Bayesian Optimization via Exact Penalty

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Abstract

Constrained optimization problems pose challenges when the objective function and constraints are nonconvex and their evaluation requires expensive black-box simulations. Recently, hybrid optimization methods that integrate statistical surrogate modeling with numerical optimization algorithms have shown great promise, as they inherit the properties of global convergence from statistical surrogate modeling and fast local convergence from numerical optimization algorithms. However, the computational efficiency is not satisfied by practical needs under limited budgets and in the presence of equality constraints. In this article, we propose a novel hybrid optimization method, called exact penalty Bayesian optimization (EPBO), which employs Bayesian optimization within the exact penalty framework. We model the composite penalty function by a weighted sum of Gaussian processes, where the qualitative components of the constraint violations are smoothed by their predictive means. The proposed method features (i) closed-form acquisition functions, (ii) robustness to initial designs, (iii) the capability to start from infeasible points, and (iv) effective handling of equality constraints. We demonstrate the superiority of EPBO to state-of-the-art competitors using a suite of benchmark synthetic test problems and two real-world engineering design problems.

Keywords: Black-box function; Expensive emulator; Hybrid optimization method; Weighted Gaussian process; Scaled expected improvement

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1 Introduction

In science and engineering, constrained optimization problems frequently arise with black-box objective function and constraints, which are expensive to evaluate. Various industries encounter such optimization tasks, as demonstrated by examples from the fine chemicals industry and early-phase oncology trials. In the fine chemicals industry, the primary goal is to maximize reaction throughput while limiting environmental waste (Felton et al., 2021). However, conducting in-depth kinetic studies to clarify mechanistic models is impractical due to the time and resource-intensive nature of reaction screening. Similarly, in early-phase oncology trials, the central goal is to identify the optimal biological dose that yields the highest efficacy while maintaining an acceptable toxicity rate (Takahashi and Suzuki, 2021). For ethical reasons, the sample size is limited and the evaluation is undoubtedly expensive. More examples include minimizing a machine learning model's validation error while ensuring that the prediction time of the learned model remains within acceptable limits (Hernández-Lobato et al., 2015; Ariafar et al., 2019), maximizing the quality of molecules while satisfying certain validity constraints (Griffiths and Hernández-Lobato, 2020), and finding optimal policy parameters by interacting with a robotic system within safety constraints (Berkenkamp et al., 2023). These diverse examples underscore the widespread need for effective solutions to address the challenges of constrained optimization with expensive black-box evaluations.

The constrained optimization problems can be generally written as

$$\min_{\boldsymbol{x}\in\mathcal{B}} f(\boldsymbol{x}) \quad \text{s.t.} \quad g_j(\boldsymbol{x}) \leqslant 0, j = 1, \ldots, J, \quad \text{and} \quad h_\ell(\boldsymbol{x}) = 0, \ell = 1, \ldots, L, \tag{1}$$

where $\mathcal{B} \subset \mathbb{R}^d$ is a known, bounded, and convex design space (e.g., a hyper-rectangle), f is the objective function, and g_js and h_ℓs are the inequality constraints and the equality constraints, respectively. Clearly, problem (1) accommodates the optimization problem with either inequality constraints or equality constraints alone (by dropping the other type). Throughout, it's assumed that a solution of problem (1) exists and that all functions are highly nonlinear, non-convex, and require black-box simulation. These simulations are not only expensive to evaluate but also do not offer any gradient information. The tacit goal is to devise a sequential design of points within $\mathcal{B}$ that efficiently locates the global optimum $\boldsymbol{x}^\star$ (up to a relaxing threshold on the equality constraints) with as few queries as possible from the expensive simulations (Pourmohamad and Lee, 2020). Meta-heuristic optimization algorithms (such as genetic algorithms and particle swarm optimization) can be used to solve high-dimensional and highly nonlinear global optimization problems (Deb and Srivastava, 2012; Parsopoulos et al., 2002; D'Angelo and Palmieri, 2021; Kumari et al., 2022). But such algorithms often require a formidably large number of evaluations of the experiment, which makes them infeasible in practice.

Constrained Bayesian optimization (CBO) has emerged as a sample-efficient sequential method to solve this problem (Gramacy et al., 2016; Gramacy, 2020; Pourmohamad and Lee, 2021; Wang et al., 2023; Garnett, 2023). The strategies of CBO can be broadly categorized into two groups (Ariafar et al., 2019). The first group focuses on modifying the acquisition function within the Bayesian optimization (BO) framework to incorporate both the feasibility of a query point and its objective value. The second group explores the development of hybrid optimization methods by combining statistical surrogate modeling and numerical optimization algorithms. Most existing works fall into the first group. See Schonlau et al. (1998), Gardner et al. (2014), Gelbart et al. (2014), Gramacy and Lee (2011), Picheny (2014), Lindberg and Lee (2015), Hernández-Lobato et al. (2015), Hernández-Lobato et al. (2016), Perrone et al. (2019), Ungredda and Branke (2021), Chen et al. (2021), Takeno et al. (2022), and the references therein. In this paper, we follow the second approach, as it possesses the properties of global convergence from statistical surrogate models and provable fast local convergence from numerical optimization algorithms (Gramacy et al., 2016; Pourmohamad and Lee, 2022).

Hybrid optimization methods have flourished since the pioneering work of Gramacy et al. (2016). The basic idea is to transform the constrained optimization problem (1) into an unconstrained one, which is subsequently tackled using an acquisition function to guide the optimization process. Gramacy et al. (2016) developed the hybrid algorithm for the optimization problem with inequality constraints by combining the augmented Lagrangian (AL) method (Nocedal and Wright, 2006) with (unconstrained) BO, called ALBO. In ALBO, two acquisition functions were proposed: predictive mean and expected improvement (EI). The predictive mean approach offers a closed-form expression but overlooks the uncertainty of the surrogate of the objective function, leading to limited exploration capabilities. On the other hand, the EI approach is not analytically tractable and needs to be evaluated numerically via Monte Carlo integration. To handle mixed (inequality and/or equality) constraints, Picheny et al. (2016) proposed a variant of ALBO called Slack-ALBO by introducing a slack variable (Nocedal and Wright, 2006). This extension simplifies EI to a one-dimensional definite integral, enabling easier numerical approximation through the quadrature method. As Picheny et al. (2016) pointed out, Slack-ALBO has a potential downside in the sense that the slack variable is chosen based solely on the posterior mean of the surrogates of the constraints, whose performance depends on the accuracy of the surrogates in representing the constraints.

Following the course of Gramacy et al. (2016), some researchers have explored and developed hybrid optimization approaches tailored to different situations. Under the condition that the objective and constraint functions can be evaluated independently, Ariafar et al. (2019) proposed to integrate BO with the alternating direction method of multipliers (ADMM) algorithm (Boyd et al., 2011). For the case where at least one of the constraints and the objective function are negatively correlated, Pourmohamad and Lee (2020) introduced the statistical filter method by employing the joint Gaussian process model (Pourmohamad and Lee, 2016) with the filter algorithm (Fletcher and Leyffer, 2002). For high-dimensional settings, Eriksson and Poloczek (2021) developed the scalable constrained BO (SCBO) method based on the trust region algorithm (Eriksson et al., 2019). To force that the design points remain within the feasible region, Pourmohamad and Lee (2022) proposed to combine BO with the interior point method (Nocedal and Wright, 2006). However, a disadvantage of this method is that it must start with some feasible initial points, which is difficult to satisfy when the feasible region is relatively small compared to the design space. While these methods address various aspects of constrained optimization, none of them can deal with equality constraints satisfactorily. Even though one can convert any equality constraint to a pair of inequality constraints (in that $h_\ell(\boldsymbol{x}) = 0$ is equivalent to $h_\ell(\boldsymbol{x}) \leqslant 0$ and $h_\ell(\boldsymbol{x}) \geqslant 0$ simultaneously), numerical issues have been reported in empirical comparisons, as the reformulation puts double-weight on equality constraints and violates certain regularity conditions (Sasena, 2002; Picheny et al., 2016; Gramacy, 2020). Consequently, there remains a gap in the existing literature for an efficient and robust hybrid optimization method capable of handling equality constraints effectively.

To overcome the aforementioned challenges and limitations in existing hybrid optimization methods, we propose a novel approach called exact penalty Bayesian optimization (EPBO), which integrates BO within the exact penalty framework (Nocedal and Wright, 2006). The exact penalty function offers distinct advantages over the augmented Lagrangian in two respects. Firstly, the *exact* property reduces the dependence on the strategy for updating the penalty parameters, leading to improved stability and performance of EPBO. Secondly, the linear penalty facilitates the representation of the surrogate model as a weighted sum of Gaussian processes, enhancing the efficiency and accuracy of the optimization process. In summary, these make the proposed algorithm possess the following features: i) closed-form acquisition functions, ii) robustness to initial designs, iii) the capability to start from infeasible points, and iv) effective handling of black-box equality constraints. These features collectively make EPBO a promising method for constrained optimization tasks, offering advantages in terms of computational efficiency, robustness, and versatility in handling various optimization scenarios.

