
Poisson Process for Bayesian Optimization

Xiaoxing Wang^{1†} Jiaying Li^{2†} Chao Xue^{3*} Wei Liu⁴ Weifeng Liu² Xiaokang Yang¹
Junchi Yan¹ Dacheng Tao⁴

¹Department of Computer Science and Engineering, and MoE Key Lab of Artificial Intelligence, Shanghai Jiao Tong University

²College of Control Science and Engineering, China University of Petroleum (East China)

³JD Explore Academy

⁴The University of Sydney

[†]Equal Contributions. This work was done while the authors were interns at JD Explore Academy.

^{*} Corresponding Author

Abstract Bayesian Optimization (BO) is a sample-efficient black-box optimizer, and extensive methods have been proposed to build the absolute function response of the black-box function through a probabilistic surrogate model, including Tree-structured Parzen Estimator (TPE), random forest (SMAC), and Gaussian process (GP). However, few methods have been explored to estimate the relative rankings of candidates, which can be more robust to noise and have better practicality than absolute function responses, especially when the function responses are intractable but preferences can be acquired. To this end, we propose a novel ranking-based surrogate model based on the Poisson process and introduce an efficient BO framework, namely Poisson Process Bayesian Optimization (PoPBO). Two tailored acquisition functions are further derived from classic LCB and EI to accommodate it. Compared to the classic GP-BO method, our PoPBO has lower computation costs and better robustness to noise, which is verified by abundant experiments. The results on both simulated and real-world benchmarks, including hyperparameter optimization (HPO) and neural architecture search (NAS), show the effectiveness of PoPBO.

1 Introduction

Bayesian optimization (BO) (Mockus et al., 1978) is a popular black-box optimization paradigm and has achieved great success in a number of challenging fields, such as robotic control (Calandra et al., 2016), biology (González et al., 2015), and hyperparameter tuning for complex learning tasks (Bergstra et al., 2011). A standard BO routine usually consists of two alternate steps: 1) Train a probabilistic surrogate model to build the response surface of a black-box function $f(x)$; 2) Suggest the next query by optimizing an acquisition function according to the learned response surface. Popular surrogate models for the first step include random forest (SMAC) (Hutter et al., 2011), Tree-structure Parzen Estimator (TPE) (Bergstra et al., 2011; Tiao et al., 2021; Song et al., 2022), Gaussian Process (GP) (Snoek et al., 2012) and Bayesian Neural Network (BNN) (Springenberg et al., 2016; Snoek et al., 2015), aiming to estimate the distribution of function values for each candidate. Classic acquisition functions for the second step include Expected Improvement (EI) (Mockus, 1994), Thompson Sampling (TS) (Chapelle and Li, 2011; Agrawal and Goyal, 2013) and Upper/Lower Confidence Bound (UCB/LCB) (Srinivas et al., 2012), aiming at the exploration and exploitation trade-off. Most of the prior BO methods (Bergstra et al., 2011; Hutter et al., 2011; Snoek et al.,

2012) attempt to build an absolute response surface¹ of a black-box function based on the observed function values, and few have been explored to build a relative response surface.

However, absolute metrics can have the following shortcomings. **1) Absolute response can be difficult to obtain or even unavailable in some practical scenarios**, such as sports games and recommender systems where only relative response can be provided by pairwise comparison He et al. (2022). **2) Absolute response can be sensitive to noise**, as pointed out by Rosset et al. (2005). Such an issue will affect the performance of BO in noisy real-world scenarios. **3) It can be challenging to directly transfer the surrogate models for absolute response surfaces**. In particular, multi-fidelity metrics usually require multiple absolute responses for the same candidate. It is hard to utilize history observations on a coarse-fidelity metric to warm up the training of surrogate models on a fine-grained-fidelity one. Similarly, in hyperparameter optimization (HPO) and neural architecture search (NAS) tasks, it is hard to transfer the performance across different datasets.

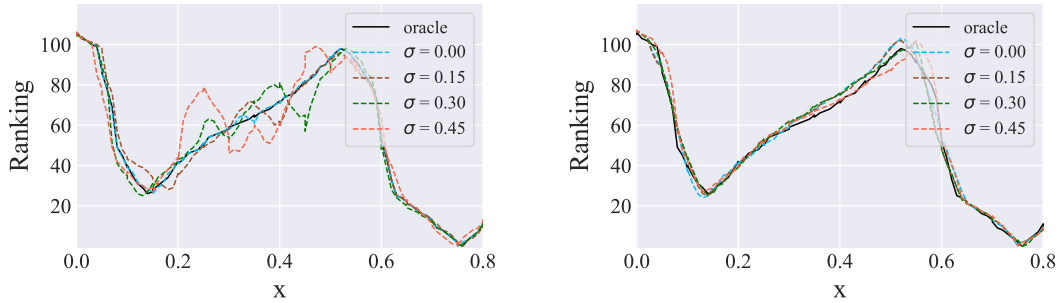
On the contrary, relative metrics can be effective cures for the above issues. **1) Relative response such as ranking has better practicality** since the information about candidate preferences can be more easily acquired than raw value (González et al., 2017; Kahneman and Tversky, 2013; Brusilovsky et al., 2007; González et al., 2017). **2) Relative response is more robust to noise than absolute response** since relation such as ranking between candidates is hard to be disrupted by noise, which is verified by Nguyen et al. (2021); Salinas et al. (2020). In this work, we also analyze the better robustness of rankings against absolute response in Sec. 3.1 under the common additive Gaussian noise assumption. **3) Relative response has better transferability**, such as rankings between candidates, since they are usually comparable among multi-fidelity metrics or evaluations across different datasets for the same candidate. It is also demonstrated by (Salinas et al., 2020; Nguyen et al., 2021; Feurer et al., 2018).

Some BO methods utilize the relative responses. Preferential BO (González et al., 2017; Mikkola et al., 2020; Lin et al., 2022) attempts to capture the relative preference by pairwise comparison. However, they either rely on a computationally-expensive soft-Copeland score (PBO) or need to optimize EI by the projective preferential query (PPBO) to propose the next query. Nguyen et al. (2021) extend the pairwise comparison to comparison among k samples, but it requires building an absolute response through the Gaussian Process and capturing the local ranking among a fixed number of neighbors via a multi-nominal logit model.

In contrast, we propose to capture the global ranking of each candidate among the whole feasible domain (search space) and model the relative response. On the one hand, we can directly search the optimum based on our relative response surface and obtain the next query without computationally expensive procedure. On the other hand, we directly build a ranking-based relative response surface without building an absolute response surface first. Specifically, we adopt Poisson Process (PP) to capture the global ranking, which is naturally suitable since the ranking of a candidate can be figured out by counting the number of better candidates. Verified experiments on the Forrester function with various degrees of additive Gaussian noise are conducted to show the robustness of our response surface capturing the global ranking. Comparison with GP-BO is illustrated in Fig. 1. The detailed settings can be found in the caption and Appendix C.1. Our contributions can be summarized as follows:

1) Ranking-based Response Surface based on Poisson Process. Unlike the prior absolute response surface (Bergstra et al., 2011; Snoek et al., 2012), nor those (Nguyen et al., 2021) using relative evidence likelihood based on absolute responses, this work is the first to directly capture the global ranking over a feasible domain via Poisson process. The robustness against noise is also analyzed in Sec. 3.1 and illustrated in Fig. 1.

¹In this work, ‘absolute response’ of a black-box function estimate as the raw values at candidate points. ‘relative response’ of a black-box function estimates the ranking of candidate points, which can be computed by pairwise comparing.



(a) Response Surface of GP (value-based model) (b) Response Surface of PP (ranking-based model)

Figure 1: We compare the sensitivity of additive Gaussian noise between GP (value-based) response surface and PoPBO (ranking-based response surface) on the Forrester function. Based on the function value, the solid black line (oracle) indicates actual rankings over 100 points evenly spaced from 0 to 0.8. We draw lines between the 100 predictions by linear interpolation for a clear illustration. The dashed lines indicate predicted rankings over the 100 points by (a) Gaussian process and (b) Poisson process on observations with varying degrees of noise whose standard deviation σ ranges from 0 to 0.45. Each response surface is trained on the same 15 queries. Note that GP performs worse as the standard deviation of noise increases. In contrast, PP performs consistently well due to its great robustness against noise.

2) Tailored Acquisition Function for Ranking-based Response Surface. Two acquisition functions for our response surface, named R-LCB and ERI, are deduced from the vanilla LCB and EI for better exploitation-exploration trade-off. Gradients of the proposed acquisition functions w.r.t. candidates are also derived, so the next query can be optimized by ADAM.

3) Computationally-efficient Bayesian Optimization Framework. The proposed ranking-based response surface and acquisition functions form an efficient and novel Bayesian optimization framework: Poisson Process Bayesian Optimization (PoPBO). The computational complexity of PoPBO is $O(N^2)$, much lower than that of GP-BO ($O(N^3)$). Comparison is shown in Fig. 3.

4) Extensive Empirical Study with Strong Performance. Our method outperforms many prior BO methods on both simulated functions and real-world benchmarks, including HPO and NAS.

