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ORIGINAL PAPER

Fluctuation free multivariate integration based logarithmic HDMR in multivariate function representation

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Abstract This paper focuses on the Logarithmic High Dimensional Model Representation (Logarithmic HDMR) method which is a divide–and–conquer algorithm developed for multivariate function representation in terms of less-variate functions to reduce both the mathematical and the computational complexities. The main purpose of this work is to bypass the evaluation of N–tuple integrations appearing in Logarithmic HDMR by using the features of a new theorem named as Fluctuationlessness Approximation Theorem. This theorem can be used to evaluate the complicated integral structures of any scientific problem whose values can not be easily obtained analytically and it brings an approximation to the values of these integrals with the help of the matrix representation of functions. The Fluctuation Free Multivariate Integration Based Logarithmic HDMR method gives us the ability of reducing the complexity of the scientific problems of chemistry, physics, mathematics and engineering. A number of numerical implementations are also given at the end of the paper to show the performance of this new method.

Keywords High dimensional model representation · Multivariate functions · Approximation

1 Introduction

Dealing with the numerical calculations of multivariate functions in chemical, physical or engineering applications may become a serious problem especially in computer based applications because of the memory and time restrictions. These limitations urge

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the researchers to develop certain divide–and–conquer methods where we desire to deal with less variate functions instead of a given multivariate function in the considered problem. One of these methods is named as High Dimensional Model Representation (HDMR) and was first proposed by I.M. Sobol [1] and then more generalized by H. Rabitz [2–4] and M. Demiralp [5]. In literature, this method is also known as Sobol HDMR or Plain HDMR. In this work, we call it as Plain HDMR and we will use that philosophy in our new HDMR based algorithm.

The Plain HDMR method has a finite expansion including a constant term, N univariate terms, $N(N-1)/2$ bivariate terms and so on. The total number of terms of the expansion is 2^N. To reduce the computational complexity needed to obtain all these components, in general, only the first few terms are taken into consideration, that is, truncation approximations are constructed to represent a multivariate function in terms of less-variate functions. To control the quality of this approximation additivity measurers [5] were defined by M. Demiralp. These measurers which are monotonously increasing measurers having values in the interval, [0, 1], allow us to make an error analysis for the obtained HDMR approximant of the given multivariate function.

Many other HDMR based methods have been developed by different researchers for various areas [6–15].

Since the expansion structure of the Plain HDMR method has an additive nature, this method works well as the function under consideration is sufficiently additive and becomes poor as the multiplicativity of the original function increases. To overcome the problems coming from multiplicativity, two different HDMR methods have been devoleped. They are Factorized HDMR method [16,17] and Logarithmic HDMR method [18].

The Factorized HDMR method works well for the multiplicative type multivariate functions as the structure of the method's expansion has an multiplicative nature. However, there exists a number of disadvantages for this algorithm. One of them is the impossibility of constructing monotonously increasing measurers like the additivity measurers of plain HDMR [5]. This makes the quality control very difficult. This is because of the multiplicative nature of the Factorized HDMR. The other disadvantage is the effect of the cumulative approximation errors coming from the truncation of the expansion at a level. This effect is again a result of the multiplicative nature of the algorithm's expansion.

The Logarithmic HDMR method is based on evaluating the integral of natural logarithm of the given multivariate function. This feature makes this method not easily applicable to the considered problems since it becomes too complicated to evaluate these integrals. Hence, in this work, we try to bypass these integral evaluations of Logarithmic HDMR and to construct more simple algorithm with the help of the Fluationlessness Approximation Theorem which was first proposed by M. Demiralp [19–21]. This mentioned theorem was also applied to different problems [22,23].

There exist another work from the authors of this work about Enhanced Multivariance Product Representation method [24]. This method was developed again for the representation of the multivariate functions having dominantly of purely multiplicative natures. The philosophy of that work is different from these mentioned HDMR based methods, that is, the method includes support functions to increase the performance of the HDMR expansion.

This paper is organized as follows. The second section describes the details of the Logarithmic HDMR method. After that, in the third section, the Fluctuationlessness Approximation Theorem is given. The Fluctuation Free Integration method is given in a detailed way in the fourth section while the new form of the Logarithmic HDMR method developed with the help of the fluctuation free integration is explained in the fifth section. Next section covers the numerical implementations to show the performance of our new method. Finally, the concluding remarks are presented in the last section of the paper.