The remainder of the paper is organized as follows. Section 2 introduces two fundamental building blocks for the proposed hybrid optimization method. Section 3 contains the main results of the proposed method, which embeds BO within the exact penalty framework and uses a novel surrogate model. Section 4 presents numerical studies to demonstrate the superior performance of the proposed method to the state-of-the-art CBO methods through three synthetic test problems and two real-world engineering design problems. Section 5 concludes the paper with some discussion. Technical details and additional numerical studies are deferred in the Supplement. An R package is provided in the web appendix and also on GitHub: `https://github.com/Jiangyan-Zhao/EPBO`.

2 Elements of Hybrid Optimization Method

In this section, we will offer a concise review of two essential components that form the cornerstone of our hybrid optimization method.

2.1 Bayesian Optimization

Bayesian optimization (BO) is a sample-efficient sequential design strategy used to tackle global optimization problems characterized by an expensive-to-evaluate black-box objective function. The modern BO can be traced back to Mockus et al. (1978). This method consists of two key components: a statistical surrogate model and an acquisition function. The surrogate model, based on cumulated function evaluations, characterizes the unknown objective function and undergoes continual refinement with each new evaluation. The Gaussian process (GP) has been the canonical choice due to its flexibility, analytical tractability, and ability to quantify uncertainty at unobserved inputs (Rasmussen and Williams, 2006; Gramacy, 2020; Garnett, 2023). An acquisition function is employed to identify the next query point to maximally enrich the model toward a global minimizer. Improvement-based acquisition functions are the most commonly used and have demonstrated practical effectiveness across a wide range of optimization problems. (Shahriari et al., 2016; Noè and Husmeier, 2018; Zhan and Xing, 2020).

Denote $\mathcal{D}_n = \{\boldsymbol{x}_i, f(\boldsymbol{x}_i)\}_{i=1}^n$. Let $f_{\min} = \min\{f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_n)\}$ be the best objective value achieved so far. A GP surrogate model $Y_f(\boldsymbol{x})$ is trained on $\mathcal{D}_n$. Let Φ and ϕ denote the distribution function and density of the standard normal variable, respectively. Denote the posterior mean and posterior standard deviation of the predictive distribution of $Y_f(\boldsymbol{x})$ by $\mu(\boldsymbol{x})$ and $\sigma(\boldsymbol{x})$, respectively, i.e., $Y_f(\boldsymbol{x})|\mathcal{D}_n \sim \mathcal{N}(\mu(\boldsymbol{x}), \sigma^2(\boldsymbol{x}))$. Denote $d(\boldsymbol{x}) = \{f_{\min} - \mu(\boldsymbol{x})\}/\sigma(\boldsymbol{x})$. Schonlau (1997) defined the potential for improvement over $f_{\min}$ at an input point $\boldsymbol{x}$ as $I(\boldsymbol{x}) = \max\{0, f_{\min} - Y_f(\boldsymbol{x})\}$. The expectation of $I(\boldsymbol{x})$ over $Y_f(\boldsymbol{x})$ has a closed form given by

$$\mathrm{EI}(\boldsymbol{x}) = \mathbb{E}\{I(\boldsymbol{x})\} = \sigma(\boldsymbol{x})[d(\boldsymbol{x})\Phi\{d(\boldsymbol{x})\} + \phi\{d(\boldsymbol{x})\}],$$

which reveals how exploitation ($\mu(\boldsymbol{x})$ under $f_{\min}$) and exploration (large $\sigma(\boldsymbol{x})$) are balanced (Jones et al., 1998). And the variance of $I(\boldsymbol{x})$ is (Noè and Husmeier, 2018)

$$\mathbb{V}\{I(\boldsymbol{x})\} = \sigma^2(\boldsymbol{x})[\{d^2(\boldsymbol{x}) + 1\}\Phi\{d(\boldsymbol{x})\} + d(\boldsymbol{x})\phi\{d(\boldsymbol{x})\}] - \mathrm{EI}^2(\boldsymbol{x}).$$

To mitigate the over-exploitative behaviour of expected improvement (EI) (Calandra et al., 2014), Noè and Husmeier (2018) proposed the scaled expected improvement (ScaledEI) acquisition function

$$\mathrm{ScaledEI}(\boldsymbol{x}) = \mathrm{EI}(\boldsymbol{x})/[\mathbb{V}\{I(\boldsymbol{x})\}]^{1/2}. \tag{2}$$

By maximizing the ScaledEI criterion, the optimization process selects the next query point at which the improvement is expected to be large with a large probability. The ScaledEI criterion encourages exploration in regions of the search space with higher uncertainty than the standard EI criterion (Alvi, 2019). On the other hand, locating the global maximum is more challenging since the multimodal surface becomes more intricate compared to its counterpart under the EI criterion.

2.2 Exact Penalty Framework

One thing that makes the ALBO method (Gramacy et al., 2016) inefficient is that the quadratic penalty in the augmented Lagrangian penalty function prevents a closed-form expression for the acquisition function. To circumvent the obstacle, we turn to the exact penalty (EP) function method, with the penalty in a linear form (Nocedal and Wright, 2006). This transition enables the development of a novel surrogate model, as presented in Section 3.1, and consequently leads to the derivation of a closed-form acquisition function, as described later in (8).

To address problem (1), Zangwill (1967) and Pietrzykowski (1969) introduced the exact penalty function

$$\mathcal{P}(\boldsymbol{x};\boldsymbol{\rho}) = f(\boldsymbol{x}) + \rho \sum_{j=1}^{J} v_{g_j}(\boldsymbol{x}) + \rho \sum_{\ell=1}^{L} v_{h_\ell}(\boldsymbol{x}),$$

where $\rho > 0$ is a penalty parameter, $v_{g_j}(\boldsymbol{x}) = \max\{0, g_j(\boldsymbol{x})\}$ and $v_{h_\ell}(\boldsymbol{x}) = |h_\ell(\boldsymbol{x})|$ are inequality and equality constraint violations, respectively. Here, the term "exact" means that, for a sufficiently large penalty parameter ρ, the (local) minimum value of the (unconstrained) penalty function yields the exact (local) solution to the original (constrained) problem (1). This property is highly desirable because it makes the performance of the penalty method less dependent on the strategy of updating the penalty parameter (Nocedal and Wright, 2006, Chapter 17).

In practice, determining a suitable and sufficiently large ρ can be a non-trivial task, especially for the non-convex problem, as the penalty function can become challenging to minimize if ρ is excessively large. To address this challenge, Barbosa and Lemonge (2002) proposed an adaptive strategy that leverages information from the dataset, such as the average of the objective function and the degree of violation of each constraint, to adaptively scale the penalty parameter for each constraint. Therefore, the original constrained optimization problem (1) is reformulated in an adaptive fashion:

$$\min_{\boldsymbol{x}\in\mathcal{B}} \left\{ \mathcal{P}(\boldsymbol{x};\boldsymbol{\rho}) = f(\boldsymbol{x}) + \sum_{j=1}^{J} \rho_{g_j} v_{g_j}(\boldsymbol{x}) + \sum_{\ell=1}^{L} \rho_{h_\ell} v_{h_\ell}(\boldsymbol{x}) \right\}, \tag{3}$$

where $\boldsymbol{\rho} = (\rho_{g_1}, \ldots, \rho_{g_J}, \rho_{h_1}, \ldots, \rho_{h_L})^\top$ is the collection of penalty parameters with

$$\rho_m = \langle |f(\boldsymbol{x})| \rangle_n \frac{\langle v_m(\boldsymbol{x}) \rangle_n}{\sum_m \{\langle v_m(\boldsymbol{x}) \rangle_n\}^2}, \quad m \in \{g_1, \ldots, g_J, h_1, \ldots, h_L\}, \tag{4}$$

and $\langle a(\boldsymbol{x}) \rangle_n = n^{-1} \sum_{i=1}^{n} a(\boldsymbol{x}_i)$ denotes the average of function $a(\boldsymbol{x})$ up to the n-th point. Each penalty parameter is updated in a way that prevents any value decline. The underlying idea is that the values of the penalty parameters should be allocated so that the harder-to-satisfy constraints have a proportionally larger penalty coefficient (Lemonge et al., 2010). It is worth noting that the strategy of Barbosa and Lemonge (2002) does not explicitly consider the exact property of penalty parameters. We will propose a modified version of this strategy in Section 3.2.

Although the exact penalty function method has been widely criticized for its non-differentiability in certain optimization contexts, we want to point out that this drawback is not relevant to the problem considered in this paper, as the gradient information of objective and constraints is not involved in the BO framework. Moreover, we will propose a novel surrogate model in Section 3.1 to smooth the problem (3).

