

000 LOCAL ENTROPY SEARCH OVER DESCENT SEQUENCES 001 FOR BAYESIAN OPTIMIZATION

002 **Anonymous authors**

003 Paper under double-blind review

004 ABSTRACT

005 Searching large and highly complex design spaces for a global optimum can
006 be infeasible and unnecessary. A practical alternative is to iteratively refine the
007 neighborhood of an initial design using local optimization methods such as gradient
008 descent. We propose local entropy search (LES), a Bayesian optimization paradigm
009 that explicitly targets the solutions reachable by the descent sequences of arbitrary
010 iterative optimizers. The algorithm propagates the posterior belief over the objective
011 through the optimizer, yielding a probability distribution over descent sequences.
012 It then selects the next evaluation by maximizing mutual information with that
013 distribution, using a practical combination of analytic entropy calculations and
014 Monte-Carlo sampling of descent sequences. Empirical results on high-complexity
015 synthetic objectives and benchmark problems show that LES achieves strong
016 sample efficiency compared to existing local and global Bayesian optimization
017 methods.

018 1 INTRODUCTION

019 Many practical optimization problems can be solved to the desired accuracy by relying solely on
020 iterative search strategies such as gradient descent, quasi-Newton methods, or evolutionary algorithms.
021 These methods do not necessarily discover a global minimizer, but refine the current solution. Local
022 optimization has repeatedly demonstrated its effectiveness in finding good solutions particularly in
023 high-dimensional and complex search spaces. Indeed, gradient-based methods remain state-of-the-art
024 for solving extreme-scale problems such as training deep neural networks with billions of parameters
025 (Chowdhery et al., 2023). However, those local optimization methods cannot directly be applied to
026 expensive-to-evaluate black-box functions due to their poor sample-efficiency.

027 Bayesian optimization (BO) (Garnett, 2023) methods are popular for expensive-to-evaluate black-box
028 functions, yet they typically aim to minimize regret relative to the global optimum. Global search
029 requires reducing uncertainty across the entire domain, which can be intractable in large and high-
030 dimensional spaces (Hvarfner et al., 2024; Xu et al., 2025). Thus, the emphasis on global search in
031 BO stands in contrast to the demonstrated effectiveness of local optimization for complex problems.

032 We introduce local entropy search (LES)¹, an information-theoretic framework for local BO that
033 transfers the idea of iterative local optimizers to the expensive-to-evaluate black-box setting. LES
034 explicitly targets the solution obtainable by an iterative optimizer starting from an initial design. LES
035 propagates the uncertainty of a Gaussian process (GP) surrogate through the local optimizer, yielding
036 a distribution over the descent sequence and the local optimum (see Fig. 1). At each iteration, LES
037 chooses the next evaluation to maximize the mutual information with the distribution over the descent
038 sequence, thereby reducing its uncertainty.

039 While several recent efforts (see Sec. 2.1) have brought local strategies to BO framework, acquisition
040 functions have so far provided only partial use of the iterative descent structure or have focused on
041 special cases. Our approach builds directly on entropy search principles (Hennig & Schuler, 2012) but
042 shifts the focus from the global optimum to the reachable local optimum as defined by the optimizer’s
043 descent trajectory.

044
045
046
047
048
049
050
051
052
053
1 Code available in the supplementary material.

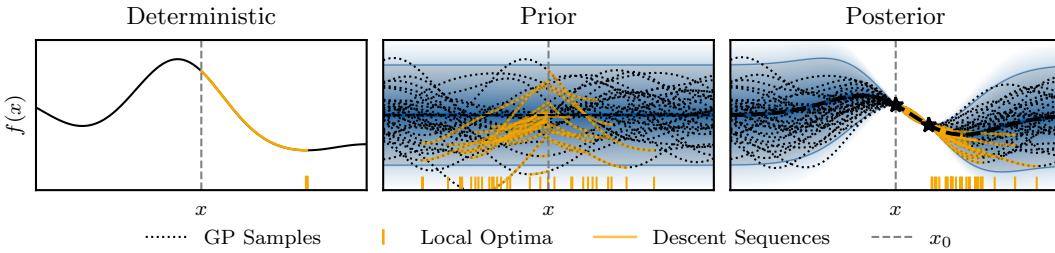


Figure 1: **Distribution over Descent Sequences:** *Left:* Local optimization on the unknown objective function. *Middle:* The prior over the objective function induces a belief over descent sequences. *Right:* After sampling data points the distributions over descent sequences and local optimum approach the deterministic ones. In LES the next query minimizes the entropy of the descent sequences.

To ensure tractability, LES combines analytic predictive entropy calculations with Monte-Carlo conditioning over sampled descent sequences. We evaluate LES against state-of-the-art local and global BO methods on higher-dimensional synthetic objectives with varying complexity and policy search tasks. LES achieves lower simple and cumulative regret with fewer evaluations especially in high-complexity tasks. In summary, our contributions are:

- We formulate *local entropy search* (LES) as an information-theoretic Bayesian optimization paradigm that targets the terminal iterate of an arbitrary optimizer, making LES the first entropy-based approach explicitly focusing on local optima rather than the global optimum.
- We present a computationally lightweight instantiation of LES as an active learning problem over descent sequences by propagating the posterior belief through the optimizer via Monte-Carlo approximation based on efficient GP sampling (Wilson et al., 2020).
- We provide empirical evidence that this LES instantiation surpasses both global entropy-search baselines and existing local BO methods on high-complexity benchmarks.

In addition, we adapt a recent stopping criterion for BO (Wilson, 2024) to the LES setting, guaranteeing a probabilistic *local regret* bound (see Appx. E).

2 PRELIMINARIES

In this section, we discuss the related work on local BO and entropy search and briefly introduce GPs and an analytical approximation of their sampling paths.

2.1 RELATED WORK

Bayesian optimization is a popular method for many challenging real-world applications such as AutoML (Barbudo et al., 2023), drug discovery (Colliandre & Muller, 2023), and policy search (Paulson et al., 2023). For a recent introduction and overview see (Garnett, 2023). Below we present related work in entropy search and local BO – the two BO subfields most relevant to LES.

Entropy Search Global entropy search acquisition functions use an information-theoretic perspective to select the next BO query point (See Appx. A for a detailed introduction). They find a point that maximizes the expected information gain about properties of the global optimum. The original entropy search (ES) (Hennig & Schuler, 2012) and predictive entropy search (PES) (Hernández-Lobato et al., 2014) maximize the information gain about the *location* of the optimum. In contrast, max-value entropy search (MES) (Wang & Jegelka, 2017) maximize the information gain about the *function value* of the optimum. MES is computationally more efficient than both ES and PES. Joint entropy search (Hvorfner et al., 2022; Tu et al., 2022) maximizes the information gain about the joint distribution of *location* and *function value* of the optimum. Entropy search has been extended to constrained (Perrone et al., 2019), multi-objective (Belakaria et al., 2020), and multi-fidelity (Marco et al., 2017) optimization. With LES we propose the first local version of entropy search by targeting a local optimum instead of a global one.

108 **Local BO** There are two main approaches commonly used for local BO, *trust regions* (Akrour
 109 et al., 2017; Fröhlich Lukas P. et al., 2019; Eriksson et al., 2019) and line search (Kirschner et al.,
 110 2019; Müller et al., 2021; Nguyen et al., 2022; Wu et al., 2023; Fan et al., 2024). Trust-region BO
 111 such as TuRBO (Eriksson et al., 2019) explicitly maintain a subset of the search space \mathcal{X} and restricts
 112 queries to be within this subset. In contrast, BO methods based on line search maintain an incumbent
 113 solution and iteratively choose a search direction and step size to improve the candidate. For example,
 114 gradient information BO (GIBO) (Müller et al., 2021) leverages the GP model of the objective’s
 115 gradient ∇f to find its search direction and step size. Similar to these methods, LES starts its search
 116 from an incumbent solution but in contrast to GIBO and its variants does not use the learned gradient
 117 to update it but instead learns about the entire descent sequence. The local BO methods above have
 118 been shown to outperform global BO methods in high-complexity tasks.
 119

120 Recent works showed that vanilla Bayesian optimization can solve high-dimensional problems if
 121 model complexity, specifically length scales of the GP kernel, is chosen appropriately (Hvarfner et al.,
 122 2024; Xu et al., 2025). While assumed model complexity is an important consideration for BO, the
 123 design of suitable prior assumption can benefit local and global BO methods and the acquisition
 124 strategy is mostly orthogonal. In Section 6, we show empirically that local BO and especially LES
 125 outperforms global BO for complex and higher-dimensional tasks.
 126

127 2.2 GPS AND EFFICIENT POSTERIOR GP SAMPLING

128 In this paper, BO uses a Gaussian Process (GP) (Rasmussen & Williams, 2006) as a fast-to-evaluate
 129 probabilistic surrogate for the unknown scalar function $f(\mathbf{x})$. We denote a GP as
 130

$$p(f) = \mathcal{GP}(f; \mu, k), \quad (1)$$

131 where $\mu : \mathcal{X} \rightarrow \mathbb{R}$ is the prior mean and $k : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is the prior covariance function, with
 132

$$\mu(\mathbf{x}) = \mathbb{E}[f(\mathbf{x}) | \mathbf{x}], \quad k(\mathbf{x}, \mathbf{x}') = \mathbb{E}[(f(\mathbf{x}) - \mu(\mathbf{x}))(f(\mathbf{x}') - \mu(\mathbf{x}'))], \quad (2)$$

133 where \mathbb{E} is the expectation. Without loss of generality, we assume $\mu(\mathbf{x}) = 0$. Given a dataset of noisy
 134 observations $y(\mathbf{x}) = f(\mathbf{x}) + \epsilon_t$, where the noise realization ϵ_t is modeled as a draw from a normal
 135 distribution $\mathcal{N}(0, \sigma_n^2)$, denoted as $\mathcal{D}_t = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_t, y_t)\}$ the posterior belief over a function
 136 value $f(\mathbf{x})$ is a normal distribution denoted as
 137

$$p(f(\mathbf{x}) | \mathcal{D}_t) = \mathcal{N}(f(\mathbf{x}); \mu(\mathbf{x} | \mathcal{D}_t), k(\mathbf{x}, \mathbf{x} | \mathcal{D}_t)). \quad (3)$$

138 Here, we denote $\mu(\mathbf{x} | \mathcal{D}_t)$ as the posterior mean and $k(\mathbf{x}, \mathbf{x}' | \mathcal{D}_t)$ as the posterior covariance
 139 between two points \mathbf{x} and \mathbf{x}' . The predictive variance for a noisy observation is $\sigma_y^2(\mathbf{x} | \mathcal{D}_t) =$
 140 $k(\mathbf{x}, \mathbf{x} | \mathcal{D}_t) + \sigma_n^2$. See (Rasmussen & Williams, 2006) for details on GP regression.
 141

142 To draw samples from the posterior distribution of objective functions $p(f | \mathcal{D}_k)$ we follow the
 143 analytical approximation proposed by (Wilson et al., 2020) that relies on Matheron’s rule (Journel &
 144 Huijbregts, 1978) (see Appx. C.1). We denote f_t^l as a sample from $p(f | \mathcal{D}_t)$:
 145

$$f_t^l(\cdot) = \underbrace{\sum_{i=1}^I w_i^l \phi_i(\cdot)}_{\text{weight-space prior}} + \underbrace{\sum_{j=1}^t v_j k(\cdot, \mathbf{x}_j)}_{\text{function-space update}}, \quad (4)$$

146 where w_i^l are randomly drawn weights, $\phi_i(\cdot)$ are basis functions and v_j is calculated from the training-
 147 data covariance matrix. The sample approximations of (4) are analytic which means we can easily
 148 differentiate with respect to \mathbf{x} and apply iterative optimizers such as gradient descent. LES can be
 149 applied to other probabilistic models from which we can efficiently draw posterior samples, e.g.,
 150 variational Bayesian last layer models (Brunzema et al., 2024).
 151

152 3 PROBLEM STATEMENT

153 The local black-box optimization problem is to find the best reachable solution from a given initial
 154 design \mathbf{x}_0
 155

$$\text{given } \mathbf{x}_0 \in \mathcal{X}, \text{ find } \mathbf{x}^* = \arg \min_{\mathbf{x} \in \mathcal{X}(\mathbf{x}_0) \subseteq \mathcal{X}} f(\mathbf{x}), \quad (5)$$

162 where $f : \mathcal{X} \rightarrow \mathbb{R}$ is the black-box objective function and $\mathcal{X}(\mathbf{x}_0)$ is some neighborhood around \mathbf{x}_0 .
 163

164 We consider local optimization where an iterative (and possibly stochastic) optimization routine \mathcal{O}
 165 generates a sequence of iterates – the *descent sequence* – converging to a local optimum \mathbf{x}^* as

$$\mathcal{O}_{\mathbf{x}_0} : \mathcal{F}(\mathcal{X}) \longrightarrow \mathcal{X}^N, \quad \mathcal{O}_{\mathbf{x}_0}(f) := (\mathbf{z}_0 = \mathbf{x}_0, \mathbf{z}_1, \dots) \subset \mathcal{X} \quad (6)$$

167 where

$$\mathbf{x}^* = \lim_{n \rightarrow \infty} \mathbf{z}_n, \quad (7)$$

168 or $\mathbf{x}^* = \mathbf{z}_N$ for finite descent sequences. We assume that the chosen optimizer converges for all
 169 sample paths of the GP prior (1). For instance, under suitable assumptions, gradient descent with an
 170 appropriate step size η produces the convergent sequence
 171

$$\text{GD}_{\mathbf{x}_0}(f) := \{\mathbf{z}_0 = \mathbf{x}_0, \mathbf{z}_1 = \mathbf{z}_0 - \eta \nabla f(\mathbf{z}_0), \mathbf{z}_2 = \mathbf{z}_1 - \eta \nabla f(\mathbf{z}_1), \dots\}. \quad (8)$$

172 When f is known we can directly apply \mathcal{O} . However, we are in the standard BO black-box setting,
 173 where we cannot directly create this sequence. We instead consider the bandit setting with sequential
 174 queries to an expensive-to-evaluate black-box function with noisy zero-order evaluations $y_t =$
 175 $f(\mathbf{x}_t) + \epsilon_t$ at locations \mathbf{x}_t . Therefore, the objective of this work is to find a practical strategy that best
 176 approximates the solution to (5) in a data-efficient manner by learning about the descent sequence.
 177

179 4 ENTROPY MINIMIZATION OF UNCERTAIN DESCENT SEQUENCES

180 **Overview.** We aim to apply the entropy search principle not to the global optimum but to the *descent*
 181 *sequence* started from \mathbf{x}_0 . **Goal:** Choose the next query \mathbf{x} that most reduces uncertainty about the
 182 entire descent sequence starting from \mathbf{x}_0 , i.e., the sequence generated by an iterative optimizer \mathcal{O} .
 183 Once we know the descent sequence, we also know the local optimum \mathbf{x}^* . **Idea:** Treat the descent
 184 sequence itself as the object of interest and apply the entropy-search principle to it: select \mathbf{x} to
 185 maximize information gain about that sequence. We target the mutual information between $(\mathbf{x}, y(\mathbf{x}))$
 186 and the random descent sequence induced by the GP posterior and \mathcal{O} . The remainder of this section
 187 formalizes this idea. After the formalization we give a practical algorithm in Sect. 5.
 188

189 Given $p(f)$ as a distribution over functions, applying an optimizer O from \mathbf{x}_0 induces a random
 190 descent sequence with observations R , as
 191

$$Q_{\mathbf{x}_0} = ((\mathbf{z}_0, R_0), (\mathbf{z}_1, R_1), \dots). \quad (9)$$

192 where \mathbf{z}_n are iterates and R_n are some observation of the objective function f at \mathbf{x} depending
 193 on O . Examples are function values $R_n := f(\mathbf{z}_n)$ (e.g., hill climbing) or gradient information
 194 $R_n := \nabla f(\mathbf{z}_n)$ (e.g. gradient descent). Reducing the uncertainty about $Q_{\mathbf{x}_0}$ also reduces uncertainty
 195 about the local optimum \mathbf{x}^* (see Fig. 1).
 196

197 To apply the entropy search framework (Hennig & Schuler, 2012) to this problem, we minimize
 198 the entropy $H(Q_{\mathbf{x}_0})$ of the descent sequence. Minimizing the entropy with a new observation is
 199 equivalent to maximizing the mutual information between the new observation $(\mathbf{x}, y(\mathbf{x}))$ and the
 200 descent sequence $Q_{\mathbf{x}_0}$ conditioned on the current data \mathcal{D}_t . Therefore, in LES we reduce entropy over
 201 $Q_{\mathbf{x}_0}$ by selecting queries that maximize mutual information with this distribution, as

$$\alpha_{\text{LES}}(\mathbf{x}) = I((\mathbf{x}, y(\mathbf{x})); Q_{\mathbf{x}_0} | \mathcal{D}_t), \quad (10)$$

202 which we reformulate into a tractable form in Sect. 5. Note, that the observations R needs to contain
 203 the information the iterative optimizer requires to determine the next iterate. Therefore, (10) requires
 204 knowledge about the inner workings of the iterative optimizer to determine Q . We will discuss the
 205 case of gradient descent sequences as an example at the end of this section.
 206

207 *Remark 1.* An alternative formulation for LES is to define the random variable $O_{\mathbf{x}_0}^*$ directly over the
 208 *local optimum* \mathbf{x}^* of $\mathcal{O}_{\mathbf{x}_0}(f)$. The distribution of $O_{\mathbf{x}_0}^*$ is the push-forward of $p(f)$ under $\mathcal{O}_{\mathbf{x}_0}$ and
 209 taking the limit as in (7). Unfortunately, the mutual information

$$I((\mathbf{x}, y(\mathbf{x})); O_{\mathbf{x}_0}^* | \mathcal{D}_t). \quad (11)$$

210 is not tractable in the general case since we would need to condition a GP on the event $O_{\mathbf{x}_0}^* = \mathbf{x}^*$
 211 which involves the entire descent sequences (see Appx. B.1). We propose and evaluate an alternative
 212 approximation in Appx. F.2.
 213

214 A tractable special case is gradient descent that terminates after the first step. The resulting acquisition
 215 function is GIBO (Müller et al., 2021) with entropy instead of the trace of the covariance matrix (see
 216 Appx. B.2).

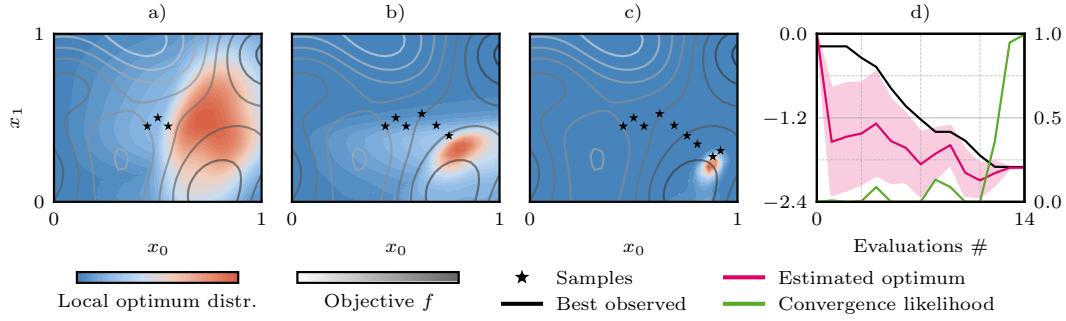


Figure 2: **Illustration of LES on a 2D example:** *a)* After three initial evaluations, the distribution over reachable local optima is wide. *b, c)* As LES selects new points, evaluations concentrate near the descent sequence, and the distribution of the local optimum narrows. *d)* Convergence behavior of LES. After 14 evaluations, the convergence criterion (see Appx. E.1) stops the optimization.

Local Entropy Search with Gradient Descent Sequences. Before we move on to the next section, we discuss the LES acquisition function for the gradient descent algorithm. The descent sequence is defined through the initial design \mathbf{x}_0 and the gradient of the function ∇f at the locations \mathbf{z}_n as $\mathbf{x}^* = \lim_{n \rightarrow \infty} \sum_{i=0}^n \mathbf{z}_i - \eta \nabla f(\mathbf{z}_i)$.

Since we can easily condition a GP on gradient information (Rasmussen & Williams, 2006) a LES acquisition function for local optimization via gradient descent is

$$\alpha_{\text{LES-GD}}(\mathbf{x}) = I((\mathbf{x}, y(\mathbf{x})); Q_{\mathbf{x}_0} \mid \mathcal{D}_t), \quad (12)$$

with $Q_{\mathbf{x}_0} = ((\mathbf{z}_0 = \mathbf{x}_0, \nabla f(\mathbf{z}_0)), (\mathbf{z}_1, \nabla f(\mathbf{z}_1)), \dots)$. In words: We are looking for the query whose outcome will reveal the most information about *gradients* of the function at the (distribution of) locations of the descent sequence. Generally, the design of the sequence $Q_{\mathbf{x}_0}$ is dependent on the optimizer choice \mathcal{O} and the properties of the GP samples (see Appx. C.2). The performance and computational burden of LES depends on the design choices. We investigate alternative choices for gradient descent in Section 6.

Remark 2. For GPs with a squared exponential kernel the push-forward of gradient-descent sequences is dense in \mathcal{X} . This means, in principle, there can be sequences arbitrarily close to any point in the domain and no region is a priori ‘‘forbidden.’’ In addition, all descent sequences are possible under this prior. For details, see Appx. G.2.

5 LOCAL ENTROPY SEARCH

This section casts the general local entropy search paradigm (Sec. 4) into a practical algorithm; see Fig. 2 for an illustrative example and Algorithm 1. We first derive the acquisition function (Sec. 5.1), afterwards we describe how to approximate the distribution of gradient descent sequences and how to condition on them (Sec. 5.2).

