Expert Systems with Applications 38 (2011) 14117–14126

Contents lists available at ScienceDirect

Expert Systems with Applications

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

Adaptive MLS-HDMR metamodeling techniques for high dimensional problems

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ARTICLE INFO

Keywords:
Metamodeling
HDMR
MLS
Sampling
DIRECT

ABSTRACT

Metamodeling technique is to represent the approximation of input variables and output variables. With the exponential increase of dimension of assigned problems, accurate and robust model is difficult to achieve by popular regression methodologies. High-dimensional model representation (HDMR) is a general set of metamodel assessment and analysis tools to improve the efficiency of deducing high dimensional underlying system behavior. In this paper, a new HDMR, based on moving least square (MLS), termed as MLS-HDMR, is introduced. The MLS-HDMR naturally explores and exploits the linearity/nonlinearity and correlation relationships among variables of the underlying function, which is unknown or computationally expensive. Furthermore, to improve the efficiency of the MLS-HDMR, an intelligent sampling strategy, DIviding RECTangles (DIRECT) method is used to sample points. Multiple mathematical test functions are given to illustrate the modeling principles, procedures, and the efficiency and accuracy of the MLS-HDMR models with problems of a wide scope of dimensionalities.

1. Introduction

In the past two decades, approximation methods and approximation-based optimization have attracted intensive attention. This type of approximation model is often termed as metamodel. A metamodel is an approximation of the input/output (I/O) function that is implied by the underlying simulation model. Metamodels are fitted to the I/O data produced by the experiment with the simulation model. Metamodeling involves (a) choosing an experimental design for generating data, (b) choosing a model to represent the data, and then (c) fitting the model to the observed data (Simpson, Peplinski, Koch, & Allen, 2001). Commonly used metamodeling techniques recent year are listed in Table 1 summarized by Wang and Shan (2007).

Although certain progress has been made to improve the efficiency and accuracy of the metamodeling techniques, the present state of metamodeling technique is that the most of low dimensional problems can be done well approximation methodologies (Shan & Wang, 2009). However, the major problem associated with these models (e.g. RBF, polynomial, Kriging) or methodologies is that the modeling effort or resource demand, in order to obtain acceptable accuracy, grows exponentially with the dimensionality of the black-box problems. Therefore, these popular techniques would be inappropriate, or even prohibitive, for modeling high dimensional problems. With the growing of the complexity and dimension of real-life problems, high dimensional approximation problems widely exist in various disciplines. High dimensional black-box problems urgently need to be addressed.

A general set of quantitative model assessment and analysis tool, termed high-dimensional model representation (HDMR), has been introduced recently for high dimensional input–output systems. The HDMR is a particular family of representations where each term in the representation reflects the independent and cooperative contributions of the inputs upon the output HDMR. This method is based on optimization and projection operator theory, which can dramatically reduce the sampling effort for learning the IO behavior of high dimensional systems (i.e., a reduction of effort from exponential scaling to only polynomic complexity) (Li, Rosenthal, & Rabitz, 2001; Li, Wang, Rosenthal, & Rabitz, 2001). Therefore, the HDMR is potential for high dimensional problems.

In this paper, in order to conquer the bottleneck for highly dimensional approximation problems, a HDMR coupled with local approximate method, moving least square (MLS) is proposed, termed as MLS-HDMR. We hope such combination can achieve robust and accurate model efficiently. Furthermore, to improve the efficiency of the metamodeling procedure, an intelligent sampling strategy, DIviding RECTangles (DIRECT) is integrated to generate sample points in each iteration. Therefore, the proposed metamodeling technique is so called adaptive MLS-HDMR method.

The rest of this paper is organized as follows. Section 2 introduces the theoretical bases including HDMR and MLS. Section 3 proposed adaptive-MLS-HDMR method. Performance metrics are introduced in Section 4. In Section 5, various nonlinear high dimensional mathematical functions are used to test the performance of the proposed method. Section 6 gives conclusions finally.

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doi:10.1016/j.eswa.2011.04.220

Table 1
Commonly used metamodeling techniques (Wang & Shan, 2007).

Experimental design/sampling methods	Metamodel choice	Model fitting
• Classic methods – (Fractional) factorial – Central composite – Box-Behnken – Alphabetical optimal – Plackett-Burman • Space-filling methods – Simple grids – Latin hypercube – Orthogonal arrays – Hammersley Sequence – Uniform designs – Minimax and MaximinHybrid methods • Random or humans selection • Importance sampling • Directional simulation • Discriminative sampling • Sequential or adaptive methods	• Polynomial (linear. quadratic, or higher) • Splines (linear, cubic, NURBS) • Multivariate adaptive regression splines (MARS) • Gaussian process • Kriging • Radial basis functions (RBF) • Least interpolating polynomials • Artificial neural network (ANN) • Knowledge base or decision tree • Support vector machine (SVM) • Hybrid models	• (Weighted) Least squares regression • Best linear unbiased predictor (BLUP) • Best linear predictor • Log-likelihood • Multipoint approximation (MPA) • Sequential or adaptive metamodeling • Back propagation (for ANN) • Entropy (inf.-theoretic. for inductive learning on decision tree)

2. Theoretical bases

2.1. HDMR

HDMR is a general set of quantitative model assessment and analysis tools for capturing the high dimensional relationships between input variables and response functions. Let the N-dimensional vector $\boldsymbol{X} = [x_1, x_2, \ldots x_N]^T \in R^N$ with N which represents the input variables of the assigned model, and the output function $f(\boldsymbol{X})$.