3 Exact Penalty Bayesian Optimization

We now extend the notation of the cumulated data up to the n-th evaluation, encompassing the values of constraints, denoted as $\mathcal{D}_n = \{\boldsymbol{x}_i, f(\boldsymbol{x}_i), g_1(\boldsymbol{x}_i), \ldots, g_J(\boldsymbol{x}_i), h_1(\boldsymbol{x}_i), \ldots, h_L(\boldsymbol{x}_i)\}_{i=1}^n$. In light of Gramacy et al. (2016), we separately model the components of the EP function by independent surrogate models denoted as $Y_f(\boldsymbol{x})$, $Y_{g_j}(\boldsymbol{x})$, and $Y_{h_\ell}(\boldsymbol{x})$ for the objective function, inequality constraints, and equality constraints, respectively. Although correlations between objective and constraints can be taken into account, e.g. through a joint GP model (Pourmohamad and Lee, 2016), the independent approach is preferred due to its simplicity and ease of implementation.

With the surrogate models, we can model the EP function (3) by

$$Y_p(\boldsymbol{x}) = Y_f(\boldsymbol{x}) + \sum_{j=1}^{J} \rho_{g_j} \max\{0, Y_{g_j}(\boldsymbol{x})\} + \sum_{\ell=1}^{L} \rho_{h_\ell} |Y_{h_\ell}(\boldsymbol{x})|. \tag{5}$$

However, due to the presence of maximum and absolute value operators, the distribution of (5) is complicated, which causes difficulty in constructing the acquisition function with a closed-form expression like ScaledEI (2). While it is possible to evaluate the non-closed-form acquisition function using the Monte Carlo method, as demonstrated by Gramacy et al. (2016), this approach introduces additional computational errors and significantly increases the computational time required. Supplement SM§5 provides details on the Monte Carlo approximation of the ScaledEI acquisition function for model (5). We will use it later for comparison with the proposed method in terms of the computational cost and the quality of the solutions.

3.1 Novel Surrogate Model

To fix the aforementioned computation issue, we first propose a sensible approximation to the surrogate model of EP in (5). It serves as a stepping stone for building the acquisition function given in Section 3.2.

Observe that for $j = 1, \ldots, J$ and $\ell = 1, \ldots, L$, the constraint violation models of (5) can be expressed as

$$\max\{0, Y_{g_j}(\boldsymbol{x})\} = \mathbb{1}\{Y_{g_j}(\boldsymbol{x}) > 0\} \cdot Y_{g_j}(\boldsymbol{x}), \quad |Y_{h_\ell}(\boldsymbol{x})| = [2\mathbb{1}\{Y_{h_\ell}(\boldsymbol{x}) > 0\} - 1] \cdot Y_{h_\ell}(\boldsymbol{x}), \tag{6}$$

where $\mathbb{1}\{\cdot\}$ is the indicator function. In both decompositions, the two factors represent the qualitative component and the quantitative part, respectively. The qualitative factor essentially signifies the violation of the constraint when it is non-zero. However, due to its inherent discontinuity, it introduces distributional challenges. To circumvent this obstacle, we simply replace the two qualitative components with their respective predictive means given by

$$\omega_{g_j}(\boldsymbol{x}) = \mathbb{E}[\mathbb{1}\{Y_{g_j}(\boldsymbol{x}) > 0\}] = \Pr\{Y_{g_j}(\boldsymbol{x}) > 0\} = \Phi\left\{\frac{\mu_{g_j}(\boldsymbol{x})}{\sigma_{g_j}(\boldsymbol{x})}\right\},$$
$$\omega_{h_\ell}(\boldsymbol{x}) = \mathbb{E}[2\mathbb{1}\{Y_{h_\ell}(\boldsymbol{x}) > 0\} - 1] = 2\Phi\left\{\frac{\mu_{h_\ell}(\boldsymbol{x})}{\sigma_{h_\ell}(\boldsymbol{x})}\right\} - 1.$$

These replacements help to create a smoother and more manageable constraint violation models and simplify the subsequent analysis. A similar idea is seen in Schonlau et al. (1998), where the acquisition function is $\mathrm{EIC}(\boldsymbol{x}) = \mathrm{EI}(\boldsymbol{x}) \prod_{j=1}^{J}\{1 - \omega_{g_j}(\boldsymbol{x})\}$. At the same time, we keep the quantitative components, which represent the magnitude of the constraint violations, unchanged.

In summary, we have introduced novel surrogate models $\omega_{g_j}(\boldsymbol{x})Y_{g_j}(\boldsymbol{x})$ and $\omega_{h_\ell}(\boldsymbol{x})Y_{h_\ell}(\boldsymbol{x})$ to represent the constraint violation functions $\max\{0, g_j(\boldsymbol{x})\}$ and $|h_\ell(\boldsymbol{x})|$, respectively. It is worth mentioning that Biswas et al. (2022) smoothed the rectified linear unit activation function $\max(0, x)$ for the deep neural network via $\Phi(\alpha x)x$ with a positive parameter α. Our smoothing substitution of $\max\{0, Y_{g_j}(\boldsymbol{x})\}$ by $\Phi\{\mu_{g_j}(\boldsymbol{x})/\sigma_{g_j}(\boldsymbol{x})\}Y_{g_j}(\boldsymbol{x})$ can be seen as a randomized version of Biswas et al. (2022) with the adaptive parameter $\sigma_{g_j}^{-1}(\boldsymbol{x})$. On one hand, this substitution interpolates $\max\{0, Y_{g_j}(\boldsymbol{x})\}$. On the other hand, as the number of design points increases, the uncertainty of the surrogate model $Y_{g_j}(\boldsymbol{x})$ reduces to zero and the smoothing model converges to the actual model $\max\{0, Y_{g_j}(\boldsymbol{x})\}$. Figure 1 shows the prediction performance of the proposed novel surrogate model for the inequality constraint violation $g^+(x) = \max\{0, g(x)\}$, where $g(x) = \exp(-1.4x)\cos(7\pi x/2)$, in comparison with that of the vanilla surrogate model (Gramacy et al., 2016). It is seen that the predictive mean function (dashed line), given by $\omega_g(x)\mu_g(x)$, converges to the true constraint violation (solid line). In contrast, the vanilla surrogate model, which is directly built on the data $\{x_i, g^+(x_i)\}_{i=1}^n$, fits worse especially in the feasible regions, as the max operator creates kinks in the surface. Similar results are seen in an example with equality constraint violation in Supplement SM§1.

Then, the model (5) is approximated by

$$\widetilde{Y}_p(\boldsymbol{x}) = Y_f(\boldsymbol{x}) + \sum_{j=1}^{J} \rho_{g_j}\omega_{g_j}(\boldsymbol{x})Y_{g_j}(\boldsymbol{x}) + \sum_{\ell=1}^{L} \rho_{h_\ell}\omega_{h_\ell}(\boldsymbol{x})Y_{h_\ell}(\boldsymbol{x}), \tag{7}$$

which is a weighted sum of $J + L + 1$ GPs, therefore a GP with mean and variance respectively given by

$$\mu_p(\boldsymbol{x}) = \mu_f(\boldsymbol{x}) + \sum_{j=1}^{J} \rho_{g_j}\omega_{g_j}(\boldsymbol{x})\mu_{g_j}(\boldsymbol{x}) + \sum_{\ell=1}^{L} \rho_{h_\ell}\omega_{h_\ell}(\boldsymbol{x})\mu_{h_\ell}(\boldsymbol{x}),$$
$$\sigma_p^2(\boldsymbol{x}) = \sigma_f^2(\boldsymbol{x}) + \sum_{j=1}^{J} \rho_{g_j}^2\omega_{g_j}^2(\boldsymbol{x})\sigma_{g_j}^2(\boldsymbol{x}) + \sum_{\ell=1}^{L} \rho_{h_\ell}^2\omega_{h_\ell}^2(\boldsymbol{x})\sigma_{h_\ell}^2(\boldsymbol{x}).$$

This approximation provides a reasonable surrogate model, as the novel surrogate model (7) interpolates the EP function (3) while also providing uncertainty quantification for unobserved inputs. While it sacrifices a minimum amount of exactness of model (5), it offers a significant advantage by transforming the problem into a stationary GP model compatible with the most readily available GP modeling tools (Gramacy et al., 2016; Gramacy, 2020; Pourmohamad and Lee, 2022). Another advantage of model (7) is that it can be seamlessly integrated into any (unconstrained) fast-to-evaluate acquisition function (Garnett, 2023), including but not limited to the improvement-based ones introduced in Section 2.1.