5.1 THE LES ACQUISITION FUNCTION

The LES acquisition function follows the entropy-search principle: ask where an observation $(\mathbf{x}, y(\mathbf{x}))$ would tell us most about the optimizer’s descent sequence $Q_{\mathbf{x}_0}$ – their mutual information. In practice this means comparing two entropies: (i) the predictive entropy at \mathbf{x} , which measures the overall uncertainty about $y(\mathbf{x})$ under the GP, and (ii) the expected entropy that remains if we condition on how \mathbf{x} would influence the descent sequences drawn from the GP posterior.

$$\begin{aligned} \alpha_{\text{LES}}(\mathbf{x}) &= I((\mathbf{x}, y(\mathbf{x})); Q_{\mathbf{x}_0} \mid \mathcal{D}_t) \\ &= \underbrace{H[y(\mathbf{x}) \mid \mathcal{D}_t]}_{\text{predictive entropy}} - \mathbb{E}_f \underbrace{H[y(\mathbf{x}) \mid \mathcal{D}_t, Q_{\mathbf{x}_0}]}_{\text{conditional entropy}}. \end{aligned} \quad (13)$$

The predictive entropy (see Fig. 3, b)) can be calculated in closed form, as

$$H[y(\mathbf{x}) \mid \mathcal{D}_t] = \frac{1}{2} \log (2\pi e \sigma_y^2(\mathbf{x} \mid \mathcal{D}_t)). \quad (14)$$

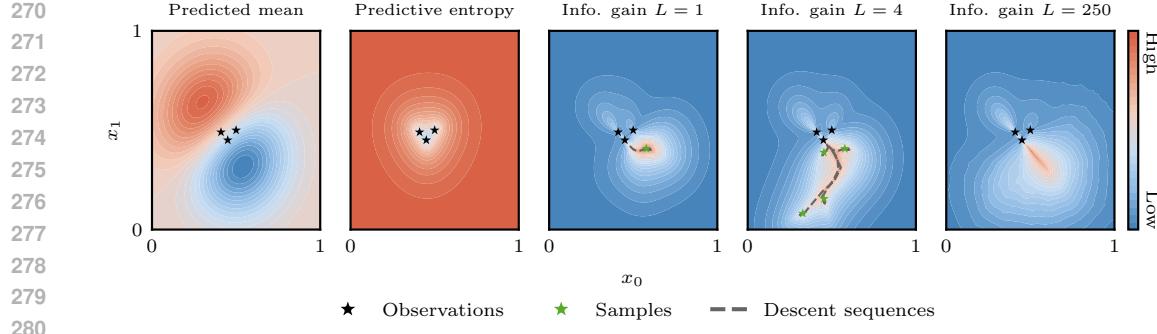


Figure 3: **Illustration of the LES acquisition function after three evaluations:** *Left:* The GP posterior mean after conditioning on the observations. *Second:* The predictive entropy is high in regions with large posterior variance. *Third to fifth:* The information gain between sampled descent sequences and query locations in \mathcal{X} (the LES acquisition function) is high at points that are far from existing observations and aligned with likely descent sequences.

The expectation over the conditional entropy is more challenging. We do not have a closed form expression of the distribution of $Q_{\mathbf{x}_0}$ as this would mean to apply the optimization routine \mathcal{O} to the distribution $p(f|\mathcal{D}_t)$. Thus, we cannot analytically calculate the expectation from it. Therefore, we approximate it by L Monte-Carlo samples:

$$\mathbb{E}_f [H[p(y(\mathbf{x}) | \mathcal{D}_t, Q_{\mathbf{x}_0})]] \approx \frac{1}{L} \sum_{l=1}^L H[p(y(\mathbf{x}) | \mathcal{D}_t, Q_{\mathbf{x}_0}^l)]. \quad (15)$$

To approximate $Q_{\mathbf{x}_0}$, we first draw L sample paths from the posterior GP according to (4) to retrieve samples f_t^1, \dots, f_t^L . Then we apply the optimization routine \mathcal{O} to each sample to retrieve the descent sequences $Q_{\mathbf{x}_0}^l = ((\mathbf{x}_0, R_0^l), (\mathbf{x}_1^l, R_1^l), \dots)$ and the local optima $\mathbf{x}^{l,*}$.

For example, in the case of gradient descent, we get $Q_{\mathbf{x}_0}^l = ((\mathbf{z}_0^l = \mathbf{x}_0, R_0^l = \nabla f^l(\mathbf{x}_0)), (\mathbf{z}_1^l = \mathbf{x}_0 - \nabla f^l(\mathbf{x}_0), R_1^l = \nabla f^l(\mathbf{z}_1^l)), \dots)$.

To condition on the parameter observation pairs $Q_{\mathbf{x}_0}^l$, we add them to the already existing observations and analytically compute the predictive posterior variance and entropy. Note that we approximate $Q_{\mathbf{x}_0}^l$ with a finite sequence to compute (15) (see Sec. 5.2). By inserting (14) and the approximation (15) into (13) we get the final LES acquisition function (see Fig. 3):

$$\alpha_{\text{LES}}(\mathbf{x}) \approx \frac{1}{2} \log(2\pi e \sigma_y^2(\mathbf{x} | \mathcal{D}_t)) - \frac{1}{L} \sum_{l=1}^L \frac{1}{2} \log(2\pi e \sigma_y^2(\mathbf{x} | \mathcal{D}_t \cup Q_{\mathbf{x}_0}^l)). \quad (16)$$

Extension of the LES acquisition function to the batch case is straight forward (see Appx. C.3).

Algorithm 1 Local Entropy Search with stopping rule

```

1: Input: initial design and corresponding observation  $\mathcal{D}_1 = (\mathbf{x}_0, y_0)$ , local optimizer  $\mathcal{O}$ 
2: for  $t \in 1, 2, \dots$  do
3:    $\mathcal{GP}_t \leftarrow$  fit GP model of  $f(\mathbf{x})$  using  $\mathcal{D}_t$  with MAP hyperparameter optimization
4:    $\hat{\mathbf{x}}_t^*, \hat{f}_t^* \leftarrow$  identify current optimum from  $\mathcal{D}_t$ 
5:    $f^1, \dots, f^L \leftarrow$  draw  $L$  samples from  $\mathcal{GP}_t$  ▷ cf. (4)
6:   for  $l \in 1, \dots, L$  do  $Q^l \leftarrow$  apply  $\mathcal{O}$  to  $f^l$  starting from  $\hat{\mathbf{x}}_t^*$ 
7:    $\mathbf{x}_{t+1} = \text{argmax}_{\mathbf{x} \in Q^1, \dots, Q^L} \alpha_{\text{LES}}(\mathbf{x})$  ▷ Maximize LES acquisition function cf. Sec. 5.1
8:   for  $l \in 1, \dots, L$  do  $r_t^l = f^l(\hat{\mathbf{x}}_t^*) - f^l(\mathbf{x}^{l,*})$  ▷ Estimate local regret
9:   if  $\sum_{l=1}^L \mathbb{1}(r_t^l \leq \epsilon) \geq k_{\text{max}}$  do stop ▷ Stopping rule for probabilistic regret. See Appx. E.
10:   $y_{t+1} \leftarrow$  evaluate objective with  $\mathbf{x}_{t+1}$ 
11:   $\mathcal{D}_{t+1} \leftarrow \mathcal{D}_t \cup \{(\mathbf{x}_{t+1}, y_{t+1})\}$ 
12: end for
13: return  $\hat{\mathbf{x}}^*$ 

```

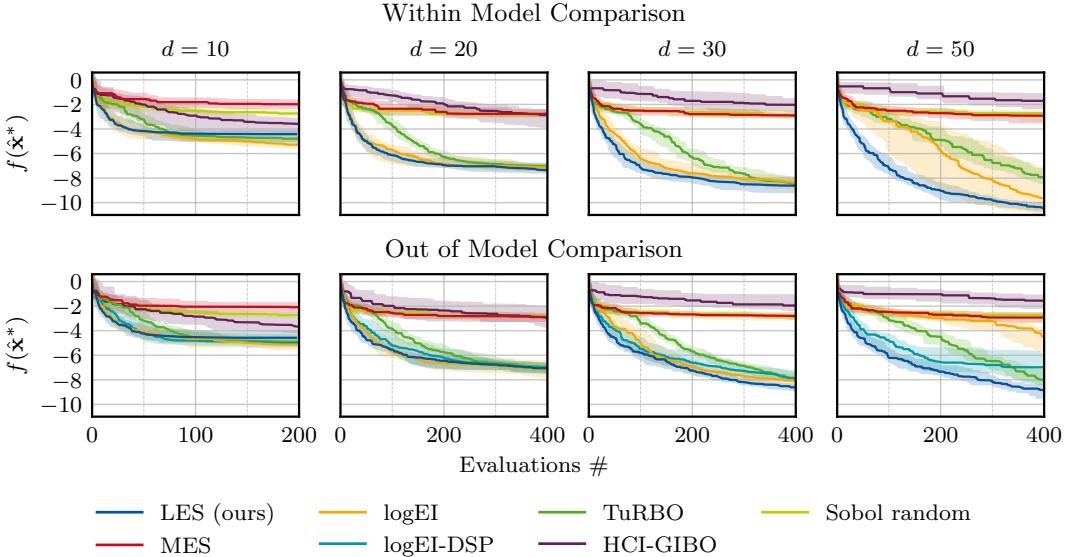


Figure 4: **Optimizing Gaussian Process Samples:** Median, 25-, and 75-percent quantiles for the best function values found for 20 sampled objective functions with medium complexity (see Tab. 1). LES outperforms baselines as dimensionality increases.

5.2 ADDITIONAL APPROXIMATIONS AND IMPLEMENTATION DETAILS

To make LES a practical algorithm we introduce additional approximations and design choices. For hyperparameter values, we refer to Appx. D.1. To solve the original problem (see Sec. 3) we need to apply the local optimizer from a fixed initial design \mathbf{x}_0 . However, in practice, we always start the descent sequence from the current best guess $\hat{\mathbf{x}}_t^*$. Additionally, instead of ensuring convergence of the local optimizer, we simply stop all the iterative optimizers after finitely many steps. Still, conditioning on all elements in $Q_{\mathbf{x}_0}^l$ can be prohibitively expensive. Thus, we choose to only condition on P equally spaced elements along the interpolated descent sequence. Additionally, we condition on function values instead of gradient observations which reduces runtime while achieving similar performance (see Appx. D.5). Optimizing any acquisition function is challenging in high-dimensions as it is non-convex (see Fig. 3). Fortunately, the approximation of $Q_{\mathbf{x}_0}$ gives us access to promising candidates. Thus we optimize the acquisition function under the finite candidate set $Q_{\mathbf{x}_0}^1, \dots, Q_{\mathbf{x}_0}^L$ with L times P candidate points.

Practical LES in one paragraph (i) Draw L posterior GP samples. (ii) For each sample, run \mathcal{O} for a finite number of steps starting at the current incumbent $\hat{\mathbf{x}}_t^*$ to obtain a descent sequence; discretize each sequence to P support points. (iii) Compute the predictive entropy at candidate \mathbf{x} and the average conditional entropy after conditioning on those discretized sequences; their difference is the acquisition function in (16) (Fig. 2). (iv) To keep optimization tractable, maximize the acquisition over the finite candidate set given by the union of all discretized sequences. (v) Evaluate, update the GP, and repeat (Alg. 1).

6 EMPIRICAL RESULTS

In this section, we empirically evaluate LES and compare it against other local and global BO variants (additional results in Appx. D). As objectives, we use GP-samples with varying lengthscales to increase complexity as well as synthetic and application-oriented benchmarks.

6.1 ABLATIONS AND BENCHMARK ALGORITHMS

LES Variants We evaluate LES with three local optimization algorithms: gradient descent, ADAM (Kingma & Ba, 2015), and covariance matrix adaptive evolutionary search (CMA-ES) (Hansen

378
 379 **Table 1: Within-Model Comparisons:** Median final objective for LES, logEI, TuRBO, and Sobol
 380 random sampling. Bold indicates performance not statistically significantly below the best. *Hyper-
 381 prior as in (Hvarfner et al., 2024).

Complexity	Method	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
high: $p(l; d) = \log(-2.5\sqrt{2} + \log\sqrt{d}, \sqrt{3}/5)$ $E[p(l; 50)] = 0.25$	LES (ours)	-2.8	-4.8	-7.4	-9.0	-10.8
	logEI	-3.9	-4.4	-2.9	-3.2	-2.9
	TuRBO	-3.5	-4.8	-7.2	-8.0	-7.1
	Sobol random	-2.4	-2.7	-2.8	-3.2	-3.0
medium: $p(l; d) = \log(-2.0\sqrt{2} + \log\sqrt{d}, \sqrt{3}/4)$ $E[p(l; 50)] = 0.52$	LES (ours)	-2.9	-4.4	-7.3	-8.6	-10.4
	logEI	-3.6	-5.3	-7.1	-8.4	-9.6
	TuRBO	-3.1	-4.8	-7.0	-8.5	-7.9
	Sobol random	-2.5	-2.7	-2.8	-2.9	-2.7
low: $p(l; d) = \log(-1.0\sqrt{2} + \log\sqrt{d}, \sqrt{3}/2)$ $E[p(l; 50)] = 2.65$	LES (ours)	-2.1	-3.7	-5.5	-6.8	-8.8
	logEI	-2.9	-4.1	-5.8	-6.6	-8.5
	TuRBO	-2.4	-3.6	-5.5	-6.5	-8.1
	Sobol random	-2.0	-2.3	-2.9	-2.8	-3.0
extremely low*: $p(l; d) = \log(1.0\sqrt{2} + \log\sqrt{d}, \sqrt{3})$ $E[p(l; 50)] = 96.2$	LES (ours)	-0.6	-0.8	-1.2	-1.5	-3.0
	logEI	-0.6	-0.9	-1.3	-1.5	-3.0
	TuRBO	-0.6	-0.8	-1.2	-1.5	-2.8
	Sobol random	-0.5	-0.7	-1.0	-1.0	-1.5

& Ostermeier, 2001). Results show that LES-ADAM and LES-GD perform best depending on problem complexity, while LES-CMA-ES shows a more global search behavior which is beneficial for low dimensional problems (see Appx. D.6). Additionally, we show that the more accurate the acquisition function approximation (higher L and P), the better the performance at the cost of higher runtime. Below, we investigate LES-ADAM with a medium approximation accuracy resulting in an average runtime of 17.8 sec per iteration in 50 dimensions excluding hyperparameter optimization (see Appx. D.5 for runtime comparisons).

Baselines We compare LES-ADAM to two other local BO paradigms: TuRBO (Eriksson et al., 2019) is based on trust-regions and high-confidence improvement Bayesian optimization (HCI-GIBO) is a gradient-based approach. HCI-GIBO (He et al., 2025) is a recent GIBO (Müller et al., 2021) extension. As a global ES alternative we choose max-value entropy search (MES) (Wang & Jegelka, 2017). Additionally, we compare to logEI (Ament et al., 2023) and Sobol random sampling.

Other Local Information-Theoretic Strategies We propose and evaluate two other search strategies as special cases of the LES paradigm: local Thompson sampling and conditioning only on the final point of the descent sequence. They empirically perform worse confirming that conditioning on the whole sequences and Monte-Carlo sampling (see Appx. F.2).

6.2 GAUSSIAN PROCESS SAMPLES

Model Complexity Recent work by (Hvarfner et al., 2024) highlights model complexity as a key factor in high-dimensional BO performance. The assumed difficulty of the problem – encoded through the model complexity in the form of length scale priors – determines global BO performance. Smaller length scales yield more complex functions with more local optima (Adler, 2010, Chapt. 6). Building on this insight, we construct benchmark functions with varying problem difficulty by sampling functions from a GP with different model complexities. Specifically, we generate functions by scaling the log-normal length scale prior $p(l)$ proposed in (Hvarfner et al., 2024). We consider four complexity levels across 5 to 50 dimensions (see Tab.1) where the lowest model complexity corresponds to the one used in (Hvarfner et al., 2024).

Within Model Comparison To assess the performance of the proposed acquisition function independently of the effects of hyperparameter optimization, we first use known hyperparameters in all evaluated BO algorithms. Results on medium model complexity (Fig. 4) show that, after 400 evaluations, LES outperforms all baselines as dimensionality increases. The asymptotical

432 Table 2: **Out-Of-Model Comparisons:** Median final objective for LES, logEI-DSP, TuRBO, and
 433 Sobol random sampling. Bold indicates performance not statistically significantly below the best.
 434

Complexity	Method	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
high: $p(l; d) = \log(-2.5\sqrt{2} + \log\sqrt{d}, \sqrt{3}/5)$ $E[p(l; 50)] = 0.25$	LES	-2.9	-5.0	-7.2	-8.5	-7.8
	TuRBO	-3.7	-5.0	-7.1	-8.2	-7.1
	logEI-DSP	-3.7	-4.1	-4.0	-4.0	-4.1
	Sobol	-2.4	-2.7	-2.8	-3.2	-3.0
medium: $p(l; d) = \log(-2.0\sqrt{2} + \log\sqrt{d}, \sqrt{3}/4)$ $E[p(l; 50)] = 0.52$	LES	-3.0	-4.6	-7.1	-8.6	-8.8
	TuRBO	-3.1	-4.9	-7.0	-7.9	-8.0
	logEI-DSP	-3.6	-5.0	-7.0	-7.9	-7.0
	Sobol	-2.5	-2.7	-2.8	-2.9	-2.7
low: $p(l; d) = \log(-1.0\sqrt{2} + \log\sqrt{d}, \sqrt{3}/2)$ $E[p(l; 50)] = 2.65$	LES	-2.1	-3.7	-5.2	-6.6	-8.5
	TuRBO	-2.4	-3.7	-5.4	-6.4	-7.7
	logEI-DSP	-2.9	-4.1	-5.7	-6.6	-8.1
	Sobol	-2.0	-2.3	-2.9	-2.8	-3.0
extremely low: $p(l; d) = \log(1.0\sqrt{2} + \log\sqrt{d}, \sqrt{3})$ $E[p(l; 50)] = 96.2$	LES	-0.6	-0.8	-1.2	-1.5	-2.9
	TuRBO	-0.6	-0.8	-1.2	-1.5	-2.9
	logEI-DSP	-0.6	-0.9	-1.3	-1.5	-3.0
	Sobol	-0.5	-0.7	-1.0	-1.0	-1.5

451
 452 performance benefits of searching globally with logEI is only seen for $d = 10$. MES, the global
 453 entropy search benchmark is not competitive. For other problem complexities the same trends can
 454 be observed (see Tab.1 and Appx. D.3). Performance differences increase with increasing problem
 455 complexity with LES clearly outperforming other methods for high complexity tasks in higher
 456 dimensions (see Appx. D.3).
 457

458 **Out-Of-Model Comparison** The out-of-model setup is identical to the within-model one except
 459 that GP hyperparameters are now estimated via MAP. All methods use the hyperprior that is used to
 460 sample from the GP, except for logEI-DSP, which was recently proposed by Hvarfner et al. (2024)
 461 and assumes a hyperprior with longer length scales. Appx. D.3 reports additional detailed results.
 462

463 The results mirror the within-model case. Interestingly, logEI performs better when using the wrong
 464 (less complex) hyperprior, as in logEI-DSP which supports the claims made in (Hvarfner et al., 2024).
 465

466 **Cumulative Regret** The local search behavior inherent to LES leads to a substantially lower
 467 empirical cumulative regret for all problems except for $d = 5$ and the lowest complexity (Appx. D.3).
 468

469 **A Stopping Criterion for Local Entropy Search** We incorporate a probabilistic stopping rule for
 470 LES that assesses whether the current solution is locally optimal. Following the Monte-Carlo test of
 471 Wilson (2024), we estimate the probability that the local simple regret falls below a user-specified
 472 tolerance and terminate once this criterion is met. The full formulation, assumptions, and theoretical
 473 guarantees, along with empirical stopping-time results, are provided in Appx. E. When compared
 474 to the results in (Wilson, 2024) these results show that the local optimization needs fewer samples
 475 before stopping, reinforcing the intuition that reaching a local optimum is easier
 476

477 6.3 SYNTHETIC AND APPLICATION-ORIENTED OBJECTIVE FUNCTIONS

478 We evaluate LES on additional analytic benchmarks (Fig. 5) and application-oriented tasks, with
 479 further results in Appx. D.4. On single-optimum functions (square), all methods reliably identify
 480 the solution, though LES and TuRBO achieve lower cumulative regret, highlighting the conservative
 481 exploration behavior inherent to local search. On the 30-d Ackley function, LES and TuRBO
 482 outperform global methods but LES shows high run-to-run variance due to the many local optima.
 483 For the rover (Wang et al., 2018) and Mopta08 (Jones, 2008) tasks, LES, logEI, and TuRBO perform
 484 similarly, with LES best on rover and logEI best on Mopta08.
 485

Additional experiments, including benchmarks designed to expose weaknesses of local search are
 presented in Appx. D.4. In these cases, LES frequently gets trapped in local optima, leading to high

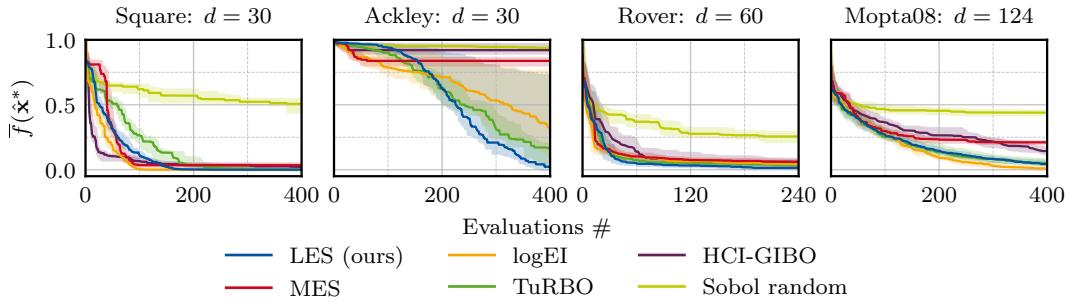


Figure 5: **Synthetic and Application-Oriented Objective Functions:** Median, 25-, and 75-percent quantiles for the best (normalized) function values found. Additional results in Appx. D.4.

run-to-run variance and overall poor performance relative to global methods. These results highlight the limitations of LES on highly multimodal landscapes with hard-to-escape local optima.

7 LIMITATIONS

We show that LES is beneficial especially in the high-dimensionality and high-complexity case. However, the focus on locality is also its most obvious constraint. Once the algorithm commits to a basin, it possesses no intrinsic mechanism for escape; achieving coverage of the full design space therefore requires globalization strategies. Furthermore, in real-world use cases it may be difficult to determine the problem complexity a-priori. Therefore, multi-starts, more advanced incumbent search, e.g., based on (Adebiyi et al., 2025), or switching heuristics between local and global optimization based on estimated objective complexity are interesting directions for future research. The stopping rule introduced in Appx. E.1 can be used to trigger a restart instead of stopping.

LES inherits the strengths and weaknesses of its surrogate. All acquisition decisions are driven by posterior samples; if the model is misspecified, the algorithm will exploit the wrong belief. Moreover, approximating the mutual information in (16) at each iteration requires drawing and optimizing posterior samples, with the number of samples increasing with dimensionality and model complexity.

The present formulation tackles unconstrained, single-objective optimization. LES is entropy-search based and therefore future work can naturally extend LES to more complex settings, such as multi-fidelity, constrained, batch (see Appx. C.3), or asynchronous optimization.

