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ORIGINAL PAPER

Constancy maximization based weight optimization in high dimensional model representation for multivariate functions

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Abstract High Dimensional Model Representation (HDMR) method is a technique that represents a multivariate function in terms of less-variate functions. Even though the method has a finite expansion, to determine the components of this expansion is very expensive due to integration based natures of the components. Hence, the HDMR expansion is generally truncated at certain multivariance level and such approximations are produced to represent the given multivariate function approximately. The weight function selection becomes an important issue for the HDMR based applications when it is desired to give different importances to function values at different points. An appropriately chosen weight function may increase the quality of the approximation incredibly. This work aims at a multivariate weight function optimization to obtain high quality approximations through the HDMR method to represent multivariate functions. The proposed optimization considers constancy measurer maximization which produces a quadratic vector equation to be solved. Another contribution of this work is to use a recently developed method, fluctuation free integration, with HDMR, to solve this equation easily. This work is an extension of a previous work about weight optimization in HDMR for univariate functions.

Keywords High Dimensional Model Representation · Multivariate functions · Approximation · Optimization · Fluctuation expansion

1 Introduction

High Dimensional Model Representation (HDMR) method which is a divide-and-conquer algorithm is used to represent a multivariate function in terms of less variate

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functions such as univariate, bivariate or higher variate functions. This method was first proposed by I.M. Sobol in 1993 [1] with constant unit weight and unit interval, [0, 1], and it was used for sensitivity analysis of such problems in which the Monte Carlo based algorithms are being applied. After Sobol, Rabitz [2–4] and his group extended the structure of the method by introducing a weight function which is product of some univariate weight functions each of which depends on a separate independent variable and a general interval definition into the algorithm to develop more generalized HDMR based methods for random sampling, chemical modeling and so on. In the same time period, M. Demiralp [5–16] and his group worked on HDMR and developed several methods for multivariate interpolation problems, algebraic eigenvalue problem modelling, Schrödinger's equation, optimal control of harmonic oscillator, exponential matrix evaluation and so on.

Many other HDMR based methods for various research areas have been also developed by many other scientists [17–26].

The HDMR expansion has the following finite sum

$$f(x_1, \ldots, x_N) = f_0 + \sum_{i_1=1}^{N} f_{i_1}(x_{i_1}) + \sum_{\substack{i_1,i_2=1 \\ i_1<i_2}}^{N} f_{i_1 i_2}(x_{i_1}, x_{i_2}) + \ldots + f_{12\ldots N}(x_1, \ldots, x_N) \tag{1}$$

where the determination of the general structures of the right hand side components is the main purpose of the method. These mentioned structures can be determined under a weight function and a number of integrals. There exist 2^N components at the right hand side of this expansion and to represent a multivariate function exactly through this expansion we need to evaluate all the components. This results in high mathematical and computational complexity. The mostly used solution to bypass this disadvantage is to take few components of the expansion into consideration and to obtain an approximation as the representation of the given multivariate function. In literature, at most bivariate terms are used for the representation of the given multivariate functions for practical purposes. However, this time the quality of the proposed approximations becomes the most important point for a successful representation. As a result, an appropriate weight function selection for the given problem plays an important role to increase the performance of this approximation since it is only stakeholder of the determination process of the HDMR components given in (1).

A study about the weight function optimization to construct the appropriate weight function for dominating less variate terms in HDMR has been quite recently realized just for the univariate functions by the authors [27]. However, we have multi para meters in real life problems of chemistry, physics, engineering and so on to model the situation. Hence, we need a more generalized structure for the weight optimization process in HDMR. This corresponds to a multivariate weight function optimization procedure for the HDMR method to represent the given multivariate function of a real life problem.

Now, this paper focuses on the HDMR's constancy optimization for a given multivariate function to construct the best weight function producing highest dominancy in the less variate terms. The details of the constancy measurer optimization for HDMR truncation approximation are given in the third section. Nonlinear algebraic equations appearing in the optimization process can be approximately solved via fluctuation free matrix representation which was first proposed by M. Demiralp [28–31].

The paper is organized as follows. The second section covers a brief information for the HDMR method. The third section involves the description of the fluctuationlessness approximation which will be needed in the solution process of the nonlinear algebraic equations obtained as the result of the next section while the weight optimization through constancy measurer for multivariate functions is given in the fourth section. Several numerical implementations to show the performance of our new method are constructed in the fifth section. Finally, the concluding remarks are given in the last section of this paper.

2 High Dimensional Model Representation (HDMR)

This method is used for representing a given multivariate function of N independent variables, say $f(x_1, x_2, \ldots, x_N)$ as the sum of a constant term, N number of univariate terms, $N(N-1)/2$ number of bivariate terms and so on as in (1). If all terms on the right hand side of (1) are involved, a given multivariate function can be represented exactly.

