and hence it holds

$$H[q_x] = \sum_x q_x \ln(1/q_x) \leq \ln(n).$$

Only once n exceeds $|\mathcal{X}|$ can entropy estimation using TS-MC span the full range of valid values $[0, \ln(|\mathcal{X}|)]$. As such, a runtime that scales in $\Theta(|\mathcal{X}|^3)$ would be required, which becomes prohibitive for large domains. In contrast, the exponential convergence of LITE allows efficient entropy estimation in $\Theta(|\mathcal{X}| \log(|\mathcal{X}|))$.

In our experiments, we report on the root mean squared relative error of PoM entropy estimation

	1-dim GP	2-dim GP (E.2)	DropWave (E.3)	Quadcopter
EST	215.5 (195.4, 233.9)	36.3 (27.5, 43.3)	5.4 (4.9, 5.8)	3.4 (2.9, 3.9)
VAPOR	169.4 (158.4, 179.7)	33.7 (26.9, 39.4)	8.2 (5.9, 10.0)	3.8 (3.4, 4.2)
F-LITE (ours)	35.9 (34.7, 37.0)	12.4 (10.8, 13.9)	5.3 (4.8, 5.7)	2.6 (1.9, 3.2)
A-LITE (ours)	44.9 (42.8, 47.0)	11.0 (9.5, 12.4)	4.7 (4.2, 5.1)	3.0 (2.4, 3.5)
INDEP. ASSUM.	18.4 (17.8, 18.9)	4.9 (4.4, 5.4)	4.6 (4.2, 5.1)	2.4 (1.6, 3.0)

Table 2: Empirical root mean squared relative error of entropy in percentage % (along with confidence bands). A-LITE and F-LITE consistently outperform competing efficient estimators of PoM. The confidence bands correspond to the square root of mean \pm standard error of the squared relative error (averaged across BO-steps).

across multiple seeds of optimization, defined as

$$\sqrt{\frac{1}{m} \sum_{i=1}^m \left(\frac{H[E | \mathcal{D}^i] - H[X^* | \mathcal{D}^i]}{H[X^* | \mathcal{D}^i]} \right)^2}.$$

The ground-truth $H[X^* | \mathcal{D}^i]$ is estimated based on expensive TS-MC, whereas $H[E | \mathcal{D}^i]$ denotes the entropy estimation according to the PoM estimator at hand. The relative error is a natural performance criterion, ensuring normalization across different stages of optimization and across various ground-truths f_{true} .

As Table 2 demonstrates, the entropy of X^* can be faithfully estimated based on the INDEPENDENCE ASSUMPTION. Whereas the two variants of LITE remain competitive with the INDEPENDENCE ASSUMPTION, VAPOR and EST are often much worse in their estimation of entropy. Here, the experimental setups correspond to Section 5.1. In particular, the 1-dim GP experiment is described in Appendix D.5, the 2-dim GP experiment in Appendix E.2, DropWave in Appendix E.3, and Quadrotor in Appendix D.6.

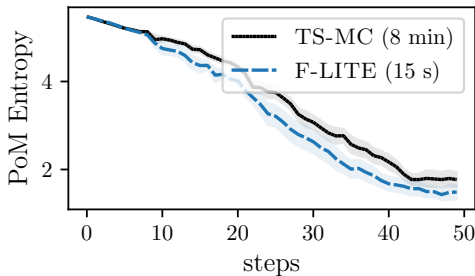


Figure 5: Entropy Search with LITE admits better computational and statistical efficiency than with TS-MC. We describe the setup in Appendix D.2.

5.3 Applications of PoM Entropy Estimation

Entropy Search (Hennig and Schuler 2012) is a widely used strategy in Bayesian optimization, which queries the reward at the point $x \in \mathcal{X}$ promising

(in expectation) the largest reduction in entropy of Gaussian PoM. In Figure 5, we run calibrated Entropy Search on a 1-dimensional Gaussian process with squared exponential kernel, discretized to a domain of size $|\mathcal{X}| = 250$. Simply replacing the standard PoM estimator (TS-MC) with LITE results in significantly shorter runtimes and better optimization trajectories, already for moderately large domains \mathcal{X} . This indicates that LITE can be used to markedly improve the scalability of Entropy Search.

Finally, through its almost-linear time and memory complexity, the estimation of PoM entropy with LITE can be used to better understand the state of Bayesian optimization in large-scale settings where previous approaches for PoM entropy estimation would become intractable. To capture such a large-scale setting, we consider an objective f_{true} set to a hyperplane in 1'000 dimensions sampled to a finite domain with $|\mathcal{X}| = 10'000$ points. On an NVIDIA A100 GPU, compared to the INDEPENDENCE ASSUMPTION and thus also TS-MC, LITE *reduces computation time from 21 days to 30 seconds*. We describe details in Appendix D.3.

6 FUTURE WORK

Generalization of LITE. The developed methodology can be extended to distributions other than Gaussians. In fact, the INDEPENDENCE ASSUMPTION has a generalization to arbitrary distributions in the form of Proposition 8 in Appendix F. Moreover, the variational approximation of LITE, which allows analytical integration, can be extended to any Lévy alpha stable distribution: let $\mathbb{P}[F_x \leq f] = G((f - \mu_{F_x})/\sigma_{F_x})$ for a stable G , then approximating $g^x(f)$ with $G((f - m_x)/s_x)$ results in an analytical expression for PoM. Together, this indicates that LITE can be generalized to a much larger class of distributions than just Gaussians. In this work, we emphasize Gaussians due to their ubiquity across many applications domains and leave a more general analysis to future work.

Learning heteroscedastic reward models. Given a random reward vector over actions, the data likelihood of (reward-maximizing) experts picking any one is precisely equal to PoM (Luce 2005; Christiano et al. 2017; Bradley and Terry 1952; Thurstone 1927). Through its closed-form derivatives stated in Proposition 3.2, LITE could allow efficient end-to-end learning of a (parametrized) reward model that simultaneously indicates the expected reward of an action, as well as its associated uncertainty. In contrast to Bradley-Terry and Thurstone, LITE naturally extends to heteroscedastic rewards, which could prove essential for faithful modeling of epistemic uncertainty.

7 CONCLUSION

In LITE, we developed estimators of Gaussian probability of maximality (PoM) that operate in near-linear efficiency with respect to the size of the Gaussian vector considered. In contrast, previous methods scale polynomially and thus quickly become computationally infeasible for moderately-sized vectors. Our empirical observations in multiple settings demonstrate that LITE, in comparison to EST and VAPOR, delivers more accurate PoM estimates and results in better PoM entropy estimation. Theoretically, we revealed connections between F-LITE and the Bayesian optimization literature, spanning PI, EST, entropy-regularized UCB, and VAPOR. Based on a variational formulation of LITE, we uncovered how Thompson sampling achieves exploration by relying simultaneously on optimism and decision uncertainty, and how these two principles, unexpectedly, guide optimal behavior in a pure exploitation task.

Finally, we demonstrated that the achieved efficiency gains translate to better performance at down-stream objectives such as recall-optimal control of bandits and Entropy Search. We envision that the scalability improvements achieved in this work inspire further development of algorithms that leverage the now-tractable notion of Gaussian PoM to tackle challenges in domains such as high-dimensional Bayesian optimization and reinforcement learning.

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Checklist

1. For all models and algorithms presented, check if you include:
 - (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model. [Yes]
 - (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm. [Yes]
 - (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries. [Yes]
2. For any theoretical claim, check if you include:
 - (a) Statements of the full set of assumptions of all theoretical results. [Yes]
 - (b) Complete proofs of all theoretical results. [Yes]
 - (c) Clear explanations of any assumptions. [Yes]
3. For all figures and tables that present empirical results, check if you include:
 - (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL). [Yes]
 - (b) All the training details (e.g., data splits, hyperparameters, how they were chosen). [Yes]
 - (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). [Yes]
 - (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). [Yes]
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
 - (a) Citations of the creator If your work uses existing assets. [Not Applicable]
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 - (d) Information about consent from data providers/curators. [Not Applicable]
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5. If you used crowdsourcing or conducted research with human subjects, check if you include:
 - (a) The full text of instructions given to participants and screenshots. [Not Applicable]
 - (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. [Not Applicable]
 - (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. [Not Applicable]

LITE: Efficiently Estimating Gaussian Probability of Maximality Supplementary Materials

Contents of Appendix

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A THOMPSON SAMPLING MONTE CARLO

Thompson sampling (TS) (Thompson 1933; Russo and Van Roy 2016; Russo et al. 2018; Chapelle and Li 2011) is a strategy for Bayesian optimisation that naturally incorporates an *exploration-exploitation trade-off* (Auer 2002). By directly sampling from the posterior probability of maximality $\mathbb{P}[x \in X^* | \mathcal{D}]$, Thompson sampling effectively incorporates the knowledge of $F | \mathcal{D}$ that is relevant for Bayesian optimization: it efficiently explores when the position of the maximizer X^* is unknown given the data \mathcal{D} , otherwise it exploits.

As a strategy for Bayesian optimization, Thompson sampling uses the fact that sampling from probability of maximality is much easier than computing it. Indeed, since X^* is a function of F , to produce samples from X^* it suffices to take the argmax of samples from F . Since by assumption the domain \mathcal{X} is finite, we may represent F as

$$F \stackrel{d}{=} \mu_F + \mathcal{L}\epsilon \sim \mathcal{N}(\mu_F, \Sigma_F), \quad (7)$$

where \mathcal{L} is the Cholesky decomposition of Σ_F and $\epsilon \sim \mathcal{N}(0, I_{|\mathcal{X}| \times |\mathcal{X}|})$. Exhaustive Thompson sampling explicitly computes \mathcal{L} and uses Equation (7) to produce a sample $f \sim p(F)$, which is subsequently processed into a sample from probability of maximality through $x^* = \arg \max_{x \in \mathcal{X}} f(x) \sim \mathbb{P}[x \in X^*]$. As a result, it costs $\Theta(|\mathcal{X}|^3 + n|\mathcal{X}|^2)$ to draw n independent Thompson samples. In contrast, as we will see shortly, using Thompson sampling to numerically approximate $\mathbb{P}[x \in X^*]$ costs $\Theta(|\mathcal{X}|^4)$ due to requiring $n \in \Theta(|\mathcal{X}|^2)$ independent samples. Note that this supralinear scaling persists, even under more efficient methods of drawing Thompson samples such as parametrising F via Random Fourier Features (Rahimi and Recht 2007).

A.1 From Thompson Sampling to Thompson Sampling Monte Carlo

TS-MC is the standard method for computing Gaussian probability of maximality (Hennig and Schuler 2012), since it is both simple and delivers unbiased and consistent estimates of the *probability of maximality*. As such, it represents the ground-truth against which all other estimators are empirically compared. Given access to n Thompson samples, one uses histogram binning to estimate PoM with each $x \in \mathcal{X}$ having its separate bin. More precisely, *probability of maximality* is estimated through

$$\mathbb{P}[x \in X^*] = \mathbb{E}[\mathbb{1}_{x \in X^*}] \approx \frac{1}{n} \sum_{i=1}^n \mathbb{1}_{x \in x_i^*} \quad \text{with samples } x_i^* \sim p(x^*).$$

Each Thompson sample of X^* provides simultaneously a sample of $\mathbb{1}_{x \in X^*}$ for all $x \in \mathcal{X}$, amortising the cost of computation. As is customary for Monte Carlo based approaches, the accuracy is in $\Theta(n^{-1/2})$ ⁷. Indeed, given independent samples $X_i^* \sim p(x^*)$, Hoeffding’s inequality guarantees that

$$\mathbb{P}\left[\left|\frac{1}{n} \sum_{i=1}^n \mathbb{1}_{x \in X_i^*} - \mathbb{P}[x \in X^*]\right| \geq \epsilon\right] \leq 2 \exp(-2n\epsilon^2).$$

Hence, for $n \geq \ln(2/\delta)/(2\epsilon^2)$ the probability that TS-MC deviates more than ϵ from the ground truth at any fixed $x \in \mathcal{X}$ is at most δ . Figure 6 shows the estimates of TS-MC and indicates the least required samples. The number of samples n must scale in $\Theta(|\mathcal{X}|^2)$ to reach an acceptable relative accuracy.

Algorithm 2 PoM estimation with EXHAUSTIVE TS-MC

Require: $\mu_F, \Sigma_F, \epsilon, \delta$
 $U, D \leftarrow \text{eig}(\Sigma_F)$ \triangleright C: $\Theta(|\mathcal{X}|^3)$, M: $\Theta(|\mathcal{X}|^2)$
 $\Sigma_F^{1/2} \leftarrow U D^{1/2}$
 $\text{counts} \leftarrow (0)_{k=1}^{|\mathcal{X}|}$
 $n \leftarrow \lceil \frac{\ln(2/\delta)}{2\epsilon^2} \rceil$
for $i = 1, \dots, n$ **do**
 $f \leftarrow \mu_F + \Sigma_F^{1/2} \cdot \varepsilon$ for $\varepsilon \sim \mathcal{N}(0, I_{|\mathcal{X}| \times |\mathcal{X}|})$ \triangleright C: $\Theta(|\mathcal{X}|^2)$, M: $\Theta(|\mathcal{X}|)$
 $\text{idx} \leftarrow \arg \max_{x \in \mathcal{X}} f_x$
 $\text{counts}_{\text{idx}} \leftarrow \text{counts}_{\text{idx}} + 1$
end for
 $p_x \leftarrow \text{counts}/n$
return $(p_x)_{x \in \mathcal{X}}$

A.2 The High Variance of Thompson Sampling Monte Carlo

Estimating probability of maximality (PoM) using TS-MC requires many samples to bring down the variance. While the central limit theorem already dictates that the error scale is in $\Theta(n^{-1/2})$, Figure 6 demonstrates empirically that going above $|\mathcal{X}|^2$ samples is indeed required for a smooth PoM estimate of high fidelity.

Here, the domain is a 50×50 grid resulting in $|\mathcal{X}| = 2'500$. f_{true} is sampled from a centered Gaussian process with exponential kernel (length scale 0.02, amplitude 1.0). The prior belief over f_{true} is a centered Gaussian process with exponential kernel (length scale 0.02, amplitude 2.0). f_{true} is observed at 10 regularly selected locations with homoscedastic additive centered Gaussian noise ($\sigma_{\text{noise}} = 0.5$). We vary $1/(\epsilon \cdot |\mathcal{X}|) =: \alpha \in \{0.02, 0.4, 1.0, 5.0\}$ to observe the fidelity of EXHAUSTIVE TS-MC. Finally, to mimic a probability density function, we divide the estimated *probability of maximality* by $1/50^2$.

⁷This is a direct consequence of the central limit theorem and verified empirically in Section A.2.

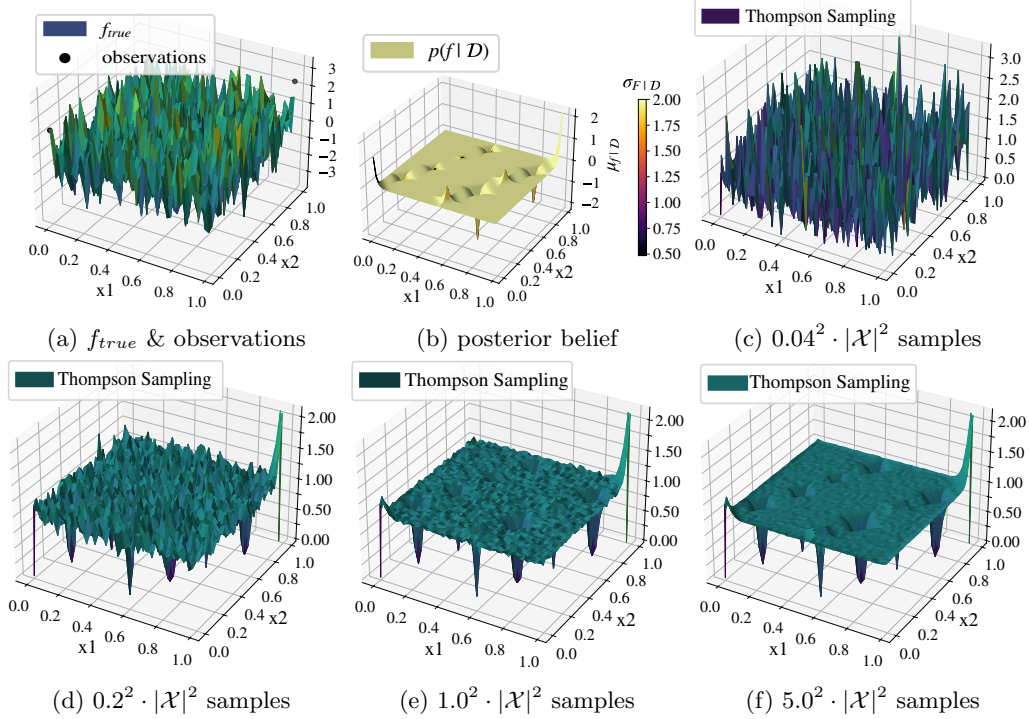


Figure 6: Demonstrating that $n \in \Theta(|\mathcal{X}|^2)$ samples are required (equivalently that $\epsilon \in \Theta(1/|\mathcal{X}|)$ is needed).

B BIAS INTRODUCED BY NEGLECTING DEPENDENCY STRUCTURE

Let us develop some intuition on the estimation bias introduced by falsely assuming uncorrelated entries in the Gaussian reward vector (Assumption 2). To that end, we consider some examples of discretized Gaussian processes that violate the independence assumption. Figure 7 considers posteriors with varying degree of concentration of measure, covering different stages of Bayesian optimization. The figure demonstrates that PoM estimation based on Assumption 2 qualitatively captures the ground-truth PoM (here estimated using TS-MC). The degeneracies at the border of the ground-truth PoM correspond to dirac-deltas of the probability density function of PoM, but have small effective measure and as such are of little concern. Theoretically, the dominant effect of falsely assuming independence can be understood by considering Slepian’s lemma (Slepian 1962), which implies that if $F \sim \mathcal{N}(\mu, \Sigma)$ and $\tilde{F} \sim \mathcal{N}(\mu, \text{diag}(\Sigma))$ with $\Sigma_{i,j} \geq 0 \forall i, j$, it holds that

$$\mathbb{P}[F^* > t] \leq \mathbb{P}[\tilde{F}^* > t] \quad \forall t \in \mathbb{R} \implies \mathbb{E}[F^*] \leq \mathbb{E}[\tilde{F}^*].$$

In light of this, the minor differences that can be observed in Figure 7 between the PoM under Assumption 2 and the ground-truth PoM are explained as follows: Assumption 2 leads to over-estimating the maximum reward F^* (Slepian’s lemma), which results in overly-cautious estimation of PoM, in particular under-estimating regions associated with promising observations. However, we stress that despite this bias towards uniformity, estimation under the INDEPENDENCE ASSUMPTION still manages to qualitatively capture the ground-truth PoM.

The experimental details of Figure 7 are as follows: the domain consists of $|\mathcal{X}| = 200$ equidistant points on which f_{true} , a sample from a centered Gaussian process \mathcal{GP} with squared exponential kernel (length scale 0.02, amplitude 1.0), is evaluated. The prior belief over f_{true} coincides with \mathcal{GP} except for the doubling of the amplitude to 2.0. f_{true} is observed at $|\mathcal{D}|$ regularly selected locations with homoscedastic additive centered Gaussian noise ($\sigma_{noise} = 0.5$). We set the accuracy parameter to $\epsilon = 1/(5|\mathcal{X}|)$. The estimated probability mass functions (of PoM) are rescaled by $1/|\mathcal{X}|$ to simulate a probability density function.