Finally, LES currently lacks finite-time regret guarantees of the GP-UCB type (Srinivas et al., 2012), and the current theoretical claims are limited to the high-probability certificate of local optimality offered by the stopping test. In addition, a bound on the difference between local and global regret for GP sample paths would bridge the current theoretical gap between local and global BO.

8 DISCUSSION AND CONCLUSION

This paper introduces LES, the first entropy-search paradigm tailored to local optimization. By propagating the GP posterior through the optimizer’s descent sequence, LES selects each evaluation to maximize mutual information with that sequence, thereby reducing uncertainty over possible descent sequences.

Empirically, LES delivers strong sample efficiency. Across high-complexity GP samples and policy-search benchmarks, the ADAM-based variant consistently attains lower simple regret than global entropy-search baselines and other local BO strategies, especially as dimensionality and complexity grows. Additionally, we show in Appx. D.4 that local search has a more conservative exploration behavior than global BO. This can be a great asset when optimizing outside of simulated environments, as e.g., in real-world robot learning. A probabilistic stopping rule guarantees bounded local regret by detecting convergence to a local optimum without additional overhead by reusing the samples from the acquisition step (Appx. E).

540 REPRODUCIBILITY STATEMENT
541542 All code necessary to reproduce the results is available in the supplementary material and will be
543 published upon publication. Additionally, we elaborate on approximations and implementation details
544 in Sec. 5.2. We report hyperparameter values in Appx. D.
545546 REFERENCES
547548 Taiwo Adebisi, Bach Do, and Ruda Zhang. Optimizing posterior samples for Bayesian optimization
549 via rootfinding. In *The Thirteenth International Conference on Learning Representations*, 2025.550 Robert J Adler. *The geometry of random fields*. SIAM, 2010.552 Riad Akrou, Dmitry Sorokin, Jan Peters, and Gerhard Neumann. Local Bayesian optimization of
553 motor skills. In *Proceedings of the 34th International Conference on Machine Learning*, volume 70,
554 pp. 41–50, 2017.556 Sebastian Ament, Samuel Daulton, David Eriksson, Maximilian Balandat, and Eytan Bakshy. Unex-
557 pected improvements to expected improvement for bayesian optimization. In *Advances in Neural*
558 *Information Processing Systems*, volume 36, pp. 20577–20612, 2023.559 Maximilian Balandat, Brian Karrer, Daniel Jiang, Samuel Daulton, Ben Letham, Andrew G Wilson,
560 and Eytan Bakshy. BoTorch: A framework for efficient Monte-Carlo Bayesian optimization. In
561 *Advances in Neural Information Processing Systems*, volume 33, pp. 21524–21538, 2020.563 Rafael Barbudo, Sebastián Ventura, and José Raúl Romero. Eight years of AutoML: categorisation,
564 review and trends. *Knowledge and Information Systems*, 65(12):5097–5149, 2023. doi: 10.1007/
565 s10115-023-01935-1.566 Syrine Belakaria, Aryan Deshwal, and Janardhan Rao Doppa. Max-value entropy search for multi-
567 objective Bayesian optimization with constraints. *Workshop on Machine Learning and the Physical*
568 *Sciences (NeurIPS)*, 2020.569 Greg Brockman, Vicki Cheung, Ludwig Pettersson, Jonas Schneider, John Schulman, Jie Tang, and
570 Wojciech Zaremba. Openai gym, 2016.572 Paul Brunzema, Mikkel Jordahn, John Willes, Sebastian Trimpe, Jasper Snoek, and James Harrison.
573 Variational last layers for Bayesian optimization. In *NeurIPS 2024 Workshop on Bayesian Decision-
574 making and Uncertainty*, 2024.576 Aakanksha Chowdhery, Sharan Narang, Jacob Devlin, Maarten Bosma, Gaurav Mishra, Adam
577 Roberts, Paul Barham, Hyung Won Chung, Charles Sutton, Sebastian Gehrmann, Parker Schuh,
578 Kensen Shi, Sasha Tsvyashchenko, Joshua Maynez, Abhishek Rao, Parker Barnes, Yi Tay, Noam
579 Shazeer, Vinodkumar Prabhakaran, Emily Reif, Nan Du, Ben Hutchinson, Reiner Pope, James
580 Bradbury, Jacob Austin, Michael Isard, Guy Gur-Ari, Pengcheng Yin, Toju Duke, Anselm Lev-
581 skaya, Sanjay Ghemawat, Sunipa Dev, Henryk Michalewski, Xavier Garcia, Vedant Misra, Kevin
582 Robinson, Liam Fedus, Denny Zhou, Daphne Ippolito, David Luan, Hyeontaek Lim, Barret Zoph,
583 Alexander Spiridonov, Ryan Sepassi, David Dohan, Shivani Agrawal, Mark Omernick, Andrew M.
584 Dai, Thanumalayan Sankaranarayana Pillai, Marie Pellat, Aitor Lewkowycz, Erica Moreira, Rewon
585 Child, Oleksandr Polozov, Katherine Lee, Zongwei Zhou, Xuezhi Wang, Brennan Saeta, Mark
586 Diaz, Orhan Firat, Michele Catasta, Jason Wei, Kathy Meier-Hellstern, Douglas Eck, Jeff Dean,
587 Slav Petrov, and Noah Fiedel. PaLM: Scaling language modeling with pathways. *Journal of*
588 *Machine Learning Research*, 24(240):1–113, 2023.589 Lionel Colliandre and Christophe Muller. Bayesian optimization in drug discovery. In *High*
590 *Performance Computing for Drug Discovery and Biomedicine*, pp. 101–136. Springer, 2023.
591 doi: 10.1007/978-1-0716-3449-3_5.592 Bach Do, Nafeezat A Ajenifuja, Taiwo A Adebisi, and Ruda Zhang. Sampling from Gaussian
593 processes: A tutorial and applications in global sensitivity analysis and optimization. *arXiv*
594 *preprint arXiv:2507.14746*, 2025.

594 David Eriksson, Michael Pearce, Jacob Gardner, Ryan D Turner, and Matthias Poloczek. Scalable
 595 global optimization via local Bayesian optimization. In *Advances in Neural Information Processing*
 596 *Systems*, pp. 5496–5507, 2019.

597

598 Zheyi Fan, Wenyu Wang, Szu Hui Ng, and Qingpei Hu. Minimizing ucb: a better local search strategy
 599 in local Bayesian optimization. In *Advances in Neural Information Processing Systems*, volume 37,
 600 pp. 130602–130634, 2024.

601 Fröhlich Lukas P., Klenske Edgar D., Daniel Christian G., and Zeilinger Melanie N. Bayesian
 602 optimization for policy search in high-dimensional systems via automatic domain selection. In
 603 *2019 IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS)*, pp. 757–764,
 604 2019. doi: 10.1109/IROS40897.2019.8967736.

605

606 Roman Garnett. *Bayesian Optimization*. Cambridge University Press, 2023.

607

608 Nikolaus Hansen and Andreas Ostermeier. Completely derandomized self-adaptation in evolution
 609 strategies. *Evolutionary Computation*, 9(2):159–195, 2001. doi: 10.1162/106365601750190398.

610 Shiming He, Alexander von Rohr, Dominik Baumann, Ji Xiang, and Sebastian Trimpe. Simulation-
 611 aided policy tuning for black-box robot learning. *IEEE Transactions on Robotics*, 41:2533–2548,
 612 2025. doi: 10.1109/TRO.2025.3539192.

613

614 Philipp Hennig and Christian J. Schuler. Entropy search for information-efficient global optimization.
 615 *Journal of Machine Learning Research*, 13(6), 2012.

616

617 José Miguel Hernández-Lobato, Matthew W. Hoffman, and Zoubin Ghahramani. Predictive entropy
 618 search for efficient global optimization of black-box functions. In *Advances in Neural Information
 Processing Systems*, volume 27, 2014.

619

620 Carl Hvarfner, Frank Hutter, and Luigi Nardi. Joint entropy search for maximally-informed Bayesian
 621 optimization. In *Advances in Neural Information Processing Systems*, volume 35, pp. 11494–11506,
 622 2022.

623

624 Carl Hvarfner, Erik Orm Hellsten, and Luigi Nardi. Vanilla Bayesian optimization performs great
 625 in high dimensions. In *Proceedings of the 41st International Conference on Machine Learning*,
 626 volume 235, pp. 20793–20817, 2024.

627

628 D. Jones. Large-scale multi-disciplinary mass optimization in the auto industry, 2008. Presented at
 the Modeling and Optimization: Theory and Applications (MOPTA) 2008 Conference.

629

630 A. G. Journel and C. J. Huijbregts. *Mining Geostatistics*. Academic Press, London, 1978.

631

632 Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. In *Proceedings of
 the 3rd International Conference on Learning Representations*, 2015.

633

634 Johannes Kirschner, Mojmir Mutny, Nicole Hiller, Rasmus Ischebeck, and Andreas Krause. Adaptive
 635 and safe Bayesian optimization in high dimensions via one-dimensional subspaces. In *Proceedings
 of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine
 Learning Research*, pp. 3429–3438, 2019.

636

637 Alonso Marco, Felix Berkenkamp, Philipp Hennig, Angela P. Schoellig, Andreas Krause, Stefan
 638 Schaal, and Sebastian Trimpe. Virtual vs. real: Trading off simulations and physical experiments in
 639 reinforcement learning with Bayesian optimization. In *IEEE International Conference on Robotics
 and Automation*, pp. 1557–1563, 2017. doi: 10.1109/ICRA.2017.7989186.

640

641 Sarah Müller, Alexander von Rohr, and Sebastian Trimpe. Local policy search with Bayesian
 642 optimization. In *Advances in Neural Information Processing Systems*, volume 34, pp. 20708–
 643 20720, 2021.

644

645 Quan Nguyen, Kaiwen Wu, Jacob Gardner, and Roman Garnett. Local Bayesian optimization
 646 via maximizing probability of descent. In *Advances in Neural Information Processing Systems*,
 647 volume 35, pp. 13190–13202, 2022.

648 Joel A. Paulson, Farshud Sorourifar, and Ali Mesbah. A tutorial on derivative-free policy learning
 649 methods for interpretable controller representations. In *American Control Conference*, pp. 1295–
 650 1306, 2023. doi: 10.23919/ACC55779.2023.10156412.

651

652 Valerio Perrone, Iaroslav Shcherbatyi, Rodolphe Jenatton, Cedric Archambeau, and Matthias Seeger.
 653 Constrained Bayesian optimization with max-value entropy search, 2019.

654

655 Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian Processes for Machine Learning*.
 656 MIT Press, 2006. doi: 10.7551/mitpress/3206.001.0001.

657

658 Niranjan Srinivas, Andreas Krause, Sham M. Kakade, and Matthias W. Seeger. Information-theoretic
 659 regret bounds for Gaussian process optimization in the bandit setting. *IEEE Transactions on
 Information Theory*, 58(5):3250–3265, 2012. doi: 10.1109/TIT.2011.2182033.

660

661 Wei-Ting Tang and Joel A. Paulson. CAGES: Cost-aware gradient entropy search for efficient local
 662 multi-fidelity Bayesian optimization. In *IEEE 63rd Conference on Decision and Control*, pp.
 1547–1552, 2024. doi: 10.1109/CDC56724.2024.10886516.

663

664 Ben Tu, Axel Gandy, Nikolas Kantas, and Behrang Shafei. Joint entropy search for multi-objective
 665 Bayesian optimization. In *Advances in Neural Information Processing Systems*, volume 35, pp.
 9922–9938, 2022.

666

667 A.W. Vaart, van der and J.H. Zanten, van. *Reproducing kernel Hilbert spaces of Gaussian priors*, pp.
 668 200–222. 2008. doi: 10.1214/074921708000000156.

669

670 Zi Wang and Stefanie Jegelka. Max-value entropy search for efficient Bayesian optimization. In
 671 *Proceedings of the 34th International Conference on Machine Learning*, volume 70, pp. 3627–3635,
 2017.

672

673 Zi Wang, Clement Gehring, Pushmeet Kohli, and Stefanie Jegelka. Batched large-scale Bayesian
 674 optimization in high-dimensional spaces. In *Proceedings of the Twenty-First International Con-
 675 ference on Artificial Intelligence and Statistics*, volume 84 of *Proceedings of Machine Learning
 676 Research*, pp. 745–754, 2018.

677

678 James Wilson, Viacheslav Borovitskiy, Alexander Terenin, Peter Mostowsky, and Marc Deisenroth.
 679 Efficiently sampling functions from Gaussian process posteriors. In *Proceedings of the 37th
 680 International Conference on Machine Learning*, volume 119, pp. 10292–10302, 2020.

681

682 James T. Wilson. Stopping Bayesian optimization with probabilistic regret bounds. In *The Thirty-
 683 eighth Annual Conference on Neural Information Processing Systems*, 2024.

684

685 Kaiwen Wu, Kyurae Kim, Roman Garnett, and Jacob Gardner. The behavior and convergence of
 686 local Bayesian optimization. In *Advances in Neural Information Processing Systems*, volume 36,
 687 pp. 73497–73523, 2023.

688

689 Zhitong Xu, Haitao Wang, Jeff M. Phillips, and Shandian Zhe. Standard Gaussian process is all you
 690 need for high-dimensional Bayesian optimization. In *The Thirteenth International Conference on
 691 Learning Representations*, 2025.

692

693

694

695

696

697

698

699

700

701

702 **Supplementary Material for “Local Entropy Search over Descent** 703 **Sequences for Bayesian Optimization”**

706 A Introduction to Bayesian Optimization with Entropy Search	15
707	
708 B Exact Information Gain Maximization of the Local Optimizer	16
709	
710 B.1 Impracticability in the General Case	16
711 B.2 Exact Information Gain Maximization in Entropy-Based GIBO	16
712	
713 C Additional Details on LES	18
714	
715 C.1 GP-sample Approximation Strategies	18
716 C.2 Relationship Between Properties of Target Function, Model Samples and Local Optimizer	18
717	
718 C.3 qLES: Batched Local Entropy Search	18
719	
720 D Empirical Evaluation	19
721	
722 D.1 LES Algorithm hyperparameter	19
723 D.2 Benchmark Algorithm Hyperparameter	19
724 D.3 Additional Details and Results on GP Samples	19
725	
726 D.4 Additional Details and Results on Synthetic and Application-Oriented Objective Functions	32
727 D.5 Ablations on Approximation Accuracies and Runtime	35
728	
729 D.6 Comparing Different Iterative Optimizers	36
730	
731 E A Stopping Criterion for Local Entropy Search	39
732	
733 E.1 Method	39
734	
735 E.2 Results	39
736	
737 F Alternative Information-Theoretic Local Acquisition Functions	40
738	
739 F.1 Local Thompson Sampling	40
740	
741 F.2 Conditioning only on the Local Optimum	40
742	
743 F.3 Results	41
744	
745 G Theoretical Results	42
746	
747 G.1 LES queries are dense	42
748	
749 G.2 Gradient descent paths under a GP prior with a squared exponential kernel	42

748 Following is the technical appendix. Note that all citations here are in the bibliography of the main
 749 document and similarly for many of the cross-references.

750
 751
 752
 753
 754
 755

756 A INTRODUCTION TO BAYESIAN OPTIMIZATION WITH ENTROPY SEARCH
757

758 Because evaluating $f(\mathbf{x})$ is costly, BO leverages all data obtained until iteration t to choose the next
759 parametrization \mathbf{x}_{t+1} in Domain \mathcal{X} . After t_{init} random samples are evaluated, BO takes two steps
760 to maximize the utility of the next experiment. First, a GP is trained on all past observations to
761 approximate $f(\mathbf{x})$. Second, this model is used in an acquisition function to balance exploration and
762 exploitation. The acquisition function α uses the probabilistic GP predictions to calculate the utility
763 of an experiment. It is maximized to find the next query:

$$764 \quad \mathbf{x}_{t+1} = \operatorname{argmax}_{\mathcal{X}} \alpha(\mathcal{GP}_k). \quad (17)$$

766 Approximately solving (17) is much easier than the original problem because only the fast-to-evaluate
767 GP model needs to be evaluated. This new query is evaluated, new data is received, and the next
768 iteration is started by again updating the GP model. This way, the GP model is iteratively refined in
769 promising regions. We refer to (Garnett, 2023) for a detailed introduction to BO.

770 Global entropy search methods use an information-theoretic perspective to select where to evaluate.
771 They find a query point that maximizes the expected information gain about the global optimum
772 $\mathbf{x}_g^* = \arg \max \mathbf{x} \in \mathcal{X} f(\mathbf{x})$ whose value $f^* = f(\mathbf{x}^*)$ achieves the global maximum of the function
773 f .

774 The original entropy search (ES) (Hennig & Schuler, 2012) and predictive entropy search (PES)
775 (Hernández-Lobato et al., 2014) maximize the information gain about the *location* of the optimum:

$$776 \quad \alpha_t(\mathbf{x}) = I(\{\mathbf{x}, y(\mathbf{x})\}; \mathbf{x}_g^* | D_t) \quad (18)$$

777 The random variable $y(\mathbf{x})$ denotes the predictive distribution of the noisy observation at the query
778 location \mathbf{x} and \mathbf{x}_g^* denotes the estimated distribution of the global optimizer. The information gain
779 can be expressed as the difference between predictive entropy of noisy observation at the query
780 location, $H(p(\mathbf{x}_g^* | D_t))$ and the expectation of the predictive conditioned on the distribution of
781 minimizers $\mathbb{E}[H(p(\mathbf{x}_* | D_t \cup \{\mathbf{x}, y\})])$. Calculating those terms requires expensive approximations
782 that do not scale well especially in high dimensions.

783 Max-value entropy search (MES) (Wang & Jegelka, 2017) maximize the information gain about the
784 *function value* of the optimum:

$$785 \quad \alpha_t(\mathbf{x}) = I(\{\mathbf{x}, y\}; f_g^* | D_t) \quad (19)$$

786 This approach is computationally significantly more efficient than ES and PES, because the expectation
787 and entropy need to be only calculated over the one dimensional distribution of optimum
788 values.

789 Joint entropy search (JES) (Hvarfner et al., 2022; Tu et al., 2022) maximizes the information gain
790 about the joint distribution of location *location* and *function value* of the optimizer

$$791 \quad \alpha_{\text{JES}}(\mathbf{x}) = I((\mathbf{x}, y); (\mathbf{x}_g^*, f_g^*) | \mathcal{D}_n) \quad (20)$$

792 This paper applies the entropy search paradigm to local BO. Up to here, we only discussed entropy
793 search for single objective optimization. It can be extended to other BO paradigms such as constrained
794 (Perrone et al., 2019), multi-objective (Belakaria et al., 2020), and multi-fidelity (Marco et al., 2017)
795 optimization.

801
802
803
804
805
806
807
808
809

810 B EXACT INFORMATION GAIN MAXIMIZATION OF THE LOCAL OPTIMIZER
811

812 In LES, we do not directly minimize the entropy of the solution of the local optimization algorithm but
813 instead minimize the entropy of the descent sequence. This section shows why directly minimizing
814 the entropy of the solution is not possible in general. Furthermore, we show that the entropy search
815 version of GIBO is a special case for one step gradient descent, where it actually is possible.
816

817 B.1 IMPRACTICABILITY IN THE GENERAL CASE
818

819 Suppose we want to directly minimize the entropy of the local optimizer:

$$820 \max_{\mathbf{x} \in \mathcal{X}} I((\mathbf{x}, y(\mathbf{x})); O_{\mathbf{x}_0}^* | \mathcal{D}_t). \quad (21)$$

822 One way of going forward is to reformulate it in the standard entropy search way:

$$823 \begin{aligned} I((\mathbf{x}, y(\mathbf{x})); O_{\mathbf{x}_0}^* | \mathcal{D}_t) \\ 824 = \underbrace{H[y(\mathbf{x}) | \mathcal{D}_t]}_{\text{predictive entropy}} - \mathbb{E}_f \underbrace{[H[y(\mathbf{x}) | \mathcal{D}_t, O_{\mathbf{x}_0}^*]]}_{\text{conditional entropy}}. \end{aligned} \quad (22)$$

827 After Monte-Carlo approximation we get:

$$829 \mathbb{E}_f [H[p(y(\mathbf{x}) | \mathcal{D}_t, O_{\mathbf{x}_0}^*)]] \approx \frac{1}{L} \sum_{l=1}^L H[p(y(\mathbf{x}) | \mathcal{D}_t, O_{\mathbf{x}_0}^{*,l})]. \quad (23)$$

831 Unfortunately, we can condition a GP efficiently only on point-wise observations of, for example,
832 function values or gradients by adding them to the original data set as virtual points. It is not possible
833 to condition a GP directly on $O_{\mathbf{x}_0}^{*,l}$ being a location that can be reached by gradient descent from \mathbf{x}_0 .
834 In Appendix F.2 we show how we can condition on $O_{\mathbf{x}_0}^{*,l}$ being a local optimum with zero gradient
835 and positive Hessian. However, this loses information about the sequence to the local optimum. An
836 alternative approach would be the following reformulation:

$$837 \begin{aligned} \alpha(\mathbf{x}) &= I((\mathbf{x}, y(\mathbf{x})); O_{\mathbf{x}_0}^* | \mathcal{D}_t) \\ 838 &= \underbrace{H[O_{\mathbf{x}_0}^* | \mathcal{D}_t]}_{\text{predictive entropy}} - \mathbb{E}_{y(\mathbf{x})} \underbrace{[H[O_{\mathbf{x}_0}^* | \mathcal{D}_t, y(\mathbf{x})]]}_{\text{conditional entropy}}. \end{aligned} \quad (24)$$

842 In principle, we can approximate the conditional entropy in (24) with Monte-Carlo approximation
843 because we only have to condition a GP on realizations of $y(\mathbf{x})$. However, this is prohibitively
844 expensive because it would require a new Monte-Carlo approximation of $O_{\mathbf{x}_0}^*$ to evaluate α at a new
845 query location \mathbf{x} . Therefore, we do not consider this possibility any further.
846

847 B.2 EXACT INFORMATION GAIN MAXIMIZATION IN ENTROPY-BASED GIBO

848 This paragraph shows that the information theoretic version CAGES (Tang & Paulson, 2024) of the
849 GIBO (Müller et al., 2021) acquisition function can be seen as a special case of LES (11). This
850 special case arises when considering a one step gradient descent algorithm that produces the following
851 descent sequence

$$852 \text{GS}_{\mathbf{x}_0}(f) := \{\mathbf{z}_0 = \mathbf{x}_0, \mathbf{z}_1 = \mathbf{z}_0 - \eta \nabla f(\mathbf{z}_0)\}. \quad (25)$$

853 Now suppose that the local optimum is the last element of that sequence $O_{\mathbf{x}_0}^* = \mathbf{x}_0 - \eta \nabla f(\mathbf{x}_0)$.
854 Inserting in equation (24) yields:

$$856 \begin{aligned} \alpha_{\text{GES}}(\mathbf{x}) &= H[O_{\mathbf{x}_0}^* | \mathcal{D}_t] - \mathbb{E}_{y(\mathbf{x})} [H[O_{\mathbf{x}_0}^* | \mathcal{D}_t, y(\mathbf{x})]] \\ 857 &= H[\mathbf{x}_0 - \eta \nabla f(\mathbf{x}_0) | \mathcal{D}_t] - \mathbb{E}_{y(\mathbf{x})} [H[\mathbf{x}_0 - \eta \nabla f(\mathbf{x}_0) | \mathcal{D}_t, y(\mathbf{x})]] \end{aligned} \quad (26)$$

858 Since \mathbf{x}_0 and η are non-random variables, we get:

$$860 \alpha_{\text{GES}}(\mathbf{x}) = H[\nabla f(\mathbf{x}_0) | \mathcal{D}_t] - \mathbb{E}_{y(\mathbf{x})} [H[\nabla f(\mathbf{x}_0) | \mathcal{D}_t \cup (\mathbf{x}, y(\mathbf{x}))]] \quad (27)$$

861 Inserting the entropy of a multivariate normal distribution, we get the original GES acquisition
862 function (Tang & Paulson, 2024, Eq. (8)):

$$863 \alpha_{\text{GES}}(\mathbf{x}) = \frac{1}{2} \log |\Sigma'(\mathbf{x}_0 | \mathcal{D}_t)| - \frac{1}{2} \log |\Sigma'(\mathbf{x}_0 | \mathcal{D}_t \cup (\mathbf{x}, y(\mathbf{x})))| \quad (28)$$

864 The covariance of the gradient at location x_0 given data \mathcal{D}_t is denoted as $\Sigma'(\mathbf{x}_0 \mid \mathcal{D}_t)$. Note that the
865 expectation over $y(\mathbf{x})$ can be ignored because the predictive variance of the gradient is independent
866 of $y(\mathbf{x})$ and only depends on \mathbf{x} . The small difference between the CAGES and the GIBO acquisition
867 function is that the GIBO acquisition function uses the trace operator instead of the determinant
868 operator $|\cdot|$ in (28).