2 Preliminaries and Background

Bayesian Optimization. Consider minimizing a black-box function $x^* = \arg \min_{x \in X} f(x)$, where $f(\cdot): X \rightarrow \mathbb{R}$, defined on a d -dimensional feasible domain $X \subset \mathbb{R}^d$. The observations have additive noise. Bayesian optimization (BO) is an efficient method to solve such a problem, especially when the black-box function is expensive to be evaluated and has no closed-form expression (Brochu et al., 2010; Perrone et al., 2018). It alternately trains a surrogate model to estimate the response surface of the black-box function based on the observed samples and suggest the next query based on a acquisition function balancing the exploitation and exploration. Gaussian process is one of the most classic and popular surrogate models, which assumes a GP prior to the black-box function and computes the posterior conditioned on the observations. SMAC (Hutter et al., 2011) introduces random forests for regression, which can be used to handle categorical hyperparameters. TPE (Bergstra et al., 2011) models two densities for each sample: $l(x) = p(y < \alpha|x, D)$ and $g(x) = p(y > \alpha|x, D)$ via kernel density estimator, and then optimize the ratio $l(x)/g(x)$ to suggest the next query. Recently, Bayesian neural network is also introduced into BO framework (Snoek et al., 2015) to estimate the response surface. Springenberg et al. (2016) improves the robustness by evaluating the posterior via a stochastic gradient MCMC method (Chen et al., 2014).

After building the response surface via a surrogate model, BO suggests the next query via an acquisition function considering the trade-off between exploitation and exploration. Popular acqui-

sition functions include expected improvement, Thompson sampling, and upper/lower confidence bound due to their ease of use and strong performance.

BO with Relative Metrics. The relative metric does not have to utilize absolute responses of the black-box function. Some methods focus on the cases where the function evaluation is not directly accessible (Brusilovsky et al., 2007; González et al., 2017; Mikkola et al., 2020; Siivola et al., 2021). Absolute responses can be difficult to obtain or even unavailable in some practical scenarios, such as sports games and recommender systems (Brusilovsky et al., 2007) where only relative evaluation can be provided by pairwise comparisons. *Preferential Bayesian Optimization* (PBO) (González et al., 2017) captures correlations between different inputs to find the optimal value of a latent function, which requires limited comparisons. To handle a high-dimensional black-box function, *Projective Preferential Bayesian Optimization* (PPBO) (Mikkola et al., 2020) proposes a projective preferential query allowing for the feedback given by human interaction. However, they ignore the tie situations and have to rely on a computationally expensive procedure to suggest the next query. Nguyen et al. (2021) extend the above method by comparing k samples but have to model the absolute response surface by Gaussian Process and assume the noise obeys Gumbel distribution. In addition, ranking-based methods (Feurer et al., 2018; Salinas et al., 2020) can also facilitate the identification of similar runs for transfer learning, reusing insights from past similar experiments. This work, on the contrary, makes the first attempt to directly capture the global ranking of candidates based on Poisson process and derive a novel Bayesian Optimization framework named PoPBO. We analyze the robustness of relative metric (ranking) against noise and show the outstanding performance of our method on various simulated benchmarks and real-world datasets.

3 Poisson Process for Bayesian Optimization

3.1 Ranking-based Metric

Consider a black-box objective function $f(\cdot)$ defined on a feasible domain X . Given a sample $x \in X$ and a subset of the feasible domain $S \subset X$, we define a set $S_x = \{y | y \in S, f(y) < f(x)\}$, consisting of the better candidates than x in S . Hence, we can estimate the superiority of x for $f(\cdot)$ against the points in set S by measuring S_x . Specifically, consider two points x_1, x_2 , if S_{x_1} has a larger measure value than S_{x_2} , it represents that there are more points in S better than x_1 compared to those better than x_2 , so x_1 is worse than x_2 . We would like to capture the ranking of each candidate x over a domain S . However, S usually contains a large number of candidates making it intractable to obtain the true ranking. Therefore, we sample a set \hat{S} from the search space X and attempt to capture the ranking of x over $S \cap \hat{S}$, i.e., $|S_x \cap \hat{S}|$.

Robustness Analysis. Consider two queries x_1, x_2 with observations y_1, y_2 . Suppose observations of the black-box function are subject to additive Gaussian noisy $y = f(x) + \epsilon, \epsilon \sim \mathcal{N}(0, \sigma^2)$. We assume $f(x_1) < f(x_2)$ without loss of generality, the probability of correctly ranking x_1, x_2 is:

$$P(y_1 < y_2) = P(\epsilon_1 - \epsilon_2 < f(x_2) - f(x_1)). \quad (1)$$

Since $\epsilon_1, \epsilon_2 \sim \mathcal{N}(0, \sigma^2)$ are independent, $\Delta\epsilon = \epsilon_1 - \epsilon_2 \sim \mathcal{N}(0, 2\sigma^2)$. According to three-sigma rule of thumb, if $f(x_2) - f(x_1) > \sqrt{2}\sigma$, the probability of correctly ranking x_1, x_2 is larger than 82.63%; If $f(x_2) - f(x_1) > 2\sqrt{2}\sigma$, the probability of correctly ranking x_1, x_2 is larger than 97.72%. Even if observations are noisy, the ranking of candidates is hard to be disrupted.

Hence, we conclude the ranking metric is robust to noise and assume the observed ranking noiseless in this work. Results of our ranking-based surrogate model on Forrester function with varying degrees of additive noises confirm our analysis, as shown in Fig. 1b. Specifically, despite that no prior of noise is considered on the observed ranking when training the PP (ranking-based) surrogate model, it can still capture the oracle ranking (the line of ground truth in black) properly even with noisy observations. In contrast, although the GP (value-based) surrogate model considers the prior of noise, it performs worse.

Algorithm 1 PoPBO: Bayesian Optimization with Poisson Process

Require: 1) A function $Rank(\{\cdot\})^\dagger$ to rank samples based on a black-box function $f(\cdot)$; 2) A feasible domain (search space) X ; 3) An acquisition function α ; 4) The number of initial points N ; 5) the number of total training iterations T .

- 1: Randomly sample N initial points $\hat{S} := \{x_j\}_{j=1}^N$ from X ;
- 2: Initialize the parameters θ of $\lambda_\xi(x)$;
- 3: **for** $t := \text{from } 1 \text{ to } T$ **do**
- 4: Get their rankings $\hat{R} := Rank(\hat{S})$;
- 5: Train θ based on points \hat{S} and \hat{R} by minimizing Eq. 4 through ADAM;
- 6: Get the next query x^* by minimizing acquisition function α ;
- 7: Update the set of points $\hat{S} := \hat{S} \cup \{x^*\}$
- 8: **end for**
- 9: Get the best query x_{opt} in history based on $Rank(\hat{S})$;

Output: The best point x_{opt} in history.

\dagger : A sorting function can serve as the $Rank(\cdot)$.

3.2 Capturing the Ranking via Poisson Process

Given a sample x and a set \hat{S} , we utilize a random process $\hat{R}_x(S)$, $\forall S \subset X$ to capture the ranking x . Note that $\hat{R}_x(S)$ also depends on \hat{S} , we omit it for conciseness. In particular, we define $\hat{R}_x \triangleq \hat{R}_x(X)$ to denote the ranking of x over the whole feasible domain X , which is a random variable. We assume the rankings of x over two disjoint areas are independent, i.e., $\hat{R}_x(S_1) \perp \hat{R}_x(S_2)$, $\forall S_1, S_2 \subset X, S_1 \cap S_2 = \emptyset$ since the function $f(x)$ is black-box. Hence, we can model $\hat{R}_x(S)$, $\forall S \subset X$ as an independent increment counting process. Moreover, $\hat{R}_x(S)$ has the following properties: 1) $\hat{R}_x(\emptyset) = 0$ and 2) $\lim_{\Delta s \rightarrow 0} P(\hat{R}_x(S + \Delta s) - \hat{R}_x(S) \geq 2) = 0$, $\forall S \subset X$. Detailed discussion is provided in Appendix A. Since the supremum of $\hat{R}_x(S)$ is $|\hat{S}|$, $\hat{R}_x(S)$ obeys a truncated non-homogeneous Poisson process (Yigiter and Inal, 2006) as Eq. 2 with parameter $\lambda(s, x)$, $s \in X$.

$$\hat{R}_x(S) \sim \text{Poisson} \left(\int_S \lambda(s, x) ds \right). \quad (2)$$

Hence, the ranking of x over the whole feasible domain is $\hat{R}_x = \hat{R}_x(X)$, the probability of $\hat{R}_x = k$ is:

$$P(\hat{R}_x = k | x, \hat{S}) = \frac{\left(\int_X \lambda(s, x) ds \right)^k}{k! \cdot Z(x)} \exp \left(- \int_X \lambda(s, x) ds \right) = \frac{(\lambda_\xi(x) |X|)^k}{k! \cdot Z(x)} \exp(-\lambda_\xi(x) |X|), \quad (3)$$

where $Z(x) = \sum_{k=0}^{|\hat{S} \setminus \{x\}|} \left[\frac{(\lambda(\xi, x) |X|)^k}{k!} \exp(-\lambda(\xi, x) |X|) \right]$ is the normalized coefficient and $|\hat{S} \setminus \{x\}|$ is the number of samples without x . There exists $\xi \in X$ satisfying $\int_X \lambda(s, x) ds = \lambda_\xi(x) |X|$ according to the mean value theorem for integrals. We can approximate $\lambda_\xi(x)$ by a multi-layer perceptron (MLP) $\lambda_\xi(x; \theta)$ with parameter θ .