2 The logarithmic HDMR method

The Logarithmic HDMR Method is simply based on the Plain HDMR philosophy. The basic formula for Plain HDMR of a given multivariate function, $f(x_1,\ldots,x_N)$, is given as follows [1].

$$f(x_1,\ldots,x_N) = f_0+\sum_{i_1=1}^{N} f_{i_1}(x_{i_1})+\sum_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N} f_{i_1i_2}(x_{i_1},x_{i_2})+\cdots+f_{1\ldots N}(x_1,\ldots,x_N) \tag{1}$$

The Logarithmic HDMR Method is based on the idea of expanding the natural logarithm of a nonnegative multivariate function to HDMR instead of the function's itself. The Logarithmic HDMR formula which defines a product type representation for a given multivariate function can be expressed as follows

$$\begin{aligned} ln\left[f\left(x_1,\ldots,x_N\right)-\phi\left(x_1,\ldots,x_N\right)\right] = \varphi_0 + \sum_{i_1=1}^{N}\varphi_{i_1}\left(x_{i_1}\right) + \sum_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\varphi_{i_1i_2}\left(x_{i_1},x_{i_2}\right) \\ +\cdots+\varphi_{1\ldots N}(x_1,\ldots,x_N) \end{aligned} \tag{2}$$

where $\phi\left(x_1,\ldots,x_N\right)$ is a minorant function to the given function, $f\left(x_1,\ldots,x_N\right)$ to produce a nonnegative or preferably positive core function for the logarithm. We call this entity "Reference Function" since it takes somehow the role of the origin in the space of the functions. For simplicity, the following assumption will be used in the rest of the relations of the work.

$$h\left(x_1,\ldots,x_N\right) = ln\left[f\left(x_1,\ldots,x_N\right)-\phi\left(x_1,\ldots,x_N\right)\right] \tag{3}$$

If the equation given in (2) is reorganized the following representation formula for Logarithmic HDMR is obtained.

$$f\left(x_1,\ldots,x_N\right)=\phi\left(x_1,\ldots,x_N\right)+\mathrm{e}^{\varphi_0}\left[\prod_{i_1=1}^{N}\mathrm{e}^{\varphi_{i_1}\left(x_{i_1}\right)}\right]\left[\prod_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\mathrm{e}^{\varphi_{i_1i_2}\left(x_{i_1},x_{i_2}\right)}\right]\times\cdots \tag{4}$$

The main important point here is to determine the general structures of the right hand side components of the Logarithmic HDMR expansion given in (2). These components such as φ_0, φ_{i_1} and so on can be uniquely obtained by imposing mutual orthogonality amongst these components [5,18]

$$(\varphi_{i_1 i_2 \ldots i_k}, \varphi_{i_1 i_2 \ldots i_l}) = 0, \quad \{i_1, i_2, \ldots, i_k\} \not\equiv \{i_1, i_2, \ldots, i_l\}, \quad 1 \le k, l \le N \tag{5}$$

where

$$(u, v) \equiv \int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N)\, u(x_1, \ldots, x_N) v(x_1, \ldots, x_N) \tag{6}$$

Here, $u(x_1, \ldots, x_N)$ and $v(x_1, \ldots, x_N)$ are arbitrary square integrable multivariate functions. 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.

$$W(x_1, \ldots, x_N) \equiv \prod_{j=1}^{N} W_j(x_j), \qquad x_j \in \left[a_j\, ,\, b_j\right], \qquad 1 \le j \le N \tag{7}$$

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

$$\int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, \ldots, x_N) \varphi_{i_1}(x_{i_1}) = 0, \qquad 1 \le i_1 \le N \tag{8}$$

For the determination of the right hand side components of the Logarithmic HDMR expansion certain projection operators are defined. The following projection operator which maps from the Hilbert space of N variate integrable functions to the same space's constant function subspace is defined for the determination of the constant term, φ_0.

$$\mathscr{P}_0 g\,(x_1, \ldots, x_N) \equiv \int_{a_1}^{b_1} dx_1 W_1\,(x_1) \times \cdots \times \int_{a_N}^{b_N} dx_N W_N\,(x_N)\, g\,(x_1, \ldots, x_N) \tag{9}$$

If $\mathscr{P}_0$ is applied on both sides of Eq. (2), all the higher than zero variate components of Logarithmic HDMR vanish because of the vanishing property (proposed by Sobol) given in (8) and we can write the following equation for the constant term.

$$\varphi_0 = \mathscr{P}_0 h\,(x_1, \ldots, x_N) \tag{10}$$

This gives the following general relation for the constant component

$$\varphi_0 = \int_{a_1}^{b_1} dx_1 W_1(x_1) \times \cdots \times \int_{a_N}^{b_N} dx_N W_N(x_N)\, h(x_1, \ldots, x_N) \tag{11}$$

where the weight function should be product type as we mentioned before, to avoid inconsistencies in the construction. To determine the univariate Logarithmic 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 $1 \le i_1 \le N$.