Finally, to further argue for our method of neglecting dependency structure, we next demonstrate that the computational complexity of any unbiased estimator of PoM is lower bounded by the number of entries in Σ_F , i.e., it lies in $\Omega(|\mathcal{X}|^2)$. Lemma 1, through construction of a simple synthetic example with closed-form *probability of maximality*, shows that in general knowledge on all entries in Σ_F would be required. Note that the Lemma

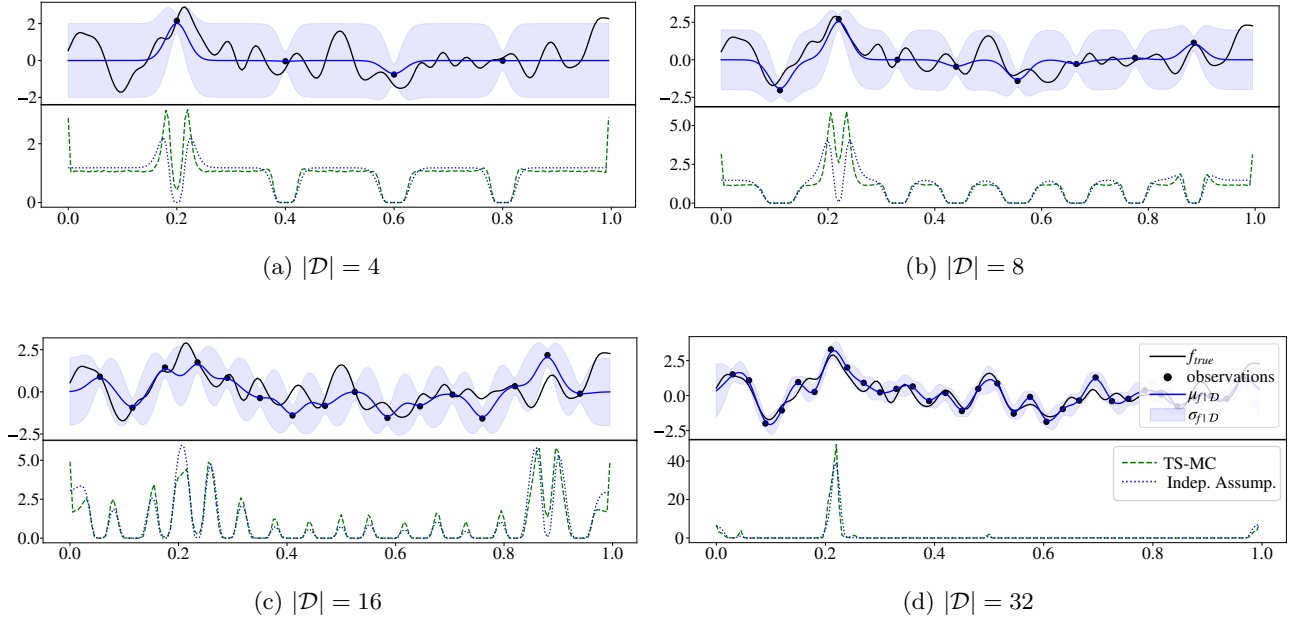


Figure 7: Falsely relying on Assumption 2 does not qualitatively change the estimation of Gaussian PoM, but rather leads to a more conservative prediction, underestimating the maximality of entries near the best observations. This can be understood as a consequence of Slepian’s lemma (Slepian 1962).

applies to all unbiased estimators, not just TS-MC, which under $\Theta(|\mathcal{X}|^2)$ samples scales in $\Theta(|\mathcal{X}|^4)$.

Lemma 1 (Example to illustrate necessity of knowing the full covariance matrix for unbiased estimation). *Consider $F \sim \mathcal{N}(0, I + s(e_i e_j^T + e_j e_i^T))$ in $\mathbb{R}^{|\mathcal{X}|}$, where $(e_i)_j = \mathbb{1}_{i=j}$, $i < j$, and $s \in [0, 1)$. Then it holds that*

$$\lim_{s \rightarrow 1^-} \mathbb{P}[k \in \arg \max_h F_h] = \begin{cases} \frac{1}{|\mathcal{X}| - 1} & k \neq i \wedge k \neq j \\ \frac{1}{2} & \text{otherwise} \end{cases}.$$

As is apparent, knowledge of the position (i, j) of the non-zero (upper) off-diagonal entry is essential for an unbiased prediction of the probability of maximality as $s \rightarrow 1^-$. Without a sparse representation of Σ_F , obtaining the pair (i, j) would require checking all upper diagonal entries in $\Omega(|\mathcal{X}|^2)$. In less synthetic examples sparsity may not be present—hence, in general, an unbiased estimator of *probability of maximality* really requires at least $\Omega(|\mathcal{X}|^2)$ compute. As such, neglecting dependency structure in the covariance matrix is an essential ingredient for obtaining *almost-linear* runtime in the size of the Gaussian reward vector $|\mathcal{X}|$: unless this bias is adopted the runtime would scale at least quadratically in $|\mathcal{X}|$.

C A-LITE

A-LITE is our *accurate* instantiation of LITE, which relies on nested binary search to match quartiles. So, we want to determine m_x and s_x such that for all $x \in \mathcal{X}$ it holds that

$$\mathbb{P}[x \in \tilde{X}^*] = \mathbb{E}[g^x(F_x)] \approx \mathbb{E}[\Phi(\frac{F_x - m_x}{s_x})].$$

Since g^x , by virtue of being a *cumulative distribution function* of a continuous random variable $\max_{z \neq x} \tilde{F}_z$, is continuous and monotonously increasing, we could efficiently find its first and third quartiles q_1 and q_3 to any accuracy using binary search. Then, we could select m_x and s_x such that the Gaussian approximation has matching quartiles. However, with evaluations of g^x costing $\Theta(|\mathcal{X}|)$, repeating the procedure for each $x \in \mathcal{X}$ would lead to a total cost in $\Omega(|\mathcal{X}|^2)$, already exceeding the desired budget.

To get around this conundrum, we approximate in a first step $g(f) := \prod_z \mathbb{P}[F_z \leq f]$ with $\Phi((f - m)/s)$ based on quartile matching, before $\forall x \in \mathcal{X}$ matching quartiles of a separate normal distribution $\Phi((f - m_x)/s_x)$ to $\Phi((f - m)/s) / \mathbb{P}[F_x \leq f] \approx g^x(f) := \prod_{z \neq x} \mathbb{P}[F_z \leq f]$. To ensure stability we operate in log-space.

Step 1: Quartile matching s.t. $\Phi(\frac{f - m}{s}) \approx g(f) := \prod_z \mathbb{P}[F_z \leq f]$.

Step 2: Quartile matching $\forall x \in \mathcal{X}$ s.t. $\Phi(\frac{f - m_x}{s_x}) \approx \Phi(\frac{f - m}{s}) / \mathbb{P}[F_x \leq f] \approx g^x(f)$.

At both stages, once the quartiles q_1 and q_3 are known, the selection of mean m and standard deviation s can be done in closed form, since $\Phi(\frac{q_1 - m}{s}) = 0.25$ and $\Phi(\frac{q_3 - m}{s}) = 0.75$ directly imply the value of m and s through⁸

$$m = \frac{q_3 + q_1}{2} \quad \text{and} \quad s = \frac{q_3 - q_1}{2\Phi^{-1}(0.75)}.$$

However, there is a caveat. $\tilde{g}^x(f) := \Phi((f - m)/s) / \Phi((f - \mu_{F_x})/\sigma_{F_x})$ is not a *cumulative distribution function*, an unfortunate consequence of approximating g by the normal $\Phi((f - m)/s)$. Although it always holds that $m > \mu_{F_x} \forall x \in \mathcal{X}$ ⁹, s can be both larger and smaller than σ_{F_x} . As Figure 8 shows, in the latter case \tilde{g}^x may not even cross the quartiles 0.25 and 0.75. The former case is more benign, admitting a continuous monotonously increasing section with range $(0, 1]$, outside of which \tilde{g}^x always exceeds 1¹⁰. As such, a binary search procedure can still be used to efficiently find its "quartiles", i.e. f such that $\tilde{g}^x(f) = 0.25$ or $\tilde{g}^x(f) = 0.75$.

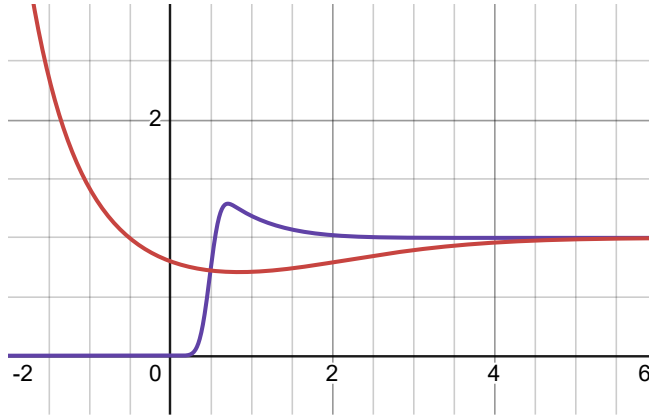


Figure 8: The graph of $\Phi(\frac{f-0.5}{2})/\Phi(\frac{f-1}{1})$ (red line) and $\Phi(\frac{f-0.5}{0.1})/\Phi(\frac{f-1}{1})$ (purple line). Unless $s \leq \sigma_{F_x}$, $\Phi(\frac{f-m}{s})/\Phi(\frac{f-\mu_{F_x}}{\sigma_{F_x}})$ blows up as $f \rightarrow -\infty$ and as a consequence may not even cross 0.25 and 0.75.

So, to ensure termination of quartile matching, we instead match $\Phi(\frac{f-m_x}{s_x})$ to $\Phi(\frac{f-m}{\min(s, \sigma_{F_x})})/\Phi(\frac{f-\mu_{F_x}}{\sigma_{F_x}})$ before predicting $\mathbb{P}[x \in X^*] \approx \Phi((\mu_{F_x} - m_x)/\sqrt{\sigma_{F_x}^2 + s_x^2})$, a method we call A-LITE-II due to its reliance on two consecutive steps of quartile matching.

If $\sigma_{F_x} \ll s$, A-LITE-II can lead to a vast underestimation of *probability of maximality*¹¹. Fortunately, there is an alternative method of approximation. As explained in Figure 9, using g instead of g^x usually does not introduce significant error except for points $x \in \mathcal{X}$ so likely maximising that they dominate the shape of g .

⁸Basic algebra and symmetry of Φ yield $m - q_1 = s\Phi^{-1}(0.75)$ and $q_3 - m = s\Phi^{-1}(0.75)$ from which the result follows swiftly by subtracting and adding the equations.

⁹Given $|\mathcal{X}| > 1$ and $\sigma_{F_x} > 0 \forall x \in \mathcal{X}$, this follows from $\mathbb{P}[\tilde{F}^* \leq q] < \mathbb{P}[F_x \leq q]$ implying $0.75 < \mathbb{P}[F_x \leq q_3]$ and $0.25 < \mathbb{P}[F_x \leq q_1]$. As such, $\mu_{F_x} = (q_3^{F_x} + q_1^{F_x})/2 < (q_3 + q_1)/2 = m$.

¹⁰This was verified for a large variety of m, μ_{F_x}, s , and σ_{F_x} , but not analytically.

¹¹For $m > \mu_{F_x}$, decreasing s always decreases $\mathbb{E}[\Phi((F_x - m)/s)/\Phi((F_x - \mu_{F_x})/\sigma_{F_x})] \approx \mathbb{P}[x \in X^*]$ because $\phi((F_x - \mu_{F_x})/\sigma_{F_x})/\sigma_{F_x} \cdot 1/\Phi((F_x - \mu_{F_x})/\sigma_{F_x})$ is dominant to the left of $\mu_{F_x} < m$, which is weighted less in the integral as $s \rightarrow 0$.

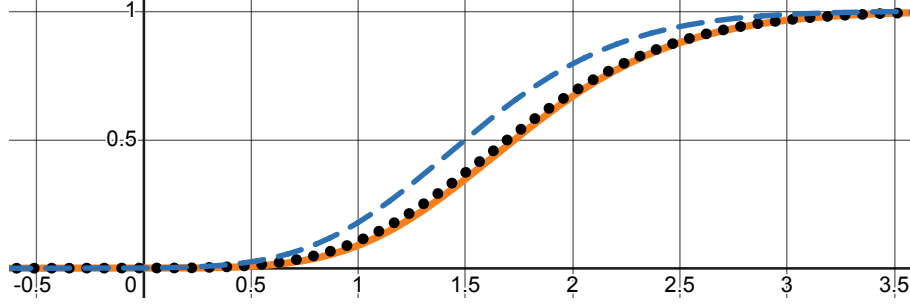


Figure 9: Illustration of the approximation error of using $g(f) = \Phi(f)^{10}\Phi(f-1)$ (orange solid line) instead of $g^{x_1} = \Phi(f)^{10}$ (blue dashed) and $g^{x_2} = \Phi(f)^9\Phi(f-1)$ (black dotted). We underestimate g^x for the likely maximiser x_1 , leading to an overly conservative (under)estimation of *probability of maximality*. Contrastingly, g^{x_2} is well approximated by g for the unlikely maximiser x^2 .

A-LITE-I exploits this observation by only relying on the initial quartile matching, where we approximated $g(f) \approx \Phi((f-m)/s)$. That is, it directly predicts PoM as $\mathbb{P}[x \in X^*] \approx \Phi((\mu_{F_x} - m)/\sqrt{\sigma_{F_x}^2 + s^2})$. As in the case of A-LITE-II, here the approximation of using g instead of g^x biases the *probabilities of maximality* towards 0.

For the most accurate estimation, we combine A-LITE-I and A-LITE-II by taking the element-wise maximum of their respective predicted PoMs, i.e., $\mathbb{P}[x \in X^*] \approx \max(\Phi((\mu_{F_x} - m_x)/\sqrt{\sigma_{F_x}^2 + s_x^2}), \Phi((\mu_{F_x} - m)/\sqrt{\sigma_{F_x}^2 + s^2}))$. Whereas A-LITE-I is targeted at unlikely maximizers with $\mu_{F_x} \ll m$, A-LITE-II is built for the opposite case where $\mu_{F_x} \approx m$. Together, they solve both cases well. Taking the maximum is justified since both A-LITE-I and A-LITE-II involve approximations that lower their predicted *probabilities of maximality*. As a final step, we add a global normalization to 1, once again relying on Assumption 1. We remark that this final step typically does not significantly affect the estimation accuracy since the estimated PoM is already almost normalized.

The complete procedure for estimation with A-LITE is described in Algorithm 3, along with its sub-procedures in Algorithms 4-7. The logarithmic search windows for the two stages of quartile matching are selected according to the results in Proposition 6 and Proposition 7 (plugging in $b \in \{0.25, 0.75\}$), while additionally taking into account that for the second stage we do not have access to the ground-truth quartiles of g and hence its statistics m and s (we only have upper and lower bounds from the first stage). The algorithm runs in $\Theta(\sum_{l=1}^{\log_2 k} 2^l |\mathcal{X}|) = \Theta(k|\mathcal{X}|)$ where k denotes the final depth that is needed for uniform convergence of the lower and upper bounds on p_x .

Proposition 6 (Logarithmic \tilde{F}^* -quantile search). *Let $b \in [0.25, 1)$ and $\tilde{F} \sim \mathcal{N}(\mu_F, \text{diag}(\sigma_{F_1}^2, \dots, \sigma_{F_{|\mathcal{X}|}}^2))$ with $|\mathcal{X}| > 1$. Assume $\exists x : \sigma_{F_x} > 0$. Define $g(f) := \Pi_z \mathbb{P}[\tilde{F}_z \leq f]$, which is continuous and strictly monotonously increasing. Then $\exists \bar{f} \in \mathbb{R}$ s.t. $g(\bar{f}) = b$. It can be found efficiently using logarithmic search with search window*

$$\mu_F^{\min} + \sigma_F^{\min} \Phi^{-1}(b^{1/|\mathcal{X}|}) \leq \bar{f} \leq \mu_F^{\max} + \sigma_F^{\max} \Phi^{-1}(b^{1/|\mathcal{X}|}).$$

The size of the search window is bounded by $\mu_F^{\max} - \mu_F^{\min} + \Phi^{-1}(b^{1/|\mathcal{X}|})\sigma_F^{\max} \in \Theta(\sqrt{\log |\mathcal{X}|})$. Run k steps of binary search resulting in best approximant \bar{f}^k . Then

$$|\bar{f} - \bar{f}^k| \leq \frac{\mu_F^{\max} - \mu_F^{\min} + \Phi^{-1}(b^{1/|\mathcal{X}|})\sigma_F^{\max}}{2^{k+1}},$$

i.e. we obtain exponential convergence with linear order. So, to ensure $|\bar{f} - \bar{f}^k| \leq \nu$, $k = \log_2((\mu_F^{\max} - \mu_F^{\min} + \Phi^{-1}(b^{1/|\mathcal{X}|})\sigma_F^{\max})/(2\nu)) \in \Theta(\log(\log(|\mathcal{X}|)/\nu))$ steps suffice.

Proposition 7 (Logarithmic $\tilde{F}^{*\setminus x}$ -quantile search). *Let $b \in (0, 1)$, $m, \mu_{F_x} \in \mathbb{R}$, and $s, \sigma_{F_x} \in \mathbb{R}_+$ such that $m > \mu_{F_x}$ and $s \leq \sigma_{F_x}$. Define $\tilde{g}^x(f) := \Phi((f - m)/s)/\Phi((f - \mu_{F_x})/\sigma_{F_x})$, which is continuous and strictly monotonously increasing on a section with range $(0, 1]$ and exceeds 1 elsewhere. Then $\exists! \bar{f}_x \in \mathbb{R}$ s.t. $\tilde{g}^x(\bar{f}_x) = b$. It can be found efficiently using logarithmic search with search window*

$$\min(\mu_{F_x} - \sqrt{2}\sigma_{F_x}, \max(\frac{m + \mu_{F_x}}{2} - \frac{\sigma_{F_x}^2 \ln(2/b)}{m - \mu_{F_x}}, m - \sqrt{\frac{2 \ln(2/b)}{1 - s^2/\sigma_{F_x}^2}}s)) \leq \bar{f}_x \leq m + \Phi^{-1}(b) \cdot s$$

The size Δ of the search window is independent of $|\mathcal{X}|$, i.e. $\Delta \in \Theta(1)$. Run k steps of binary search resulting in best approximant \bar{f}_x^k . Then $|\bar{f}_x - \bar{f}_x^k| \leq \frac{\Delta}{2^{k+1}}$, i.e., we obtain exponential convergence with linear order. So, to ensure $|\bar{f}_x - \bar{f}_x^k| \leq \nu$, $k = \log_2(\Delta/(2\nu)) \in \Theta(\log(1/\nu))$ steps suffice.

Algorithm 3 A-LITE

Require: $\mu_F, \sigma_F, \epsilon$

$max_error \leftarrow \epsilon$

$d \leftarrow 1$

while $max_error \geq \epsilon$ **do**

$d \leftarrow d \cdot 2$

$(m^{up}, m^{low}, s^{up}, s^{low}) \leftarrow \text{A-LITE-I-S}(d, \mu_F, \sigma_F)$

 ▷ C: $\Theta(d|\mathcal{X}|)$, M: $\Theta(1)$

$(m_x^{up}, m_x^{low}, s_x^{up}, s_x^{low})_{x \in \mathcal{X}} \leftarrow \text{A-LITE-II-S}(d, m^{up}, m^{low}, s^{up}, s^{low}, \mu_F, \sigma_F)$

 ▷ C: $\Theta(d|\mathcal{X}|)$, M: $\Theta(|\mathcal{X}|)$

if $s^{low} < 0$ or $\min_x s_x^{low} < 0$ **then**

 jump to the top of this while-loop

end if

$$(p_x^{I,up})_{x \in \mathcal{X}} \leftarrow \left(\Phi\left(\max\left(\frac{\mu_{F_x} - m^{low}}{\sqrt{\sigma_{F_x}^2 + (s^{low})^2}}, \frac{\mu_{F_x} - m^{low}}{\sqrt{\sigma_{F_x}^2 + (s^{up})^2}}\right)\right) \right)_{x \in \mathcal{X}}$$

$$(p_x^{I,low})_{x \in \mathcal{X}} \leftarrow \left(\Phi\left(\min\left(\frac{\mu_{F_x} - m^{up}}{\sqrt{\sigma_{F_x}^2 + (s^{low})^2}}, \frac{\mu_{F_x} - m^{up}}{\sqrt{\sigma_{F_x}^2 + (s^{up})^2}}\right)\right) \right)_{x \in \mathcal{X}}$$

$$(p_x^{II,up})_{x \in \mathcal{X}} \leftarrow \left(\Phi\left(\max\left(\frac{\mu_{F_x} - m_x^{low}}{\sqrt{\sigma_{F_x}^2 + (s_x^{low})^2}}, \frac{\mu_{F_x} - m_x^{low}}{\sqrt{\sigma_{F_x}^2 + (s_x^{up})^2}}\right)\right) \right)_{x \in \mathcal{X}}$$

$$(p_x^{II,low})_{x \in \mathcal{X}} \leftarrow \left(\Phi\left(\min\left(\frac{\mu_{F_x} - m_x^{up}}{\sqrt{\sigma_{F_x}^2 + (s_x^{low})^2}}, \frac{\mu_{F_x} - m_x^{up}}{\sqrt{\sigma_{F_x}^2 + (s_x^{up})^2}}\right)\right) \right)_{x \in \mathcal{X}}$$

$$(p_x^{up}, p_x^{low})_{x \in \mathcal{X}} \leftarrow (\max(p_x^{I,up}, p_x^{II,up}), \max(p_x^{I,low}, p_x^{II,low}))_{x \in \mathcal{X}}$$

$$max_error \leftarrow \max_{x \in \mathcal{X}} p_x^{up} - p_x^{low}$$

end while

$$(p_x)_{x \in \mathcal{X}} \leftarrow ((p_x^{up} + p_x^{low})/2)_{x \in \mathcal{X}}$$

return $(p_x / \sum_{z \in \mathcal{X}} p_z)_{x \in \mathcal{X}}$

The shared final depth k of the nested binary search procedures is actually quite small. Indeed, as explained in Proposition 6, to ensure the quartiles q_1 and q_3 of g are determined up to accuracy ν it suffices to run $k \in \Theta(\log(\log(|\mathcal{X}|)/\nu))$ steps. This describes the efficiency of A-LITE-I. Similarly, according to Proposition 7, the second stage of binary search produces ν -accurate quartiles in just $k = \log_2(\Delta/(2\nu)) \in \Theta(\log(1/\nu))$ steps. Stacking the two will result in ν -accurate quartiles of $\Phi((f - m)/s)/\Phi((f - \mu_{F_x})/\sigma_{F_x})$ at a shared depth k scaling in $\Theta(\log(\log(|\mathcal{X}|)/\nu))$. This describes the efficiency of A-LITE-II.