The HDMR expresses the response function $f(\boldsymbol{X})$ as a hierarchical correlated function expansion in terms of input variables as

$$f(\boldsymbol{X}) = f_0 + \sum_{i=1}^{N} f_i(x_i) + \sum_{1<i\leqslant j\leqslant N} f_{ij}(x_i, x_j) + \sum_{1<i\leqslant j\leqslant k\leqslant N} f_{ijk}(x_i, x_j, x_k) + \cdots + \sum_{1<i_1\leqslant\cdots\leqslant i_l\leqslant N} f_{i_1 i_2 \cdots i_l(x_{i_1}, x_{i_2}, \ldots, x_{i_l})} + \cdots + f_{12\cdots N}(x_1, x_2, \ldots x_N), \tag{1}$$

where f_0 denotes a constant term representing the 0th order effect to $f(\boldsymbol{X})$. The function $f_i(x_i)$ is a first-order term expressing the effect of variable x_i acting alone, although generally nonlinearly, upon the output response $f(\boldsymbol{X})$. The function $f_{ij}(x_i, x_j)$ is a second-order term that describes the cooperative effects of the variables x_i and x_j upon the output response $f(\boldsymbol{X})$. The higher order terms give the cooperative effects of increasing numbers of input variables acting together to influence the output $f(\boldsymbol{X})$. The last term $f_{12\ldots N}(x_1, x_2, \ldots, x_N)$ contains any residual dependence of all input variables locked together in a cooperative way to influence the output response $f(\boldsymbol{X})$. Once all the relevant component functions in Eq. (1) are determined, the component functions constitute an HDMR, thereby replacing the original computationally expensive method of calculating $f(\boldsymbol{X})$ by the computationally efficient model. Usually the higher order terms in Eq. (1) are negligible such that the HDMR with only low order correlations to second-order amongst input variables is typically used to represent the behavior of output response. The HDMR expansion has a finite number of terms 2^N and is always exact. The HDMR discloses the hierarchy of correlations among the input variables. Each component function of the HDMR has distinct mathematical meaning. At each new level of the HDMR, higher order correlated effects of the input variables are introduced. While there is no correlation term between input variables, only the constant component f_0 and the function terms $f_i(x_i)$ will exist in the HDMR model. Furthermore, it can be proved that $f_0 = f(X_0)$ is the constant term of the Taylor series; the first order function $f_i(x_i)$ is the sum of all the Taylor series terms which only contain variables x_i, while the second order function $f_{ij}(x_i, x_j)$ is the sum of all the Taylor series terms which only contain variables x_i and x_j and so on. There are two particular HDMR expansions: random sampling HDMR (RS-HDMR) and cut-HDMR. The RS-HDMR is useful for measuring the contributions of the variance of individual component functions to the overall variance of the output, and this version is based on the mean value of $f(\boldsymbol{X})$ over entire domain. On the other hand, cut-HDMR expansion is an exact representation of the output $f(\boldsymbol{X})$ in the hyperplane passing through a cut point in the design space. In this study, cut-HDMR algorithm is used to construct metamodel. Using the cut-HDMR, a cut point X_c is defined in the design space. In the convergence limit, cut-HDMR is invariant to the choice of cut point X_c. In practice, X_c is chosen within the neighborhood of interest in the design space. The response function is determined by evaluating the I/O responses of the system relative to the defined cut point X_c along associated lines, planes and sub-volumes, etc. (i.e. cuts) in the design space. This process reduces to the following relationship (Eqs. (2)–(6)) for the component functions in Eq. (1).

$$f_0 = f(\boldsymbol{X}_c), \tag{2}$$

$$f_i(x_i) = f(x_i, \boldsymbol{X}_c^i) - f_0, \tag{3}$$

$$f_{ij}(x_i, x_j) = f(x_i, x_j, \boldsymbol{X}_c^{ij}) - f_i(x_i) - f_j(x_j) - f_0, \tag{4}$$

$$f_{ij}(x_i, x_j, x_k) = f(x_i, x_j, x_k, \boldsymbol{X}_c^{ijk}) - f_{ij}(x_i, x_j) - f_{ik}(x_{ik}) - f_{ik}(x_i, x_k) - f_{jk}(x_j, x_k) - f_i(x_i) - f_j(x_j) - f_k(x_k) - f_0, \tag{5}$$

$$\ldots$$

$$f_{12\cdots N}(x_1, x_2, \ldots, x_N) = f(\boldsymbol{X}) - f_0 - \sum_i f_i(x_i) - \sum_{ij} f_{ij}(x_i, x_j) - \sum_{ijk} f_{ijk}(x_i, x_j, x_k) - \cdots, \tag{6}$$

where $\boldsymbol{X}_c^i$, $\boldsymbol{X}_c^{ij}$, $\boldsymbol{X}_c^{ijk}$ are respectively X_c without terms x_i, x_i, x_j, and x_i, x_j, x_k. The higher order terms are evaluated as cuts in the design space through the cut point. Therefore, each first-order term $f_i(x_i)$ is evaluated along its variable axis through the center point. Each second-order term $f_{ij}(x_i, x_j)$is evaluated in a plane defined by the binary set of input variables x_i, x_j through the cut point; etc. The process of subtracting the lower order expansion functions removes their dependence to assure a unique contribution from the new expansion function.

If each input variable is sampled at s different values, the required number of model runs to construct the $f_i(x_i), f_{ij}(x_i, x_j), \ldots$ can be obtained by