Computers and Structures 178 (2017) 58–70

Contents lists available at ScienceDirect

Computers and Structures

journal homepage: www.elsevier.com/locate/compstruc

# A proper infill sampling strategy for improving the speed performance of a Surrogate-Assisted Evolutionary Algorithm

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ARTICLE INFO

*Article history:*
Received 18 March 2016
Accepted 4 October 2016

*Keywords:*
Surrogate model
Evolutionary algorithm
Model updating
Differential evolution
Infill sampling strategy

ABSTRACT

In the present paper, an improved Surrogate-Assisted Evolutionary Algorithm is proposed. It combines the Differential Evolution algorithm with a quadratic surrogate approximation and a proper infill sampling strategy to choose appropriate sample points. The selection of the new candidate points is arranged to enhance both the local accuracy and the global optimum search. A comparison between performances of different evolutionary algorithms is carried out by searching the global minimum of two benchmark functions, by solving a dynamic identification problem of a three floor frame and by calibrating the non-linear stress-crack opening relation for Fibre-Reinforced Concrete specimens starting from experimental data.



## 1. Introduction

Model updating and inverse analyses are widely employed to develop accurate models representing real structures in the framework of optimization design [1], damage identification [2] and structural health monitoring [3,4]. The basic procedure is to adjust some parameters of the structure so that the model responses agree as closely as possible with the measurements. The set of unknown parameters is obtained solving an optimization problem where the objective function is defined as the difference between measured data and numerical predictions. Since the objective functions are generally implicitly defined and they may often exhibit multiple local optima, the efficiency of the optimization algorithm plays a crucial role in the success of the optimization problems especially with reference to computationally expensive linear or non-linear numerical models. The goal is thus to find an accurate solution with a limited number of function evaluations.

Genetic and evolutionary algorithms are widely used for solving global optimization problems. Their architecture is designed for large-scale problems and it allows to escape from local minima. The main drawback is that the convergence is often reached after a large number of function evaluations. Surrogate-Assisted Evolutionary Strategies use efficient computational models, as response surface (RS) [5,6], high polynomial functions [7] or Kriging models [8–10], to approximate the objective function. Recently, they received considerably increasing interest in reducing the computational effort in optimization problems, mainly when the evaluation of the objective function is highly time consuming [7,11]. The most straightforward idea is to evaluate those individuals that potentially have a good prediction of the objective function value [12]. Even if several surrogate assisted evolutionary algorithms are proposed (see for instance [7,11,13]), the strategy for properly managing the surrogates (that is when and how to use the surrogate model) is a serious challenge and it still remains an interesting research topic.

The introduction of a second-order surrogate in the Differential Evolution (DE) algorithm [14] is reported in [15]. In this algorithm, named DE-Q, both the performances in terms of speed rate are improved by introducing a quadratic approximation of the objective function and the accuracy of results is preserved.

In the present paper, a proper infill sampling strategy is introduced in the DE-Q algorithm to further reduce the number of objective function evaluations. The updated algorithm is called DE-S. The aim is to evaluate the objective function only at a limited number of selected points. The candidate points are chosen trying to find a compromise between local and global search, that is to enhance both the accuracy in the region of the optimum predicted by the surrogate (local exploitation) and global exploration. Therefore, the proposed method assigns a score to each candidate in order to identify the best search points to be evaluated. The score depends on both the distances of the candidate from the overall population and the objective function value predicted by the surrogate model.

The paper is structured as follows. In Section 2 a brief state of the art of Surrogate-Assisted Evolutionary Algorithms is presented.

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http://dx.doi.org/10.1016/j.compstruc.2016.10.004
0045-7949/

Section 3 recalls some basic information concerning the original Differential Evolution (DE) algorithm and it briefly describes the architecture of the DE-Q algorithm. In Section 4 the algorithmic scheme of the proposed DE-S is reported and the introduced infill sampling strategy is described. Afterwards, some results on the minimization of two analytical benchmark functions are reported in Section 5 in order to compare the performances of the DE, the DE-Q and the DE-S algorithms. Moreover, results of some sensitivity analyses are performed to illustrate the role played by the main parameters governing the proposed algorithm. Finally, in Sections 6 and 7 the results of optimization procedures based on two case studies are presented. The first numerical example concerns the dynamic identification of mechanical and geometrical properties of a three floor frame where the modal parameters are considered as the reference solution. Concerning the second case study, inverse analyses are performed to find the parameters governing the non-linear stress-crack opening relation for Fibre-Reinforced Concrete (FRC) specimens with reference to experimental results reported in [16].