869 This observation highlights that GIBO-style acquisition functions learn about one step of the gradient
870 descent sequence, whereas LES maximizes the information gain about the whole descent sequence.
871

872

873

874

875

876

877

878

879

880

881

882

883

884

885

886

887

888

889

890

891

892

893

894

895

896

897

898

899

900

901

902

903

904

905

906

907

908

909

910

911

912

913

914

915

916

917

918 C ADDITIONAL DETAILS ON LES

920 C.1 GP-SAMPLE APPROXIMATION STRATEGIES

922 In this work, we approximate GP sample paths using the decoupled method of (Wilson et al., 2020)
 923 (Eq. (4)), which we regard as state-of-the-art and computationally attractive. It has been shown to
 924 outperform alternatives, is readily available in TensorFlow and PyTorch, and is still recommended
 925 in recent tutorials on GP sampling (Do et al., 2025). We therefore do not empirically investigate
 926 alternative sampling strategies for LES.

927 By contrast, the GP-sample benchmarks in GIBO (Müller et al., 2021) and follow-up work (Nguyen
 928 et al., 2022) adopt a different approach: they sample the posterior at fixed locations and then re-
 929 interpolate these points with a GP. In our preliminary experiments, this led to overly smooth sample
 930 functions in low dimensions.

931 Exploring how different sampling strategies affect LES remains an interesting direction for future
 932 work, both to assess robustness and to better understand potential biases introduced by approximation
 933 schemes.

935 C.2 RELATIONSHIP BETWEEN PROPERTIES OF TARGET FUNCTION, MODEL SAMPLES AND 936 LOCAL OPTIMIZER

938 The choice of local optimizer \mathcal{O} is constrained by the properties of the GP sample paths and practically
 939 by their approximations. For instance, if \mathcal{O} is gradient-based, the sample paths f^l must be at least
 940 once differentiable. More generally, the samples need to be differentiable to the same order required
 941 by \mathcal{O} . LES, however, is not limited to gradient-based methods: zeroth-order optimizers such as hill
 942 climbing or pattern search can be used when samples are non-differentiable. We illustrate this in
 943 Appx. D.6 with LES-CMAES, which employs a zeroth-order evolutionary optimizer.

944 Different kernels also practically affect optimizer choice. For example, Matérn-1/2 or Matérn-3/2
 945 kernels often generate sample paths with many shallow local minima. In such cases, an optimizer
 946 that incorporates momentum (e.g., Adam) may help to avoid undesired convergence to these minima.

947 Crucially, these requirements apply to the GP sample paths, not to the true objective. Indeed, GPs
 948 can approximate sub-gradients of non-differentiable functions, as shown in (Wu et al., 2023).

950 C.3 QLES: BATCHED LOCAL ENTROPY SEARCH

952 The LES paradigm can be straightforwardly extended to the batch case. This serves as an example
 953 of the versatility of entropy search methods and their potential for local optimization. We simply
 954 maximize the mutual information between the joint predictive distribution of multiple samples
 955 $y(\mathbf{x}_1), \dots, y(\mathbf{x}_q)$ and the distribution of descent sequences. Equation (13) becomes:

$$\begin{aligned} \alpha_{\text{qLES}}(\mathbf{x}_1, \dots, \mathbf{x}_q) &= I(\mathbf{x}_1, \dots, \mathbf{x}_q, y(\mathbf{x}_1), \dots, y(\mathbf{x}_q); Q_{\mathbf{x}_0} \mid \mathcal{D}_t) \\ &= \underbrace{H[y(\mathbf{x}_1), \dots, y(\mathbf{x}_q) \mid \mathcal{D}_t]}_{\text{predictive entropy}} - \underbrace{\mathbb{E}_f [H[y(\mathbf{x}_1), \dots, y(\mathbf{x}_q) \mid \mathcal{D}_t, Q_{\mathbf{x}_0}]]}_{\text{conditional entropy}}. \end{aligned} \quad (29)$$

960 With this, the only change to the acquisition function calculation is the entropy calculation. The
 961 entropy of the predictive and conditional entropies can still be calculated in closed form and omitting
 962 the intermediate steps, the acquisition function (16) becomes:

$$\begin{aligned} \alpha_{\text{qLES}}(\mathbf{x}_1, \dots, \mathbf{x}_q) &\approx \frac{1}{2} \log \det(\Sigma_y(\mathbf{x}_1, \dots, \mathbf{x}_q \mid \mathcal{D}_t)) \\ &\quad - \frac{1}{L} \sum_{l=1}^L \frac{1}{2} \log \det(\Sigma_y(\mathbf{x}_1, \dots, \mathbf{x}_q \mid \mathcal{D}_t \cup Q_{\mathbf{x}_0}^l)). \end{aligned} \quad (30)$$

968 The term $\Sigma_y(\mathbf{x}_1, \dots, \mathbf{x}_q \mid \mathcal{D}_t)$ denotes the predictive covariance matrix of the posterior GP at the
 969 query locations $\mathbf{x}_1, \dots, \mathbf{x}_q$ given data \mathcal{D}_t .

971 Optimizing (30) becomes more computationally expensive as q increases. However, we expect this
 972 increase to be relatively minor. The most expensive parts of the LES formalisms, i.e., generating L

972 GP samples, locally optimizing them and then conditioning L GPs on the descent sequences have to
 973 be done only once, independently of q .
 974

975 D EMPIRICAL EVALUATION 976

977 This section gives additional results and details on the empirical evaluation. Most notably, we show
 978 that the local exploration behavior results in reduced cumulative cost (D.3,D.4) and show extended
 979 results on GP-samples with varying problem complexity for the within and out of model comparison
 980 setting (D.3). Additional results are the impact of the discretizations on runtime and quality (D.5)
 981 and the impact of the local optimizer choice (D.6).
 982

983 D.1 LES ALGORITHM HYPERPARAMETER 984

985 Table 3 summarizes the main LES hyperparameter. In summary, LES has four types of hyper
 986 parameters: (a) GP-hyperparameter as any other BO algorithm (see Tab. 4, 10). (b) L and P that
 987 govern the accuracy of the acquisition function approximation. They should be chosen as large as
 988 computational resources permit (see Appx. D.5) (c) parameter of the stopping rule of the stopping
 989 rule (see Appx. E) (d) the local optimizer and its parameters (see Appx. D.6).
 990

991 Table 3: Default hyperparameter of LES

992 Name	993 Description	994 Value
994	995 Number of initial uniform random samples	996 2
995	996 L Monte-Carlo samples of gradient descent sequences	997 250
996	997 P discretizations of the gradient descent sequences	998 8
997	998 M prior features of the GP posterior sampling	999 1024
998	1000 ϵ stopping criterion optimality	1001 0.1, 0.01
999	1001 δ total risk	1002 0.05
1000	1002 δ_{est} estimation risk	1003 0.0025
1001	1003 T_{dec} samples between each decision	1004 25
1002	1005 Local Optimizer	1006 ADAM
1003	1006 Number of Local Optimization Steps	1007 500
1004	1007 Learning Rate	1008 0.002
1005	1008 Momentum Parameters	1009 Keras Default

1008 D.2 BENCHMARK ALGORITHM HYPERPARAMETER 1009

1010 For HCI-GIBO we choose $\alpha = 0.9$ and perform hyperparameter optimization after each gradient
 1011 step. We use the BoTorch (Balandat et al., 2020) implementations of MES, logEI, and TuRBO. MES
 1012 uses a candidate set of 5000 points and both MES and TuRBO use default parameters of the BoTorch
 1013 implementation. Again, all algorithm use identical GP parameters with the exception of logEI-DSP,
 1014 where the hyperprior of (Hvarfner et al., 2024) is chosen.
 1015

1016 D.3 ADDITIONAL DETAILS AND RESULTS ON GP SAMPLES 1017

1018 **General Setup.** Table 4 summarizes the GP hyperparameters used in the GP-sample experiments.
 1019 Following (Hvarfner et al., 2024), we employ a log-normal hyperprior $p(l)$ for the length scales
 1020 and assume a constant, known measurement noise distribution. Test functions are generated by first
 1021 sampling length scales from the hyperprior and then drawing functions according to (4). To vary
 1022 problem difficulty, we scale the log-normal hyperpriors of (Hvarfner et al., 2024) (see Sec. 6.2);
 1023 expected length scales are reported in Table 5. Note that the original hyperprior assumes very large
 1024 average length scales, whereas in the high-complexity scenario the expected length scale at $d = 50$ is
 1025 $E[p(l)] = 0.25$, which is still reasonable.

1025 Across all experiments, data is not standardized, each algorithm is evaluated on 20 random seeds, and
 the two initial points are chosen randomly.

1026

1027

1028

1029

1030

1031

1032

1033

1034

1035

1036

1037

1038

1039

1040

1041

1042

1043

1044

1045

1046

1047

1048

1049

1050

1051

1052

1053

1054

1055

1056

1057

1058

1059

1060

1061

1062

1063

1064

1065

1066

1067

1068

1069

1070

1071

1072

1073

1074

1075

1076

1077

1078

1079

Table 4: GP hyperparameters for out of model comparison on GP samples

Name	Description	Value
$k(\cdot, \cdot)$	kernel	SE-ARD
$p(l; d)$	length-scale hyper prior	Log Normal (see Tab. 5)
σ_n	observation noise	fixed at 0.002
σ_k	GP output scale	variable - init at 1
l_{init}	length scale initialization	$E[p(l; d)]$
	hyperparameter optimization frequency	after every sample ²
	standardize data	yes

Table 5: Expected length scales $E[p(l; d)]$ for the different hyperpriors.

Complexity	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
high: $p(l; d) = \log(-2.5\sqrt{2} + \log\sqrt{d}, \sqrt{3}/5)$	0.08	0.11	0.15	0.19	0.25
medium: $p(l; d) = \log(-2.0\sqrt{2} + \log\sqrt{d}, \sqrt{3}/4)$	0.16	0.23	0.33	0.4	0.52
low: $p(l; d) = \log(-1.0\sqrt{2} + \log\sqrt{d}, \sqrt{3}/2)$	0.83	1.19	1.67	2.05	2.65
extremely low (Hvarfner et al., 2024): $p(l; d) = \log(1.0\sqrt{2} + \log\sqrt{d}, \sqrt{3})$	21.86	30.92	34.73	53.56	69.15

Within-Model Comparison. In this setting, all BO algorithms are given access to the sampled ground-truth hyperparameters (length scales, output scale, and noise variance). Tables 6 and 7 summarize the results, with statistical significance determined by the signed rank test. Entries not in bold are statistically significantly worse than the best-performing algorithm. Figures 6–13 show the convergence curves.

LES achieves statistically significant improvements in higher-dimensional, high-complexity settings, particularly in terms of cumulative regret. Global BO methods only outperform LES in high-complexity, low-dimensional cases.

²Except for the GIBO variants, where we optimize the hyperparameter only after each step.

1080 Table 6: Best achieved function value after full budget for within model comparison on GP samples.
 1081 Entries not in bold are statistically significantly worse than the best preforming algorithm. Smaller is
 1082 better.

Complexity	Method	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
high	LES (ours)	-2.8	-4.8	-7.4	-9.0	-10.8
	MES	-2.4	-2.6	-3.0	-2.9	-2.8
	logEI	-3.9	-4.4	-2.9	-3.2	-2.9
	TuRBO	-3.5	-4.8	-7.2	-8.0	-7.1
	HCI-GIBO	-2.7	-2.0	-2.3	-1.8	-0.7
	Sobol random	-2.4	-2.7	-2.8	-3.2	-3.0
medium	LES (ours)	-2.9	-4.4	-7.3	-8.6	-10.4
	MES	-3.4	-2.0	-2.8	-2.9	-2.9
	logEI	-3.6	-5.3	-7.1	-8.4	-9.6
	TuRBO	-3.1	-4.8	-7.0	-8.5	-7.9
	HCI-GIBO	-2.9	-3.6	-2.9	-2.0	-1.7
	Sobol random	-2.5	-2.7	-2.8	-2.9	-2.7
low	LES (ours)	-2.1	-3.7	-5.5	-6.8	-8.8
	MES	-2.9	-4.0	-4.9	-4.6	-3.9
	logEI	-2.9	-4.1	-5.8	-6.6	-8.5
	TuRBO	-2.4	-3.6	-5.5	-6.5	-8.1
	HCI-GIBO	-2.1	-3.4	-5.0	-5.9	-7.3
	Sobol random	-2.0	-2.3	-2.9	-2.8	-3.0
extremely low	LES (ours)	-0.6	-0.8	-1.2	-1.5	-3.0
	MES	-0.6	-0.9	-1.3	-1.5	-2.7
	logEI	-0.6	-0.9	-1.3	-1.5	-3.0
	TuRBO	-0.6	-0.8	-1.2	-1.5	-2.8
	HCI-GIBO	-0.6	-0.8	-1.1	-1.3	-2.7
	Sobol random	-0.5	-0.7	-1.0	-1.0	-1.5

1107 Table 7: Cumulative observed function values after full budget for within model comparison on GP
 1108 samples. Entries not in bold are statistically significantly worse than the best preforming algorithm.
 1109 Smaller is better.

Complexity	Method	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
high	LES (ours)	-260.1	-842.1	-2515.1	-2938.4	-3214.3
	MES	35.8	22.3	0.1	1.1	4.0
	logEI	-176.6	-230.6	-17.1	-0.8	6.5
	TuRBO	-247.9	-672.5	-1783.3	-1503.0	-977.9
	HCI-GIBO	-59.5	-28.3	-16.6	-19.8	-24.7
	Sobol random	1.5	-1.7	-7.2	7.2	3.7
medium	LES (ours)	-272.8	-811.4	-2464.3	-2861.7	-3159.1
	MES	-97.1	167.3	288.4	6.5	-0.6
	logEI	-163.7	-645.5	-2111.3	-2071.3	-1378.3
	TuRBO	-246.7	-697.6	-1876.0	-1924.9	-1375.1
	HCI-GIBO	-114.5	-121.3	-51.4	-27.4	-4.2
	Sobol random	6.4	3.0	0.6	5.3	1.3
low	LES (ours)	-192.9	-685.7	-2059.5	-2415.1	-2969.3
	MES	-97.6	-358.9	-682.8	-276.7	337.6
	logEI	-88.1	-434.0	-1679.0	-2144.8	-2795.6
	TuRBO	-201.8	-637.6	-1916.6	-2048.7	-2390.1
	HCI-GIBO	-169.8	-581.9	-1638.9	-1874.3	-2224.6
	Sobol random	7.1	1.7	-42.8	-0.2	-1.5
extremely low	LES (ours)	-56.8	-160.5	-471.9	-591.0	-1142.4
	MES	-13.0	-7.5	-132.2	-69.1	-252.3
	logEI	-51.0	-122.5	-357.4	-320.6	-581.0
	TuRBO	-57.1	-152.3	-456.3	-516.8	-896.0
	HCI-GIBO	-54.3	-145.2	-420.7	-496.1	-913.7
	Sobol random	-1.9	21.1	-74.3	61.9	-88.9

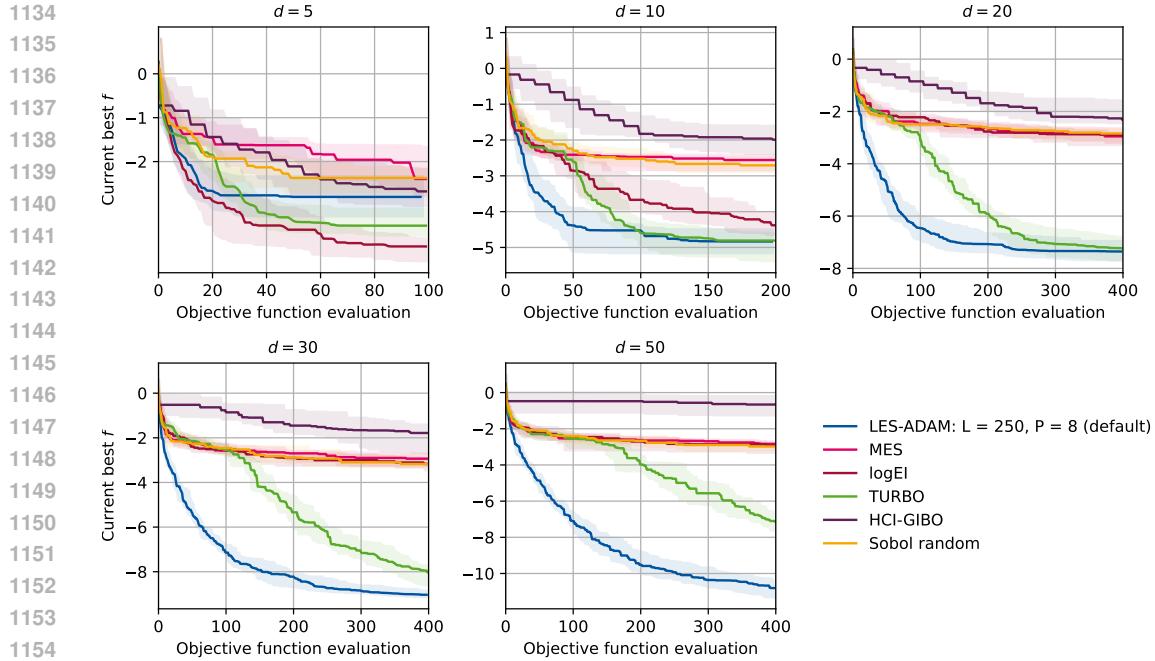


Figure 6: **Within Model Comparison, Complexity - high:** Median, 25-, and 75-percent quantiles - detailed results

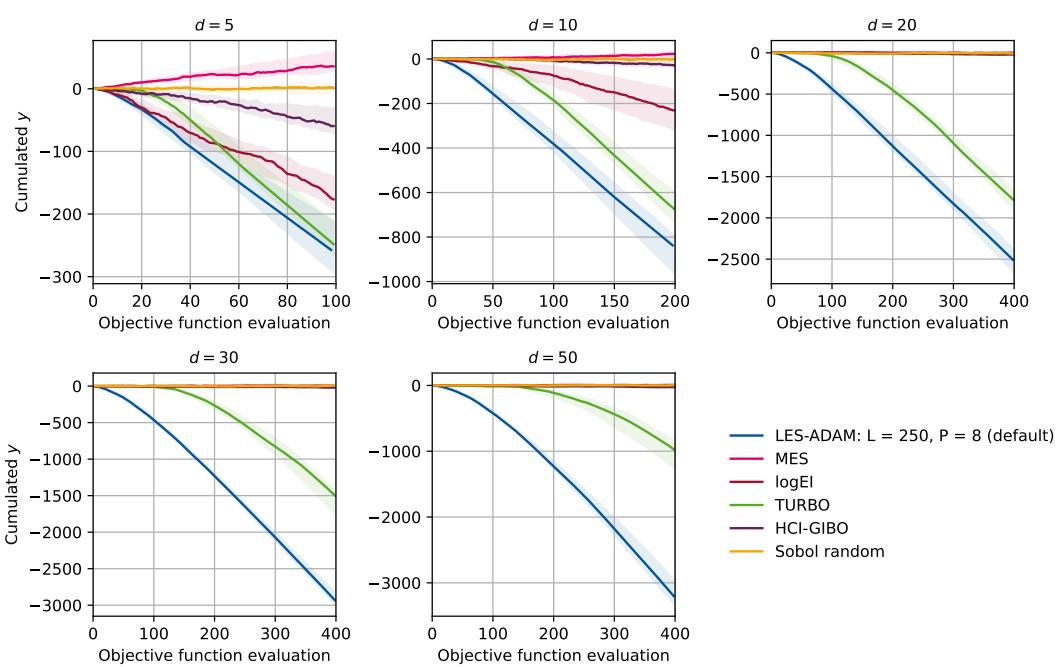


Figure 7: **Within Model Comparison, Complexity - high:** Median, 25-, and 75-percent quantiles - detailed results