To train θ , we resort to the maximized loglikelihood estimation (MLE). Give $N (\geq 2)$ samples $\hat{S} = \{x_j\}_{j=1}^N$, the ranking of each sample over \hat{S} is $\hat{K} = \{\hat{k}_{x_j}\}_{j=1}^N$. Similar to (Salinas et al., 2020), the log-likelihood $\log L(\hat{K} | \hat{S}; \theta)$ can be approximated as follows and θ can be optimized through ADAM.

$$\sum_{j=1}^N \left\{ \hat{k}_{x_j} \log(\lambda_\xi(x_j; \theta) |X|) - \log(\hat{k}_{x_j}!) - \log \left[\sum_{i=0}^{N-1} \frac{(\lambda_\xi(x_j; \theta) |X|)^i}{i!} \right] \right\}. \quad (4)$$

Once θ is determined after training on the observations (\hat{S}, \hat{K}) , the ranking of a new sample x^* over the whole feasible domain X can be predicted, where Z is the normalized coefficient by Eq. 3.

$$P\left(\hat{R}_{x^*}(X) = k | \theta, x^*, \hat{S}\right) = \frac{(\lambda_{\xi}(x^*; \theta) | X)^k}{k! \cdot Z(x^*)} \cdot \exp(-\lambda_{\xi}(x^*; \theta) | X). \quad (5)$$

The proposed Bayesian optimization framework with Poisson process (PoPBO) is outlined in Alg. 1. The acquisition function is introduced in the next section.

4 Tailored Acquisition Functions for PoPBO

The existing acquisition functions are designed for absolute response surface considering independent mean and variance, which can be improper for our ranking-based response surface since the mean of Poisson distribution is the same as the variance. Directly applying these acquisition functions to our PoPBO will cause the over-exploitation issue. To this end, we introduce a series of acquisition functions, named rectified upper confidence bound (R-UCB) and expected ranking improvement (ERI), derived from vanilla UCB and EI, respectively.

4.1 Rectified Lower Confidence Bound (R-LCB)

Ranking of the point x obeys Poisson distribution as Eq. 5, with expectation $\mu(x) = \lambda_{\xi}(x) | X | \cdot \frac{\sum_{i=0}^{N-1} (\lambda_{\xi}(x) | X |)^i / i!}{\sum_{i=0}^N (\lambda_{\xi}(x) | X |)^i / i!}$ and standard deviation $\sigma(x) = \sqrt{\mu(x)}$ according to the property of Poisson distribution. Thus the vanilla LCB of each point is:

$$\alpha_{\text{LCB}}(x) = \mu(x) - \beta \sigma(x) = \sqrt{\mu(x)} \left(\sqrt{\mu(x)} - \beta \right). \quad (6)$$

However, Poisson distribution with a large expectation also has a large variance, indicating less confidence in the ranking prediction. The vanilla LCB will be trapped into an over-exploitation issue. Hence, we propose a rectified LCB (R-LCB) to restrict the lower value to a threshold:

$$\alpha_{\text{R-LCB}}(x) = \begin{cases} \alpha_{\text{LCB}}(x) & \text{if } \lambda_{\xi}(x; \theta) | X | < q |\hat{S}| \\ \epsilon_x, \epsilon_x \sim U[0, 1] & \text{Otherwise} \end{cases}, \quad (7)$$

where ϵ_x is a uniform random variable for reparameterization, and q is a pre-defined quantile of the number of samples. The threshold $q |\hat{S}|$ can be adaptively adjusted during the BO process. To minimize R-UCB, we randomly sample a set of start points and adopt a LBFGS (Liu and Nocedal, 1989) optimizer. In particular, LBFGS will not update the samples whose predicted ranking is larger than $q |\hat{S}|$, and they have a probability of being selected as the next query if the sampled ϵ_x is very small. Results in Fig. 5 show the advantage of our R-UCB against UCB.

4.2 Expected Ranking Improvement (ERI)

Inspired by EI, we introduce ERI to maximize the expected improvement on ranking over the worst tolerable ranking K_m . We set $K_m = 5$ by default.

$$\alpha_{\text{ERI}}(x) = \sum_{k=0}^{K_m} (K_m - k) \cdot P\left(\hat{R}_x = k | \theta, x\right), \quad (8)$$

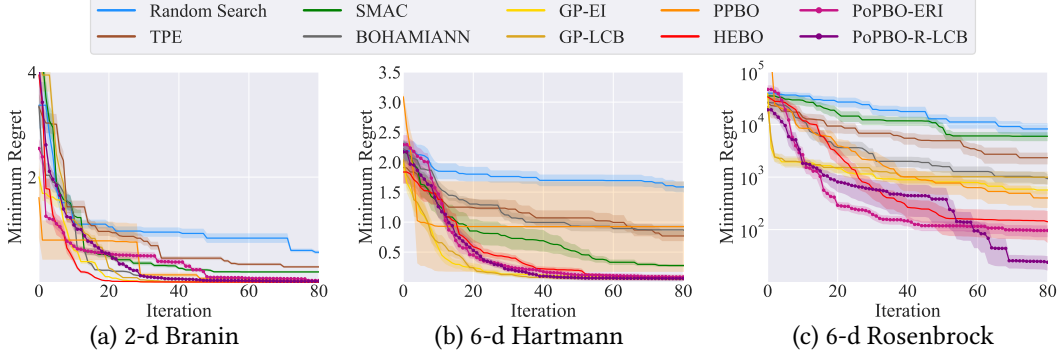


Figure 2: Performance of black-box optimization methods on three simulation functions. Y-axis is the residual of the optimum function value and the incumbent. We run each method ten times and plot the average performance and standard error as the line and shadow.

where $P(\hat{R}_x = k | \theta, x)$ is defined in Eq. 5 representing the prediction of ranking of x . The gradient of ERI w.r.t. x is defined as follows, where $\lambda_\xi(x) = \lambda_\xi(x; \theta)$.

$$\begin{aligned} \frac{\partial \alpha_{\text{ERI}}(x)}{\partial x} &= \sum_{k=0}^{K_m} \left[\frac{K_m - k}{k!} \frac{\partial}{\partial x} \left(\frac{(\lambda_\xi(x)|X|)^k}{k! \cdot Z(x)} \cdot \exp(-\lambda_\xi(x)|X|) \right) \right] \\ &= \sum_{k=0}^{K_m} \left\{ \frac{(K_m - k) (\lambda_\xi(x)|X|)^{k-1} |X|}{k! \left(\sum_{i=0}^N \frac{(\lambda_\xi(x)|X|)^i}{i!} \right)^2} \left[k \sum_{i=0}^N \frac{(\lambda_\xi(x)|X|)^2}{i!} - \lambda_\xi(x)|X| \sum_{i=0}^{N-1} \frac{(\lambda_\xi(x)|X|)^2}{i!} \right] \right\}. \end{aligned} \quad (9)$$

Hence, we can get the next query x^* by minimizing $\alpha_{\text{ERI}}(x)$ through a LBFGS optimizer. Similar to R-LCB, we also apply the rectified technique in Eq. 7 to ERI.

5 Empirical Analysis

Benchmarks. We verify the efficacy of PoPBO on both simulated and real-world benchmarks, including HPO and NAS. For the simulated benchmark, we select three simulation functions, including 2-d Branin, 6-d Hartmann, and 6-d Rosenbrock. For the HPO task, we test on the tabular benchmark HPO-Bench (Eggenberger et al., 2021). For the NAS task, we test on on NAS-Bench-201 (Dong and Yang, 2020). Details of the benchmarks can be found in the Appendix C.2

Baselines. We compare against random search (RS) (Bergstra and Bengio, 2012) and various value-based Bayesian optimization methods, including GP (Snoek et al., 2012), TPE (Bergstra et al., 2011), SMAC (Hutter et al., 2011), BOHAMIANN (Springenberg et al., 2016), and HEBO (Cowen-Rivers et al., 2022). For GP methods, we use EI and LCB as acquisition functions, which are optimized by LBFGS, and adopt the Matérn 5/2 covariance function to be the kernel function. We also compare with PPBO (Mikkola et al., 2020), one of state of the art preferential BO methods. Detailed settings of the baselines are provided in Appendix C.3.

Settings. We run all the methods for 80 iterations with 12 initial points by default. For the Rosenbrock-6d simulation function, we run all methods for 80 iterations with 30 initial points due to its complex search space. The MLP $\lambda_\xi(x; \theta)$ used to approximate the parameter of the Poisson process has three hidden layers with 128 nodes and a ReLU activation function. The MLP is trained for 100 steps by ADAM Tian and Parikh (2022) with 64 batch sizes and a 0.01 initial learning rate multiplied by 0.2 every 30 steps. All methods are evaluated

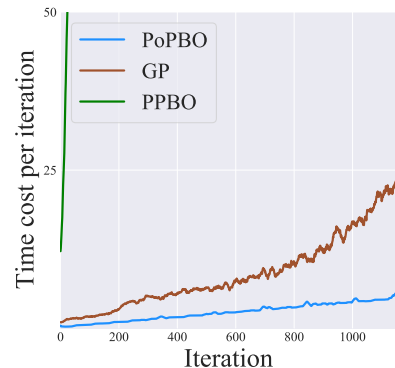


Figure 3: Time cost of GP-BQ, PPBO (Mikkola et al., 2020) and PoPBO. All the methods are applied to optimize 6-d