The main task in the algorithm of the method is to uniquely determine the general structures of the HDMR components. This determination process is based on vanishing conditions and projection operators under a product type weight function (the product of univariate functions each of which depends on a different independent variable). The general structures of the vanishing conditions which were first imposed by Sobol [1] are as follows

$$\int_{a_{i_k}}^{b_{i_k}} dx_{i_k} W_{i_k}(x_{i_k}) f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) = 0, \qquad i_1 \le i_k \le i_s \tag{2}$$

These conditions correspond to the following orthogonality conditions as first noticed by Demiralp and Rabitz and published by Rabitz [2–4]

$$\int_{a_1}^{b_1} dx_1 W_1(x_1) \cdots \int_{a_N}^{b_N} dx_N W_N(x_N) f_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) f_{j_1 \ldots j_\ell}(x_{j_1}, \ldots, x_{j_\ell}) = 0$$
$$(s \ne \ell) \vee [(i_1 \ne j_1) \vee \ldots \vee (i_s \ne j_s)] \tag{3}$$

which mean that any two of HDMR components are mutually orthogonal in the Hilbert space of functions under the inner product weighed by the HDMR weight function over the HDMR geometry. The properties of the weight function, $W(x_1, \ldots, x_N)$, appearing in the vanishing conditions are

$$W(x_1,\ldots,x_N) \equiv \prod_{i_1=1}^{N} W_{i_1}(x_{i_1}), \quad \int_{a_{i_1}}^{b_{i_1}} dx_{i_1} W_{i_1}(x_{i_1}) = 1,$$
$$x_{i_1} \in \left[a_{i_1}\, ,\, b_{i_1} \right], \quad 1 \le i_1 \le N \tag{4}$$

where each factor of the product is assumed to be normalized to give 1 value under integration through the related geometry and the weighing. In this work, to obtain approximate representations for the multivariate functions, we use at most the univariate HDMR approximant and this necessitates the evaluation of the constant and the univariate HDMR components only. To this end, the following projection operators are needed

$$\mathscr{P}_0 g\left(x_1,\ldots,x_N\right) \equiv \int_{a_1}^{b_1} dx_1 \ldots \int_{a_N}^{b_N} dx_N W\left(x_1,\ldots,x_N\right) g\left(x_1,\ldots,x_N\right) \tag{5}$$

$$\begin{aligned}\mathscr{P}_{i_1} g(x_1,\ldots,x_N) \equiv & \int_{a_1}^{b_1} dx_1 W_1(x_1) \times \cdots \times \int_{a_{i_1-1}}^{b_{i_1-1}} dx_{i_1-1} W_{i_1-1}(x_{i_1-1}) \\ & \times \int_{a_{i_1+1}}^{b_{i_1+1}} dx_{i_1+1} W_{i_1+1}(x_{i_1+1}) \\ & \times \cdots \times \int_{a_N}^{b_N} dx_N W_N(x_N) g(x_1,\ldots,x_N)\end{aligned} \tag{6}$$

where $1 \le i_1 \le N$. Here $\mathscr{P}_0$ and $\mathscr{P}_{i_1}$ operators are defined for the determination of the constant and univariate HDMR components respectively. If these projection operators are applied to the both sides of the HDMR expansion given in (1), the following structures are obtained as the constant and the univariate HDMR components.

$$\begin{aligned} f_0 &= \mathscr{P}_0 f(x_1,\ldots,x_N) \\ f_{i_1}(x_{i_1}) &= \mathscr{P}_{i_1} f(x_1,\ldots,x_N) - f_0, \qquad 1 \le i_1 \le N \end{aligned} \tag{7}$$

The higher terms of the method can be evaluated by using some other projection operators that are defined in the same manner. Although the utilization of at most univariate components reduces the mathematical and computational complexity, the representation becomes an approximation. The constant and the univariate HDMR approximants now can be written as follows

$$\begin{aligned} s_0(x_1,\ldots,x_N) &= f_0 \\ s_1(x_1,\ldots,x_N) &= f_0 + \sum_{i_1=1}^{N} f_{i_1}(x_{i_1}) \end{aligned} \tag{8}$$

respectively.

The important point here is to observe the quality of these approximations. A number of measurers, named as “Additivity Measurers”, are defined for this purpose [5]

$$
\begin{aligned}
\sigma_0 &\equiv \frac{1}{\|f\|^2}\|f_0\|^2\\
\sigma_1 &\equiv \frac{1}{\|f\|^2}\sum_{i_1=1}^{N}\left\|f_{i_1}\right\|^2+\sigma_0\\
&\vdots\\
\sigma_N &\equiv \frac{1}{\|f\|^2}\|f_{12\ldots N}\|^2+\sigma_{N-1}
\end{aligned}
\tag{9}
$$

which form a well-ordered sequence as mathematically stated below

$$0 \le \sigma_0 \le \cdots \le \sigma_N = 1 \tag{10}$$

Since we are dealing with at most univariate approximation, only the constancy, σ_0, and the first order additivity, σ_1, measurers will be used in our new method and in its numerical implementations. This well-ordered sequence lets us know that the closer the σ_{i_1} $(1 \le i_1 \le N)$ is to one, the better the quality of the i_1-th approximation.

In this case, the expectation is to get the capability of success fully representing the given multivariate function as much as possible. One way is to select the most appropriate weight function for the problem. This selection’s success depends on how sufficient we know the problem’s nature. To construct a more general and appropriate weight function selection in the HDMR based representations for the multivariate problems, this work proposes a weight function optimization scheme for multivariate functions. This optimization scheme is developed with the help of the fluctuation free matrix representation theory and the next section involves the relevant details.