$$\begin{aligned}\mathscr{P}_{i_1} g(x_1, \ldots, x_N) &\equiv \int_{a_1}^{b_1} dx_1 W_1(x_1) \times \cdots \times \int_{a_{i_1-1}}^{b_{i_1-1}} dx_{i_1-1} W_{i_1-1}(x_{i_1-1}) \\ &\times \int_{a_{i_1+1}}^{b_{i_1+1}} dx_{i_1+1} W_{i_1+1}(x_{i_1+1}) \times \cdots \times \int_{a_N}^{b_N} dx_N W_N(x_N) g(x_1, \ldots, x_N)\end{aligned} \tag{12}$$

This operator maps from the entire Hilbert space to its subspace of relevant univariate functions. If we apply $\mathscr{P}_{i_1}$ on both sides of (2) and take the Sobol's vanishing conditions or equivalently Demiralp's orthogonality conditions into consideration then we can write the general structure of the univariate Logarithmic HDMR components as follows

$$\varphi_{i_1}\left(x_{i_1}\right) = \mathscr{P}_{i_1} h(x_1, \ldots, x_N) - \varphi_0, \quad 1 \le i_1 \le N \tag{13}$$

The following general expression for the univariate Logarithmic HDMR components can be then written.

$$\begin{aligned}\varphi_{i_1}\left(x_{i_1}\right) &= \int_{a_1}^{b_1} dx_1 W_1(x_1) \times \cdots \times \int_{a_{i_1-1}}^{b_{i_1-1}} dx_{i_1-1} W_{i_1-1}(x_{i_1-1}) \int_{a_{i_1+1}}^{b_{i_1+1}} dx_{i_1+1} W_{i_1+1}(x_{i_1+1}) \\ &\times \cdots \times \int_{a_N}^{b_N} dx_N W_N(x_N) h(x_1, \ldots, x_N) - \varphi_0, \qquad 1 \le i_1 \le N\end{aligned} \tag{14}$$

The structure of the bivariate Logarithmic HDMR components can be determined in the similar way. Hence, we give only the final form of this structure as

$$
\begin{aligned}
\varphi_{i_1 i_2}\left(x_{i_1}, x_{i_2}\right) = & \int_{a_1}^{b_1} dx_1 W_1(x_1) \times \cdots \times \int_{a_{i_1-1}}^{b_{i_1-1}} dx_{i_1-1} W_{i_1-1}(x_{i_1-1}) \\
& \times \int_{a_{i_1+1}}^{b_{i_1+1}} dx_{i_1+1} W_{i_1+1}(x_{i_1+1}) \times \cdots \times \int_{a_{i_2-1}}^{b_{i_2-1}} dx_{i_2-1} W_{i_2-1}(x_{i_2-1}) \\
& \times \int_{a_{i_2+1}}^{b_{i_2+1}} dx_{i_2+1} W_{i_2+1}(x_{i_2+1}) \times \cdots \times \int_{a_N}^{b_N} dx_N W_N(x_N) h\left(x_1, \ldots, x_N\right) \\
& -\varphi_{i_1}\left(x_{i_1}\right) - \varphi_{i_2}\left(x_{i_2}\right) - \varphi_0
\end{aligned} \tag{15}
$$

where $1 \leq i_1 < i_2 \leq N$. The determination of higher variate Logarithmic HDMR components can be realised by defining other projection operators which maps to the subspaces of higher variate functions in the same manner.

Logarithmic HDMR is in fact a finite sum and it can be truncated at some level of variance 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 Logarithmic HDMR by $\pi_i\left(x_1, \ldots, x_N\right)$ where i denotes the level of multivariance. The cases $i = 0, i = 1, i = 2$ correspond to the constant, univariate and bivariate Logarithmic HDMR approximants respectively. They are given below by using the relation given in (4) under the assumption that the minorant function, $\phi\left(x_1, \ldots, x_N\right)$, is vanishing for simplicity (otherwise they will be more complicated although a recursive structure can be constructed).

$$
\begin{aligned}
\pi_0(x_1, \ldots, x_N) &= \mathrm{e}^{\varphi_0} \\
\pi_1(x_1, \ldots, x_N) &= \pi_0(x_1, \ldots, x_N) \prod_{i_1=1}^{N} \mathrm{e}^{\varphi_{i_1}\left(x_{i_1}\right)} \\
\pi_2(x_1, \ldots, x_N) &= \pi_1(x_1, \ldots, x_N) \prod_{\substack{i_1, i_2=1 \\ i_1 < i_2}}^{N} \mathrm{e}^{\varphi_{i_1 i_2}\left(x_{i_1}, x_{i_2}\right)}
\end{aligned} \tag{16}
$$

