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Hybrid HDMR method with an optimized hybridity parameter in multivariate function representation

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Abstract High Dimensional Model Representation (HDMR) based methods are used to generate an approximation for a given multivariate function in terms of less variate functions. This paper focuses on Hybrid HDMR which is composed of Plain HDMR and Logarithmic HDMR. The Plain HDMR method works well for representing multivariate functions having additive nature. If the function under consideration has a multiplicative nature, then the Logarithmic HDMR method produces better approximation. Hybrid HDMR method aims to successfully represent a multivariate function having neither purely additive nor purely multiplicative nature under a hybridity parameter. The performance of the Hybrid HDMR method strongly depends on the value of this hybridity parameter because this parameter manages the contribution level of Plain and Logarithmic HDMR expansions. The main purpose of this work is to optimize the hybridity parameter to get the best approximations. Fluctuationlessness Approximation Theorem is used in this optimization process and in evaluating the multiple integrals appearing in HDMR based methods. A number of numerical implementations are given at the end of the paper to show the performance of our proposed method.

Keywords High dimensional model representation · Multivariate functions · Approximation by polynomials · Fluctuation expansion · Optimization

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1 Introduction

Dealing with multivariate functions may become a serious problem for the numerical and analytical calculations in scientific and engineering problems of physics, chemistry and the other research areas of applied mathematics such as atmospheric modelling, atmospheric dynamics, source-sinks of trace gases, operational models, stratospheric chemical kinetics, multivariate data modelling, financial applications and so on. To overcome these difficulties, researchers work on developing divide-and-conquer based methods to deal with less variate functions instead of a given multivariate function. High Dimensional Model Representation (HDMR) based methods are of type divide-and-conquer.

HDMR was first proposed by Sobol [1] and now it is named as Sobol HDMR or Plain HDMR. After Sobol's innovative work, Plain HDMR method was more generalized by Rabitz [2–4] and Demiralp [5]. Furthermore, Demiralp and his group [5–12] developed several HDMR based methods for different scientific engineering problems to increase its power and efficiency.

The Plain HDMR method is an expansion with 2^N terms. This expansion can be described as finite summation of a constant term, N univariate terms, $N(N-1)/2$ bivariate terms and so on. If all these 2^N terms are used in the expansion then a given multivariate function can be represented exactly. However, to reduce the mathematical and computational complexity, it is not preferred to use all HDMR terms. Only the first few terms are taken into consideration from the expansion and it is sufficient to make an approximation to represent the given multivariate function. How well the multivariate function is represented through HDMR approximant is determined by using additivity measurers. These measurers were defined by Demiralp [5] and these are monotonously increasing entities having values in the unit interval, [0, 1]. We can make an error analysis for the obtained HDMR approximant of the given multivariate function by using additivity measurers.

In literature, there are several HDMR based methods to obtain a better approximation for different types of multivariate functions. Plain HDMR method works well when the function under consideration is purely or dominantly additive and it becomes poor as the multiplicativity of the original function increases. Factorized HDMR [6,7] and Logaritmic HDMR [8,9] methods work well as the function under consideration is purely or dominantly multiplicative and they become poor as the additivity increases.

If the multivariate function under consideration is neither dominantly additive nor dominantly multiplicative then we need a new HDMR algorithm. For this purpose, Hybrid HDMR method was developed with an expansion having the combination of Plain HDMR and Factorized HDMR expansions under an hybridity parameter [10,11]. On the other hand, it is known that the measurers defined for the Factorized HDMR method have no monotonously increasing nature because of its multiplicative expansion. That is, there is no warranty to get a better approximation when a higher variate component is used in representing the multivariate function under consideration. To this end, another combination for the Hybrid HDMR expansion can be considered. This results in combining Plain HDMR and Logarithmic HDMR expansions again under an hybridity parameter [12]. The most important issue of this study is to optimize this parameter. To increase the efficiency of the Hybrid HDMR expansion, it is critical to select the most appropriate value for the hybridity parameter because this parameter manages the contribution level of two expansions to the resulting expansion of Hybrid HDMR. Hence, the main purpose of this work is to combine the two HDMR based methods, Plain and Logarithmic HDMRs under the optimized hybridity parameter to get a better representation for the given multivariate function.

The HDMR based methods have multiple integrals to be evaluated to obtain the structures of the components appearing in the expansion. One way is to evaluate the integrals analytically. This increases the mathematical and computational complexity because of the incapabilities of standard numerical methods, computer based algebraic tools and computer hardware features. In addition, the Logarithmic HDMR method includes integrals of natural logarithm of the given function which is usually a problematic case. To bypass these disadvantages, another way is to apply the Fluctuationlessness Approximation Theorem, which was first proposed by Demiralp [13–16], in the algorithm to gain ability of evaluating these integrals. This theorem facilitates the numerical evaluation of complicated integral structures whose values can not be easily obtained analytically. Besides, it allows us to obtain the results of the integrals even that cannot be evaluated analytically. The theorem is also used to evaluate the multiple integrals of the Plain HDMR algorithm to get the results easily.

