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Incremental modeling of a new high-order polynomial surrogate model

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ABSTRACT

This study will develop a new high-order polynomial surrogate model (HOPSM) to overcome routines of expensive computer simulations in engineering. The proposed HOPSM is expected to keep advantages of the traditional low-order polynomial models in efficiency, transparency and simplicity, while avoid their disadvantage in accuracy. The zeros of Chebyshev polynomials having the highest allowable order will be utilized as the sampling candidates to improve stability and accuracy of the approximation. In the numerical process, a space-filling scheme is used to generate the initial set of samples, and then an incremental method based on the *maximin* principle is established to select more samples from all candidates. At the same time, the order of HOPSM is sequentially updated by using an order incremental scheme, to adaptively increase the polynomial order along with the increase of the sample size. After the order increment, the polynomial with the largest adjusted R-square is determined as the final HOPSM. Several typical test functions and two engineering applications are used to demonstrate the effectiveness of the proposed surrogate modeling method.

1. Introduction

Numerical simulations using accurate models for many real world problems in engineering often become unaffordable, as they involve routine evaluations of a large number of cost-prohibitive computations. A surrogate model is an engineering method for approximation of practical design problems, to avoid computation extensive simulations. For example, the finite element analysis of vehicle crashworthiness will usually take tens of hours to run one simulation, while the whole crashworthiness will take hundreds and even thousands of iterations to complete. Furthermore, the simulation model is in general a black box, with little or no additional information available for its inner mechanism except for the output it generates [1]. It is hard to explore, optimize or gain insight into the system. Hence, the surrogate models have been widely used as inexpensive approximation for computationally expensive models [2]. The surrogate model, also termed as meta-model, response surface or emulator, refers to any relatively simple relationship between parameters and response often based on limited data [3]. There are two main steps involved in the construction of a surrogate model: (1) the sampling or design of experiment (DOE) and (2) metamodeling via interpolation or regression algorithms after the sampling.

There have been several types of surrogate models, including the traditional response surface (low order polynomials) [4], radial basic function (RBF) [5], Kriging [6,7], multivariate adaptive regression splines (MARS) [8], support vector regression (SVR)

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[9,10], high dimensional model representation (HDMR) [11,12], or the combination of these surrogate models [13–15]. For example, Jin et al. [16] studied several surrogate models based on the multiple performance criteria, including accuracy, robustness, efficiency, transparency, and conceptual simplicity. Their results showed that the polynomial surrogate models may have advantages in efficiency, transparency, and conceptual simplicity over other models. They also noted that the performance of a surrogate model is influenced by sampling. Simpson et al. [17] showed that the approximations of Kriging and RBF models for high-order nonlinear problems are more accurate, while quadratic polynomials are better for low-order nonlinear functions. At the same time, Rijpkema et al. [18] shown that the Kriging model was less stable than the polynomials regression model in some cases. Hence, there is no one surrogate model suitable for all problems over different sampling schemes and different sample sizes. Further studies about the comparison of different kinds of surrogate models can be found in references [19–22].

As aforementioned, the low-order polynomials have been applied to many engineering problems due to their advantages, especially efficiency and transparency. However, due to low accuracy in fitting high-order nonlinear functions, the low-order polynomials have difficulty for problems with high nonlinearity. To keep the merits of low-order polynomials while overcome their weakness for building surrogate models, the high-order polynomials [23] can be applied to establish surrogate models, such as, the Bernstein polynomials [24,25], Chebyshev polynomials [26,27] and Gegenbauer functions [28]. However, how to build surrogate models using high-order polynomials is seldom studied in engineering, mainly because of two reasons: the first is the numerical instabilities, e.g. the Runge phenomena, and the second is the large number of samples for estimation of the unknown coefficients, particularly for high-dimensional problems [29]. In fact, the first can be avoided by selecting new samples to improve stability and accuracy, e.g. the zeros of the first kind Chebyshev polynomials [30–34]. The second can be improved by using a suitable expression of polynomials (e.g. the simplex), which may reduce the number of high-order coefficients to be estimated in the model. It is noted that the required number of samples is more influenced by the extent of complexity and dimension of the function rather than the type of surrogate models. Thus, the required sampling size will increase with the increase of complexity and dimension, no matter which type of surrogate models is used.

