A Survey of Surrogate Approaches for Expensive Constrained Black-Box Optimization

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Abstract. Numerous practical optimization problems involve black-box functions whose values come from computationally expensive simulations. For these problems, one can use surrogates that approximate the expensive objective and constraint functions. This paper presents a survey of surrogate-based or surrogate-assisted methods for computationally expensive constrained global optimization problems. The methods can be classified by type of surrogate used (e.g., kriging or radial basis function) or by the type of infill strategy. This survey also mentions algorithms that can be parallelized and that can handle infeasible initial points and high-dimensional problems.

Keywords: Global optimization · Black-box optimization · Constraints · Surrogates · Kriging · Radial basis functions

1 Introduction

Many engineering optimization problems involve black-box objective or constraint functions whose values are obtained from computationally expensive finite element (FE) or computational fluid dynamics (CFD) simulations. Moreover, for some of these problems, the calculation of the objective or constraint functions might fail at certain inputs, indicating the presence of hidden constraints. For such optimization problems, a natural approach involves using surrogate models that approximate the expensive objective or constraint functions. Commonly used surrogates include kriging or Gaussian process models and Radial Basis Function (RBF) models. In the literature, various strategies for selecting sample points where the objective and constraint functions are evaluated (also known as *infill strategies*) have been proposed, including those for problems with expensive black-box constraints and cheap explicitly defined constraints.

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This paper provides a survey of approaches for computationally expensive constrained optimization problems of the following general form:

$$\begin{aligned} &\min\ f(x) \\ \text{s.t.}\quad & x \in \mathbb{R}^d,\ \ell \le x \le u \\ & g_i(x) \le 0,\ i = 1, \ldots, m \\ & h_j(x) = 0,\ j = 1, \ldots, p \\ & x \in \mathcal{X} \subseteq \mathbb{R}^d \end{aligned} \tag{1}$$

where $\ell, u \in \mathbb{R}^d$, $m \ge 0$, $p \ge 0$, at least one of the objective or constraint functions $f, g_1, \ldots, g_m, h_1, \ldots, h_p$ is black-box and computationally expensive, and $\mathcal{X} \subseteq \mathbb{R}^d$ is meant to capture the region where hidden constraints are not violated. Here, we allow for the possibility that $m = 0$ or $p = 0$ (no inequality or no equality constraints or both). Also, we allow $\mathcal{X} = \mathbb{R}^d$ (no hidden constraints). In general, hidden constraints cannot be relaxed (i.e., *hard constraints*) while the above inequality and equality constraints can be relaxed (i.e., *soft constraints*). Note that in a practical problem, there might be a mixture of expensive black-box constraints and cheap explicitly defined constraints. It is also possible that the objective may be cheap to evaluate and only some (or all) of the constraints are black-box and expensive. These problems are referred to *grey-box* models [7]. Most of the algorithms discussed here are meant for problems with expensive objective and inequality constraint functions (no equality and hidden constraints).

Define the vector-valued functions $G(x) := (g_1(x), \ldots, g_m(x))$ and $H(x) := (h_1(x), \ldots, h_p(x))$, and let $[\ell, u] := \{x \in \mathbb{R}^d : \ell \le x \le u\}$, and let $\mathcal{D} := \{x \in [\ell, u] \cap \mathcal{X} : G(x) \le 0,\ H(x) = 0\}$ be the feasible region of (1). Here, $[\ell, u] \subseteq \mathbb{R}^d$ is the *search space* of problem (1), and one *simulation* for a given input $x \in [\ell, u] \cap \mathcal{X}$ yields the values of $f(x)$, $G(x)$ and $H(x)$. In the computationally expensive setting, one wishes to find the global minimum of (1) (or at least a feasible solution with good objective function value) given a relatively limited number of simulations. If $\mathcal{D} \ne \emptyset$, f, $g_1, \ldots, g_m$, $h_1, \ldots, h_p$ are all continuous functions on $[\ell, u]$ and $\mathcal{X} = \mathbb{R}^d$ (or $\mathcal{X}$ contains the region defined by all the constraints), then $\mathcal{D}$ is a compact set and f is guaranteed to have a global minimizer in $\mathcal{D}$. Now some of the black-box objective and constraint functions may not be continuous in practice, but it is helpful to consider situations when a global minimizer is guaranteed to exist.

