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Review on Surrogate-Based Global Optimization with Biomedical Applications

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ABSTRACT

Time and accuracy are two key elements that have a significant impact on an algorithm brilliance in many engineering applications. Consequently, many algorithms aim to improve precision and cut down computational costs when resolving contemporary real-life problems. Optimization based on surrogates is considered as an efficient way to keep pace with ever growing problems encountered in modern systems. The design of prosthetic de- vices for people with disabilities involve challenging optimization problems. In such design problems, the relation between the design parameters and the overall performance of the device is complex. Thus, surrogate-based optimization plays an essential role in solving them. This paper reviews the key issues of surrogate-based global optimization starting with the fundamental models used as surrogates, then contemporary research on sampling approaches, and infill criteria with an eye on biomedical applications. Finally, challenges facing surrogate based optimization are discussed.

Keywords: Surrogate Model; Black Box Function; Sampling Technique; Prosthetic Devices, Engineering Applications; Global Optimization

Abbreviations: GA: Genetic Algorithms; SA: Simulated Annealing; SBGO: Surrogate-Based Global Optimization; DOE: Design of Experiments; RBF: Radial Basis Function; MARS: Multivariate Adaptive Regression Splines; MADS: Mesh Adaptive Direct Search; RBDO: Reliability-Based Design Optimization; EI: Expected Improvement; PLRS: Potential Lipschitz Constants and Response Surfaces; AMGO: Adaptive Metamodel Based Global Optimization; MSSR: Multi-Start Space Reduction; CFD: Computational Fluid Dynamics; DBN: Deep Belief Network; EMO: Evolutionary Multi-Objective Optimization; ASO: Aerodynamic Shape Optimization

Introduction

Many of today's design problems involve multiple objectives and computationally expensive analysis and simulations to evaluate a given design. For instance, the design of a prosthetic device requires complex simulations to determine the optimal parameters of the device needed to reach target functionality to aid a disabled person. Design problems need to be formulated mathematically as optimization problems in order to find adequate techniques for solving them. An optimization problem formulation involves deciding on control variables and a criterion or more for evaluating a design. The evaluation criterion is referred to as the problem objective function. Optimization algorithms can be divided into two categories: deterministic (for instance, gradient descent method) and stochastic or sometimes called metaheuristics. For instance, genetic algorithms (GA) [1], the simulated annealing (SA) algorithm [2] and particle swarm optimization (PSO) algorithm [3] are pioneering metaheuristic algorithms. The recent ones include the cuckoo search algorithm [4], the bee colony optimization algorithm [5,6], the firefly algorithm [7], the grey wolf algorithm [8], and the whale optimization algorithm [9,10]). These algorithms are derivative-free and may perform better than the conventional derivative-free optimization methods like the coordinate search method. The search for the global optimal solution usually requires thousands of objective function evaluations. In many

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engineering applications, the objective function is a black-box function, which is evaluated using complicated time-consuming computer simulations. This renders determinitic gradient-based optimization techniques inadequate for use. Moreover, the huge number of objective function evaluations required by meta- heuristics encouraged researchers to use surrogate models to replace the expensive black-box objective function by another cheap model.

Surrogate-based global optimization (SBGO) is regarded as a good method with a number of advantages over the conventional optimization approaches. The following are some of SBGO's distinctive merits. First, it needs fewer computaional resources and less time owing to the ap- proximation process. Second, it provides fast approximations of the objective function at new design points making postoptimality studies and sensitivity analysis feasible. Third, the information obtained from the available samples through interacting with the system can help the designer gain insight into the system under study. The three basic stages for SBGO are: design of experiments (DOE), approaches for surrogate modeling and infill criteria. The first stage in the SBGO is referred to as the design of experiments (DOE) stage, which defines the samples plan in the design space. The original black-box function is evaluated at these sample points. Nobody can argue that the selection of the sample candidate points has a substantial impact on the surrogate model accuracy. Clearly, if the sample candidate points are well-chosen, then this can help reduce the huge computational cost as discussed in [11,12]. There are two types of experiments that can be used in this stage: i) design of physical experiments, and ii) com- puter experiments. In physical experiments, the samples plan construction strategies include factorial designs as in [13] and [14] and central composite designs such as [15]. As for computer experiments, the samples plan designs include uniform designs [16] and latin hypercube designs [17,18]. Simpson, et al. [19] confirmed that the conventional physical experiments designs are inefficient or even improper for computer experiments.

