Metamodeling for High Dimensional Simulation-based Design Problems

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Abstract

Computational tools such as finite element analysis and simulation are widely used in engineering. But they are mostly used for design analysis and validation. If these tools can be integrated for design optimization, it will undoubtedly enhance a manufacturer's competitiveness. Such integration, however, faces three main challenges: 1) high computational expense of simulation, 2) the simulation process being a black-box function, and 3) design problems being high dimensional. In the past two decades, metamodeling has been intensively developed to deal with expensive black-box functions, and has achieved success for low dimensional design problems. But when high dimensionality is also present in design, which is often found in practice, there lacks of a practical method to deal with the so-called High-dimensional, Expensive, and Black-box (HEB) problems. This paper proposes the first metamodel of its kind to tackle the HEB problem. This work integrates Radial Basis Function (RBF) with High Dimensional Model Representation (HDMR) into a new model, RBF-HDMR. The developed RBF-HDMR model offers an explicit function expression, and can reveal the 1) contribution of each design variable, 2) inherent linearity/nonlinearity with respect to input variables, and 3) correlation relationships among input variables. An accompanying algorithm to construct the RBF-HDMR has also been developed. The model and the algorithm fundamentally

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change the exponentially growing computation cost to be polynomial. Testing and comparison confirm the efficiency and capability of RBF-HDMR for HEB problems.

Key words: response surface, metamodel, large-scale, high dimension, design optimization, simulation-based design

1. Introduction

Metamodel is a "model of model," which is used to approximate a usually expensive analysis or simulation process; metamodeling refers to the techniques and procedures to construct such a metamodel. In the last two decades, research on metamodeling has been intensive and roughly along one of the four directions, including sampling and evaluation, metamodel development and evaluation, model validation, and metamodel-based optimization. Recently the authors [1] reviewed the applications of metamodeling techniques in the context of engineering design and optimization. Chen [2] summarized pros and cons of the design of experiments methods and approximation models. Simpson *et al.* [3] reviewed the history of metamodeling in the last two decades and presented an excellent summary on what have been achieved in the area thus far and challenges ahead.

It can be seen from the recent reviews that metamodels have been successfully applied to solve low dimensional problems in many disciplines. One major problem associated with these models (e.g., polynomial, RBF and Kriging) and metamodeling methodologies, however, is that in order to reach acceptable accuracy the modeling effort grows exponentially with the dimensionality of the underlying problem. Therefore, the modeling cost will be prohibitive for

these traditional approaches to model high-dimensional problems. In the context of design engineering, according to references [3-6], the dimensionality larger than ten ($d > 10$) is considered high if model/function evaluation is expensive, and such problems widely exist in various disciplines [6-10]. Due to its computational challenge for modeling and optimization, the high dimensionality problem is referred as the notorious "curse of dimensionality" in the literature. For combating the "curse of dimensionality," Friedman and Stuetzle [11] developed projection pursuit regression, which worked well with dimensionality $d \leq 50$ with large data sets. Friedman [12] proposed multivariate adaptive regression splines (MARS) model, which potentially makes improvement over existing methodology in settings involving $3 \leq d \leq 20$, with moderate sample size, $50 \leq N \leq 1000$. Sobol [13] has proved the theorem that an integrable function can be decomposed into summands of different dimensions. This theorem indicates that there exists a unique expansion of high-dimensional model representation (HDMR) for any function $f(\boldsymbol{x})$ integrable in space Ω^d. This HDMR is exact and of finite order and has a hierarchical structure. A family of HDMRs with different characters has since been developed, studied, and applied for various purposes [14-21].

In our recent review of modeling and optimization strategies of high dimensional problems [22], it is found that the research on this topic has been scarce, especially in engineering. In engineering design, there is no metamodel developed to directly tackle HEB problems. Currently available metamodels are not only limited to low dimensional problems, and are also derived in separation from the characteristics of the underlying problem. A different model type is therefore needed for HEB problems. This paper proposes the RBF-HDMR model in response to such a need.

As part of the metamodeling methodology, an adaptive sampling method is also developed to support the proposed RBF-HDMR model. In the research of sampling for metamodeling, sequential and adaptive sampling has gained popularity in recent years, mainly due to the difficulty of knowing the "appropriate" sampling size *a priori*. Lin [23] proposed a sequential exploratory experiment design (SEED) method to sequentially generate new sample points. Jin *et a.l.* [24] applied Enhanced Stochastic Evolution to generate optimal sampling points. Sasena *et al.* [25] used the Bayesian method to adaptively identify sample points that gave more information. Wang [26] proposed an inheritable Latin Hypercube design for adaptive metamodeling. Jin *et al.* [27] compared a few different sequential sampling schemes and found that sequential sampling allows engineers to control the sampling process and it is generally more efficient than one-stage sampling. In this work, we develop an adaptive sampling method that is rooted in the RBF-HDMR model format. Section 4 will describe the method in detail.

Before we introduce the RBF-HDMR and its metamodeling method, the premise of this paper is that are given as below: 1) there exists a unique expansion of HDMR and the full expansion is exact for a high dimensional function, and 2) for most well-defined physical systems, only relatively low-order correlations among input variables are expected to have a significant impact upon the output; and high-order correlated behavior among input variables is expected to be weak [15]. The order of correlation refers to the number of correlated variables, e.g., bivariate correlation is considered low order while multivariate (e.g. five-variable) correlation is high. Premise 1 was proven in Sobol [13]. Broad evidence supporting Premise 2 comes from the multivariate statistical analysis of many systems where significant covariance of highly-correlated input variables rarely appears [6, 15]. Owen [28] observed that high dimensional

functions appearing in the documented success stories did not have full d-dimensional complexity. The rapid dying-off of the order of correlations among input variables does not, however, eliminates non-linear influence of variables, or strong variable dependence, or even the possibility that all the variables are important. These premises pave the way for this work to tackle the "curse of dimensionality".

This paper is organized as follows. Section 2 introduces HDMR. Section 3 proposes the RBF-HDMR model. Section 4 discusses how we address the high dimensionality challenge and describes in detail the metamodeling approach for RBF-HDMR. A modeling example is also given for the ease of understanding of RBF-HDMR and its metamodeling approach. Section 5 studies the behavior of RBF-HDMR with respect to dimensionality through a study problem and testing on a suite of high dimensional problems. The test results are also compared with those from other metamodels based on Latin Hypercube samples. Conclusions are drawn in Section 6.

2. Basic Principle of HDMR

A HDMR represents the mapping between input variables $\boldsymbol{x} = [x_1, x_2, \cdots, x_d]^T$ defined in the design space and the output $f(\boldsymbol{x})$. A general form of HDMR [13,15] is shown as follows:

$$f(\boldsymbol{x}) = f_0 + \sum_{i=1}^{d} f_i(x_i) + \sum_{1\le i<j\le d} f_{ij}(x_i, x_j) + \sum_{1\le i<j<k\le d} f_{ijk}(x_i, x_j, x_k) + \cdots + \sum_{1\le i_1<\cdots<i_l\le d} f_{i_1 i_2 \cdots i_l}(x_{i_1}, x_{i_2}, \cdots, x_{i_l}) + \cdots + f_{12\cdots d}(x_1, x_2, \cdots, x_d) \quad (1)$$

Where the component f_0 is a constant representing the zero-th order effect to $f(\boldsymbol{x})$; the component function $f_i(x_i)$ gives the effect of the variable x_i acting independently upon the output $f(\boldsymbol{x})$ (the first order effect), and may have an either linear or non-linear dependence on x_i. The component function $f_{ij}(x_i, x_j)$ describes the correlated contribution of variables x_i and

x_j upon the output $f(\boldsymbol{x})$ (the second order effect) after the individual influences of x_i and x_j are discounted, and $f_{ij}(x_i, x_j)$ could be linear or nonlinear as well. The subsequent terms reflect the effects of increasing numbers of correlated variables acting together upon the output $f(\boldsymbol{x})$. The last term $f_{12\cdots d}(x_1, x_2, \cdots x_d)$ represents any residual dependence of all the variables locked together to influence the output $f(\boldsymbol{x})$ after all the lower-order correlations and individual influence of each involved x_i (i =1,…,d) have been discounted. As the order of the component function increases, the residual impact of higher correlations decreases. If the impact of an l-th order component function is negligible, the impact of higher order (>l-th) component functions will be even smaller and thus negligible as well. For example if $f_{ij}(x_i, x_j)$ is negligible, then $f_{ijk}(x_i, x_j, x_k)$ will be negligible since it is the residual impact after the influences of $f_i(x_i)$ and $f_{ij}(x_i, x_j)$ are modeled. It is known that the HDMR expansion has a finite number of terms 2^d (d is the number of variables, or dimensionality) and is always exact [13].