3 Fluctuationlessness approximation for multivariate functions

The fluctuationlessness approximation is based on matrix representations of independent variables of a multivariate function on Hilbert space, $\mathscr{H}$ in which multivariate functions are square integrable over the hyperprism whose edges are represented by the intervals $[\,a_i, b_i\,]$ $(1 \le i \le N)$. This can be written as a theorem as follows [31]

Theorem 1 *The matrix representation of an algebraic multiplication operator multiplying its operand by $f\,(x_1,\ldots,x_N)$, a multivariate function which is analytic on the hyperprism whose edges are located on the intervals $[\,a_i, b_i\,]$ $(1 \le i \le N)$, over H_n is the image of the matrix representation of the independent variables over H_n under the function f at the fluctuationlessness limit.*

That is, we can write

$$\mathbf{F}^{(n)} \approx f\left(\widehat{\mathbf{X}}_1^{(n)},\ldots,\widehat{\mathbf{X}}_N^{(n)}\right) \tag{11}$$

where

$$\mathbf{F}^{(n)} = \left(\mathbf{w}, \widehat{f}\mathbf{w}^T\right), \quad \widehat{\mathbf{X}}_i^{(n)} = \left(\mathbf{w}, \widehat{x_i}\mathbf{w}^T\right), \quad \mathbf{w} = \mathbf{w}_1 \otimes \cdots \otimes \mathbf{w}_N, \quad 1 \le i \le N \qquad (12)$$

Here, $\widehat{\mathbf{X}}_i^{(n)}$ and $\mathbf{F}^{(n)}$ are the matrix representations of the ith independent variable operator, $\widehat{x_i}$, which multiplies its operand by the independent variable x_i and the function operator $\widehat{f}$ which multiplies its operand by the function $f(x_1, \ldots, x_N)$ respectively. $\mathbf{w}$ appearing in the above relations is an n $(n = n_1 \times n_2 \times \cdots \times n_N)$ element vector whose elements are multivariate functions, and it is constructed through the direct product of the vectors composed of orthogonal univariate basis functions. Each $\mathbf{w}_k$s is an n_k element vector where k lies between 1 and N.

Using the direct product properties, the following expression can be written

$$\begin{aligned}
&\widehat{\mathbf{X}}_i^{(n)} \\
&= \left(\mathbf{w}, \widehat{x_i}\mathbf{w}^T\right) = \left(\left(\mathbf{w}_1 \otimes \cdots \otimes \mathbf{w}_i \otimes \cdots \otimes \mathbf{w}_N\right), \widehat{x_i}\left(\mathbf{w}_1 \otimes \cdots \otimes \mathbf{w}_i \otimes \cdots \otimes \mathbf{w}_N\right)^T\right) \\
&= \left(\mathbf{w}_1, {\mathbf{w}_1}^T\right) \otimes \cdots \otimes \left(\mathbf{w}_i, \widehat{x_i}{\mathbf{w}_i}^T\right) \otimes \cdots \otimes \left(\mathbf{w}_N, {\mathbf{w}_N}^T\right) \\
&= \mathbf{I}_{n_1} \otimes \cdots \otimes \mathbf{X}_i \otimes \cdots \otimes \mathbf{I}_{n_N} \qquad (13)
\end{aligned}$$

where $1 \le i \le N$ and $\mathbf{I}_{n_i}$ is the $n_i \times n_i$ type identity matrix and $\mathbf{X}_i$ shows $n_i \times n_i$ type (square) symmetric matrix which corresponds to the matrix representation of $\widehat{x_i}$ over the subspace spanned by the element functions of the vector $\mathbf{w}_i$

$$\mathbf{X}_i = \left(\mathbf{w}_i, \widehat{x_i}\mathbf{w}_i^T\right), \qquad 1 \le i \le N \qquad (14)$$

Theorem 1 states that it is easier to evaluate $f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)$ in stead of matrix representation of the given multivariate function, $\mathbf{F}^{(n)}$. Thus, by using the approximate structure coming from this theorem, the right hand side of the relation (11) can be approximately obtained. However the result is in a quite closed form and for the sake of more explicity, the following spectral relation can be considered to obtain $f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)$

$$f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right) = \sum_{i_1=1}^{n_1} \cdots \sum_{i_N=1}^{n_N} f\left(\lambda_{i_1}^{(1)}, \ldots, \lambda_{i_N}^{(N)}\right) \mathbf{V}_{i_1 \cdots i_N} {\mathbf{V}_{i_1 \cdots i_N}}^T \qquad (15)$$

where

$$\mathbf{V}_{i_1 \cdots i_N} = \mathbf{v}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{v}_{i_N}^{(N)} \qquad (16)$$

and $\lambda_{i_\ell}^{(\ell)}$ $(1 \le \ell \le N, 1 \le i_\ell \le n_\ell)$ stands for the i_ℓth eigenvalue while $\mathbf{v}_{i_\ell}^{(\ell)}$ denotes the corresponding eigenvector of the matrix, $\mathbf{X}_\ell$ [31].

Here, to evaluate the expression $f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)$, the eigenvalues and the corresponding eigenvectors of the matrix representation of each independent variable must be obtained. Although this process seems to appear quite awkward at the first glance it is not so cumbersome in reality, since the eigenvalues and the eigenvectors of the universal matrix representations are rather lower dimensional in comparison with the global matrix dimensionality [31] and this task will be performed only once because of the universality without increasing the computational complexity of each individual application.