On the other side, when the best sample candidate points are determined, we attempt to create the surrogate model (or response surface). The purpose of the surrogate model is to create an approximation of the original objective function over a particular design space. The most important step is deciding on the best surrogate model. The mathematical characteristics and nature of the surrogate model that is chosen actually depends on the mathematical properties of the problem objective function. Unfortunately, in real-life applications, these mathematical properties are unknown in advance when we try to solve the problem.

How the performance of the surrogate model can be enhanced is the next issue that needs to be resolved. The answer is based on methods for selecting new promising sample points referred to as infill criteria. Combining exploitation and exploration help define infill criteria. On one side, the exploitation strategy concentrates the search on the area in the close vicinity of the best point discovered so far. This current optimum location, where the search is concentrated around, might not be the global or local minimum, or even not a stationary point of the original objective function. Therefore, this will likely result in falling into a local optimum. On the other hand, the exploration strategy always investigates unexplored regions within the design space. Various infill criteria have been developed for choosing the new sample points in recent years. The basic stages of the SBGO must be repeated until some specific criteria are achieved such as: a specific maximum number of iterations or function evaluations, a specific amount of CPU time, or the relative error of the required function drops to be less than or equal to a specific value.

Surrogate Models

There is a variety of types of surrogate models which can be classified into interpolating surrogate models; such as Radial Basis Function (RBF) [20-22] and Kriging (K) (see [23])) and non-interpolating surrogate models; such as Polynomial Regression Models (PRM) [24], and Multivariate Adaptive Regression Splines (MARS) [25]. Several research articles, such as [25-29], developed comprehensive studies to investigate the effectiveness and the accuracy of various surrogate models. However, we cannot find an agreement on the dominance of one specific model over other models. In the past few years, numerous novel surrogate models have been proposed; for instance, in [20], a new approach for setting up radial basis function artificial neural network is proposed by letting the bias be defined a priori using a corresponding regression model. The authors have shown that the RBF with a priori bias works perfect for optimizing surrogate-based designs, because it gathers both coarse and dense features of the underlying original model simultaneously. Surrogates can be constructed by using simplified physics, or by relaxing internal tolerances within the black-box simulation. These surrogates are often provided by the designer of the simulation. We refer to these as static surrogates.

Surrogates can also be built and updated as the optimization progresses. Interpolation or regression methods can be applied to mimic the output of the simulation using quadratic [30,31] or polynomial [32] approximations, DACE Kriging [33-35], treed Gaussian processes [36], LOWESS models [37], radial basis functions [38-41] or even ensembles of surrogates [42]. We refer to these as dynamic models. The surrogate management framework in [11] details how to exploit a surrogate model to reduce the overall computational optimization time. Research on surrogate-assisted direct search optimization usually involves the use of either static or dynamic models. In [43] proposed a way to combine a static surrogate as input for a quadratic model of an optimization problem, to be used within the poll step of the Mesh Adap- tive Direct Search (MADS) algorithm [44]. Some authors have studied a combination of both static and dynamic surrogate models. For example, the authors in [45] propose additive and multiplicative ways of combining static surrogates with dynamic ones. The objective of their research was to propose a hybrid strategy to build a quadratic model whose input is not only the optimization variables, but also a supplementary variable taking the value of the static surrogate model into account. This yields flexible models that

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inherit the global properties of the static surrogate model and the local precision of quadratic models. A novel radial basis function surrogate model assisted evolutionary algorithm for high- dimensional expensive optimization problems (RSAEH) was proposed in [46].

Specifically, the proposed algorithm consists of a local search part and a surrogate-guided pre-screening part. In the local search part, a local surrogate is built using radial basis functions with the most promis- ing training sample points, and the optima (or near-optima) are located by the optimizer to carry out exact function evaluation at these points. In the surrogate-guided pre-screening part, the current best sample point is refined using sequential quadratic programming, thus guiding the mutation direction by using differential evolution operator with the original objective function being evaluated at promising offspring.

Reliability-based design optimization (RBDO) [47] has been used for optimizing engineering systems with uncertainties in design variables and system parameters. However, moment-based RBDO is inefficient for problems with many random variables and sensitivity is not defined properly at certain design points. To make the moment-based RBDO more efficient and prac- tical, a Kriging metamodel or surrogate model with an active constraint strategy was proposed to resolve this issue. The use of constraints based on surrogates complicates the optimization problem as the uncertainty within the design space influences both the objective and constraint functions. While some optimization methods consider the mean prediction for the constraints, several methods have been reported on ways to include the uncertainty into the constraints. One way is to use a probability of feasibility to account for the mean prediction and its uncertainty. This approach is explored in [48] to evaluate its feasibility and compared to other alternative methods documented in the literature.