As a final detail, we do not seek ν -accurate quartiles, but rather ϵ -converged predictions of *probability of maximality*. The error propagation from quartiles to predictions is provided in Lemma 2. It presents the required ν such that A-LITE-I is ϵ accurate to the analytical A-LITE-I, which is based on the actual quartiles ($k \rightarrow \infty$). According to the lemma it suffices to take $\nu = \epsilon \cdot \bar{s}^2 / (\max_x |\mu_{F_x} - \bar{m}| + \bar{s})$, where \bar{m} and \bar{s} describe the mean and standard deviation implied by the true quartiles. By using m_x, \bar{m}_x and s_x, \bar{s}_x instead of m, \bar{m} and s, \bar{s} , Lemma 2

applies directly to A-LITE-II as well. Due to the linear propagation of error from ϵ to ν predicted by Lemma 2, we obtain a total runtime complexity in $\Theta(|\mathcal{X}| \log(\log(|\mathcal{X}|)/\epsilon))$ and memory consumption $\Theta(|\mathcal{X}|)$. In terms of asymptotic efficiency we are on par with F-LITE, being essentially independent of ν and linear in $|\mathcal{X}|$. However, in practice the constant factor is quite a bit worse, as can be observed in Figure 2.

Lemma 2 (A-LITE error propagation). *Let $\mu_F \in \mathbb{R}^{|\mathcal{X}|}$, $\sigma_F \in \mathbb{R}_+^{|\mathcal{X}|}$, and $\epsilon > 0$. Let $\bar{q}_1, \bar{q}_3 \in \mathbb{R}$ and $q_1, q_3 \in \mathbb{R}$ be pairs of quartiles such that $|\bar{q}_1 - q_1| \leq \nu$ and $|\bar{q}_3 - q_3| \leq \nu$ for $\nu = \epsilon \cdot \bar{s}^2 / (\max_x |\mu_{F_x} - \bar{m}| + \bar{s})$. Then with $m = (q_3 + q_1)/2$ and $\bar{m} = (\bar{q}_3 + \bar{q}_1)/2$ the means and $s = (q_3 - q_1)/(2\Phi^{-1}(0.75))$ and $\bar{s} = (\bar{q}_3 - \bar{q}_1)/(2\Phi^{-1}(0.75))$ the standard deviations of quartile-matched Gaussians, it holds that for all $x \in \mathcal{X}$*

$$\left| \Phi\left(\frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + s^2}}\right) - \Phi\left(\frac{\mu_{F_x} - \bar{m}}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}}\right) \right| \leq \epsilon + \mathcal{O}(\epsilon^2). \quad (8)$$

Algorithm 4 A-LITE-I-S(earch)

Require: d, μ_F, σ_F
 $(q_1^{low}, q_1^{up}, q_3^{low}, q_3^{up}) \leftarrow \text{A-LITE-I-SW}(\mu_F, \sigma_F)$ \triangleright C: $\Theta(|\mathcal{X}|)$, M: $\Theta(1)$
for $1, \dots, d$ **do**
 $q_1 \leftarrow (q_1^{up} + q_1^{low})/2$
 $q_3 \leftarrow (q_3^{up} + q_3^{low})/2$
 $g_1 = \prod_z \Phi\left(\frac{q_1 - \mu_{F_z}}{\sigma_{F_z}}\right)$ \triangleright C: $\Theta(|\mathcal{X}|)$, M: $\Theta(1)$
 $g_3 = \prod_z \Phi\left(\frac{q_3 - \mu_{F_z}}{\sigma_{F_z}}\right)$ \triangleright C: $\Theta(|\mathcal{X}|)$, M: $\Theta(1)$
 $(q_1^{up}, q_1^{low}) \leftarrow \begin{cases} (q_1, q_1^{low}) & g_1 > 0.25 \\ (q_1^{up}, q_1) & \text{otherwise} \end{cases}$
 $(q_3^{up}, q_3^{low}) \leftarrow \begin{cases} (q_3, q_3^{low}) & g_3 > 0.75 \\ (q_3^{up}, q_3) & \text{otherwise} \end{cases}$
end for
 $(m^{up}, m^{low}) \leftarrow \left(\frac{q_3^{up} + q_1^{up}}{2}, \frac{q_3^{low} + q_1^{low}}{2} \right)$
 $(s^{up}, s^{low}) \leftarrow \left(\frac{q_3^{up} - q_1^{low}}{2\Phi^{-1}(0.75)}, \frac{q_3^{low} - q_1^{up}}{2\Phi^{-1}(0.75)} \right)$
return $(m^{up}, m^{low}, s^{up}, s^{low})$

Algorithm 5 A-LITE-I-S(earch)W(indow)

Require: μ_F, σ_F
 $q_1^{low} \leftarrow \mu_F^{min} + \sigma_F^{min} \Phi^{-1}(0.25^{1/|\mathcal{X}|})$
 $q_1^{up} \leftarrow \mu_F^{max} + \sigma_F^{max} \Phi^{-1}(0.25^{1/|\mathcal{X}|})$
 $q_3^{low} \leftarrow \mu_F^{min} + \sigma_F^{min} \Phi^{-1}(0.75^{1/|\mathcal{X}|})$
 $q_3^{up} \leftarrow \mu_F^{max} + \sigma_F^{max} \Phi^{-1}(0.75^{1/|\mathcal{X}|})$
return $(q_1^{low}, q_1^{up}, q_3^{low}, q_3^{up})$

Algorithm 6 A-LITE-II-S(earch)

Require: $d, m^{up}, m^{low}, s^{up}, s^{low}, \mu_F, \sigma_F$

$$(\tilde{m}^{up}, \tilde{m}^{low}) \leftarrow (\max(m^{up}, \mu_F^{max}), \max(m^{low}, \mu_F^{max}))$$

$$(\tilde{s}_x^{up}, \tilde{s}_x^{low})_{x \in \mathcal{X}} \leftarrow (\min(s_x^{up}, \sigma_{F_x}), \min(s_x^{low}, \sigma_{F_x}))_{x \in \mathcal{X}}$$

$$(q_{x,1}^{low}, q_{x,1}^{up}, q_{x,3}^{low}, q_{x,3}^{up})_{x \in \mathcal{X}} \leftarrow \text{A-LITE-II-SW}(\tilde{m}^{up}, \tilde{m}^{low}, \tilde{s}^{up}, \tilde{s}^{low}, \mu_F, \sigma_F)$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$
for $1, \dots, d$ **do**

$$(q_{x,1})_{x \in \mathcal{X}} \leftarrow ((q_{x,1}^{up} + q_{x,1}^{low})/2)_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(q_{x,3})_{x \in \mathcal{X}} \leftarrow ((q_{x,3}^{up} + q_{x,3}^{low})/2)_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(g_{x,1}^{up})_{x \in \mathcal{X}} \leftarrow (\max(\Phi(\frac{q_{x,1} - \tilde{m}^{low}}{\tilde{s}_x^{up}})/\Phi(\frac{q_{x,1} - \mu_{F_x}}{\sigma_{F_x}}), \Phi(\frac{q_{x,1} - \tilde{m}^{low}}{\tilde{s}_x^{low}})/\Phi(\frac{q_{x,1} - \mu_{F_x}}{\sigma_{F_x}}))_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(g_{x,1}^{low})_{x \in \mathcal{X}} \leftarrow (\min(\Phi(\frac{q_{x,1} - \tilde{m}^{up}}{\tilde{s}_x^{up}})/\Phi(\frac{q_{x,1} - \mu_{F_x}}{\sigma_{F_x}}), \Phi(\frac{q_{x,1} - \tilde{m}^{up}}{\tilde{s}_x^{low}})/\Phi(\frac{q_{x,1} - \mu_{F_x}}{\sigma_{F_x}}))_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(g_{x,3}^{up})_{x \in \mathcal{X}} \leftarrow (\max(\Phi(\frac{q_{x,3} - \tilde{m}^{low}}{\tilde{s}_x^{up}})/\Phi(\frac{q_{x,3} - \mu_{F_x}}{\sigma_{F_x}}), \Phi(\frac{q_{x,3} - \tilde{m}^{low}}{\tilde{s}_x^{low}})/\Phi(\frac{q_{x,3} - \mu_{F_x}}{\sigma_{F_x}}))_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(g_{x,3}^{low})_{x \in \mathcal{X}} \leftarrow (\min(\Phi(\frac{q_{x,3} - \tilde{m}^{up}}{\tilde{s}_x^{up}})/\Phi(\frac{q_{x,3} - \mu_{F_x}}{\sigma_{F_x}}), \Phi(\frac{q_{x,3} - \tilde{m}^{up}}{\tilde{s}_x^{low}})/\Phi(\frac{q_{x,3} - \mu_{F_x}}{\sigma_{F_x}}))_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(q_{x,1}^{up}, q_{x,1}^{low})_{x \in \mathcal{X}} \leftarrow \left(\begin{cases} (q_{x,1}, q_{x,1}^{low}) & g_{x,1}^{low} \geq 0.25 \\ (q_{x,1}^{up}, q_{x,1}) & g_{x,1}^{up} \leq 0.25 \\ (q_{x,1}^{up}, q_{x,1}^{low}) & \text{otherwise} \end{cases} \right)_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$

$$(q_{x,3}^{up}, q_{x,3}^{low})_{x \in \mathcal{X}} \leftarrow \left(\begin{cases} (q_{x,3}, q_{x,3}^{low}) & g_{x,3}^{low} \geq 0.75 \\ (q_{x,3}^{up}, q_{x,3}) & g_{x,3}^{up} \leq 0.75 \\ (q_{x,3}^{up}, q_{x,3}^{low}) & \text{otherwise} \end{cases} \right)_{x \in \mathcal{X}}$$

 $\triangleright \text{C: } \Theta(|\mathcal{X}|), \text{M: } \Theta(|\mathcal{X}|)$
end for

$$(m_x^{up}, m_x^{low})_{x \in \mathcal{X}} \leftarrow \left(\frac{q_{x,3}^{up} + q_{x,1}^{up}}{2}, \frac{q_{x,3}^{low} + q_{x,1}^{low}}{2} \right)_{x \in \mathcal{X}}$$

$$(s_x^{up}, s_x^{low})_{x \in \mathcal{X}} \leftarrow \left(\frac{q_{x,3}^{up} - q_{x,1}^{low}}{2\Phi^{-1}(0.75)}, \frac{q_{x,3}^{low} - q_{x,1}^{up}}{2\Phi^{-1}(0.75)} \right)_{x \in \mathcal{X}}$$

return $(m_x^{up}, m_x^{low}, s_x^{up}, s_x^{low})_{x \in \mathcal{X}}$
Algorithm 7 A-LITE-II-S(earch)W(indow)

Require: $\tilde{m}^{up}, \tilde{m}^{low}, \tilde{s}^{up}, \tilde{s}^{low}, \mu_F, \sigma_F$

$$(q_{x,1}^{low})_{x \in \mathcal{X}} \leftarrow (\min(\mu_{F_x} - \sqrt{2}\sigma_{F_x}, \max(\frac{\tilde{m}^{low} + \mu_{F_x}}{2} - \frac{\sigma_{F_x}^2 \ln(2/0.25)}{\tilde{m}^{low} - \mu_{F_x}}, \tilde{m}^{low} - \sqrt{\frac{2 \ln(2/0.25)}{1 - (\tilde{s}_x^{up}/\sigma_{F_x})^2} \tilde{s}_x^{up}}))_{x \in \mathcal{X}}$$

$$(q_{x,1}^{up})_{x \in \mathcal{X}} \leftarrow \tilde{m}^{up} + \Phi^{-1}(0.25)\tilde{s}_x^{low}$$

$$(q_{x,3}^{low})_{x \in \mathcal{X}} \leftarrow (\min(\mu_{F_x} - \sqrt{2}\sigma_{F_x}, \max(\frac{\tilde{m}^{low} + \mu_{F_x}}{2} - \frac{\sigma_{F_x}^2 \ln(2/0.75)}{\tilde{m}^{low} - \mu_{F_x}}, \tilde{m}^{low} - \sqrt{\frac{2 \ln(2/0.75)}{1 - (\tilde{s}_x^{up}/\sigma_{F_x})^2} \tilde{s}_x^{up}}))_{x \in \mathcal{X}}$$

$$(q_{x,3}^{up})_{x \in \mathcal{X}} \leftarrow \tilde{m}^{up} + \Phi^{-1}(0.75)\tilde{s}_x^{up}$$

return $(q_1^{low}, q_1^{up}, q_3^{low}, q_3^{up})$

D EXPERIMENTAL DETAILS

D.1 Figure 1

As a realistic posterior distribution over a large set of candidates, we use the posterior distribution of the final iteration of our quadcopter experiment (see Appendix D.6 for details). This posterior distribution over a 4-dimensional space of feedback control parameters captures our current estimate of the quadcopters’ performance under any of those feedback parameters. Our goal is to select a small set of feedback parameters for final testing that contain the best-performing feedback parameters with high probability. Figure 1 shows that our PoM estimator outperforms previous methods for recall-optimal candidate selection and Figure 10 quantifies the impact of using a faithful PoM estimator over a less-faithful one for this task. We report on expected recall and its standard error.

	Area Under Curve
TS-MC	$83.7 \pm 3.4 \%$
INDEP. ASSUM.	$83.2 \pm 3.5 \%$
A-LITE	$83.3 \pm 3.5 \%$
F-LITE	$82.9 \pm 3.4 \%$
EST	$82.3 \pm 3.4 \%$
VAPOR	$81.4 \pm 3.3 \%$
TS	$75.0 \pm 2.8 \%$
MEANS	$67.5 \pm 4.1 \%$

Figure 10: Faithful estimators to PoM perform marginally better than less faithful ones. As such, the computational efficiency improvements achieved in this work dominate the drop in sample efficiency compared to TS-MC. In contrast, the performance drop to heuristics such as TS and MEANS is much more pronounced.

D.2 Figure 5

We sample the objective function f_{true} from a centered Gaussian process on the line segment $[0,1]$ with a squared exponential kernel (length scale 0.02, amplitude 1.0). We assume an observation model with independent homoscedastic centered additive Gaussian noise where $\sigma_{noise} = 0.2$. We run calibrated Entropy Search for 50 steps after evenly discretizing the domain to $|\mathcal{X}| = 250$ points. The experiment is repeated 10 times and we report on the mean and standard error of the entropy of PoM, which is the objective that Entropy Search seeks to minimize. We use five samples to condition on hypothetical observations. For each conditioning, the PoM entropy reduction is estimated either with F-LITE for convergence parameter $\epsilon = 1/(10|\mathcal{X}|)$, or using TS-MC. Running TS-MC to convergence would lead to an exploding runtime, so we always use the fixed budget of 4 samples. Note that we cannot decrease the cost much further, since for a single Monte Carlo sample the entropy would always degenerate to 0. Even so, on an NVIDIA TITAN RTX GPU a full run of Entropy Search using LITE takes just 15.4 seconds, whereas using the TS-MC backend, it takes 8.2 minutes. This difference becomes much more pronounced as the size of the Gaussian reward vector is increased.

D.3 Estimating the State of Large-Scale Bayesian Optimization

To demonstrate that LITE can truly be scaled to large-scale industrial settings, we run uncalibrated Bayesian optimization with a linear kernel for 800 steps using both the GP-upper confidence bound (Srinivas et al. 2010) (UCB) and the expected improvement (EI) acquisition function. Here, the ground-truth objective function is described by a (random) hyperplane in 1’000 dimensions, sampled at 10’000 points on the unit-sphere. A comparison between LITE and a ground-truth surrogate for PoM such as TS-MC is not possible here: even estimation under the INDEPENDENCE ASSUMPTION would require 500 hours (21 days) on an NVIDIA A100 GPU to compute PoMs across the BO-path for a single seed. In contrast, LITE only takes a few seconds (about 30 seconds), i.e., it is about 60’000 times faster. Our results confirm that LITE can be used to interpret the state of convergence of Bayesian optimization and to compare competing optimization schemes in terms of their information-theoretic performance, particularly in large-scale settings where standard approaches fail.

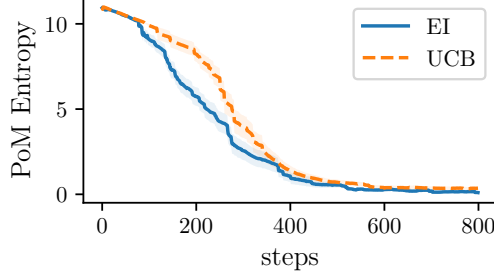


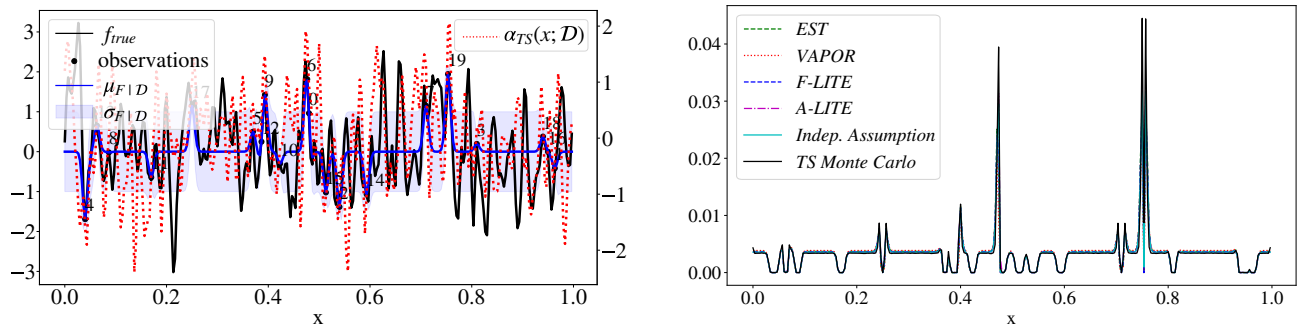
Figure 11: PoM entropy estimation with LITE allows tracking the state of large-scale Bayesian optimization. On an NVIDIA A100 GPU, LITE reduces time of computation from more than 21 days to 30 seconds.

D.4 Figure 2

We densely discretise the drop-wave function $f_{true}(x_1, x_2) := (1 + \cos(12\sqrt{x_1^2 + x_2^2})) / ((x_1^2 + x_2^2)/2 + 2)$ on the rectangle $[-5, 4]^2$ using a grid with $300^2 = 90'000$ nodes. To obtain different domain sizes, we subsample the grid uniformly at random (without repetition). Next, we run Bayesian optimisation using the *expected improvement* (over best observation) acquisition function. The posterior is derived based on a Gaussian process prior fitted at each step with marginal likelihood maximisation (we fit the length scale and amplitude of a Matern 5/2 kernel, the constant mean function, and σ_{noise}). To jump start the kernel selection, we make 50 random observations prior to starting Bayesian optimisation. We assume additive centred Gaussian noise with $\sigma_{noise} = 0.1$. We report on the mean and standard deviation of the runtime averaged across 100 steps of Bayesian optimisation for 5 seeds. All estimators use $\alpha = 1$. We cancel runs exceeding a computational budget of 6 hours (216 seconds per step), which is why TS-MC and EST do not have values at all time steps.