Since we are dealing with the Logarithmic HDMR approximants, we need to examine the quality of these approximations. For this purpose, the following relative error analysis relation is defined

$$
\mathcal{N}_{\pi_k} = \frac{\| f - \pi_k \|}{\| f \|}, \qquad 1 \leq k \leq N \tag{17}
$$

where π_k stands for the k-th order Logarithmic HDMR approximant. In this work, we only evaluate the $\mathcal{N}_{\pi_0}$, $\mathcal{N}_{\pi_1}$ and $\mathcal{N}_{\pi_2}$ error values since we are dealing at most the bivariate Logarithmic HDMR approximant. The error values getting close to zero, the higher quality of our Logarithmic HDMR approximant. The performance of the Logarithmic HDMR approximants decreases while this relative error value begins to approach to 1.

3 Fluctuationlessness approximation theorem

In this section, we give some information about a new method which is called Fluctuationlessness Approximation [19–21] and a related theorem for the univariate functions.

We can consider the Hilbert space $\mathscr{H}$ and its n-dimensional subspace $\mathscr{H}_n$. The difference between the unit matrix of $\mathscr{H}$ and $\mathscr{H}_n$ is called "Fluctuation Operator "in the proof of the following theorem which was given together with its proof in Demiralp's paper [21].

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* [21].

$$\mathbf{F}^{(n)} \approx f\left(\mathbf{X}^{(n)}\right) \tag{18}$$

Here $\mathbf{X}^{(n)}$ is the matrix representation of the multiplication operator $(\hat{x})$ which multiplies its operand by the independent variable, x. It is explicitly given below

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

where the $w_j(x)$ functions are the members of an orthonormal basis set to span the Hilbert space $\mathscr{H}$ under consideration and the matrix representation of the function $f(x)$, denoted by $\mathbf{F}^{(n)}$ here, can be given as follows

$$\mathbf{F}^{(n)} \equiv \begin{bmatrix} F_{11}^{(n)} & \cdots & F_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ F_{n1}^{(n)} & \cdots & F_{nn}^{(n)} \end{bmatrix}, \qquad F_{jk}^{(n)} \equiv \left(w_j, \widehat{f} w_k\right), \quad 1 \le j, k \le n \tag{20}$$

Here $\hat{f}$ stands for the algebraic operator which multiplies its operand by the function $f(x)$.

The multivariate counterpart of this theorem is also proven by M. Demiralp [26]. There we replace the single independent variable x by N number of independent variables, $x_1,\ldots,x_N$ and the function $f(x)$ should be replaced by its N–variate counterpart, $f(x_1,\ldots,x_N)$. Then, we can write

$$\mathbf{F}^{(n)} \approx f\left(\mathbf{X}_1^{(n_1)},\ldots,\mathbf{X}_N^{(n_N)}\right) \tag{21}$$

Here, the main idea is 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. So the right hand side of the Eq. (21) can be given as follows by using the spectral representations of matrices.

$$\mathbf{F}^{(n)} \approx f(\mathbf{X}_1,\ldots,\mathbf{X}_N) = \sum_{i_1=1}^{n_1}\cdots\sum_{i_N=1}^{n_N} f\left(\lambda_{i_1}^{(1)},\ldots,\lambda_{i_N}^{(N)}\right)\alpha_{i_1\cdots i_N}\alpha_{i_1\cdots i_N}{}^T \tag{22}$$

Here $\lambda_{i_j}^{(k)}$ $(1 < j < N)$ is the i_j–th eigenvalue of the matrix representation of the independent variable x_k. The definition of the $\alpha_{i_1,\ldots,i_N}$ vector is given as follows

$$\alpha_{i_1\cdots i_N} = \alpha_{i_1}^{(1)}\otimes\cdots\otimes\alpha_{i_N}^{(N)} \tag{23}$$

where $\alpha_{i_j}^{(k)}$s are the corresponding eigenvectors of i_j–th eigenvalues. The operator $\otimes$ appearing in the above relation corresponds to direct product operation.

4 Fluctuation free integration

The Fluctuation Free Integration method produces an approximation by using the universal matrix which is the matrix representation of the independent variable and the fluctuationlessness theorem instead of evaluating the integral of the given function analytically.

In this section, this method will be explained for the univariate function, $f(x)$ and then the utilization of fluctuation free integration in Logarithmic HDMR for the multivariate functions will be given in the next section.