There is a family of HDMRs with different features [14, 18-20]. Among these types, the Cut-HDMR [15, 16] involves only simple arithmetic computation and presents the least costly model with similar accuracy as other HDMR types. Therefore Cut-HDMR is chosen as our basis for the proposed RBF-HDMR. A Cut-HDMR [14-15] expresses $f(\boldsymbol{x})$ by a superposition of its values on lines, planes and hyper-planes (or cuts) passing through a "cut" center $\boldsymbol{x}_0$ which is a point in the input variable space. The Cut-HDMR expansion is an exact representation of the output $f(\boldsymbol{x})$ along the cuts passing through $\boldsymbol{x}_0$. The location of the center $\boldsymbol{x}_0$ becomes irrelevant if the expansion is taken out to convergence [15]. On the other hand, if HDMR expansion did not reach convergence, i.e., the model omits significant high order components in the underlying

function, a poor choice of $\boldsymbol{x}_0$ may lead to large error [21]. Sobol [21] suggests using the point as $\boldsymbol{x}_0$ that has the average function value; the average is taken from function values of a certain number of randomly sampled points. The component functions of the Cut-HDMR are listed as follows:

$$f_0 = f(x_0) \tag{2}$$

$$f_i(x_i) = f\left(x_i, \boldsymbol{x}_0^i\right) - f_0 \tag{3}$$

$$f_{ij}\left(x_i, x_j\right) = f\left(x_i, x_j, \boldsymbol{x}_0^{ij}\right) - f_i(x_i) - f_j\left(x_j\right) - f_0 \tag{4}$$

$$f_{ijk}\left(x_i, x_j, x_k\right) = f\left(x_i, x_j, x_k, \boldsymbol{x}_0^{ijk}\right) - f_{ij}\left(x_i, x_j\right) - f_{ik}(x_i, x_k) - f_{jk}\left(x_j, x_k\right) - f_i(x_i) - f_j\left(x_j\right) - f_k(x_k) - f_0 \tag{5}$$

. . .

$$f_{12\cdots d}(x_1, \cdots x_d) = f(x) - f_0 - \sum_i f_i(x_i) - \sum_{ij} f_{ij}(x_i, x_j) - \cdots \tag{6}$$

where $\boldsymbol{x}_0^i$, $\boldsymbol{x}_0^{ij}$, and $\boldsymbol{x}_0^{ijk}$ are respectively $\boldsymbol{x}_0$ without elements x_i; x_i, x_j; and x_i, x_j, x_k. For the convenience of later discussions, the points $\boldsymbol{x}_0$, $\left(x_i, \boldsymbol{x}_0^i\right) = [x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_{d_0}]^T$, $(x_i, x_j, \boldsymbol{x}_0^{ij}) = [x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_j, \cdots, x_{d_0}]^T$, … , are respectively called as the zero-th order, first order, second order model-constructing point(s), respectively. Accordingly, $f(\boldsymbol{x}_0)$ is the value of $f(\boldsymbol{x})$ at $\boldsymbol{x}_0$; $f\left(x_i, \boldsymbol{x}_0^i\right)$ is the value of $f(\boldsymbol{x})$ at point $\left(x_i, \boldsymbol{x}_0^i\right)$.

The HDMR discloses the hierarchy of correlations among the input variables. Each component function of the HDMR has distinct mathematical meaning. At each new order of HDMR, a higher order variable correlation than the previous level is introduced. While there is no correlation among input variables, only the constant component f_0 and the function terms $f_i(x_i)$ exist in the HDMR model. It can be proven that $f_0 = f(\boldsymbol{x}_0)$ 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 [14]. These component functions are optimal choices tailored to $f(\boldsymbol{x})$ over the entire *d*-dimensional space because these component functions are orthogonal to each other, the influence of each component term is independently captured by the model, and the component functions lead to minimum approximation error defined by $\|f(\boldsymbol{x})-f_{\text{model}}(\boldsymbol{x})\|^2$ [14, 15].

Although Cut-HDMR has demonstrated good properties, the model at its current stage only offers a check-up table, lacks of a method to render a complete model, and also lacks of accompanying sampling methods to support it. This work proposes to integrate RBF to model the component functions of HDMR.

3. RBF-HDMR

In order to overcome the drawbacks of HDMR, this work employs RBF to model each component function of the HDMR. Among a variety of RBF formats, this work chooses the one composed of a sum of thin plate spline plus a linear polynomial. The details of the chosen RBF format are in the Appendix. Without losing generality, the simple linear RBF format is used for the ease of description and understanding. In RBF-HDMR, RBF models are used to approximate component functions in Eqs. (3-6), as follows:

$$\hat{f}_i(x_i) = \sum_{k=1}^{m_i} \alpha_{i_k} \left| (x_i, \boldsymbol{x}_0^i) - (x_{i_k}, \boldsymbol{x}_0^i) \right|, \text{where } (x_i, \boldsymbol{x}_0^i) = [x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_{d_0}]^T \quad (7)$$

$$\hat{f}_{ij}(x_i, x_j) = \sum_{k=1}^{m_{ij}} \alpha_{ij_k} \left| (x_i, x_j, \boldsymbol{x}_0^{ij}) - (x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij}) \right| \text{ , where}$$

$$(x_i, x_j, \boldsymbol{x}_0^{ij}) = [x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_j, \cdots, x_{d_0}]^T, i \neq j \tag{8}$$

…

$$\hat{f}_{12\cdots d}(x_1, x_2, \cdots, x_d) = \sum_{k=1}^{m_{12\cdots d}} \alpha_{12\cdots d_k} |\boldsymbol{x} - \boldsymbol{x}_k| \tag{9}$$

Where $\left(x_{i_k}, \boldsymbol{x}_0^i\right), i = 1, \ldots, d$ are points $\left(x_i, \boldsymbol{x}_0^i\right) = \left[x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_{d_0}\right]^T$ evaluated at $k = 1, \ldots, m_i$ along each x_i component; similarly $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij}), k = 1, \cdots, m_{ij}$ are points $[x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_j, \cdots, x_{d_0}]^T$ evaluated at x_i, i=1,…,m_i, and x_j, j=1,…,m_j, that are used to construct the first-order component functions; $\boldsymbol{x}_k$= $[x_{1_k}, x_{2_k}, \cdots, x_{i_k}, \cdots, x_{j_k}, \cdots, x_{d_k}]^T$, k=1,…, $m_{12\cdots d}$, are the points built from evaluated $\boldsymbol{x}$ components for lower order component functions.