D.5 Figure 3b

f_{true} is sampled from a centred Gaussian process \mathcal{GP} with squared-exponential kernel (length scale 0.005, amplitude 1.0) on the interval $[0, 1]$ discretised with $|\mathcal{X}| = 300$ points. The prior belief over f_{true} coincides with \mathcal{GP} . A Bayesian optimisation scheme according to Thompson sampling is run for 200 steps with observations $Y_x = f_{true}(x) + \varepsilon$ for i.i.d. $\varepsilon \sim \mathcal{N}(0, 0.1^2)$. All estimators are ensured to converge to within $\epsilon = 1/(10 \cdot |\mathcal{X}|)$ of their analytical expressions. We report on the mean and standard error of TV-distance to the ground-truth PoM (estimated using TS-MC) based on 50 different seeds of optimisation. Figure 12 illustrates the setup along with a possible set of estimated PoMs.



(a) Example f_{true} with associated $p(f|D)$ and $\alpha_{TS}(x; D)$ after 20 queries to f_{true} .

(b) $\mathbb{P}[x \in X^*|D]$ according to different PoM estimators after 20 queries to example f_{true}

Figure 12: Illustration of the setup for Figure 3b.

D.6 Figure 3c

Based on a simulator of the dynamics of a quadcopter, we are able to measure how close the quadcopter got to stabilisation at a target position when starting at a separate fixed location. We use the same experimental setup as (Hübötter et al. 2024), with the quadcopter simulation of (Chandra 2023). The quadcopter is steered through a controller with 8 degrees of freedom, which describe the unknown perturbation to the system. The task is to use Bayesian optimisation to identify the disturbance parameters through feedback from the simulator (with additive centred Gaussian noise at a standard deviation of $\sigma_{noise} = 0.1$). The unknown perturbation is sampled element-wise according to a χ^2 -distribution, resulting in a distribution over f_{true} . Due to 4 degrees of freedom removed using a heuristic, Bayesian optimisation must be performed in 4-dimensional space. To obtain a tractably finite domain, we sample 400 discrete points uniformly at random in the hypercube $[0, 20]^4$. We run Bayesian optimisation for 175 steps using the *expected improvement* (over best observation) acquisition function. The posterior is derived based on a Gaussian process prior fitted at each step with marginal likelihood maximisation (we fit the length scale and amplitude of a Matern 5/2 kernel, the constant mean function, and σ_{noise}). To jump start the kernel selection, we make 25 random observations prior to starting Bayesian optimisation. We also leave out the first 5 steps of Bayesian optimisation (warmup steps), during which the estimation of the parameters of the Gaussian process prior are highly volatile. All reported PoM estimators are run to ϵ -convergence for $\epsilon = 1/|\mathcal{X}|$. The ground-truth is estimated using TS-MC with $\epsilon = 1/(10 \cdot |\mathcal{X}|)$.

D.7 Figure 4

We coarsely discretise the drop-wave function $f_{true}(x_1, x_2) := (1 + \cos(12\sqrt{x_1^2 + x_2^2})) / ((x_1^2 + x_2^2)/2 + 2)$ on the rectangle $[-2.5, 2]^2$ using a grid with $25^2 = 625$ nodes. We run Bayesian optimisation for 30 steps using the *expected improvement* (over best observation) acquisition function. The posterior is derived based on a Gaussian process prior fitted at each step with marginal likelihood maximisation (we fit the length scale and amplitude of a Matern 5/2 kernel, the constant mean function, and σ_{noise}). To jump start the kernel selection, we make 10 random observations prior to starting Bayesian optimisation. We assume additive centred Gaussian noise with $\sigma_{noise} = 0.1$. Figure 13 shows the posteriors and probabilities of maximality belonging to step 10 of Bayesian optimisation at seed 0.

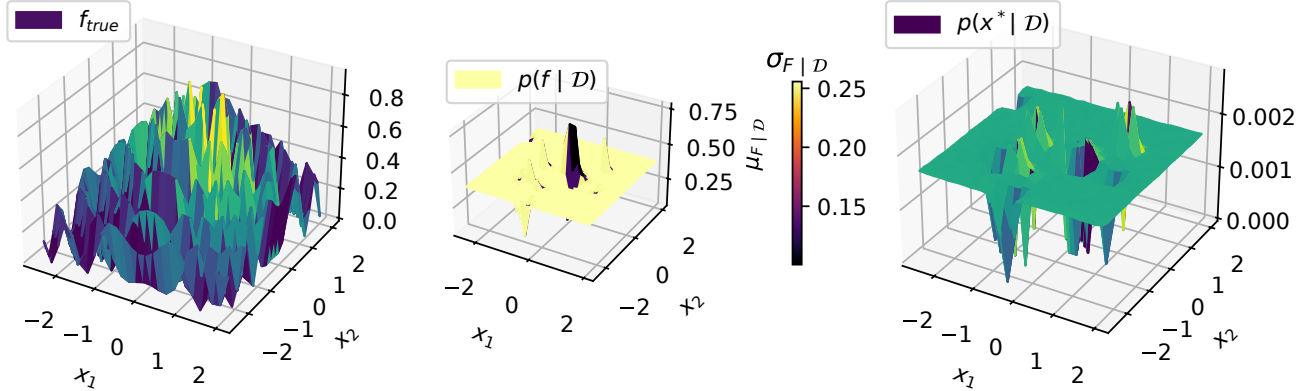


Figure 13: Problem setting for the accuracy/runtime operating points plot in Figure 4

We report on the mean and standard error of the runtime and TV-distance averaged across steps 11 – 30 of Bayesian optimisation for 5 different seeds (the first 10 warm-up steps are removed to obtain a more decisive picture). To evaluate the estimators under different convergence requirements, $\alpha = 1/(\epsilon \cdot |\mathcal{X}|)$ is swept through $\{0.01, 0.03, 0.1, 0.3, 1.0, 3.0, 10.0\}$. The ground-truth is estimated using TS-MC with $\alpha = 10.0$, which runs in 915 seconds (per optimisation step) on an NVIDIA TITAN RTX GPU.

D.8 Total Variation Distance

The total variation distance d_{TV} is the central fidelity metric in our experiments. Formally, it is defined as

Definition 1 (Total variation distance). *Let P, Q be probability distributions over a measurable space (Ω, \mathcal{E}) . Then the total variation distance between P and Q is defined as*

$$d_{TV}(P, Q) := \sup_{A \in \mathcal{E}} |P(A) - Q(A)|.$$

Alternatively, it corresponds to the metric derived from the L^1 norm over the space of probability mass functions:

Proposition 8 (Total variation distance as L^1 -norm induced metric). *Let P, Q be probability measures over a measurable space (Ω, \mathcal{E}) and μ a σ -finite measure over (Ω, \mathcal{E}) s.t. $P, Q \ll \mu$. Then d_{TV} can be characterised by*

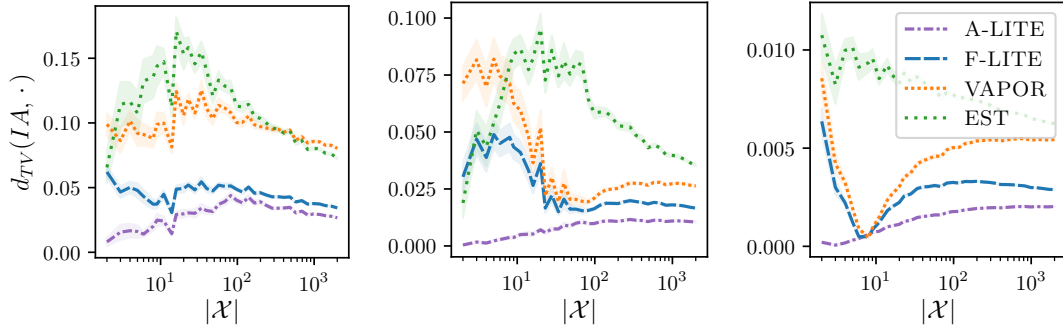
$$d_{TV}(P, Q) = \frac{1}{2} \left\| \frac{dP}{d\mu} - \frac{dQ}{d\mu} \right\|_{L^1(\Omega, \mathcal{E}, \mu)},$$

where $\frac{dP}{d\mu}$ and $\frac{dQ}{d\mu}$ denote Radon-Nykodym derivatives of P and Q with respect to the base measure μ . Important cases are when μ is the Lebesgue measure or when it is the counting measure leading to a formulation for probability density functions and probability mass functions, respectively.

E ADDITIONAL EXPERIMENTS

E.1 Alternative Synthetic Experiments

To add to the results presented in Figure 3a, we sample μ_F and σ_F according to other distributions. Figure 14 reports the TV-distance between the estimated PoM and a ground-truth according to the INDEPENDENCE ASSUMPTION. As in Figure 3a, μ_{F_x} and σ_{F_x} are sampled i.i.d. across $x \in \mathcal{X}$. All estimators are ensured to converge to within $\epsilon = 1/(200 \cdot |\mathcal{X}|)$. The experiments are repeated across 20 seeds to report the mean and standard error. Notice how A-LITE and F-LITE consistently outperform EST and VAPOR across a variety of μ_F and σ_F .



(a) $\mu_{F_x} \sim \mathcal{U}(0, 5)$, $\sigma_{F_x} \sim \mathcal{U}(\frac{1}{2}, 2)$ (b) $\mu_{F_x} \sim \mathcal{U}(0, 5)$, $\sigma_{F_x} = \frac{1}{2}$ (c) $\mu_{F_x} \sim \mathcal{U}(0, \frac{1}{10})$, $\sigma_{F_x} = \frac{1}{2}$

Figure 14: TV-distance under alternative synthetic posteriors. As in the main text, LITE significantly outperforms competing methods from the literature.

E.2 f_{true} Sampled from Alternative Gaussian Process

Instead of the one-dimensional Gaussian process with squared exponential kernel that was prominently featured in Figures 3b with a detailed description in Section D.5, we may instead use a two-dimensional Gaussian process with exponential kernel. Accordingly, we sample the test function f_{true} from a centred Gaussian process \mathcal{GP} with exponential kernel (length scale 0.1, amplitude 1.0) on $[0, 1]^2$ discretised to $|\mathcal{X}| = 400$ points. To ensure calibrated Bayesian optimisation, the prior belief over f_{true} coincides with \mathcal{GP} . We run Bayesian optimisation based on Thompson sampling, where the observations are generated as $Y_x = f_{true}(x) + \epsilon$ for i.i.d. $\epsilon \sim \mathcal{N}(0, 0.1^2)$. Figure 15 illustrates the setup.

Figure 16 reports on the accuracy of the PoM estimators during Bayesian optimisation. We ensure convergence of all estimators to within $\epsilon = 1/(10 \cdot |\mathcal{X}|)$ of their analytical expressions, including TS-MC, which is used

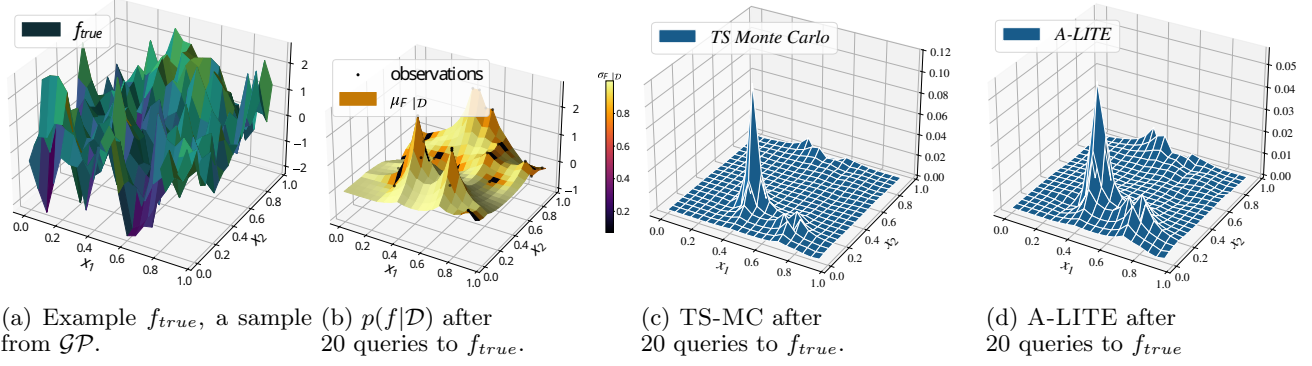


Figure 15: Illustration of the setup for Bayesian optimisation with f_{true} sampled from 2-dimensional Gaussian process with exponential kernel.

as a ground-truth. To derive the mean and standard error at each step we use 50 different seeds of Bayesian optimisation.

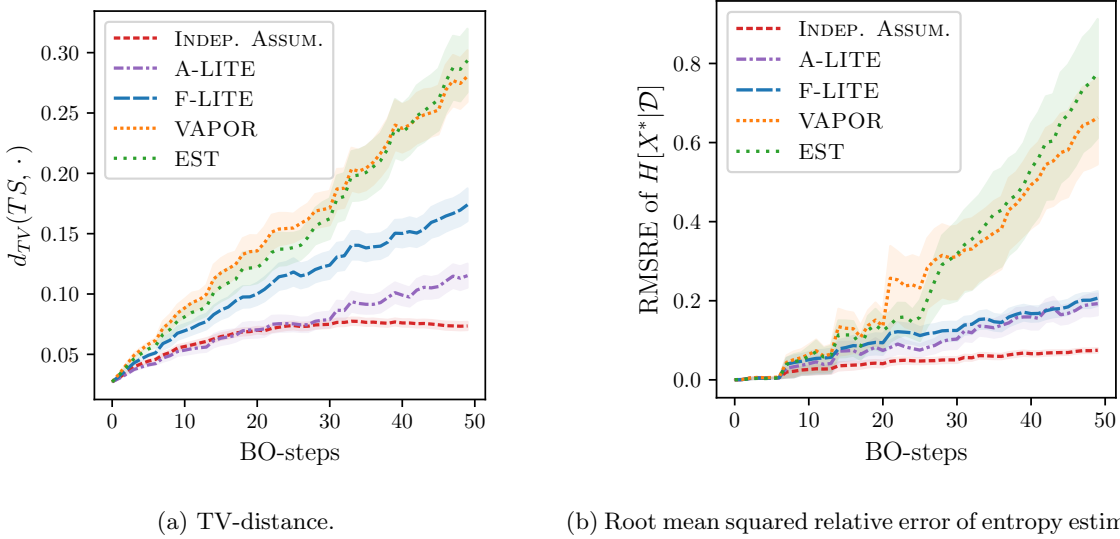
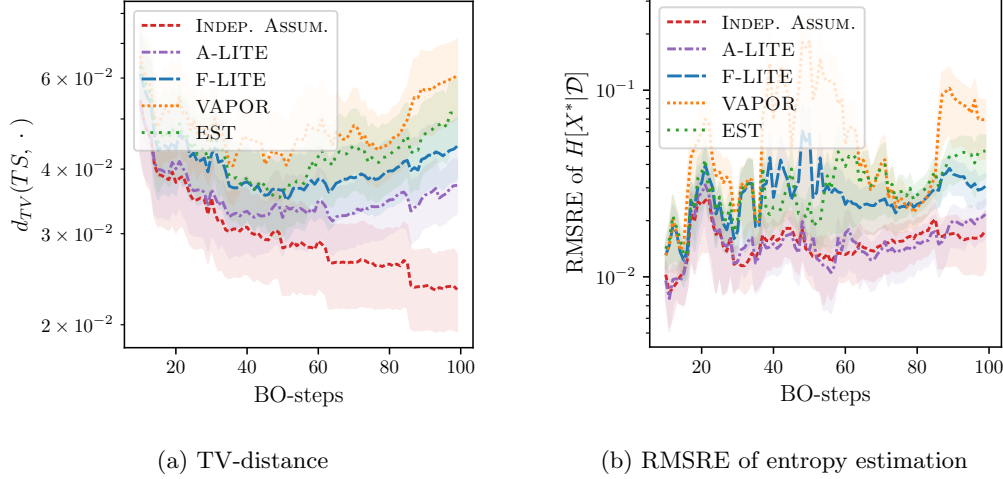


Figure 16: Fidelity of PoM estimates during Bayesian optimisation with f_{true} sampled from 2-dimensional Gaussian process with exponential kernel.

E.3 Drop-Wave

While the drop-wave function $f_{true}(x_1, x_2) := (1 + \cos(12\sqrt{x_1^2 + x_2^2})) / ((x_1^2 + x_2^2)/2 + 2)$ is featured in the main text, there we do not report on the evolution during Bayesian optimisation of the PoM fidelity and relative error of entropy estimation. Recall the setting in Section D.7, but now running Bayesian optimisation for 100 steps instead of 30. Then Figure 17a reports the mean and standard error of the TV-distance to ground-truth PoM during 50 seeds of Bayesian optimisation. Here, we exclude the first 10 steps of Bayesian optimisation (warmup steps) and all estimators, including TS-MC for the ground-truth, are ensured to converge to within $\epsilon = 1/|\mathcal{X}|$ of their analytical expression

Likewise, Figure 17b reports on the mean and standard error of the root mean squared relative error of entropy estimation based on 50 repetitions of Bayesian optimisation. Still, convergence of all estimators to within $\epsilon = 1/|\mathcal{X}|$ of their analytical expression is ensured, including the estimator for ground-truth (based on TS-MC).


 Figure 17: Fidelity of PoM estimates during Bayesian optimisation with f_{true} set to drop-wave.

F PROOFS

F.1 Assumptions

Assumption 1. X^* is almost surely unique, which is equivalently expressed as $\sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^*] = 1$.