There are also some other works about applying the HDMR philosophy to scientific problems. These studies are about stochastic finite element analysis [17], reliability analysis [18], sensitivity analysis [19].

This paper is organized as follows. The second section includes the mathematical background of Plain HDMR, Logarithmic HDMR, Hybrid HDMR and the Fluctuationlessness Approximation Theorem. The usage of the Fluctuationlessness Approximation Theorem in Hybrid HDMR is given in the third section. The fourth section covers the hybridity parameter optimization process of Hybrid HDMR. The numerical implementations to show the performance of our new method are discussed in the fifth section. Finally, the concluding remarks are mentioned in the last section of the paper.

2 Mathematical background

This section covers the details of the HDMR based methods and the Fluctuationlessness Approximation Theorem that are used in this study. Since the expansion of the Hybrid HDMR method consists of Plain HDMR and Logarithmic HDMR, the first two subsections are about the algorithm of how to represent a multivariate function by using Plain HDMR and Logaritmic HDMR respectively. The third subsection describes the details of the Hybrid HDMR method. The efficiency of this method is managed through a hybridity parameter. This parameter identifies the contribution level of Plain and Logarithmic HDMR expansions to the representation of the given multivariate function. One of the most important tasks of this study is to optimize the value of this parameter to obtain better approximations. For this purpose, the details of the Fluctuationlessness Approximation Theorem are given in last subsection.

2.1 The Plain HDMR Method

The basic formula for Plain HDMR to represent a given multivariate function, $f(x_1, \ldots, x_N)$, is given as

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

The right hand side components of the above equation can be uniquely obtained by imposing mutual orthogonality amongst these components [5]

$$(f_{i_1 i_2 \ldots i_k}, f_{i_1 i_2 \ldots i_l}) = 0, \quad \{i_1, i_2, \ldots, i_k\} \not\equiv \{i_1, i_2, \ldots, i_l\}, \quad 1 \le k, l \le N \tag{2}$$

where

$$(u, v) \equiv \int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N)\, u(x_1, \ldots, x_N) v(x_1, \ldots, x_N) \tag{3}$$

The weight function appearing in the abovementioned orthogonality conditions is assumed to be a product of univariate functions each of which depends on a different independent variable

$$W(x_1, \ldots, x_N) \equiv \prod_{j=1}^{N} W_j(x_j), \quad x_j \in \left[a_j, b_j\right], \quad 1 \le j \le N \tag{4}$$

These orthogonality conditions are equivalent to the following Sobol's vanishing conditions

$$\int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N) f_{i_1}(x_{i_1}) = 0, \quad 1 \le i \le N \tag{5}$$

For the determination of the right hand side components of the Plain HDMR expansion certain projection operators are defined. The following projection operator is defined for the determination of the constant HDMR term, f_0

$$\mathscr{P}_0 g(x_1, \ldots, x_N) \equiv \int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N)\, g(x_1, \ldots, x_N) \tag{6}$$

If $\mathscr{P}_0$ is applied on both sides of Eq. (1), all the higher than zero variate components of Plain HDMR vanish because of the vanishing property (proposed by Sobol and revised by Rabitz) given in (5) and we can write the following equation for the constant term

$$f_0 = \mathscr{P}_0 f\,(x_1, \ldots, x_N) \tag{7}$$

To determine the univariate HDMR terms, we need to define other projection operators denoted by $\mathscr{P}_{i_1}$ $(1 \le i_1 \le N)$. They are equivalent to $\mathscr{P}_0$'s new form obtained after removing the integration over x_{i_1} and discarding the univariate weight function factor $W_{i_1}\left(x_{i_1}\right)$ where $1 \le i_1 \le N$

$$\begin{aligned} \mathscr{P}_{i_1} g(x_1, \ldots, x_N) \equiv & \int_{a_1}^{b_1} dx_1 W_1(x_1) \cdots \int_{a_{i_1-1}}^{b_{i_1-1}} dx_{i_1-1} W_{i_1-1}(x_{i_1-1}) \\ & \times \int_{a_{i_1+1}}^{b_{i_1+1}} dx_{i_1+1} W_{i_1+1}(x_{i_1+1}) \cdots \int_{a_N}^{b_N} dx_N W_N(x_N) g(x_1, \ldots, x_N) \end{aligned} \tag{8}$$

If we apply $\mathscr{P}_{i_1}$ on both sides of (1) and take the Sobol's vanishing conditions or equivalently Demiralp's orthogonality conditions into consideration then we may write the general structure of the univariate Plain HDMR components as follows

$$f_{i_1}\left(x_{i_1}\right) = \mathscr{P}_{i_1} f\,(x_1, \ldots, x_N) - f_0, \quad 1 \le i_1 \le N \tag{9}$$

The determination of higher multivariate Plain HDMR components can be realised by defining other projection operators in the same manner.