4 Weight optimization through constancy measurer for multivariate functions

The HDMR expansion given in (1) represents the considered multivariate function exactly when we use all the right hand side components of the expansion. Since this increases the complexity of the representation process, only a few components of the expansion are generally taken into consideration as approximation. This necessitates the maximization of the quality of these component contributions. When the HDMR algorithm is examined carefully, it is seen that the weight function of HDMR plays an important role in the determination of the HDMR component structures. Hence, this work aims at the maximization of the contribution of the retained components with respect to this weight function. This results in multivariate weight optimization in the truncated HDMR approximation. In this work, we deal with at most univariate HDMR components, that is, we obtain the univariate HDMR approximant to represent the given multivariate function. This means, we need to maximize the qualities of the constant and the univariate component contributions. For this purpose, a maximization procedure is developed through the constancy measurer given in (9) to optimize the multivariate weight function of HDMR. When we optimize the weight function through the constancy measurer first the contribution of the constant HDMR term becomes more qualified. Because of the well-ordered sequence relation between the additivity measurers as given in (10), the quality of the univariate component contributions also increase. As a result, the quality of the total representation of the given multivariate function through the univariate HDMR approximant increases.

The first step in weight optimization process is to define a general expression for the multivariate weight function to be optimized. For this purpose, a linear combination of functions are selected as

$$W\left(x_1, \ldots, x_N\right) = \left(\sum_{j=1}^{n} \alpha_j w_j\left(x_1, \ldots, x_N\right)\right)^2 \tag{17}$$

where the $w_j\left(x_1, \ldots, x_N\right)$ functions are members of an orthonormal basis set spanning the Hilbert space $\mathscr{H}$ under consideration. In fact, Hilbert space is assumed to be spanned by infinite number of the $w_j\left(x_1, \ldots, x_N\right)$ functions. We denote the subspace of the Hilbert space spanned via first n elements of the basis set spanning the entire Hilbert space by $\mathscr{H}_n$. The α_j parameters appearing in this relation are the basic unknowns of the weight function optimization through the constancy measurer. Since HDMR's vanishing conditions need to use true weight functions which must be positive everywhere except a finite number of points where they can vanish, the squares of the linear combinations of the functions mentioned above are taken into consideration to guarantee this positiveness.

The next step is to determine the general structure of the constant HDMR component under this proposed weight. The projection operator defined to determine the general structure of the constant component is reorganized by using the abovementioned weight function and the relation given in (7) for the constant component can be rewritten explicitly as follows

$$f_0 = \int_{a_1}^{b_1} dx_1 \ldots \int_{a_N}^{b_N} dx_N \left(\sum_{j=1}^{n} \alpha_j w_j (x_1, \ldots, x_N) \right)^2 f(x_1, \ldots, x_N) \tag{18}$$

The following more compact form can also be obtained to this end.

$$f_0 = \sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_j \alpha_k \int_{a_1}^{b_1} dx_1 \ldots \int_{a_N}^{b_N} dx_N w_j (x_1, \ldots, x_N) w_k (x_1, \ldots, x_N) f(x_1, \ldots, x_N) \tag{19}$$

Since the weight optimization is conducted through the constancy measurer, we need to evaluate $\| f_0 \|^2$ and $\| f \|^2$. After evaluating these norms, the structure of the constancy measurer is obtained as follows.

$$\sigma_0 = \frac{\left(\sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_j \alpha_k \int_{a_1}^{b_1} dx_1 \ldots \int_{a_N}^{b_N} dx_N w_j (x_1, \ldots, x_N) w_k (x_1, \ldots, x_N) f(x_1, \ldots, x_N) \right)^2}{\sum_{j=1}^{n} \sum_{k=1}^{n} \alpha_j \alpha_k \int_{a_1}^{b_1} dx_1 \ldots \int_{a_N}^{b_N} dx_N w_j (x_1, \ldots, x_N) w_k (x_1, \ldots, x_N) f(x_1, \ldots, x_N)^2} \tag{20}$$

The right hand side of the above expression can be put into more amenable form by using Rayleigh quotients. For this purpose, we will use the matrix representations of the functions such as

$$\mathbf{F}^{(n)} = \left(\mathbf{w}, \widehat{f} \mathbf{w}^T \right), \qquad \mathbf{F}_1^{(n)} = \left(\mathbf{w}, \widehat{f}^2 \mathbf{w}^T \right) \tag{21}$$

Relation (20) which is given for the constancy measurer can be written by taking the expressions defined in relation (21) into consideration and the following general structure for σ_0 is obtained

$$\sigma_0 = \frac{\left(\alpha^T \mathbf{F}^{(n)} \alpha \right)^2}{\alpha^T \mathbf{F}_1^{(n)} \alpha} \tag{22}$$

This relation is in quadratic form and cannot be solved analytically except for very specific cases due to its nonlinearity. To by pass this difficulty and to evaluate, at least approximately, the α vectors which is the main task of the weight optimization, the first step is to apply the fluctuationlessness approximation theorem to the above relation by using the approximation given in (11). As a result, the following structure is determined

$$\sigma_0 \approx \frac{\left[\alpha^T f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)\alpha\right]^2}{\alpha^T f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)^2 \alpha} \tag{23}$$