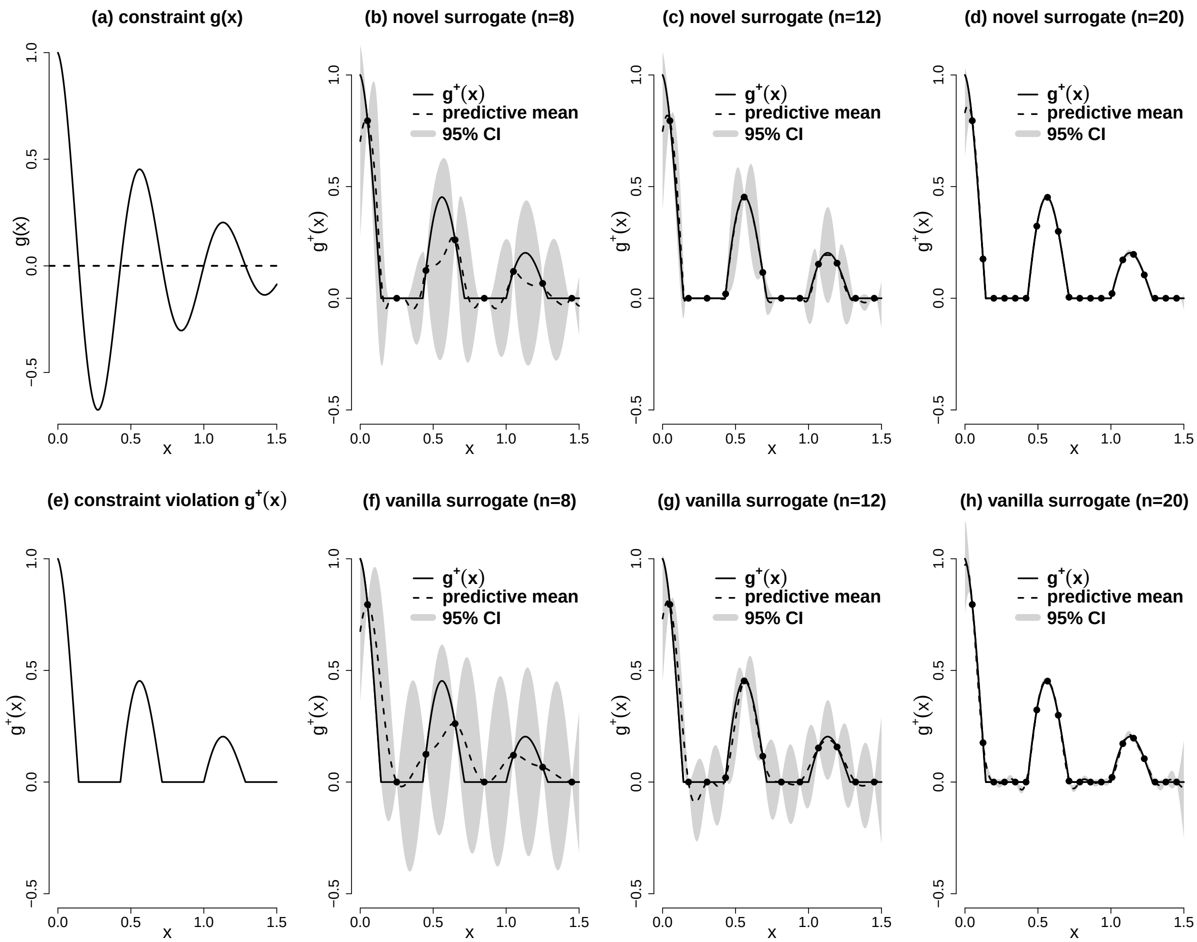

Figure 1: (a): True constraint function $g(x) = \exp(-1.4x)\cos(7\pi x/2)$; (b)–(d): the proposed novel surrogate model based on 8, 12 and 20 equally spaced samples in [0.05, 1.45], respectively, where the solid line is the true constraint violation, the dashed line is the predictive mean of the surrogate model, and the shaded areas are the corresponding 95% confidence intervals (CI) given by $\mu(x) \pm 1.96\sigma(x)$; (e): constraint violation function $g^+(x) = \max\{0, g(x)\}$; (f)–(h): counterparts of (b)–(d) obtained by the vanilla surrogate model.

3.2 Algorithm

Based on the novel surrogate model (7), there are two key issues that need to be carefully dealt with for the EPBO algorithm. They are (i) how to initialize and update the penalty parameters $\boldsymbol{\rho}$ and (ii) how to efficiently solve the problem (3) within the BO framework.

To answer the question (i), we first introduce a softened definition of feasible solutions in the presence of equality constraints, since it is often impractical to strictly satisfy equality constraints in practical problems. A solution $\boldsymbol{x}$ is considered feasible, within a small user-specified tolerance $\varepsilon > 0$, if it satisfies all inequality constraints and $|h_\ell(x)| \leqslant \varepsilon$ for all $\ell =$

$1, \ldots, L$.

Note that the adaptive updating strategy of penalty parameters in (4) may not precisely adhere to an exact penalty approach as $\boldsymbol{\rho}$ may not be sufficiently large. To address this, we propose a modified strategy as follows. If there is no infeasible solution in the sequential design, the denominator of (4) is not defined. In such case, we set all penalty parameters to zero, as all constraints are inactive. On the other hand, if the sequential design contains some infeasible solutions and the minimizer $\widehat{\boldsymbol{x}} = \mathrm{argmin}_{\boldsymbol{x} \in \mathcal{D}_n} \{\mathcal{P}(\boldsymbol{x}, \boldsymbol{\rho})\}$ does not satisfy some constraints, then the penalty parameters associated with these unsatisfied constraints are doubled successively until $\widehat{\boldsymbol{x}}$ becomes feasible. Additionally, when equality constraints are present, (4) does not distinguish the tolerance level of equality constraints. Clearly, the smaller the tolerance level, the harder it is for the equality constraints to be satisfied. Therefore, we set a lower bound and replace the penalty parameters ρ_{h_ℓ} in (4) by $\max\{\rho_{h_\ell}, (L\varepsilon)^{-1}\}$.

To answer the question (ii), it is crucial to tailor another key component of BO, i.e., the acquisition function. Similar to the ALBO algorithm (Gramacy et al., 2016), we also provide two acquisition functions: ScaledEI and predictive mean. Let $y_{\min} = \min\{\mathcal{P}(\boldsymbol{x}_i; \boldsymbol{\rho}) : i = 1, \ldots, n\}$ be the best value of the EP function achieved so far. Let $I_p(\boldsymbol{x}) = \max\{0, y_{\min} - \widetilde{Y}_p(\boldsymbol{x})\}$ be the improvement at $\boldsymbol{x}$. The ScaledEI acquisition function (2) can be directly applied to the problem (3), again with the closed form given by

$$\mathrm{ScaledEI_p}(\boldsymbol{x}) = \mathbb{E}\{I_p(\boldsymbol{x})\}/[\mathbb{V}\{I_p(\boldsymbol{x})\}]^{1/2}, \tag{8}$$

where the terms $f_{\min}$, $\mu(\boldsymbol{x})$, $\sigma(\boldsymbol{x})$, and $d(\boldsymbol{x})$ in (2) are replaced by $y_{\min}$, $\mu_p(\boldsymbol{x})$, $\sigma_p(\boldsymbol{x})$, and $d_p(\boldsymbol{x}) = \{y_{\min} - \mu_p(\boldsymbol{x})\}/\sigma_p(\boldsymbol{x})$, respectively.

Note that ScaledEI can be exactly zero for an uncountably infinite subset of the search space $\mathcal{B}$. Therefore, finding regions of positive ScaledEI can be challenging, especially in later iterations when the penalty parameters $\boldsymbol{\rho}$ are large. If no non-zero ScaledEI region can be found, switch to the predictive mean approach (9), as recommended by Picheny et al. (2016), Gramacy (2020, Section 7.3.6), and Picheny et al. (2021).

The predictive mean of the surrogate model (5) is

$$\mathbb{E}\{Y_p(\boldsymbol{x})\} = \mu_f(\boldsymbol{x}) + \sum_{j=1}^{J} \rho_{g_j} \mathrm{EV}_{g_j}(\boldsymbol{x}) + \sum_{\ell=1}^{L} \rho_{h_\ell} \mathrm{EV}_{h_\ell}(\boldsymbol{x}), \tag{9}$$

where

$$\mathrm{EV}_{g_j}(\boldsymbol{x}) = \mathbb{E}[\max\{0, Y_{g_j}(\boldsymbol{x})\}] = \mu_{g_j}(\boldsymbol{x})\Phi\left\{\frac{\mu_{g_j}(\boldsymbol{x})}{\sigma_{g_j}(\boldsymbol{x})}\right\} + \sigma_{g_j}(\boldsymbol{x})\phi\left\{\frac{\mu_{g_j}(\boldsymbol{x})}{\sigma_{g_j}(\boldsymbol{x})}\right\},$$

Algorithm 1 EPBO: exact penalty Bayesian optimization

Input: Search space $\mathcal{B}$, initial design size n_0, maximum design size N, tolerance $\varepsilon > 0$ for equality constraints

1: Generate an initial experimental design of size n_0 and obtain cumulated data $\mathcal{D}_{n_0}$
2: Initialize the penalty parameters $\boldsymbol{\rho}$
3: **for** $n = n_0, \ldots, N-1$ **do**
4: Fit or update GP models for the objective and constraints based on $\mathcal{D}_n$
5: Construct the surrogate model (7) for the exact penalty function (3)
6: Select the next query point $\boldsymbol{x}_{n+1}$ by maximizing ScaledEI (8) or minimizing predictive mean (9)
7: Append the evaluation results of the objective and constraints at $\boldsymbol{x}_{n+1}$ to $\mathcal{D}_n$
8: Update the penalty parameters $\boldsymbol{\rho}$
9: **end for**