## 2. Related works

Research on Surrogate-Assisted Evolutionary computation began over a decade ago and it received considerably increasing interest in recent years. Surrogate models, also known as meta-models, have proved successful for finding the global optima of computationally expensive continuous optimization problems and they have been employed for solving real world applications. Surrogate-Assisted Evolutionary Strategies use several different categories of surrogate models [17–20] to approximate the objective function to solve engineering design problems [21,22], including the polynomial-based response surface models [10,23], the neural networks (NNs) based surrogate models [24,25], the Radial Basis Function (RBF) models [7] and the Kriging models [20].

Surrogate models can be applied to almost all operations of evolutionary algorithms, such as population initialization, crossover, mutation, local search and objective function evaluations [11]. A surrogate can then be used for filtering out poor solutions in population initialization or for pre-screening candidate solutions before the objective function evaluations. Moreover, the introduction of surrogate models in mutation or crossover operations [26] can reduce the randomness in the genetic operators.

In literature, many surrogate models are based on Gaussian processes, also known as Kriging models [8–10]. These surrogates provide an estimate of both the objective function shape and the model uncertainty. However, the computational cost for constructing Gaussian processes can be very high when a large number of sample points is used. In [18] a robust archived differential evolution (RADE) algorithm is combined with a Kriging surrogate model to reduce the total number of evaluations in the shape optimization of an aeroengine turbine disc. A Kriging model is constructed starting from data collected by evaluating the objective and constraint functions at a few initial points. At each iteration the Kriging model is repeatedly updated by the robust archived differential evolution algorithm to estimate the location of the optimum and to suggest points to achieve a global exploration.

Kitayama [27] proposes a Sequential Approximate Optimization (SAO) procedure using a RBF network to construct a response surface. The Gaussian function is employed as the basis function. The optimum of the response surface is taken as a new sample point for a local approximation while a function called density function is constructed using the RBF network to achieve a global exploration. The global minimum of the density function is taken as the new sample point. Unlike the classical approximation-based optimization procedure summarized by Kitayama, the sequential approximate optimization approach proposed by [28] first conducts a small-size design of experiment, using various approximate techniques to construct a surrogate. The global optimum of the surrogate is then found by optimization methods such as evolutionary algorithms.

Mueller [7,29] introduces a surrogate model based algorithm for computationally expensive global optimization problems. A RBF model is used to select candidates at which the objective function is to be evaluated. The algorithm iteratively evaluates the objective function at chosen points of the variable domain and it updates the surrogate model. For each iteration four perturbation methods are used to diversify the selection of candidates for the next evaluations and the best point of each group is chosen based on scoring criteria that allow to establish a balance of local and global search.

A polynomial-based response surface model is the most widely used surrogate model due to its simplicity and effectiveness [30]. Several examples of high-order polynomial surrogate models are proposed to globally approximate the objective function (see for instance [7]). If these kinds of surrogate models are chosen, an expensive computational complexity is usually needed especially to minimize the high-dimensional surrogate itself. On the other hand, if second-order polynomial models are adopted, the computational effort to minimize the surrogate is significantly reduced but the objective function can be only locally fitted.

As a matter of fact, a large category of Surrogate-Assisted Evolutionary Algorithms use surrogates in local search only [31,32]. Khoo and Chen [33] propose to integrate the response surface methodology with genetic algorithms (GAs) to realize a GA-based prototype system for the determination of near optimal values in response surface designs. The memetic algorithms [34] are evolutionary algorithms equipped with a local search module to perform local improvement of individual solutions. Many local surrogate models can be built to assist the local search process of the memetic algorithms instead of building a global model. The main advantage of this local search is the combination of the power of an evolutionary operator and the local search with the purpose to explore and to exploit the search space, respectively.

The introduction of a second-order surrogate in the Differential Evolution (DE) algorithm [14] is reported in [15]. In this algorithm, named DE-Q, both the performances in terms of speed rate are improved by introducing a quadratic approximation of the objective function and the accuracy of results is preserved. In the present paper, a proper infill sampling strategy is introduced in the DE-Q algorithm to further reduce the number of objective function evaluations. To better understand the main stages of the proposed DE-S algorithm, the next section recalls some basic information concerning the Differential Evolution (DE) algorithm and it describes the architecture of the DE-Q algorithm.

## 3. Differential evolution algorithm with a second-order response surface

Differential Evolution (DE) algorithm is a parallel direct search method and it is widely used in the field of numerical optimization [35,36], model updating [37–39] and inverse analyses [40,41]. The basic procedure is reported in details in [14,42] and it is briefly summarized in the following.

*NP* vectors collecting the unknown parameters are simultaneously adopted in the optimization process. Each vector $\mathbf{x}_{i,G}$ contains a number $D$ of optimization parameters, where subscript $G$ indicates the $G$-th generation, and it connects a search point with the origin of the parameter domain. First, the initial generation of points is randomly chosen in the search space and the associated objective function values $H$ are evaluated. Starting from the initial