The approximation accuracy of a surrogate model is not only determined by the type of surrogate models but also by sampling information. The accuracy of a surrogate model will be improved when more data points are sampled. However, it is impossible to choose too many sample points due to the computational cost. How to evaluate the unknown information only in terms of a limited number of sampling points, to maintain a well trade-off between computational cost and accuracy is an important issue for sampling (or DOE). Traditionally, the DOE can be categorized as Factor Design (FD) [35], Central Composite Design (CCD) [35], Pseudo-Monte Carlo Sampling [36] (PMCS, e.g. the Latin Hypercube sampling [37], and Orthogonal Sampling [38]) and Quasi-Monte Carlo Sampling (QMCS) [3,36,39]. The FD and CCD, belonging to the classical DOE [3], are usually employed for laboratory experiments where the random errors are assumed to exist, while the modern DOE (PMCS and QMCS) are used in deterministic computer simulations without random errors [36].

The above sampling methods can be classified as “one-shot” sampling schemes, as the samples are chosen once and fixed in the fitting process [1]. These methods can be easily implemented and provide a good coverage of the design space without incorporating any prior knowledge of the system. However, the “one-shot” DOE may suffer from its inflexibility to learn the special characteristics of the shape of the response surface [40], and the number of sampling points is easily over or under estimated.

To improve flexibility and efficiency of sampling, the sequential sampling strategy (e.g. the adaptive sampling [41] and incremental sampling [42]) has been developed. Sequential sampling analyses the data from samples and surrogate models in order to select new samples from the regions that are difficult to approximate, resulting in a more efficient distribution of samples in the entire design space compared to the traditional one-shot sampling scheme. That is, in the sequential sampling, a surrogate model is first built using an initial set of samples and then sequentially updated by adding new sample points. There are two schemes used in the sequential sampling: the first is the global exploration, which scatters samples in regions containing no sampling points, and the second is the local exploitation [43] which adds more samples to regions identified to be interesting. The exploration selects sampling points to fill the entire design space, which is mainly used to build global surrogate models, while the exploitation is mainly used in the surrogate model-based optimization. Furthermore, some studies combined exploration with exploitation to build global surrogate models, e.g. [1,40,43].

The exploration aims to place samples in the entire design space uniformly, which is the same as some modern DOEs. However, most QMCS and PMCS are non-incremental sampling methods, as augmenting the number of samples implies a completely different sampling of the parameter space with all new point-locations [44], which will be too expensive to be used. Romero et al. [42] used the Progressive Lattice Sampling (PLS) incremental sampling designs to construct the progressive response surface. However, the PLS allows only a quantized increment M of samples to be added to an existing PLS level (point set) to achieve to a new level. This quantized incremental cost M accelerates quickly with the increase of the PLS level and dimension of the parameter space. To make the sequential sampling more flexible, Romero et al. [44] suggested to use the Halton points to build the progressive response surface, because Halton sampling does not suffer from the cost-scaling problems that the PLS does. Halton [45] is a lower discrepancy (degree of the nonuniformity) sequence method and has a hierarchical structure. The Halton points will be used to compare with the sampling scheme proposed in this paper.

This study will focus on the proposal of a new global surrogate model using high-order polynomials, which can retain the merits of traditional low-order polynomial models while improving approximation accuracy. The sampling points will be sequentially and incrementally selected from a candidate set which is comprised of the zeros of first kind Chebyshev polynomials, to make the surrogate model more stable. In building the surrogate model, only some of the candidate samples are chosen as the required sampling points by using a sequential sampling scheme based on the *maximin* principle [46]. Since the initial samples,