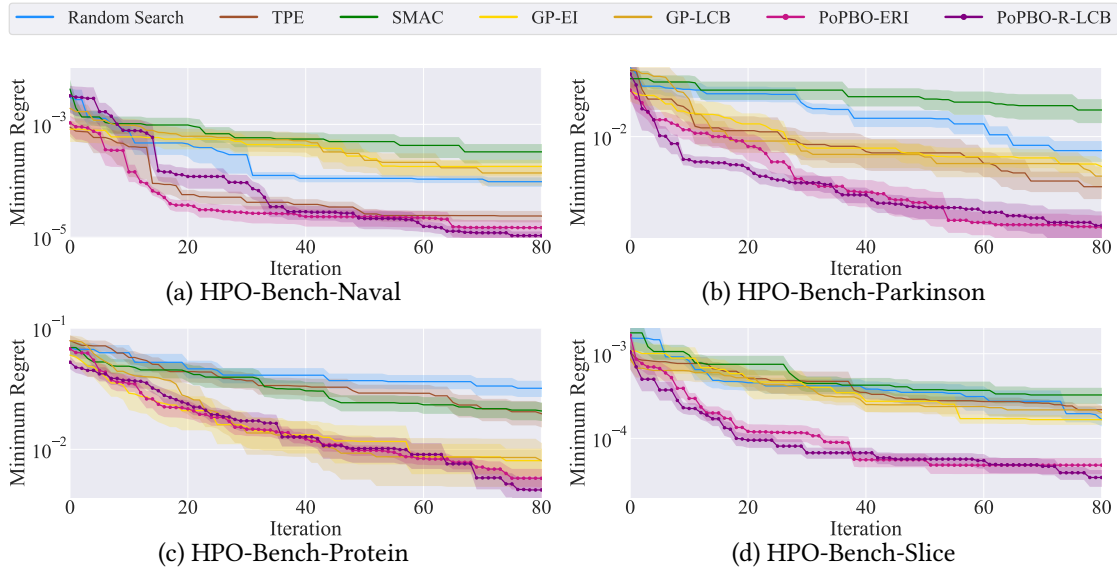


Figure 4: Minimum regret comparison with random search and various Bayesian optimization methods on tabular datasets in HPO-Bench. Y-axis indicates the residual between the optimum function value and the incumbent. We run each method ten times and plot the average performance and standard error of the incumbent as the line and shadow. Our PoPBO can quickly discover good samples and achieves the best performance (lowest regret).

ten times independently on an Intel(R) Xeon(R) Silver 4210R CPU.

5.1 Performance on the Simulated Benchmarks

Fig. 2 compares PoPBO and baselines on 2-d Branin, 6-d Hartmann, and 6-d Rosenbrock simulation benchmarks. Hartmann has higher dimensions than Branin and thus is more difficult to optimize. As shown in Fig. 2b, although the standard GP temporarily outperforms others in the early stage, our PoPBO achieves the best at around 40-th iterations and takes the lead till the end. In particular, PPBO performs great in the early stage but falls into a local optimum after ten iterations. Optimizing the Rosenbrock function is much more complicated than Branin and Hartmann since its global optimum lies in a narrow valley (Picheny et al., 2013) as well as a more extensive search space. Hence, we increase the initial points to 30 for a better preview of the Rosenbrock landscape for all methods. Fig. 2c shows that our PoPBO can quickly find the valley and significantly outperforms other BO methods.

Computational Cost. Fig. 3 compares the time cost (wall-clock time) of three peer methods, showing that the cost of GP-BO and PPBO are much higher than PoPBO as the number of observations increases. Specifically, GP has to compute the inverse of a covariance matrix resulting in a $O(N^3)$ computational complexity. PPBO is also based on GP and requires computing another covariance matrix of size $J \times J$, where J is the number of random samples. In contrast, the computational bottleneck of PoPBO lies in the training of an MLP, which is $O(N^2)$ as shown in Eq. 4. Notice that the units are wall-clock times. Nevertheless, in our experiment, the evaluation of candidates can be negligible compared with the training of the surrogate model and the optimization of acquisition. Therefore, the wall-clock time has little difference from the CPU time.

Table 1: Top-1 mean accuracy (%) for classification on NAS-Bench-201. The first block shows the performance of non-parameter sharing algorithms and various Bayesian optimization methods. The second block shows the performance of PoPBO with ERI and R-LCB acquisition functions. †: Results are obtained from NAS-Bench-201. Otherwise, we independently run the method for ten times. The best mean accuracy in each column is in bold.

Methods	CIFAR-10		CIFAR-100		ImageNet-16-120	
	valid	test	valid	test	valid	test
REINFORCE (Williams, 1992) [†]	91.09±0.37	93.85±0.37	71.61±1.12	71.71±1.09	45.05±1.02	45.24±1.18
REA (Real et al., 2019) [†]	91.19±0.31	93.92±0.30	71.81±1.12	71.84±0.99	45.15±0.89	45.54±1.03
Random Search (Bergstra and Bengio, 2012)	91.00±0.38	93.83±0.31	71.29±1.29	71.47±1.16	44.83±1.11	45.05±1.14
BOHB (Falkner et al., 2018) [†]	90.82±0.53	93.61±0.52	70.74±1.29	70.85±1.28	44.26±1.36	44.42±1.49
TPE (Bergstra et al., 2011)	91.06±0.38	93.90±0.34	71.29±1.29	71.85±1.13	45.04±1.23	45.27±1.49
SMAC (Hutter et al., 2011)	91.09±0.38	93.95±0.28	71.40±1.23	71.66±1.11	45.11±0.99	45.32±1.09
GP (EI) (Snoek et al., 2012)	91.40±0.18	94.23±0.15	72.67±0.83	72.75±0.47	45.83±0.45	46.20±0.63
GP (LCB) (Snoek et al., 2012)	91.30±0.25	93.98±0.22	72.00±0.80	72.05±0.76	45.37±0.83	45.60±0.94
BOHAMIANN (Springenberg et al., 2016)	91.36±0.16	94.13±0.23	72.36±0.82	72.38±0.81	45.93±0.66	46.18±0.60
PoPBO (ERI)	91.52±0.05	94.35±0.03	73.21±0.29	73.25±0.18	46.27±0.36	46.54±0.19
PoPBO (R-LCB)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32

5.2 Performance on the Real-world Benchmarks

HPO-Bench. we run each method for ten times and plot the trend of minimum regret during the BO procedure. Fig. 4 compares PoPBO with advanced Bayesian optimization methods and random search on HPO-Bench (Eggensperger et al., 2021), showing that our PoPBO achieves the best on all the four datasets. In contrast, other methods are unable to perform consistently well and even worse than random search. Moreover, the performance of our method has a lower standard error than other methods, indicating its outstanding stability. The numerical performance of all methods on the four datasets are provided in Table 2 in Appendix C.4.

NAS-Bench-201. Table 1 reports the performance on the NAS task. The first block shows the performance of prior non-parameter-sharing-based NAS methods, including random search, evolution algorithm, reinforcement learning, and Bayesian optimization. We adopt the same initial observations when testing Random Search, GP-BO, and our PoPBO for a fair comparison. As for SMAC and TPE, we directly run the open-source codes, which have different sampling implementations from ours, making it hard to sample the same initial observations as ours even under the same random seed. Our method achieves the best performance on the three datasets and, in particular, outperforms the state-of-the-art Bayesian optimization methods BOHB (Falkner et al., 2018) and BOHAMIANN (Springenberg et al., 2016). Additionally, we plot the performance trend of various methods on the validation and test set of CIFAR-10, CIFAR-100, and ImageNet16-120 in Fig. 6 in Appendix C.4.

5.3 Effectiveness of the Rectified Technique

The quantile parameter q in Eq. 7 trades off the exploration and exploitation, i.e., a smaller q has better exploration ability. On the one hand, the method degrades to random search when $q \rightarrow 0$, with weak exploitation ability, so it is undesirable to set q as a rather small value. On the other hand, it degrades to the vanilla acquisition functions when $q \rightarrow 1$, with weak exploration ability as our analysis in Sec. 4. Fig. 5 evaluates the effect of quantile parameters q on both R-LCB and ERI on 6-d Rosenbrock benchmark. The best setting of the quantile parameter q for R-LCB is 0.6, and the best for ERI is 0.4. We also conduct the ablation study on NAS-Bench-201, which verify that this setting could provide a good balance between exploration and exploitation. The results on NAS-Bench-201 can be found in Appendix C.7.

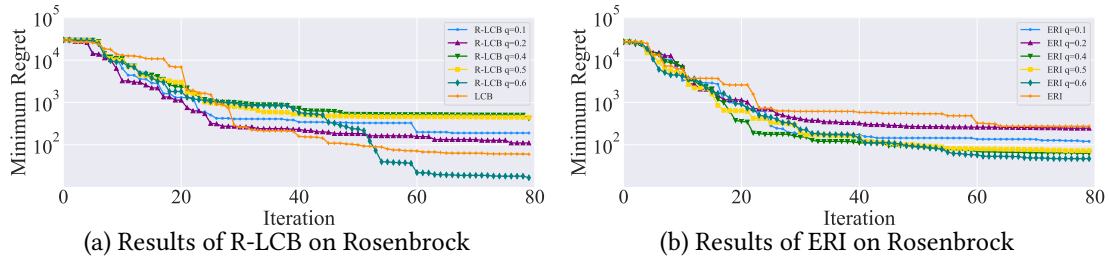


Figure 5: Ablation study on hyperparameter q , which controls the exploitation-exploration trade-off. We test on the Rosenbrock simulation function and show the effect of q on (a) R-LCB and (b) ERI. For each setting, we run ten times and plot the average performance of the incumbent.

6 Conclusion

We have proposed a novel Bayesian Optimization framework, named PoPBO, for optimizing black-box functions with relative responses, being more robust to noise than absolute responses. Specifically, we introduce a relative response surface to capture the global ranking of candidates based on the Poisson process that is suitable for modeling discrete count events. We give the likelihood and posterior forms of ranking under the general assumption of a non-homogeneous Poisson process. To balance the trade-off between exploration and exploitation, we design two acquisition functions, namely Rectified Lower Confidence Bound (R-LCB) and Expected Ranking Improvement (ERI), for our ranking-based response surface. Our method enjoys a lower computational complexity of $O(N^2)$ compared to GP’s $O(N^3)$ and performs competitively on both simulated and real-world benchmarks.