Sampling Techniques

The sampling criterion determines which points to add to the sample plan generated using a specific design of experiments methodology. The choice is based on either the built model or the given sample points. The infill criterion or sampling criterion is an essential component of the surrogate-based global optimization (SBGO) procedure. In SBGO, similar to metaheuristic algorithms, this criterion is used to perform sequential addition of sample points, gradually leading to the global optimum. The sampling criteria can be divided into two categories: a single-phase criterion and a multi- phase criterion. The distinction between a single-phase and multi-phase sampling criterion is based on whether the exploitation and exploration criteria are united or separate. For one- phase criterion, the exploitation and exploration goals are achieved together from a single sub- optimization problem. In contrast, the multi-phase criterion completely separates the phases of exploitation and exploration. The expected improvement (EI) criterion is a classic example of a single-phase criterion. The EI standard measure determines the predicted value of the improvement numerically. The ex- pected improvement introduced in [49,50] and its modified versions including weighted expected improvement [51], augmented expected improvement [52], and the probability of expected im- provement [53], are widely used as infill criteria. This step to select further designs that offer improvement is iterative till a certain convergence criterion or termination criterion is reached. More examples of a single-phase criterion can be found in [54] that use an RBF surrogate model.

In [55], Bjorkman and Holmstrom generalized the EI measure which is used to optimize a certain bumpiness function. The potential Lipschitz constants and response surfaces (PLRS) technique was proposed by Liu et al. in [56] as a tunable algorithm that balances between exploration and exploitation. The adaptive metamodel based global optimization (AMGO) algorithm [57] is an SBGO that combines the Kriging and RBF models. It is effective only for a certain sort of optimization problems, problems that have a few modes. But when this technique is used on complicated problems, it does not perform well due to that is used a single-phase criterion, where it sometimes favors exploration over exploitation or vice versa; meaning that they affect one another. To decipher this dilemma, most of recently developed techniques belong to multi-phase criteria. For instance, the super-EGO (efficient global optimization) technique, developed by Sasena [58], has multi-phase criteria not only two phase criteria for exploration and exploitation; but, there is also another one for insuring that the new sample point is feasible. Moreover, the multi-start space reduction (MSSR) algorithm [59] is a multi-phase sampling technique. It uses the kriging function as a surrogate model, divides the design space into three design sub-spaces GS (global space), MS (medium space), and finally LS (local space). In every iteration of this technique, at least three sample points are selected from the design sub-spaces. While these algorithms make use of several phases, but the transitions between phases are repetitive and not adaptable.

The ARSM-ISES algorithm [60] involves multi-phase criteria and is adaptive. It employs the maximum distance criterion as an exploration criterion and utilizes the exploita- tion of the surrogate model as an exploitation criterion. Multiple-phase criteria are utilized in the AMP-SBGO technique [61] to construct an efficient SBGO sampling algorithm. To select a point and progressively acquire the global optimum, the sampling criterion involves two distinct stages that search a localized region of interest and a global design domain. This is a sampling technique with tight transfer requirements from one phase to another. An adaptive sampling optimization technique based on the complex method was proposed by Xu et al. in [62]. The adaptive sampling strategy couples the process of adding points with the optimization process. An initial kriging surrogate model is generated using the initial sample points as well as one or more complex shapes. The kriging surrogate model and the complex shapes are then utilized to yield new replacement points. In this method, the replacement point of a complex shape is determined to efficiently capture the information of the optimization direction. Next, the replacement point is added to the initial sample set as a new sample in the optimization process

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to update the surrogate model. It is worth noting that when several complex shapes are used concurrently, numerous complex forms occasionally search in the same optimization direction, resulting in a decreased computational efficiency.