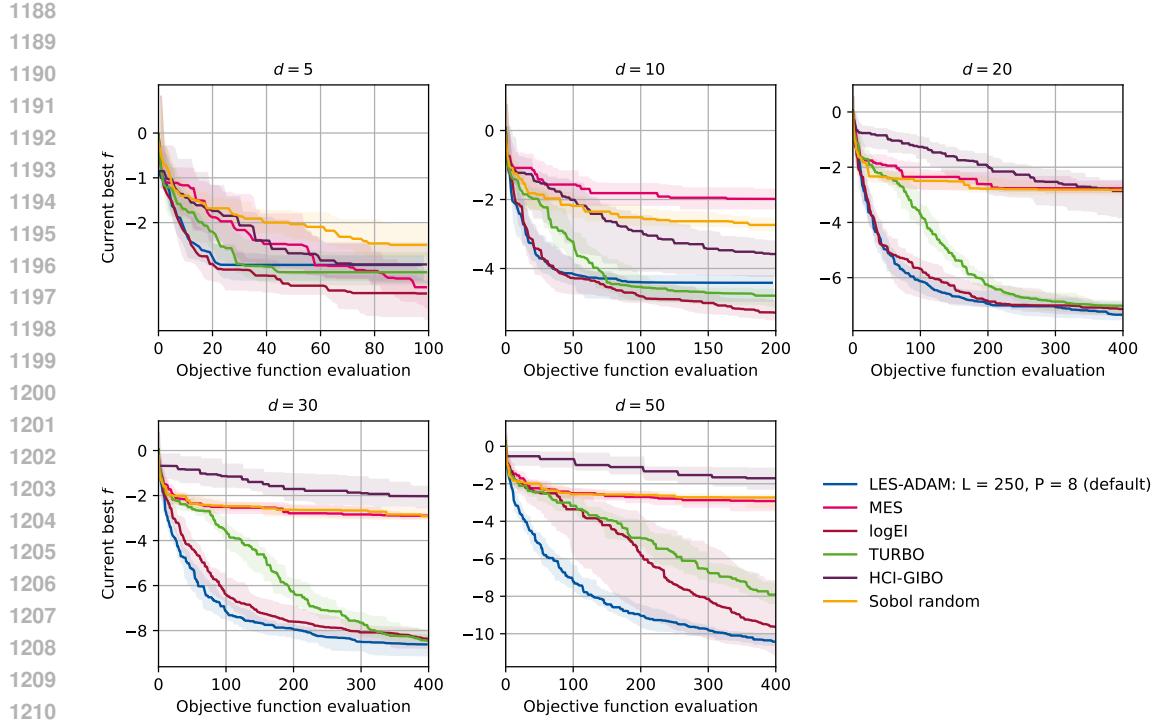


Figure 8: **Within Model Comparison, Complexity - medium:** Median, 25-, and 75-percent quantiles - detailed results

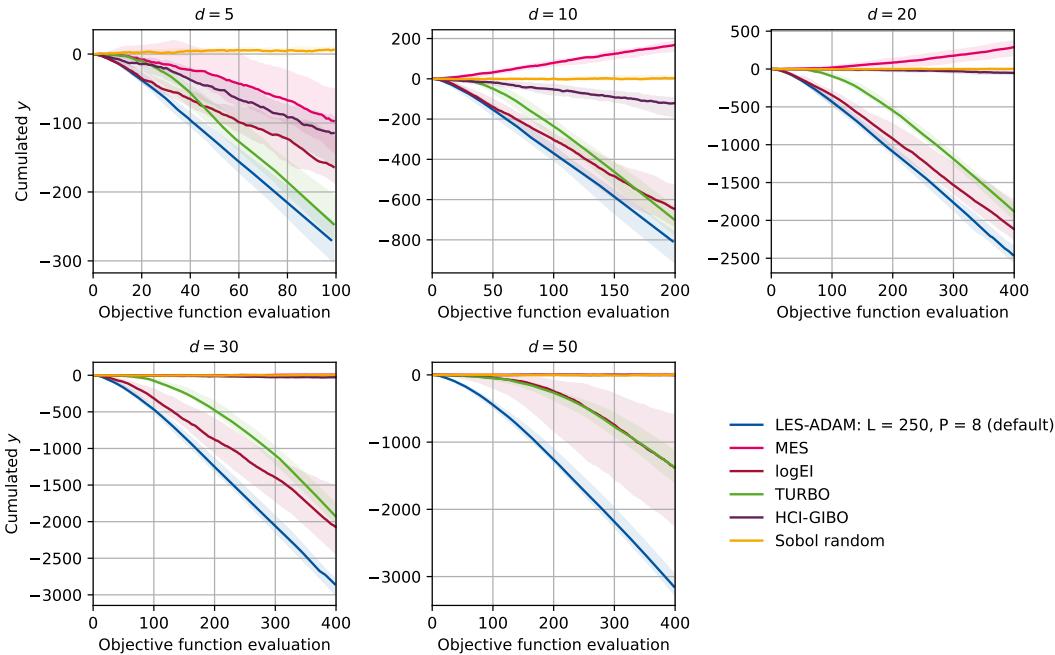


Figure 9: **Within Model Comparison, Complexity - medium:** Median, 25-, and 75-percent quantiles - detailed results

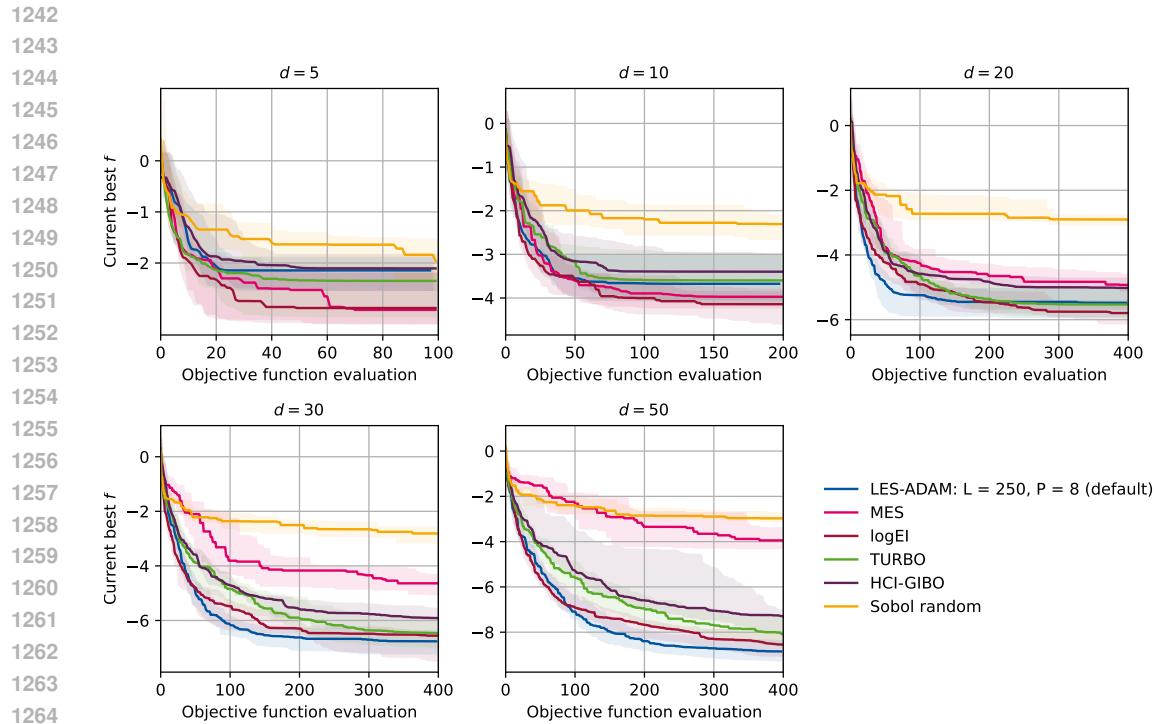


Figure 10: **Within Model Comparison, Complexity - low:** Median, 25-, and 75-percent quantiles - detailed results

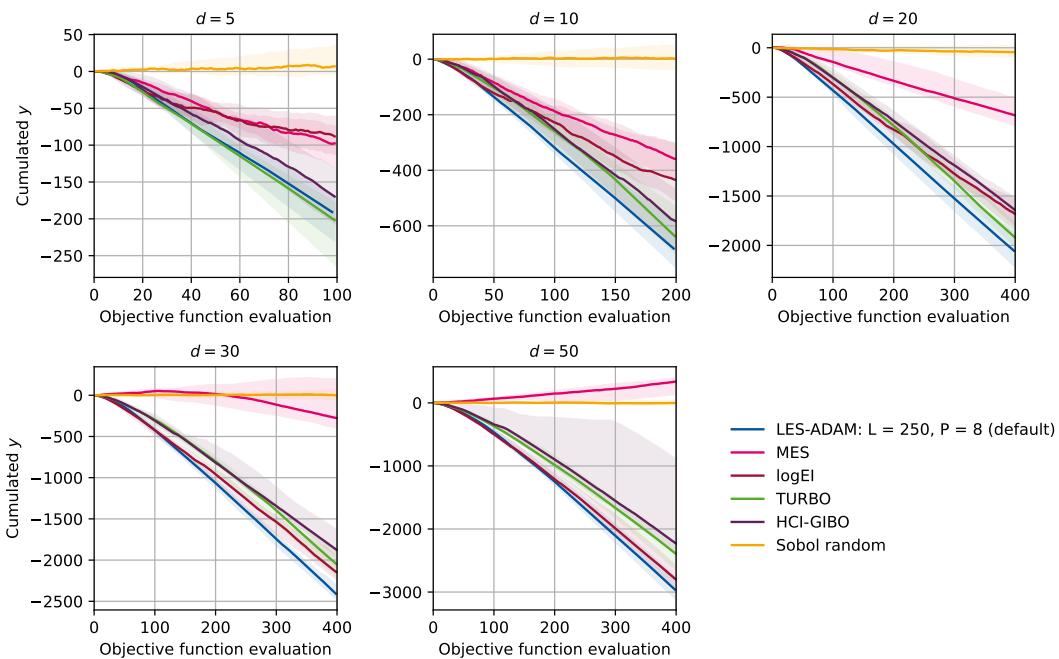


Figure 11: **Within Model Comparison, Complexity - low:** Median, 25-, and 75-percent quantiles - detailed results

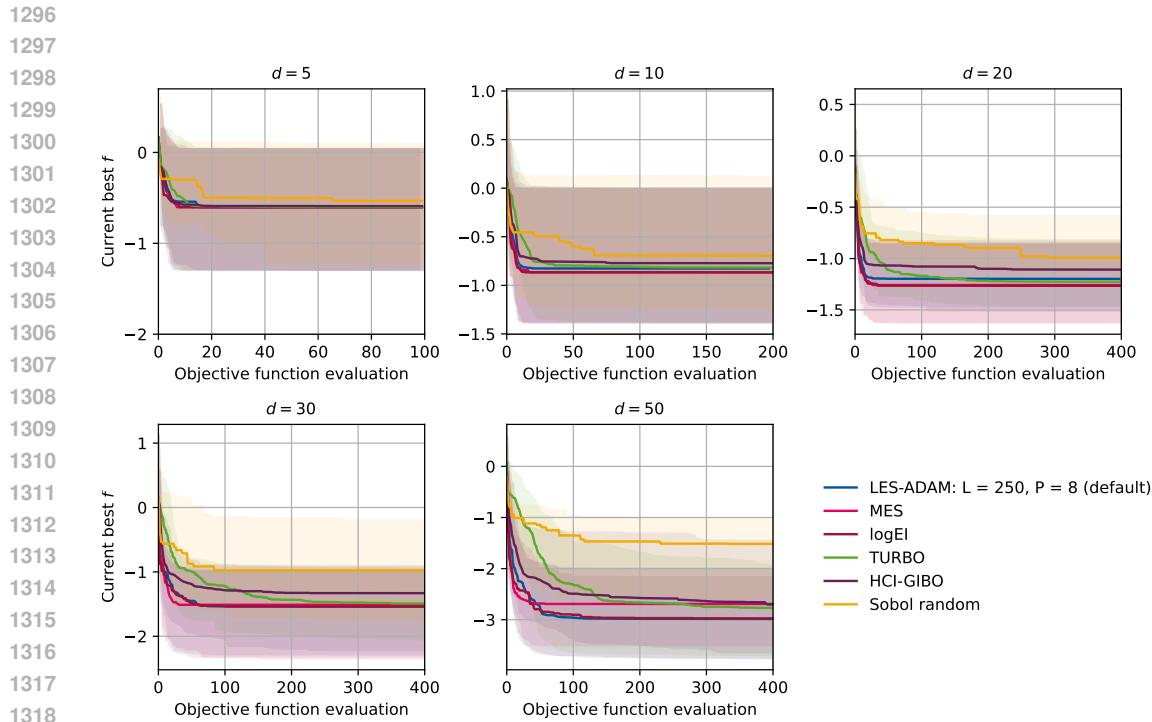


Figure 12: **Within Model Comparison, Complexity - extremely low:** Median, 25-, and 75-percent quantiles - detailed results

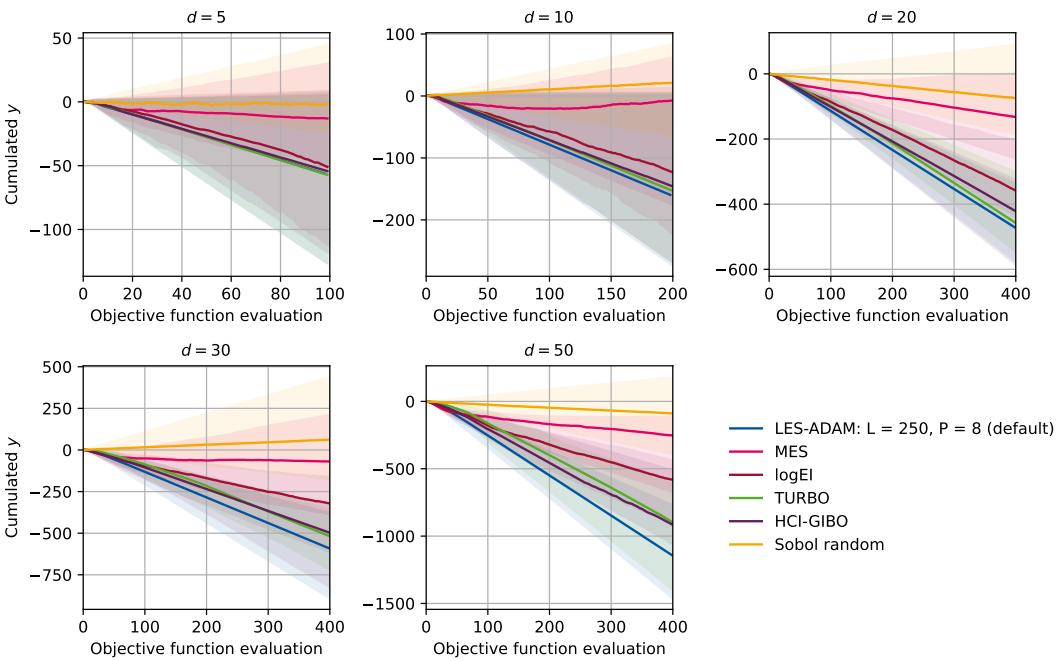


Figure 13: **Within Model Comparison, Complexity - extremely low:** Median, 25-, and 75-percent quantiles - detailed results

1350
 1351 **Out of Model Comparison.** The out-of-model setup is identical to the within-model one except
 1352 that GP hyperparameters are now estimated via MAP according to Table 4. Tables 8 and 9 report best
 1353 and cumulative evaluations, and Figures 14–21 show the corresponding progress in optimization over
 1354 the number of queries.

1355 Table 8: Best achieved function value after full budget for out-of-model comparison on GP samples.
 1356 Entries not in bold are statistically significantly worse than the best performing algorithm. Smaller is
 1357 better.

	Complexity	Method	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
1359	high	LES (ours)	-2.9	-5.0	-7.2	-8.5	-7.8
		MES	-1.9	-2.5	-2.8	-2.8	-3.0
		logEI	-4.0	-4.3	-2.8	-2.9	-3.0
		logEI-DSP	-3.7	-4.1	-4.0	-4.0	-4.1
		TuRBO	-3.7	-5.0	-7.1	-8.2	-7.1
		HCI-GIBO	-2.3	-2.2	-1.9	-2.0	-1.8
1360	medium	Sobol random	-2.4	-2.7	-2.8	-3.2	-3.0
		LES (ours)	-3.0	-4.6	-7.1	-8.6	-8.8
		MES	-3.6	-2.1	-2.9	-2.8	-2.9
		logEI	-3.6	-5.1	-7.2	-8.1	-4.5
		logEI-DSP	-3.6	-5.0	-7.0	-7.9	-7.0
		TuRBO	-3.1	-4.9	-7.0	-7.9	-8.0
1361	low	HCI-GIBO	-2.9	-3.7	-2.9	-2.0	-1.6
		Sobol random	-2.5	-2.7	-2.8	-2.9	-2.7
		LES (ours)	-2.1	-3.7	-5.2	-6.6	-8.5
		MES	-2.9	-4.0	-5.1	-5.4	-3.7
		logEI	-2.9	-4.1	-5.7	-6.4	-8.4
		logEI-DSP	-2.9	-4.1	-5.7	-6.6	-8.1
1362	extremely low	TuRBO	-2.4	-3.7	-5.4	-6.4	-7.7
		HCI-GIBO	-2.2	-3.5	-4.9	-5.9	-7.5
		Sobol random	-2.0	-2.3	-2.9	-2.8	-3.0
		LES (ours)	-0.6	-0.8	-1.2	-1.5	-2.9
		MES	-0.6	-0.9	-1.2	-1.4	-2.5
		logEI	-0.6	-0.9	-1.3	-1.5	-3.0
1363	extremely low	logEI-DSP	-0.6	-0.9	-1.3	-1.5	-3.0
		TuRBO	-0.6	-0.8	-1.2	-1.5	-2.9
		HCI-GIBO	-0.6	-0.7	-1.3	-1.5	-2.5
		Sobol random	-0.5	-0.7	-1.0	-1.0	-1.5

1404
 1405
 1406
 1407
 1408
 1409
 1410
 1411
 1412
 1413
 1414
 1415

1416 Table 9: Cumulative observed function values after full budget for out of model comparison on GP
 1417 samples. Entries not in bold are statistically significantly worse than the best preforming algorithm.
 1418 Smaller is better.

Complexity	Method	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
high	LES (ours)	-259.0	-867.2	-2298.3	-2482.5	-2081.9
	MES	56.9	13.6	11.6	-0.2	10.7
	logEI	-172.9	-197.7	0.4	3.4	2.8
	logEI-DSP	-130.4	-169.4	-128.1	-127.2	-119.3
	TuRBO	-257.0	-649.4	-1789.6	-1565.5	-927.9
	HCI-GIBO	-50.6	-24.5	-27.7	-18.1	-8.9
medium	Sobol random	1.5	-1.7	-7.2	7.2	3.7
	LES (ours)	-269.6	-819.0	-2267.5	-2494.5	-2427.1
	MES	-111.1	176.1	34.3	-3.5	-5.4
	logEI	-172.8	-667.3	-1949.7	-1597.4	-110.1
	logEI-DSP	-150.1	-524.4	-1912.4	-1644.4	-652.1
	TuRBO	-250.9	-673.5	-1900.0	-1737.7	-1352.6
low	HCI-GIBO	-160.1	-109.0	-40.8	-15.1	-19.9
	Sobol random	6.4	3.0	0.6	5.3	1.3
	LES (ours)	-182.3	-662.1	-1883.7	-2183.6	-2572.6
	MES	-102.5	-373.0	-666.8	-443.0	317.9
	logEI	-101.7	-448.3	-1639.7	-2049.2	-2691.8
	logEI-DSP	-88.9	-380.8	-1563.4	-1966.1	-2604.0
extremely low	TuRBO	-204.1	-620.1	-1764.8	-1848.2	-2151.1
	HCI-GIBO	-148.5	-456.3	-1454.9	-1783.2	-2128.8
	Sobol random	7.1	1.7	-42.7	-0.1	-1.5
	LES (ours)	-54.2	-146.5	-475.7	-580.9	-1063.6
	MES	-22.8	-10.7	-147.1	-84.6	-243.6
	logEI	-43.6	-102.3	-338.4	-318.6	-629.5

1447
 1448
 1449
 1450
 1451
 1452
 1453
 1454
 1455
 1456
 1457

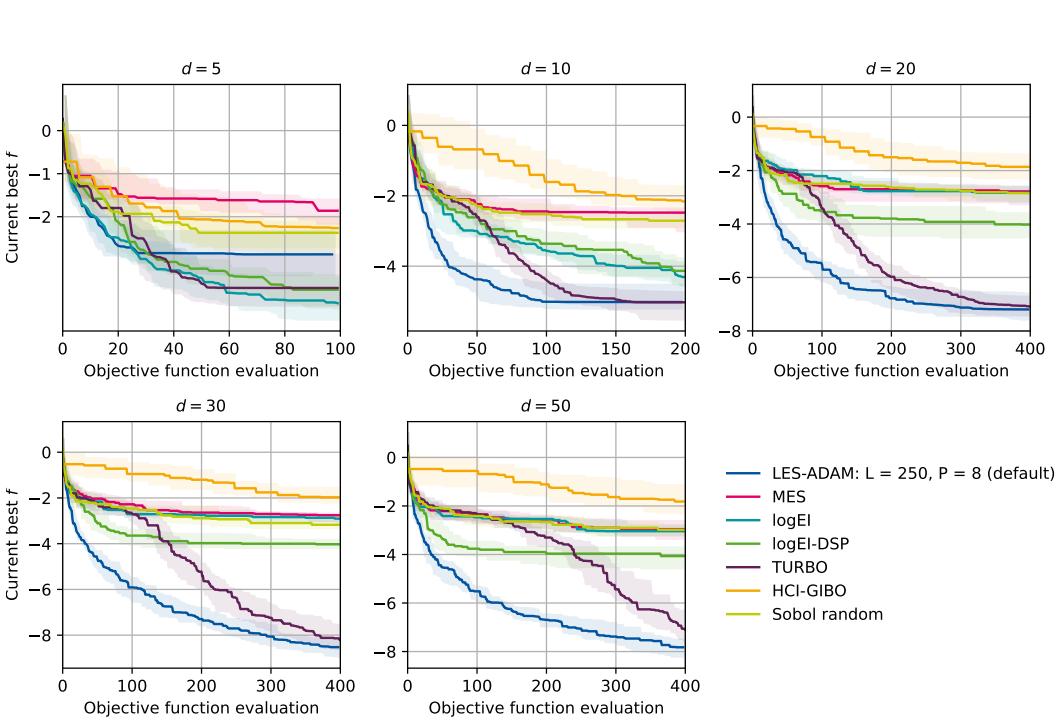


Figure 14: **Out of model comparison, complexity - high:** Median, 25-, and 75-percent quantiles - detailed results