This paper is organized as follows. Section 2 provides the general structure of surrogate methods for constrained optimization. Section 3 provides two widely used surrogates, Radial Basis Functions and Kriging. Section 4 discusses some of the infill strategies for constrained optimization. An *infill strategy* is a way to select sample points for function evaluations. Finally, Sect. 5 provides a summary and some future directions for surrogate-based constrained optimization.

2 General Structure of Surrogate Methods for Constrained Optimization

Surrogate-based methods for expensive black-box optimization generally follow the same structure. There is an *initialization phase* where the objective and constraint functions are evaluated at initial points, typically from a space-filling design such as a Latin hypercube design. After the initial sample points are obtained, the initial surrogates are built. Here, a *sample point* refers to a point in the search space (i.e., $x \in [\ell, u]$) where the objective and constraint function values ($f(x)$, $G(x)$ and $H(x)$) are known. Depending on the type of method, the surrogates may be *global surrogates* in the sense that all sample points are used or *local surrogates* in that only a subset of sample points are used.

After initialization, the method enters a *sampling phase* where the surrogates and possibly additional information from previous sample points are used to select one or more new points where the simulations will take place. The sampling phase is typically where various algorithms differ. Some methods solve optimization subproblems to determine new points while others select points from a randomly generated set of points, where the probability distribution is chosen in a way that makes it more likely to generate feasible points with good objective function values.

After the sampling phase, simulations are run on the chosen point(s), yielding new data points. The surrogates are then updated with the new information obtained and the process iterates until some termination condition is satisfied. In practice, the method usually terminates when the computational budget, in terms of maximum number of simulations allowed, is reached.

In the case of constrained black-box optimization, one major consideration is finding feasible sample points to begin with. For problems where the feasible region is relatively small in relation to the search space, it is not easy to obtain a feasible initial point by uniform random sampling. In this situation, part of the iterations could be devoted first to finding a good feasible point and then the remaining iterations are used to improve on this feasible point.

3 Surrogates for Constrained Black-Box Optimization

3.1 Radial Basis Function Model

The Radial Basis Function (RBF) interpolation model described in Powell [17] has been successfully used in various surrogate-based methods for constrained optimization, including some that can handle high-dimensional problems with hundreds of decision variables and many black-box inequality constraints [18–20]. Below we describe the procedure for building this RBF model.

Let $u(x)$ be the objective function or one of the constraint functions g_i or h_j for some i or j. Given n distinct sample points $(x_1, u(x_1)), \ldots, (x_n, u(x_n)) \in R^d \times \mathbb{R}$, we use an interpolant of the form

$$s_n(x) = \sum_{i=1}^{n} \lambda_i \phi(\|x - x_i\|) + p(x), \; x \in \mathbb{R}^d. \tag{2}$$

Here, $\|\cdot\|$ is the Euclidean norm, $\lambda_i \in \mathbb{R}$ for $i = 1, \ldots, n$ and $p(x)$ is a polynomial in d variables. In some surrogate-based methods ϕ has the *cubic* form ($\phi(r) = r^3$) and $p(x)$ is a linear polynomial. Other possible choices for ϕ include the thin plate spline, multiquadric and Gaussian forms (see [17]).

To build the above RBF model in the case where the tail $p(x)$ is a linear polynomial, define the matrix $\Phi \in \mathbb{R}^{n\times n}$ by: $\Phi_{ij} := \phi(\|x_i - x_j\|), \quad i, j = 1, \ldots, n$. Also, define the matrix $P \in \mathbb{R}^{n\times(d+1)}$ whose i^{th} row is $[1, x_i^T]$. Now, the RBF model that interpolates the sample points $(x_1, u(x_1)), \ldots, (x_n, u(x_n))$ is obtained by solving the linear system