Test Problems and Applications

There is a variety of benchmark test functions that must be investigated to evaluate the performance of any new surrogate-based optimization technique; for instance, the authors in [63] collect several non-smooth unconstrained, bound constrained, and inequality constrained test problems. More test problems; some of which are unconstrained, and others are linearly con- strained minimax optimization problems, can be found in [64]. Applications of SGBO to aeronautics over the past decades are vast [65-67], especially when involving expensive computational fluid dynamics (CFD) simulations of airfoils and wings [68]. More efforts are exerted to reduce the need for expensive DOE through adaptive sam- pling [69,70]. Connventionally, a Kriging-based method is employed to build a surrogate model, although other models such as RBFs [71] and the Gaussian Process [72] have been also used. Ma- chine learning models such as deep neural networks [73-75], Generative Adversarial Networks (GAN) [76,77] and Deep Belief Network (DBN) [78] are other types of surrogates that have been employed for aerodynamic shape optimization (ASO) of airfoils [73-75] and wings [76,78,75]. In [79], it is demonstrated that evolutionary multi-objective optimization(EMO) and RBF network with a priori bias are powerful tools for performing multi-objective optimization of multi-physics systems such as a disc brake system of a heavy truck. Additionally, different surrogate models are used to optimize the performance of an air impulse turbine for ocean wave energy harvesting by CFD analysis [80]. More interesting are the applications of surrogate-based modeling and optimization in the field of biomedical systems. For instance, Srinivas et al. used kriging model for building response surfaces for two-dimensional flow of blood in [81]. Coronary stents are cardiovascular medical devices vastly used in the treatment of coronary heart disease. In [82], the authors used multi-ojective optimization and SGBO for finding new geometric designs of coronary stents with the goal of achieved improved biomechanical performance.

In [83], Tammareddi et al. ad- ditionally included uncertainties in their optimal design seeking procedure to yield more robust stent designs minimizing possible risks. On the other hand, the authors in [84] investigated the use of non-uniform rational basis splines (NURBS) in representing the stent geometry and demonstrated its effectiveness in the results of their shape optimization procedure. G. Alaimo et al. in [85] proposed a methodology for designing Nitinol stents that combines structural finite element analysis with a multi-objective genetic algorithm based on a kriging surrogate model. They resorted to the use of surrogates to reduce the computational complexity of their proposed approach. Other efforts in the field of stent geometry optimization include the work presented by Putra, et al. in [86]. They considered both triangular and rectangular struts in their study. SGBO based on a kriging model has been used with the objective of maximizing the expected hypervolume improvement. Other prosthetic devices design optimization problems include hip prosthesis design. In [87], cementless hip prosthesis design optimization is formulated as a multi-objective, reliability-based optimization problem. They employed finite element analysis and surrogate based optimization. The constructed kriging surrogate models are validated and tested using several measures. More- over, the optimization of stimulus energy for cochlear implants is another challenging problem. In [88], a convolutional neural network surrogate model of an auditory nerve fiber is constructed to avoid conducting simulations with a realistic biophysical system, which is a time-consuming process.

Major Challenges

Designers face numerous challenges in the seek of the best design under given constraints. One major challenge is the selection of the design evaluation criteria or design objectives. Usually, there is more than one objective to be satisfied. The issue is that the design criteria are conflicting goals and there is a need for a good trade-off between them. Another challenge related to the design objectives appearing in many applications is that their evaluation involves a complicated and computationally expensive procedure. They are mostly in the form of black-box functions relating the design parameters and the system response. Even for problems with a small dimension, the optimization problem may consume a long time to find its solution due to the complex simulations required to evaluate the design. Both types of challenges are faced by designers that need to solve shape optimization problems encountered in aeronautics and prosthetic devices design. The use of derivative-free optimization techniques with surrogate models has become a popular solution methodology in such applications. However, the design of a surrogate-based optimization algorithm is not an easy task. The selection of an appropriate surrogate model is a key step in such an algorithm. There is a variety of surrogate models that range from simple regression models to complex machine-learning based models. Moreover, the choice of the initial sample points plan can have a significant role in cutting down the overall running time of the optimization algorithm. Building consistent surrogate models that conform with the original objective function is crucial to finding the true optimal designs. Development of an adaptive sampling strategy, which carefully adds new sample points at which the expensive function is evaluated, is yet another challenging step. From the above review, it is apparent that there is still for improvement in the design of new sampling strategies to balance between exploration and exploitation. Producing reliable designs in the presence of uncertainties is a challenging issue to be considered by designers. Appropriate statistical tools should be incorporated within the optimization procedure to ensure reliability of obtained designs. It is noteworthy that somehow the suitability of a SBGO strategy is problem-dependent and thus the designer needs to be aware of the different strategies to address a problem in hand.

Conclusion

In this article, surrogate-based optimization has been briefly explained with an eye on biomedical applications. Prosthetic devices design and stimulus energy optimization are two interesting applications of surrogate-based optimization. The stages involved in a surrogate-based optimization procedure have been discussed and commonly used surrogate models have been reviewed. The main challenges faced by designers when solving a practical optimization problem have also been highlighted.

Conflict of Interest

The authors report there is no any economic interest or any conflict of interest exists.

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