Proof. Being an assumption, we only have to show the equivalence between almost sure uniqueness and integration to 1. Denote by $\mathcal{E} = \{|\arg \max_{x \in \mathcal{X}} F_x| = 1\}$. Then

$$\begin{aligned} \sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^* | \mathcal{D}] &= \sum_{x \in \mathcal{X}} \mathbb{P}[\{x\} = X^*, \mathcal{E} | \mathcal{D}] + \sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^* | \mathcal{D}, \mathcal{E}^c] \mathbb{P}[\mathcal{E}^c | \mathcal{D}] \\ &= \mathbb{P}[\mathcal{E} | \mathcal{D}] + (1 - \mathbb{P}[\mathcal{E} | \mathcal{D}]) \sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^* | \mathcal{D}, \mathcal{E}^c] \\ &\geq \mathbb{P}[\mathcal{E} | \mathcal{D}] + 2(1 - \mathbb{P}[\mathcal{E} | \mathcal{D}]) = 2 - \mathbb{P}[\mathcal{E} | \mathcal{D}] \end{aligned}$$

with equality if $\mathbb{P}[\mathcal{E} | \mathcal{D}] = 1$. □

F.2 Propositions

Proposition 1. Let $\tilde{F} \sim \mathcal{N}(\mu_F, \text{diag}(\sigma_1^2, \dots, \sigma_{|\mathcal{X}|}^2))$, let $\epsilon \in (0, 1/4]$, and define $\tilde{\epsilon} := -\Phi^{-1}(2\epsilon)$. Then for

$$n = \left\lceil \frac{\mu_F^{\max} - \mu_F^{\min} + 2\tilde{\epsilon}\sigma_F^{\max}}{\epsilon \cdot 2\sqrt{2\pi}\sigma_F^{\min}} \right\rceil + 2 \in \Theta(\sqrt{\log(1/\epsilon)}/\epsilon)$$

integration points at positions $f_0 = -\infty$, $f_n = \infty$, and $f_i = \mu_F^{\min} - \tilde{\epsilon}\sigma_F^{\max} + \frac{i-1}{n-2}(\mu_F^{\max} - \mu_F^{\min} + 2\tilde{\epsilon}\sigma_F^{\max})$ for $0 < i < n$, it holds for all $x \in \mathcal{X}$ that

$$\left| \tilde{p}_x - \sum_{i=0}^{n-1} \frac{g^x(f_{i+1}) + g^x(f_i)}{2} \mathbb{P}[\tilde{F}_x \in (f_i, f_{i+1}]] \right| \leq \epsilon.$$

Proof. The proposition follows from Proposition 8 by refining the conditions

$$\max_{x \in \mathcal{X}} \mathbb{P}[\tilde{F}_x \leq f_1] \leq 2\epsilon, \quad \max_{x \in \mathcal{X}} \mathbb{P}[\tilde{F}_x > f_{l-1}] \leq 2\epsilon, \quad \text{and} \quad \max_{x \in \mathcal{X}} \mathbb{P}[\tilde{F}_x \in (f_i, f_{i+1}]] \leq 2\epsilon \quad \forall i = 1, \dots, l-2$$

for the Gaussian case (with $\epsilon \leq 1/4$) to the stronger assumptions

$$f_1 \leq \mu_F^{\min} + \Phi^{-1}(2\epsilon)\sigma_F^{\max}, \quad f_{l-1} \geq \mu_F^{\max} - \Phi^{-1}(2\epsilon)\sigma_F^{\max}, \quad \text{and} \quad f_{i+1} - f_i \leq 2\sqrt{2\pi}\sigma_F^{\min}\epsilon \quad \forall i = 1, \dots, l-2.$$

To satisfy these assumptions, we select equidistantly placed f_1, \dots, f_{l-1} :

$$f_i = \mu_F^{\min} + \Phi^{-1}(2\epsilon)\sigma_F^{\max} + \frac{i-1}{l-2} (\mu_F^{\max} - \mu_F^{\min} - 2\Phi^{-1}(2\epsilon)\sigma_F^{\max}) \quad \forall i = 1, \dots, l-1,$$

where we ensure sufficiently small steps $f_{i+1} - f_i$ by taking

$$l = \left\lceil \frac{\mu_F^{\max} - \mu_F^{\min} - 2\Phi^{-1}(2\epsilon)\sigma_F^{\max}}{2\sqrt{2\pi}\sigma_F^{\min}\epsilon} \right\rceil + 2.$$

Finally, the asymptotic scaling of n follows from Lemma 3. \square

Proposition 2. Let $F \sim \mathcal{N}(\mu_F, \Sigma_F)$, $\sigma_{F_i}^2 = \Sigma_{ii} \quad \forall i = 1, \dots, |\mathcal{X}| > 1$, and $\kappa^* \in \mathbb{R}$ s.t. $s(\kappa^*) := \sum_{x \in \mathcal{X}} \mathbb{P}[F_x \geq \kappa^*] = 1$. Then $s(\cdot)$ is cont. monot. decreasing and $\mu_F^{\min} + \sigma_F^{\min} \cdot \Phi^{-1}(\frac{1}{|\mathcal{X}|}) \leq \kappa^* \leq \mu_F^{\max} + \sigma_F^{\max} \cdot \Phi^{-1}(\frac{1}{|\mathcal{X}|})$. The search window scales in $\Theta(\sqrt{\log |\mathcal{X}|})$ and $\forall x \in \mathcal{X}$

$$|\mathbb{P}[F_x \geq \kappa^*] - \mathbb{P}[F_x \geq \kappa^k]| \leq \frac{\mu_F^{\max} - \mu_F^{\min} - \Phi^{-1}(|\mathcal{X}|^{-1})\sigma_F^{\max}}{2^{k+1}\sqrt{2\pi}\sigma_{F_x}},$$

where κ^k is the estimate at step k according to Algorithm 1. Hence, $k = \log_2((\mu_F^{\max} - \mu_F^{\min} - \Phi^{-1}(|\mathcal{X}|^{-1})\sigma_F^{\max})/(2\epsilon)) \in \Theta(\log(\log(|\mathcal{X}|)/\epsilon))$ steps suffice to ensure that for all $x \in \mathcal{X}$ it holds that $|\mathbb{P}[F_x \geq \kappa^*] - \mathbb{P}[F_x \geq \kappa^k]| \leq \epsilon$.

Proof. This proposition follows swiftly from Lemma 4 and Lemma 5 by restricting our attention from general stochastic processes to Gaussian processes, i.e. by using $\mathbb{P}[F_x \geq \kappa] = \Phi(\frac{\mu_{F_x} - \kappa}{\sigma_{F_x}})$ with Lipschitz constant $1/(\sqrt{2\pi}\sigma_{F_x})$. A direct consequence of Equation (16) in Lemma 4 is that $\kappa^* \leq \mu_F^{\max} - \Phi^{-1}(1/|\mathcal{X}|)\sigma_F^{\max}$, since otherwise $\mathbb{P}[F_z \geq \kappa^*] < \frac{1}{|\mathcal{X}|}$ for all $z \in \mathcal{X}$. Similarly, $\kappa^* \geq \mu_F^{\min} - \Phi^{-1}(1/|\mathcal{X}|)\sigma_F^{\min}$ since otherwise $\mathbb{P}[F_z \geq \kappa^*] > \frac{1}{|\mathcal{X}|}$ for all $z \in \mathcal{X}$. So, we have proven the validity of the initialisation of the logarithmic search window. The asymptotic behaviour of the search window follows immediately from Lemma 3. The error bounds after running k steps of binary search follow from Lemma 5 when taking into account the Lipschitz constant of the Gaussian cdf. \square

Proposition 3. Let $h_x := \phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \frac{1}{\sigma_{F_x}}$. Then

$$\frac{dq_x}{d\mu_{F_z}} = h_x \cdot \left(\mathbb{1}_{x=z} - \frac{h_z}{\sum_{w \in \mathcal{X}} h_w} \right) \quad (3)$$

$$\frac{dq_x}{d\sigma_{F_z}} = h_x \cdot \left(\mathbb{1}_{x=z} - \frac{h_z}{\sum_{w \in \mathcal{X}} h_w} \right) \cdot \frac{\kappa^* - \mu_{F_z}}{\sigma_{F_z}}. \quad (4)$$

Proof. According to the chain rule of differentiation we have

$$\frac{dp_\theta(x)}{d\theta_i} = \frac{d\Phi(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}})}{d\theta_i} = \phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \frac{d}{d\theta_i} \frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}.$$

Specialising θ_i to either μ_{F_z} or σ_{F_z} , we get

$$\begin{aligned} \frac{dp_\theta(x)}{d\mu_{F_z}} &= \phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \frac{\mathbb{1}_{x=z} - \frac{d\kappa^*}{d\mu_{F_z}}}{\sigma_{F_x}} \\ \frac{dp_\theta(x)}{d\sigma_{F_z}} &= \phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \frac{-\frac{d\kappa^*}{d\sigma_{F_z}}\sigma_{F_x} + (\kappa^* - \mu_{F_x})\mathbb{1}_{x=z}}{\sigma_{F_x}^2}. \end{aligned} \quad (9)$$

So, we are only left to find an expression for $\frac{d\kappa^*}{d\mu_{F_z}}$ and $\frac{d\kappa^*}{d\sigma_{F_z}}$. To that end, notice how κ^* is an implicit function of $\theta = (\mu_F, \sigma_F) \in \mathbb{R}^{2|\mathcal{X}|}$. Indeed, κ^* was defined as the unique real number (dependent on θ) such that

$$g(\theta, \kappa^*) := \sum_{x \in \mathcal{X}} \Phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) - 1 \stackrel{!}{=} 0,$$

where g is a continuously differentiable function. We may then use the multi-variate chain rule to derive an explicit formula for $\frac{d\kappa^*(\theta)}{d\theta_i}$:

$$\begin{aligned} \theta \mapsto \frac{d}{d\theta_i} \overbrace{g(\theta, \kappa^*(\theta))}^{\stackrel{!}{=} 0} &= \frac{dg(\theta, b)}{d\theta} \Big|_{b=\kappa^*(\theta)} \frac{d\theta}{d\theta_i} + \frac{dg(\theta, b)}{db} \Big|_{b=\kappa^*(\theta)} \frac{d\kappa^*(\theta)}{d\theta_i} \stackrel{!}{=} 0 \\ &\iff \\ \frac{d\kappa^*(\theta)}{d\theta_i} &= - \frac{dg(\theta_1, \dots, \theta_{2|\mathcal{X}|}, b)}{d\theta_i} \Big|_{b=\kappa^*(\theta)} / \frac{dg(\theta, b)}{db} \Big|_{b=\kappa^*(a)}. \end{aligned} \quad (10)$$

Next, we evaluate Equation (10) for $\frac{d\kappa^*}{d\mu_{F_z}}$ and $\frac{d\kappa^*}{d\sigma_{F_z}}$, which result in

$$\begin{aligned} \frac{d\kappa^*}{d\mu_{F_z}} &= \phi\left(\frac{\mu_{F_z} - \kappa^*}{\sigma_{F_z}}\right) \frac{1}{\sigma_{F_z}} / \sum_{w \in \mathcal{X}} \phi\left(\frac{\mu_{F_w} - \kappa^*}{\sigma_{F_w}}\right) \frac{1}{\sigma_{F_w}} = h_z / \sum_{w \in \mathcal{X}} h_w, \\ \frac{d\kappa^*}{d\sigma_{F_z}} &= \phi\left(\frac{\mu_{F_z} - \kappa^*}{\sigma_{F_z}}\right) \left(-\frac{\mu_{F_z} - \kappa^*}{\sigma_{F_z}^2}\right) / \sum_{w \in \mathcal{X}} \phi\left(\frac{\mu_{F_w} - \kappa^*}{\sigma_{F_w}}\right) \frac{1}{\sigma_{F_w}} \\ &= -\frac{\mu_{F_z} - \kappa^*}{\sigma_{F_z}} \frac{d\kappa^*}{d\mu_{F_z}}. \end{aligned} \quad (11)$$

where $h_z := \phi\left(\frac{\mu_{F_z} - \kappa^*}{\sigma_{F_z}}\right) \frac{1}{\sigma_{F_z}}$. Combining Equation (9) with Equation (11), we get the statement in the theorem. \square

Proposition 4. *Define the variational objective*

$$\mathcal{W}(p) := \sum_{x \in \mathcal{X}} p_x \cdot \left(\mu_{F_x} + \underbrace{\sqrt{2\tilde{I}(p_x)} \cdot \sigma_{F_x}}_{\text{exploration bonus}} \right), \quad (5)$$

with the quasi-surprisal $\tilde{I}(u) := (\phi(\Phi^{-1}(u))/u)^2/2$. Then the maximizer of \mathcal{W} among elements of the probability simplex is given by F-LITE, i.e., by q with

$$q_x := \Phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right) \text{ with } \kappa^* \text{ s.t. } \sum_x q_x = 1.$$

Proof. First notice that by the definition of \tilde{I} , we obtain the easier objective to work with:

$$\mathcal{W}(r) = \sum_{x \in \mathcal{X}} r_x \mu_{F_x} + \phi(\Phi^{-1}(r_x)) \sigma_{F_x}.$$

Next, we show that $\mathcal{W}(r)$ is concave by computing the Hessian:

$$\begin{aligned} \frac{\partial}{\partial r_x} \mathcal{W}(r) &= \mu_{F_x} - \sigma_{F_x} \Phi^{-1}(r_x) \phi(\Phi^{-1}(r_x)) \frac{d}{dr_x} \Phi^{-1}(r_x) \\ &= \mu_{F_x} - \sigma_{F_x} \Phi^{-1}(r_x) \\ \frac{\partial^2}{\partial r_x \partial r_z} \mathcal{W}(r) &= -\sigma_{F_x} \mathbb{1}_{x=z} \frac{1}{\phi(\Phi^{-1}(r_x))} \begin{cases} < 0 & x = z \\ = 0 & x \neq z \end{cases}, \end{aligned}$$

where the inverse function rule was employed twice. From negative definiteness strict concavity follows immediately. We show next that $r^* \in \text{relint}(\Delta(\mathcal{X}))$, the relative interior of the probability simplex. Indeed, at the border of the probability simplex the partial derivatives explode:

$$\frac{\partial}{\partial r_x} \mathcal{W}(r) = \mu_{F_x} - \sigma_{F_x} \Phi^{-1}(r_x) = \begin{cases} \infty & r_x \rightarrow 0^+ \\ \text{finite} & r_x \in (0, 1) \\ -\infty & r_x \rightarrow 1^- \end{cases}.$$

Together with the concavity of $\mathcal{W}(\cdot)$ this ensures that $r^* \in \text{relint}(\Delta(\mathcal{X}))$. Hence, r^* is a local optimiser of $\mathcal{W}(r)$ on the plane defined by $\sum_{x \in \mathcal{X}} r_x = 1$. Consequently, we obtain the Lagrangian function

$$\mathcal{L}(r, \kappa) : (0, 1)^{|\mathcal{X}|} \times \mathbb{R} \rightarrow \mathbb{R} \quad r \mapsto \mathcal{W}(r) + \kappa(1 - \sum_{x \in \mathcal{X}} r_x).$$

Setting its partial derivatives equal to zero, we derive the closed-form solution:

$$0 = \mu_{F_x} - \sigma_{F_x} \Phi^{-1}(r_x^*) - \kappa^* \iff r_x^* = \Phi\left(\frac{\mu_{F_x} - \kappa^*}{\sigma_{F_x}}\right),$$

where κ^* ensures a normalised distribution, i.e. $\sum_{x \in \mathcal{X}} r_x^* = 1$. □

Proposition 5. *The maximizer to Equation (6) on the probability simplex admits the closed-form expression*

$$v_x := v\left(\frac{\mu_{F_x} - \nu^*}{\sigma_{F_x}}\right) \text{ with } \nu^* \text{ such that } \sum_x v_x = 1,$$

where $v(c) := \exp(-(\sqrt{c^2 + 4} - c)^2/8)$. Moreover, to find ν^* we can use binary search with $k \in \Theta(\log(\sqrt{\log |\mathcal{X}|}/\epsilon))$ iterations, ensuring that the k -th iterate v^k satisfies $\|v^* - v^k\|_\infty < \epsilon$.

Proof. We show first that $r^* \in \text{relint}(\Delta(\mathcal{X}))$. Indeed, at the border of the probability simplex the partial derivatives explode:

$$\frac{\partial}{\partial r_x} \mathcal{V}(r) = \mu_{F_x} + \sigma_{F_x} \left(\sqrt{-2 \ln r_x} - \frac{1}{\sqrt{-2 \ln r_x}} \right) = \begin{cases} \infty & r_x \rightarrow 0^+ \\ \text{finite} & r_x \in (0, 1) \\ -\infty & r_x \rightarrow 1^- \end{cases}$$

which together with the concavity of $\mathcal{V}(\cdot)$, shown in Proposition 10, ensures that $r^* \in \text{relint}(\Delta(\mathcal{X}))$. Hence, r^* is a local optimiser of $\mathcal{V}(r)$ on the plane defined by $\sum_{x \in \mathcal{X}} r_x = 1$. Consequently, we obtain the Lagrangian function

$$\mathcal{L}(r, \nu) : (0, 1)^{|\mathcal{X}|} \times \mathbb{R} \rightarrow \mathbb{R} \quad r \mapsto \mathcal{V}(r) + \nu \left(1 - \sum_{x \in \mathcal{X}} r_x \right).$$

Setting its partial derivatives equal to zero we derive the closed-form solution:

$$\begin{aligned} 0 &= \mu_{F_x} + \sigma_{F_x} \left(\sqrt{-2 \ln r_x} - \frac{1}{\sqrt{-2 \ln r_x}} \right) - \nu \iff 0 = \sqrt{-2 \ln r_x}^2 + \sqrt{-2 \ln r_x} \overbrace{\frac{\mu_{F_x} - \nu}{\sigma_{F_x}}}^{c_x} - 1 \\ \iff \sqrt{-2 \ln r_x} &= \frac{-c_x + \sqrt{c_x^2 + 4}}{2} \iff r_x^* = \exp(-[\sqrt{c_x^2 + 4} - c_x]^2/8) \quad \text{where } c_x = \frac{\mu_{F_x} - \nu}{\sigma_{F_x}}. \end{aligned} \quad (12)$$

Being a Lagrange multiplier, ν automatically ensures a normalised probability distribution, i.e. $\sum_{x \in \mathcal{X}} r_x^* = 1$.

To show that ν^* can be found with binary search using $k \in \Theta(\log(\sqrt{\log |\mathcal{X}|}/\epsilon))$ steps while ensuring $\|r^* - r^k\|_\infty < \epsilon$, it suffices to demonstrate that $v^* \mapsto \sum_{x \in \mathcal{X}} v\left(\frac{\mu_{F_x} - \nu^*}{\sigma_{F_x}}\right)$ is continuous and monotonously decreasing, $v^{-1}(r_x) = 1/\sqrt{-2 \ln r_x} - \sqrt{-2 \ln r_x}$, $\mu_F^{\min} - v^{-1}(\frac{1}{|\mathcal{X}|})\sigma_F^{\min} \leq \nu^* \leq \mu_F^{\max} - v^{-1}(\frac{1}{|\mathcal{X}|})\sigma_F^{\max}$, and that $v(\cdot)$ is Lipschitz continuous.

Lipschitz continuity follows immediately from a bounded derivative

$$\frac{d}{dc} v(c) = \exp(-[\sqrt{c^2 + 4} - c]^2/8) \frac{\sqrt{c^2 + 4} - c}{4} \left(\frac{2c}{2\sqrt{c^2 + 4}} - 1 \right) \in [0, 0.4).$$

Since $\nu \mapsto c_x$, $c_x \mapsto (\sqrt{c_x^2 + 4} - c_x)^2$, and $z \mapsto \exp(-z/8)$ are each monotonously decreasing, their composition $\nu \mapsto r_x^\nu$ is also monotonously decreasing. As the sum of decreasing functions $\nu \mapsto \sum_{x \in \mathcal{X}} p_x^\nu$ is monotonously decreasing. The binary search window is initialised based on the insight that

$$\begin{aligned} 1 &\stackrel{!}{=} \sum_{x \in \mathcal{X}} r_x^* \leq |\mathcal{X}|v(c_u) \implies c_u \geq v^{-1}(1/|\mathcal{X}|) \\ 1 &\stackrel{!}{=} \sum_{x \in \mathcal{X}} r_x^* \geq |\mathcal{X}|v(c_l) \implies c_l \leq v^{-1}(1/|\mathcal{X}|) \end{aligned}$$

Finally, from the equivalences in Equation (12) we obtain an inverse to $v(c)$, i.e.

$$v^{-1}(r_x) = \frac{1}{\sqrt{-2 \ln r_x}} - \sqrt{-2 \ln r_x},$$

which we remark fulfills $v^{-1}(1/k) \leq 0 \ \forall k \geq 2$. As a direct consequence we obtain $\nu \leq \mu_F^{max} - v^{-1}(1/|\mathcal{X}|)\sigma_F^{max}$, since otherwise $c_z < v^{-1}(1/|\mathcal{X}|)$ for all $z \in \mathcal{X}$. Similarly, it holds that $\nu \geq \mu_F^{min} - v^{-1}(1/|\mathcal{X}|)\sigma_F^{min}$, since otherwise $c_z > v^{-1}(1/|\mathcal{X}|)$ for all $z \in \mathcal{X}$. Hence,

$$\nu \in [\mu_F^{min} - v^{-1}(1/|\mathcal{X}|)\sigma_F^{min}, \mu_F^{max} - v^{-1}(1/|\mathcal{X}|)\sigma_F^{max}].$$

□

Proposition 6 (Logarithmic \tilde{F}^* -quantile search). *Let $b \in [0.25, 1)$ and $\tilde{F} \sim \mathcal{N}(\mu_F, \text{diag}(\sigma_{F_1}^2, \dots, \sigma_{F_{|\mathcal{X}|}}^2))$ with $|\mathcal{X}| > 1$. Assume $\exists x : \sigma_{F_x} > 0$. Define $g(f) := \Pi_z \mathbb{P}[\tilde{F}_z \leq f]$, which is continuous and strictly monotonously increasing. Then $\exists \bar{f} \in \mathbb{R}$ s.t. $g(\bar{f}) = b$. It can be found efficiently using logarithmic search with search window*

$$\mu_F^{min} + \sigma_F^{min} \Phi^{-1}(b^{1/|\mathcal{X}|}) \leq \bar{f} \leq \mu_F^{max} + \sigma_F^{max} \Phi^{-1}(b^{1/|\mathcal{X}|}).$$

The size of the search window is bounded by $\mu_F^{max} - \mu_F^{min} + \Phi^{-1}(b^{1/|\mathcal{X}|})\sigma_F^{max} \in \Theta(\sqrt{\log |\mathcal{X}|})$. Run k steps of binary search resulting in best approximant \bar{f}^k . Then

$$|\bar{f} - \bar{f}^k| \leq \frac{\mu_F^{max} - \mu_F^{min} + \Phi^{-1}(b^{1/|\mathcal{X}|})\sigma_F^{max}}{2^{k+1}},$$

i.e. we obtain exponential convergence with linear order. So, to ensure $|\bar{f} - \bar{f}^k| \leq \nu$, $k = \log_2((\mu_F^{max} - \mu_F^{min} + \Phi^{-1}(b^{1/|\mathcal{X}|})\sigma_F^{max})/(2\nu)) \in \Theta(\log(\log(|\mathcal{X}|)/\nu))$ steps suffice.

