Fluctuation Free Matrix Representation Based Univariate Integration in Hybrid High Dimensional Model Representation (HHDMR) Over Plain and Factorized HDMR

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Abstract: High Dimensional Model Representation (HDMR) which was first proposed fifteen years ago is still under development for the construction of its new varieties. It is a finite term representation of a multivariate function in terms of less variate functions. Its truncation at certain level of variance serves as an approximation to the target function and the truncation level is preferred to be kept at most bivariance for practical applications. Plain HDMR is used for the functions highly additive while the Factorized HDMR is designed for dominantly multiplicative functions. The Hybrid HDMR (HHDMR) combines these two HDMR varieties into a new version of HDMR and is expected to work more efficiently than plain HDMR and FHDMR. The construction of HHDMR basically uses the components of plain HDMR since FHDMR does the same. The definite integrals appearing in the definition of these components are efficiently approximated by using the fluctuation free matrix representation method which was recently developed by M. Demiralp.

Key–Words: Multivariate Functions, High Dimensional Model Representation, Approximation, Fluctuation Free Matrix Representation.

1 Introduction

A multivariate function $f(x_1, ..., x_N)$ can be expressed as a sum of a constant term, univariate terms, bivariate terms and so on via High Dimensional Model Representation (HDMR) [1–4] as follows

$$\begin{aligned} f(x_1, ..., x_N) &= f_0 + \sum_{i_1=1}^{N} f_{i_1}(x_{i_1}) \\ &+ \sum_{\substack{i_1,i_2=1 \\ i_1<i_2}}^{N} f_{i_1,i_2}(x_{i_1}, x_{i_2}) + \cdots \\ &+ f_{12\cdots N}(x_1, \cdots, x_N) \end{aligned} \quad (1)$$

To obtain the right hand side HDMR components a multiplicative weight functions is used

$$\begin{aligned} &W(x_1, \ldots, x_N) \equiv \prod_{j=1}^{N} w_i(x_i), \\ &x_i \in [\,a_i\,,\, b_i\,], \qquad 1 \le i \le N \end{aligned} \quad (2)$$

where each univariate factor should satisfy the normalization condition

$$\int_{a_i}^{b_i} dx_i w_i(x_i) = 1, \qquad a_i \le x_i \le b_i \quad (3)$$

HDMR components must also satisfy the condition

$$\int_{a_j}^{b_j} dx_j w_j(x_j) f_{i_1 i_2 \ldots i_k}(x_{i_1}, x_{i_2}, \ldots, x_{i_k}) = 0 \quad (4)$$

for $x_j \in \{x_{i_1}, x_{i_2}, \ldots, x_{i_N}\}$, $1 \le j \le k \le N$. This is called "vanishing under integration"condition and it really means that all HDMR components are orthogonal to each other through an appropriately defined inner product. If we assume that $u(x_1, \ldots, x_N)$ and $v(x_1, \ldots, x_N)$ are two arbitrary square integrable multivariate functions, the inner product of these two functions can be defined as

$$\begin{aligned} (u, v) &\equiv \int_{a_1}^{b_1} dx_1 w_1(x_1) \ldots \int_{a_N}^{b_N} dx_N w_N(x_N) \\ &\times \; u(x_1, \ldots, x_N) v(x_1, \ldots, x_N) \end{aligned} \quad (5)$$

With the help of the weight function $W(x_1, \cdots, x_N)$ given in (2) and the normalization condition (3) together with orthogonality condition (4), the components of the right hand side of the expansion in (1) can be obtained as follows

$$\begin{aligned} f_0 &= \int_{a_1}^{b_1} dx_1 w_1(x_1) \ldots \int_{a_N}^{b_N} dx_N w_N(x_N) \\ &\times f(x_1, \ldots, x_N) \end{aligned} \tag{6}$$

$$\begin{aligned} f_i(x_i) &= \int_{a_1}^{b_1} dx_1 w_1(x_1) \ldots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} \\ &\times w_{i-1}(x_{i-1}) \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} w_{i+1}(x_{i+1}) \\ \ldots &\times \int_{a_N}^{b_N} dx_N w_N(x_N) f(x_1, \ldots, x_N) - f_0 \\ & 1 \le i \le N \end{aligned} \tag{7}$$