Eqs. (7-9) are referred as the modeling lines, planes, and hyper-planes. Substituting the above approximation expressions into the HDMR in Eq. (1), we have the following:

$$f(\boldsymbol{x}) \cong f_0 + \sum_{i=1}^{d} \sum_{k=1}^{m_i} \alpha_{i_k} \left|\left(x_i, \boldsymbol{x}_0^i\right) - \left(x_{i_k}, \boldsymbol{x}_0^i\right)\right| + \sum_{1 \le i < j \le d} \sum_{k=1}^{m_{ij}} \alpha_{ij_k} \left|(x_i, x_j, \boldsymbol{x}_0^{ij}) - (x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij})\right| + \cdots + \sum_{k=1}^{m_{12\cdots d}} \alpha_{12\cdots d_k} |\boldsymbol{x} - \boldsymbol{x}_k| \tag{10}$$

The above approximation in Eq. (10) is called the RBF-HDMR model. Inheriting the hierarchy of HDMR, RBF-HDMR distinctly represents the correlation relationship among the input variables in the underlying function, and provides an explicit model with a finite number of terms. The component functions of multiple RBFs in the model approximate the univariates, bivariates, triple-variates, etc., respectively. The RBF-HDMR approximation of the underlying function $f(\boldsymbol{x})$ is global. Since the HDMR component functions are orthogonal in the design space [14], approximation of HDMR component functions such as RBF-HDMR likely provides

the simplest and also the most efficient model to approximate $f(\boldsymbol{x})$ over the entire d-dimensional design space.

For typical underlying functions, RBF-HDMR expands to the second order as follows

$$f(\boldsymbol{x}) \cong f_0 + \sum_{i=1}^{d} f_i(x_i) + \sum_{1\le i<j\le d} f_{ij}(x_i, x_j)$$
$$\cong f_0 + \sum_{i=1}^{d}\sum_{k=1}^{m_i} \alpha_{i_k}\left|(x_i, \boldsymbol{x}_0^i) - (x_{i_k}, \boldsymbol{x}_0^i)\right| + \sum_{1\le i<j\le d}\sum_{k=1}^{m_{ij}} \alpha_{ij_k}\left|(x_i, x_j, \boldsymbol{x}_0^{ij}) - (x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij})\right| \quad (11)$$

The RBF-HDMR in Eq. (11) neglects higher order component terms based on the assumption that the residual impact of the high order correlation is small after the impact of individual variables and their lower order correlations has been captured. The second model, however, does include all input variables and is capable of capturing high nonlinearity of the underlying function through nonlinear component functions.

As we know RBF is an interpolative function, each component function will go through its own model construction points. But since RBF-HDMR is a summand of these component functions, the question is: "will the resultant RBF-HMDR go through all of the evaluated model construction points?"

Lemma:

A RBF-HDMR model passes through all the prescribed sample points used for constructing zero-th order to the current order component functions.

For clarity, the prescribed, as compared to arbitrarily selected, model-constructing points are explained as follows. For the zero-th order component, the model-constructing point is $\boldsymbol{x}_0$; for

the first order components, the model-construction points include $\boldsymbol{x}_0$ and $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$; for the second order components, its model-construction points are $\boldsymbol{x}_0, \left(x_{i_k}, \boldsymbol{x}_0^i\right), \left(x_{j_k}, \boldsymbol{x}_0^j\right)$ and $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij}), i \neq j$.

The lemma is proved as follows. Assuming $\boldsymbol{x}_0$ is the cut center, the RBF-HDMR at first-order is defined as $f(\boldsymbol{x}) = f_0 + f_i(x_i)$. Its first order component function $f_i(x_i)$ is approximated by one dimensional RBF function $\sum_{k=1}^{m_i} \alpha_{i_k} \left|\left(x_i, \boldsymbol{x}_0^i\right) - \left(x_{i_k}, \boldsymbol{x}_0^i\right)\right|$ by using the function values computed from $f_i\left(x_{i_k}\right) = f\left(x_{i_k}, \boldsymbol{x}_0^i\right) - f_0$, where x_{i_k} is the k-th model-constructing point along x_i, and $f\left(x_{i_k}, \boldsymbol{x}_0^i\right)$ is the true function value at point $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$. Since f_0 is a constant and $f_i(x_i)$ interpolates all model constructing points, the RBF-HDMR model $f(\boldsymbol{x})$ will interpolate all the model constructing points $\boldsymbol{x}_0$ and $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$.

For the second order components, the function values of these components are computed from $f_{ij}\left(x_i, x_j\right) = f\left(x_i, x_j, \boldsymbol{x}_0^{ij}\right) - f_i(x_i) - f_j\left(x_j\right) - f_0$, and $f_{ij}\left(x_i, x_j\right)$ is then approximated by a two-dimensional RBF function $\sum_{k=1}^{m_{ij}} \alpha_{ij_k} \left|\left(x_i, x_j, \boldsymbol{x}_0^{ij}\right) - \left(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij}\right)\right|$ with points $\boldsymbol{x}_0$, $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$, $\left(x_{j_k}, \boldsymbol{x}_0^j\right)$, and $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij}), i \neq j$. It is easy to see $f_{ij}\left(x_i, x_j\right)$ pass through all the evaluated points since they all participated in modeling $f_{ij}\left(x_i, x_j\right)$. For first order component functions, which are functions of only x_i and orthogonal to each other, they will have zero error at $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij})$ since each $f_i(x_i)$ goes through x_i. Therefore all first-order component functions, and therefore the resultant RBF-HDMR model, will pass through all model constructing points to the second order component function, i.e., $\boldsymbol{x}_0$, $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$, $\left(x_{j_k}, \boldsymbol{x}_0^j\right)$, and $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij}), i \neq j$.

Similarly the RBF-HDMR model passes their model-constructing points till the *d*-th component. As the RBF-HDMR has a finite number of terms and each of its component function is exact on these prescribed model-constructing (or evaluated sample) points, the RBF-HDMR model will pass through all sample points. The lemma is proved.

The above lemma not only reveals an important feature of RBF-HDMR, it is also a great help to answer the following question, "if the RBF-HDMR model is built at the *l*-th order, how to identify if there is still (*l*+1)-th order component that need to be modeled?"

Let's start with *l*=1, which indicates that all the zero-th and first order component functions have been modeled using points $\boldsymbol{x}_0$ and $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$. If the second order component functions are to be built, we will use the elements in these existing points to create new sample points $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij})$ for modeling. According to the lemma, the to-be-built second order RBF-HDMR model is then expected to go through these sample points $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij})$. If the first-order RBF-HDMR model cannot accurately predict the function value at the new sample point $(x_{i_k}, x_{j_k}, \boldsymbol{x}_0^{ij})$, it indicates that there must exist second order and/or higher order correlation that has not been modeled, since the approximation error is zero for the first order component functions at points $(x_{i_k}, \boldsymbol{x}_0^i)$ and $(x_{j_k}, \boldsymbol{x}_0^j)$..

To generalize the above discussion, we create a point $\boldsymbol{x}_k = [x_{1_k}, x_{2_k}, \cdots, x_{i_k}, \cdots, x_{j_k}, \cdots, x_{d_k}]^T, k \neq 0$ by random combining the sampled values x_i in the first order component construction for each input variable (i.e., $x_i,\ i = 1,..., d$ and evaluated at

$(x_i, \boldsymbol{x}_0^i)$, respectively). According to the lemma, the complete RBF-HDMR model in Eq. (10) should interpolate this point, $\boldsymbol{x}_k$. If an *l*-th order RBF-HDMR model does not interpolate this point, it indicates that there is higher order (>*l*-th) component functions need to be modeled to decrease the prediction error, and the metamodeling should therefore continue until convergence. This fact has been incorporated in the metamodeling algorithm, which is to be detailed in Section 4.2.