$$\begin{pmatrix} \Phi & P \\ P^T & 0_{(d+1)\times(d+1)} \end{pmatrix} \begin{pmatrix} \lambda \\ c \end{pmatrix} = \begin{pmatrix} U \\ 0_{d+1} \end{pmatrix}, \tag{3}$$

where $0_{(d+1)\times(d+1)} \in \mathbb{R}^{(d+1)\times(d+1)}$ is a matrix of zeros, $U = (u(x_1), \ldots, u(x_n))^T$, $0_{d+1} \in \mathbb{R}^{d+1}$ is a vector of zeros, $\lambda = (\lambda_1, \ldots, \lambda_n)^T \in \mathbb{R}^n$ and $c = (c_0, c_1, \ldots, c_d)^T \in \mathbb{R}^{d+1}$ consists of the coefficients for the linear function $p(x)$. The coefficient matrix in (3) is nonsingular if and only if $\text{rank}(P) = d + 1$ (Powell [17]). This condition is equivalent to having a subset of $d + 1$ affinely independent points among the points $\{x_1, \ldots, x_n\}$.

3.2 Kriging Model

A widely used kriging surrogate model is described in Jones et al. [13] and Jones [12] (sometimes called the DACE model) where the values of the black-box function f are assumed to be the outcomes of a stochastic process. That is, before f is evaluated at any point, assume that $f(x)$ is a realization of a Gaussian random variable $Y(x) \sim N(\mu, \sigma^2)$. Moreover, for any two points x_i and x_j, the correlation between $Y(x_i)$ and $Y(x_j)$ is modeled by

$$Corr[Y(x_i), Y(x_j)] = \exp\left(-\sum_{\ell=1}^{d} \theta_\ell |x_{i\ell} - x_{j\ell}|^{p_\ell}\right), \tag{4}$$

where $\theta_\ell, p_\ell (\ell = 1, \ldots, d)$ are parameters to be determined. This correlation model is only one of many types of correlation functions that can be used in kriging metamodels. Note that when x_i and x_j are close, $Y(x_i)$ and $Y(x_j)$ will be highly correlated according to this model. As x_i and x_j become farther apart, the correlation drops to 0.

Given n points $x_1, \ldots, x_n \in \mathbb{R}^d$, the uncertainty about the values of f at these points can be modeled by using the random vector $Y = (Y(x_1), \ldots, Y(x_n))^T$. Note that $E(Y) = J\mu$, where J is the $n\times 1$ vector of all ones, and $\text{Cov}(Y) = \sigma^2 R$, where R is the $n \times n$ matrix whose (i, j) entry is given by (4).

Suppose the function f has been evaluated at the points $x_1, \ldots, x_n \in \mathbb{R}^d$. Let $y_1 = f(x_1), \ldots, y_n = f(x_n)$ and let $y = (y_1, \ldots, y_n)^T$ be the vector of observed function values. Fitting the kriging model in [12] through the data points $(x_1, y_1), \ldots, (x_n, y_n)$ involves finding the maximum likelihood estimates

(MLEs) of the parameters $\mu, \sigma^2, \theta_1, \ldots, \theta_d, p_1, \ldots, p_d$. The MLEs of these parameters are typically obtained by solving a numerical optimization problem. Now the value of the kriging predictor at a new point x^* is provided by the formula [12]

$$\widehat{y}(x^*) = \widehat{\mu} + r^T R^{-1}(y - J\widehat{\mu}), \tag{5}$$

where $\widehat{\mu} = \dfrac{J^T R^{-1} y}{J^T R^{-1} J}$ and $r = (\mathrm{Corr}[Y(x^*), Y(x_1)], \ldots, \mathrm{Corr}[Y(x^*), Y(x_n)])^T$. Moreover, a measure of error of the kriging predictor at x^* is given by

$$s^2(x) = \widehat{\sigma}^2 \left[1 - r^T R^{-1} r + \frac{(1 - r^T R^{-1} r)^2}{J^T R^{-1} J} \right], \tag{6}$$

where $\widehat{\sigma}^2 = \frac{1}{n}(y - J\widehat{\mu})^T R^{-1}(y - J\widehat{\mu})$.