Let $f(x)$ be an univariate and analitic function and $\mathscr{I}$ be the integral of this function in the interval of [0, 1].

$$\mathscr{I} = \int_0^1 dx f(x) \tag{24}$$

To build an approximation to this integral, at first we have to determine the matrix representation of the independent variable x, that is, we need to construct the fluctuation matrix [21,25]. To obtain the matrix representation of the independent variable, we need to select the basis functions, $w_j(x)$ spanning the Hilbert space under consideration. Since we are dealing with the integral evaluation the constraint, $w_1(x) = 1$ choice is preferred on the first element of the basis set. The reason of this constraint is to rewrite the integral structure given in (24) as follows by using the fluctuationlessness approximation theorem.

$$\mathscr{I} = \int_0^1 dx f(x) \equiv \int_0^1 dx w_1(x) f(x) w_1(x) = (w_1, f(\widehat{x}) w_1) \tag{25}$$

Only constant function choice enables us to do so.

If we consider that the expression $(w_1, f(\widehat{x})w_1)$ is an inner product and the fact that (j, k)-th element of the n dimensional matrix representation of the analytical function $f(x)$, is $\left(w_j, f\left(\widehat{x}\right) w_k\right)$, $1 \le j, k \le n$, then the following relation can be written

$$(w_1, f(\widehat{x})w_1) = \mathbf{e_1}^{(n)^T} \mathbf{F}^{(n)} \mathbf{e_1}^{(n)} \tag{26}$$

where $\mathbf{e_1}^{(n)}$ is the n dimensional unit cartesian vector whose only nonzero element, 1, is located at the first position. For this case, we can rewrite the relation (25) as follows.

$$\mathscr{I} = \int_0^1 dx f(x) \equiv \int_0^1 dx w_1(x) f(x) w_1(x) = (w_1, f(\widehat{x})w_1) = \mathbf{e_1}^{(n)^T} \mathbf{F}^{(n)} \mathbf{e_1}^{(n)} \tag{27}$$

When the fluctuationlessness approximation theorem is taken into consideration, the following relation is obtained by using the relation given in (18).

$$\mathbf{e_1}^{(n)^T} \mathbf{F}^{(n)} \mathbf{e_1}^{(n)} \approx \mathbf{e_1}^{(n)^T} f\left(\mathbf{X}^{(n)}\right) \mathbf{e_1}^{(n)} \tag{28}$$

To obtain the value of the given integral, finally we can write the image of the spectral decomposition of the $\mathbf{X}^{(n)}$ matrix under the function, f, as follows

$$f\left(\mathbf{X}^{(n)}\right) = \sum_{i=1}^{n} f\left(\xi_i\right) \alpha_i \alpha_i^T \tag{29}$$

and the approximate value of the given integral by using this image is obtained as

$$\mathscr{I} \approx \sum_{i=1}^{n} f\left(\xi_i\right) \mathbf{e_1}^{(n)^T} \alpha_i \alpha_i^T \mathbf{e_1}^{(n)} = \sum_{i=1}^{n} f\left(\xi_i\right) \left(\mathbf{e_1}^{(n)^T} \alpha_i\right)^2 \tag{30}$$

By this way, to evaluate the given integral, we deal with the eigenvalues and the corresponding eigenvectors of the independent variable's n dimensional matrix representation and the image of each eigenvalue under the given function instead of the analytical determination process. This will give an approximate result for the given integral.

There exist still such integrals in the construction of the matrix representations of the independent variables. However, these matrix representations are universal for each n value. Once these matrices are constructed then they can be saved in a database and can be used in other problems having the same n value. This means, we reduce the complexity of the problem coming from integral evaluations.

When the elements of the basis set are selected as polynomials, this method becomes same as the Gauss quadrature method [27,28]. The big difference is to have the ability of selecting basis set elements different from polynomials, that is, there is no extra structural constraint on basis set selection. This feature gives an important flexibility to our new method.

5 Fluctuation free integration based logarithmic HDMR method

Since every finite interval can be converted to the unit interval [0, 1], we will use this unit interval in our method's relations. In addition to this, the weight function appearing in the integrals of the Logarithmic HDMR method is unit constant weight function to get weight function integral unity.

$$W_i(x_i) = 1, \quad 1 \le i \le N \quad \Longrightarrow \quad W(x_1, \ldots, x_N) = \prod_{i=1}^{N} W_i(x_i) = 1 \tag{31}$$

Hence, we can rewrite the structure of the constant Logarithmic HDMR component given in (11) as follows.

$$\varphi_0 = \int_0^1 dx_1 \cdots \int_0^1 dx_N h\left(x_1, \ldots, x_N\right) \tag{32}$$