4. Metamodeling for RBF-HDMR

4.1 Strategies for High Dimensionality

From the recent review [22], the authors find that the cost of modeling an underlying function is affected by multiple factors including the function's dimensionality, linearity/nonlinearity, ranges of input variables, and convergence criteria. Generally speaking, the cost increases as the dimensionality and nonlinearity rise, the ranges of input variables become larger, and as the convergence criteria become stricter. This section describes four strategies associated with the proposed metamodeling method for RBF-HDMR that help to circumvent/alleviate the computational difficulty brought by the increase of dimensionality without the loss of sampling resolution.

First, a RBF-HDMR model has a hierarchical structure from zero-th order to *d*-th order components. If this structure can be identified progressively, the cost of constructing higher-order components in HDMR can be saved. The computational cost (i.e. the number of sampling points) of generating a Cut-HDMR up to the *l*-th level is given by [15, 16]

$$c = \sum_{i=0}^{l} \frac{d!}{(d-i)!i!}(s-1)^i = 1 + d(s-1) + \frac{d(d-1)}{2!}(s-1)^2 + \frac{d(d-1)(d-2)}{3!}(s-1)^3 + \cdots$$

$$+ \frac{d(d-1)(d-2)\cdots(d-l+1)}{l!}(s-1)^l \quad (12)$$

Where s is the number of sample points taken for each x_i. The cost of Cut-HDMR is related to the highest order of the Cut-HDMR expansion where the convergence is reached. Each term in Eq. (12) represents the computational cost for constructing the corresponding order of component functions. The cost relates to three factors—the dimensionality d, the number of sampling points s for each variable (i.e., take s levels for each variable), and the highest order of the component functions l. The highest order, l, of component functions represents the maximum number of correlated input variables. As mentioned before, only relatively low-order correlations of the input variables are expected to have an impact upon the output and high-order correlated behavior of the input variables is expected to be weak. Typically $l \leq 3$ has been found to be quite adequate [6]. Considering $l \ll d$, a full space resolution $1/s$ is obtained at the computational cost less than $[d(s-1)]^l/(l-1)!$. Thus the exponentially increasing difficulty s^d is transformed into a polynomial complexity, s^l. This strategy exploits a superposition of functions of a suitable set of low dimensional variables to represent a high dimensional underlying function.

Second, for components of the same order, e.g., at the second order with bivariate correlations, not all possible bivariate correlations may present in the underlying function. Therefore some of the non-existing correlations among input variables can be identified and eliminated from modeling to further reduce the cost. The coefficients in Eq. (12), for example, $\frac{d(d-1)}{2!}$, $\frac{d(d-1)(d-2)}{3!}$, respectively denote the maximum number of probable combinations of the correlated terms at

second and third order component levels. While the number of dimensionality, d, cannot be changed, the number of these coefficients can be reduced if the non-existing correlations can be identified and eliminated and the modeling cost associated with those terms can therefore be saved. The developed metamodeling algorithm for RBF-HDMR adaptively identifies such non-existing correlations and models the underlying function accordingly, which will be described in the next section.

Third, although the number of sample points, *s,* for each variable cannot be reduced in order to keep a certain sampling resolution 1/*s*, these sample points can be reused for modeling higher-order component functions. For example, while modeling second-order component functions, sample points on the reference axes, or hyper-planes, such as $\boldsymbol{x}_0$, $\left(x_{i_k}, \boldsymbol{x}_0^i\right)$, and $\left(x_{j_k}, \boldsymbol{x}_0^j\right)$ are re-used.

Lastly, the number of sample points, *s*, relates to the degree of the nonlinearity of the underlying function with respect to the input variable x_i . The higher the degree of the nonlinearity, the more sample points along x_i are needed to meet the required accuracy. For a linear component, two sample points are enough to accurately model it. The developed metamodeling algorithm for RBF-HDMR gradually explores the non-linearity of the component functions and thus conservatively allocates such cost.

In summary, the RBF-HDMR model naturally helps to transform an exponentially increasing computational difficulty into a polynomial one by neglecting higher order component functions. The proposed metamodeling method will also adaptively explore the linearity/nonlinearity of

each component function, identify non-existing variable correlations, and reuse sample points to further reduce the modeling costs.

4.2 Sampling and Model Construction

Based on the proposed RBF-HDMR model, a sampling and model construction algorithm is developed. The algorithm steps are described as follows:

1. Randomly choose a point $\boldsymbol{x}_0 = \left[x_{1_0}, x_{2_0}, \cdots, x_{d_0}\right]^T$ in the modeling domain as the cut center. Evaluating $f(\boldsymbol{x})$ at $\boldsymbol{x}_0$, we then have f_0.

2. Sample for the first order component functions $f_i(x_i) = f\left([x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_{d_0}]^T\right) - f_0$ in the close neighbourhood of the two ends of x_i (lower and upper limits) while fixing the rest of x_j ($j \neq i$) components at $\boldsymbol{x}_0$. In this work, a neighborhood is defined as one percent of the variable range which is in the design space and near a designated point. Evaluating these two end points, we got the left point value $f_{iL}(x_i) = f\left([x_{1_0}, x_{2_0}, \cdots, x_{i_L}, \cdots, x_{d_0}]^T\right) - f_0$ and the right point value $f_{iR}(x_i) = f\left([x_{1_0}, x_{2_0}, \cdots, x_{i_R}, \cdots, x_{d_0}]^T\right) - f_0$ and model the component function as $\hat{f}_i(x_i)$ by a one dimensional RBF model for each variable x_i .

3. Check the linearity of $f_i(x_i)$. If the approximation model $\hat{f}_i(x_i)$ goes through the center point, $\boldsymbol{x}_0$, $f_i(x_i)$ is considered as linear. In this case, modeling for this component terminates. Otherwise, use the center point $\boldsymbol{x}_0$ and the two end points to re-construct $\hat{f}_i(x_i)$. Then a random value along x_i is generated and combined with the rest of x_j ($j \neq i$) components at $\boldsymbol{x}_0$ to form a new point to test $\hat{f}_i(x_i)$. If $\hat{f}_i(x_i)$ is not sufficiently accurate (the relative prediction error is larger than a given criterion, e.g. 0.1), the test point and all the evaluated points will be used to re-construct $\hat{f}_i(x_i)$. This sampling-remodeling process iterates till convergence. This process is to

capture the nonlinearity of the component function with one sample point at a time. Step 3 repeats for all of the first order component functions to construct the first order terms of RBF-HDMR model.

4. Form a new point, $(x_i, x_j, \cdots x_d)_k = [x_{1_k}, x_{2_k}, \cdots, x_{i_k}, \cdots, x_{j_k}, \cdots, x_{d_k}]^T, k \neq 0$ by random combining the sampled value x_i in the first order component construction for each input variable (i.e., x_i, $i = 1, \ldots, d$ and evaluated at $(x_i, \boldsymbol{x}_0^i)$, respectively). This new point is then evaluated by expensive simulation and the first order RBF-HDMR model. The function values from expensive simulation and model prediction are compared. If the two values are sufficiently close (the relative error is less than a small value, e.g. 0.1), it indicates that no higher-order terms exist in the underlying function, the modeling process terminates. Otherwise, go to the next Step.

