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Simulation optimization based on Taylor Kriging and evolutionary algorithm

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A B S T R A C T

This paper develops a simulation optimization algorithm based on Taylor Kriging and evolutionary algorithm (SOAKEA) for simulation models with high computational expenses. In SOAKEA, an evolutionary algorithm is used to search for optimal solutions of a simulation model, and Taylor Kriging temporarily serves as a surrogate fitness function of this evolutionary algorithm to evaluate solutions. Taylor Kriging is an enhanced version of Kriging where Taylor expansion is used to approximate the drift function of Kriging, and it improves the interpolation accuracy of Kriging. The structures and properties of SOAKEA are analyzed. A combination correction strategy is created, and it effectively reduces the computational expense of SOAKEA. The empirical comparison of SOAKEA with some other well-known metaheuristics is conducted, and the proposed SOAKEA uses particle swam optimization, a population-based evolutionary algorithm, to solve four simulation problems based on multimodal benchmark functions. The results indicate that SOAKEA has significant advantages in optimizing simulation models with high computational expenses.

1. Introduction

Evolutionary algorithms (EAs) are effective simulation optimization tools due to their features of stochastic optimization and independence of the properties of optimized models. The typical evolutionary algorithms include Evolutionary Programming [1], Evolution Strategy (ES) [2], Genetic Algorithm (GA) [3], Particle Swarm Optimization (PSO) [4], Ant Colony Optimization [5], Differential Evolution [6], and Estimation of Distribution Algorithm [7]. To obtain a comprehensive introduction to these algorithms, readers can refer to the related references [1–8]. Fig. 1 gives the basic process of optimization operations of these algorithms. An EA uses a fitness function to calculate fitness values of candidate solutions, and use these values as a standard to evaluate the quality of solutions. According to fitness values, an EA performs evolutionary operations to generate new evolved solutions. Part of the evolved solutions and current solutions are chosen to construct next generation solutions. The algorithm continues this loop until a stopping criterion is satisfied.

In EAs, fitness functions need to be frequently evaluated. For simulation optimization, an evaluation implies to run a simulation model once and is called a simulation evaluation in this paper. Due to the complexity of real-world systems, the simulation models of systems are often computer expensive based on the time of Central Processing Unit (CPU). When a simulation model is computationally too costly, EAs will encounter essential difficulties because of computer limitations such as memory capacity and processor speed. For example, when running a simulation model for one time needs 30 min and the number of simulation evaluations needed in an EA are 1000, the EA will spend about 21 days to find optimal solutions ($30/(60 \times 24) \times 1000 \approx 24$). Influenced by costly computational expenses, evolutionary operations will be stopped due to insufficient fitness values, as indicated by the dash lines in Fig. 1.

This paper explores how to introduce a metamodel to assist in evolutionary optimization while an EA is used to optimize a simulation model with high computational expenses. A Simulation Optimization Algorithm based on Taylor Kriging and Evolutionary Algorithm (SOAKEA) is thus developed. The advantages of metamodels are that they are computational inexpensive, and searching for their optimal solutions is easy. Simulation models consider more details and constraints of systems and thus need higher computational expenses. The fundamental idea of SOAKEA is that in evolutionary optimization, a metamodel fitted by known observations temporarily replaces a simulation model to evaluate simulation inputs such that simulation evaluations can be reduced, and the computational expense caused by simulation evaluations can be limited. Taylor Kriging (TK) is the chosen metamodel due to its accurate interpolation feature, and is used to assist in evolutionary optimization. TK is an enhanced version of Kriging by introducing Taylor expansion to serve as a drift function. Kriging is an accurate nonlinear interpolation tool and named after Daniel G. Krige, a mining engineer in South Africa [9].

The rest of paper is organized as follows. In Section 2, the literature review of Kriging applications in simulation and optimization