To evaluate these integrals with the help of the fluctuation free integration, first we construct the matrix representations of each independent variable. For this purpose, to evaluate the N dimensional integral structure having N independent variables, N number of matrix representations will be obtained. The dimension of each matrix is given as $n_k \times n_k$, $(1 \le k \le N)$ and these values may be chosen all different. Using the fluctuation free integration philosophy, the first step to obtain the structure of the constant Logarithmic HDMR component in terms of the matrix representation features of each independent variable can be given as

$$\varphi_0 \approx \int_0^1 dx_1 \cdots \int_0^1 dx_{N-1} \mathbf{e_1}^{(n_N)^T} \sum_{k_n=1}^{n_N} h\left(x_1, \ldots, x_{N-1}, \lambda_N^{(k_N)}\right) \xi_{k_N}^{(N)} \xi_{k_N}^{(N)^T} \mathbf{e_1}^{(n_N)} \tag{33}$$

where $\lambda_N^{(k_N)}$ stands for the eigenvalues of the $n_N \times n_N$ dimensional X_N matrix representation of the independent variable x_N and $\xi_{k_N}^{(N)}$ stand for the corresponding eigenvectors of the eigenvalues. Since the given multivariate function is analytical the above relation can be rewritten as

$$\varphi_0 \approx \sum_{k_n=1}^{n_N} \left(\mathbf{e_1}^{(n_N)^T} \xi_{k_N}^{(N)} \right)^2 \int_0^1 dx_1 \cdots \int_0^1 dx_{N-1} h\left(x_1, \ldots, x_{N-1}, \lambda_N^{(k_N)}\right) \tag{34}$$

and if the above approximation procedure is repeated for the remaining integrations in the same manner, the following final structure of the constant component is obtained.

$$\varphi_0 \approx \sum_{k_1=1}^{n_1} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{i=1}^{N} \left(\mathbf{e_1}^{(n_i)^T} \xi_{k_i}^{(i)} \right)^2 \right] h\left(\lambda_1^{(k_1)}, \ldots, \lambda_N^{(k_N)}\right) \tag{35}$$

The next step is to determine the univariate Logarithmic HDMR structures by using the same philosophy. As a result the following structure for the univariate components is determined

$$\begin{aligned} \varphi_{i_1}(x_{i_1}) \approx & \sum_{k_1=1}^{n_1} \cdots \sum_{k_{i_1-1}=1}^{n_{i_1-1}} \sum_{k_{i_1+1}=1}^{n_{i_1+1}} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{\substack{m=1\\ m\neq i_1}}^{N} \left(\mathbf{e_1}^{(n_m)^T} \xi_{k_m}^{(m)} \right)^2 \right] \\ & \times h\left(\lambda_1^{(k_1)}, \ldots, \lambda_{i_1-1}^{(k_{i_1-1})}, x_{i_1}, \lambda_{i_1+1}^{(k_{i_1+1})}, \ldots, \lambda_N^{(k_N)}\right) - \varphi_0 \end{aligned} \tag{36}$$

where $1 \le i_1 \le N$. Since we are dealing with at most bivariate Logarithmic HDMR components the last relation for this section is given for these components as follows

$$\begin{aligned} \varphi_{i_1 i_2}(x_{i_1}, x_{i_2}) \approx & \sum_{k_1=1}^{n_1} \cdots \sum_{k_{i_1-1}=1}^{n_{i_1-1}} \sum_{k_{i_1+1}=1}^{n_{i_1+1}} \cdots \sum_{k_{i_2-1}=1}^{n_{i_2-1}} \sum_{k_{i_2+1}=1}^{n_{i_2+1}} \cdots \sum_{k_n=1}^{n_N} \left[\prod_{\substack{m=1\\ m\neq i_1 \wedge m\neq i_2}}^{N} \left(\mathbf{e_1}^{(n_m)^T} \xi_{k_m}^{(m)} \right)^2 \right] \\ & \times h\left(\lambda_1^{(k_1)}, \ldots, \lambda_{i_1-1}^{(k_{i_1-1})}, x_{i_1}, \lambda_{i_1+1}^{(k_{i_1+1})}, \ldots, \lambda_{i_2-1}^{(k_{i_2-1})}, x_{i_2}, \lambda_{i_2+1}^{(k_{i_2+1})}, \ldots, \lambda_N^{(k_N)}\right) \\ & - \varphi_{i_1}(x_{i_1}) - \varphi_{i_2}(x_{i_2}) - \varphi_0 \end{aligned} \tag{37}$$

where $1 \le i_1 < i_2 \le N$. After all these terms are obtained, the equation given in (16) is used to make an approximation to the given multivariate function.