5. Use the values of x_i and x_j, $i \neq j$ that exist in thus-far evaluated points $\left(x_i, \boldsymbol{x}_0^i\right) = [x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_{d_0}]^T$, and $\left(x_j, \boldsymbol{x}_0^j\right) = [x_{1_0}, x_{2_0}, \cdots, x_j, \cdots, x_{d_0}]^T$ to form new points of the form $(x_i, x_j, \boldsymbol{x}_0^{ij}) = [x_{1_0}, x_{2_0}, \cdots, x_i, \cdots, x_j, \cdots, x_{d_0}]^T$. Randomly select one of the points from these new points to test the first-order RBF-HDMR model. If the model passes through the new point, it indicates that x_i and x_j are not correlated and the process continues with the next pair of input variables. This is to save the cost of modeling non-existing or insignificant correlations. Otherwise, use this new point and the evaluated points $\left(x_i, \boldsymbol{x}_0^i\right)$ and $\left(x_j, \boldsymbol{x}_0^j\right)$ to construct the second order component function, $\hat{f}_{ij}\left(x_i, x_j\right)$. This sampling-remodeling process iterates for all possible two-variable correlations until convergence (e.g., the relative prediction error is less than 0.1). Step 5 is repeated for all pairs of input variables.

Theoretically, Step 5 applies to all higher-order terms in RBF-HDMR model, Eq. (10), in a similar manner. In this work, the process proceeds towards the end of the second order terms based on the Premise 2 in the introduction section. The identification of correlations in Steps 4 and 5 is supported by the discussions in Section 3.

4.3 An Example for Metamodeling RBF-HDMR

For the ease of understanding, consider the following mathematical function with $d = 3$

$$f(x) = x_2^2 + x_1 x_3 + x_1 - 4,\ 0 \le x_i \le 1 \tag{13}$$

Table 1 shows the modeling processes – finding f_0, modeling the first order components $f_i(x_i), i = 1, \cdots, 3$, detecting and exploiting linearity and correlation relationship in the underlying function, and modeling higher order components, $f_{ij}, i \neq j$, if they exist. This process continues until convergence. The first and last rows list the original function and the corresponding RBF-HDMR model, respectively. Each middle row demonstrates the modeling process in hierarchy. The detailed steps are as follows.

Step 1. Randomly sample the cut center $\boldsymbol{x}_0$ in the neighbourhood of the center of the design space, in this case, $\boldsymbol{x}_0 = [0.5, 0.5, 0.5]^T$ and then find $f_0 = f(\boldsymbol{x}_0)$.

Step 2. Randomly sample x_i at its two ends, and form two new points $(x_i, \boldsymbol{x}_0^i)$ (one per end) and evaluate them. Model the component functions using the two end points. For example, for x_1, two values 0 and 1 are sampled; we can use the function values [f (0, 0.5, 0.5)-f_0] and [f (1, 0.5, 0.5)-f_0] as their function values for 0 and 1, respectively to model $f_1(x_1)$. Note that the special

RBF format as in the Appendix is used rather than the simple linear spline format to avoid matrix singularity.

Step 3. Detect the linearity of the output function with respect to each variable x_i by comparing $f(\boldsymbol{x}_0)$ and $\hat{f}(\boldsymbol{x}_0)$. If nonlinearity exists, model $f_i(x_i), i = 1, \cdots, 3$ till convergence. The $f_2(x_2)$ component function, for instance, is a nonlinear function. In addition to the two end points 0 and 1, two more new sample points are generated at 0.19 and 0.81 to capture its nonlinearity. All of the component functions are plotted with a distance f_0 in the last column in Table 1.

Step 4. Identify if correlation exists. If no, terminate modeling. Otherwise, go to Step 5. In this case, since there exists correlation between x_1 and x_3, the modeling process continues.

Step 5. Identify the correlated terms according to Step 5 of the algorithm described in Section 4.2. If correlation exists in the underlying function, model the identified correlated terms. In this case, only the correlated term $x_1 x_3$ exists, which needs to be modeled as a component function. Repeat Step 5 until convergence.

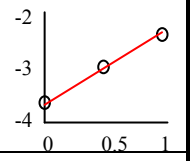
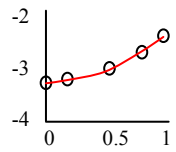
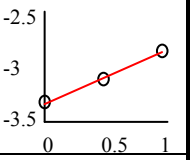
To better understand Table 1, let us take modeling $f_2(x_2)$ as an example. When modeling $f_2(x_2)$, five values along x_2 are generated, i.e., 0, 1, 0.5, 0.19, 0.81, according to the sampling algorithm described in Section 4.2. By combining these values with other $\boldsymbol{x}_0$ component values except for x_2, we have five new points and their function values are evaluated. Deducted the f_0 value from their function values, we obtain the component function $f_2(x_2)$ values for these five points are, respectively, -0.25, 0.75, 0.0, -0.2139, 0.4061. Employing these five points and their function values to fit the RBF function as defined in the Appendix, one can have the RBF model for $f_2(x_2)$, with five nonlinear terms and two polynomial terms, as shown in the last row of Table 1.

In Table 1, $f_3(x_3)$ is especially noteworthy. One can see from the original function expression that there is no separate x_3 term in the function, but an x_1x_3 term. Why is $f_3(x_3)$ not zero? This is because HDMR first finds the first order influence of x_3, the residual then goes to the second order component function $f_{13}(x_1, x_3)$. Therefore, it would be wrong to mechanically match the component functions with the terms in the underlying function. As a matter of fact, the x_1x_3 term in the original function has been expressed by $f_3(x_3)$ and $f_{13}(x_1, x_3)$, as well as partially by $f_1(x_1)$.

Figure 1 shows the distribution of all sample points in the modeling space. It can be seen that most sampled points are located on the lines and planes across the cut center $\boldsymbol{x}_0$. Points $\boldsymbol{x}_{12}, \boldsymbol{x}_{13}, \boldsymbol{x}_{23}$ and $\boldsymbol{x}_{123}$ were used to identify the correlation among the variables, respectively between x_1 and x_2, x_1 and x_3, x_2 and x_3, as well as the existence of correlations among all variables x_1, x_2 and x_3 of the underlying function. It is to note that these sample points are generated as needed according to the aforementioned sampling and model construction method.