The remaining higher order terms can be calculated in a similar manner. The right hand side of (1) can be truncated at a desired level of terms for approximation. These truncated representations are called HDMR approximants and are given as below

$$\begin{aligned} s_0(x_1, ..., x_N) &\equiv f_0 \\ s_1(x_1, ..., x_N) &\equiv s_0(x_1, ..., x_N) + \sum_{i=1}^{N} f_i(x_i) \\ &\vdots \\ s_N(x_1, ..., x_N) &\equiv s_{N-1}(x_1, ..., x_N) \\ & \quad + f_{i_1 \ldots i_N}(x_{i_1}, ..., x_{i_N}) \end{aligned} \tag{8}$$

2 Factorized HDMR

If a given multivariate function $f(x_1, \ldots, x_N)$ has dominantly multiplicative structure, Factorized High Dimensional Model Representation, FHDMR, is recommended. FHDMR expansion of a multivariate function $f(x_1, \ldots, x_N)$ is given as follows

$$\begin{aligned} f(x_1, \ldots, x_N) &= r_0 \left[\prod_{i_1=1}^{N} (1 + r_{i_1}(x_{i_1})) \right] \\ &\times \left[\prod_{\substack{i_1, i_2=1 \\ i_1 < i_2}}^{N} (1 + r_{i_1 i_2}(x_{i_1, i_2})) \right] \times \\ &\ldots \times \left[(1 + r_{1 \cdots N}(x_1, \ldots, x_N)) \right] \end{aligned} \tag{9}$$

If a given multivariate function is purely multiplicative then the following FHDMR terms survive in the above product by leaving all factors containing the other FHDMR terms having the value 1. That is,

$$r_0 = f_0 \tag{10}$$

$$r_i(x_i) = \frac{f_i(x_i)}{f_0} \tag{11}$$

Using (10) and (11)

$$f(x_1, \ldots, x_N) = r_0 \left[\prod_{i_1=1}^{N} (1 + r_{i_1}(x_{i_1})) \right] \tag{12}$$

is obtained, so HDMR expansion given in (1) is shaped in factorized form. If (12) is generalized, it is clear that (9) will appear. It is also possible to truncate the product in (9) at some level as we have already done in HDMR expansion (1). If k-th order truncation is shown as p_k, FHDMR approximants are defined as follows

$$\begin{aligned} p_0 &= f_0 \\ p_1 &= p_0 \left[\prod_{i_1=1}^{N} (1 + r_{i_1}(x_{i_1})) \right] \\ &\vdots \\ p_N &= p_{N-1} \left[(1 + r_{12 \cdots N}(x_1, x_2, \ldots, x_N)) \right] \end{aligned} \tag{13}$$

3 Hybrid HDMR using HDMR and FHDMR

If the given multivariate function which is being worked on is neither solely additive nor solely multiplicative, Hybrid HDMR method is expected to approximate the function better than plain HDMR or FHDMR does. Obviously the following idendity holds for any parameter α

$$\begin{aligned} f(x_1, \ldots, x_N) &= \alpha f(x_1, \ldots, x_N) \\ &+ (1 - \alpha) f(x_1, \ldots, x_N) \end{aligned} \tag{14}$$

If we replace the first f at the right hand side of (14) with (1) and the second f with (9) the following expression is obtained.

$$\begin{aligned} f(x_1, \ldots, x_N) &= \alpha \left[f_0 + \sum_{i_1=1}^{N} f_{i_1}(x_{i_1}) + \cdots \right] \\ &+ (1 - \alpha) \left[r_0 \prod_{i_1=1}^{N} (1 + r_{i_1}(x_{i_1})) \cdots \right] \end{aligned} \tag{15}$$