6 Numerical implementations

In this section, we present certain implementations to test the performance of fluctuation free integration based Logarithmic HDMR method. All computations for this purpose are done by using MuPAD, Computer Algebra System [29], with 10 decimal digit precision. The program codes are run under Linux (Ubuntu 7.10) Operating System.

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

$$
\begin{aligned}
& f_1(x_1,\ldots,x_5)=\sum_{i=1}^{5} x_i, && f_2(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5} x_i\right]^3, \\
& f_3(x_1,\ldots,x_5)=\left[\sum_{i=1}^{5} x_i\right]^6, && f_4(x_1,\ldots,x_5)=\prod_{i=1}^{5} x_i \\
& f_5(x_1,\ldots,x_4)=x_1x_3\cos(x_2x_4), && f_6(x_1,\ldots,x_5)=\mathrm{e}^{x_1+x_2+x_3+x_4+x_5}
\end{aligned}
\tag{38}
$$

The first four testing functions are polynomial type functions while the fifth one is trigonometric and the last one is an exponential. The first testing function is a purely additive function, the second one is dominantly additive and the other polynomial functions are dominantly and purely multiplicative functions respectively. The last two functions are given here to test the performance of our new method in different function types, that is, in different types of scientific problems.

Relations (35), (36) and (37) are used to determine the constant, univariate and the bivariate structures of each testing function and then these components are inserted into the approximants given in (16) to obtain the constant, univariate and the bivariate Logarithmic HDMR approximants. Since the obtained representations of the given multivariate testing functions are approximants, we need to measure the quality of them. Hence, we use relation (17) to evaluate a relative error value for each approximant to observe the performance success of our new method.

The relative error values for each testing implementation obtained through the Fluctuation Free Multivariate Integration based Logarithmic HDMR method are given with respect to the Plain HDMR method in Table 1. The integrals of the Plain HDMR method are also evaluated with the help of the Fluctuationlessness Theorem in this work. The table covers $\mathcal{N}_{s_0}$, $\mathcal{N}_{s_1}$ and $\mathcal{N}_{s_2}$ standing for the relative error values of the constant, univariate and the bivariate Plain HDMR approximants while $\mathcal{N}_{\pi_0}$, $\mathcal{N}_{\pi_1}$ and $\mathcal{N}_{\pi_2}$ corresponding to the relative error values of the constant, univariate and the bivariate Logarithmic HDMR approximants respectively. The best relative error value obtained for each implementation is marked as boldface.

It is clear that the Plain HDMR method has an additive type expansion to represent the given multivariate function. Hence, we expect that the Plain HDMR method will represent the multivariate functions having additive natures well. On the other hand, as the additivity dominance of the given function decreases while the multiplicativity dominance increases, the performance of the Plain HDMR method becomes worse and it is easily seen that the performance of the Logarithmic HDMR method which is supported by the Fluctuationlessness Approximation Theorem becomes impressive. This result can be observed when we examine the error values given in Table 1 obtained

Table 1 Relative error values of the testing implementations obtained for HDMR and logarithmic HDMR

	f_1	f_2	f_3	f_4	f_5	f_6
$\mathscr{N}_{s_0}$	0.25	0.58280	0.86329	0.87332	0.66440	0.56552
$\mathscr{N}_{s_1}$	**0.0**	0.17263	0.55561	0.60596	0.25730	0.21750
$\mathscr{N}_{s_2}$	**0.0**	**0.01978**	0.24538	0.32174	0.03411	0.06034
$\mathscr{N}_{\pi_0}$	0.25246	0.61832	0.89731	0.93280	0.71027	0.58598
$\mathscr{N}_{\pi_1}$	0.04943	0.23351	0.88168	**0.0**	0.04718	**0.0**
$\mathscr{N}_{\pi_2}$	0.01242	0.04944	**0.13991**	**0.0**	**0.0**	**0.0**

for especially the third and the fourth testing functions since the natures of these functions are dominantly and purely multiplicative. The relative error value obtained for the bivariate Fluctuation Free Multivariate Integration based Logarithmic HDMR approximant of the third testing function is approximately 14% while the error for the bivariate Plain HDMR approximant is 25%. The fourth testing function is purely multiplicative and the univariate approximant obtained through our new method represents that function exactly. The bivariate Plain HDMR approximant of the same function can represent the same function with an error value of 32%. These values prove our expectations that our new method can represent the given multiplicative functions impressively better than the Plain HDMR.