Proof. Continuity and monotonicity of $g(f)$ follows from continuity and monotonicity of $\mathbb{P}[\tilde{F}_z \leq f]$ for all $z \in \mathcal{X}$. The existence and uniqueness of \bar{f} follows swiftly, since $g(f) = \mathbb{P}[\tilde{F}^* \leq f]$ ¹², as a cumulative distribution function, has range $(0, 1)$. Let us derive the search window. It holds that

$$\Phi^{|\mathcal{X}|}\left(\frac{f - \mu_F^{max}}{\sigma_2}\right) \leq \prod_{x \in \mathcal{X}} \Phi\left(\frac{f - \mu_F^{max}}{\sigma_{F_x}}\right) \leq \underbrace{\prod_{x \in \mathcal{X}} \Phi\left(\frac{f - \mu_{F_x}}{\sigma_{F_x}}\right)}_b \leq \prod_{x \in \mathcal{X}} \Phi\left(\frac{f - \mu_F^{min}}{\sigma_{F_x}}\right) \leq \Phi^{|\mathcal{X}|}\left(\frac{f - \mu_F^{min}}{\sigma_1}\right)$$

where $\sigma_1 = \sigma_F^{min}$ if $f \geq \mu_F^{min}$ and $\sigma_1 = \sigma_F^{max}$ otherwise, and $\sigma_2 = \sigma_F^{max}$ if $f \geq \mu_F^{max}$ and $\sigma_2 = \sigma_F^{min}$ otherwise. Equivalently, it then holds that

$$\frac{f - \mu_F^{max}}{\sigma_2} \leq \Phi^{-1}(b^{1/|\mathcal{X}|}) \leq \frac{f - \mu_F^{min}}{\sigma_1} \iff \mu_F^{min} + \sigma_1 \Phi^{-1}(b^{1/|\mathcal{X}|}) \leq f \leq \mu_F^{max} + \sigma_2 \Phi^{-1}(b^{1/|\mathcal{X}|}).$$

Now, since by assumption $b \geq \frac{1}{4}$ and $|\mathcal{X}| \geq 2$, it holds that $b^{1/|\mathcal{X}|} \geq \frac{1}{2}$ and hence $\Phi^{-1}(b^{1/|\mathcal{X}|}) \geq 0$. Consequently, we obtain the desired search window

$$\mu_F^{min} + \sigma_F^{min} \Phi^{-1}(b^{1/|\mathcal{X}|}) \leq f \leq \mu_F^{max} + \sigma_F^{max} \Phi^{-1}(b^{1/|\mathcal{X}|}).$$

¹²Recall, that here we are in the independent Gaussian process setting.

Regarding the scaling of the search window, notice that the window size is given by $\mu_F^{max} - \mu_F^{min} + (\sigma_F^{max} - \sigma_F^{min})\Phi^{-1}(b^{1/|\mathcal{X}|})$. Now, we may apply Lemma 3, which states that

$$\Phi^{-1}(y) \sim \sqrt{-2\ln(1-y)} \text{ as } y \rightarrow 1^-.$$

Plugging in $b^{1/|\mathcal{X}|}$ for y then gives us

$$\Phi^{-1}(b^{1/|\mathcal{X}|}) \sim \sqrt{-2\ln(1-b^{1/|\mathcal{X}|})} \text{ as } |\mathcal{X}| \rightarrow \infty. \quad (13)$$

According to the L'Hôpital-Bernoulli rule, it holds that $\lim_{a \rightarrow 1} \frac{1-a}{1-\ln(a)} = \lim_{a \rightarrow 1} a = 1$. Since $b^{1/|\mathcal{X}|} \rightarrow 1^-$ as $|\mathcal{X}| \rightarrow \infty$, we equivalently get

$$1 - b^{1/|\mathcal{X}|} \sim -\ln(b^{1/|\mathcal{X}|}) = \ln(1/b)/|\mathcal{X}| \text{ as } |\mathcal{X}| \rightarrow \infty.$$

Combining this with Equation (13), we obtain

$$\Phi^{-1}(b^{1/|\mathcal{X}|}) \sim \sqrt{2\ln(|\mathcal{X}|) - 2\ln(\ln(1/b))}.$$

Hence, the search window scales in

$$\Theta(\mu_F^{max} - \mu_F^{min} + (\sigma_F^{max} - \sigma_F^{min})\Phi^{-1}(b^{1/|\mathcal{X}|})) = \Theta(\sqrt{\ln|\mathcal{X}|}).$$

Finally, k steps of binary search divide the search window by 2^k resulting in an accuracy of

$$|\bar{f} - \bar{f}^k| \leq \frac{\mu_F^{max} - \mu_F^{min} + (\sigma_F^{max} - \sigma_F^{min})\Phi^{-1}(b^{1/|\mathcal{X}|})}{2^{k+1}} \iff k \leq \log_2 \left(\frac{\mu_F^{max} - \mu_F^{min} + (\sigma_F^{max} - \sigma_F^{min})\Phi^{-1}(b^{1/|\mathcal{X}|})}{2|\bar{f} - \bar{f}^k|} \right).$$

Therefore, for $k = \log_2((\mu_F^{max} - \mu_F^{min} + (\sigma_F^{max} - \sigma_F^{min})\Phi^{-1}(b^{1/|\mathcal{X}|}))/(\nu))$ it must hold that $|\bar{f} - \bar{f}^k| \leq \nu$. Inserting the asymptotic scaling of the search window finishes the proof. \square

Proposition 7 (Logarithmic $\tilde{F}^{* \setminus x}$ -quantile search). *Let $b \in (0, 1)$, $m, \mu_{F_x} \in \mathbb{R}$, and $s, \sigma_{F_x} \in \mathbb{R}_+$ such that $m > \mu_{F_x}$ and $s \leq \sigma_{F_x}$. Define $\tilde{g}^x(f) := \Phi((f - m)/s)/\Phi((f - \mu_{F_x})/\sigma_{F_x})$, which is continuous and strictly monotonously increasing on a section with range $(0, 1]$ and exceeds 1 elsewhere. Then $\exists! \bar{f}_x \in \mathbb{R}$ s.t. $\tilde{g}^x(\bar{f}_x) = b$. It can be found efficiently using logarithmic search with search window*

$$\min(\mu_{F_x} - \sqrt{2}\sigma_{F_x}, \max(\frac{m + \mu_{F_x}}{2} - \frac{\sigma_{F_x}^2 \ln(2/b)}{m - \mu_{F_x}}, m - \sqrt{\frac{2\ln(2/b)}{1-s^2/\sigma_{F_x}^2}}s)) \leq \bar{f}_x \leq m + \Phi^{-1}(b) \cdot s$$

The size Δ of the search window is independent of $|\mathcal{X}|$, i.e. $\Delta \in \Theta(1)$. Run k steps of binary search resulting in best approximant \bar{f}_x^k . Then $|\bar{f}_x - \bar{f}_x^k| \leq \frac{\Delta}{2^{k+1}}$, i.e., we obtain exponential convergence with linear order. So, to ensure $|\bar{f}_x - \bar{f}_x^k| \leq \nu$, $k = \log_2(\Delta/(2\nu)) \in \Theta(\log(1/\nu))$ steps suffice.

Proof. Since \tilde{g}^x is continuous and strictly monotonously increasing on a section with range $(0, 1]$ and larger than 1 elsewhere, see the illustration in Figure 8, it follows immediately that for $b \in (0, 1)$ $\exists! \bar{f}_x \in \mathbb{R}$ s.t. $\tilde{g}^x(\bar{f}_x) = b$. Let us next establish an upper bound on \bar{f}_x . It holds that

$$\tilde{g}^x(\bar{f}_x) = \Phi\left(\frac{\bar{f}_x - m}{s}\right)/\Phi\left(\frac{\bar{f}_x - \mu_{F_x}}{\sigma_{F_x}}\right) > \Phi\left(\frac{\bar{f}_x - m}{s}\right) \geq b$$

for $\bar{f}_x \geq m + \Phi^{-1}(b) \cdot s$, directly implying the upper bound on the search window in this theorem. For the lower bound we make use of Lemma 3, which states that $\forall a < 0$ one has

$$\phi(a) \left(\frac{1}{-a} - \frac{1}{-a^3} \right) \leq \Phi(a) \leq \frac{\phi(x)}{-a}. \quad (14)$$

Assuming $f \leq \mu_{F_x} - \sqrt{2}\sigma_{F_x}$, which is automatically less than m , one has $1 - 1/(\frac{f - \mu_{F_x}}{\sigma_{F_x}})^2 \geq \frac{1}{2}$. Together with Equation (14), we then get

$$\tilde{g}^x(f) = \frac{\Phi\left(\frac{f-m}{s}\right)}{\Phi\left(\frac{f-\mu_{F_x}}{\sigma_{F_x}}\right)} \leq \frac{\phi\left(\frac{f-m}{s}\right)}{\phi\left(\frac{f-\mu_{F_x}}{\sigma_{F_x}}\right)} \frac{2\frac{f-\mu_{F_x}}{\sigma_{F_x}}}{\frac{f-m}{s}} \leq 2 \frac{\phi\left(\frac{f-m}{s}\right)}{\phi\left(\frac{f-\mu_{F_x}}{\sigma_{F_x}}\right)}, \quad (15)$$

where in the last inequality we used that for $f \leq \mu_{F_x} < m$ it holds that $\frac{f - \mu_{F_x}}{f - m} = \frac{\mu_{F_x} - f}{m - f} < 1$ and that for $s \leq \sigma_{F_x}$ it holds that $\frac{s}{\sigma_{F_x}} \leq 1$. We want to figure out for what f the right hand side of Equation (15) cannot reach b , i.e.

$$b > 2 \exp((f - \mu_{F_x})^2 / 2\sigma_{F_x}^2 - (f - m)^2 / 2s^2),$$

which is implied by either of the conditions below:

$$\begin{aligned} \ln(b/2) &> (f - \mu_{F_x})^2 / 2\sigma_{F_x}^2 - (f - m)^2 / 2\sigma_{F_x}^2 = \frac{(f - \mu_{F_x})^2 - (f - m)^2}{2\sigma_{F_x}^2} \\ \ln(b/2) &> (f - m)^2 / 2\sigma_{F_x}^2 - (f - m)^2 / 2s^2 = (f - m)^2 \cdot \left(\frac{1}{2\sigma_{F_x}^2} - \frac{1}{2s^2} \right). \end{aligned}$$

These conditions, in turn, are satisfied for

$$f < \frac{\sigma_{F_x}^2 \ln(b/2)}{m - \mu_{F_x}} + \frac{m + \mu_{F_x}}{2} \quad \text{and} \quad f < m - \sqrt{\ln(b/2) / \left(\frac{1}{2\sigma_{F_x}^2} - \frac{1}{2s^2} \right)},$$

leading to the stated lower bound on the search window in this theorem. Clearly, the size of the search window only depends on b, m, s, μ_F , and σ_F , i.e., it is independent of $|\mathcal{X}|$. The rest of the theorem follows immediately. \square

Proposition 8. Suppose an independent stochastic process¹³ $\{F_x : \Omega \rightarrow \mathbb{R} \mid x \in \mathcal{X}\}$ on a finite domain \mathcal{X} . Let $\epsilon > 0$ and assume $f_0, \dots, f_l \in \overline{\mathbb{R}}$ with $f_i \leq f_{i+1}$ such that $f_0 = -\infty$, $f_l = \infty$, $\max_{x \in \mathcal{X}} \mathbb{P}[F_x \leq f_1] \leq 2\epsilon$, $\max_{x \in \mathcal{X}} \mathbb{P}[F_x > f_{l-1}] \leq 2\epsilon$, and $\max_{x \in \mathcal{X}} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \leq 2\epsilon \forall i = 1, \dots, l-2$. Then it holds for $X^* = \arg \max_{z \in \mathcal{X}} F_z$ that

$$\left| \mathbb{P}[x \in X^*] - \sum_{i=0}^{l-1} \frac{g_x(f_{i+1}) + g_x(f_i)}{2} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \right| \leq \epsilon,$$

where $g_x(f) := \prod_{z \in \mathcal{X} \setminus \{x\}} \mathbb{P}[F_z \leq f]$.

Proof. First, recall that mutually independent random variables Z_1, \dots, Z_n are characterized by $\mathbb{P}[Z_1 \in \mathcal{A}_1, \dots, Z_n \in \mathcal{A}_n] = \prod_{i=1}^n \mathbb{P}[Z_i \in \mathcal{A}_i]$ for any Borel sets $\mathcal{A}_1, \dots, \mathcal{A}_n$. Hence, conditionals $Z_2, \dots, Z_n | Z_1$ are also mutually independent:

$$\begin{aligned} \mathbb{P}[Z_2 \in \mathcal{A}_2, \dots, Z_n \in \mathcal{A}_n | Z_1 \in \mathcal{A}_1] &= \mathbb{P}[Z_1 \in \mathcal{A}_2, \dots, Z_n \in \mathcal{A}_n] / \mathbb{P}[Z_1 \in \mathcal{A}_1] \\ &= \prod_{i=1}^n \mathbb{P}[Z_i \in \mathcal{A}_i] / \mathbb{P}[Z_1 \in \mathcal{A}_1] = \prod_{i=2}^n \mathbb{P}[Z_i \in \mathcal{A}_i]. \end{aligned}$$

Conditional independence then allows us to derive a tractable integral for $\mathbb{P}[x \in X^*]$, which we write as a sum of integrals over an l -piece partition of \mathbb{R} :

$$\begin{aligned} \mathbb{P}[x \in X^*] &= \mathbb{P}[F_z \leq F_x \forall z \in \mathcal{X} \setminus \{x\}] = \mathbb{E}[\mathbb{P}[F_z \leq F_x \forall z \in \mathcal{X} \setminus \{x\} | F_x]] = \mathbb{E}\left[\prod_{z \in \mathcal{X} \setminus \{x\}} \mathbb{P}[F_z \leq F_x | F_x]\right] \\ &= \mathbb{E}[g_x(F_x)] = \int_{\mathbb{R}} g_x(f) d\mathbb{P}[F_x \in \cdot] = \sum_{i=0}^{l-1} \int_{(f_i, f_{i+1}]} g_x(f) d\mathbb{P}[F_x \in \cdot]. \end{aligned}$$

Each of these integrals can then be numerically evaluated using the trapezoidal rule. Moreover, we can upper bound the approximation error of numerical integration. Indeed, due to the triangle inequality, the fact that g_x

¹³That is, for any $x_1, \dots, x_n \subseteq \mathcal{X}$ it holds that F_{x_1}, \dots, F_{x_n} are mutually independent.

increases monotonously, and through a telescoping sum, one has

$$\begin{aligned}
 & \left| \mathbb{P}[x \in X^*] - \sum_{i=0}^{l-1} \frac{g_x(f_{i+1}) + g_x(f_i)}{2} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \right| \\
 & \leq \sum_{i=0}^{l-1} \left| \int_{(f_i, f_{i+1}]} g_x(f) d\mathbb{P}[F_x \in \cdot] - \frac{g_x(f_{i+1}) + g_x(f_i)}{2} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \right| \\
 & \leq \sum_{i=0}^{l-1} \frac{g_x(f_{i+1}) - g_x(f_i)}{2} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \leq \sum_{i=0}^{l-1} \frac{g_x(f_{i+1}) - g_x(f_i)}{2} \max_{i=0, \dots, l-1} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \\
 & = \max_{i=0, \dots, l-1} \frac{\mathbb{P}[F_x \in (f_i, f_{i+1}]]}{2}.
 \end{aligned}$$

Finally, for the partitioning $\mathbb{R} = (-\infty, f_1] \cup \bigcup_{i=1}^{l-2} (f_i, f_{i+1}] \cup (f_{l-1}, \infty)$ to ensure that $\mathbb{P}[F_x \in (f_i, f_{i+1}]] \leq 2\epsilon$ for all $x \in \mathcal{X}$ simultaneously, we require that

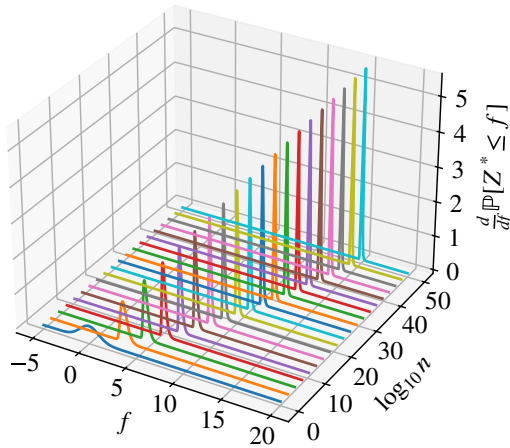
$$\max_{x \in \mathcal{X}} \mathbb{P}[F_x \leq f_1] \leq 2\epsilon, \quad \max_{x \in \mathcal{X}} \mathbb{P}[F_x > f_{l-1}] \leq 2\epsilon, \quad \text{and} \quad \max_{x \in \mathcal{X}} \mathbb{P}[F_x \in (f_i, f_{i+1}]] \leq 2\epsilon \quad \forall i = 1, \dots, l-2.$$

These are exactly the conditions that the Theorem demands. \square

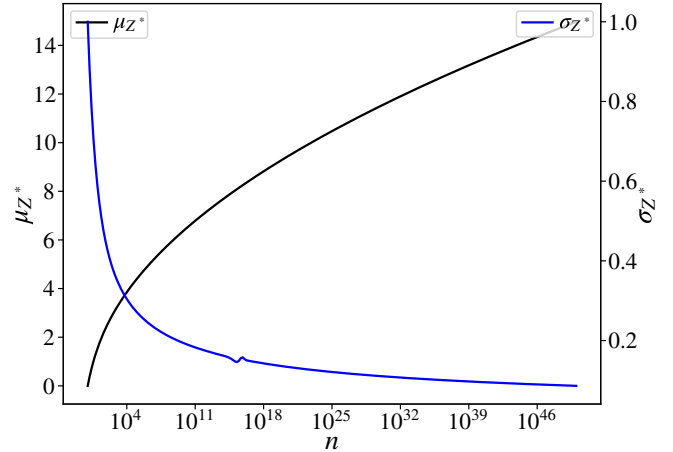
Proposition 9. Assume i.i.d. $Z_1, Z_2, \dots \sim \mathcal{N}(\mu, \sigma^2)$. Then $\exists (a_n)_{n \in \mathbb{N}}$ s.t.

$$\forall \epsilon > 0 \quad \lim_{n \rightarrow \infty} \mathbb{P}[\max_{i \leq n} Z_i - a_n > \epsilon] = 0.$$

One such sequence is given by $a_n = \mu + \sigma \cdot \Phi^{-1}(1 - \frac{1}{n})$. The rate of convergence is illustrated in Figure 18.



(a) Probability density function of maximum of i.i.d. standard normals.



(b) Mean and standard deviation of maximum of i.i.d. standard normals.

Figure 18: The distribution of the maximum of i.i.d. $Z_1, Z_2, \dots, Z_n \sim \mathcal{N}(0, 1)$ very slowly approaches that of a deterministic quantity as n is increased.

