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Survey paper

Surrogate-assisted evolutionary computation: Recent advances and future challenges

Yaochu Jin

Department of Computing, University of Surrey, Guildford, Surrey, GU2 7XH, UK

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ABSTRACT

Surrogate-assisted, or meta-model based evolutionary computation uses efficient computational models, often known as surrogates or meta-models, for approximating the fitness function in evolutionary algorithms. Research on surrogate-assisted evolutionary computation began over a decade ago and has received considerably increasing interest in recent years. Very interestingly, surrogate-assisted evolutionary computation has found successful applications not only in solving computationally expensive single- or multi-objective optimization problems, but also in addressing dynamic optimization problems, constrained optimization problems and multi-modal optimization problems. This paper provides a concise overview of the history and recent developments in surrogate-assisted evolutionary computation and suggests a few future trends in this research area.

1. Introduction

In most evolutionary algorithms, it is often implicitly assumed that there exists a means for evaluating the fitness value of all individuals in a population. In general, the fitness value of an individual can be computed using an explicit fitness function, a computational simulation, or an experiment. In practice, however, fitness evaluations may become non-trivial. Such situations typically occur when evolutionary algorithms are employed to solve expensive optimization problems, where either the computational simulation for each fitness evaluation is highly time-consuming, or the experiments for fitness estimation are prohibitively costly, or an analytical function for fitness evaluations simply does not exist.

Surrogate-assisted evolutionary computation was mainly motivated from reducing computational time in evolutionary optimization of expensive problems, such as aerodynamic design optimization [1] or drug design [2], where complex computational simulations are involved.

In principle, surrogates should be used together with the real fitness function, as long as such a fitness function exists to prevent the evolutionary algorithm from being misled by a false minimum introduced by the surrogates [3]. A strategy for properly using the surrogates is often known as model management or evolution control. In surrogate-assisted evolutionary optimization of expensive problems, in particular when the problems are of high-dimension, the development of a model management strategy remains a challenging research topic.

The remainder of the paper is organized as follows. Section 2 takes a brief look back at the history of surrogate-assisted evolutionary computation starting from the late 1990s. Representative model management strategies are discussed in Section 3, which distinguish themselves into managing a single surrogate, homogeneous multiple surrogates, and heterogeneous multiple surrogates. Application of surrogates to addressing problems other than expensive optimization in evolutionary computation is presented in Section 4. Application examples of meta-model based evolutionary optimization are briefly accounted in Section 5. A few promising yet challenging research topics are suggested in Section 4. The paper concludes with a brief summary in Section 7.

2. A brief look back

Research on evolutionary optimization using approximate fitness evaluations was first reported in the mid-1980s [4], and sporadic yet increasing research results on evolutionary optimization using computational models for fitness estimation appeared after the mid-1990s [5–9]. The first event devoted to research on using surrogates in evolutionary optimization was a workshop held in 2002 within the Genetic and Evolutionary Computation Conference (GECCO) [10]. Since then, a series of special sessions and workshops have been organized on the major conferences including GECCO and IEEE Congress on Evolutionary

E-mail address: yaochu.jin@surrey.ac.uk.

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Computation, and journal special issues have also been edited. An overview of the research on surrogated-assisted evolutionary optimization reported in various fields was first presented in a conference paper [11], and then a journal paper in a special issue [12]. A first tutorial on fitness approximation on evolutionary optimization was given at the GECCO in 2005. Most recently, an edited book on the use of surrogates in evolutionary computation was also published [13].

In the review paper [12], the importance of managing surrogates was emphasized for the first time to prevent the evolutionary algorithms from being misled to a false optimum that can be introduced in a surrogate. In that review, methods for managing surrogates in evolutionary computation were divided into three categories, namely, individual-based, generation-based and population-based strategies. A variety of computational models, including polynomials (also known as response surface methodologies in the field of traditional design optimization), Gaussian processes (also known as Kriging in traditional design optimization), neural networks, together with data sampling techniques such as design of experiments, active learning and boosting were also presented. Practically, fitness inheritance from parents or fitness imitation from siblings [14–16] can be seen as a sort of simplified yet effective interpolation technique. General issues such as the global and local approximation, approximation of nonlinear constraints and the use of multiple surrogates having various fidelities were discussed. Theoretical analysis of the convergence properties was also raised.

Since the review paper [12], very encouraging research progresses have been made in many of the areas, whereas some issues remain unsolved, in particular with respect to a rigorous theoretical support for the benefit for using surrogates in evolutionary computation. Note that this paper focuses on surrogates in evolutionary computation. Readers interested in recent developments of surrogate-assisted design and analysis methods are referred to [17,18].