4 Infill Strategies for Constrained Optimization

4.1 Radial Basis Function Methods

One effective infill strategy for problems with expensive black-box objective and inequality constraints (no equality constraints and no hidden constraints) is provided by the COBRA algorithm [19]. COBRA uses the above RBF model to approximate the objective and constraint functions though one can use other types of surrogates with its infill strategy. It treats each inequality constraint individually instead of combining them into a penalty function and builds/updates RBF surrogates for the objective and constraints in each iteration. Moreover, it handles infeasible initial sample points using a two-phase approach where Phase I finds a feasible point while Phase II improves on this feasible point. In Phase I, the next iterate is a minimizer of the sum of the squares of the predicted constraint violations (as predicted by the RBF surrogates) subject only to the bound constraints. In Phase II, the next iterate is a minimizer of the RBF surrogate of the objective subject to RBF surrogates of the inequality constraints within some small margin and also satisfying a distance requirement from previous iterates. That is, the next iterate x_{n+1} solves the optimization subproblem:

$$\begin{array}{c} \min_x \ s_n^{(0)}(x) \\ \text{s.t.} \quad x \in \mathbb{R}^d, \ \ell \le x \le u \\ s_n^{(i)}(x) + \epsilon_n^{(i)} \le 0, \ i = 1, 2, \ldots, m \\ \|x - x_j\| \ge \rho_n, \ j = 1, \ldots, n \end{array} \tag{7}$$

Here, $s_n^{(0)}(x)$ is the RBF model of $f(x)$ while $s_n^{(i)}(x)$ is the RBF model of $g_i(x)$ for $i = 1, \ldots, m$. Moreover, $\epsilon_n^{(i)} > 0$ is the margin for the ith constraint and ρ_n is the distance requirement given the first n sample points. The margins are meant to facilitate the generation of feasible iterates. The ρ_n's are allowed to cycle from large values meant to enforce global search and small values that promote local search. In the original implementation, the optimization subproblem in (7) is solved using Matlab's gradient-based *fmincon* solver from a good starting point obtained by a global search scheme, but one can also combine this with a multistart approach. COBRA performed well compared to alternatives on 20 test problems and on the large-scale 124-D MOPTA08 benchmark with 68 black-box inequality constraints [11].

One issue with COBRA [19] observed by Koch et al. [14] is that sometimes the solution returned by the solver for the subproblem is infeasible. Hence, they developed a variant called COBRA-R [14] that incorporates a repair mechanism that guides slightly infeasible points to the feasible region (with respect to the RBF constraints). Moreover, another issue with COBRA is that its performance can be sensitive to the choice of the distance requirement cycle (DRC) that specifies the ρ_n's in (7). To address this, Bagheri et al. [3] developed SACOBRA (Self-Adjusting COBRA), which includes an automatic DRC adjustment and selects appropriate ρ_n values based on the information obtained after initialization. In addition, SACOBRA re-scales the search space to $[-1, 1]^d$, performs a logarithmic transformation on the objective function, if necessary, and normalizes the constraint function values. Numerical experiments in [3] showed that SACOBRA outperforms COBRA with different fixed parameter settings.

An alternative to COBRA [19] is the ConstrLMSRBF algorithm [18], which also uses RBF models of the objective and constraint functions though one can also use other types of surrogates. ConstrLMSRBF is a heuristic that selects sample points from a set of randomly generated candidate points, typically from a Gaussian distribution centered at the current best point. In each iteration, the sample point is chosen to be the best candidate point according to two criteria (predicted objective function value and minimum distance from previous sample points) from among the candidate points with the minimum number of predicted constraint violations. When it was first introduced at ISMP 2009, ConstrLMSRBF was the best known algorithm for the MOPTA08 problem [11].

The original ConstrLMSRBF [18] assumes that there is a feasible point among the initial points. Extended ConstrLMSRBF [19] was developed to deal with infeasible initial points by following a similar two-phase structure as COBRA [19] where Phase I searches for a feasible point while Phase II improves the feasible point found. In Phase I of Extended ConstrLMSRBF, the next sample point is the one with the minimum number of predicted constraint violations among the candidate points, with ties being broken by using the maximum predicted constraint violation as an additional criterion.