Output: The recommended solution $\widehat{\boldsymbol{x}}$

$$\mathrm{EV}_{h_\ell}(\boldsymbol{x}) = \mathbb{E}[|Y_{h_\ell}(\boldsymbol{x})|] = \mu_{h_\ell}(\boldsymbol{x}) \left[2\Phi\left\{\frac{\mu_{h_\ell}(\boldsymbol{x})}{\sigma_{h_\ell}(\boldsymbol{x})}\right\} - 1 \right] + 2\sigma_{h_\ell}(\boldsymbol{x})\phi\left\{\frac{\mu_{h_\ell}(\boldsymbol{x})}{\sigma_{h_\ell}(\boldsymbol{x})}\right\}.$$

Here, we adopt the concept of the expected violation (EV) of Audet et al. (2000) for equality constraints. The positive partial derivatives of EVs with respect to σ, given by

$$\frac{\partial \mathrm{EV}_{g_j}(\boldsymbol{x})}{\sigma_{g_j}(\boldsymbol{x})} = \phi\left\{\frac{\mu_{g_j}(\boldsymbol{x})}{\sigma_{g_j}(\boldsymbol{x})}\right\}, \quad \frac{\partial \mathrm{EV}_{h_\ell}(\boldsymbol{x})}{\sigma_{h_\ell}(\boldsymbol{x})} = 2\phi\left\{\frac{\mu_{h_\ell}(\boldsymbol{x})}{\sigma_{h_\ell}(\boldsymbol{x})}\right\},$$

reveal that the approach through the predictive mean acquisition function is purely exploitative. However, the predictive mean approach will not make the search stuck at local minimizers, as it is only adopted later in the iteration when the uncertainty of the surrogate model (7) becomes very small (Gramacy, 2020, Section 7.3.6).

We are now in a position to state our proposed algorithm, which we refer to as exact penalty Bayesian optimization (EPBO). The complete description of our proposed EPBO method is summarized in Algorithm 1. On line 1, the algorithm begins by generating an initial experimental design using a space-filling design, such as the Latin hypercube design (LHD) (McKay et al., 1979), and obtains the corresponding values of objective and constraints. After initializing the penalty parameters (line 2), EPBO iterates its main loop until the budget has been exhausted (lines 3–9). In each iteration, EPBO fits or updates the GP models for the objective and constraints separately from the cumulated data (line 4) and constructs the surrogate model for the exact penalty function (line 5). Line 6 is the key step of EPBO, showing how to select the next query experiment point $\boldsymbol{x}_{n+1}$ according to the acquisition function (8) or (9). Both strategies have closed-form representations, which enable fast implementation using standard numerical optimization methods, e.g., initializing local L-BFGS-B searches (Byrd et al., 1995) from the best point of the random candidate grid (Gramacy, 2016; Picheny et al., 2016). In lines 7–8, EPBO augments the cumulated data and updates the penalty parameters by evaluating the objective and constraints at the query point $\boldsymbol{x}_{n+1}$. Finally, EPBO reports the recommended solution

$$\widehat{\boldsymbol{x}} = \underset{\boldsymbol{x}\in\mathcal{D}_N}{\operatorname{argmin}}\{f(\boldsymbol{x}) : g_j(\boldsymbol{x}) \leqslant 0, |h_\ell(\boldsymbol{x})| \leqslant \varepsilon, j = 1, \ldots, J, \ell = 1, \ldots, L\},$$

where ε is a pre-specified tolerance level for the equality constraints.

4 Empirical Comparison

In this section, we present empirical comparisons of the proposed EPBO method with six state-of-the-art CBO methods, namely, EIC (Schonlau et al., 1998), ALBO (Gramacy et al., 2016), Slack-ALBO (Picheny et al., 2016), the asymmetric entropy (AE) method (Lindberg and Lee, 2015), SCBO (Eriksson and Poloczek, 2021), and the barrier method (BM) (Pourmohamad and Lee, 2022). As a reference, we include the results obtained by the random search using the Latin hypercube design (LHD) of a sufficiently large number of points (depending on the precision needed) (McKay et al., 1979). The comparison is conducted on a set of benchmark synthetic test problems (Gramacy, 2020; Pourmohamad and Lee, 2022) and two real-world engineering design problems (Pourmohamad and Lee, 2021; Felton et al., 2021).

Assume that all black-box objective and constraints are modeled by independent GP priors with zero mean and squared exponential kernel, as commonly used in GP modeling (Rasmussen and Williams, 2006; Gramacy, 2020). The implementations of ALBO, Slack-ALBO, and EIC are readily available through the `laGP` package in R (Gramacy, 2016). The implementation of SCBO is available via the `BoTorch` package in Python (Balandat et al., 2020). For the proposed EPBO method, as well as AE and BM, we have prepared an R package available in the web supplement and also on GitHub. See more details in Supplement SM§2.

To make a fair comparison, we employ the same random initial design of size $n_0 = 10d$ across all methods. (Recall that d is the dimension of the space.) The initial design is generated by the LHD method through the `tgp` package of R (Gramacy and Taddy, 2010). The $10d$ rule-of-thumb is recommended by Jones et al. (1998) and Loeppky et al. (2009). We have more discussion about the size of initial design in Section 5. We set the number of replications for the synthetic test problems and the real-world engineering design problems to be 100 and 30, respectively, under random initializations to ensure a robust and statistically meaningful assessment of the performance (Gramacy et al., 2016; Pourmohamad and Lee, 2022).

Table 1: Comparison of the mean and IQR of the BFOVs at the final evaluation obtained by the seven competing methods and the LHD-based random search for the HSQ and MTP problems.

		LHD	EIC	AE	ALBO	Slack	SCBO	BM	EPBO
HSQ	Mean	-1.0930	-1.0930	-1.0823	-1.0931	-1.0739	-1.0776	-1.0933	-1.0934
	IQR ($\times 10^{-4}$)	4.47	4.25	52.9	2.28	325	325	1.35	0.07
MTP	Mean	-1.9589	-2.0059	-2.0101	-2.0142	-1.7115	-1.9508	-2.0045	-2.0212
	IQR ($\times 10^{-2}$)	5.49	1.59	1.24	0.79	1.98	0.68	2.03	0.22

We employ the metric of the average of the best feasible objective value (BFOV) over iterations to evaluate the performance of convergence to the global minimum. When only inequality constraints are involved, we examine the distribution (via boxplot) of BFOV at the final evaluation to assess the performance of the robustness with respect to the initial design (Gramacy et al., 2016). When equality constraints are present, we report the proportion of successfully finding feasible solutions (as a challenge in this context) over iterations (Picheny et al., 2016).

4.1 Synthetic Test Problems

We first present the comparison on three synthetic test problems, where the first two involve only inequality constraints and the third one includes mixed constraints. The detailed description and visualization for each problem are given in Supplement SM§3.

4.1.1 Inequality Constrained Problems

Consider the inequality constrained problem from Gramacy (2016) that is composed by the "Herbie's tooth" objective (Lee et al., 2011), a sinusoidal inequality constraint, and a quadratic inequality constraint. It is referred to as the HSQ problem. It is a challenging problem as both objective function and constraints are highly non-linear and there are several local minima within the feasible set. The problem is further complicated by the fact that the difference between the local minimum (-1.0609) and the global minimum (-1.0934) is very small and their spatial separation is large (exceeding 40% of the maximum distance of the search space), as shown in Panel (a) of Figure SM.2 and Figure SM.3. See more details in the `demo("ALfhat")` of the `laGP` package of R and Gramacy (2020, Section 7.3.7).

Panel (a) of Figure 2 shows the average progress in BFOVs of the competing methods over 120 iterations. It is seen that EPBO, EIC, ALBO, and BM perform well in identifying the global minimum after 120 iterations. EPBO yields the fastest convergence in about 60 iterations. However, BM, EIC, and ALBO converge in about 80 to 100 iterations. AE performs