Although this step cannot eliminate the mentioned nonlinearity, it brings an alternative solution process such as we can use the spectral decomposition of matrices. To this end, the first step is to write the following eigenequations of each $\mathbf{X}_\ell$, $1 \le \ell \le N$ as

$$\begin{aligned} \mathbf{X}_1\mathbf{x}_{i_1}^{(1)} &= \xi_{i_1}^{(1)}\mathbf{x}_{i_1}^{(1)}, \qquad 1 \le i_1 \le n_1 \\ \mathbf{X}_2\mathbf{x}_{i_2}^{(2)} &= \xi_{i_2}^{(2)}\mathbf{x}_{i_2}^{(2)}, \qquad 1 \le i_2 \le n_2 \\ &\vdots \\ \mathbf{X}_N\mathbf{x}_{i_N}^{(N)} &= \xi_{i_N}^{(N)}\mathbf{x}_{i_N}^{(N)}, \qquad 1 \le i_N \le n_N \end{aligned} \tag{24}$$

where $\xi_{i_\ell}^{(\ell)}$ and $\mathbf{x}_{i_\ell}^{(\ell)}$ stand for the i_ℓth eigenvalue and the corresponding normalized eigenvector of the matrix, $\mathbf{X}_\ell$. Then, we obtain the following relation from (24) by taking the Theory of Matrices and the direct product properties into consideration.

$$f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)\mathbf{x}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{x}_{i_N}^{(N)} = f\left(\xi_{i_1}^{(1)}, \ldots, \xi_{i_N}^{(N)}\right)\mathbf{x}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{x}_{i_N}^{(N)} \tag{25}$$

$$f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)^2\mathbf{x}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{x}_{i_N}^{(N)} = f\left(\xi_{i_1}^{(1)}, \ldots, \xi_{i_N}^{(N)}\right)^2\mathbf{x}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{x}_{i_N}^{(N)} \tag{26}$$

To obtain more concise forms in the following relations, the direct product of the normalized eigenvectors is defined as

$$\nu_{i_1\cdots i_N} = \mathbf{x}_{i_1}^{(1)} \otimes \cdots \otimes \mathbf{x}_{i_N}^{(N)} \tag{27}$$

and if we multiply the relations (25) and (26) by ${\nu_{i_1\cdots i_N}}^T$ through left hand side, we obtain

$${\nu_{i_1\cdots i_N}}^T f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)\nu_{i_1\cdots i_N} = f\left(\xi_{i_1}^{(1)}, \ldots, \xi_{i_N}^{(N)}\right){\nu_{i_1\cdots i_N}}^T \nu_{i_1\cdots i_N} \tag{28}$$

$${\nu_{i_1\cdots i_N}}^T f\left(\widehat{\mathbf{X}}_1^{(n)}, \ldots, \widehat{\mathbf{X}}_N^{(n)}\right)^2 \nu_{i_1\cdots i_N} = f\left(\xi_{i_1}^{(1)}, \ldots, \xi_{i_N}^{(N)}\right)^2 {\nu_{i_1\cdots i_N}}^T \nu_{i_1\cdots i_N} \tag{29}$$

Since the eigenvectors appearing in the direct product of relation (27) are normalized eigenvectors, their norms are equal to 1. Therefore, the norm of $\nu_{i_1\cdots i_N}$ which is direct product of these eigenvectors is 1, that is, ${\nu_{i_1\cdots i_N}}^T \nu_{i_1\cdots i_N} = 1$.

Then, the relations (28) and (29) are rewritten as follows

$$f\left(\xi_{i_1}^{(1)},\ldots,\xi_{i_N}^{(N)}\right)=\nu_{i_1\cdots i_N}{}^T f\left(\widehat{\mathbf{X}}_1^{(n)},\ldots,\widehat{\mathbf{X}}_N^{(n)}\right)\nu_{i_1\cdots i_N} \tag{30}$$

$$f\left(\xi_{i_1}^{(1)},\ldots,\xi_{i_N}^{(N)}\right)^2=\nu_{i_1\cdots i_N}{}^T f\left(\widehat{\mathbf{X}}_1^{(n)},\ldots,\widehat{\mathbf{X}}_N^{(n)}\right)^2\nu_{i_1\cdots i_N} \tag{31}$$

After both sides of relation (30) are squared, the ratio of relations (30) and (31) becomes 1. Since we try to maximize the constancy measurer and make it close to 1, we can write the following relation for σ_0 by using the mentioned ratio

$$\sigma_0 \approx \frac{\left[\nu_{i_1\cdots i_N}{}^T f\left(\widehat{\mathbf{X}}_1^{(n)},\ldots,\widehat{\mathbf{X}}_N^{(n)}\right)\nu_{i_1\cdots i_N}\right]^2}{\nu_{i_1\cdots i_N}{}^T f\left(\widehat{\mathbf{X}}_1^{(n)},\ldots,\widehat{\mathbf{X}}_N^{(n)}\right)^2\nu_{i_1\cdots i_N}}=1 \tag{32}$$

When relations (23) and (32) are ta ken into consideration, the vectors, $\nu_{i_1\cdots i_N}$ which are composed of direct product of $\mathbf{x}_{i_1}^{(1)},\ldots,\mathbf{x}_{i_N}^{(N)}$ which are eigenvectors of the mat rices, $\mathbf{X}_1,\ldots,\mathbf{X}_N$ approximately maximize the constancy measurer within the fluctuationlessness limit. Although this constancy measurer relation is obtained in fluctuation lessness limit, it still contains nonlinearity. Hence, we cannot say that these vectors are the only possible vectors approximately maximize the constancy measurer. However, it can be proven that these vectors are the only possible vectors that satisfy our maximization process through the constancy measurer [27]. This means that the only possible vector values for the unknown vector, α are the direct product of eigenvectors of the matrices, $\mathbf{X}_1,\ldots,\mathbf{X}_N$ which correspond to $\nu_{i_1\cdots i_N}$.