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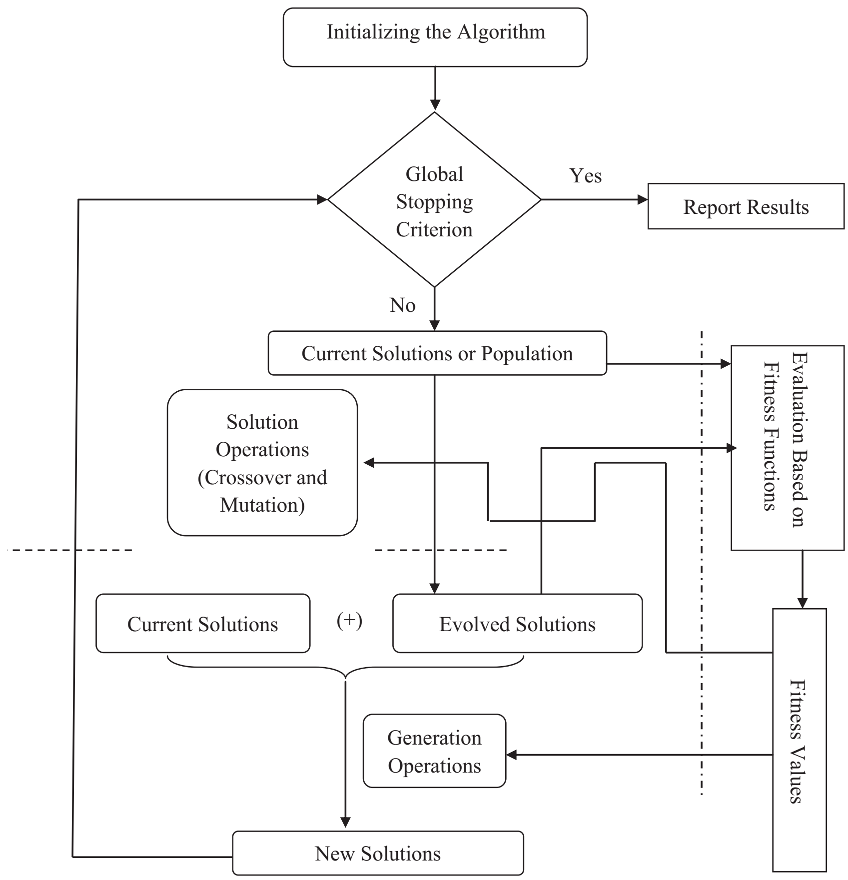

Fig. 1. Basic evolutionary operations of evolutionary algorithms.

is presented. In Section 3, the Taylor Kriging methodology is introduced. In Section 4, SOAKEA is developed, and its structures and properties are analyzed. In Section 5, the computational experience is provided, and a combination correction strategy is created. Finally, summary and conclusion are given.

2. Literature review

Kriging is a spatial statistical technique. Its early application was mainly in geological settings [10]. In recent years Kriging has been widely applied to other areas such as engineering design [11], economic sensitivity analysis and cost estimation [12–14], energy modeling [15], simulation interpolation [16–18], and optimization [19–21].

The application of Kriging to simulation interpolation first occurred in the area of deterministic simulation. The classic reference refers to [16] who considers the computer experiments which are computationally expensive to run and whose outputs are deterministic. Mitchell and Morris [22] investigate Kriging as an alternative to the conventional response surface methodology for use in simulation experiments. The application of Kriging to random simulations is proposed by Barton [17]. The recent representative work of the Kriging applications to simulation interpolation is given by Kleijnen and van Beers [18,23,24]. The literature shows that Kriging has accurate advantages for simulation interpolation over other methods such as regression and response surface method. And this is the main reason why Kriging is chosen to serve as a surrogate fitness function of EA. Note that Kriging models mainly adopted in the literature focused on Ordinary Kriging (OK). However, the drift function of OK is a constant. It is difficult for it to capture the non-constant mean drift of data in complex simulation models. Although some references used Universal Kriging (UK), the drift function of UK is a general polynomial, and its base functions are not clearly identified. There exist difficulties in choosing specific base functions for UK.

Kriging has been applied to optimization. The applications of Kriging in optimization are also based on its interpolation accuracy, and can be divided into two types. One is that Kriging is used to assist in evolutionary optimization by acting as temporal fitness functions; the other is called Sequential Kriging Optimization (SKO) where Kriging itself serves as an optimization tool to search for optimization solutions. The application of Kriging in evolutionary optimization was initially conducted by Ratle [25,26]. Ratle proposes a hybrid algorithm by integrating Kriging and a real-coded GA. El-Beltagy et al. [27] investigate the same problem and suggest that the issue of balancing the concerns of optimization with those of experiment design should be addressed. Zhou et al. [28] give a hierarchical surrogate-assisted evolutionary optimization framework. Another form of the Kriging applications to optimization, SKO, is also called the efficient global optimization method. The related references can be referred in [19–21,29]. Note that the integration application of Kriging and EAs to optimization was just starting and the related research is in the preliminary stage but the obtained results indicate some promise [30]. The deep analysis and investigation on the structures and properties of the integration algorithm are necessary.

3. Kriging methodology

3.1. Basic Kriging principles

Suppose a stochastic process has the following form:

$$Z(\boldsymbol{X}) = \mu(\boldsymbol{X}) + \varepsilon(\boldsymbol{X}) \tag{1}$$