HDMR is in fact a finite sum and it can be truncated at some level of multivariance to get an approximation since it becomes quite difficult to calculate all the right hand side components as the multivariance increases. Hence we can denote the truncated sums of Plain HDMR by $s_i\,(x_1, \ldots, x_N)$ where i denotes the level of multivariance

$$\begin{aligned} s_0(x_1, \ldots, x_N) &= f_0 \\ s_1(x_1, \ldots, x_N) &= s_0(x_1, \ldots, x_N) + \sum_{i_1=1}^{N} f_{i_1}(x_{i_1}) \\ s_2(x_1, \ldots, x_N) &= s_1(x_1, \ldots, x_N) + \sum_{\substack{i_1, i_2=1 \\ i_1 < i_2}}^{N} f_{i_1 i_2}(x_{i_1}, x_{i_2}) \end{aligned} \tag{10}$$

Here, the cases $i = 0, i = 1$ and $i = 2$ correspond to the constant, univariate and bivariate HDMR approximants respectively.

2.2 The logarithmic HDMR method

Logarithmic HDMR method was developed by using Plain HDMR philosophy. This method is based on expanding the natural logarithm of a given nonnegative multivariate function to HDMR instead of the function itself [8,9]. The Logarithmic HDMR formula for a given multivariate function can be expressed as follows

$$\begin{aligned} & ln\left[f\left(x_1,\ldots,x_N\right)-\phi\left(x_1,\ldots,x_N\right)\right] \\ & \quad=\varphi_0+\sum_{i_1=1}^{N}\varphi_{i_1}\left(x_{i_1}\right)+\sum_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\varphi_{i_1 i_2}\left(x_{i_1},x_{i_2}\right)+\cdots \end{aligned} \tag{11}$$

where $\phi\left(x_1,\ldots,x_N\right)$ is called as "Reference Function" and it is used for producing a nonnegative or preferably positive core function for the logarithm. The right hand side components of (11) are mutualy orthogonal and can be determined by tracing the basic rule of the HDMR method.

If basic Logarithmic HDMR expansion given in (11) is rearranged, the following formula is obtained for Logarithmic HDMR

$$f\left(x_1,\ldots,x_N\right)=\phi\left(x_1,\ldots,x_N\right)+\mathrm{e}^{\varphi_0}\left[\prod_{i_1=1}^{N}\mathrm{e}^{\varphi_{i_1}\left(x_{i_1}\right)}\right]\left[\prod_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\mathrm{e}^{\varphi_{i_1 i_2}\left(x_{i_1},x_{i_2}\right)}\right]\times\cdots \tag{12}$$

The explicit expressions of Logarithmic HDMR approximants can be written as follows when the reference function is assumed to be vanishing for simplicity

$$\begin{aligned} \pi_0(x_1,\ldots,x_N) &= \mathrm{e}^{\varphi_0} \\ \pi_1(x_1,\ldots,x_N) &= \pi_0(x_1,\ldots,x_N)\prod_{i_1=1}^{N}\mathrm{e}^{\varphi_{i_1}\left(x_{i_1}\right)} \\ \pi_2(x_1,\ldots,x_N) &= \pi_1(x_1,\ldots,x_N)\prod_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\mathrm{e}^{\varphi_{i_1 i_2}\left(x_{i_1},x_{i_2}\right)} \end{aligned} \tag{13}$$

where indexed π s stand for the Logarithmic HDMR approximants. The other approximants including the higher variate components of the Logarithmic HDMR expansion can be written in the same manner. We can determine the structures of the right hand side components of relation (11) by using the steps of the Plain HDMR method. Then, we use this Logarithmic HDMR expansion in our new form of Hybrid HDMR expansion.

2.3 The hybrid HDMR method

The general expansion for Hybrid HDMR which is the combination of Plain HDMR and Logarithmic HDMR can be given as follows

$$f(x_1,\ldots,x_N)=\alpha\left(f_0+\sum_{i_1=1}^{N}f_{i_1}(x_{i_1})+\cdots\right)$$
$$+(1-\alpha)\left(\phi\left(x_1,\ldots,x_N\right)+e^{\varphi_0}\left[\prod_{i_1=1}^{N}e^{\varphi_{i_1}\left(x_{i_1}\right)}\right]\times\cdots\right) \quad (14)$$

where α is named as hybridity parameter. The reference function, $\phi\left(x_1,\ldots,x_N\right)$, will be assumed to be vanishing as stated in the previous subsection.

Using relation (14), the following general structure for the Hybrid HDMR approximants can be defined as

$$f(x_1,\ldots,x_N)\approx h_{jk}(x_1,\ldots,x_N;\alpha)\equiv\alpha s_j(x_1,\ldots,x_N)+(1-\alpha)\pi_k(x_1,\ldots,x_N) \quad (15)$$

where $1\le j,k\le N$. Here, $s_j(x_1,\ldots,x_N)$ and $\pi_k(x_1,\ldots,x_N)$ correspond to the j-th order Plain HDMR approximant and the k-th order Logarithmic HDMR approximant respectively. The hybridity parameter, α, plays an important role to determine the best approximation through Hybrid HDMR. To this end, we need a mechanism to specify a value for this parameter. In this study, an algorithm for this purpose is constructed and the details of this algorithm is given in the fourth section.