The next section provides a brief overview of recent advances in the research on surrogate-assisted evolutionary optimization, emphasizing on the progresses made after the review paper [12]. Research on using surrogates beyond solving expensive problems is discussed in Section 4. A few challenging topics for future research are suggested in Section 6. A summary of the paper is given in Section 7.

3. Strategies for managing surrogates

In most real-world optimization problems, no analytical fitness function exists for accurately evaluating the fitness of a candidate solution. Instead, there are only more accurate and less accurate fitness estimation methods, which often trade off accuracy with computational costs, as illustrated in Fig. 1. For example, in evolutionary optimization of aerodynamic structures [1], wind tunnel experiments may provide the most accurate estimation of the quality of candidate designs. The cost of such experiments is often prohibitively high. In addition, three-dimensional (3-D) computational fluid dynamic (CFD) simulations using Navier–Stokes equations may provide very accurate fitness evaluations. Unfortunately, such CFD simulations are highly time-consuming, which can take hours or even days for one single fitness evaluation. Computationally more efficient simulations can be achieved by 2-D full simulations or even incomplete simulations. By incomplete simulation, we mean that a simulation process is stopped before it converges. The computationally most efficient way for estimating fitness is the use of machine learning models, i.e., surrogates. Note, however that this graphic only shows a simplified version of actual levels of accuracy.

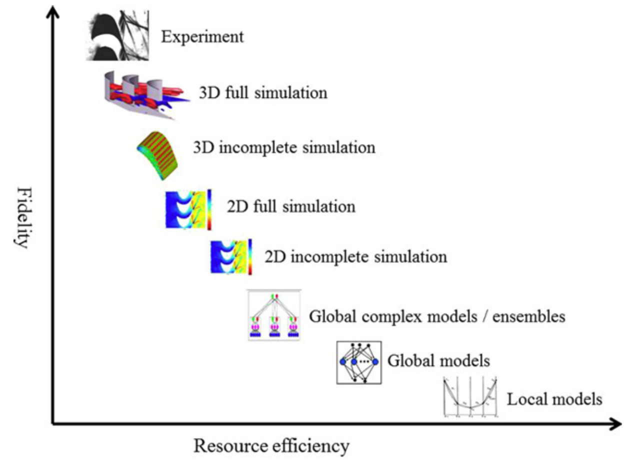

Fig. 1. An illustration of a trade-off between fidelity (approximation accuracy) and computational cost. Usually, high-fidelity fitness evaluations are more time-consuming. By contrast, low-fidelity fitness evaluations are often less time-consuming.

In the research of surrogate-assisted evolutionary optimization, most algorithms have been developed based on benchmark problems, where it is assumed that fully accurate fitness evaluations can be provided. Such fitness functions are often termed "real fitness function" or "original fitness function". In the following, we use surrogates for denoting computational models constructed with data, whereas other approximate fitness techniques such as full or incomplete 2-D CFD simulations are called problem approximations as termed in [12]. In addition, we do not distinguish between surrogate-assisted single objective optimization and surrogate-assisted multi-objective optimization if the method for model management does not differ.

In the early work on surrogate-assisted evolutionary optimization, the evolutionary search is based solely on a surrogate, assuming that the surrogate can provide sufficiently accurate fitness evaluations. However, such assumptions can give rise to serious problems if the surrogate introduces optima that do not exist in the original optimization problem. This issue was first explicitly raised in [3] to stress the importance of model management in surrogate-assisted evolutionary optimization, mainly by using the surrogate together with the real fitness function.

Surrogates can be applied to almost all operations of evolutionary algorithms, such as population initialization, cross-over, mutation, local search and fitness evaluations, as illustrated in Fig. 2. For instance, a surrogate can be used for filtering out poor solutions in population initialization, crossover [19] or mutation [20]. The use of surrogates in initialization, mutation or crossover [21] can reduce the randomness in the genetic operators, thus termed informed operators. Most recently, a similar approach is adopted for multi-objective optimization [22], where a single, aggregated meta-model is built to pre-screen candidate solutions before fitness evaluation. The requirement on the quality of surrogates is minimum, as an estimated fitness that is better than a random guess is adequate.

Techniques for managing surrogates for fitness evaluations can generally be divided into individual-based, generation-based and population-based [12]. By generation-based, we mean that surrogates are used for fitness evaluations in some of the generations, while in the rest of the generations, the real fitness function is used [8,23,24,7]. By contrast, in individual-based model management techniques, the real-fitness function is used for fitness evaluations for some of the individuals in a generation [25,3,23]. In population-based approaches, more than one subpopulation co-evolves, each using its own surrogate for fitness