Fig. 1 Distribution of sample points for the example problem

Table 1 Process of modeling RBF-HDMR for the example problem

Function	$f(\boldsymbol{x}) = x_2^2 + x_1x_3 + x_1 - 4, \quad 0 \le x_i \le 1$					
f_0	$f(\boldsymbol{x}_0) = f([0.5, 0.5, 0.5]^T) = -3$					
$f_i(x_i)$	Linearity	Samples x_i	Observed $f(\boldsymbol{x})$	$f(x_i, \bar{x}^i) - f_0$	RBF coefs	Component Function Plot
	$f_1(x_1)$ (linear)	0 1 0.5	-3.75 -2.25 -3	-0.75 0.75 0	0 0 0 -0.75 1.5	
	$f_2(x_2)$ (non-linear)	0 1 0.5 0.19 0.81	-3.25 -2.25 -3 -3.2139 -2.5939	-0.25 0.75 0 -0.2139 0.4061	0.6796 0.6796 -0.1754 -0.5918 -0.5918 -0.3977 1	
	$f_3(x_3)$ (linear)	0 1 0.5	-3.25 -2.75 -3	-0.25 0.25 0	0 0 0 -0.25 0.5	
$f_{ij}(x_i, x_j)$	Correlation Relationship	Sampling $[x_i, x_j]^T$	Observed $f(\boldsymbol{x})$	$f(x_1, x_3, \boldsymbol{x}_0^{ij}) - f_1(x_1) - f_3(x_3) - f_0$		RBF coefs
	$f_{12}(x_1, x_2)$	null	null	null		null
	$f_{13}(x_1, x_3)$	(0.5,0.5); (0,0.5); (1,0.5); (0.5,0); (0.5, 1); (0,0); (1,1); (0,1); (1,0);	-3 -3.75 -2.25 -3.25 -2.75 -3.75 -1.75 -3.75 -2.75	0 0 0 0 0 0.25 0.25 -0.25 -0.25		0;0;0;0;0; 0.3607; 0.3607; -0.3607; -0.3607; 0;0;0
	$f_{23}(x_2, x_3)$	null	null	null		null
$\hat{f}(\boldsymbol{x})$	$\overbrace{-3}^{f_0} \overbrace{-0.75 + 1.5x_1}^{f_1} + \overbrace{0.6796\lvert x_2\rvert^2 \log\lvert x_2\rvert + 0.6796\lvert x_2 - 1\rvert^2 \log\lvert x_2 - 1\rvert - 0.1754\lvert x_2 - 0.5\rvert^2 \log\lvert x_2 - 0.5\rvert - 0.5918\lvert x_2 - 0.19\rvert^2 \log\lvert x_2 - 0.19\rvert - 0.5918\lvert x_2 - 0.81\rvert^2 \log\lvert x_2 - 0.81\rvert - 0.3977 + x_2}^{f_2} \overbrace{-0.25 + 0.5x_3}^{f_3} + \overbrace{0.3607 \begin{vmatrix} x_1 \\ x_3 \end{vmatrix}^2 \log \begin{vmatrix} x_1 \\ x_3 \end{vmatrix} + 0.3607 \begin{vmatrix} x_1 - 1 \\ x_3 - 1 \end{vmatrix}^2 \log \begin{vmatrix} x_1 - 1 \\ x_3 - 1 \end{vmatrix} - 0.3607 \begin{vmatrix} x_1 - 0 \\ x_3 - 1 \end{vmatrix}^2 \log \begin{vmatrix} x_1 - 0 \\ x_3 - 1 \end{vmatrix} - 0.3607 \begin{vmatrix} x_1 - 1 \\ x_3 - 0 \end{vmatrix}^2 \log \begin{vmatrix} x_1 - 1 \\ x_3 - 0 \end{vmatrix}}^{f_{13}}$				

Given the metamodel as expressed in the last row of Table 1, one can observe that all first order functions are linear except for f_2, which indicates that x_2 has a nonlinear influence to the overall f function while others have linear effects. For the second order components, only a nonlinear f_{13} is present, indicating other variables are not correlated.

5. Testing of RBF-HDMR

Problems from literature are used for testing the proposed RBF-HDMR and its metamodeling method. The modeling efficiency is indicated by the number of (expensive) sample points. The modeling accuracy is evaluated by three performance metrics. A comparison of the RBF-HDMR model with other metamodels is also given.

5.1 Performance Metrics

There are various commonly-used performance metrics for approximation models that are given in [22]. To the authors' knowledge, however, there are no specially defined performance metrics for high dimensional approximation models in the open literature. In mathematics, where the high dimensional problems are mostly (and yet not adequately) studied, the percentage relative error is often used as a metric for model validation. It is found, however, when the absolute errors of the metamodels are quite small, their percentage relative errors could be extremely large when the function value is close to zero. The percentage relative error measure is also dependent on the problem scale, which makes the comparison between problems disputable. In the engineering design, the cross-validation method is currently a popular method for model validation. However, Lin [23] found that the cross-validation is an insufficient measurement for metamodel accuracy. The cross-validation is actually a measurement for degrees of insensitivity

of a metamodel to lost information at its data points, while an insensitive metamodel is not necessarily accurate. To be consistent with Ref. [5], which will be used for result comparison, this work employs three commonly used performance metrics —R square, relative average absolute error (RAAE) and relative maximum absolute error (RMAE) —for validating approximation models. After the RBF-HDMR modeling process is terminated, additional 10,000 new random sample points are used to evaluate the model against the three performance metrics by Monte Carlo simulation. The values of these performance metrics show the prediction capability of the RBF-HDMR on new points. It is to be noted that these three metrics all need a fairly large number of validation points to be meaningful but for High dimensional, Expensive, Black-box (HEB) problems such information are too costly to obtain. This is in contrast to high dimensional problems studied in mathematics where those are inexpensive problems and a large quantity of validation points is affordable. Validation methodology for HEB problems is therefore worth further research. Since this work also chose mathematical problems for testing and comparison, we can still employ the three metrics with Monte Carlo simulations for validation. These metrics are described as below:

1) R Square:

$$R^2 = 1 - \frac{\sum_{i=1}^{m}[f(x_i)-\hat{f}(x_i)]^2}{\sum_{i=1}^{m}[f(x_i)-\bar{f}(x_i)]^2} \tag{14}$$

Where $\bar{f}(x_i)$ denotes the mean of function on m sample points. This metrics indicates the overall accuracy of an approximation model. The closer the value of R square approaches one, the more accurate is the approximation model. Note that R^2 is evaluated on the new validation points, not on the modeling points. The same is true for RAAE and RMAE.

2) Relative Average Absolute Error (RAAE):

$$RAAE = \frac{\sum_{i=1}^{m} |f(x_i) - \hat{f}(x_i)|}{m * STD} \tag{15}$$

where *STD* stands for standard deviation. Like R square, this metric shows the overall accuracy of an approximation model. The closer the value of RAAE approaches zero, the more accurate is the approximation model.

3) Relative Maximum Absolute Error (RMAE):

$$RMAE = \frac{\max\left(|f(x_1) - \hat{f}(x_1)|, |f(x_2) - \hat{f}(x_2)|, \cdots, |f(x_m) - \hat{f}(x_m)|\right)}{STD} \tag{16}$$

This is a local metric. A RMAE describes error in a sub-region of the design space. Therefore, a small value of RMAE is preferred.

5.2 Study Problem

A problem for large-scale optimization in Matlab™ optimization toolbox is chosen to study the performance of RBF-HDMR and its metamodeling method as a function of the dimensionality, *d*.

$$f(\boldsymbol{x}) = \sum_{i=1}^{d-1} [(x_i^2)^{(x_{i+1}^2+1)} + (x_{i+1}^2)^{(x_i^2+1)}], \ 0 \le x_i \le 1 \tag{17}$$

This highly nonlinear problem was tested with *d*=30, 50, 100, 150, 200, 250 and 300. For each *d*, ten runs have been taken and the mean values of R square, RAAE and RMAE are charted in Fig. 3.

Fig. 2 Performance metrics mean with respect to *d* (x-axis) for the study problem

As seen from Fig. 2, although the three accuracy performance metrics deteriorate slightly as *d* increases, they demonstrate that the RBF-HDMR model fits well the high dimensional

underlying function. The minimum (worst) value of R square is close to 0.9, the maximum (worst) values of RAAE is about 0.32 and the maximum (worst) value of RMAE is about 0.54. The data explains the RBF-HDMR model has a good fit of the underlying function.

Regarding to modeling cost, assuming five samples are taken along each axes ($s = 5$), we list the number of evaluations for RBF-HDMR model, full second order expansion of the HDMR (polynomially increasing cost), and the full factorial design of experiments (exponentially increasing cost) for various dimensionality d in Table 2. The comparison clearly shows the computational advantage of the proposed RBF-HDMR. The efficiency of the proposed method will be further studied in comparison with Latin Hypercube samples in the next section.