Proof. By shifting and scaling we can assume without loss of generality that $\mu = 0$ and $\sigma = 1$. Furthermore,

$$\lim_{x \rightarrow \infty} \frac{1 - \Phi(x + \epsilon)}{1 - \Phi(x)} = \lim_{x \rightarrow \infty} \frac{\phi(x + \epsilon)}{\phi(x)} = \lim_{x \rightarrow \infty} \exp\left(-\frac{(x + \epsilon)^2 - x^2}{2}\right) = \lim_{x \rightarrow \infty} \exp(-\epsilon x - \epsilon^2/2) = 0 \quad \forall \epsilon > 0$$

where L'Hôpital's rule was applied. We now directly apply Lemma 7. \square

F.3 Lemmas

Lemma 1 (Example to illustrate necessity of knowing the full covariance matrix for unbiased estimation). Consider $F \sim \mathcal{N}(0, I + s(e_i e_j^T + e_j e_i^T))$ in $\mathbb{R}^{|\mathcal{X}|}$, where $(e_i)_j = \mathbf{1}_{i=j}$, $i < j$, and $s \in [0, 1]$. Then it holds that

$$\lim_{s \rightarrow 1^-} \mathbb{P}[k \in \arg \max_h F_h] = \begin{cases} \frac{1}{|\mathcal{X}| - 1} & k \neq i \wedge k \neq j \\ \frac{1/2}{|\mathcal{X}| - 1} & \text{otherwise} \end{cases}.$$

Proof. We first verify that $\Sigma_F^s := I + s(e_i e_j^T + e_j e_i^T)$ is indeed symmetric positive semi-definite. Symmetry is trivial. On the other hand, positive semi-definiteness follows from

$$z^T \Sigma_F z = \|z\|^2 + 2s \cdot z^T e_i \cdot e_j^T z = 1 + 2s z_i z_j \geq 0 \quad \forall z : \|z\| = 1$$

where we have used that $z_i^2 + z_j^2 \leq 1$ implies $|z_i| \leq \sqrt{1 - z_j^2}$ which in turn gives $|z_i| \cdot |z_j| \leq \sqrt{z_j^2 - z_j^4} \leq \frac{1}{2}$ for any $z_j \in [-1, 1]$. The more general case allowing $\|z\| \neq 1$ follows from linearity. Next, let us verify the *probability of maximality* in the limit. To that end, consider the explicit Cholesky decomposition of Σ_F^s given by

$$(\Sigma_F^s)^{1/2} = I + s \cdot e_i e_j^T + (\sqrt{1 - s^2} - 1) \cdot e_i e_i^T,$$

which can be verified by evaluating $(\Sigma_F^s)^{1/2}((\Sigma_F^s)^{1/2})^T$ to Σ_F^s through rigorous algebra. Alternatively, we may consider the element-wise representation as

$$((\Sigma_F^s)^{1/2})_{k,h} = \begin{cases} 1 & (k, h) \in \{(a, a) : a \neq i\} \\ \sqrt{1 - s^2} & (k, h) = (i, i) \\ s & (k, h) = (i, j) \\ 0 & \text{otherwise} \end{cases}.$$

So, for $\varepsilon \sim \mathcal{N}(0, I)$ it holds that $F \stackrel{d}{=} (\Sigma_F^s)^{1/2} \varepsilon$, which can be parsed as $F_z = \varepsilon_z$ for all $z \neq i$ and $F_i = \sqrt{1 - s^2} \cdot \varepsilon_i + s \cdot \varepsilon_j$. Now it should be clear that as $s \rightarrow 1^-$, $F_i \rightarrow \varepsilon_j = F_j$. However, for any $s < 1$ the maximiser X^* is almost surely unique. Consequently, the probability of maximality will be evenly distributed in the limit of $s \rightarrow 1^-$ except for the halving of the probability mass among index i and j , since up to an infinitesimally small perturbation in the form of ε_i the entries F_i and F_j are identical. This proves the Lemma. \square

Lemma 2 (A-LITE error propagation). Let $\mu_F \in \mathbb{R}^{|\mathcal{X}|}$, $\sigma_F \in \mathbb{R}_+^{|\mathcal{X}|}$, and $\epsilon > 0$. Let $\bar{q}_1, \bar{q}_3 \in \mathbb{R}$ and $q_1, q_3 \in \mathbb{R}$ be pairs of quartiles such that $|\bar{q}_1 - q_1| \leq \nu$ and $|\bar{q}_3 - q_3| \leq \nu$ for $\nu = \epsilon \cdot \bar{s}^2 / (\max_x |\mu_{F_x} - \bar{m}| + \bar{s})$. Then with $m = (q_3 + q_1)/2$ and $\bar{m} = (\bar{q}_3 + \bar{q}_1)/2$ the means and $s = (q_3 - q_1)/(2\Phi^{-1}(0.75))$ and $\bar{s} = (\bar{q}_3 - \bar{q}_1)/(2\Phi^{-1}(0.75))$ the standard deviations of quartile-matched Gaussians, it holds that for all $x \in \mathcal{X}$

$$\left| \Phi\left(\frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + s^2}}\right) - \Phi\left(\frac{\mu_{F_x} - \bar{m}}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}}\right) \right| \leq \epsilon + \mathcal{O}(\epsilon^2). \quad (8)$$

Proof. We start by noting that with $p := 1/\Phi^{-1}(0.75) \approx 1.48$ it holds that

$$\begin{aligned} |m - \bar{m}| &\leq \frac{1}{2}(|q_3 - \bar{q}_3| + |q_1 - \bar{q}_1|) \leq \nu, \\ |s - \bar{s}| &\leq \frac{1}{2\Phi^{-1}(0.75)}(|q_3 - \bar{q}_3| + |q_1 - \bar{q}_1|) \leq p\nu, \\ |s^2 - \bar{s}^2| &= (s + \bar{s}) \cdot |s - \bar{s}| \leq (s + \bar{s})p\nu \leq 2\bar{s}p\nu + p^2\nu^2. \end{aligned}$$

We will use these inequalities at various places throughout this proof. By a Taylor series expansion around $\delta = 0$ we have

$$\left| \frac{1}{\sqrt{1+z}} - \frac{1}{\sqrt{1+z+\delta}} \right| = \frac{|\delta|}{2(1+z)^{3/2}} + \mathcal{O}\left(\frac{\delta^2}{(1+z)^{5/2}}\right).$$

Setting $z = \bar{s}^2/\sigma_{F_x}^2$, $\delta = \frac{s^2 - \bar{s}^2}{\sigma_{F_x}^2}$, and multiplying with $1/\sigma_{F_x}$ yields

$$\begin{aligned} \left| \frac{1}{\sqrt{\sigma_{F_x}^2 + s^2}} - \frac{1}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}} \right| &= \frac{|s^2 - \bar{s}^2|}{2(\sigma_{F_x}^2 + \bar{s}^2)^{3/2}} + \mathcal{O}\left(\frac{(s^2 - \bar{s}^2)^2}{(\sigma_{F_x}^2 + \bar{s}^2)^{5/2}}\right) \leq \frac{|s^2 - \bar{s}^2|}{2\bar{s}^3} + \mathcal{O}\left(\frac{(s^2 - \bar{s}^2)^2}{\bar{s}^5}\right) \\ &\leq \frac{p}{\bar{s}^2}\nu + \mathcal{O}(\nu^2) = \varepsilon_1. \end{aligned}$$

Now we can directly get a hold on the difference between the entries of Φ in Equation (8) using the triangle inequality of the absolute value:

$$\begin{aligned} \varepsilon_2 &= \left| \frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + s^2}} - \frac{\mu_{F_x} - \bar{m}}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}} \right| = \left| \frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + s^2}} - \frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}} + \frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}} - \frac{\mu_{F_x} - \bar{m}}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}} \right| \\ &\leq \varepsilon_1 |\mu_{F_x} - m| + |m - \bar{m}|/\sqrt{\sigma_{F_x}^2 + \bar{s}^2} \leq \varepsilon_1 (|\mu_{F_x} - \bar{m}| + \nu) + |m - \bar{m}|/\bar{s} \\ &\leq p \frac{|\mu_{F_x} - \bar{m}| + \bar{s}}{\bar{s}^2} \nu + \mathcal{O}(\nu^2) \leq p\epsilon + \mathcal{O}(\epsilon^2) \end{aligned}$$

Finally, by the mean value theorem, $\exists c \in [\frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + s^2}}, \frac{\mu_{F_x} - \bar{m}}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}}]$ such that

$$\left| \Phi\left(\frac{\mu_{F_x} - m}{\sqrt{\sigma_{F_x}^2 + s^2}}\right) - \Phi\left(\frac{\mu_{F_x} - \bar{m}}{\sqrt{\sigma_{F_x}^2 + \bar{s}^2}}\right) \right| \leq \varepsilon_2 \phi(c) \leq \varepsilon_2 / \sqrt{2\pi} \leq \epsilon + \mathcal{O}(\epsilon^2).$$

□

Lemma 3 (Asymptotics of Gaussian cumulative distribution function and its inverse). *For all $x < 0$ it holds that*

$$\phi(x) \left(\frac{1}{-x} - \frac{1}{-x^3} \right) \leq \Phi(x) \leq \frac{\phi(x)}{-x}.$$

Moreover, we have the following asymptotic behavior:

$$\begin{aligned} \Phi(x) &\sim \frac{\phi(x)}{-x} \text{ as } x \rightarrow -\infty, \\ \Phi^{-1}(y) &\sim -\sqrt{-2 \ln y} \text{ as } y \rightarrow 0^+, \\ \Phi^{-1}(y) &= -\Phi^{-1}(1-y) \sim \sqrt{-2 \ln(1-y)} \text{ as } y \rightarrow 1^-, \end{aligned}$$

where $a_n \sim b_n \iff \lim_{n \rightarrow \infty} b_n/a_n = 1$.

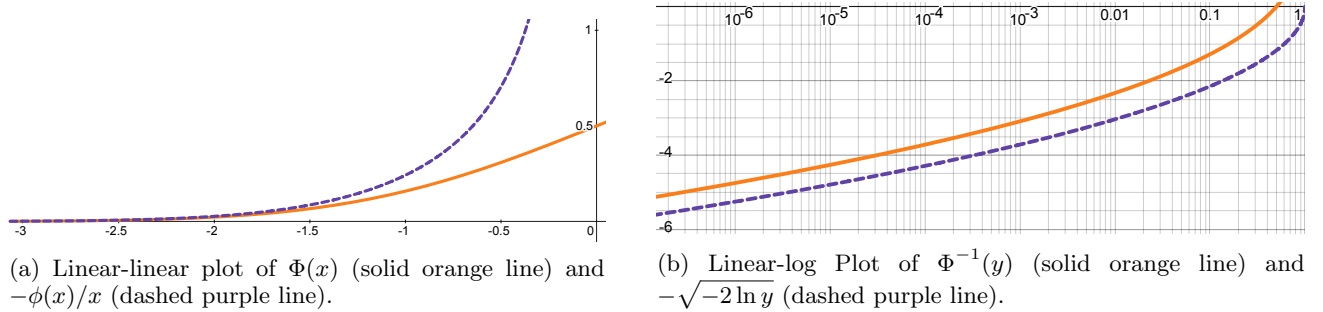


Figure 19: Finite-value behavior of the Gaussian cumulative distribution function and its inverse compared against their respective asymptotics.

Proof. Integration by parts provides upper and lower bounds on $\Phi(x)$ for $x < 0$:

$$\begin{aligned}\Phi(x) &= \int_{-\infty}^x \phi(s) ds = \int_{-\infty}^x \frac{\frac{d}{ds}\phi(s)}{-s} ds = \frac{\phi(x)}{-x} - \underbrace{\int_{-\infty}^x \frac{\phi(s)}{s^2} ds}_{\geq 0} \\ &= \frac{\phi(x)}{-x} - \int_{-\infty}^x \frac{\frac{d}{ds}\phi(s)}{-s^3} ds = \frac{\phi(x)}{-x} - \frac{\phi(x)}{-x^3} + 3 \underbrace{\int_{-\infty}^x \frac{\phi(s)}{s^4} ds}_{\geq 0}.\end{aligned}$$

Regarding $\Phi^{-1}(x)$ we perform a change of variable based on $\lim_{x \rightarrow -\infty} \Phi(x) = 0$:

$$\lim_{y \rightarrow 0^+} \frac{-\sqrt{-2 \ln y}}{\Phi^{-1}(y)} = \lim_{x \rightarrow -\infty} \frac{-\sqrt{-2 \ln \Phi(x)}}{\Phi^{-1}(\Phi(x))} = \lim_{x \rightarrow -\infty} \frac{-\sqrt{-2 \ln \Phi(x)}}{x}.$$

Now, since $-2 \ln \phi(x) = x^2 + \ln 2\pi$ one may reuse the upper and lower bounds on Φ to obtain that $\lim_{y \rightarrow 0^+} -\sqrt{-2 \ln y} / \Phi^{-1}(y) = 1$. Finally, by point symmetry $y = \Phi(x) = 1 - \Phi(-x)$ and hence $\Phi^{-1}(y) = x$ and $-\Phi^{-1}(1 - y) = x$, which together give the last equation of the theorem. \square

Lemma 4. Let $\{F_x : x \in \mathcal{X}\}$ be a stochastic process with $1 < |\mathcal{X}| < \infty$. In order to find $\kappa^* \in \mathbb{R}$ such that $\sum_{x \in \mathcal{X}} \mathbb{P}[F_x \geq \kappa^*] \stackrel{!}{=} 1$, we can use logarithmic search with search window derived from

$$\max_{z \in \mathcal{X}} \mathbb{P}[F_z \geq \kappa^*] \geq \frac{1}{|\mathcal{X}|} \text{ and } \min_{z \in \mathcal{X}} \mathbb{P}[F_z \geq \kappa^*] \leq \frac{1}{|\mathcal{X}|}. \quad (16)$$

Proof. Due to $\kappa \mapsto \mathbb{P}[F_x \geq \kappa]$ being monotonously decreasing $\forall x \in \mathcal{X}$, it follows that $\kappa \mapsto \sum_{x \in \mathcal{X}} \mathbb{P}[F_x \geq \kappa]$ is also monotonously decreasing. Consequently, logarithmic search allows one to quickly find the normalising κ^* . The search window is initialised based on the insight that

$$|\mathcal{X}| \min_{z \in \mathcal{X}} \mathbb{P}[F_z \geq \kappa] \leq \underbrace{\sum_{x \in \mathcal{X}} \mathbb{P}[F_x \geq \kappa]}_{\stackrel{!}{=} 1} \leq |\mathcal{X}| \max_{z \in \mathcal{X}} \mathbb{P}[F_z \geq \kappa]$$

\square

Lemma 5. Let $\{F_x : x \in \mathcal{X}\}$ be a stochastic process with L_x -Lipschitz continuous $\kappa \mapsto \mathbb{P}[F_x \geq \kappa]$ and $1 < |\mathcal{X}| < \infty$. Let $\kappa^* \in \mathbb{R}$ be unknown such that $\sum_{x \in \mathcal{X}} \mathbb{P}[F_x \geq \kappa^*] = 1$. Run k steps of binary search based on a search window $\kappa^* \in [a, b]$ according to Lemma 4 resulting in best approximant $\kappa^{(k)}$. Then

$$\begin{aligned}|\kappa^* - \kappa^{(k)}| &\leq \frac{b - a}{2^{k+1}} \\ |\mathbb{P}[F_x \geq \kappa^*] - \mathbb{P}[F_x \geq \kappa^{(k)}]| &\leq L_x \frac{b - a}{2^{k+1}} \quad \forall x \in \mathcal{X}, \\ \left| \sum_{x \in \mathcal{X}} \mathbb{P}[F_x \geq \kappa^{(k)}] - 1 \right| &\leq |\mathcal{X}| L_x \frac{b - a}{2^{k+1}}.\end{aligned}$$

Proof. Binary search reduces the size of the search window after k steps to $\frac{b-a}{2^k}$. Define $\kappa^{(k)}$ as the half-point of the search interval giving $|\kappa^* - \kappa^{(k)}| \leq \frac{b-a}{2^{k+1}}$. Then the Lemma follows immediately by definition of Lipschitz continuity and the triangle inequality of the absolute value. \square

Lemma 6. The quasi-surprisal shares the asymptotics of the surprisal, i.e.

$$\tilde{I}(1) = 0 = -\ln(1) \text{ and } \tilde{I}(r_x) \sim -\ln r_x \text{ as } r_x \rightarrow 0^+.$$

Proof. By the definition of \tilde{I} it holds that $\tilde{I}(r_x) := \frac{1}{2}(\phi(\Phi^{-1}(r_x))/r_x)^2$. Since $t_x := \Phi^{-1}(r_x) \rightarrow -\infty$ as $r_x \rightarrow 0^+$ and according to Lemma 3 both $\phi(t_x) \sim -t_x \Phi(t_x)$ as $t_x \rightarrow -\infty$ and $\Phi^{-1}(r_x) \sim -\sqrt{-2 \ln r_x}$ as $r_x \rightarrow 0^+$ it follows that

$$\phi(\Phi^{-1}(r_x))/r_x \sim -\Phi^{-1}(r_x)/r_x \sim \sqrt{-2 \ln r_x} \text{ as } r_x \rightarrow 0^+.$$

□

Lemma 7 (Law of large numbers for maximum, see Theorem 1 in Gnedenko 1992). *Suppose i.i.d. X_1, X_2, \dots with $\mathbb{P}[X_i \leq x] = F(x) \forall i \in \mathbb{N}$, where $x \mapsto F(x)$ is continuous at all $x > x_0$ for some $x_0 \in \mathbb{R}$ and $F(x) < 1 \forall x \in \mathbb{R}$. Then*

$$\exists (a_n)_{n \in \mathbb{N}} : \forall \epsilon > 0 \lim_{n \rightarrow \infty} \mathbb{P}[\max_{i \leq n} X_i - a_n > \epsilon] = 0 \iff \forall \epsilon > 0 \lim_{x \rightarrow \infty} \frac{1 - F(x + \epsilon)}{1 - F(x)} = 0, \quad (17)$$

giving a necessary and sufficient condition for "convergence in probability to a deterministic sequence". If such a sequence exists it can be selected as $a_n = \inf F^{-1}(\{1 - \frac{1}{n}\}) \forall n \geq n_0, a_n = 0 \forall n < n_0$, where n_0 is s.t. $1 - \frac{1}{n_0} > F(x_0)$.

Proof. Define for any $n \in \mathbb{N}$ the shorthand notation $F^n(x) = (F(x))^n$. Using

$$\mathbb{P}[\max_{i \leq n} X_i - a_n > \epsilon] = \mathbb{P}[\max_{i \leq n} X_i - a_n > \epsilon] + \mathbb{P}[\max_{i \leq n} X_i - a_n < -\epsilon] = (1 - F^n(a_n + \epsilon)) + \lim_{\delta \rightarrow 0^+} F^n(a_n - \epsilon - \delta)$$

we get another representation for the left-hand-side of Equation (17) given by

$$1 \stackrel{!}{=} \lim_{n \rightarrow \infty} 1 - \mathbb{P}[\max_{i \leq n} X_i - a_n > \epsilon] = \lim_{n \rightarrow \infty} F^n(a_n + \epsilon) - \lim_{\delta \rightarrow 0^+} F^n(a_n - \epsilon - \delta),$$

which is equivalent to the conditions¹⁴

$$\begin{aligned} \lim_{n \rightarrow \infty} F^n(a_n + \epsilon) = 1 \wedge \lim_{n \rightarrow \infty} F^n(a_n - \epsilon) = 0 \\ \iff \\ \lim_{n \rightarrow \infty} n \ln F(a_n + \epsilon) = 0 \wedge \lim_{n \rightarrow \infty} n \ln F(a_n - \epsilon) = -\infty. \end{aligned}$$

Using a Taylor expansion of $x \mapsto \ln x$ around 1, i.e. $\ln F(x) = \ln(1 - (1 - F(x))) = -(1 - F(x))(1 + o(1))$, one can simplify the conditions further to

$$\lim_{n \rightarrow \infty} n(1 - F(a_n + \epsilon)) = 0 \wedge \lim_{n \rightarrow \infty} n(1 - F(a_n - \epsilon)) = \infty. \quad (18)$$

Given this simplified form, we now show both directions of the equivalence relation in Equation (17).

Let us start with sufficiency, i.e. " \Leftarrow ". Assume

$$\forall \epsilon > 0 \lim_{x \rightarrow \infty} \frac{1 - F(x + \epsilon)}{1 - F(x)} = 0.$$

Based on the continuity of the cumulative distribution function $F(x)$ for x large enough, define¹⁵ $a_n := \inf F^{-1}(\{1 - \frac{1}{n}\})$ which satisfies $\lim_{n \rightarrow \infty} a_n = \infty$. Then

$$\forall \epsilon > 0 \quad n(1 - F(a_n + \epsilon)) = \frac{1 - F(a_n + \epsilon)}{1 - F(a_n)} \rightarrow 0 \text{ as } n \rightarrow \infty$$

¹⁴Here we used that $\lim_{n \rightarrow \infty} F^n(a_n + \epsilon) = 1 \Rightarrow \lim_{n \rightarrow \infty} F(a_n + \epsilon) = 1 \Rightarrow a_n \rightarrow \infty$ and that $x \mapsto F(x)$ is continuous for $x > x_0$, thus $\lim_{\delta \rightarrow 0^+} F(a_n - \epsilon - \delta) = F(a_n - \epsilon)$ as $n \rightarrow \infty$.