It is either quite difficult or almost impossible to evaluate the N–tuple integrals of the functions like the fifth testing function by using the standard Logarithmic HDMR method in computer based algebraic tools because the method expands the natural logarithm of the given function to HDMR instead of the function's itself. Our new algorithm which uses the Fluctuationlessness Approximation Theory in the evaluation process of these integrals allows us to bypass the mentioned evaluations and to represent the given multivariate function in terms of less variate functions such as univariate and bivariate ones. The function, $f_5(x_1, \ldots, x_4)$, is a trigonometric function and it is not easy to evaluate the 4-tuple integrals of the natural logarithm of this function when we use the standard Logarithmic HDMR method to represent it. However, we have the ability of representing the same function through the Fluctuation Free Multivariate Integration based HDMR methods and it is seen that the best approximation is obtained through the bivariate approximant of our new method. In addition, one can say that the representation quality of even the univariate approximant is enough to represent that function since the obtained error value is between 4 and 5%.

When the results obtained for the exponential function, $f_6(x_1, \ldots, x_5)$, are examined, since the structure of the Logarithmic HDMR's expansion best fits the problem we get the exact representation through the univariate Logarithmic HDMR approximant.

Another advantage of our new method is to decrease the CPU time periods needed to evaluate the N–tuple integrations appearing in the HDMR based methods. The Logarithmic HDMR method supported by the Fluctuationlessness Approximation Theory allows us to obtain the results of those integrations in very short CPU time periods. To show this difference the following testing function is selected

$$f(x_1, \ldots, x_4) = \left[\sum_{i=1}^{4} x_i \right]^{15} \tag{39}$$

where the number of independent variables is 4 and the power appearing in the structure is too big. Hence, the integrations inside the standard HDMR based methods cannot be easily evaluated. They need too long CPU time periods. However, in Fluctuation Free Multivariate Integration based HDMR methods there exist universal matrix representations of multivariate functions and these matrices can be stored in look-up tables. If needed, the mentioned matrices are used in HDMR based methods. Hence the computational complexity of this part of our method is constant. The CPU time period needed to obtain the bivariate Fluctuation Free Multivariate Integration based Logarithmic HDMR approximant is 19.42 seconds while it is 267.05 for the bivariate standard Logarithmic HDMR approximant determination.

7 Concluding remarks

Modelling multivariate problems and using these models in computer based applications cause high mathematical and computational complexities. It is generally better to deal with less-variate structures instead of multivariate ones in engineering problems. This corresponds to the usage of divide–and–conquer methods in modelling. High Dimensional Model Representation based methods are these types of methods. The HDMR method has a finite sum involving a constant term, N number of univariate terms followed by $N(N-1)/2$ bivariate terms and so on. The expansion of this method has 2^N components.

Since the method has a huge number of components to be determined, our main aim is to take the constant, univariate and at most the bivariate components of this expansion into consideration. Hence, an approximate structure can be obtained as the model of the given multivariate problem.

The important point here is the Plain HDMR method works well for the representation of multivariate functions having purely or dominantly additive natures since its expansion is a finite sum. Hence, we need another method to represent the dominantly or purely multiplicative natures well. In the same philosophy with the Plain HDMR expansion to have acceptable repsentations for these types of multivariate function this method should have an finite expansion of products of less-variate components. This method is Factorized HDMR. In fact, the expansion of this method brings huge amount of errors when we deal with the Factorized HDMR approximants. For this purpose, another HDMR based method named as Logarithmic HDMR was developed. This method depends on taking the natural logarithm of the given function. This step allows us to use the Plain HDMR's expansion in the representation of the multiplicative type functions.

One of the most important points of this method is to uniquely determine the structures of the expansion's components. In the standard method there exist N–tuple integrations for the constant term, $N-1$–tuple integrations for the univariate terms, $N-2$–tuple integrations for the bivariate terms and so on. These integral structures cause mathematical and computational complexities because of analytical integral evaluation processes. Here, N stands for the number of the independent variables of the given problem and as this number increases the evaluation of the mentioned integrals become quite difficult and sometimes impossible.

To avoid the determination of these integrals analytically, this work proposes a new algorithm which uses the Fluctuationlessness Approximation Theorem. Using this algorithm, we reduce the mathematical complexity of the problems and we can obtain the results of the integrals even for the functions of which we cannot evaluate the integrals analytically.

As a result, we built a new algorithm for the HDMR based methods and named as Fluctuation Free Based Logarithmic HDMR Method. This new method includes the universal matrix representations of each independent variable and produces the structures of the Logarithmic HDMR components with the help of the eigenvalues and the corresponding eigenvectors of each matrix. When the relative error values obtained for each problem having different types of multivariate functions are examined, it is seen that the method works well especially for the dominantly and purely multiplicative, trigonometric and the exponential structures. The performance of the method is also satisfactory for the structures having additive natures.

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