Table 2 Comparison of modeling cost for the study problem

d	Cost of RBF-HDMR (second order)	Cost of a full second order expansion of HDMR $c = 1 + d(s-1) + \frac{d(d-1)}{2!}(s-1)^2$ (polynomial)	Cost of full factorial design s^d (exponential)
30	819	7081	$9.31 \text{ X } 10^{20}$
50	1830	19801	$8.88 \text{ X } 10^{34}$
100	6116	79601	$7.88 \text{ X } 10^{69}$
150	12807	179401	$7.01 \text{ X } 10^{104}$
200	22042	319201	$6.22 \text{ X } 10^{139}$
250	33762	499001	$5.53 \text{ X } 10^{174}$
300	47979	718801	$4.91 \text{ X } 10^{209}$

5.3 Testing and Comparison with Other Metamodels

In order to test the effectiveness of various models (MARS, RBF, Kriging, and polynomial), Jin et al. [5] selected 14 problems which are classified into two categories: large scale and small scale. The large scale includes one 14-variable application, one 16-variable, and four 10-variable problems. The small scale includes five two-variable problems and three three-variable problems, among which one was repeated by adding some noise to form a new problem. Therefore, in total Ref. [5] gives 13 unique problems, twelve are tested with RBF-HDMR except for the 14-variable application problem, which is unavailable to authors. Since this work deals with high dimensional problems, only the test results for the large scale problems (Problems 1-5) are reported in Table 3 with the first and second order RBF-HDMR models. These problems are listed in the Appendix. In our test, each problem runs ten times independently for robustness testing, and then takes the average of ten runs for each problem. In Table 3, NoE indicates the number of all evaluated expensive points, which include modeling points and detecting points

that used for correlation identification. The NoE for the second order modeling includes the NoE for the first order modeling.

Table 3 Modeling results for the test suite.

Problem		R Square	RAAE	RMAE	NoE
1 (d=10)	First	0.90	0.233	1.66	95
	Second	0.92	0.211	1.16	321
2 (d=10)	First	1.00	0.006	0.04	40
	Second	1.00	0.006	0.02	232
3 (d=10)	First	0.99	0.049	0.59	121
	Second	0.96	0.129	1.16	408
4 (d=10)	First	0.98	0.110	0.33	34
	Second	0.98	0.107	0.28	40
5 (d=16)	First	0.96	0.150	0.91	59
	Second	0.99	0.088	0.25	297
Mean	First	0.97	0.109	0.71	70
	Second	0.97	0.113	0.65	250

It is can be seen from Table 3 that all results of the first order RBF-HDMR are good enough for large scale problems, even though Problems 1 and 3 are highly nonlinear. The results of the second-order models show slight improvement over the first-order models for all the problems except for Problem 3, which indicates a certain degree of over fitting. Theoretically when convergence criteria or numeric tolerance for nonlinearity and correlation identification is sufficiently tight, the second order model should be more accurate than the first order. In practice, however, the errors in nonlinearity and correlation identification and RBF model construction may be larger than the influence of higher order components. In such circumstances, over-fitting of RBF may occur.

To understand the test results in Table 3, we compare the results with those from Ref. [5] in Figure 3. Ref. [5] used three different Latin Hypercube Design (LHD) sample sets for the large

scale problems. Their average numbers are 34, 112, and 250 for scarce, small, and large data sets, respectively. From Figure 3, one can see that the first order RBF-HDMR modeling requires a data set of a size falling in between those of the scarce and small data sets.

Figure 3 Comparison of NoE with Latin Hypercube points from Reference [5].

Figure 4 Model accuracy comparison. Data for models other than RBF-HDMR are from Ref. [5]; R^2 values are for large-scale problems only, while RMAE and RAAE values are for all 14 test problems.

Figure 4 shows the mean value of the same three metrics — R square, RAAE and RMAE — for the aforementioned four models applied to test problems. From Fig. 4, it can be seen that while the mean R^2 for RBF-HDMR models is 0.97, the maximum (best) value of the four models in the reference is about 0.78. Because that the exact RAAE and RMAE data for only the large-scale problems are not available in Ref. [5], we use the mean for all 14 test problems as a comparison. The RAAE and RMAE values for the 14 problems should be lower than that for the large scale problems alone. Even with these comparison values, RBF-HDMR has much smaller RAAE and RMAE values. It is also to be noted that the accuracy data from Ref. [5] is based on the average results for all data sets. The highest R^2 value for large sample sets (250 points) for the four models is slightly above 0.90, still significantly lower than 0.97, which is the R^2 value of RBF-HDMR with only 70 points.

In summary, from the comparison with the reference, the proposed RBF-HDMR model and its metamodeling method generates more accurate models with fewer sample points than conventional models such as MARS, RBF, Kriging, and polynomial functions with Latin Hypercube designs.

5.4 Discussion

This work employs RBF to model component functions of the HDMR, so that HDMR is no longer a check-up table but rather a complete equation. The proposed metamodeling approach takes advantages of properties of HDMR to make the sampling efficient. RBF was chosen because of 1) its simplicity and robustness in model construction 2) the ease of obtaining an explicit function expression, and 3) its ability to interpolate the sample points (this could be a problem for noisy data, which will be a topic of our future research). The integration of HDMR with the interpolative feature of RBF supports the developed lemma and the sampling method, especially on identification of nonlinearity, variable correlations, and higher order components. Therefore RBF helps to reduce the sample size. The choice of a specific RBF form, as shown in the Appendix, is deliberate as it is better than a simple linear spline for avoiding singularity. Exploration of other interpolative metamodels and selection of the best metamodel for component functions may be a topic for future research.

The proposed metamodeling approach takes advantage of the hierarchical structure of HDMR, adaptively models its component functions while exploring its inherent linearity/nonlinearity and correlation among variables. The sample points are thus limited and well controlled. The realized

samples spread in the design space (refer to Fig. 1), but unevenly, according to complexity of regions in the space. Regions of high nonlinearity or correlation will have more sample points while linear regions have fewer points, all according to the needs to capture the behavior of the underlying function. In contrast, the Latin Hypercube Design (LHD) has only one-dimensional uniformity and it is "blind" to the function characteristics. It is also worth noting that the metamodeling process only involves fast and simple algebraic operations, which also lends itself well for parallel computation at each order of component levels. The outputs are multitude, i.e., an explicit RBF-HDMR model, function linearity/non-linearity, correlations among variables, and so on.

The RBF-HDMR at currently stage, however, only models to the second-order components. If an underlying function has significant multivariate correlation, the method may be limited. New approaches are needed to extend beyond the second-order, whereas keeping the modeling cost low. Secondly, the proposed RBF-HDMR adaptively determines the location of sample points, which is attractive when there is no existing data and the goal is to reduce the number of function evaluations. In real practice, however, there are situations that some expensive data may have already been generated. Strategies needed to be developed to take advantage of the existing data when constructing RBF-HDMR. Thirdly, RBF-HDMR at its current stage only deals with deterministic problems while in practice the expensive model may be noisy. Future research is needed to deal with these issues.

6. Conclusion

This work proposes a methodology of metamodeling High dimensional, Expensive, and Black-box (HEB) problems. The methodology consists of the proposed RBF-HDMR metamodel, and its accompanying metamodeling method. The RBF-HDMR model inherits hierarchical structural properties of HDMR, provides an explicit expression with RBF components, and needs neither any knowledge about the underlying functions nor assumes *a priori* a parametric form. The modeling process automatically explores and makes use of the properties of the underlying functions, refines the model accuracy by iterative sampling in the subspace of nonlinearity and correlated variables, and involves only fast and simple algebraic operations that can be easily parallelized. The developed methodology alleviates or circumvents the "curse of dimensionality." Testing and comparison with other metamodels reveal that RBF-HDMR models high dimensional problems with higher efficiency and accuracy. Future research aims to extend the modeling approach to efficiently model high-order components, to use existing data, and to deal with noisy samples.