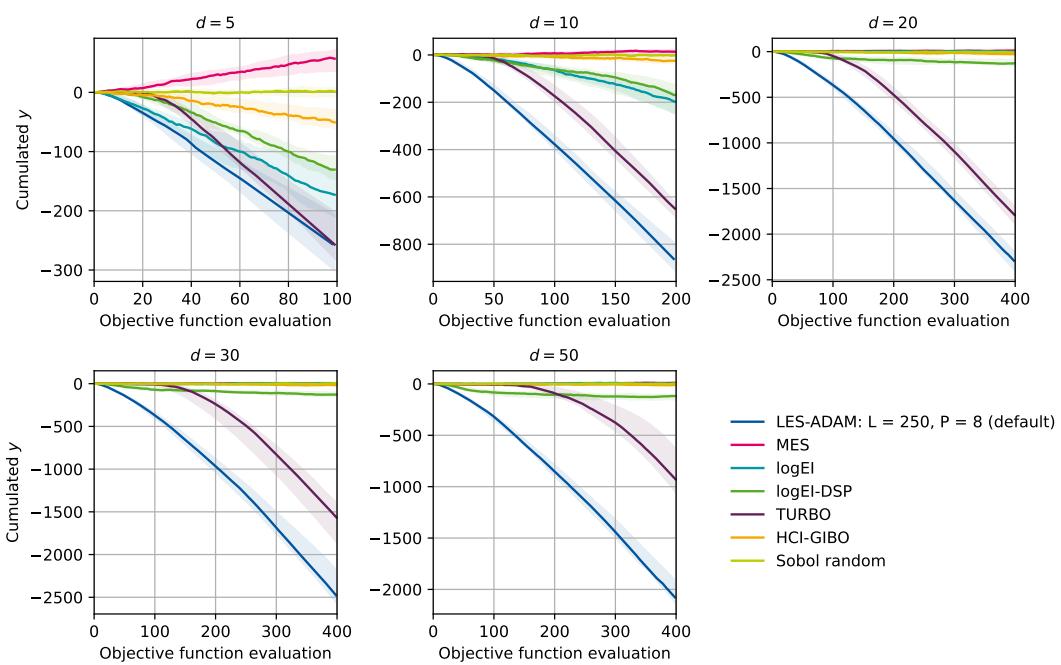


Figure 15: **Out of model comparison, complexity - high:** Median, 25-, and 75-percent quantiles - detailed results

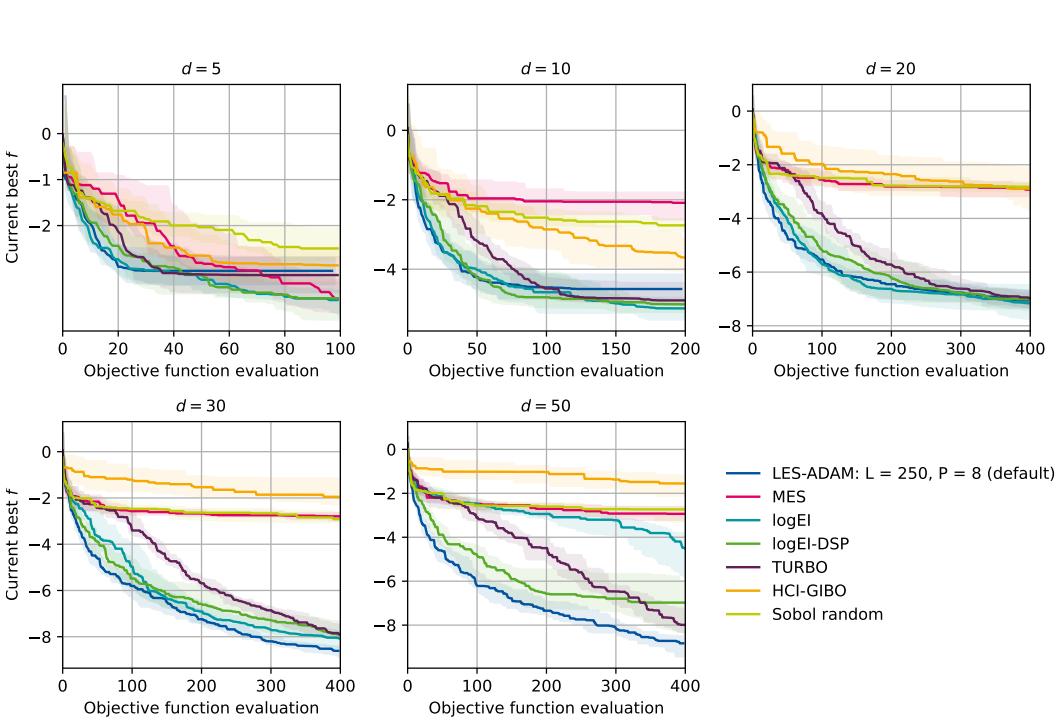


Figure 16: **Out of model comparison, complexity - medium:** Median, 25-, and 75-percent quantiles - detailed results

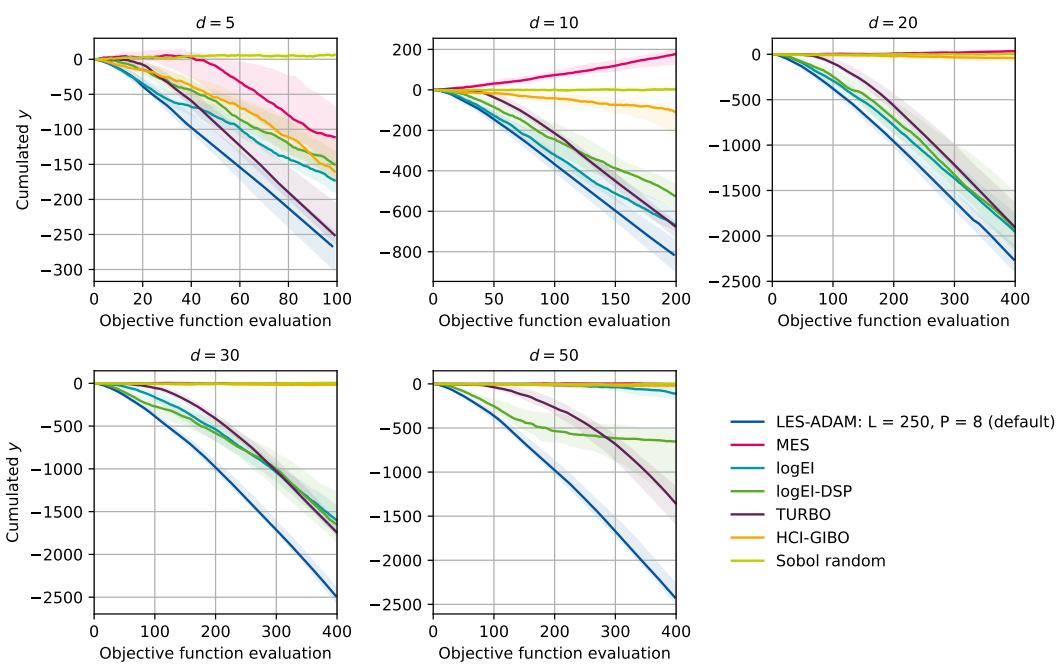


Figure 17: **Out of model comparison, complexity - medium:** Median, 25-, and 75-percent quantiles - detailed results

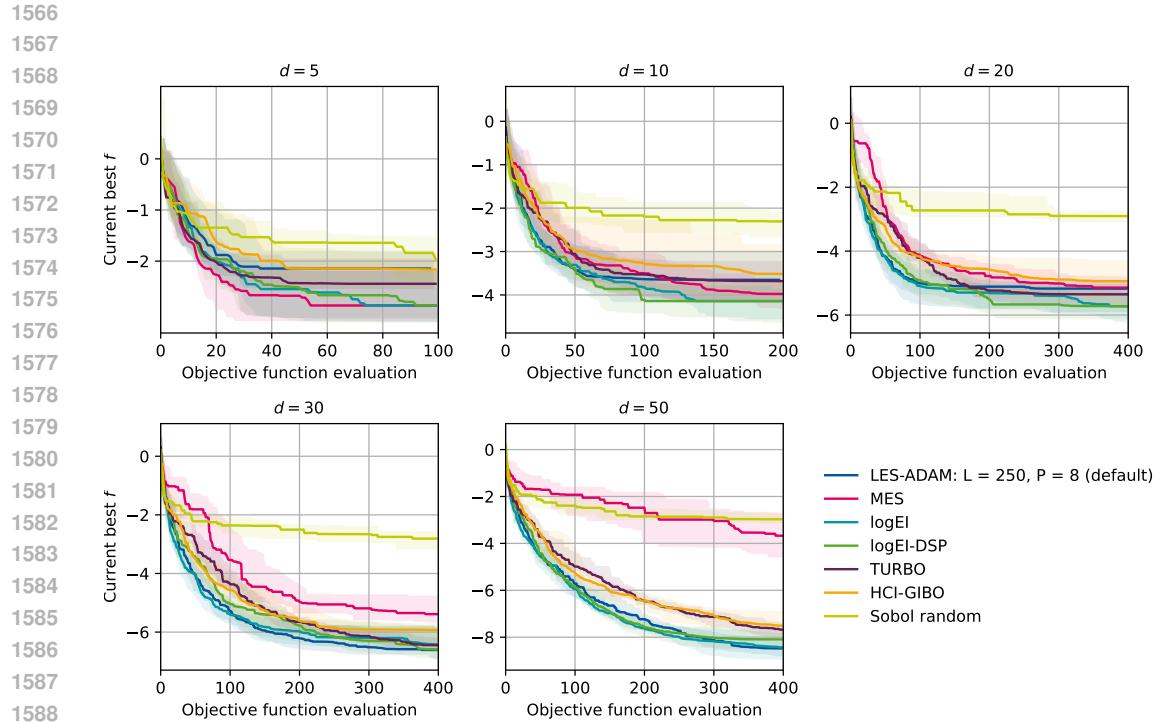


Figure 18: **Out of model comparison, complexity - low:** Median, 25-, and 75-percent quantiles - detailed results

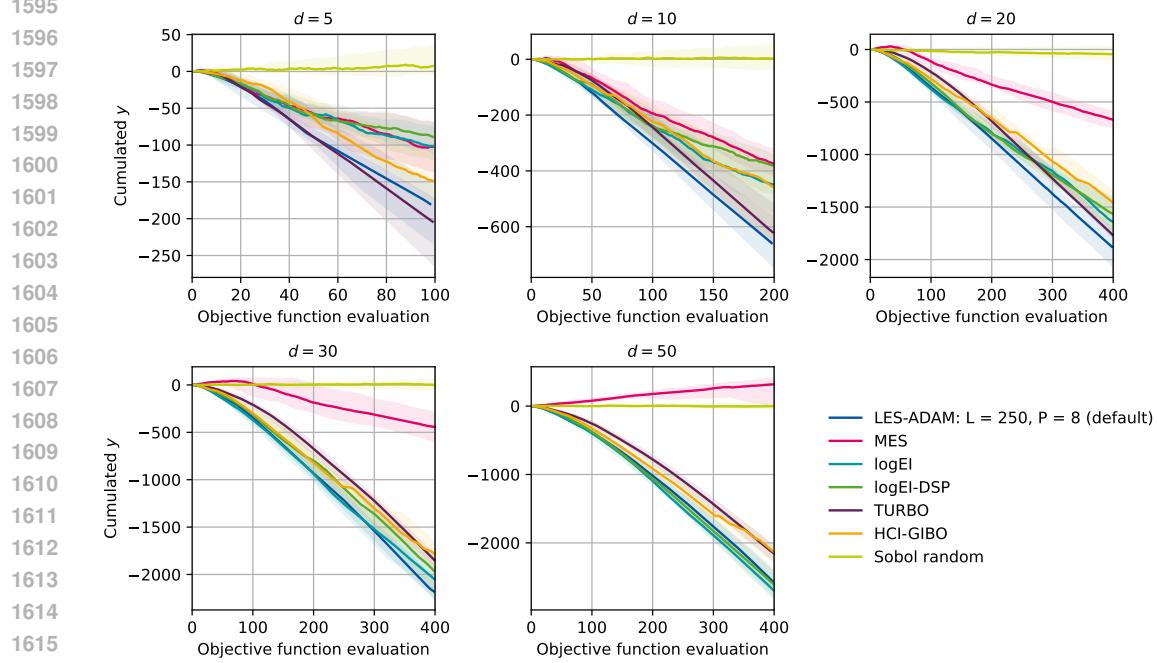


Figure 19: **Out of model comparison, complexity - low:** Median, 25-, and 75-percent quantiles - detailed results

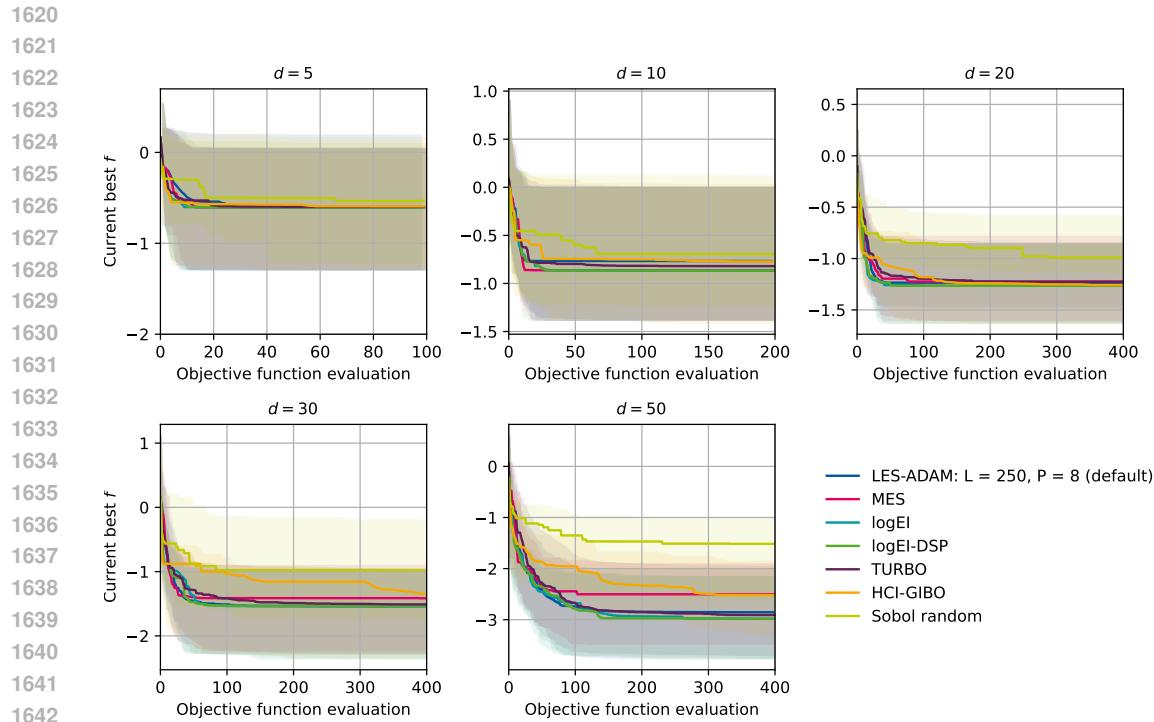


Figure 20: **Out of model comparison, complexity - extremely low:** Median, 25-, and 75-percent quantiles - detailed results

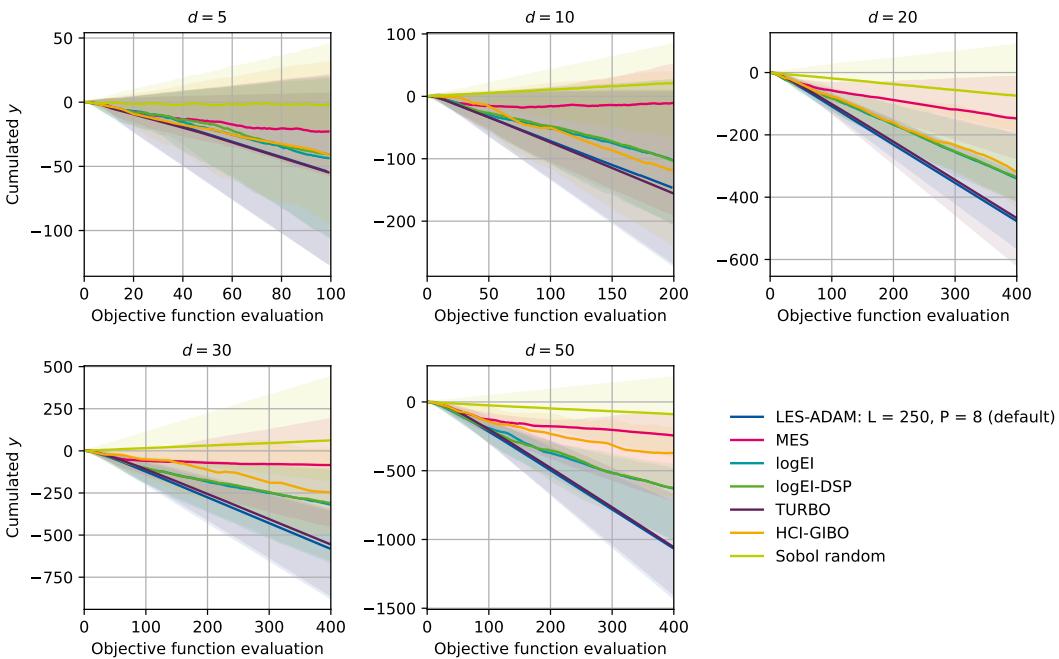


Figure 21: **Out of model comparison, complexity - extremely low:** Median, 25-, and 75-percent quantiles - detailed results

1674 **D.4 ADDITIONAL DETAILS AND RESULTS ON SYNTHETIC AND APPLICATION-ORIENTED**
1675 **OBJECTIVE FUNCTIONS**
1676

1677 In total, we evaluate LES on nine benchmark functions (Fig. 23 and 24). On functions with a single
1678 local optimum (square function $f(x) = \mathbf{x}\mathbf{x}^\top$), all methods reliably identify the optimum, though
1679 LES and TuRBO achieve lower cumulative regret, underscoring the advantage of local search in this
1680 setting. In contrast, the 5-d Ackley function – designed as a failure case for LES – leads all methods,
1681 including LES and the global baselines, to perform poorly (Appx. D.4). Surprisingly, for 30-d Ackley,
1682 LES and TuRBO outperform global methods. However, LES has a high run-to-run variance which
1683 indicates that some runs get stuck in local optima.

1684 In the rover (Wang et al., 2018) and Mopta08 (Jones, 2008) tasks, LES, logEI and TuRBO perform
1685 similarly with LES being best in the rover task and logEI being best in the Mopta08 task. In the lunar
1686 lander task (Brockman et al., 2016), LES is not competitive. The lunar lander task has multiple local
1687 optima where LES is getting stuck in some runs (see Fig. 22).

1688 The lunar lander problem (Fig. 22) and the Ackley function both contain many local minima, which
1689 makes them particularly challenging for our local method. Interestingly, LES performs still best on
1690 the 30-dimensional Ackley function. Overall, LES achieves the lowest cumulative regret – sometimes
1691 tied with other algorithms – except on low-dimensional problems with many local optima (Ackley-
1692 $d = 5$, Lunar). For logEI, high exploration costs occur only in low dimensions, which may be
1693 explained by its tendency to repeatedly sample the same location once it has found a (local) optimum.
1694 In terms of simple regret, LES matches the baselines except on the low-dimensional, multi-modal
1695 benchmarks (5-d Ackley and Lunar).

1696 All BO algorithms use the hyperparameter as presented in Table 10. Hyperparameters follow (Xu
1697 et al., 2025), using a box hyperprior and length scale initialization scaled by \sqrt{d} to favor low model
1698 complexity. Observations are generated without noise. We use 20 seeds for the policy search tasks
1699 and 10 seeds for the synthetic functions.

1700 **Table 10: Model Hyperparameters for the synthetic and application-oriented objective functions**
1701

1702

Name	Description	Value
$k(\cdot, \cdot)$	kernel	SE-ARD
$p(l)$	length-scale hyper prior	None
σ_n	observation noise	fixed at 0.001
σ_k	GP output scale	variable
l_{\max}	length scale upper bound	\sqrt{d}
l_{\min}	length scale lower bound	0.05
l_{init}	length scale initialization	$0.2\sqrt{d}$
	hyperparameter optimization frequency	after every sample ³
	standardize data	yes

1713 ⁴Except for the GIBO variants, where we optimize the hyperparameter only after each step.
1714
1715
1716
1717
1718
1719
1720
1721
1722
1723
1724
1725
1726
1727

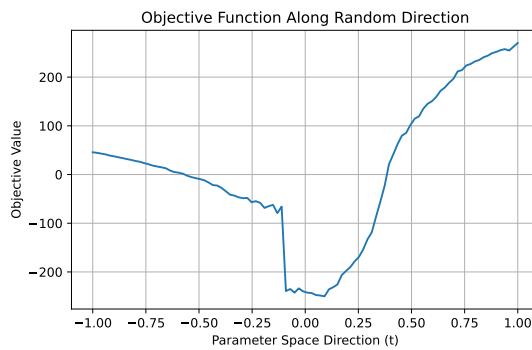


Figure 22: A random slice through the deterministic lunar lander objective function. Although the objective is deterministic, we see multiple noise-like local optima and a prominent step in the objective function landscape. Both properties are hard to model with a GP using an SE kernel with small observation noise.