To this end, we have the ability of solving the constancy measurer optimization problem, which has a nonlinear structure, with the help of the fluctuationlessness approximation. Now, we know that the solution of this problem will give us n number of σ_0 values since there exist n number of different $\nu_{i_1\cdots i_N}$ vectors. Hence, we can define the following terms

$$\overline{\sigma}_0^{(\ell)}=\frac{\left(\nu_{i_1\cdots i_N}{}^T\mathbf{F}^{(n)}\nu_{i_1\cdots i_N}\right)^2}{\nu_{i_1\cdots i_N}{}^T\mathbf{F}_1^{(n)}\nu_{i_1\cdots i_N}},\qquad 1\le i_s\le n_s,\quad 1\le s\le N,\quad 1\le\ell\le n \tag{33}$$

where they take values between 0 and 1.

Next step of our new algorithm is to find a single unique solution for this optimization problem, that is, we have to deter mine the $\nu_{i_1\cdots i_N}$ vector that maximizes the σ_0 value throughout the $\overline{\sigma}_0^{(\ell)}$ values where $1\le\ell\le n$. This $\nu_{i_1\cdots i_N}$ vector can be named as ν_{opt} in which the abbreviation *opt* stands for optimum value. Taking the relation (27) into consideration, the following relation can be written

$$\nu_{opt}=\mathbf{x}_{opt}^{(1)}\otimes\cdots\otimes\mathbf{x}_{opt}^{(N)} \tag{34}$$

where $\mathbf{x}_{opt}^{(1)},\ldots,\mathbf{x}_{opt}^{(N)}$ are the optimum eigenvectors of matrices, $\mathbf{X}_1,\ldots,\mathbf{X}_N$ that satisfy ν_{opt}.

The general structure of the HDMR's weight function can now be de fined in terms of the optimized weight factors obtained through the constancy measurer maximization process

$$W_{opt}(x_1, \ldots, x_N) \equiv \prod_{i=1}^{N} W_{i,opt}(x_i) \tag{35}$$

where

$$W_{i,opt}(x_i) = \mathbf{w}_i(x_i)^T \mathbf{x}_{opt}^{(i)}, \qquad 1 \le i \le N \tag{36}$$

and

$$\mathbf{w}_i(x_i)^T = \left[w_1(x_i)\ w_2(x_i)\ \cdots\ w_{n_i}(x_i) \right], \qquad 1 \le i \le N \tag{37}$$

In terms of (17), each element of the following vector, $\mathbf{w}(x_1, x_2, \ldots x_N)$ which is given as the direct product of $\mathbf{w}_i(x_i)$s is denoted by $w_j(x_1, \ldots, x_N)$ that belongs to the orthonormal basis set spanning the considered Hilbert space.

$$\mathbf{w}(x_1, x_2, \ldots x_N) = \mathbf{w}_1(x_1) \otimes \mathbf{w}_2(x_2) \otimes \cdots \otimes \mathbf{w}_N(x_N) \tag{38}$$

Several numerical implementations are given in the next section to show the steps that are described in this section for weight optimization.

5 Numerical implementations

This section includes various numerical implementations to examine the performance of our new method. The results are obtained by using certain program codes written in MuPAD, Multi Processing Algebra Data tool [32]. These program codes are run using 10-digit arithmetic precision. This precision can be increased by using the environmental variable, *DIGITS*, of MuPAD which takes positive integers less than 2^{31}.

To make a general error analysis approach for the obtained HDMR approximants of the given testing analytical structures, the following relative error analysis relation is used in this work

$$\mathcal{N} = \frac{||f_{org} - f_{hdmr}||}{||f_{org}||} \tag{39}$$

where f_{org} and f_{hdmr} stand for the original multivariate function and the HDMR approximant obtained through the optimized weight function which is the main task of this paper.

The first implementation is constructed to show the steps of our new algorithm clearly and in a detailed way. To this end, an exponential test function having 2 independent variables with a purely multiplicative nature is selected

$$f_1(x_1, x_2) = \mathrm{e}^{(x_1 + x_2)} \tag{40}$$

where the interval for each independent variable is $[-1, 1]$. Our new method here aims at expressing this function in terms of HDMR components. To obtain a good representation, this work proposes a weight optimization approach through constancy measurer maximization process. The fluctuation approximation theory is used in this maximization process to bypass the nonlinearity given in (22).

The basic steps of this implementation are given below to make our new algorithm more clear:

- Determine the matrix representation of each independent variable, $\mathbf{X_1}$ and $\mathbf{X_2}$, in which the types of these matrices are $n_1 \times n_1$ and $n_2 \times n_2$, where n_1 and n_2 are certain positive integers which may be same or different, respectively. Relation (14) is used for this purpose.
- Evaluate the eigenvalues and the corresponding eigenvectors of these two matrices. As a result, there exist n_1 eigenvalues and n_1 eigenvectors for the matrix, $\mathbf{X_1}$ and n_2 eigenvalues and n_2 eigenvectors for the matrix, $\mathbf{X_2}$.
- Construct the vectors through the direct product of these eigenvectors as given in (27). There will be $n_1 \times n_2$ number of $n_1 \times n_2$ element vectors.
- Evaluate the σ_0 values by using the vectors obtained in the previous step. There are $n_1 \times n_2$ number of σ_0 values since there are $n_1 \times n_2$ number of these vectors as given in (33).
- The maximum σ_0 value is selected as the appropriate σ_0 value in the maximization process.
- The vector composed of direct product of the eigenvectors of the matrices that gives the appropriate σ_0 value is ta ken into consideration. The corresponding relation is given in (34). The first eigenvector belongs to the first matrix, $\mathbf{X_1}$ and the second eigenvector belongs to the matrix, $\mathbf{X_2}$.
- The structure of each weight function component can then be determined by using relation (36).
- For instance, if we assume the dimensions of these two matrices as $n_1 = 8$ and $n_2 = 8$, the weight function components are obtained through the constancy measurer maximization process as follows