Limitations and Future Work. This work analyzes the robustness of relative response against noise and thus does not involve prior knowledge of noise. However, there exist real scenarios where the noise is too large to disrupt the ranking of observations, and we would like to leave it as our future work. Additionally, the mean of Poisson distribution is the same as variance, which has a potential over-exploitation issue as mentioned in Sec. 4. This work introduces a rectified technique to alleviate it, and we would like to explore other elegant acquisition functions in future work.

Acknowledgements

This work was supported by NSFC (U19B2035, 61972250, 61671480), the Qingdao Natural Science Foundation (23-2-1-161-zyyd-jch), and the Shandong Natural Science Foundation (ZR2023MF008).

References

- Agrawal, S. and Goyal, N. (2013). Thompson sampling for contextual bandits with linear payoffs. In *ICML*.
- Bergstra, J., Bardenet, R., Bengio, Y., and Kégl, B. (2011). Algorithms for hyper-parameter optimization. In *NeurIPS*.
- Bergstra, J. and Bengio, Y. (2012). Random search for hyper-parameter optimization. *Journal Of Machine Learning Research*.
- Brochu, E., Cora, V. M., and de Freitas, N. (2010). A tutorial on bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning. *Computer Research Repository*.
- Brusilovsky, P., Kobsa, A., and Nejdl, W., editors (2007). *The Adaptive Web, Methods and Strategies of Web Personalization*, volume 4321 of *Lecture Notes in Computer Science*. Springer.

- Calandra, R., Seyfarth, A., Peters, J., and Deisenroth, M. P. (2016). Bayesian optimization for learning gaits under uncertainty - an experimental comparison on a dynamic bipedal walker. *Annals of Mathematics and Artificial Intelligence*.
- Chapelle, O. and Li, L. (2011). An empirical evaluation of thompson sampling. In *NeurIPS*.
- Chen, T., Fox, E. B., and Guestrin, C. (2014). Stochastic gradient hamiltonian monte carlo. In *ICML*.
- Coraddu, A., Oneto, L., Ghio, A., Savio, S., Anguita, D., and Figari, M. (2016). Machine learning approaches for improving condition-based maintenance of naval propulsion plants. *Proceedings of the Institution of Mechanical Engineers, Part M: Journal of Engineering for the Maritime Environment*.
- Cowen-Rivers, A. I., Lyu, W., Wang, Z., Tutunov, R., Hao, J., Wang, J., and Bou-Ammar, H. (2022). Hebo: Pushing the limits of sample-efficient hyper-parameter optimisation. *Journal of Artificial Intelligence Research*.
- Dong, X. and Yang, Y. (2020). Nas-bench-201: Extending the scope of reproducible neural architecture search. In *ICLR*.
- Eggenberger, K., Müller, P., Mallik, N., Feurer, M., Sass, R., Klein, A., Awad, N. H., Lindauer, M., and Hutter, F. (2021). Hpobench: A collection of reproducible multi-fidelity benchmark problems for HPO. In *NeurIPS*.
- Falkner, S., Klein, A., and Hutter, F. (2018). BOHB: robust and efficient hyperparameter optimization at scale. In *ICML*.
- Feurer, M., Letham, B., and Bakshy, E. (2018). Scalable meta-learning for bayesian optimization using ranking-weighted gaussian process ensembles. In *AutoML Workshop at ICML*.
- González, J., Dai, Z., Damianou, A. C., and Lawrence, N. D. (2017). Preferential bayesian optimization. In *ICML*.
- González, J., Longworth, J., James, D. C., and Lawrence, N. D. (2015). Bayesian optimization for synthetic gene design. *arXiv preprint arXiv:1505.01627*.
- Graf, F., Kriegel, H., Schubert, M., Pölsterl, S., and Cavallaro, A. (2011). 2d image registration in CT images using radial image descriptors. In *MICCAI*.
- He, Y., Gan, Q., Wipf, D., Reinert, G., Yan, J., and Cucuringu, M. (2022). Gnnrank: Learning global rankings from pairwise comparisons via directed graph neural networks. In *ICML*.
- Hutter, F., Hoos, H. H., and Leyton-Brown, K. (2011). Sequential model-based optimization for general algorithm configuration. In *LION*.
- Kahneman, D. and Tversky, A. (2013). Prospect theory: An analysis of decision under risk. In *Handbook of the fundamentals of financial decision making: Part I*, pages 99–127. World Scientific.
- Klein, A. and Hutter, F. (2019). Tabular benchmarks for joint architecture and hyperparameter optimization. *Computer Research Repository*.
- Lin, Z. J., Astudillo, R., Frazier, P. I., and Bakshy, E. (2022). Preference exploration for efficient bayesian optimization with multiple outcomes. In *AISTATS*, volume 151, pages 4235–4258.
- Liu, D. C. and Nocedal, J. (1989). On the limited memory BFGS method for large scale optimization. *Math. Program.*, 45(1-3):503–528.

- Mikkola, P., Todorovic, M., Järvi, J., Rinke, P., and Kaski, S. (2020). Projective preferential bayesian optimization. In *ICML*.
- Mockus, J. (1994). Application of bayesian approach to numerical methods of global and stochastic optimization. *Journal of Global Optimization*.
- Mockus, J., Tiesis, V., and Zilinskas, A. (1978). The application of bayesian methods for seeking the extremum. *Towards global optimization*.
- Nguyen, Q. P., Tay, S., Low, B. K. H., and Jaillet, P. (2021). Top-k ranking bayesian optimization. In *AAAI*.
- Perrone, V., Jenatton, R., Seeger, M. W., and Archambeau, C. (2018). Scalable hyperparameter transfer learning. In *NeurIPS*.
- Picheny, V., Wagner, T., and Ginsbourger, D. (2013). A benchmark of kriging-based infill criteria for noisy optimization. *Structural and multidisciplinary optimization*.
- Rana, P. (2013). Physicochemical properties of protein tertiary structure data set. *UCI Machine Learning Repository*.
- Real, E., Aggarwal, A., Huang, Y., and Le, Q. V. (2019). Regularized evolution for image classifier architecture search. In *AAAI*.
- Rosset, S., Perlich, C., and Zadrozny, B. (2005). Ranking-based evaluation of regression models. In *ICDM*.
- Salinas, D., Shen, H., and Perrone, V. (2020). A quantile-based approach for hyperparameter transfer learning. In *ICML*.
- Siivola, E., Dhaka, A. K., Andersen, M. R., González, J., Moreno, P. G., and Vehtari, A. (2021). Preferential batch bayesian optimization. In *MLSP*.
- Snoek, J., Larochelle, H., and Adams, R. P. (2012). Practical bayesian optimization of machine learning algorithms. In *NeurIPS*.
- Snoek, J., Rippel, O., Swersky, K., Kiros, R., Satish, N., Sundaram, N., Patwary, M. M. A., Prabhat, and Adams, R. P. (2015). Scalable bayesian optimization using deep neural networks. In *ICML*.
- Song, J., Yu, L., Neiswanger, W., and Ermon, S. (2022). A general recipe for likelihood-free bayesian optimization. In *ICML*, volume 162, pages 20384–20404. PMLR.
- Springenberg, J. T., Klein, A., Falkner, S., and Hutter, F. (2016). Bayesian optimization with robust bayesian neural networks. In *NeurIPS*.
- Srinivas, N., Krause, A., Kakade, S. M., and Seeger, M. W. (2012). Information-theoretic regret bounds for gaussian process optimization in the bandit setting. *IEEE Transactions on Information Theory*.
- Tian, R. and Parikh, A. P. (2022). Amos: An adam-style optimizer with adaptive weight decay towards model-oriented scale. *CoRR*, abs/2210.11693.
- Tiao, L. C., Klein, A., Seeger, M. W., Bonilla, E. V., Archambeau, C., and Ramos, F. (2021). BORE: bayesian optimization by density-ratio estimation. In *ICML*, volume 139, pages 10289–10300. PMLR.

Tsanas, A., Little, M. A., McSharry, P. E., and Ramig, L. O. (2010). Accurate telemonitoring of parkinson’s disease progression by noninvasive speech tests. *IEEE Transactions on Biomedical Engineering*.

Williams, R. J. (1992). Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine Learning*.

Yigiter, A. and Inal, C. (2006). Right truncated homogeneous poisson process. *PAKISTAN JOURNAL OF STATISTICS-ALL SERIES-*, 22(1):69.

A Discussion on the Assumptions for $\hat{R}_x(S)$

Consider to minimize a black-box function $f(x)$. In this paper, $\hat{R}_x(S) = |S_x \cap \hat{S}|$, where \hat{S} is a set of samples and $S_x = \{y|y \in S, f(y) < f(x)\}$ is the set of better points than x . We assume $\hat{R}_x(S)$ has the following properties:

- 1) $\hat{R}_x(S_1) \perp \hat{R}_x(S_2), \forall S_1, S_2 \subset X, S_1 \cap S_2 = \emptyset$; (independent increment)
- 2) $\hat{R}_x(\emptyset) = 0$;
- 3) $\lim_{\Delta s \rightarrow 0} P(\hat{R}_x(S') + \Delta s) - \hat{R}_x(S') \geq 2) = 0, \forall S' \subset S$.