On the other hand, it is important to examine the performance of these Hybrid HDMR approximants. In other words, how well does obtaining approximant represent the given multivariate function? To measure the approximating capability of the Hybrid HDMR approximant, we have to define a measuring device. The following relative error formula is defined to measure the approximating capability of the related approximant

$$\mathscr{N}_{h_{jk}}=\frac{\left\|f-h_{jk}\right\|^2}{\|f\|^2},\quad 1\le j,k\le N \quad (16)$$

It can be easily seen that, if the value of $\mathscr{N}_{h_{jk}}$ is equal to 0 for any j and k value, the exact representation is obtained.

2.4 Fluctuationlessness approximation theorem

Fluctuationlessness Approximation Theorem for the univariate and multivariate functions were suggested by Demiralp [15,16] and a brief description of this approximation theory and its theorem are given as a summary below.

We symbolize the Hilbert space by $\mathscr{H}$ and its n-dimensional subspace by $\mathscr{H}_n$. The term, Fluctuation Operator, describes the difference between the unit matrix of $\mathscr{H}$ and $\mathscr{H}_n$. The proof of the following theorem which was given together with its proof in Demiralp's paper are given as follows

Theorem *The matrix representation of an algebraic multiplication operator multiplying its operand by $f(x)$, a univariate function which is analytic on the interval $[a, b]$, over H_n is the image of the matrix representation of the operator $\widehat{x}$, which multiplies its operand by the independent variable, over H_n under the function f at the fluctuationlessness limit* [15]

$$\mathbf{F}^{(n)} \approx f\left(\mathbf{X}^{(n)}\right) \tag{17}$$

where $\mathbf{X}^{(n)}$ is the matrix representation of the multiplication operator $\hat{x}$ which multiplies its operand by the independent variable x and $\mathbf{F}^{(n)}$ is the matrix representation of $\hat{f}$ stands for the algebraic operator which multiplies its operand by the function, $f(x)$.

The matrices $\mathbf{X}^{(n)}$ and $\mathbf{F}^{(n)}$ are given as

$$\mathbf{X}^{(n)} \equiv \begin{bmatrix} X_{11}^{(n)} & \cdots & X_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ X_{n1}^{(n)} & \cdots & X_{nn}^{(n)} \end{bmatrix}, \qquad X_{jk}^{(n)} \equiv \left(w_j, \widehat{x} w_k\right), \quad 1 \leq j, k \leq n \tag{18}$$

$$\mathbf{F}^{(n)} \equiv \begin{bmatrix} F_{11}^{(n)} & \cdots & F_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ F_{n1}^{(n)} & \cdots & F_{nn}^{(n)} \end{bmatrix}, \qquad F_{jk}^{(n)} \equiv \left(w_j, \widehat{f} w_k\right), \quad 1 \leq j, k \leq n \tag{19}$$

where $w_j(x)$ functions are the members of an orthonormal basis set to span the Hilbert space. The fluctuationlessness approximation method becomes equivalent to Gauss quadrature [20,21] when polynomial structures are used as basis. Although the Gauss quadratures always need polynomial basis set, fluctuationlessness approximation is not limited by this basis set.

The left hand side of relation (17) is given in (19). Now, we need to find the structure of the right hand side of the same relation. For this purpose, first, the spectral decomposition of the matrix, $\mathbf{X}^{(n)}$ is written as

$$\mathbf{X}^{(n)} = \sum_{i=1}^{n} \lambda_i \boldsymbol{\xi}_i \boldsymbol{\xi}_i^T \tag{20}$$

where λ_i stands for the i-th eigenvalue of $\mathbf{X}^{(n)}$ and $\boldsymbol{\xi}_i$ stands for the corresponding eigenvector. Using above relation, the right hand side of the relation given in (17) can be given as

$$f\left(\mathbf{X}^{(n)}\right) = \sum_{i=1}^{n} f\left(\lambda_i\right) \boldsymbol{\xi}_i \boldsymbol{\xi}_i^T \tag{21}$$

Since we are dealing with multivariate functions in this work, we need to use the fluctuationlessness theorem including multivariance features. The multivariate counterpart of this theorem is also proven [16] and its matematical expression is as follows

$$\mathbf{F}^{(n)} \approx f\left(\mathbf{X}_1^{(n_1)}, \ldots, \mathbf{X}_N^{(n_N)}\right) \tag{22}$$

This formula tells us that the matrix representation of the multivariate function is aproximated by the image of the matrix representations of the N number of independent variables under this function [16,22].

Here, when the spectral representations of matrices are used, the right hand side of above equation becomes as follows

$$f\left(\mathbf{X_1}, \ldots, \mathbf{X_N}\right) = \sum_{i_1=1}^{n_1} \cdots \sum_{i_N=1}^{n_N} f\left(\lambda_{i_1}^{(1)}, \ldots, \lambda_{i_N}^{(N)}\right) \boldsymbol{\xi}_{i_1 \cdots i_N} \boldsymbol{\xi}_{i_1 \cdots i_N}{}^T \tag{23}$$

where

$$\boldsymbol{\xi}_{i_1 \cdots i_N} = \boldsymbol{\xi}_{i_1}^{(1)} \otimes \cdots \otimes \boldsymbol{\xi}_{i_N}^{(N)} \tag{24}$$

Here, $\lambda_{i_k}^{(k)}$ $(1 \leq k \leq N)$ is the i_kth eigenvalue and $\boldsymbol{\xi}_{i_k}^{(k)}$s are the corresponding eigenvectors of the matrix $\mathbf{X}_k^{(n_k)}$. The operator $\otimes$ stands for the direct product operation.