Here α is called the hybridity parameter and usually takes values between zero and one inclusive. Hybrid HDMR approximants are defined using (8) and (13) at the right hand side of equation (15) as follows

$$\begin{aligned} f\left(x_1,\ldots,x_N\right) &\approx h_{jk}\left(x_1,\ldots,x_N;\alpha\right) \\ &= \alpha s_j\left(x_1,\cdots,x_N\right) \\ &+ \left(1-\alpha\right)p_k\left(x_1,\ldots,x_N\right) \end{aligned} \tag{16}$$

where s_j comes from the HDMR expansion and p_k comes from the FHDMR expansion. Hence h_{jk} is called jk-th order HHDMR approximant and enables us to form a table as follows

$$\begin{matrix} h_{00} & \cdots & h_{0N} \\ \vdots & \ddots & \vdots \\ h_{N0} & \cdots & h_{NN} \end{matrix}$$

Beside this, the qualities of these approximants are measured by the entities defined below

$$q_{jk} = \frac{\left|f-h_{jk}\right|^2}{\left|f\right|^2}, \qquad j,k=1,2,...,N \tag{17}$$

The best approximation quality for each approximant is defined by the minimum of these entities. On the other hand each of these entities depend on hybridity parameter through a quadratic function and hence gives an optimum value for the hybridity parameter. However the optimum value may not be in the interval $[\,0,1\,]$. One can expect the optimum values close to 1 for additive functions whereas the multiplicative functions may produce optimimum hybridities close to 0. As long as the hybridity parameter value remains between 0 and 1 it can be considered as a weight for additivity while its complement to 1 can be interpreted as the weight for multiplicativity. On the other hand, the existence possibility of hybridity parameters outside the interval $[\,0,1\,]$ is the signal of the existence of some other cases which can not be considered as a linear combination of additivity and multiplicativity.

4 Fluctuation Free Matrix Representation

The fluctuation free matrix representation is based on the fluctuationlessness theorem, [6–9] conjectured and proven by M. Demiralp. This theorem is given below

Theorem : *If $\widehat{f}$ is an algebraic operator multiplying its operand by $f(x)$ where $f(x)$ belongs to $\mathcal{H}$, the Hilbert space of univariate functions which are analytic and therefore square integrable on the interval $[\,a,b\,]$, and $\widehat{x}$ stands for the algebraic operator which multiplies its operand by the independent variable x then the matrix representation of $\widehat{f}$ over a finite subspace of $\mathcal{H}$ is equal to the image of the matrix representation for $\widehat{x}$, the independent variable operator, over the same subspace, under the function $f(x)$, at the fluctuationlessness limit.*

If the dimension of the subspace in this theorem increases unboundedly then its statement becomes valid without considering the fluctuations since the fluctuations are defined for the transitions between the considered finite subspace $\mathcal{H}_n$ and its complement with respect to $\mathcal{H}$ and the complementary space tends to empty space as n goes to infinity. Otherwise, it states an approximation which can be formulated as follows

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

where $\mathbf{X}^{(n)}$ denotes the matrix representation of the independent variable operator over $\mathcal{H}_n$ and its explicit definition is given below

$$\mathbf{X}^{(n)} \equiv \begin{bmatrix} X_{11}^{(n)} & \cdots & X_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ X_{n1}^{(n)} & \cdots & X_{nn}^{(n)} \end{bmatrix},$$

$$X_{jk}^{(n)} \equiv \left(u_j, \hat{x}u_k\right), \;\; 1 \le j,k \le n \tag{19}$$

The notation $\mathbf{F}^{(n)}$ introduced above symbolizes the matrix representation of the function $f(x)$ over $\mathcal{H}_n$ and its explicit definition can be given as follows

$$\mathbf{F}^{(n)} \equiv \begin{bmatrix} F_{11}^{(n)} & \cdots & F_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ F_{n1}^{(n)} & \cdots & F_{nn}^{(n)} \end{bmatrix},$$

$$F_{jk}^{(n)} \equiv \left(u_j, \hat{f}u_k\right), \;\; 1 \le j,k \le n \tag{20}$$

The functions $u_1(x),\ldots,u_n(x)$ appearing in (19) and (20) are orthonormal basis functions spanning $\mathcal{H}_n$.