¹⁵Strictly speaking the preimage could be empty. However, for $n \geq n_0$ where n_0 is such that $1 - \frac{1}{n_0} > F(x_0)$ continuity of F prevents this from occurring. Set $a_n = 0 \forall n < n_0$.

and

$$n(1 - F(a_n - \epsilon)) = \frac{1 - F(a_n - \epsilon)}{1 - F(a_n)} = 1 / \frac{1 - F(a_n)}{1 - F(a_n - \epsilon)} \rightarrow \infty \text{ as } n \rightarrow \infty,$$

which are exactly the conditions given in Equation (18).

Let us proceed with necessity, i.e. " \implies ". Assume $\exists (a_n)_{n \in \mathbb{N}}$ such that

$$\forall \epsilon > 0 \quad \lim_{n \rightarrow \infty} n(1 - F(a_n + \epsilon)) = 0 \wedge \lim_{n \rightarrow \infty} n(1 - F(a_n - \epsilon)) = \infty.$$

It follows that $\lim_{n \rightarrow \infty} F(a_n + \epsilon) = 1$ and hence $\lim_{n \rightarrow \infty} a_n = \infty$. Without loss of generality take a_n increasing. For any $x \geq a_1$ determine matching n_x s.t. $a_{n_x-1} \leq x \leq a_{n_x}$. Then $\lim_{x \rightarrow \infty} n_x = \infty$ and it holds that for any $\epsilon > 0$

$$0 \leq \frac{1 - F(x + \epsilon)}{1 - F(x - \epsilon)} \leq \frac{1 - F(a_{n_x-1} + \epsilon)}{1 - F(a_{n_x} - \epsilon)} = \frac{n_x(1 - F(a_{n_x-1} + \epsilon))}{n_x(1 - F(a_{n_x} - \epsilon))} \xrightarrow{x \rightarrow \infty} 0$$

and consequently we obtain the desired result:

$$\forall \epsilon > 0 \quad \lim_{x \rightarrow \infty} \frac{1 - F(x + \epsilon)}{1 - F(x)} = \lim_{x \rightarrow \infty} \frac{1 - F(x + \epsilon/2)}{1 - F(x - \epsilon/2)} = 0.$$

□

F.4 Theoretical Basis for VAPOR in the Bandit Setting

Definition 2 (Cumulant generating function). *Let $X : \Omega \rightarrow \mathbb{R}$ be a random variable on $(\Omega, \Sigma, \mathbb{P})$. Then we define the cumulant generating function as*

$$\Psi_X : \mathbb{D} \rightarrow [0, \infty) \quad \beta \mapsto \ln \mathbb{E}[\exp(\beta(X - \mathbb{E}[X]))]$$

where $\mathbb{D} \subseteq \mathbb{R}$ denotes the interior of the interval of well-definedness.

Proposition 10 (VAPOR, adapted from Lemma 4 in Tarbouriech et al. 2024). *Let $F \in \mathbb{R}^{|\mathcal{X}|}$ be a random vector with σ_{F_x} -sub-Gaussian entries F_x . Then the maximin optimisation problem*

$$\max_{p \in \Delta(\mathcal{X})} \min_{\tau \in \mathbb{R}_+^{|\mathcal{X}|}} \mathcal{V}_\tau(p) \text{ for } \mathcal{V}_\tau(p) := \sum_{x \in \mathcal{X}} p_x \cdot (\mu_{F_x} + \sigma_{F_x}^2 / (2\tau_x) - \ln(p_x) \cdot \tau_x) = H_\tau(p) + \sum_{x \in \mathcal{X}} p_x \cdot (\mu_{F_x} + \sigma_{F_x}^2 / (2\tau_x)) \quad (19)$$

has inner minimiser $\tau_x^* = \sigma_{F_x} / \sqrt{-2 \ln p_x}$, which simplifies the optimisation problem to

$$\max_{p \in \Delta(\mathcal{X})} \mathcal{V}(p) \text{ for } \mathcal{V}(p) := \mathcal{V}_{\tau^*}(p) = \sum_{x \in \mathcal{X}} p_x \cdot \left(\mu_{F_x} + \sqrt{2 \ln(1/p_x)} \sigma_{F_x} \right) = \left\langle p, \mu_F + \sqrt{2I(p)} \odot \sigma_F \right\rangle$$

Crucially, the objective $p \mapsto \mathcal{V}(p)$ is a concave¹⁶ functional. Finally, under Assumption 1 we get the lower bounds:

$$\max_{p \in \Delta(\mathcal{X})} \mathcal{V}(p) \geq \mathcal{V}(\mathbb{P}[\cdot \in X^*]) \geq \mathbb{E}[F^*].$$

Proof. The minimiser τ^* and the minimum $\mathcal{V}(p) = \mathcal{V}_{\tau^*}(p)$ of the (inner) minimisation in Equation (19) follow directly from Lemma 12. Let us now show (strict) concavity of $\mathcal{V}(\cdot)$. It is straightforward to show that the function $g_x(a) = a(\mu_{F_x} + \sigma_{F_x} \sqrt{-2 \ln a})$ is concave for $\sigma_{F_x} \geq 0 \forall x \in \mathcal{X}$ and strictly concave if $\sigma_{F_x} > 0 \forall x \in \mathcal{X}$. Now, let $p, q \in \Delta(\mathcal{X})$ and $\lambda \in (0, 1)$. Then

$$\mathcal{V}(\lambda p + (1 - \lambda)q) = \sum_{x \in \mathcal{X}} g_x(\lambda p_x + (1 - \lambda)q_x) \geq \sum_{x \in \mathcal{X}} \lambda g_x(p_x) + (1 - \lambda)g_x(q_x) = \lambda \mathcal{V}(p) + (1 - \lambda)\mathcal{V}(q),$$

¹⁶It is even strictly concave if $\sigma_{F_x} > 0 \forall x \in \mathcal{X}$.

where the inequality is strict given $\sigma_{F_x} > 0 \forall x \in \mathcal{X}$. We have shown (strict) concavity of the objective $\mathcal{V} : \Delta(\mathcal{X}) \rightarrow \mathbb{R}$. In order to establish $\max_{p \in \Delta(\mathcal{X})} \mathcal{V}(p)$ being lower bounded by $\mathbb{E}[F^*]$ we again invoke Lemma 12, which yields

$$\mathbb{E}[F_x | x \in X^*] \leq \mu_{F_x} + \sigma_{F_x} \sqrt{-2 \ln \mathbb{P}[x \in X^*]}$$

for any $x \in \mathcal{X}$ s.t. $\mathbb{P}[x \in X^*] > 0$. With this upper bound and the additional assumption of an almost surely unique optimum (Assumption 1), we obtain

$$\begin{aligned} \mathbb{E}[F^*] &= \mathbb{E}[E[F^* | X^*]] = \sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^*] \mathbb{E}[F_x | x \in X^*] \leq \sum_{x \in \mathcal{X}} \mathbb{P}[x \in X^*] \left(\mu_{F_x} + \sigma_{F_x} \sqrt{-2 \ln \mathbb{P}[x \in X^*]} \right) \\ &= \mathcal{V}(\mathbb{P}[\cdot \in X^*]), \end{aligned}$$

finishing the proof. \square

Lemma 8 (Variational form of the KL-divergence, generalised from Theorem 3.2 in Gray 2011, which is limited to discrete probability spaces). *Fix two probability distributions $p : \Sigma \rightarrow [0, 1]$ and $q : \Sigma \rightarrow [0, 1]$ over the measurable space (Ω, Σ) such that p is absolutely continuous with respect to q ($p \ll q$). Then*

$$D_{KL}[p||q] = \sup_X \{ \mathbb{E}_p[X] - \ln \mathbb{E}_q[\exp X] \},$$

where the supremum is taken over all measurable $X : \Omega \rightarrow \mathbb{R}$ such that $\mathbb{E}_p[X]$ and $\mathbb{E}_q[\exp X]$ are well-defined.

Proof. Since $p \ll q$, there exists a Radon-Nykodym derivative¹⁷ $\frac{dp}{dq}(\omega)$ such that $p(\mathcal{A}) = \int_{\mathcal{A}} \frac{dp}{dq}(\omega) dq(\omega)$. Setting $X(\omega) = \ln(\frac{dp}{dq}(\omega))$ gives

$$\mathbb{E}_p[X] - \ln(\mathbb{E}_q[\exp X]) = \int_{\Omega} \ln \left(\frac{dp}{dq}(\omega) \right) dp(\omega) - \ln \left(\int_{\Omega} \frac{dp}{dq}(\omega) dq(\omega) \right) = D_{KL}[p||q],$$

from which well-definedness of $\mathbb{E}_p[X]$ and $\mathbb{E}_q[\exp X]$ also follows. Hence, we derived that $D_{KL}[p||q] \leq \sup_X \{ \mathbb{E}_p[X] - \ln \mathbb{E}_q[\exp X] \}$. On the other hand, let $X : \Omega \rightarrow \mathbb{R}$ be any random variable such that $\mathbb{E}_p[X]$ and $\mathbb{E}_q[\exp X]$ are well-defined. Then

$$\begin{aligned} D_{KL}[p||q] - (\mathbb{E}_p[X] - \ln(\mathbb{E}_q[\exp X])) &= \mathbb{E}_p \left[\ln \left(\frac{dp}{dq}(\omega) \right) \right] - \mathbb{E}_p \left[\ln \frac{\exp X}{\mathbb{E}_q[\exp X]} \right] \\ &= \mathbb{E}_p \left[\ln \left(\frac{dp}{dq}(\omega) \frac{\mathbb{E}_q[\exp X]}{\exp(X)} \right) \right] = \mathbb{E}_p \left[\ln \frac{dp}{d\lambda} \right] = D_{KL}[p||\lambda] \geq 0, \end{aligned} \tag{20}$$

where we have defined the probability measure

$$\lambda(\mathcal{A}) = \int_{\mathcal{A}} \exp(X(\omega)) / \mathbb{E}_q[\exp X] dq(\omega)$$

with Radon-Nykodym derivative

$$\frac{d\lambda}{dq}(\omega) = \frac{\exp(X(\omega))}{\mathbb{E}_q[\exp X]} \text{ inducing another derivative } \frac{dq}{d\lambda}(\omega) = \frac{\mathbb{E}_q[\exp X]}{\exp(X(\omega))},$$

due to $\lambda \ll q$ and $q \ll \lambda$ holding both. The final key is that with $p \ll q \ll \lambda$ one further obtains

$$\frac{dp}{dq}(\omega) \frac{\mathbb{E}_q[\exp X]}{\exp(X)} = \frac{dp}{dq} \frac{dq}{d\lambda}(\omega) = \frac{dp}{d\lambda}(\omega),$$

justifying Equation (20). \square

¹⁷The Radon-Nykodym derivative is uniquely defined up to a set of q -measure zero.

Lemma 9 (Conditioned KL-divergence). *Consider the probability space $(\Omega, \Sigma, \mathbb{P})$ and an event $\mathcal{B} \in \Sigma$ of non-zero probability, i.e. $\mathbb{P}[\mathcal{B}] > 0$. Then*

$$D_{KL}[\mathbb{P}[\cdot | \mathcal{B}] \parallel \mathbb{P}] = -\ln \mathbb{P}[\mathcal{B}].$$

Proof. By the definition of conditional expectation it holds

$$\mathbb{P}[\mathcal{A} | \mathcal{B}] = \frac{\mathbb{P}[\mathcal{A} \cap \mathcal{B}]}{\mathbb{P}[\mathcal{B}]} = \int_{\mathcal{A}} \frac{\mathbb{1}_{\omega \in \mathcal{B}}}{\mathbb{P}[\mathcal{B}]} d\mathbb{P}(\omega) \quad \forall \mathcal{A} \in \Sigma.$$

where we recognise absolute continuity $\mathbb{P}[\cdot | \mathcal{B}] \ll \mathbb{P}$ and the Radon-Nykodym derivative

$$\frac{d\mathbb{P}[\cdot | \mathcal{B}]}{d\mathbb{P}}(\omega) = \frac{\mathbb{1}_{\omega \in \mathcal{B}}}{\mathbb{P}[\mathcal{B}]}.$$

Hence, we obtain the following expression for the Kullback-Leibler divergence:

$$D_{KL}[\mathbb{P}[\cdot | \mathcal{B}] \parallel \mathbb{P}] = \int_{\Omega} \ln \frac{d\mathbb{P}[\cdot | \mathcal{B}]}{d\mathbb{P}} d\mathbb{P}[\cdot | \mathcal{B}] = \int_{\Omega} \ln \frac{\mathbb{1}_{\omega \in \mathcal{B}}}{\mathbb{P}[\mathcal{B}]} d\mathbb{P}[\cdot | \mathcal{B}] = -\ln \mathbb{P}[\mathcal{B}]$$

□

Lemma 10 (Information theoretic upper bound on conditional expectation, see Theorem 1 in O'Donoghue and Lattimore 2021 and Lemma 11 in Tarbouriech et al. 2024). *Let $X : \Omega \rightarrow \mathbb{R}$ be a random variable on $(\Omega, \Sigma, \mathbb{P})$ such that the cumulative generating function restricted to \mathbb{R}^+*

$$\Psi_X : \mathbb{D} \subseteq \mathbb{R}^+ \rightarrow [0, \infty) \quad \beta \mapsto \ln \mathbb{E}[\exp(\beta(X - \mathbb{E}[X]))]$$

exists. Assume further that $\mathbb{P}[\mathcal{B}] > 0$ such that $\mathbb{P}[\cdot | \mathcal{B}]$ is well-defined. Then with Ψ_X^ the convex conjugate of Ψ_X it holds*

$$\mathbb{E}[X | \mathcal{B}] \leq \mathbb{E}[X] + (\Psi_X^*)^{-1}(D_{KL}[\mathbb{P}[\cdot | \mathcal{B}] \parallel \mathbb{P}]).$$

Proof. Since Given Ψ_X exists, Ψ_X^* is well-defined, as the cumulant generating function is non-negative and convex. Let us apply Lemma 8 to $p(\mathcal{E}) = \mathbb{P}[\mathcal{E} | \mathcal{B}]$, $q(\mathcal{E}) = \mathbb{P}[\mathcal{E}]$, and restrict the supremum over the random variables $\{\lambda(X - \mathbb{E}[X])\}_{\lambda \in \mathbb{R}^+}$. Then

$$\begin{aligned} D_{KL}[\mathbb{P}[\cdot | \mathcal{B}] \parallel \mathbb{P}] &\geq \sup_{\lambda \in \mathbb{R}^+} \{ \lambda \mathbb{E}[X - \mathbb{E}[X] | \mathcal{B}] - \ln \mathbb{E}[\exp(\lambda(X - \mathbb{E}[X]))] \} \\ &= \sup \{ \lambda(\mathbb{E}[X | \mathcal{B}] - \mathbb{E}[X]) - \Psi_X(\lambda) : \lambda \in \mathbb{R}^+ \} \\ &= \Psi_X^*(\mathbb{E}[X | \mathcal{B}] - \mathbb{E}[X]) \end{aligned}$$

Furthermore, since $\lambda \in \mathbb{R}^+$ it follows that Ψ_X^* is strictly increasing and thus admits a strictly increasing inverse which finishes the proof:

$$(\Psi_X^*)^{-1}(D_{KL}[\mathbb{P}[\cdot | \mathcal{B}] \parallel \mathbb{P}]) \geq \mathbb{E}[X | \mathcal{B}] - \mathbb{E}[X].$$

□

Lemma 11 (Upper bound on the inverse of Ψ^* for sub-Gaussians). *Let $X : \Omega \rightarrow \mathbb{R}$ be a σ -sub-Gaussian random variable on $(\Omega, \Sigma, \mathbb{P})$, i.e. $\mathbb{E}[\exp(\lambda(X - \mathbb{E}[X]))] \leq \exp(\sigma^2 \lambda^2 / 2) \forall \lambda \in \mathbb{R}$. Then the cumulant generating function restricted to \mathbb{R}^+ exists globally, i.e. $\Psi_X : \mathbb{R}^+ \rightarrow [0, \infty)$ is well-defined, its convex dual Ψ_X^* is strictly increasing (and hence admits a strictly increasing inverse), and it holds that*

$$(\Psi_X^*)^{-1}(\lambda) \leq \sigma \sqrt{2\lambda} \quad \forall \lambda \geq 0$$

Proof. Since X is sub-Gaussianity, then the cumulant generating function $\Psi_X : \mathbb{R}^+ \rightarrow [0, \infty)$ exists on all of \mathbb{R}^+ with

$$\Psi_X(\beta) \leq \beta^2 \sigma^2 / 2 \quad \forall \beta > 0.$$

We then get its strictly increasing convex dual

$$\Psi_X^*(\alpha) = \sup \{ \alpha \beta - \Psi_X(\beta) : \beta \in \mathbb{R}^+ \} \quad \alpha \in \mathbb{R}.$$

Consequently, $\alpha \mapsto \Psi_X^*(\alpha)$ admits an inverse derived by

$$\begin{aligned}
 \alpha = (\Psi_X^*)^{-1}(\lambda) &\iff \lambda = \sup\{\alpha\beta - \Psi_X(\beta) : \beta \in \mathbb{R}^+\} \\
 &\iff \lambda \geq \alpha\beta - \Psi_X(\beta) \quad \forall \beta \in \mathbb{R}^+ \\
 &\quad \wedge \forall \epsilon > 0 \exists \beta_\epsilon \in \mathbb{R}^+ \text{ s.t. } \lambda - \epsilon < \alpha\beta_\epsilon - \Psi_X(\beta_\epsilon) \\
 &\iff \alpha \leq \lambda/\beta + \Psi_X(\beta)/\beta \quad \forall \beta \in \mathbb{R}^+ \\
 &\quad \wedge \forall \epsilon > 0 \exists \beta_\epsilon \in \mathbb{R}^+ \text{ s.t. } \alpha + \epsilon > \lambda/\beta_\epsilon + \Psi_X(\beta_\epsilon)/\beta_\epsilon \\
 &\iff (\Psi_X^*)^{-1}(\lambda) = \alpha = \inf\{\lambda/\beta + \Psi_X(\beta)/\beta : \beta \in \mathbb{R}^+\}.
 \end{aligned}$$

Finally, plugging in Equation (F.4) we obtain

$$(\Psi_X^*)^{-1}(\lambda) \leq \inf\{\lambda/\beta + \beta\sigma^2/2 : \beta \in \mathbb{R}^+\} = \sigma\sqrt{2\lambda} \quad \forall \lambda \geq 0.$$

□

Lemma 12 (Upper bound on conditional expectation for sub-Gaussians). *Let $X : \Omega \rightarrow \mathbb{R}$ be a σ -sub-Gaussian random variable on $(\Omega, \Sigma, \mathbb{P})$, i.e. it satisfies $\mathbb{E}[\exp(\lambda(X - \mathbb{E}[X]))] \leq \exp(\sigma^2\lambda^2/2) \quad \forall \lambda \in \mathbb{R}$, and let $\mathcal{B} \in \Sigma$ such that $\mathbb{P}[\mathcal{B}] > 0$. Then*

$$\mathbb{E}[X|\mathcal{B}] \leq \mathbb{E}[X] + \sigma\sqrt{-2\ln\mathbb{P}[\mathcal{B}]} = \mathbb{E}[X] + \min\left\{\frac{\sigma^2}{2s} - s\ln\mathbb{P}[\mathcal{B}] : s > 0\right\},$$

with minimiser $s^* = \sigma/\sqrt{-2\ln\mathbb{P}[\mathcal{B}]}$.

Proof. According to Lemma 11 the cumulant generating function Ψ_X restricted to \mathbb{R}^+ exists everywhere and its convex conjugate admits an inverse with upper bound:

$$(\Psi_X^*)^{-1}(\lambda) \leq \sigma\sqrt{2\lambda}.$$

Moreover, according to Lemma 10 and Lemma 9 it holds that

$$\mathbb{E}[X|\mathcal{B}] \leq \mathbb{E}[X] + (\Psi_X^*)^{-1}(-\ln\mathbb{P}[\mathcal{B}]).$$

Combining the two equations yields the first desired statement:

$$\mathbb{E}[X|\mathcal{B}] \leq \mathbb{E}[X] + \sigma\sqrt{-2\ln\mathbb{P}[\mathcal{B}]}.$$

Finally, a separate examination of the first order condition of

$$\min\left\{\frac{\sigma^2}{2s} - s\ln\mathbb{P}[\mathcal{B}] : s > 0\right\}$$

results in the minimum $\sigma\sqrt{-2\ln\mathbb{P}[\mathcal{B}]}$ for the minimiser $s^* = \sigma/\sqrt{-2\ln\mathbb{P}[\mathcal{B}]}$.

□