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A surrogate-assisted evolution strategy for constrained multi-objective optimization



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ABSTRACT

In many real-world optimization problems, several conflicting objectives must be achieved and optimized simultaneously and the solutions are often required to satisfy certain restrictions or constraints. Moreover, in some applications, the numerical values of the objectives and constraints are obtained from computationally expensive simulations. Many multi-objective optimization algorithms for continuous optimization have been proposed in the literature and some have been incorporated or used in conjunction with expert and intelligent systems. However, relatively few of these multi-objective algorithms handle constraints, and even fewer, use surrogates to approximate the objective or constraint functions when these functions are computationally expensive. This paper proposes a surrogate-assisted evolution strategy (ES) that can be used for constrained multi-objective optimization of expensive black-box objective functions subject to expensive black-box inequality constraints. Such an algorithm can be incorporated into an intelligent system that finds approximate Pareto optimal solutions to simulation-based constrained multiobjective optimization problems in various applications including engineering design optimization, production management and manufacturing. The main idea in the proposed algorithm is to generate a large number of trial offspring in each generation and use the surrogates to predict the objective and constraint function values of these trial offspring. Then the algorithm performs an approximate non-dominated sort of the trial offspring based on the predicted objective and constraint function values, and then it selects the most promising offspring (those with the smallest predicted ranks from the non-dominated sort) to become the actual offspring for the current generation that will be evaluated using the expensive objective and constraint functions. The proposed method is implemented using cubic radial basis function (RBF) surrogate models to assist the ES. The resulting RBF-assisted ES is compared with the original ES and to NSGA-II on 20 test problems involving 2-15 decision variables, 2-5 objectives and up to 13 inequality constraints. These problems include well-known benchmark problems and application problems in manufacturing and robotics. The numerical results showed that the RBF-assisted ES generally outperformed the original ES and NSGA-II on the problems used when the computational budget is relatively limited. These results suggest that the proposed surrogate-assisted ES is promising for computationally expensive constrained multi-objective optimization.

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1. Introduction

Multi-objective optimization techniques have been successfully applied in many real-world decision problems. In general, a decision maker can make better decisions when multiple, possibly conflicting, goals or objectives are taken into account. In this situation, there are usually many, sometimes infinitely many, "optimal" solutions that are incomparable, referred to as Pareto optimal solutions. These Pareto optimal solutions obtained by a multi-objective

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optimization algorithm yield a trade-off curve or trade-off surface called the Pareto front where finding a solution that improves one objective potentially causes the deterioration of another objective. Hence, this trade-off surface shows how much a decision maker has to sacrifice in one objective if he or she wants to improve another objective. The goal of some multi-objective optimization approaches is to find all Pareto optimal solutions or at least find a representative subset of these solutions.

In this article, we develop a surrogate-assisted evolution strategy (ES) for constrained multi-objective optimization that can be used for problems with computationally expensive objective and constraint functions. Our problem setting is that the values of the

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objective functions and constraint functions for a given input vector are obtained via a time-consuming simulation that could take several seconds to many hours per simulation. Such problems are found in many engineering applications, including those that involve finite element or computational fluid dynamics simulations (e.g., Bureerat & Srisomporn, 2010; Husain, Lee, & Kim, 2011; Kunakote & Bureerat, 2011), and also simulation-based problems in production planning and manufacturing (e.g., Gansterer, Almeder, & Hartl, 2014; Güller, Uygun, & Noche, 2015). Many multi-objective optimization algorithms have been proposed in the literature and some have been incorporated or used in conjunction with expert and intelligent systems in manufacturing and engineering design applications (e.g., Kasperska & Ostwald, 2006; Lee & Kim, 1996; Redondo, Sedano, Vera, Hernando, & Corchado, 2013). Our proposed approach extends the capability of multi-objective optimization algorithms in these intelligent systems to handle constraints and computationally expensive simulation-based problems.

Our focus is on solving constrained multi-objective optimization problems of the following form:

$$\min F(x) = (f_1(x), \dots, f_k(x))$$
s.t.
$$G(x) = (g_1(x), \dots, g_m(x)) \le 0$$

$$\ell \le x \le u$$

$$(1)$$

Here, $f_i : \mathbb{R}^d \to \mathbb{R}$, i = 1, ..., k and $g_j : \mathbb{R}^d \to \mathbb{R}$, j = 1, ..., m are black-box functions whose values are obtained via an expensive but deterministic simulation. For now, we assume that there are no equality constraints and that the feasible region $\mathcal{D} := \{x \in \mathbb{R}^d : \ell \le x \le u, G(x) \le 0\}$ has a nonempty interior. Throughout the paper, we assume that one *simulation* for a given input vector $x \in [\ell, u]$ for problem (1) yields the values of all the components of the vector-valued functions F(x) and G(x).

When function evaluations are computationally expensive, a natural approach is to employ surrogate models or metamodels for the expensive functions (e.g., Forrester, Sobester, & Keane, 2008). Commonly used surrogate modeling techniques include polynomial regression (particularly, linear and quadratic models), kriging interpolation, radial basis function (RBF) interpolation, neural networks, and support vector regression. In addition, many authors have proposed ensembles of various types of surrogate models to improve the predictive capabilities of the overall approximation model (e.g., Acar, 2015).