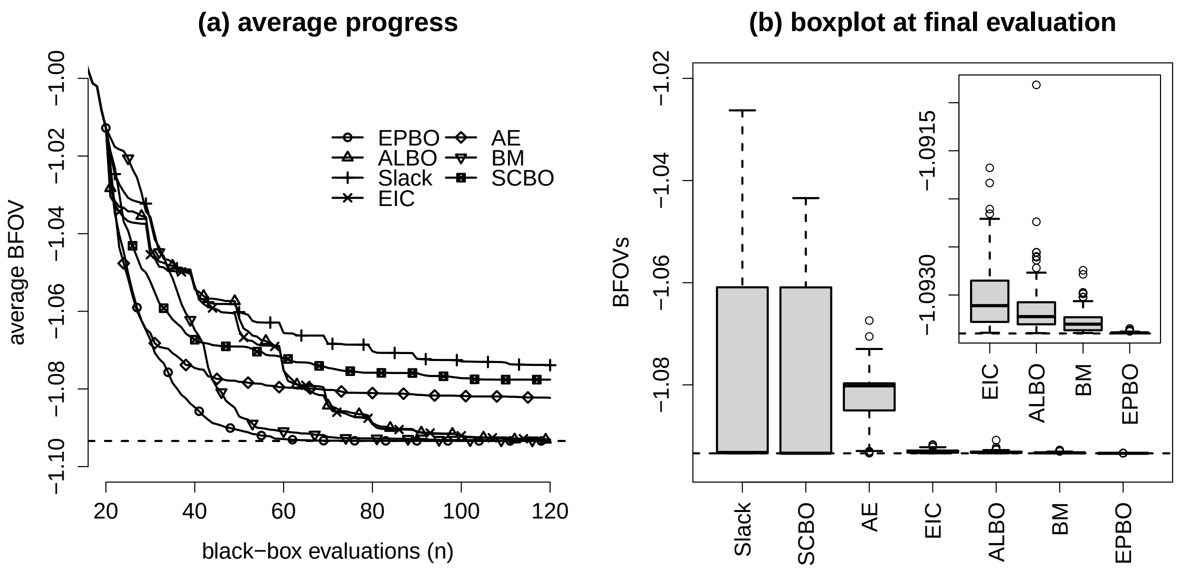

Figure 2: Comparison results for the HSQ problem. (a) average progress in BFOVs over 120 iterations, where the horizontal dashed line indicates the value of the global optimum, and (b) boxplots of the BFOVs at the final evaluation, where the sub-window displays the boxplots of the best four (in the sense of mean) in a refined scale.

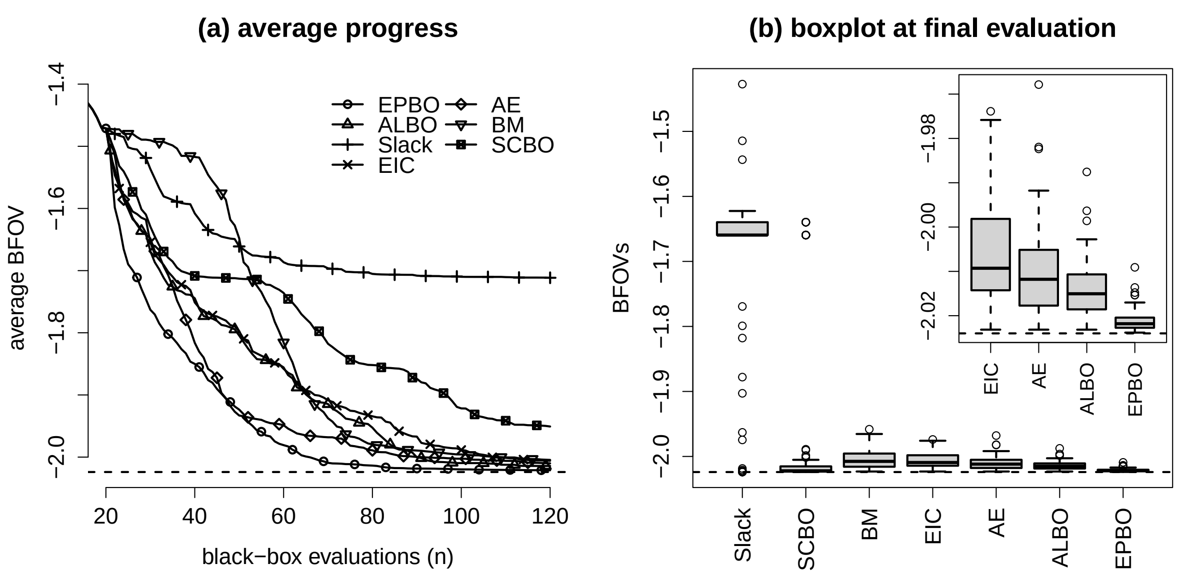

Figure 3: Comparison results for the MTP problem with the same captions as in Figure 2.

inferior to the aforementioned four methods because the optimum point does not reside along the constraint boundary. Slack-ALBO and SCBO perform the least efficiently, with noticeable gaps from the global minimum. This deficiency is due to their high probability (nearly 50%) of getting trapped in some local minimizers. Panel (b) of Figure 2 and the upper panel of Table 1 compare the distributions of the BFOVs at the final evaluation of the competing methods. The inter-quantile range (IQR) of the BFOVs of EPBO is as small as 7×10^{-6}. However, the IQRs of EIC, ALBO, and BM are 4.25×10^{-4}, 2.28×10^{-4}, and 1.35×10^{-4}, respectively. Such over 20 times reduction by EPBO reveals the great improvement in robustness against variation in the initial design. On the other hand, it takes the LHD-based random search method 10,000 points to achieve the comparable BFOVs obtained by EIC in 120 points, which is slightly inferior to EPBO. Supplement SM§4 further explains the distinctive behaviors of EPBO, AE, Slack-ALBO, and SCBO by using a graphical presentation of the distribution of design points in a single run.

The second synthetic test problem is the modified Townsend problem (MTP) from Pourmohamad and Lee (2022). It faces similar challenges as the HSQ problem. One notable difference is that, for this problem, the global optimum point of MTP is situated precisely on the boundary of the constraint.

The comparison results in Figure 3 show that EPBO outperforms other comparators in terms of both convergence and robustness. On average, all methods, except Slack-ALBO and SCBO, converge to the global optimum after 120 iterations, with EPBO being the fastest. AE converges the second fastest, as the optimum point is located along the constraint boundary. Slack-ALBO and SCBO have 80% and 20% chances, respectively, of getting stuck in some local minimizers, as told from the boxplots in Panel (b). The IQR of the BFOVs of EPBO at the final evaluation is 0.22×10^{-2} in contrast to the much larger values of 2.03×10^{-2}, 1.59×10^{-2}, 1.24×10^{-2}, and 0.79×10^{-2} by BM, EIC, AE, and ALBO, respectively (the lower panel of Table 1). This result echos the superiority of EPBO in robustness against initial designs. And the finding of the advantage of the CBO methods over random search is consistent with that in HSQ.

4.1.2 Mixed Constrained Problem

Consider the mixed constrained problem studied in Picheny et al. (2016) with one inequality and two equality constraints. The objective function is a centered and rescaled version of the "Goldstein-Price" function (Picheny et al., 2013). The inequality constraint is the sinusoidal constraint from the HSQ problem introduced in Section 4.1.1. The first equality constraint is a centered "Branin" function (Picheny et al., 2013), and the second equality constraint is taken from Parr et al. (2012). We refer to it as the GSBP problem. (More details can be found in the `demo("GSBP")` of the `laGP` package of R.)

As the EIC, AE, BM, and SCBO methods are not inherently compatible with the equality constraints, we replace the equality constraint $h(\boldsymbol{x}) = 0$ with two inequality constraints simultaneously, i.e., $h(\boldsymbol{x}) \leqslant \varepsilon$ and $h(\boldsymbol{x}) \geqslant \varepsilon$, where the tolerance parameter ε controls the closeness

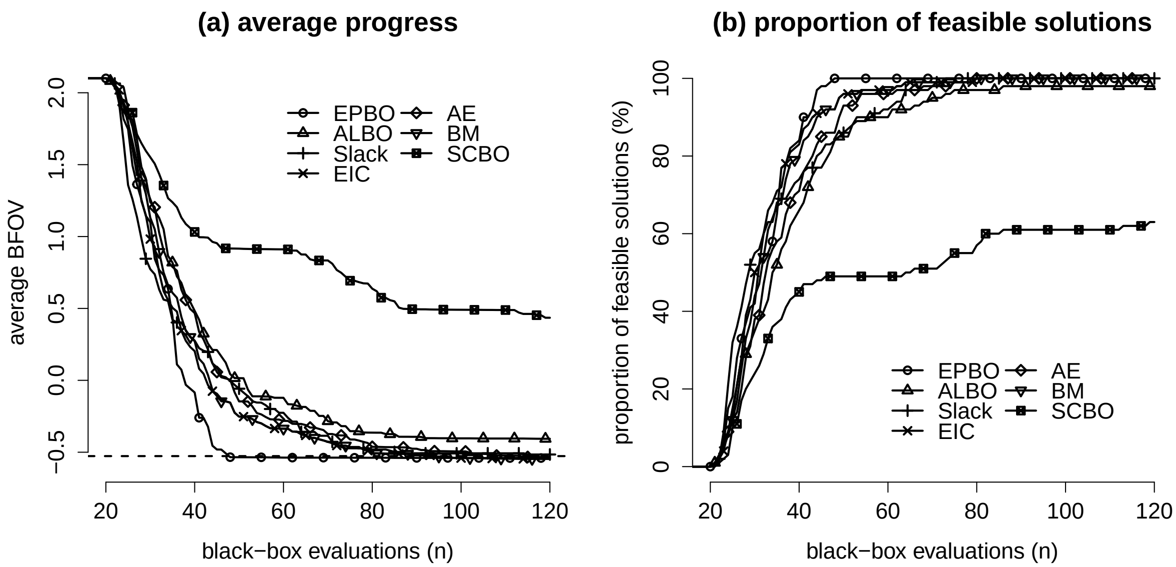

Figure 4: Comparison results over iterations for the GSBP problem under tolerance $\varepsilon = 0.01$. (a) average progress of BFOVs, where the horizontal dashed line indicates the value of the global optimum and (b) proportions of feasible solutions.

