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A complete expected improvement criterion for Gaussian process assisted highly constrained expensive optimization

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ABSTRACT

Expected improvement (EI) is a popular infill criterion in Gaussian process assisted optimization of expensive problems for determining which candidate solution is to be assessed using the expensive evaluation method. An EI criterion for constrained expensive optimization (constrained EI) has also been suggested, which requires that feasible solutions exist in the candidate solutions. However, the constrained EI criterion will fail to work in case there are no feasible solutions. To address the above issue, this paper proposes a new EI criterion for highly constrained optimization that can work properly even when no feasible solution is available in the current population. The proposed constrained EI criterion can not only exploit local feasible regions, but also explore infeasible yet promising regions, making it a complete constrained EI criterion. The complete constrained EI is theoretically validated and empirically verified. Simulation results demonstrate that the proposed complete constrained EI is better than or comparable to five existing infill criteria.

1. Introduction

Most of the science and engineering optimization problems in the real world are highly constrained. These constrained optimization problems (COPs) present serious challenges to existing optimization techniques. A general COP [36,46] can be defined as:

$$\begin{array}{ll} \min & y = f(\mathbf{x}) \\ \mathrm{st}: & \mathbf{l} \le \mathbf{g}(\mathbf{x}) = (g_1(\mathbf{x}), g_2(\mathbf{x}), \ldots, g_m(\mathbf{x})) \le \mathbf{u} \\ \mathrm{where} & \mathbf{l} = (l_1, l_2, \ldots, l_m), \mathbf{u} = (u_1, u_2, \ldots, u_m); \\ & \mathbf{x} = (x_1, x_2, \ldots, x_n) \in \mathbf{X} \\ & \mathbf{X} = \{\mathbf{x} | \mathbf{x_l} \le \mathbf{x} \le \mathbf{x_u}\} \\ & \mathbf{x_l} = (x_{l1}, x_{l2}, \ldots, x_{ln}), \mathbf{x_u} = (x_{u1}, x_{u2}, \ldots, x_{un}) \end{array} \tag{1}$$

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where $\mathbf{x}$ is a solution vector (solution for short) within the solution space $\mathbf{X}$, $\mathbf{g}(\mathbf{x})$ are constraints, $\mathbf{l}$ and $\mathbf{u}$ denote the lower and upper constraint bounds, respectively. If a solution $\mathbf{x} \in \mathbf{X}$ satisfies all constraints $\mathbf{g}(\mathbf{x})$, it is called a feasible solution; otherwise, it is called an infeasible solution.

Due to the inherent characteristics of gradient-free and insensitivity to the local optimal, evolutionary algorithms (EAs) are much preferable for various complex and non-convex optimization problems, including COPs. Constraint handling techniques based on EAs can be categorized as follows [30,47]: feasibility rules, stochastic ranking, ε constrained method, novel penalty functions, novel special operators, multi-objective concepts and ensemble of constraint-handling techniques.

Nevertheless, many engineering optimization problems require expensive computer simulations or physical experiments for evaluating candidate solutions, such as in wind turbine design [34], drug design [44], antenna design [18] and aerodynamic design [21]. Traditional EAs cannot directly solve them since a large number of function evaluations is unaffordable for this kind of problems. To address this issue, surrogate-assisted EAs (SAEAs) have been developed, where part of expensive fitness evaluations are replaced by computationally cheap approximate models often known as surrogates or meta-models. In the optimization process, computationally expensive fitness functions are replaced by some previously built surrogate models based on historical data, so that the cost of the time-consuming or resource-consuming fitness functions can be reduced.

The Gaussian process, also known as Kriging in traditional design optimization, is the most popular model when compared to others because of its ability to provide uncertainty estimation for the approximated values, and it has been increasingly employed as surrogates in evolutionary single and multi-objective optimization [2,32]. After building a GP model, how to manage the tradeoff between the accuracy and the uncertainty of surrogates is the main issue in GP-assisted EAs. Infill sampling criteria make use of the estimates of fitness and estimated uncertainty (also known as confidence level) to assess the value of a solution with respect to the optimality and uncertainty. If a point is expected to be promising according to an infill sampling criterion, it will be selected to be evaluated using the real expensive fitness function. Maximizing the expected improvement (EI) [22] is a widely-used sampling strategy used in selecting sample solutions for updating GP models. Using EI is advantageous since it is likely to be larger at unsampled areas or at under sampled areas near the global optimum and offers solutions with both exploration and exploitation of the GP model.

For expensive COPs, Schonlau [38] proposed a constrained EI by maximizing the multiplication of the EI and the probability feasibility (PF), which are both statistical measures determined by GP models of fitness and constraints. The constrained EI is based on the current best feasible solution. However, for highly constraint functions with small feasible regions, e.g., the well-known constrained benchmark test suite IEEE CEC2006 [26] consists of 24 problems, but 19 of them with the feasible ratio less than 1%, so using surrogates for these problems to obtain a feasible solution can be very challenging. When a feasible solution is not provided in the sampling data, the existing constrained EI no longer work, which means they are incomplete. To fill this gap, this study introduces a complete constrained EI as infill sampling criterion for efficiently dealing with computationally expensive COPs. The motivation of this paper is to adopt EI of constraint violation to reach feasible regions. The preliminary idea of the EI of constraint violation has presented in [19]. Note that in this paper, the objective and constraints are assumed mutually independent .

New contributions of the paper are summarized as follows:

(1) This paper is the first attempt to propose the idea that concentrating on EI of constraint violation to deal with highly constrained problems where no feasible solution is available in the sampling data for an expensive COP. Different from the maximization of the feasibility probability [3,15] in the case of no feasible point available, the proposed method adopts the EI of constraint violation as the metric for selecting a new potential solution. The level of constraint violation of a solution reflects the distance to the feasible space, hence it is often employed to handle the constraint difficulty. In addition, the maximum EI value enables the GP model to efficiently explore the optimum as well as improve the model accuracy in single-objective optimization [48]. Maximizing the EI of constraint violation will drive the search towards promising feasible regions.
(2) A suitable formulation of COP in Eq. (1) is suggested for the GP-assisted expensive optimization since the widely-used typical formulation is not suitable, since it needs to introduce additional constraints and dependencies among the objective and constraints. Handling the additional constraints and dependencies would cost additional computational resource, especially the additional dependencies are likely to degrade the performance of expensive optimization technologies, since most technologies are under the assumption of mutual independency among the objective and constraints.

The remainder of this article is organized as follows. The related work is briefly discussed in Section 2. A brief description of related techniques is provided in Section 3. The proposed method is introduced and theoretically discussed in Section 4. A surrogate-assisted evolutionary algorithm framework is presented in Section 5. Numerical results on benchmark problems and comparison with five existing infill sampling criteria are presented in Section 6. Finally, conclusions and future work are discussed in Section 7.

2. Related work

A lot of efforts and progress have been made in developing the surrogate-based EAs. Many machine learning models can be utilized to build surrogates, including: Gaussian process (GP) [22], multivariate polynomials (particularly quadratic mod-