$$\begin{aligned}
W_1(x_1) = {} & (9.918237879\, x_1^7 + 9.524382432\, x_1^6 - 9.367876187\, x_1^5 \\
& -8.995875217\, x_1^4 + 2.042531522\, x_1^3 + 1.96142175\, x_1^2 \\
& -0.05849917961\, x_1 - 0.05617611115)^2 \\
W_2(x_2) = {} & (9.918237879\, x_2^7 + 9.524382432\, x_2^6 - 9.367876187\, x_2^5 \\
& -8.995875217\, x_2^4 + 2.042531522\, x_2^3 + 1.96142175\, x_2^2 \\
& -0.05849917961\, x_2 - 0.05617611115)^2
\end{aligned} \tag{41}$$

- Using these weight components in relation (35), the general structure of the optimized weight function for the given problem is determined.

– Determine the constant and the univariate HDMR components and construct the constant and univariate approximants. The results are as follows

$$s_0(x_1, x_2) = 6.848953285$$
$$s_1(x_1, x_2) = 2.617049694\, e^{x_1} + 2.617049694\, e^{x_2} - 6.848953285 \qquad (42)$$

where $s_0(x_1, x_2)$ and $s_1(x_1, x_2)$ correspond to the constant and univariate approximants respectively.

Table 1 includes the constancy measurer and constant HDMR component values obtained through the maximization process for different n_1 and n_2 values that correspond to the matrix dimensions of $\mathbf{X_1}$ and $\mathbf{X_2}$. In addition, the relative error values, $\mathcal{N}_{s_1}$, standing for the univariate HDMR approximant evaluated with the help of the optimized weight, are given for each case. To make a comparison between a constant weight and the optimized weight, the univariate HDMR approximant with a constant weight, $\overline{s}_1$, and the relative error, $\mathcal{N}_{\overline{s}_1}$, for that HDMR approximant are also evaluated

$$\overline{s}_1(x_1, x_2) = 1.175201194\, e^{x_1} + 1.175201194\, e^{x_2} - 1.381097846$$
$$\mathcal{N}_{\overline{s}_1} = 0.056837347 \qquad (43)$$

where the constant weight is $W(x_1, x_2) = 1/4$, $(W_1(x_1) = 1/2,\ W_2(x_2) = 1/2)$ since the domain for each independent variable is given as the interval $x_1, x_2 \in [-1, 1]$ and each weight component should satisfy the criteria given in (4).

It is seen from Table 1 that as the selected dimensions increase, σ_0 value becomes close to one and this forces σ_1 value become also close to one. As a result, we obtain better approximants through the HDMR method including multivariate weight optimization. This can be examined by looking at the relative error values obtained for the HDMR approximant with the optimized weight given as the last line of Table 1. When we compare these errors with the error obtained through the constant weight given in (43), it is seen that we get approximations in excellent quality through the HDMR method including multivariate weight optimization process with respect to the one having no optimization on weight.

Figure 1 shows the performance of our new method in representing the given testing function graphically. It can be easily seen that the approximation is very successful to represent the given exponential function.

Table 1 Maximized constancy measurer and optimized constant HDMR component values for the first testing function, $f_1\,(x_1, x_2) = e^{(x_1+x_2)}$

	$n_1 = 3$, $n_2 = 4$	$n_1 = 4$, $n_2 = 4$	$n_1 = 4$, $n_2 = 5$	$n_1 = 5$, $n_2 = 6$	$n_1 = 8$, $n_2 = 8$
σ_0	0.953311264	0.969417884	0.976188742	0.98631914	0.9953495042
f_0	5.312109611	5.72519444	5.959262875	6.352571487	6.848953285
$\mathcal{N}_{s_1}$	0.000489546	0.000237462	0.000131491	0.000043261	0.000005419

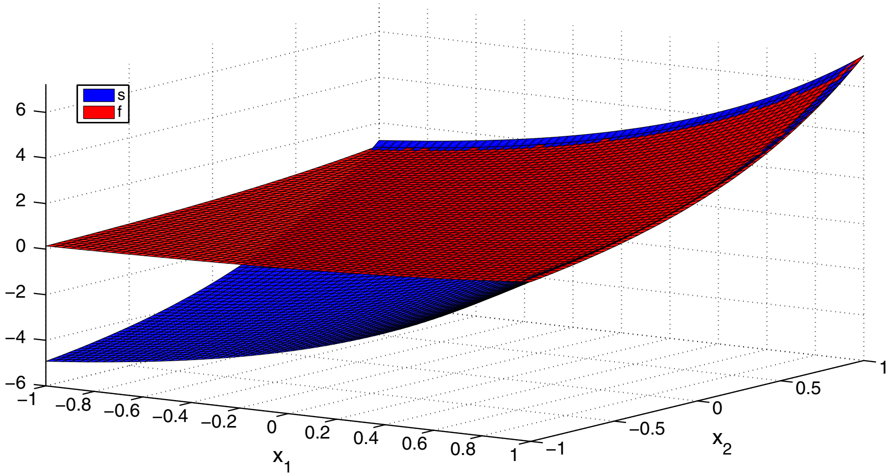

Fig. 1 The testing function, $f_1\ (x_1, x_2) = \mathrm{e}^{(x_1+x_2)}$ and the univariate HDMR approximant, $s_1(x_1, x_2)$