Surrogate models have been combined with evolutionary algorithms for computationally expensive single-objective optimization problems (e.g., Andrés, Salcedo-Sanz, Monge, and Pérez-Bellido, 2012; Bhattacharya, 2007; Regis and Shoemaker, 2004; Shi and Rasheed, 2008) and also for multi-objective optimization problems (e.g., Akhtar & Shoemaker, 2016; Isaacs, Ray, & Smith, 2009; Kanyakam & Bureerat, 2012; Knowles & Nakayama, 2008; Liu & Sun, 2013; Ray & Smith, 2006). Moreover, several authors (e.g., Couckuyt, Deschrijver, & Dhaene, 2014; Knowles, 2006; Ponweiser, Wagner, Biermann, & Vincze, 2008; Wagner, Emmerich, Deutz, & Ponweiser, 2010; Zhang, Liu, Tsang, & Virginas, 2010) developed kriging-based methods that are extensions of the Efficient Global Optimization (EGO) method by Jones, Schonlau, and Welch (1998) to multi-objective optimization. EGO is a global optimization method that uses kriging models together with an expected improvement criterion to select its iterates.

This paper proposes a multi-objective optimization approach based on an evolutionary algorithm that is assisted by surrogate models. Evolutionary algorithms simulate the process of evolution and natural selection by maintaining a population of solutions that are modified in each iteration (called a *generation*) using recombination and mutation operators. In this study, we used an evolution strategy, which is a particular type of evolutionary algorithm that evolves not just a population of solutions but also the associated parameters that control the generation of new solutions. Moreover, our proposed algorithm is based on an evolution strategy that only uses a mutation operator as will be explained later. However, there are other approaches for multi-objective optimization. Besides evolutionary algorithms such as NSGA-II, swarm intelligence algorithms such as MOPSO (Coello, Pulido, & Lechuga, 2004) are also popular. Swarm algorithms also maintain a population of solutions that simulate the behavior of a swarm of agents or particles as they collectively attempt to find an optimal state. Finally, there are also direct search methods and trust region methods that have been recently proposed for multi-objective optimization.

Our approach to solving problem (1) is to use a surrogate to assist an evolution strategy and enhance its performance on constrained multi-objective optimization problems. Although numerous multi-objective evolutionary algorithms have been proposed in the literature (Deb, Agrawal, Pratap, & Meyarivan, 2002; Knowles & Corne, 2000; Zhang & Li, 2007; Zitzler & Thiele, 1998), relatively few have directly dealt with black-box constraints without using a penalty. Moreover, although surrogate models have been combined with evolutionary algorithms for computationally expensive optimization problems, most implementations use surrogates only for a single objective function. Relatively few methods use surrogates for multiple constraint functions (e.g., Regis, 2014) or for multiple objectives (e.g., Akhtar & Shoemaker, 2016; Isaacs et al., 2009; Kanyakam & Bureerat, 2012; Knowles & Nakayama, 2008; Ray & Smith, 2006). Even fewer methods use surrogates to approximate both the objective functions and constraint functions in a multiobjective setting (e.g., Emmerich, Giannakoglou, & Naujoks, 2006; Singh, Couckuyt, Ferranti, & Dhaene, 2014). Hence, the method we propose, which uses surrogates to approximate the objective functions and constraint functions in a multi-objective setting is still somewhat rare.

The main idea in our proposed surrogate-assisted multiobjective evolution strategy (SMES) is to generate a large number of trial offspring in every generation, use surrogates for the objectives and constraints to estimate the actual objective and constraint function values from the expensive simulations, and then use a non-dominated sorting procedure to identify the most promising trial offspring solutions, which then become the actual offspring solutions where the expensive simulations will be carried out. Our method attempts to get a good approximation of the Pareto set using only a relatively limited number of function evaluations, i.e., hundreds or a few thousands evaluations rather than hundreds of thousands of evaluations commonly used with standard evolutionary algorithms. Our method substantially extends the surrogate-assisted ES by Regis and Shoemaker (2004), which was designed for single-objective problems with no blackbox constraints. Moreover, we use surrogates to approximate expensive black-box inequality constraints as in the evolutionary programming (EP) algorithm in Regis (2014). In the numerical experiments, we use radial basis function (RBF) surrogates in the SMES method and apply the resulting algorithm to 20 test problems, including four well-known benchmark problems, three instances of a robotics application problem, and two manufacturing problems. To assess performance, we compare our method with an ordinary ES for constrained multi-objective optimization and with NSGA-II on the same problems and using the same initial conditions. The results showed that the proposed RBF-assisted SMES is very promising for computationally expensive constrained multi-objective optimization problems.

The SMES approach differs from Emmerich et al. (2006) and Singh et al. (2014) in that it can be used with any type of surrogate model while these other methods use a kriging metamodel in conjunction with the multi-objective *Probability of Improvement* (*Pol*) criterion. Moreover, the method proposed by Singh et al. (2014) is a non-evolutionary method that uses a *Probability of* Download English Version:

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