Another way to generate infill points for constrained optimization using RBF surrogates is to use the CONORBIT trust region approach [23], which is an extension of the ORBIT algorithm [27]. CONORBIT uses only a subset of previous sample points that are close to current trust region center to build RBF models for the objective and constraint functions. In a typical iteration, the next sample point is obtained by minimizing the RBF model of the objective subject to RBF models of the constraints within the current trust region. As with COBRA [19], it uses a small margin for the RBF constraints.

4.2 Kriging-Based Methods

The most popular kriging-based infill strategy is the *expected improvement* criterion [25] that forms the basis of the original Efficient Global Optimization (EGO) method [9,13] for bound-constrained problems. Here, we use the notation from Sect. 3.2. In this strategy, the next sample point is the point x that maximizes the *expected improvement* function $\mathrm{EI}(x)$ over the search space where

$$\mathrm{EI}(x) = (f_{min} - \widehat{y}(x))\Phi\left(\frac{f_{min} - \widehat{y}(x)}{s(x)}\right) + s(x)\phi\left(\frac{f_{min} - \widehat{y}(x)}{s(x)}\right), \quad (8)$$

if $s(x) > 0$ and $\mathrm{EI}(x) = 0$ if $s(x) = 0$. Here, Φ and ϕ are the cdf and pdf of the standard normal distribution, respectively. Also, f_{min} is the current best objective function value. Extensions and modifications to the EI criterion include *generalized expected improvement* [25] and *weighted expected improvement* [26]. Moreover, alternatives to EI are given in [24], including the *WB2 (locating the regional extreme)* criterion, which maximizes $\mathrm{WB2}(x) = -\widehat{y}(x) + \mathrm{EI}(x)$. This attempts to minimize the kriging surrogate while also maximizing EI.

When the problem has black-box inequality constraints $g_i(x) \leq 0$, $i = 1, \dots, m$, we fit a kriging surrogate $\widehat{g}_i(x)$ for each $g_i(x)$. That is, for each i and a given x, assume that $g_i(x)$ is the realization of a Gaussian random variable $G_i(x) \sim N(\mu_{g_i}, \sigma^2_{g_i})$ where the parameters of this distribution are estimated by maximum likelihood as in Sect. 3.2. A standard way to handle these inequality constraints is to find the sample point x that maximizes a *penalized expected improvement* function obtained by multiplying the EI with the probability that x will be feasible (assuming the $G_i(x)$'s are independent) [25]:

$$\mathrm{EI}_p(x) = \mathrm{EI}(x) \prod_{i=1}^{m} P(G_i(x) \leq 0) = \mathrm{EI}(x) \prod_{i=1}^{m} \Phi\left(\frac{-\widehat{\mu}_{g_i}}{\widehat{\sigma}_{g_i}}\right), \quad (9)$$

where $\widehat{\mu}_{g_i}$ and $\widehat{\sigma}^2_{g_i}$ are the MLEs of the parameters of the random variable $G_i(x)$ and where f_{min} for the EI in (8) is the objective function value of the current best feasible solution (or the point closest to being feasible if no feasible points are available yet) [16].

Sasena et al. [24], Parr et al. [16], Basudhar et al. [4] and Bagheri et al. [2] presented extensions of EGO for constrained optimization. Moreover, Bouhlel et al. [6] developed SEGOKPLS+K, which is an extension of SuperEGO [24] for constrained high-dimensional problems by using the KPLS+K (Kriging with Partial Least Squares) model [5]. SEGOKPLS+K uses the WB2 (locating the regional extreme) criterion described above where the surrogate is minimized while also maximizing the EI criterion. Moreover, it replaces the kriging models by the KPLS(+K) models, which are more suitable for high-dimensional problems.