The rest part of this section includes a number of testing functions having 5 independent variables to show the performance of our new method in the multivariate problems. These testing functions are selected as follows

$$\begin{aligned} f_2(x_1,\ldots,x_5) &= \sum_{i=1}^{5} x_i, \qquad f_3(x_1,\ldots,x_5) = \left[\sum_{i=1}^{5} x_i\right]^3, \\ f_4(x_1,\ldots,x_5) &= \left[\sum_{i=1}^{5} x_i\right]^6, \quad f_5(x_1,\ldots,x_5) = \prod_{i=1}^{5} x_i, \\ f_6(x_1,\ldots,x_5) &= \sin\left(x_1+x_2+x_3+x_4+x_5\right) \end{aligned} \tag{44}$$

where the functions, f_2, f_3, f_4, f_5 and f_6 have purely additive, dominantly additive, dominantly multiplicative, purely multiplicative and trigonometric natures respectively. The domain for each independent variable of these testing functions is again selected as $[-1, 1]$ for simplicity. The goal is to obtain the optimized weight for each analytical structure needed in the HDMR approximant construction to represent the given multivariate function in terms of less-variate functions. In this work, we use at most the univariate HDMR approximant for this purpose.

The case that the weight optimization process is not applied to the HDMR method has the following constant weight under the criteria given in (4)

$$W(x_1,\ldots,x_5) = \frac{1}{32} \tag{45}$$

where

$$W_1(x_1) = W_2(x_2) = W_3(x_3) = W_4(x_4) = W_5(x_5) = \frac{1}{2}, \quad x_1,\ldots x_5 \in [-1, 1] \tag{46}$$

Table 2 includes the values $\mathscr{N}_{s_1}$ and $\mathscr{N}_{\bar{s}_1}$ which correspond to the relative error values for the univariate HDMR approximant with the optimized weight, and for the univariate HDMR approximant with the constant weight respectively. The optimization process is done by selecting the matrix dimensions as $n_1 = 2, n_2 = 3, n_3 = 2, n_4 = 3$ and $n_5 = 2$. Although these values seem to be quite small as matrix dimensions, the fluctuationlessness approximation method provides HDMR to produce powerfull representations for the given multivariate structures. Hence there is no need to increase these dimensions. This can be easily seen from the results given in Table 2.

Table 2 shows that relative error values for the HDMR approximants obtained through the weight optimization process are impressively better than the error values obtained for the HDMR approximants based on constant weight. Since the expansion of the HDMR method has an additive nature, the method works well for the purely additive natures. However, as the additivity dominancy of the given problem decreases and the multiplicativity becomes dominant, the approximation quality reduces and unacceptable representations are obtained. This can be observed by especially looking at the last line of Table 2 which corresponds to the relative error values of the approximants with constant weight. Multivariate weight optimization process inserted into the HDMR method prevents the mentioned disadvantage and significant results are determined. The results of Table 2 also say that our new method brings a new and a high qualified approximation technique to the classical HDMR method.

6 Conclusion

High Dimensional Model Representation Method is a widely used technique for representing a given multivariate function. This method is based on divide-and-conquer philosopy, that is, less variate functions are taken into consideration instead of given multivariate function itself. HDMR has a finite expansion, that is, it has finite number of terms in the expansion. If all these terms are used for representing a given function, the exact representation is obtained. However this approach will be quite expensive in terms of calculation. Instead, a few terms are used for representing the given function. Hence, an approximation would have made for the representation. This brings a new problem, whether the obtained approximation represents the given mutivariate function as good as possible or not.

In this paper, we have focused on increasing the performance of the High Dimensional Model Representation Method by using the weight optimization through constancy measurer. It means that, our aim is to find the appropriate weight function to

Table 2 Relative error values of univariate HDMR approximants with both optimized and constant weight ($n_1 = 2, n_2 = 3, n_3 = 2, n_4 = 3, n_5 = 2$)

	$f_2(x_1, \ldots, x_5)$	$f_3(x_1, \ldots, x_5)$	$f_4(x_1, \ldots, x_5)$	$f_5(x_1, \ldots, x_5)$	$f_6(x_1, \ldots, x_5)$
$\mathscr{N}_{s_1}$	0.0	0.0131335841	0.09226203159	0.2737548706	0.0619816713
$\mathscr{N}_{\bar{s}_1}$	0.0	0.3453744493	0.8983342051	1.0	0.3009969579

be able to obtain the best representation for a given multivariate function when the fist few terms are taken into consideration from basic HDMR expansion formula.

During the progress of the optimization process some difficulties come up. For example, the equation which is obtained from the optimization process is nonlinear. This feature makes the equation difficult to solve. To get rid of this difficulty, we use fluctuationlessness approximation method. This method includes fluctuationlessness teorem and the universal matrix representations of each independent variable to find the solution of this nonlinear problem.

Several numerical implementations were designed to show the efficiency of the new algorithms. These implementations having various functions which have different types of structure, show us a need for weight optimization in HDMR based methods.

As the final conclusion, we have constructed a new algorithm for the HDMR based method to obtain optimized weight function with the help of the Fluctuationlessness Approximation, for multivarite functions.

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