3 Fluctuation free integration based hybrid HDMR method

The determination process of either Plain HDMR or Logarithmic HDMR components consists of evaluating N-tuple integrals. One possible way is of course to evaluate the integrations analytically. However, it is usually hard to get a result for the multiple integrations even sometimes it is impossible. Hence, this work aims to evaluate these integrals by using the fluctuationlessness approximation method [9]. In general, when we apply the considered theorem to the integration, the approximate result of the integral of a univariate function under the unit interval and unit weight is obtained as follows

$$\int_0^1 dx f(x) \approx \sum_{i=1}^{n} f\left(\lambda_i\right) \left(\mathbf{e_1}^{(n)^T} \boldsymbol{\xi}_i\right)^2 \tag{25}$$

where $\mathbf{e_1}^{(n)}$ is the n dimensional unit cartesian vector whose first element is 1 and the others are 0. This result can be used to obtain the general structure of all Plain and Logarithmic HDMR components. However, the domain of each independent variable of a given multivariate function is assumed as $a_i \leq x_i \leq b_i$ where $1 \leq i \leq N$ in which N stands for the number of independent variables. This means that we should convert the given $[a_i, b_i]$ intervals to unit interval, [0, 1]. In this sense, the first step is to write the following general structure of the constant HDMR component

$$f_0 = \int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N) f(x_1, \ldots, x_N) \tag{26}$$

To determine the structure of the constant and the higher variate components, a weight selection is needed as the second step. The following weight, which also satisfies the normalization criteria, is chosen

$$W\left(x_1, \ldots, x_N\right) = \prod_{i=1}^{N} \frac{1}{b_i - a_i}, \quad 1 \le i \le N \tag{27}$$

The third step is to convert the intervals to unit interval and the following conversion is used for this purpose

$$x_i = (b_i - a_i) y_i + a_i, \quad 1 \le i \le N \tag{28}$$

When the integral evaluation process given in (25) and the interval conversion given in (28) are applied to the relation (26), the constant component of Plain HDMR method is approximately obtained as follows

$$f_0 \approx \sum_{k_1=1}^{n_1} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{i=1}^{N} \left(\mathbf{e_1}^{(n_i)^T} \xi_{k_i}^{(i)} \right)^2 \right] f\left(\lambda_1^{(k_1)}, \ldots, \lambda_N^{(k_N)} \right) \tag{29}$$

The same philosophy can be applied to the Logarithmic HDMR algorithm and the constant Logarithmic HDMR component is obtained as

$$\varphi_0 \approx \sum_{k_1=1}^{n_1} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{i=1}^{N} \left(\mathbf{e_1}^{(n_i)^T} \xi_{k_i}^{(i)} \right)^2 \right] q\left(\lambda_1^{(k_1)}, \ldots, \lambda_N^{(k_N)} \right) \tag{30}$$

where

$$q\left(x_1, \ldots, x_N\right) \equiv \ln\left[f\left(x_1, \ldots, x_N\right) - \phi\left(x_1, \ldots, x_N\right)\right] \tag{31}$$

The following univariate component structures can be determined by using the same philosophy for the Plain and Logarithmic HDMR methods

$$\begin{aligned} f_{i_1}\left(x_{i_1}\right) \approx & \sum_{k_1=1}^{n_1} \cdots \sum_{k_{i_1-1}=1}^{n_{i_1-1}} \sum_{k_{i_1+1}=1}^{n_{i_1+1}} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{\substack{m=1 \\ m \ne i_1}}^{N} \left(\mathbf{e_1}^{(n_m)^T} \xi_{k_m}^{(m)} \right)^2 \right] \\ & \times f\left(\lambda_1^{(k_1)}, \ldots, \lambda_{i_1-1}^{(k_{i_1-1})}, x_{i_1}, \lambda_{i_1+1}^{(k_{i_1+1})}, \ldots, \lambda_N^{(k_N)} \right) - f_0 \end{aligned} \tag{32}$$

$$\begin{aligned} \varphi_{i_1}\left(x_{i_1}\right) \approx & \sum_{k_1=1}^{n_1} \cdots \sum_{k_{i_1-1}=1}^{n_{i_1-1}} \sum_{k_{i_1+1}=1}^{n_{i_1+1}} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{\substack{m=1 \\ m \ne i_1}}^{N} \left(\mathbf{e_1}^{(n_m)^T} \xi_{k_m}^{(m)} \right)^2 \right] \\ & \times q\left(\lambda_1^{(k_1)}, \ldots, \lambda_{i_1-1}^{(k_{i_1-1})}, x_{i_1}, \lambda_{i_1+1}^{(k_{i_1+1})}, \ldots, \lambda_N^{(k_N)} \right) - \varphi_0 \end{aligned} \tag{33}$$

where $1 \le i_1 \le N$.