4.3 Surrogate-Assisted Methods for Constrained Optimization

An alternative approach for constrained expensive black-box optimization is to use surrogates to accelerate or enhance an existing method, typically a metaheuristic. We refer to these as *surrogate-assisted methods*. For example, CEP-RBF [20] is a Constrained Evolutionary Programming (EP) algorithm that is assisted by RBF surrogates. Recall that in a standard Constrained $(\mu + \mu)$-EP, each parent generates one offspring using only mutations (typically from a Gaussian or Cauchy distribution) and does not perform any recombination. Moreover, the offspring are compared using standard rules such as: between two feasible solutions, the one with the better objective function value wins; or a between a feasible solution and an infeasible solution, the feasible solution wins; and between two infeasible solutions, the one with the smaller constraint violation (according to some metric) wins. In each generation of CEP-RBF, a large number of trial offspring are generated by each parent. Then, RBF surrogates are used to identify the most promising among these trial offspring for each parent, and this becomes the sample point where the simulation will take place. Here, a *promising* trial offspring is the one with the best predicted objective function value from among those with the minimum number of predicted constraint violations. Once the simulation is performed and the objective and constraint function values are known, the selection of the new parent population proceeds as in a regular Constrained EP and the process iterates.

Another surrogate-assisted metaheuristic is the CONOPUS (CONstrained Optimization by Particle swarm Using Surrogates) framework [21]. In each iteration of CONOPUS, multiple trial positions for each particle in the swarm are generated, and surrogates for the objective and constraint functions are used to identify the most promising trial position where the simulations are performed. Moreover, it includes a refinement step where the current overall best position is replaced by the minimum of the surrogate of the objective within a neighborhood of that position and subject to surrogate inequality constraints with a small margin and with a distance requirement from all previous sample points.

In addition, one can also use surrogates to assist provably convergent algorithms. For example, quadratic models have been used in the direct search method NOMAD [8]. Moreover, CARS-RBF [15] is an RBF-assisted version of Constrained Accelerated Random Search (CARS), which extends the Accelerated Random Search (ARS) algorithm [1] to constrained problems. In each iteration of CARS, a sample point is chosen uniformly within a box centered at the current best point. The initial size of the box is chosen so that it covers the search space. If the sample point is worse than the current best point, then the size of the box is reduced. Otherwise, if the sample point is an improvement over the current best point, then the size of the box is reset to the initial value so that the box again covers the search space. CARS [15] has been shown to converge to the global minimum almost surely. Further, it was shown numerically to converge faster than the constrained version of Pure Random Search on many test problems. In CARS-RBF, a large number of trial points is generated uniformly at random within the current box, and as before, RBF surrogates are used to identify the most promising among these trial points using the same criteria used by ConstrLMSRBF [18]. The simulations are then carried out at this promising trial point and the algorithm proceeds in the same manner as CARS.

4.4 Parallelization and Handling High Dimensions

To make it easier to find good solutions for computationally expensive problems, one can generate multiple sample points that can be evaluated in parallel in each iteration. Metaheuristics such as evolutionary and swarm algorithms are naturally parallel, and so, the surrogate-assisted CEP-RBF [20] and CONOPUS [21] algorithms are easy to parallelize. COBRA [19] and ConstrLMSRBF [18] can be parallelized using ideas in [22]. Moreover, parallel EGO approaches are described in [10,28] and these can be extended to constrained problems.

For high-dimensional problems, RBF methods have been shown to be effective (e.g., ConstrLMSRBF [18], COBRA [19], CEP-RBF [20] and CONOPUS-RBF [21]). The standard constrained EGO, however, has difficulties with in high dimensions because of the computational overhead and numerical issues with fitting the kriging model. To alleviate these issues, Bouhlel et al. [6] introduced SEGOKPLS+K, which can handle problems with about 50 decision variables.

5 Summary and Future Directions

This paper gave a brief survey of some of the surrogate-based and surrogate-assisted methods for constrained optimization. The methods discussed are based on RBF and kriging models, though other types of surrogates and ensembles may be used. Various infill strategies were discussed. Moreover, parallel surrogate-based methods and algorithms that can handle high-dimensional problems were mentioned. Possible future directions of research for constrained expensive black-box optimization would be to develop methods that can handle black-box equality constraints. Relatively few such methods have been developed and one approach is described in [3]. Another direction is to deal with hidden constraints. Finally, it is important to develop more methods that can be proved to converge to the global minimum, or at least to first order points.

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