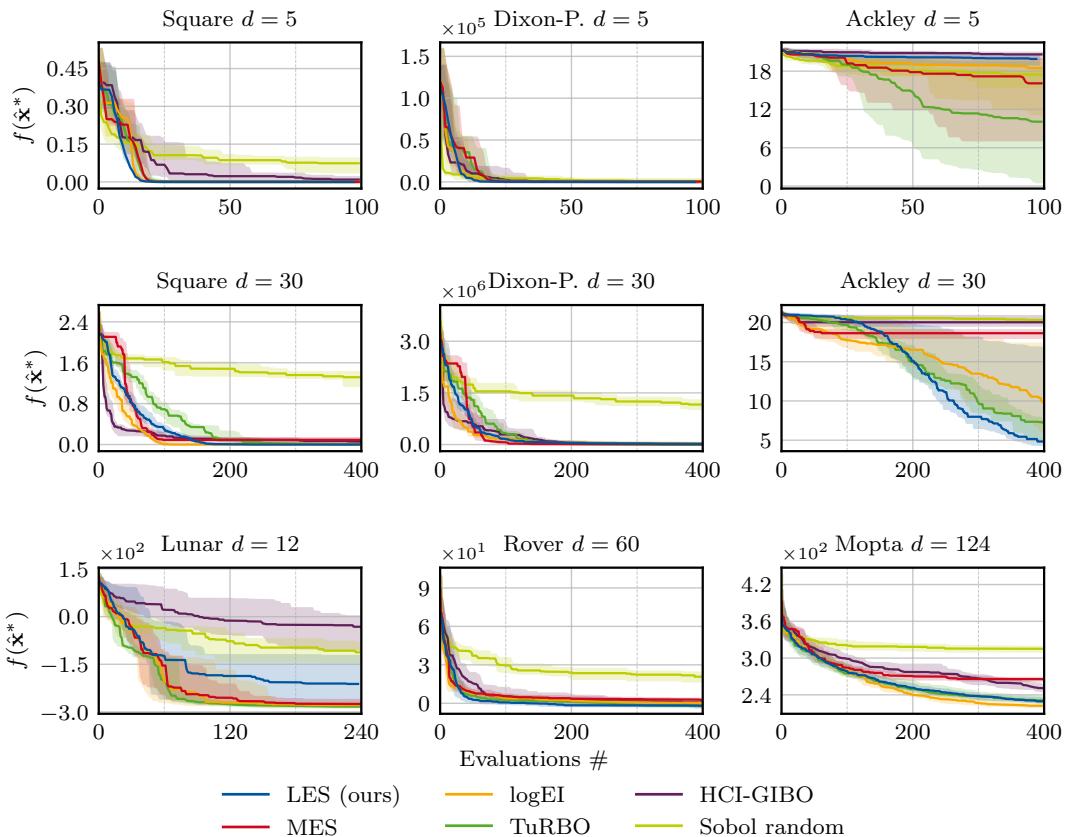
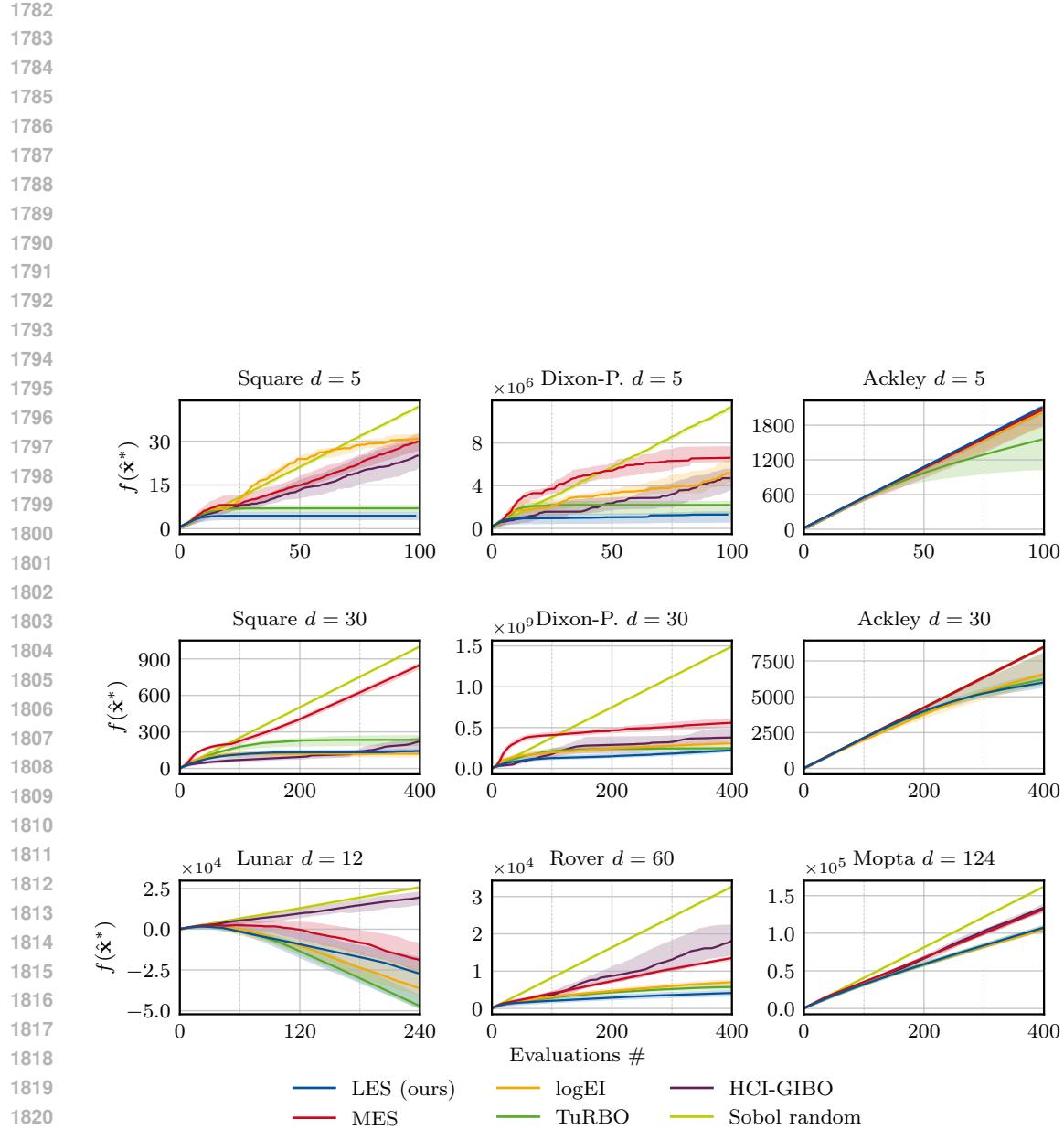


Figure 23: Median, 25-, and 75-percent quantiles - synthetic and application-oriented objective functions



1822 Figure 24: Median, 25-, and 75-percent quantiles of cumulative cost - synthetic and application-
1823 oriented objective functions

1824
1825
1826
1827
1828
1829
1830
1831
1832
1833
1834
1835

1836

D.5 ABLATIONS ON APPROXIMATION ACCURACIES AND RUNTIME

1837

1838

1839 Figure 25 illustrates the effect of the number of Monte Carlo samples L and the number of equally
 1840 spaced points P taken from each descent sequence. We evaluate this in the out-of-model GP sample
 1841 scenario with medium complexity (see Sec. 6.2). As expected, more accurate approximations yield
 1842 better performance, with the differences most pronounced in the $d = 50$ case. While $L = 250$ and
 1843 $P = 16$ performs best, we adopt $L = 250$ and $P = 8$ in our experiments as a compromise between
 1844 runtime and accuracy.

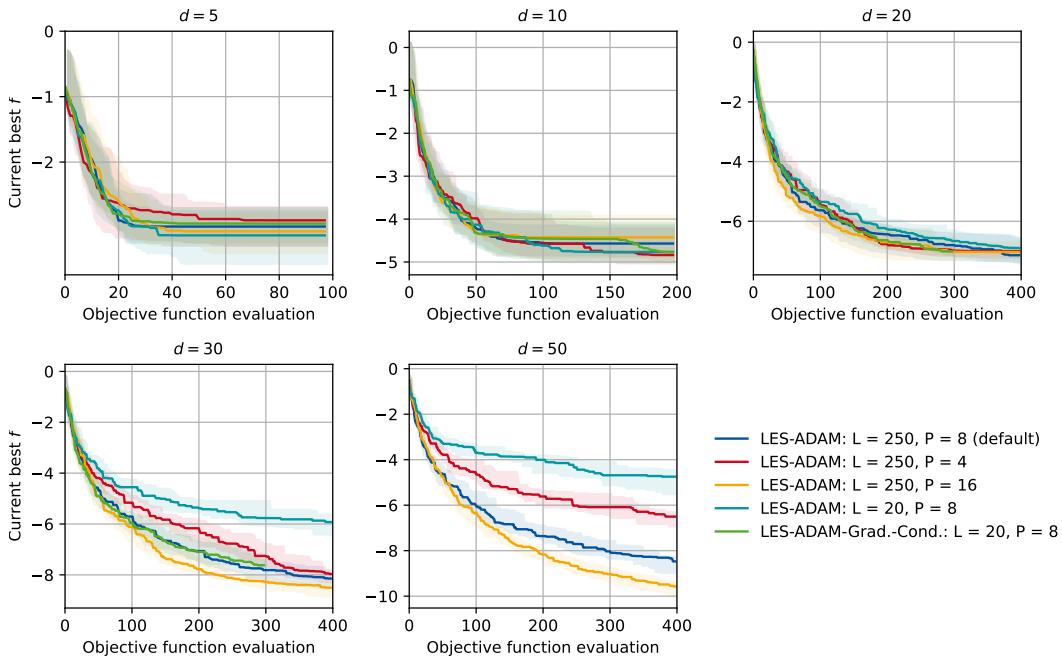
1845

1846 We further verify that conditioning on function values instead of gradients in the descent sequence
 1847 does not substantially harm performance. For runtime and memory reasons, gradient conditioning
 1848 (LES-ADAM-Grad.-Cond.) was only run with coarse discretizations, up to 300 samples and excluding
 $d = 50$.

1849

1850

1851



1872

1873 Figure 25: Comparing different acquisition function approximation accuracies - the better the
 1874 approximation (larger value of P and L) the better the results (Out-Of-Model Comparison on
 1875 GP-Samples - medium complexity).

1876

1877

1878

1879

1880

1881

1882

1883

1884

1885

1886

1887

1888

1889

The computational cost of LES is closely related to the chosen discretization, i.e., the values of L and P . To compare the influence of the acquisition function choice on overall runtime we evaluate it in the within-model comparison case. Table 11 shows the results for medium complexity. For comparison, we also include the runtime of our baselines. Additionally, Figure 26 shows the average runtime per iteration.

Our proposed approximation of LES requires roughly 10 times the wall-clock time compared to TuRBO, with an average of 17 seconds per iteration to select the next query. Notably, BoTorch’s logEI has a similar runtime.

As a caveat, runtime depends strongly on several factors, including settings for acquisition function optimization. We used the default configurations from BoTorch tutorials for all baselines and did not optimize any baseline or our implementation for speed.

1890 Table 11: Average computation time per iteration of LES-ADAM for the medium complexity within
 1891 model comparison, i.e., without GP hyperparameter optimization. Results are given in seconds and
 1892 are averaged over 20 seeds.

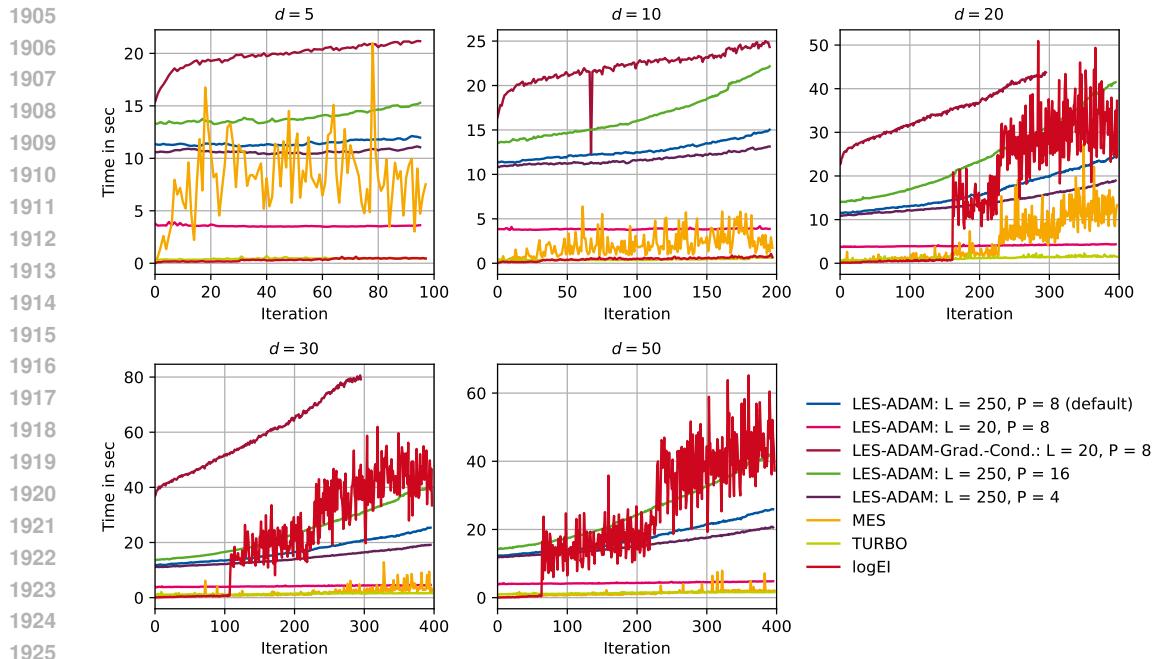
1893

1894

	$d = 5$	$d = 10$	$d = 20$	$d = 30$	$d = 50$
LES: L = 250, P = 8 (default)	11.4	12.6	16.5	17.1	17.6
LES: L = 250, P = 4	10.6	11.7	14.0	14.3	15.4
LES: L = 250, P = 16	13.8	16.6	24.5	24.1	25.3
LES: L = 20, P = 8	3.5	3.8	4.0	4.2	4.3
MES	8.2	2.1	5.1	1.8	1.3
TuRBO	0.4	0.4	1.2	1.4	1.4
logEI	0.3	0.5	15.5	23.0	24.0

1903

1904



1926

Figure 26: Evaluating LES with different local optimizers (Out-Of-Model Comparison on GP-Samples - low complexity)

1927

1928

1929

D.6 COMPARING DIFFERENT ITERATIVE OPTIMIZERS

1930

If not stated otherwise, the ADAM optimizer was employed as the local optimization algorithm throughout this work. However, the general framework is applicable to any kind of iterative optimization. Therefore, we evaluated the impact of different iterative optimization schemes on the overall performance. We use the out of model comparison GP sample scenarios (see Sec. 6.2).

1931

We expect that the performance of different inner optimizers also depends on the kernel. Sample paths from a GP with a Matérn 1/2 kernel are not continuously differentiable, making LES-ADAM and LES-GD less suitable choices. In such cases, LES with CMA-ES or other zeroth-order optimizers (e.g., hill climbing or pattern search) may perform better. We leave a more thorough evaluation of the benefits of different local optimizers in LES for future work.

1941

1942

ADAM For Adam we use 500 local optimization steps a step size of 0.002, and default Keras momentum hyperparameter ($\beta_1 = 0.9$, $\beta_2 = 0.999$). As an alternative, we also evaluate a LES-ADAM variant with less aggressive gradient smoothing ($\beta_1 = 0.5$). Instead of conditioning on the

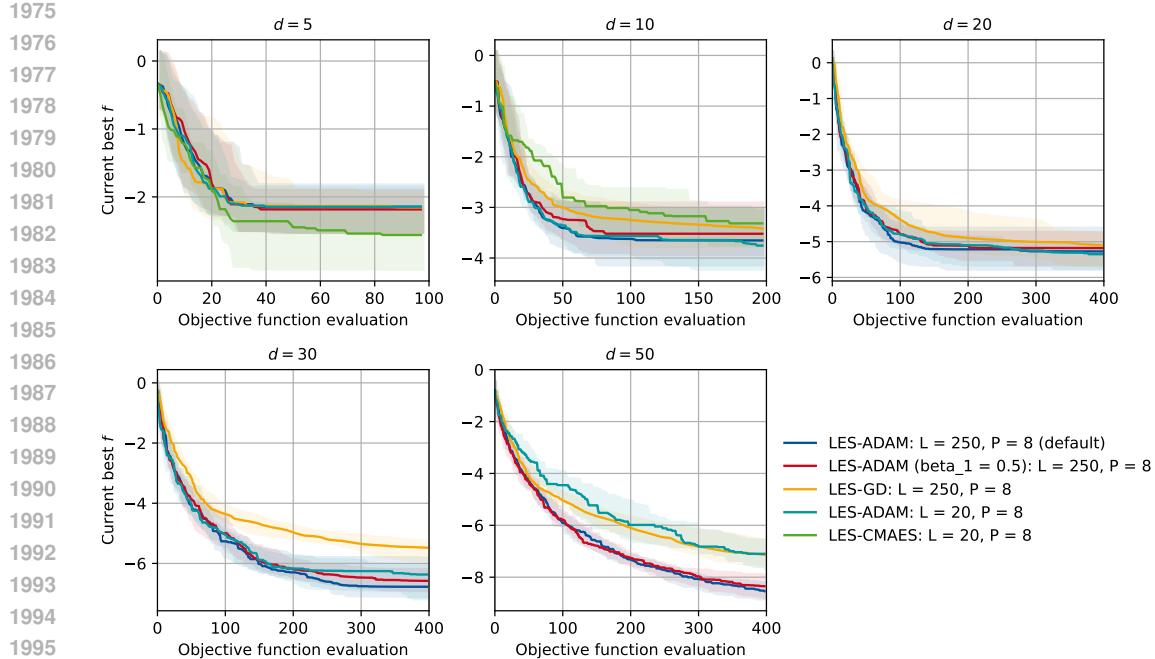
1944 gradient observations, we condition on function values. We show in Appx. D.5 that this simplification
 1945 is justified empirically.
 1946

1947 **Gradient Descent** For Gradient Descent (GD) we also use 500 local optimization steps and a
 1948 smaller learning rate of 0.0001. Preliminary results with a larger step size (the same as in ADAM)
 1949 has produced oscillating behavior. Similarly to ADAM we condition on function values instead of
 1950 gradient observations.
 1951

1952 **CMAES** As a third optimizer we choose CMAES and run it for 50 steps. We approximate the
 1953 descent sequence by the mean of the parameter distribution. The σ hyperparameter is set to 0.5 and
 1954 similar to ADAM and GD we warm-start CMAES from the best solution found so far. Due to the
 1955 high computational cost of running CMAES on multiple GP samples in each iteration, we evaluate it
 1956 only in the 5-d and 10-d case and use a coarse discretization. Note that CMAES is a zeroth-order
 1957 optimization algorithm and therefore does not require the GP-samples to be differentiable.
 1958

1959 Figures 27 to 29 show the results for low, medium, and high complexity. LES-CMAES performs
 1960 better than the other algorithms for $d = 5$ and low problem complexity. This may hint to a more
 1961 global search behavior and may indicate that the optimizer's properties on the individual samples
 1962 may carry over to the respective LES version. However, already at $d = 10$ or higher complexity LES-
 1963 CMAES falls behind. This can be attributed to the worse performing global optimization or to the
 1964 descent sequence approximation using the mean of the population not being accurate enough. Both
 1965 LES-ADAM version perform similar in all complexities. LES-GD performs worse than LES-ADAM
 1966 in the low-complexity case. However, in the medium and high complexity cases LES-GD performs
 1967 best.
 1968

1969 Overall, results highlight that investigating various local optimizers for different model properties is
 1970 an interesting direction for future research.
 1971
 1972
 1973
 1974
 1975



1996 Figure 27: Evaluating LES with different local optimizers (Out-Of-Model Comparison on GP-
 1997 Samples - low complexity)

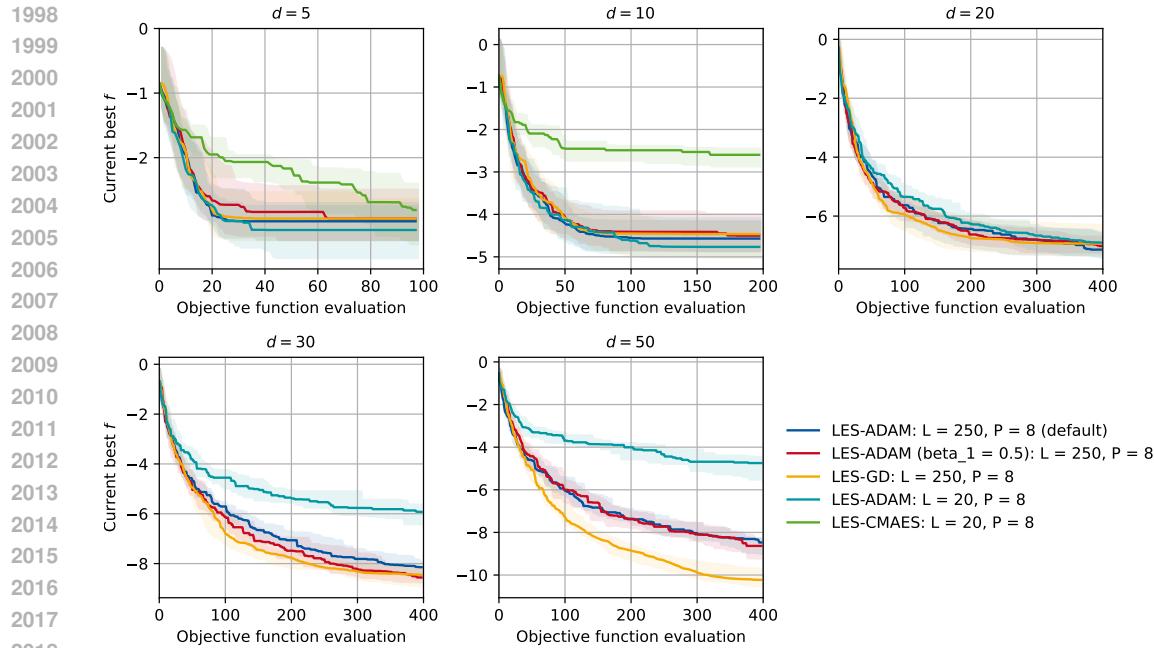


Figure 28: Evaluating LES with different local optimizers (Out-Of-Model Comparison on GP Samples - medium complexity)