We adopt the first assumption since $f(x)$ is a black-box function. Unlike GP that assume $f(x)$ is a linear function $f(x) = w^\top x$, we make no prior assumption on the form of black-box function and only assume the rankings over disjoint areas are independent. The second assumption is naturally satisfied since there are no points $x' \in \emptyset$ satisfying $y' > y$, where y indicates the observation of point x . The third assumption is also satisfied no matter if the black-box function is a discrete or continuous. Specifically, we can find a small enough Δs making $(S \cap \hat{S}) \cap \Delta s$ only contains one point, since \hat{S} is discrete.

B Algorithm Details

As the number of observations N increases, the right truncated Poisson distribution gradually approaches to the normal one(Yigiter and Inal, 2006), which has a smaller computational cost. Hence, we use normal Poisson process to model the response surface when $N \geq 12$.

B.1 Workflow of PoPBO

Suppose at t -th iteration, we have $N^{(t)}$ history queries, denoted as $\hat{S}^{(t)}$ and their observations. The detailed workflow of our PoPBO at t iteration is as follows (In the following, we omit t without loss of generality.):

1) **Get the rankings.** $\forall x \in \hat{S}$, we compute the ranking of x over \hat{S} by comparing its observation with others and obtain a ranking set $\hat{K} = \{k_x | \forall x \in \hat{S}\}$. Similar to [1], we assume the rankings between queries are independent. (Though it is not rigorous, we find it performs better than a truly independent ranking strategy, which will be analyzed later.)

2) **Compute log-likelihood on observations \hat{K} .** Since the rankings in \hat{K} are independent, we can get the log-likelihood on the observations of ranking \hat{K} as:

$$\log L(\hat{K}|\hat{S}; \theta) = \log \left\{ \prod_{x \in \hat{S}} p(\hat{R}_x = k_x | x, \hat{S}) \right\} \quad (\text{Property of independent increment}) \quad (10)$$

$$= \sum_{x \in \hat{S}} \log \left\{ \frac{(\lambda(\xi, x)|X|)^k}{k! \cdot Z(x)} \exp(-\lambda(\xi, x)|X|) \right\} \quad (\text{According to the definition of } p(\hat{R}_x = k_x | x, \hat{S}) \text{ in Eq. 3}) \quad (11)$$

$$= \sum_{x \in \hat{S}} \left\{ k_x \log(\lambda_\xi(x; \theta)|X|) - \log(k_x!) - \log \left[\sum_{i=0}^{N-1} \frac{(\lambda_\xi(x; \theta)|X|)^i}{i!} \right] \right\} \quad (\text{Derive Eq. 4}). \quad (12)$$

3) **Train the surrogate model.** We then train MLP by minimizing the log-likelihood through ADAM, whose gradient can be computed as Eq. 8.

4) **Get the next query.** We utilize R-LCB or ERI acquisition function to determine the next query. After obtaining the reward, we put the new query and its reward to the observation set \hat{S} .

B.2 Independent ranking strategy VS. Our implementation.

Given two points x_1, x_2 and a set S , their rankings over $S \setminus \{x_1, x_2\}$ are independent. Hence, we implement a truly independent ranking strategy as follows: We sample $N/2$ samples from all queries \hat{S} to build a base set B . For the left $N/2$ samples, we obtain their rankings over B and build the ranking set $\hat{K} = \{k_x, \forall x \in \hat{S} \setminus B\}$, where k_x denotes the ranking of x over B . Such a ranking strategy can guarantee that the rankings in \hat{K} are independent of each other. Then the log-likelihood of the observations of ranking \hat{K} can be computed as:

$$\begin{aligned} \log L(\hat{K}|\hat{S} \setminus B; \theta) &= \log \left\{ \prod_{x \in \hat{S} \setminus B} p(\hat{R}_x = k_x) \right\} \quad (13) \\ &= \sum_{x \in \hat{S} \setminus B} \log \left\{ \frac{(\lambda(\xi, x)|X|)^k}{k! \cdot Z(x)} \exp(-\lambda(\xi, x)|X|) \right\} \\ &= \sum_{x \in \hat{S} \setminus B} \left\{ k_x \log(\lambda_\xi(x; \theta)|X|) - \log(k_x!) - \log \left[\sum_{i=0}^{|B|-1} \frac{(\lambda_\xi(x; \theta)|X|)^i}{i!} \right] \right\} \end{aligned}$$

However, the above independent ranking strategy results in under-utilization of observations \hat{S} since it has to be divided into two sets. Moreover, candidates with different performances may get the same ranking over B , which will mislead the training of the surrogate. This work adopts a simple relaxation – We compute \hat{R} as the ranking over the whole set \hat{S} and assume independence property, which is also utilized in [1]. Our experimental results show that such a relaxation results in better performance since it can fully utilize all observations.

C Supplementary of Experiments

C.1 Experimental Settings on Robustness Analysis

We compare the sensitivity to additive Gaussian noise between GP (value-based) response surface and PoPBO (ranking-based) response surface on Forrester function. To simulate the performance of GP, we first utilize Gaussian process to fit a certain number of (15 in this paper) observed values and plot the ranking of e.g. 100 points according to the values predicted by GP as Fig. 1a. Meanwhile,

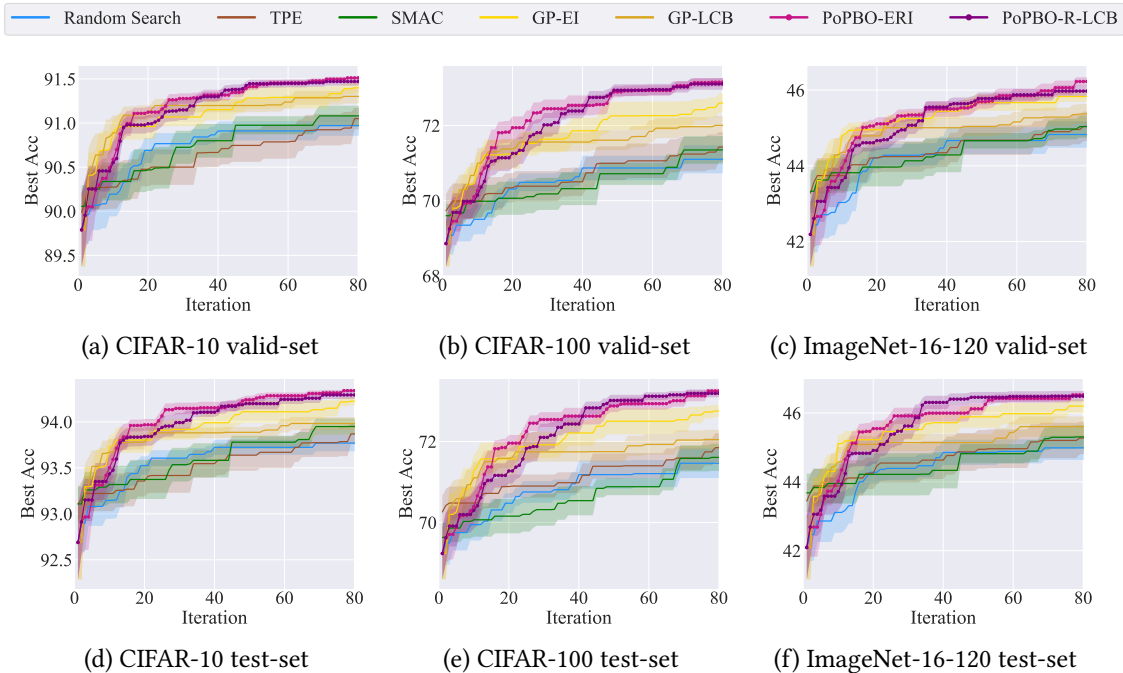


Figure 6: Performance trend of random search and Bayesian optimization methods on NAS-Bench-201.

We run 10 times for each setting and plot the mean accuracy as the lines. Note that when testing Random Search, GP-BO, and our PoPBO, we adopt the same initial random seeds for all settings at each run for fairness. Hence, the lines in each plot have the same initial point (at the 0-th iteration).

Methods	Naval	Parkinson	Protein	Slice
Random Search (Bergstra and Bengio, 2012)	$9.54 \times 10^{-5} \pm 5.76 \times 10^{-5}$	$7.99 \times 10^{-3} \pm 4.18 \times 10^{-3}$	$3.04 \times 10^{-2} \pm 1.51 \times 10^{-2}$	$1.48 \times 10^{-4} \pm 7.45 \times 10^{-5}$
TPE (Bergstra et al., 2011)	$1.67 \times 10^{-5} \pm 1.64 \times 10^{-5}$	$4.49 \times 10^{-3} \pm 2.55 \times 10^{-3}$	$1.86 \times 10^{-2} \pm 1.37 \times 10^{-2}$	$1.80 \times 10^{-4} \pm 7.10 \times 10^{-5}$
SMAC (Hutter et al., 2011)	$2.94 \times 10^{-4} \pm 3.96 \times 10^{-4}$	$1.48 \times 10^{-2} \pm 9.38 \times 10^{-3}$	$2.05 \times 10^{-2} \pm 1.14 \times 10^{-2}$	$3.16 \times 10^{-4} \pm 2.25 \times 10^{-4}$
GP (EI) (Snoek et al., 2012)	$1.79 \times 10^{-4} \pm 1.77 \times 10^{-4}$	$6.20 \times 10^{-3} \pm 2.44 \times 10^{-3}$	$8.06 \times 10^{-3} \pm 6.53 \times 10^{-2}$	$1.66 \times 10^{-4} \pm 7.00 \times 10^{-5}$
GP (LCB) (Snoek et al., 2012)	$1.38 \times 10^{-4} \pm 1.77 \times 10^{-4}$	$5.31 \times 10^{-3} \pm 2.79 \times 10^{-3}$	$8.08 \times 10^{-3} \pm 1.02 \times 10^{-2}$	$1.95 \times 10^{-4} \pm 1.30 \times 10^{-4}$
PoPBO (ERI)	$1.38 \times 10^{-5} \pm 1.59 \times 10^{-5}$	$1.92 \times 10^{-3} \pm 1.51 \times 10^{-3}$	$5.77 \times 10^{-3} \pm 3.55 \times 10^{-3}$	$4.83 \times 10^{-5} \pm 3.29 \times 10^{-5}$
PoPBO (R-LCB)	$1.07 \times 10^{-5} \pm 6.26 \times 10^{-6}$	$2.41 \times 10^{-3} \pm 1.93 \times 10^{-3}$	$4.62 \times 10^{-3} \pm 3.91 \times 10^{-3}$	$3.14 \times 10^{-5} \pm 1.74 \times 10^{-5}$

Table 2: Regret of the configuration discovered by various methods on the four datasets of HPO-Bench.