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Appendix

1. RBF model

A general radial basis functions (RBF) model [2,5] is shown as follows.

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{n} \beta_i \varphi(|\boldsymbol{x} - \boldsymbol{x}_i|) \tag{A.1}$$

Where β_i is the coefficient of the expression and $\boldsymbol{x}_i$ are the sampled points of input variables or the centers of RBF approximation. $\varphi(.)$ is a distance function or the radial basis function. $|.|$ denotes a *p*-norm distance. A RBF is a real-valued function whose value depends only on the distance from center points $\boldsymbol{x}_i$. It employs linear combinations of a radically symmetric function based on the distance to approximate underlying functions. Its advantages include: the number of sampled points for constructing approximation can be small and the approximations are good fits to arbitrary contours of response functions [2]. Consequently, RBF is a popular model for multivariate data interpolation and function approximations.

The key of RBF approach is to choose a *p*-norm and a radial basis function $\phi(.)$, both of which have multiple formats. One of the goals for choosing a format is to make the distance matrix ($A_{ij} = \varphi(|\boldsymbol{x}_i - \boldsymbol{x}_j|)$, for $1 \leq i,j \leq n$, n is the number of sample points) non-singular. The singularity of the distance matrix relates to the distribution of the sample points. It can be seen that there are many works on choosing a *p*-norm and a radial basis function $\varphi(.)$ to avoid the singularity of the distance matrix [29]. This research uses a sum of thin plate spline (the first term) plus a linear polynomial $P(\boldsymbol{x})$ (the second term) as follows.

$$\hat{f}(\boldsymbol{x}) = \sum_{i=1}^{n} \beta_i \, |\boldsymbol{x} - \boldsymbol{x}_i|^2 log|\boldsymbol{x} - \boldsymbol{x}_i| + P(\boldsymbol{x})$$

$$\textstyle\sum_{i=1}^{n} \beta_i \, \boldsymbol{p}(\boldsymbol{x}) = \boldsymbol{0}, \;\; P(\boldsymbol{x}) = \boldsymbol{p}\boldsymbol{\alpha} = [p_1, p_2, \cdots, p_q][\alpha_1, \alpha_2, \cdots, \alpha_q]^T \qquad \text{(A.2)}$$

Where $\boldsymbol{x_i}$ are the vectors of evaluated *n* sample points; the coefficients $\boldsymbol{\beta} = [\beta_1, \beta_2, \cdots, \beta_n]$ and $\boldsymbol{\alpha}$ are parameters to be found. $P(\boldsymbol{x})$ is a polynomial function, where $\boldsymbol{p}$ consists of a vector of basis of polynomials. In this work, $\boldsymbol{p}$ is chosen to be $(1, x_1, \cdots, x_d)$ including only linear variable

terms and therefore q=d+1; The side condition $\sum_{i=1}^{n} \beta_i \, \boldsymbol{p}(\boldsymbol{x}) = 0$ is imposed on the coefficients $\boldsymbol{\beta}$ to improve an under-determined system, i.e., the singularity of distance matrix $\boldsymbol{A}$ [29**]**. To calculate the coefficients $\boldsymbol{\beta}$ and $\boldsymbol{\alpha}$, Eq. (A.2) may be written in the matrix form as below

$$\begin{bmatrix} \boldsymbol{A} & \widetilde{\boldsymbol{P}} \\ \widetilde{\boldsymbol{P}}^{\boldsymbol{T}} & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta} \\ \boldsymbol{\alpha} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{0} \end{bmatrix} \tag{A.3}$$

Where, $A_{ij} = \left|\boldsymbol{x}_i - \boldsymbol{x}_j\right|^2 log\left|\boldsymbol{x}_i - \boldsymbol{x}_j\right|, \;\; i, j = 1, \cdots, n$

$$\tilde{P}_{ij} = p_j(\boldsymbol{x}_i), \;\; i = 1, \cdots, n; \;\; j = 1, \cdots, (d+1);$$

and $\boldsymbol{x_i}$ and $\boldsymbol{x}_j$ are the vectors of evaluated n sample points. The theory guarantees the existence of a unique vector $\boldsymbol{\beta}$ and a unique polynomial $P(\boldsymbol{x})$ satisfying Eq.(A.2) [29].

2. Test Problems

No.	Function	Variable Ranges
1	$f(\boldsymbol{x}) = \sum_{i=1}^{10} [[\ln(x_i - 2)]^2 + [\ln(10 - x_i)]^2] - (\prod_{i=1}^{10} x_i)^{0.2}$	$2.1 \le x_i \le 9.9,$ $i = 1, \cdots, 10$
2	$f(\boldsymbol{x}) = \sum_{i=1}^{10} x_i (c_i + ln \frac{x_i}{x_1 + \cdots + x_{10}})$	$1E-6 \le x_i \le 10, i = 1, \cdots, 10$
3	$f(\boldsymbol{x}) = \sum_{i=1}^{10} \exp(x_i) [c_i + x_i - \ln (\sum_{k=1}^{10} \exp(x_k))]$	$-10 \le x_i \le 10,$ $i = 1, \cdots, 10$
4	$f(\boldsymbol{x}) = x_1^2 + x_2^2 + x_1 x_2 - 14x_1 - 16x_2 + (x_3 - 10)^2 + 4(x_4 - 5)^2 + (x_5 - 3)^2 + 2(x_6 - 1)^2 + 5x_7^2 + 7(x_8 - 11)^2 + 2(x_9 - 10)^2 + (x_{10} - 7)^2 + 45$	$-10 \le x_i \le 11,$ $i = 1, \cdots, 10$
5	$f(\boldsymbol{x}) = \sum_{i=1}^{16} \sum_{j=1}^{16} a_{ij} (x_i^2 + x_i + 1)(x_j^2 + x_j + 1)$	$0 \le x_i, x_j \le 5,$ $i, j = 1, \cdots, 16$

For Prob. 2 and 3

$c_{i=1,\cdots,10}$
$= -6.089, -17.164, -34.054, -5.914, -24.721, -14.986, -24.100, -10.708, -26.662, -22.179$

For Prob. 5

$$[a_{ij}]_{row1-8} = \begin{bmatrix} 1\,0\,0\,1\,0\,0\,1\,1\,0\,0\,0\,0\,0\,0\,0\,1 \\ 0\,1\,1\,0\,0\,0\,1\,0\,0\,1\,0\,0\,0\,0\,0\,0 \\ 0\,0\,1\,0\,0\,0\,1\,0\,1\,1\,0\,0\,0\,1\,0\,0 \\ 0\,0\,0\,1\,0\,0\,1\,0\,0\,0\,1\,0\,0\,0\,1\,0 \\ 0\,0\,0\,0\,1\,1\,0\,0\,0\,1\,0\,1\,0\,0\,0\,1 \\ 0\,0\,0\,0\,0\,1\,0\,1\,0\,0\,0\,0\,0\,0\,1\,0 \\ 0\,0\,0\,0\,0\,0\,1\,0\,0\,0\,1\,0\,1\,0\,0\,0 \\ 0\,0\,0\,0\,0\,0\,0\,1\,0\,1\,0\,0\,0\,0\,1\,0 \end{bmatrix} \quad [a_{ij}]_{row9-16} = \begin{bmatrix} 0\,0\,0\,0\,0\,0\,0\,0\,1\,0\,0\,1\,0\,0\,0\,1 \\ 0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,1\,0\,0\,0\,0 \\ 0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,1\,0\,1\,0 \\ 0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,1\,0\,0 \\ 0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,1\,0 \\ 0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,0\,1 \end{bmatrix}$$

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