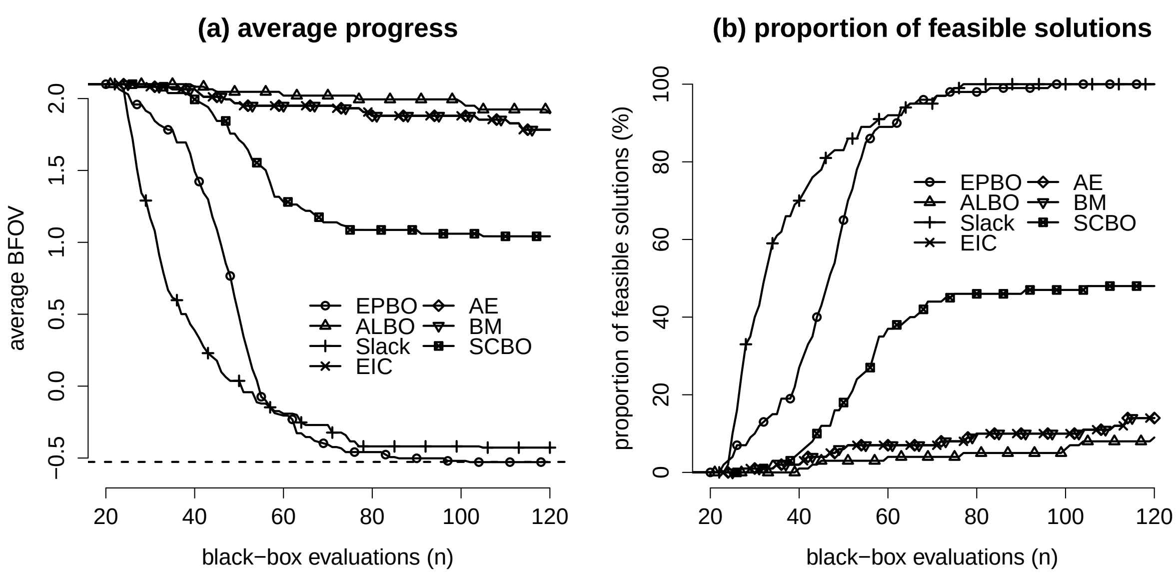

Figure 5: Comparison results over iterations for the GSBP problem under $\varepsilon = 0.001$ with the same captions as in Figure 4.

of the approximation to the equality constraint.

Figures 4 and 5 compare the seven methods in terms of the average BFOV and the proportion of finding feasible solutions under tolerance levels of 0.01 and 0.001, respectively. It is seen that EPBO performs the best in both metrics. The distinction of performances across methods is

Table 2: Proportions (in %) of finding global, local, and infeasible solutions obtained by the seven competing methods over 100 replications for the GSBP problem.

ε	method	solution		
		global	local	infeasible
0.01	SCBO	59	4	37
	ALBO	86	12	2
	AE	97	3	0
	BM	98	2	0
	EIC	98	2	0
	Slack-ABLO	96	4	0
	EPBO	100	0	0
0.001	ALBO	5	4	91
	AE	8	6	86
	BM	8	6	86
	EIC	8	6	86
	SCBO	24	24	52
	Slack-ALBO	88	12	0
	EPBO	100	0	0

more pronounced under the tolerance level of 0.001, i.e. closer to the equality constraint. SCBO does not perform well in this example primarily because none of the initial designs provide any feasible solution in the disjoint feasible regions. (SCBO aims to reduce the sum of constraint violations in the trust region alone before finding a feasible solution. It heavily relies on the initial design, though it is less dependent on the tolerance level.) In contrast, EPBO, ALBO, and Slack-ALBO strive to reduce the sum of constraint violations and objective function in the full search space, regardless of whether a feasible solution is found. Nevertheless, ALBO needs to evaluate the acquisition function numerically via Monte Carlo integration. On the other hand, the random search method needs approximately 10,000 and 90,000 points to discover a feasible solution under tolerance levels of 0.01 and 0.001, respectively. However, EPBO accomplishes this by using just 50 and 100 design points, respectively.

In addition, Table 2 reports the percentages of finding global, local, and infeasible solutions by the competing methods. EPBO demonstrates its superior performance (with a 100% success rate) in finding the global optimum. When the approximation to the equality constraint gets closer ($\varepsilon = 0.001$), the percentages of finding local or infeasible solutions rise dramatically for the other methods. This is attributed to the fact that, as the tolerance level strengthens, the softened feasible region shrinks quickly, making it more challenging to find a feasible solution.

4.2 Real-world Engineering Design Problems

We now compare the competing methods on two real-world engineering design problems. It is noted that these real-world problems involve higher dimensions than those in the synthetic test problems.

4.2.1 Nucleophilic Aromatic Substitution Reaction Problem

Our motivating example, the nucleophilic aromatic substitution reaction (SnAr) problem, is a virtual benchmark developed by Felton et al. (2021) based on Hone's kinetic model (Hone et al., 2017). The SnAr benchmark is a commonly used reaction in the fine chemical industry, involving the reaction between difluoronitrobenzene 1 and pyrrolidine 2 to produce one desired product and two undesired side-products. The reaction is carried out in a virtual flow reactor. The goal is to maximize the space-time yield $f(\boldsymbol{x})$, the mass of product formed per unit residence time, under an acceptable E-factor $g(\boldsymbol{x})$, defined as the ratio of product formed to waste produced, i.e.,

$$\min_{\boldsymbol{x} \in \mathcal{B}} \ -f(\boldsymbol{x}) \quad \text{s.t.} \quad g(\boldsymbol{x}) - 10 \leqslant 0.$$

The search space $\mathcal{B}$ involves four decision variables, corresponding to the reaction conditions: residence time ($x_1 \in [0.5, 2]$ minutes), equivalents of pyrrolidine ($x_2 \in [1, 5]$), concentration of difluoronitrobenzene ($x_3 \in [0.1, 0.5]$ M), and temperature ($x_4 \in [30, 120]$ °C).

We use the BFOV (-11376) obtained by the LHD-based random search with one million points as a reference. Figure 6 compares the performance of EPBO and the other six methods in terms of the average progress of BFOV and the boxplot of BFOV at the final evaluation over iterations. Overall, EPBO outperforms the others in both indices, showing superiority in convergence speed and robustness against the variation of initial designs. In particular, panel (a) shows that EPBO and the close runner-up SCBO need only 50 design points to achieve the reference BFOV. Their average BFOVs at the final evaluation after 150 iterations are -11560 and -11501, respectively, which are even smaller than the reference BFOV. AE, EIC, and ALBO also achieve the same level of BFOV approximately. Both Slack-ALBO and BM show slow descending in BFOV and retain remarkable gaps from the reference BFOV till the budget is exhausted. Panel (b) shows the boxplots of the BFOVs at the final evaluation. The IQR of BFOVs of EPBO is the smallest at 0.35, which is less than one percent of that (58.41) of the second best SCBO. Such substantial improvement in the robustness of EPBO over the other methods is because EPBO utilizes a random candidate grid for the acquisition function, enhanced by L-BFGS-B search (as described at the end of Section 3.2).

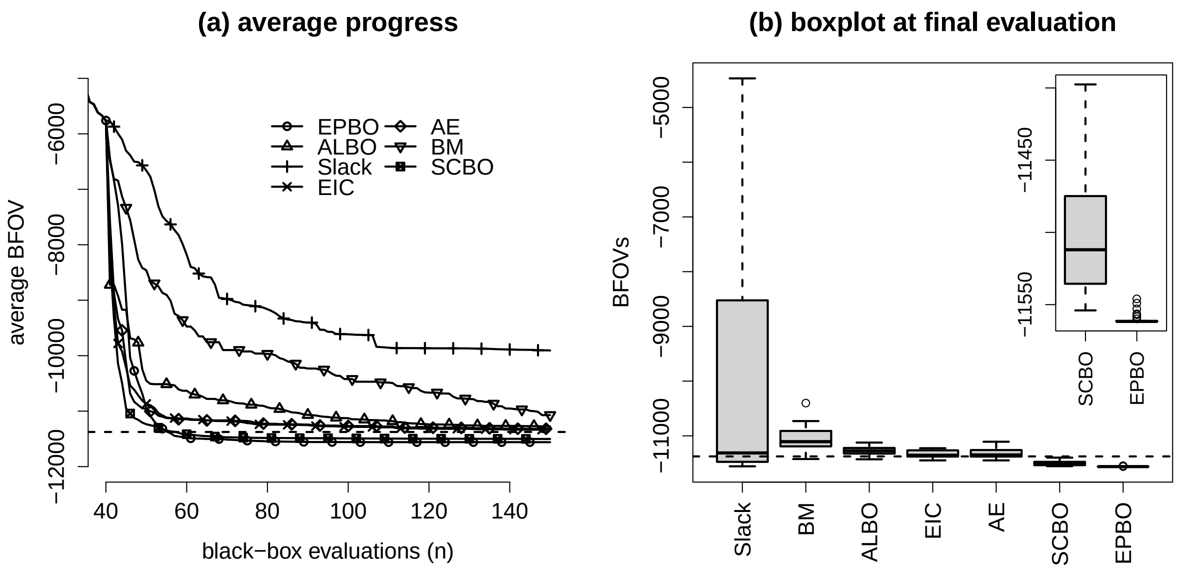

Figure 6: Comparison results over iterations for the SnAr problem. (a) average progress of BFOVs, where the horizontal dashed line indicates the reference BFOV, and (b) boxplots of the BFOVs at the final evaluation, where the sub-window displays the boxplots of SCBO and EPBO in a refined scale.