In this work, we are interested in at most bivariate Plain or Logaritmic HDMR components, so the structure of these two methods' components are given as follows

$$
\begin{aligned}
&f_{i_1 i_2}(x_{i_1}, x_{i_2}) \\
&\approx \sum_{k_1=1}^{n_1} \cdots \sum_{k_{i_1-1}=1}^{n_{i_1-1}} \sum_{k_{i_1+1}=1}^{n_{i_1+1}} \cdots \sum_{k_{i_2-1}=1}^{n_{i_2-1}} \sum_{k_{i_2+1}=1}^{n_{i_2+1}} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{\substack{m=1 \\ m \neq i_1 \wedge m \neq i_2}}^{N} \left(\mathbf{e_1}^{(n_m)^T} \xi_{k_m}^{(m)} \right)^2 \right] \\
&\quad \times f \left(\lambda_1^{(k_1)}, \ldots, \lambda_{i_1-1}^{(k_{i_1-1})}, x_{i_1}, \lambda_{i_1+1}^{(k_{i_1+1})}, \ldots, \lambda_{i_2-1}^{(k_{i_2-1})}, x_{i_2}, \lambda_{i_2+1}^{(k_{i_2+1})}, \ldots, \lambda_N^{(k_N)} \right) \\
&\quad - f_{i_1}(x_{i_1}) - f_{i_2}(x_{i_2}) - f_0
\end{aligned} \tag{34}
$$

$$
\begin{aligned}
&\varphi_{i_1 i_2}(x_{i_1}, x_{i_2}) \\
&\approx \sum_{k_1=1}^{n_1} \cdots \sum_{k_{i_1-1}=1}^{n_{i_1-1}} \sum_{k_{i_1+1}=1}^{n_{i_1+1}} \cdots \sum_{k_{i_2-1}=1}^{n_{i_2-1}} \sum_{k_{i_2+1}=1}^{n_{i_2+1}} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{\substack{m=1 \\ m \neq i_1 \wedge m \neq i_2}}^{N} \left(\mathbf{e_1}^{(n_m)^T} \xi_{k_m}^{(m)} \right)^2 \right] \\
&\quad \times q \left(\lambda_1^{(k_1)}, \ldots, \lambda_{i_1-1}^{(k_{i_1-1})}, x_{i_1}, \lambda_{i_1+1}^{(k_{i_1+1})}, \ldots, \lambda_{i_2-1}^{(k_{i_2-1})}, x_{i_2}, \lambda_{i_2+1}^{(k_{i_2+1})}, \ldots, \lambda_N^{(k_N)} \right) \\
&\quad - \varphi_{i_1}(x_{i_1}) - \varphi_{i_2}(x_{i_2}) - \varphi_0
\end{aligned} \tag{35}
$$

where $1 \leq i_1 < i_2 \leq N$.

The components obtained through (29), (32) and (34) are used to construct the Plain HDMR approximants given in (10) while the Logarithmic HDMR approximants given in (13) are determined by using relations (30), (33) and (35). Finally, these approximants allow us to obtain the Hybrid HDMR approximants given in (15). To execute this last step we need to optimize the value of the hybridity parameter. The procedure of the determination process of this optimized α parameter is given in the next section.

4 Hybridity parameter optimization process

The Hybrid HDMR method is needed to represent a multivariate function having a hybrid nature. Hybrid nature means that the multivariate function under consideration has no purely either additive or multiplicative nature. The Plain HDMR method works well when the function to be represented has a purely or dominantly additive nature. On the other hand, Logarithmic HDMR has its best performance when the given function has a purely or dominantly multiplicative nature. The Hybrid HDMR philosophy uses the expansions of these two methods in a single expansion. The mentioned combination is constructed under a parameter which is named as hybridity parameter. This parameter controls the contribution levels of the two expansions in the representation procedure of the given multivariate function through Hybrid HDMR. Hence, the most important point in this work is to optimize the hybridity parameter to make this control at its highest efficiency. This results in a better approximation through Hybrid HDMR than the other two HDMRs.