We run each method for ten times and report the mean and standard deviation. The best performance (lowest mean value and standard deviation) is in bold.

our method utilizes Poisson process to directly capture the ranking response surface based on the same 15 observations and predict the ranking of 100 points as shown in Fig. 1b. We observe that our response surface is more robust to noise and can better capture the global ranking.

C.2 Details of the Benchmarks

For the simulated benchmark, we apply PoPBO to optimize three simulation functions: 1) 2-d Branin function with the domains of each dimension are $[-5, 10]$ and $[0, 15]$ respectively; 2) 6-d Hartmann function in $[0, 1]$ for all six dimensions; 3) 6-d Rosenbrock function defined in $[-5, 10]^6$. For the HPO task, we test PoPBO on the tabular benchmark HPO-Bench (Eggenesperger et al., 2021), containing the root mean square error (RMSE) of a 2-layer feed-forward neural network (FCNET) (Klein and Hutter, 2019) trained under 62208 hyper-parameter configurations on four real-world datasets: protein structure (Rana, 2013), slice localization (Graf et al., 2011), naval propulsion (Coraddu et al., 2016) and parkinsons telemonitoring (Tsanas et al., 2010). The averaged RMSE over four independent runs under the same configuration is utilized as the performance of that configuration. For the NAS task, we test on NAS-Bench-201 (Dong and Yang, 2020) containing 15,625 architectures

in a cell search space that consists of 6 categorical parameters, and each parameter has five choices. Each architecture is evaluated on three datasets. Following the setting of (Dong and Yang, 2020), we search for the best architecture according to its performance on the CIFAR-10 validation set after 12 epochs training.

C.3 Detailed Settings of Baseline Methods

In this section, we provide the specific details of each baseline mentioned in the paper:

Random Search (RS). Following the description in Bergstra and Bengio (2012), we sample candidates uniformly at random.

BO with Gaussian Process (GP). We follow the settings that described by Snoek et al. (2012) and use the implementation of our own. We use expected improvement (EI) and lower confidence bound (LCB) as acquisition functions and adopt LBFSGS to optimize them. When the search space is completely discrete like Dong and Yang (2020), we use random sampling to find the next query, which gives the maximizer of the acquisition function among $N = 1000$ random samples. For kernel function, we use Matérn 5/2 kernel for GP. During the training process, we adopt slice sampling, an efficient Markov chain Monte Carlo (MCMC) method, to fit the hyperparameters of GP, which we find to work more robustly for GP.

Tree Parzen Estimator (TPE). Bergstra et al. (2011) adopt kernel density estimators to model the probability of points with bad and good performance respectively. Then TPE give the next query by optimizing the ratio between the two estimated likelihood, which is proved to be equivalent to optimizing EI. We use the default settings provided in hyperopt package (<https://github.com/hyperopt/hyperopt>).

SMAC. Hutter et al. (2011) adopt random forest to model the response surface of the black-box function. We use the default settings given by scikit-optimize package (<https://github.com/scikit-optimize/scikit-optimize>).

BOHAMIANN. Unlike Snoek et al. (2012), BOHAMIANN adopts Bayesian neural network to build the response surface, whose weights are sampled via a stochastic gradient Hamiltonian Monte-Carlo (SGHMC) method. We use the default settings provided in pybnn package (<https://github.com/automl/pybnn>) and use EI as the acquisition function.

PPBO. This is an effective preferential BO method based on pairwise comparisons, attempting to learn user preferences in high-dimensional spaces. We use the default settings provided by PPBO package (<https://github.com/AaltoPML/PPBO>).

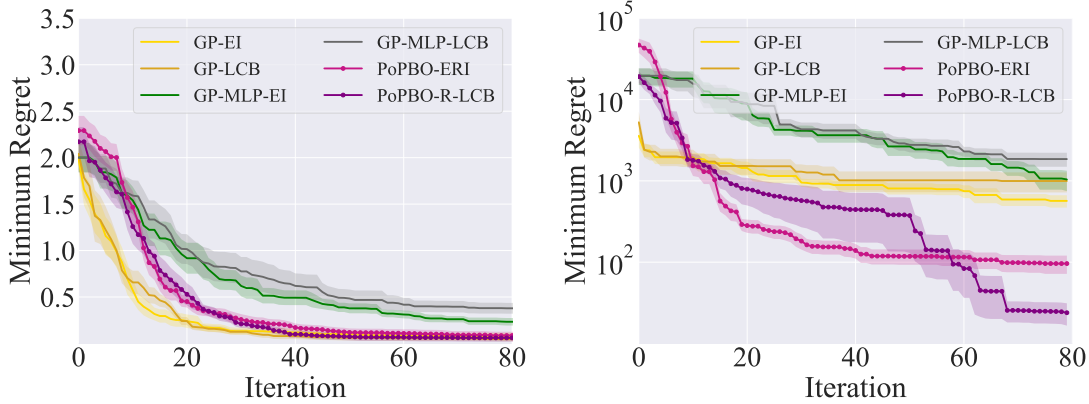
HEBO. Heteroscedastic Evolutionary Bayesian Optimisation that won the NeurIPS 2020 black-box optimisation competition. We use the default strategy and its default parameters provided in HEBO package (<https://github.com/huawei-noah/HEBO>). For a fair comparison, we use a uniform sampling strategy instead of a sobol one during initialization and candidates generation.

C.4 Detailed Results on HPO-Bench and NAS-Bench-201

Table 2 reports the numerical performance of PoPBO and other methods on the four datasets on HPO-Bench. Fig. 6 displays the performance trend of PoPBO and other methods on the validation set and test set under the search space of NAS-Bench-201.

C.5 Is the gain in performance of PoPBO due to the complex representation of MLP in the surrogate model?

We utilize the same MLP architecture and training settings as PoPBO’s to fit the Gaussian likelihood of each candidate. We denote such a setting as GP-MLP. We plot the regret of GP-MLP, GP, and our



(a) 6-d Hartmann (b) 6-d Rosenbrock
 Figure 7: Performance trend of GP, GP-MLP, and PoPBO on Hartmann and Rosenbrock simulated benchmarks.

Table 3: Ablation study about rectified hyperparameter q on NAS-Bench-201.

Methods	CIFAR-10		CIFAR-100		ImageNet-16-120	
	valid	test	valid	test	valid	test
PoPBO (ERI, $q=0.1$)	91.41±0.15	94.22±0.15	72.70±0.63	72.68±0.69	45.93±0.61	46.45±0.34
PoPBO (ERI, $q=0.2$)	91.47±0.12	94.26±0.16	72.96±0.59	73.00±0.53	45.90±0.66	46.33±0.55
PoPBO (ERI, $q=0.4$)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32
PoPBO (ERI, $q=0.5$)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32
PoPBO (ERI, $q=0.6$)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32
PoPBO (R-LCB, $q=0.1$)	91.33±0.19	94.19±0.23	72.62±0.82	72.52±0.67	45.71±0.56	46.10±0.65
PoPBO (R-LCB, $q=0.2$)	91.50±0.06	94.30±0.11	73.04±0.56	73.04±0.45	46.07±0.38	46.37±0.30
PoPBO (R-LCB, $q=0.4$)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32
PoPBO (R-LCB, $q=0.5$)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32
PoPBO (R-LCB, $q=0.6$)	91.52±0.04	94.33±0.08	73.21±0.36	73.19±0.31	46.12±0.43	46.61±0.32

PoPBO on Hartmann and Rosenbrock in Fig. 7. We observe that GP-MLP performs much worse than GP and ours, showing that the complex representation of the MLP in the surrogate model is not the main reason for the gain in performance.

C.6 Ablation Study about the Worst Tolerant Ranking K_m in ERI

Fig. 8 compares the performance of ERI under various settings for the worst tolerant ranking K_m . We observe that PoPBO-ERI is not very sensitive to K_m . Specifically, for Branin, ERI with larger K_m converges faster but ERI with various K_m have similar ultimate performance after 80 iterations. For Rosenbrock that has larger search space and more complex landscape, better exploitation ability is more important than exploration, and thus ERI with lower K_m achieves better performance.

C.7 Ablation Study about the Rectified Technique on NAS-Bench-201

Table 3 evaluates the effect of quantile parameters q on both R-LCB and ERI on NAS-Bench-201. We adopt the same ten random seeds for different settings for fair comparison. The results show that our settings of q (0.4 for ERI and 0.6 for R-LCB) perform still well on the real-world benchmark. Moreover, we observe that the results are the same when $q = 0.4, 0.5, 0.6$. We analyze that ERI and R-LCB have the same effect as the vanilla EI and LCB respectively when $q \geq 0.4$.