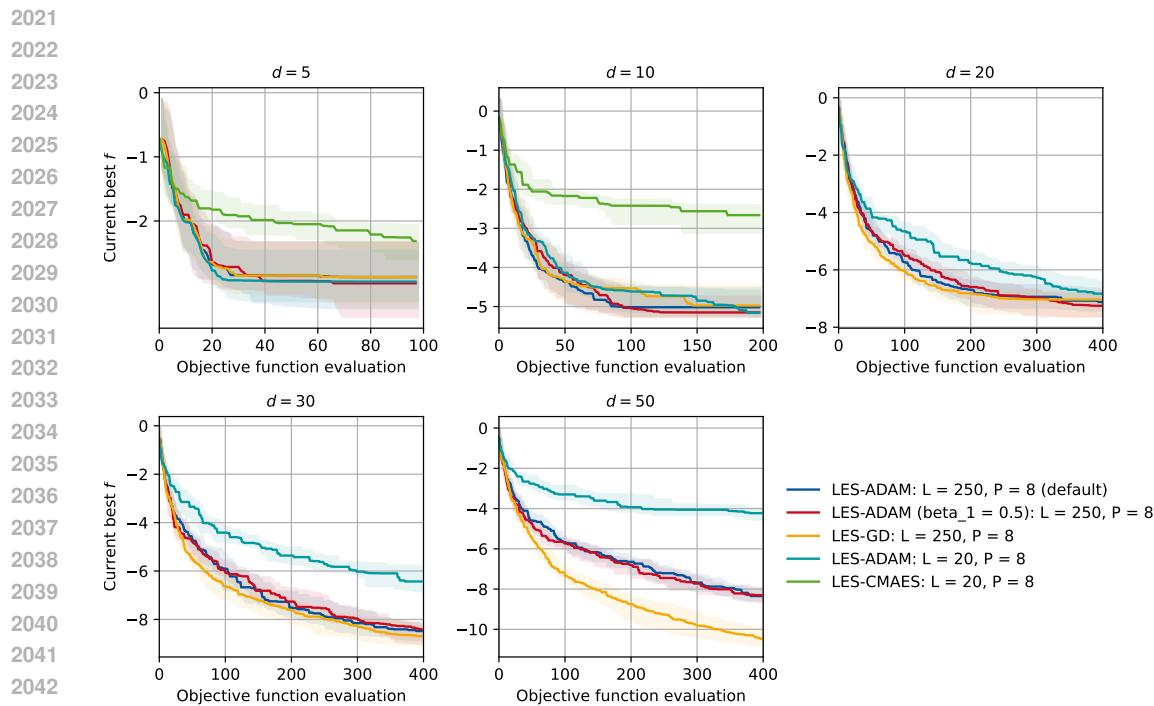


Figure 29: Evaluating LES with different local optimizers (Out-Of-Model Comparison on GP Samples - high complexity)

2052 E A STOPPING CRITERION FOR LOCAL ENTROPY SEARCH
20532054 E.1 METHOD
2055

2056 In practical applications, it is essential to determine when to terminate the optimization. In the
2057 previous section, we performed local optimization on multiple posterior samples. This enables us
2058 to adopt the Monte-Carlo-based stopping criterion proposed by (Wilson, 2024) in a local setting
2059 without incurring significant additional cost, as we can directly reuse the samples generated during
2060 the acquisition step. To achieve this we define a new notion of local regret:

2061 **Definition 1** (Local simple regret). Given the posterior GP f_t at BO step t , the *local simple regret*
2062 with respect to the model-based local optimum $f_t^* = \sup_x f_t(x)$ of a candidate point $x \in \mathcal{X}$ is
2063

$$2064 \quad r_t^{\mathcal{O}}(x) = f_t^* - f_t(x). \quad (31)$$

2066 Local regret formalizes how close we are to the best value reachable from the user’s initial guess by
2067 the optimizer \mathcal{O} . This is attractive when the global optimum is irrelevant or unattainable in practice.
2068 We stop the optimization if the current solution is within ε of the optimum with probability δ , i.e.,
2069 when it is (ε, δ) locally optimal:

2071 **Definition 2** $((\varepsilon, \delta)$ -local optimality). Fix tolerances $\varepsilon > 0$ and $\delta \in (0, 1)$. A point x observed up to
2072 step t is (ε, δ) -*locally-optimal* (with respect to x_0 and optimizer \mathcal{O}) if
2073

$$2074 \quad \Pr[r_t^{\mathcal{O}}(x) \leq \varepsilon] \geq 1 - \delta. \quad (32)$$

2076 We estimate the probability of the regret being smaller than epsilon using Monte-Carlo sampling:

$$2079 \quad \Pr(r_t \leq \varepsilon) \approx \frac{1}{L} \sum_{l=1}^L \mathbb{1}(r_t^l \leq \varepsilon) = \frac{1}{L} \sum_{l=1}^L \mathbb{1}(f^l(\hat{x}_t^*) - f^l(x_t^{l,*}) \leq \varepsilon). \quad (33)$$

2082 We follow (Wilson, 2024) and design a probabilistic stopping rule that leads to bounded *local* regret
2083 (31) with high (within-model) probability. Next, we restate the formal results from (Wilson, 2024)
2084 for LES.

2085 **Assumption 1.**

- 2087 • The search space is the unit hyper-cube $\mathcal{X} = [0, 1]^D$.
- 2088 • There exists a constant $L_k > 0$ so that $\forall x, x' \in \mathcal{X}, |k(x, x) - k(x, x')| \leq L_k \|x - x'\|_{\infty}$.
- 2089 • The sequence of query locations (x_t) is almost surely dense in \mathcal{X} .

2090 We show in Appx. G.1 that LES fulfills the third assumption for specific kernels.

2092 **Theorem 1** (Proposition 2, (Wilson, 2024)). *Assume 1. Given a risk tolerance $\delta > 0$, define
2093 non-zero probabilities δ_{mod} and δ_{est} such that $\delta_{\text{mod}} + \delta_{\text{est}} \leq \delta$ and let $(\delta_{\text{test}}^t)_{t \geq 0}$ be a positive
2094 sequence so that $\sum_{t=0}^{\infty} \delta_{\text{test}}^t \leq \delta_{\text{est}}$. For any regret bound $\varepsilon > 0$, if the Monte-Carlo test of (Wilson,
2095 2024, Alg. 2) is run at each step $t \in \mathbb{N}_0$ with tolerance δ_{test}^t to decide whether a point satisfies
2096 $\Pr[r_t^{\mathcal{O}}(x) \leq \varepsilon] \geq 1 - \delta_{\text{mod}}$, then LES almost surely terminates and returns a solution with
2097 probabilistic regret that satisfies Definition 2.*

2100 E.2 RESULTS
2101

2102 The stopping times (Sec. E.1) for LES on the out-of-model comparison with low model complexity
2103 are in Tab. 12. For $d \geq 30$ fewer than half the runs stop within the budget of 400 evaluations. When
2104 compared to the results in (Wilson, 2024) these results show that the local optimization needs fewer
2105 samples before stopping. These results reinforce the intuition that reaching a local optimum is easier
than reaching a global one – even in black-box optimization problems.

2106 Table 12: Median stopping times with decision every 25 queries ($\delta = 0.05$) - out of model comparison.
2107
2108

ε	$d = 5$	$d = 10$	$d = 20$
0.1	50	150	325
0.01	50	175	350

2115 Table 13 summarizes the results for the stopping rule in the within model comparison case with low
2116 problem complexity. For comparison, (Wilson, 2024) reported an average stopping time after 100
2117 queries for the 4-d within-model case. Note that we choose the results of (Wilson, 2024) for the low
2118 noise case, since it is most fitting to our experiments. The parameters reported in Table 3 lead to a
2119 BO run being stopped after $k_{\max} = 248$ out of $L = 250$ samples show local regret smaller than ε .

2120 Table 13: Number of queries until half of the runs are stopped ($\delta = 0.05$). Decision every 25 queries
2121 - within model comparison.
2122

ε	$d = 5$	$d = 10$	$d = 20$
0.1	50	150	275
0.01	50	175	300

2130

F ALTERNATIVE INFORMATION-THEORETIC LOCAL ACQUISITION 2131 FUNCTIONS

2133 We propose two additional information-theoretic local acquisition functions that are closely related
2134 to the local entropy search paradigm: Local Thompson sampling and local-optimum LES. Both are
2135 conceptually more straight forward and easier to compute than LES but perform worse.
21362138

F.1 LOCAL THOMPSON SAMPLING

2140 In local Thompson sampling (L-TS) we sample only one path from the GP, which we then minimize
2141 locally using the ADAM optimizer and query at its minimum. This method proves to be significantly
2142 more computationally efficient than the entropy search approach, as it avoids the need for the relatively
2143 costly Monte Carlo approximation outlined in equation (16).2144 We assess local Thompson sampling to better understand the benefits of considering the distribution
2145 over descent sequences at each iteration, as implemented in LES. We expect that L-TS may not
2146 perform as well as LES, since L-TS optimizes a single descent sequence in a greedy manner. In
2147 contrast, LES recognizes that multiple descent sequences exist and seeks to maximize information
2148 gain across all of them.
21492150

F.2 CONDITIONING ONLY ON THE LOCAL OPTIMUM

2152 In Appx. B.1, we have shown that directly conditioning on the local optimum is not possible in
2153 general. That is, we cannot condition a GP on $O_{\mathbf{x}_0}^{*,l}$ in
2154

2155
$$\mathbb{E}_f [H[p(y(\mathbf{x}) | \mathcal{D}_t, O_{\mathbf{x}_0}^*)]] \approx \frac{1}{L} \sum_{l=1}^L H[p(y(\mathbf{x}) | \mathcal{D}_t, O_{\mathbf{x}_0}^{*,l})]. \quad (34)$$

2156 We cannot encode that the local optimum at location $\mathbf{x}^{*,l}$ was reached through a local optimizer from
2157 point \mathbf{x}_0 . What we can encode is that $\mathbf{x}^{*,l}$ is a local optimum defined by a gradient of zero and a
2158

positive (known) Hessian:

$$\begin{aligned} & \frac{1}{L} \sum_{l=1}^L H[p(y(\mathbf{x}) \mid \mathcal{D}_t, O_{\mathbf{x}_0}^l)] \\ & \approx \frac{1}{L} \sum_{l=1}^L H[p(y(\mathbf{x}) \mid \mathcal{D}_t \cup (\mathbf{x}^{*,l}, f^l(\mathbf{x}^{*,l})), (\mathbf{x}^{*,l}, \nabla f^l(\mathbf{x}^{*,l})), (\mathbf{x}^{*,l}, \Delta f^l(\mathbf{x}^{*,l})))] \end{aligned} \quad (35)$$

Note that the exact values of the observations again are irrelevant for the conditional entropy. This gives rise to the LES-ADAM Opt. Cond. acquisition function.

We evaluate LES-ADAM Opt. Cond. because we aim to demonstrate that the sequence leading to the local optima contains valuable information; merely conditioning on the local optimum—the final point of this descent sequence—is insufficient.

F.3 RESULTS

Figure 30 shows that LES-ADAM outperforms the other information-theoretic approaches, with the performance gap widening in higher dimensions. The experiments are conducted in the out-of-model GP sample scenario with medium complexity (see Sec. 6.2). Overall, the results indicate that considering multiple descent sequences per iteration, as well as the entire descent sequence rather than only the distribution of local optima, improves performance.

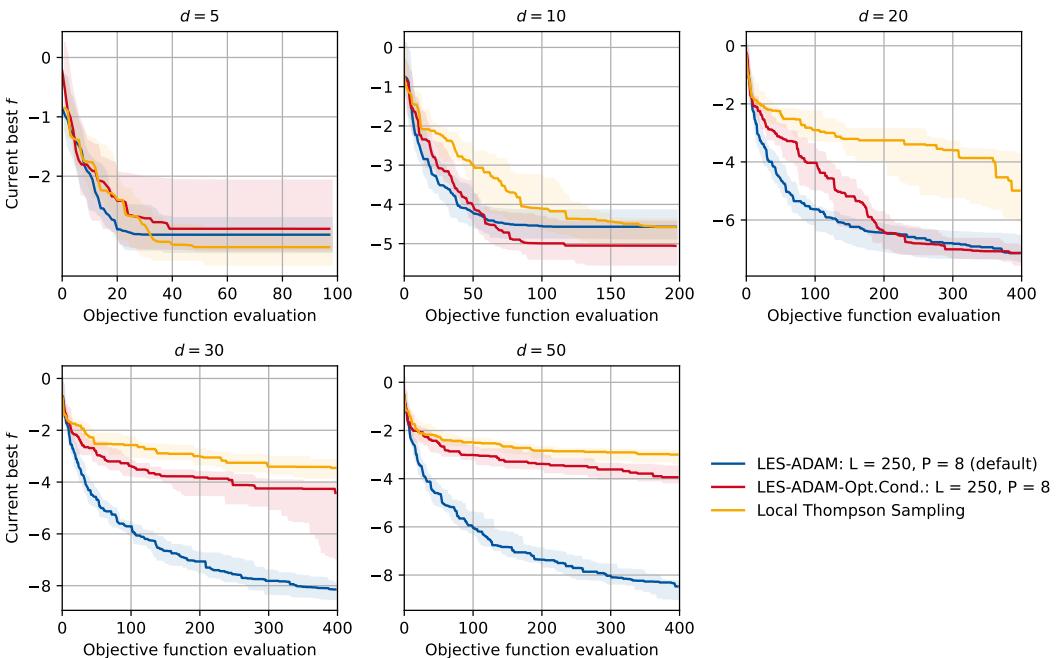


Figure 30: Median, 25-, and 75-percent quantiles, out-Of-model comparison on GP-Samples - medium complexity).

2214

G THEORETICAL RESULTS

2215

2216 This section contains some theoretical results in support of the main claims of the paper. We use the
2217 notational shorthand $k_t(\cdot, \cdot) = k(\cdot, \cdot \mid \mathcal{D}_t)$.
2218

2219

G.1 LES QUERIES ARE DENSE

2220

2221 **Lemma 1** (Density of LES maximizers). *Assume $\mathcal{X} = [0, 1]^D$ and let $k_t : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ be a
2222 continuous, positive-definite kernel that admits the no-empty-ball property (Wilson, 2024, Definition
2223 3), $\forall \mathbf{x}, \mathbf{x}' \notin \mathcal{D}_t$ $k(\mathbf{x}, \mathbf{x}') > 0$, and the descent sequence (\mathbf{z}_n) contains at least one $\mathbf{z} \notin \mathcal{D}_t$ almost
2224 surely. Fix a noise variance $\gamma^2 \geq 0$ and denote by k_t, σ_t^2 the posterior covariance and predictive
2225 variance after t evaluations. Then, for every $t \in \mathbb{N}$ and all $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$,*

2226
$$k_t(\mathbf{x}, \mathbf{x}) > k_t(\mathbf{x}', \mathbf{x}') = 0 \implies \alpha_{\text{LES}, t}(\mathbf{x}) > \alpha_{\text{LES}, t}(\mathbf{x}') \quad (36)$$
2227

2228 Consequently the sequence (\mathbf{x}_t) of maximizers $\mathbf{x}_t \in \arg \max_{\mathbf{x} \in \mathcal{X}} \alpha_{\text{LES}, t}(\mathbf{x})$ form a dense sequence
2229 in \mathcal{X} almost surely.

2230 *Proof.* If $k_t(\mathbf{x}', \mathbf{x}') = 0$, positive-semidefiniteness implies $k_t(\mathbf{x}', \mathbf{z}) = 0$ for every $\mathbf{z} \in \mathcal{X}$. Hence,
2231 $\sigma_t^2(\mathbf{x}') = \sigma_{t \mid X_{\text{DS}}}^2(\mathbf{x}') = \gamma^2$ for every Monte-Carlo draw X_{DS} , so $\alpha_{\text{LES}, t}(\mathbf{x}') = 0$.

2232 Take \mathbf{x} with $k_t(\mathbf{x}, \mathbf{x}) > 0$. Because the the descent sequence (\mathbf{z}_n) contains at least one $\mathbf{z} \notin \mathcal{D}_t$
2233 almost surely the posterior covariance is not zero the covariance vector $k_t(\mathbf{x}, X_{\text{DS}})$ is non-zero. The
2234 GP variance update gives

2235
$$\sigma_{t \mid X_{\text{DS}}}^2(\mathbf{x}) = \sigma_t^2(\mathbf{x}) - k_t(\mathbf{x}, X_{\text{DS}})[K_t(X_{\text{DS}}, X_{\text{DS}}) + \gamma^2 I]^{-1}k_t(X_{\text{DS}}, \mathbf{x}), \quad (37)$$
2236

2237 and the quadratic form on the right is strictly positive, hence $\sigma_{t \mid X_{\text{DS}}}^2(\mathbf{x}) < \sigma_t^2(\mathbf{x})$. Therefore each
2238 logarithm inside $\alpha_{\text{LES}, t}(\mathbf{x})$ is positive and their expectation is strictly positive $\alpha_{\text{LES}, t}(\mathbf{x}) > 0$.

2239 Density of the query points now follow from (Wilson, 2024, Proposition 4). \square

2240

G.2 GRADIENT DESCENT PATHS UNDER A GP PRIOR WITH A SQUARED EXPONENTIAL 2241 KERNEL

2242

2243 In this section we zoom in on a specific instantiation of LES that samples candidate points by running
2244 gradient-descent (8) on functions drawn from a squared-exponential (SE) GP prior. This section
2245 explains why that particular pairing is a sensible starting point. We show, with a suitably step size, a
2246 gradient descent sequence starting from an initial design can reach any subset of the domain with
2247 positive prior probability. In addition, for any finite horizon the distribution of such sequences has full
2248 support on the corresponding product space and can therefore realize any finite sequence. Importantly,
2249 these reachability and support guarantees ensure that no part of the search space is ruled out by
2250 construction in this setting.

2251 **Assumption 2** (Design domain). The search space $\mathcal{X} \subset \mathbb{R}^d$ is non-empty, compact, convex, and has
2252 non-empty interior.

2253 We formalize the assumptions as follows.

2254 **Assumption 3** (Step size). Let $\mathcal{X} \subset \mathbb{R}^D$ be compact. For every realized objective $f \in \mathcal{C}^1(\mathcal{X})$ denote
2255 by $L(f)$ the global Lipschitz constant of its gradient. Choose a step size $\eta(f) > 0$ satisfying

2256
$$\eta(f) L(f) < 1.$$

2257 With this choice the gradient-descent map $\Phi_f(\mathbf{x}) = \mathbf{x} - \eta(f) \nabla f(\mathbf{x})$ is a strict contraction on \mathcal{X} .

2258 **Assumption 4** (Squared-exponential prior). The objective is a random draw from $p(f) \sim$
2259 $GP(0, k_{\text{SE}})$, so that $f \in C^\infty(\mathcal{X})$ almost surely and the associated RKHS is dense in $C^\infty(\mathcal{X})$
2260 with the C^1 -norm.

2261 **Lemma 2** (Open-set reachability of GD paths). *Let Assumption 2, 3, 4 hold. Define the gradient-descent iterates as in (8) so that*

2262
$$\mathbf{z}_0 \in \mathcal{X}, \quad \mathbf{z}_{n+1} = \mathbf{z}_n - \eta \nabla f(\mathbf{z}_n), \quad n \geq 0. \quad (38)$$
2263

2268 Then for every non-empty open set $U \subset \mathcal{X}$
 2269

$$\Pr_f[(\mathbf{z}_n) \cap U \neq \emptyset] > 0. \quad (39)$$

2272 *Proof.* Fix $U \neq \emptyset$ open and choose $u \in U$ and a horizon $m \in \mathbb{N}$.
 2273

2274 Since the map $\Phi_f(\mathbf{z}) = \mathbf{z} - \eta \nabla f(\mathbf{z})$ is a contraction (Assumption 3) one can constructs a smooth
 2275 function $f^* \in C^\infty(\mathcal{X})$ such that

$$\mathbf{z}_m(f^*) = u, \quad \|\nabla f^*\|_{\text{Lip}} \leq L_*. \quad (40)$$

2278 Since the RKHS $\mathcal{H}_{k_{\text{SE}}}$ of the squared-exponential kernel is dense in $C^\infty(\mathcal{X})$, every C^1 -ball
 2279 $B_\varepsilon(f^*) = \{f : \|f - f^*\|_{C^1} < \varepsilon\}$ contains at least one element of $\mathcal{H}_{k_{\text{SE}}}$. By the Gaussian-measure
 2280 support theorem (Vaart, van der & Zanten, van, 2008, Lem. 5.1), every open set that intersects $\mathcal{H}_{k_{\text{SE}}}$
 2281 has positive prior probability, hence

$$\Pr_f[\|f - f^*\|_{C^1} < \varepsilon] > 0. \quad (41)$$

2285 The mapping $C^1(\mathcal{X}) \ni g \mapsto \Phi_g^{(m)}(\mathbf{x}_0)$ is continuous in the C^1 -norm when $\eta L_* < 1$. Hence there
 2286 exists $\varepsilon > 0$ such that $\|f - f^*\|_{C^1} < \varepsilon \implies \mathbf{x}_m(f) \in U$.

2287 Combining this with (41) gives $\Pr_f[\mathbf{x}_m(f) \in U] > 0$, which implies (39). \square
 2288

2289 **Corollary 1** (Full support of finite GD paths). *Fix an integer horizon $N \geq 0$ and define*

$$\mathcal{O} : C^1(\mathcal{X}) \longrightarrow \mathcal{X}^{N+1}, \quad \mathcal{O}(f) := (\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N), \quad (42)$$

2292 where (\mathbf{x}_t) are obtained by gradient descent. Under Assumptions 2–4, the push-forward measure
 2293 $\mathcal{O}_\sharp[GP(0, k_{\text{SE}})]$ has full support on \mathcal{X}^{N+1} ; i.e., for every open cylinder set $U_0 \times \dots \times U_N \subset \mathcal{X}^{N+1}$
 2294 with all U_t open and non-empty,

$$\Pr_f[(\mathbf{x}_0, \dots, \mathbf{x}_N) \in U_0 \times \dots \times U_N] > 0. \quad (43)$$

2298 *Proof.* Proceed inductively on N .
 2299

2300 *Base case $N = 0$:* trivial because \mathbf{x}_0 is fixed.

2301 *Inductive step:* Assume the claim holds up to horizon $N - 1$. Given open U_0, \dots, U_N , the induction
 2302 hypothesis provides a function f^* and $\varepsilon > 0$ such that $\|f - f^*\|_{C^1} < \varepsilon$ implies $(\mathbf{x}_0, \dots, \mathbf{x}_{N-1}) \in$
 2303 $U_0 \times \dots \times U_{N-1}$. Apply Lemma 2 with starting point $\mathbf{x}_{N-1}(f^*)$ and target open set U_N to obtain
 2304 a further refinement ε' . Choose $\delta = \min\{\varepsilon, \varepsilon'\}$ and use the support property (41) to conclude the
 2305 probability is positive. \square

2306 As long as $k_t(\mathbf{x}, \mathbf{x}) > 0 \ \forall \mathbf{x} \in \mathcal{X}$ the same applies to the posterior. The proofs are identical because
 2307 conditioning on finitely many points does not change the RKHS nor the support of the measure; it
 2308 only shifts the mean.

2310 In summary, Lemmas 2 and 1 together show that, in the SE-prior/GD instantiation of LES, the
 2311 candidate-generation mechanism is fully expressive: no open region is inaccessible and no finite GD
 2312 sequence is excluded.

2313
 2314
 2315
 2316
 2317
 2318
 2319
 2320
 2321