When the relation given in (15) is examined carefully, it is easily seen that if the hybridity parameter, α, is equal to 0 then all contributions come from Logaritmic

HDMR expansion while if α parameter is equal to 1 then all contributions come from Plain HDMR expansion for the approximation. However, the most important purpose of the Hybrid HDMR method is to let these two expansions be effective on the representation of the given multivariate function. This means that there should be a process to specify the best α value to get the best representation. For this purpose, a functional is defined as

$$G(\alpha) \equiv \left\| f - h_{jk}(\alpha)) \right\|^2 \tag{36}$$

where f and $h_{jk}(\alpha)$ stand for the given multivariate function and the Hybrid HDMR approximant given in (15) respectively. The explicit form of the right hand side of this relation is

$$\begin{aligned} \left\| f - h_{jk}(\alpha)) \right\|^2 = &\int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N) \\ &\times \left[f\left(x_1, \ldots, x_N\right) - h_{jk}\left(x_1, \ldots, x_N; \alpha\right) \right]^2 \end{aligned} \tag{37}$$

where $1 \leq j, k \leq N$. When the fluationlessness theorem is applied to this N-tuple integration, the following approximate relation is obtained as the result of the above-mentioned integral structure

$$\begin{aligned} G(\alpha) \approx &\sum_{k_1=1}^{n_1} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{i=1}^{N} \left(\mathbf{e_1}^{(n_i)^T} \xi_{k_i}^{(i)} \right)^2 \right] \\ &\times \left[f\left(\lambda_1^{(k_1)}, \ldots, \lambda_N^{(k_N)} \right) - h_{jk}\left(\lambda_1^{(k_1)}, \ldots, \lambda_N^{(k_N)}; \alpha \right) \right]^2 \end{aligned} \tag{38}$$

Now, we have a polynomial structure in terms of α parameter. Next step is to determine the α value that minimizes the value of this norm. This minimization criterion can be given as follows

$$\frac{\partial G}{\partial \alpha} = 0 \tag{39}$$

Using the value for α obtained from this relation in the Hybrid HDMR expansion, the best Hybrid HDMR approximant can be determined for the given multivariate function. Any value inside or outside the interval [0, 1] may be obtained as the hybridity parameter value at the end of this optimization procedure.

Now, the Hybrid HDMR approximants can be constructed through the Plain and Logarithmic HDMR components given in the previous section under the optimized hybridity parameter whose value is obtained through the relation (39).

5 Numerical implementations

In this section, we present certain implementations to test the performance of Hybrid HDMR approximants obtained through the optimization process of the hybridity parameter with the help of the Fluctuationlessness Approximation Theorem. To show the efficiency of the Hybrid HDMR method more clearly, the testing functions are chosen as functions having different types of structures and Hybrid HDMR approximants are obtained for these various testing functions. To measure the performance of the Hybrid HDMR approximants, we use the relative error relation given in (16).

All computations are done by using MuPAD, Computer Algebra System [23], with 10 decimal digits precision. The program codes are run under Linux (Ubuntu 7.10) Operating System. On the other hand, all the numerical results are given within 4-digits precision for simplicity.

The following multivariate functions are chosen to construct numerical implementations for the performance examination

$$
\begin{aligned}
&f_1(x_1,\ldots,x_5)=\sum_{i=1}^{5}x_i, && f_2(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5}x_i\right]^3,\\
&f_3(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5}x_i\right]^5, && f_4(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5}x_i\right]^8,\\
&f_5(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5}x_i\right]^{15}, && f_6(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5}x_i\right]^{20},\\
&f_7(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5}x_i\right]^{25}, && f_8(x_1,\ldots,x_5)=\prod_{i=1}^{5}x_i,\\
&f_9(x_1,\ldots,x_5)=\mathrm{e}^{(x_1+x_2+x_3+x_4+x_5)}, && f_{10}(x_1,\ldots,x_5)=\sin^2(x_1+x_2+x_5)\\
& && \quad+\cos^2(x_3+x_4)
\end{aligned}
\tag{40}
$$

where they all have 5 independent variables. The first testing function, f_1, has a purely additive nature while the testing function, f_8, has a purely multiplicative nature. The other functions from f_2 to f_7 have hybridity nature at different levels. The last two testing functions, f_9 and f_{10} are exponential and trigonometric structures respectively.

We know from the previous works that the Plain HDMR method works well for approximating purely and dominantly additive functions and the Logarithmic HDMR method works well in representing purely and dominantly multiplicative structures. Hybrid HDMR aims to successfully approximate the multivariate functions having hybrid nature which means the functions that are neither dominantly additive nor dominantly multiplicative. When we examine the relative error values given in Table 1, these concluding remarks are proven through numerical examples. The first nine columns of Table 1 are about the relative error values obtained for the Hybrid HDMR