C.8 More iterations on 6-d Rosenbrock for GP and PoPBO

Since 6-d Rosenbrock has a large search space and is hard to converge, we run GP and PoPBO for more iterations (200 queries) and plot the regret in Fig. 9. We observe that PoPBO consistently

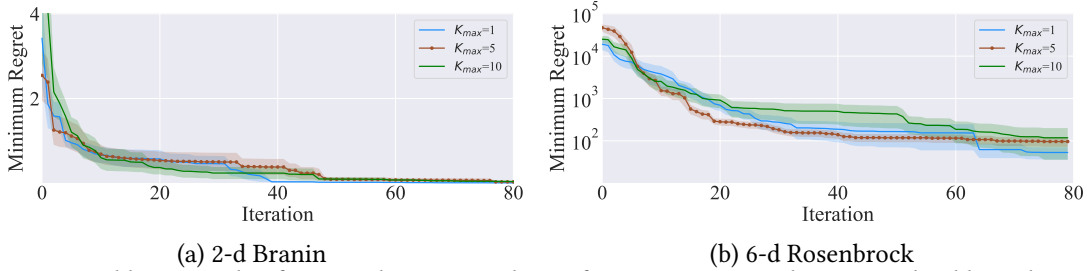


Figure 8: Ablation study of ERI on the two simulation functions. K_{max} is the worst tolerable ranking, and a higher K_{max} leads to a higher rate of exploration.

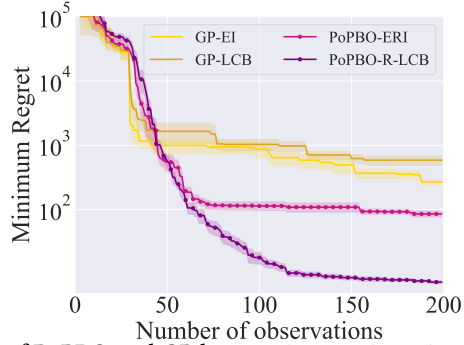


Figure 9: Performance trend of PoPBO and GP by running 200 iterations on 6-d Rosenbrock. For each setting, we conduct replicated experiments for six times with various random seeds.

outperforms GP after 50 epochs. Moreover, both PoPBO-ERI and PoPBO-R-LCB have lower variance than GP-EI and GP-LCB.

C.9 Fewer Initial Points on 6-d Rosenbrock

We set the number of initial points to 30 for a better preview of the Rosenbrock landscape for all methods. To demonstrate the sample efficiency of our algorithm, we use fewer initial points (7 points for each algorithm) and compare PoPBO with GP-based BO, SMAC and TPE on 6-d Rosenbrock benchmark. The results can be found in Fig. 11.

C.10 Robustness to various noise level

In our settings, the observations in the simulation function are noiseless, while the observations in the real-world benchmark (HPO-Bench and NAS-Bench-201) are noisy. For HPO-Bench, the performance of each configuration (hyperparameters of FCNet) is evaluated 4 times under different random seeds. In the experiment settings of HPO-Bench, the average performance is used as the observation, which is naturally noisy. NAS-Bench-201 attempts to search for a neural architecture that performs best after 200 training epochs. However, following the experiment settings of NAS-Bench-201, only the validation accuracy after 12 training epochs of each architecture can be queried, making the observations noisy.

To verify the robustness to noise of PoPBO on simulated benchmarks, we add Gaussian noises with zero mean and various standard deviation (σ) to Hartmann, Branin, and Rosenbrock simulation functions and run GP-BO and PoPBO separately. Trends of average regret among six parallel tests are plotted in Fig. 10, showing that GP performs worse with the increment of noise level. In contrast, PoPBO performs much more stable. Moreover, PoPBO outperforms GP when the objective function has large noise ($\sigma = 0.1$ for Hartmann, $\sigma = 5$ for Branin and Rosenbrock). The results demonstrate the robustness of PoPBO to noise.

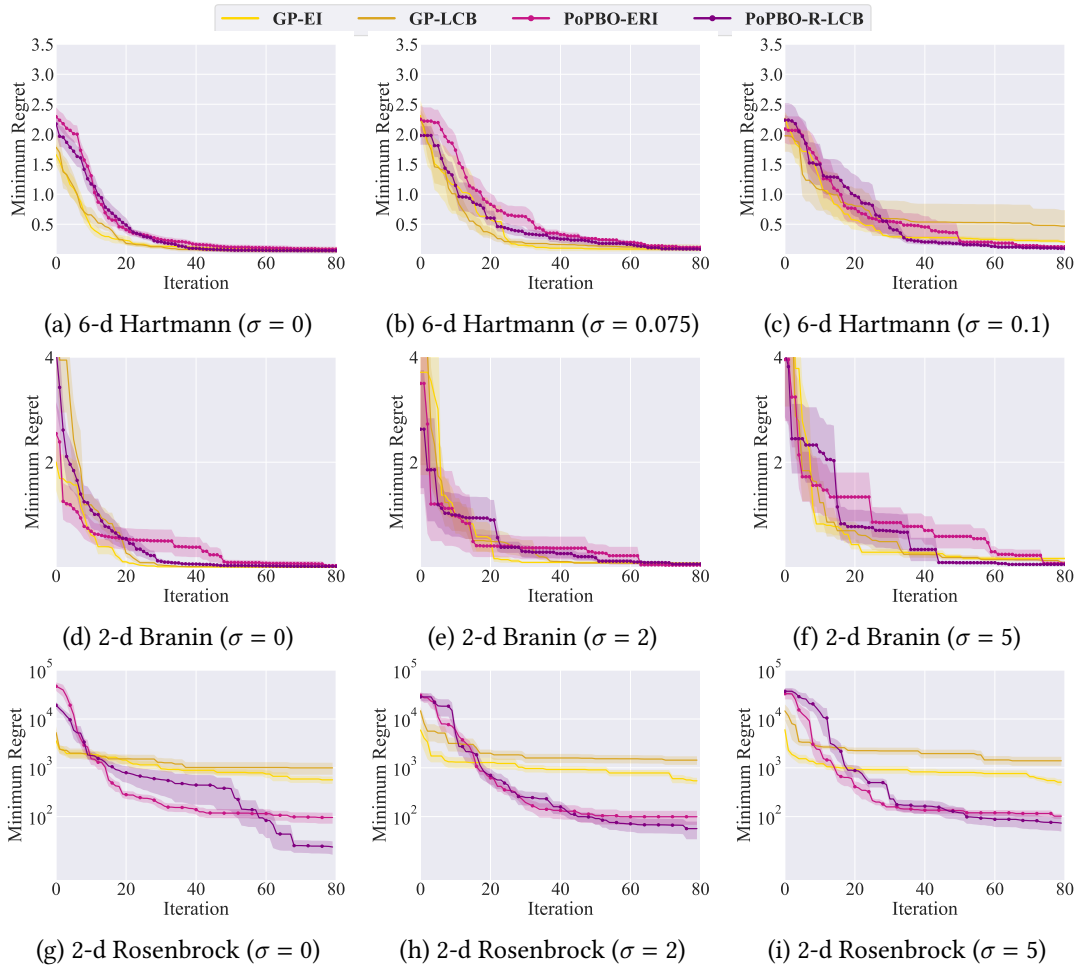


Figure 10: Comparison of the robustness to noise between GP-BO and PoPBO. We add Gaussian noises with zero mean and various standard deviation σ to the objective function. Notice that Branin and Rosenbrock have much larger range of value than Hartman, so we add noises with larger variance to them.

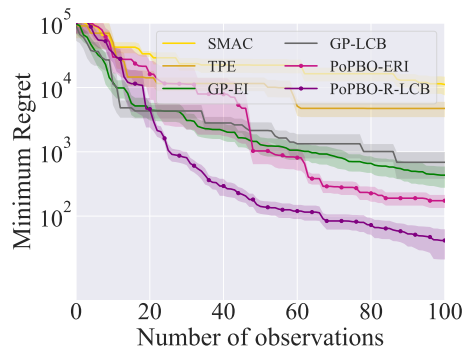


Figure 11: Performance on 6-d Rosenbrock with fewer initial points (dimension + 1 = 7 points). For each setting, we conduct replicated experiments for six times with various random seeds.

D Notations

- 1 X is the whole feasible domain (search space). If X is continuous, $|X|$ is the volume of X . While X is discrete, $|X|$ is the cardinality of it.
- 2 $S_x = \{y | y \in S, f(y) < f(x)\}$ is the set of better points than x in $S \subset X$, where S can be any continuous domain or discrete set.
- 3 \hat{S} is a discrete set containing both initial samples for BO and the history queries.
- 4 Given a specific S , $\hat{R}_x(S)$ is a random variable denoting possible ranking of x over a discrete set $\hat{S}_x \cap \hat{S}$. Hence, $\hat{R}_x(S)$ depends on \hat{S} , we utilize a hat symbol $\hat{\cdot}$ on R_x to omit \hat{S} for conciseness.

E Broader Impact and Limitations

This paper addresses the problem of Bayesian Optimization (BO) to enable efficient and effective black-box optimization. It has broad applications in perception tasks, especially computer vision, robotic control and biology. This, on the one hand, would facilitate our daily life, and on the other hand, we shall be careful about their abuse which may break one's privacy. In this sense, privacy-protection BO is also needed for development, and our techniques can also be of specific help for its generality.