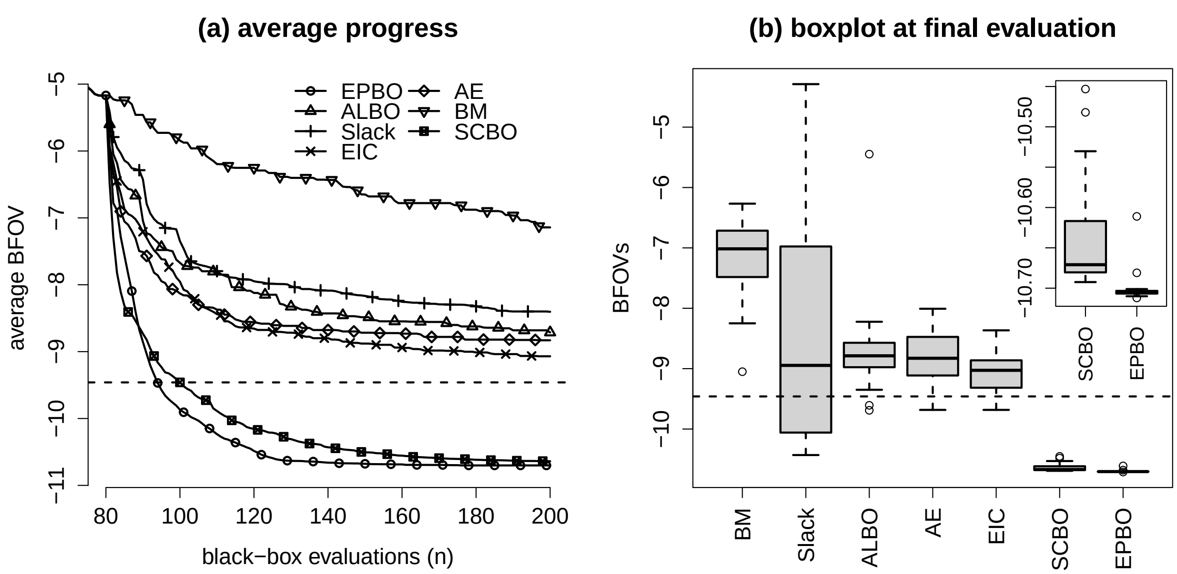

Figure 7: Comparison results over iterations for the Sprinkler problem with the same captions as in Figure 6.

4.2.2 Constrained Sprinkler Computer Model

The garden sprinkler computer model is a classical multi-objective engineering optimization problem. It was initially investigated by Siebertz et al. (2010) and later adapted to a black-box computer model in the framework of constrained optimization by Pourmohamad and Lee (2021). The problem aims to maximize the range of the garden sprinkler $f(\boldsymbol{x})$ while adhering to the constraint that the water consumption $g(\boldsymbol{x})$ does not exceed five, i.e.,

$$\min_{\boldsymbol{x}\in\mathcal{B}} \; -f(\boldsymbol{x}) \quad \text{s.t.} \quad g(\boldsymbol{x}) - 5 \leqslant 0.$$

The search space $\mathcal{B}$ involves eight decision variables: vertical ($x_1 \in [0, 90]^\circ$) and tangential ($x_2 \in [0, 90]^\circ$) nozzle angles, nozzle profile ($x_3 \in [2\text{e-}6, 4\text{e-}6]\text{m}^2$), diameter of the sprinkler head ($x_4 \in [0.1, 0.2]$mm), dynamic ($x_5 \in [0.01, 0.02]$Nm) and static ($x_6 \in [0.01, 0.02]$Nm/s) friction moments, entrance pressure ($x_7 \in [1, 2]$bar), and diameter of the flow line ($x_8 \in [5, 10]$mm). More details are available in the `CompModels` package in R (Pourmohamad, 2021). Pourmohamad and Lee (2021) showed that the reference BFOV of the random search with one million design points is -9.46.

Figure 7 shows similar comparison results of the seven methods as in Figure 6 for the SnAr problem. EPBO and SCBO outstand themselves by quickly reaching the reference BFOV in about 95 and 100 design points, respectively. The average BFOVs of EPBO and SCBO at the final evaluation are -10.70 and -10.64, respectively, much smaller than the reported BFOV (-9.46). In contrast, BM, Slack-ALBO, ALBO, AE, and EIC exhibit noticeable gaps from the reference BFOV till the budget is exhausted. The magnified window in Panel (b) shows that the IQR of BFOVs of EPBO (0.0029) is significantly smaller than that (0.0634) of the runner-up SCBO. Such superiority in robustness is consistent with what is seen in the SnAr example.

5 Discussion

We propose a novel hybrid optimization method, called exact penalty Bayesian optimization (EPBO), to tackle constrained optimization problems featuring expensive black-box objective and constraints. We integrate (unconstrained) BO into the exact penalty framework to effectively balance global exploration, local exploitation, and feasibility of design points. By expressing the surrogate model of the exact penalty function as a weighted sum of GPs, EPBO enjoys the closed-form acquisition functions, which significantly save computational cost while enhancing convergence speed and solution quality. EPBO not only handles the case involving inequality constraints alone but also naturally accommodates mixed (inequality and/or equality) constraints.

While the squared exponential kernel is used as the default, we show in Supplement SM§6.1 that the proposed EPBO is insensitive to the choice of kernel. We also demonstrate that EPBO can start at infeasible points and is robust to variation in the size of initial design in Supplement SM§6.2. The latter offers great convenience when the budget of initial design (based on a space-filling design) is limited.

Through a series of test problems, EPBO exhibits its superiority over popular competitors in convergence speed and solution quality. To further examine the performance of EPBO, we make comparisons on additional test problems involving (i) disjoint feasible regions, (ii) challenges in estimating global GP surrogate models, and (iii) high dimensionality. For the sake of space, we present the results in Supplement SM§7. It is found that EPBO shows consistent superiority for problems (i) and (ii) and great promise when combined with other strategies, such as the trust region strategy, for the problem (iii). As our test problems are far from exhaustive, more investigation of the theoretical properties of EPBO is needed. In summary, we recommend EPBO for general CBO problems of low dimension, particularly when local minima are highly deceptive, such as the HSQ and MTP problems.

On the other hand, we believe there is still room for improvement for EPBO. Firstly, EPBO requires a joint evaluation of the objective function and constraints at a candidate point in each step. However, the objective function and the constraints can be evaluated independently for a wide class of problems known as "decoupled" problems (Hernández-Lobato et al., 2016; Ariafar et al., 2019). This can be particularly effective in situations where some black-box functions are significantly more complicated than others. Handling the expensive black-box optimization problem with mixed constraints in a decoupled manner is worth investigating. Secondly, developing hybrid optimization methods in the presence of measurement noise is another avenue for future research, especially when the noise level is comparable to the magnitude of the objective and/or constraints (Letham et al., 2019). Thirdly, we note that statistical models in hybrid optimization methods offer a global search for solutions to constrained optimization problems. However, the convergence behavior of hybrid optimization methods, including EPBO, is still an open problem (Pourmohamad and Lee, 2022). Understanding and improving the convergence properties of hybrid optimization techniques represent an important aspect of future research efforts. Lastly, while Supplement SM§7 offers insights into the potential of EPBO when combined with the trust region strategy in high-dimensional constrained problems, more algorithmic development and empirical comparisons are needed to fully explore and harness this potential.

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Supplementary Materials

1 A supplementary document contains (i) the prediction performance of the proposed novel surrogate model for the equality constraint violation, (ii) the implementation details for comparators, (iii) the visualizations and mathematical definitions of the synthetic test problems, (iv) the distributional behaviors of design points obtained by various methods in a single run, (v) an examination of the discrepancy between the closed-form and the Monte Carlo ScaledEI acquisition function, (vi) the sensitivity analysis of EPBO concerning the choice of kernel function and the size of the initial design, and (vii) the additional empirical comparisons and discussions regarding various real-world challenges. (.pdf file)

2 An R-package, called `EPBO`, implements the proposed EPBO method as well as the AE and BM methods. The R code, `generate_figure_4.R`, reproduces Figure 4. For detailed instructions, please refer to the README file provided in the base directory. (GNU zipped tar file)

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