Table 1 Relative error values obtained for the testing functions

	$\mathcal{N}_{h_{00}}$	$\mathcal{N}_{h_{10}}$	$\mathcal{N}_{h_{20}}$	$\mathcal{N}_{h_{01}}$	$\mathcal{N}_{h_{02}}$	$\mathcal{N}_{h_{11}}$	$\mathcal{N}_{h_{12}}$	$\mathcal{N}_{h_{21}}$	$\mathcal{N}_{h_{22}}$	$\mathcal{N}_{s_2}$	$\mathcal{N}_{\pi_2}$
f_1	0.0625	0.0	0.0	0.0019	0.0002	0.0	0.0	0.0	0.0	0.0	0.0002
f_2	0.3403	0.0298	0.0004	0.0161	0.0023	0.0047	0.0021	0.0003	0.0003	0.0004	0.0025
f_3	0.5883	0.1486	0.0135	0.0485	0.0089	0.0265	0.0079	0.0078	0.0106	0.0135	0.0116
f_4	0.8054	0.3942	0.0980	0.0967	0.0258	0.0767	0.0270	0.0464	0.0474	0.9800	0.0476
f_5	0.9561	0.7551	0.4074	0.0882	0.0578	0.1128	0.1109	0.1459	0.2185	0.4074	0.2200
f_6	0.9789	0.8511	0.5528	0.0522	0.0635	0.0923	0.1948	0.1713	0.3583	0.5528	0.3584
f_7	0.9872	0.8945	0.6351	0.0282	0.0694	0.0740	0.2998	0.1793	0.4773	0.6351	0.4795
f_8	0.7627	0.3672	0.1035	0.0	0.0	0.0	0.0	0.0	0.0	0.1035	0.0
f_9	0.3217	0.0479	0.0037	0.0	0.0	0.0	0.0	0.0	0.0	0.0037	0.0
f_{10}	0.0945	0.0321	0.0006	0.0324	0.0029	0.0316	0.0027	0.0006	0.0005	0.0006	0.0038

Table 2 Optimized α values for each testing function

	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8	f_9	f_{10}
α	1.0	0.9602	0.8916	−0.2008	−0.7388	0.9602	0.9825	0.0	0.0	0.8475

approximants while the last two columns are for the bivariate Plain HDMR and Logarithmic HDMR approximants respectively. Since this work proposes an optimization process for obtaining the most appropriate hybridity parameter to get best approximations, the value evaluated for α becomes very important issue in the numerical implementations. Table 2 includes the optimized hybridity parameter values for each implementation. These values are the α values evaluated for the Hybrid HDMR approximant which gives the best representation of the testing function under consideration.

Now, the following discussions are given by taking the results of Tables 1 and 2 into consideration. The first testing function is successfully represented by bivariate HDMR approximant. This is also true for some Hybrid HDMR approximants under the hybridity parameter value 1.0 which means that only the Plain HDMR approximant is used in the representation process because of the nature of the Hybrid HDMR expansion given in (15). The second testing function has a dominantly additive nature. Hence, the Plain HDMR works well for representing this function. In addition, some Hybrid HDMR approximants also work well as a result of the optimization of the hybridity parameter and the α value is obtained as 0.9602 in this implementation. The Hybrid HDMR approximants h_{21}, h_{02}, h_{02}, h_{01} and h_{01} are the best representations for the testing functions f_3, f_4, f_5, f_6 and f_7 respectively. The relative error values obtained for these testing functions are extremely better than the bivariate Plain HDMR and Logarithmic HDMR approximants. These results show us that the optimization of the hybridity parameter significantly effects the efficiency of Hybrid HDMR. The function, f_8, has a purely multiplicative nature and the Logarithmic HDMR approximant works well in the representation of this function. Under the α value 0.0 which means the only contribution comes from the Logarithmic HDMR expansion, some Hybrid HDMR approximants can also exactly represent the given function. The ninth testing function is an exponential one and the methods react in the same way that is seen in the testing function, f_8 which is purely multiplicative. The last testing function is a trigonometric function and h_{22} is the best representation for this trigonometric function. In the last example, the obtained α value is equal to 0.8475, which means that the highest contribution comes from bivariate Plain HDMR approximant while less contribution comes from the bivariate Logarithmic HDMR approximant.

6 Conclusion

In this work, we tried to represent a multivariate function having hybrid nature by using Hybrid HDMR method with an optimized hybridity parameter. Hybrid HDMR expansion is composed of two expansions. One of these expansions is selected as Plain HDMR since it works well in representing the multivariate functions having purely or dominantly additive nature. The second expansion is selected as an expansion of an HDMR based method which works well in expressing functions having purely or dominantly multiplicative nature. In this study, Logarithmic HDMR expansion is inserted into the Hybrid HDMR expansion.

It is well known that taking all components of HDMR based methods increases the mathematical and computational complexity of the method. In this sense, at most the bivariate approximants are used to represent the given multivariate function through Plain, Logarithmic and Hybrid HDMR methods. Truncation at a level in Hybrid HDMR may decrease the representation quality of the given function. To handle this difficulty, the hybridity parameter, which manages the contribution level of each expansion to the Hybrid HDMR structure, plays an important role. This results in a need to optimize this parameter. The numerical results given in the previous section show us that the optimized hybridity parameter dramatically effects the performance of the Hybrid HDMR method. The optimization process of this work with the help of the Fluctuationlessness Approximation Theorem is a successful attempt to get high quality approximations for representing the multivariate functions.

In addition, a problematic case in the HDMR based methods is the evaluation process of multiple integrals coming from the nature of method. The integrals appearing in the Logarithmic HDMR method consists of natural logarithm of the given function and this makes these integrals either hard or impossible to evaluate analytically. To overcome this problem, we use the Fluctuationlessness Approximation Theorem. The numerical results given in Table 1 also show the success of this theorem in the Hybrid HDMR method.

In conclusion, a new algorithm including hybridity parameter optimization for the Hybrid HDMR philosophy is developed in this work. The numerical results support the satisfactory and acceptable performance of this new method.

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