5 HDMR With Fluctuation Free Integrals

In this section we will try to compute the integrals encountered while calculating the components of (1). As it was mentioned in the first section, a weight function satisfying the conditions (2) and (3) can be considered for HDMR. For simplicity, the weight function will be chosen as the constant function taking the value 1. We also use the interval $[0,1]$ without any remarkable loss of generality in finite intervals since any finite interval can be transformed to this universal interval through an affine transformation. On the other hand, we will focus on univariate integrals although the HDMR integrals are in general multivariate, since our main goal here to simply show the efficiency of the fluctuation free matrix representation in the integration. So, the integral to be calculated can be expressed as follows

$$I \equiv \int_0^1 dx f(x) \tag{21}$$

Our aim is to approximate this integral with the help of the fluctuation free matrix representation given in (18).

Using the definitions in (19) and (20), the $\mathbf{F}^{(n)}$ and $\mathbf{X}^{(n)}$ matrix elements at the intersection of the i-th row and j-th column can be expressed as follows

$$\begin{aligned} \mathbf{e}_i^{(n)^T}\mathbf{F}^{(n)}\mathbf{e}_j^{(n)} &= \int_0^1 dx u_i(x) f(x) u_j(x) \\ \mathbf{e}_i^{(n)^T}\mathbf{X}^{(n)}\mathbf{e}_j^{(n)} &= \int_0^1 dx u_i(x) x u_j(x) \end{aligned} \tag{22}$$

where $\mathbf{e}_i^{(n)}$ is i-th standard unit cartesian vector whose element in the i-th position is 1 and all the other elements are 0.

u_i basis functions can be obtained from the monic polynomials set 1, x, x^2,..., x^n via an appropriate orthonormalization procedure by taking these terms into the procedure in ascending powers. If this is done then this orthonormalization will obviously leave u_1 as the constant function 1. With this tricky idea the original integral is transformed into its new form as follows

$$\begin{aligned} I &\equiv \int_0^1 dx u_1(x) f(x) u_1(x) = \left(u_1, \hat{f} u_1\right) \\ &= \left(u_1, f\left(\hat{x}\right) u_1\right) \approx \mathbf{e}_1^{(n)^T} f\left(\mathbf{X}^{(n)}\right) \mathbf{e}_1^{(n)} \end{aligned} \tag{23}$$

The symmetry in $\mathbf{X}^{(n)}$ locates its spectrum on the real axis. Beyond this, its spectrum is confined to the interval $[0,1]$ since $\mathbf{X}^{(n)}$ is the matrix representation of $\hat{x}$. If we denote the i-th eigenvalue and related eigenvector by λ_i and $\boldsymbol{\xi}_i$ respectively then the spectral decomposition of $\mathbf{X}^{(n)}$ can be expressed as follows

$$\mathbf{X}^{(n)} = \sum_{i=1}^{n} \lambda_i \boldsymbol{\xi}_i \boldsymbol{\xi}_i^T \tag{24}$$

which enables us to write

$$f\left(\mathbf{X}^{(n)}\right) = \sum_{i=1}^{n} f(\lambda_i) \boldsymbol{\xi}_i \boldsymbol{\xi}_i^T \tag{25}$$

If (25) is premultiplied by $\mathbf{e}_1^{(n)^T}$ and postmultiplied by $\mathbf{e}_1^{(n)}$ then the approximation to the integral in (21) can be expressed as follows

$$I \approx \sum_{i=1}^{n} f\left(\lambda_i\right) \left(\mathbf{e}_i^{(n)^T} \boldsymbol{\xi}_i\right)^2 \tag{26}$$

(26) leads us to understand the fact that we can approximate the integral of a univariate function by using the matrix representation of its independent variable. So, we approximate a hard-to-compute integral with the help of the fluctuationlessness approximation in inner products.

6 Implementation

In this section, we try to approximately compute the integrals appearing in High Dimensional Model Representation components via Fluctuation Free Matrix Representation Approximation. To measure the efficiency of this method, numerical evaluations are performed for a few univariate functions having different kind of structures. These functions are e^x, $sin(x)$ and $\sqrt{1-x^2}$ respectively. As it can be seen from (16), there will be no contribution provided by plain HDMR when the hybridity parameter α is zero. This means that all contribution to HHDMR expansion will come from FHDMR portion. On the other hand when α is one, FHDMR will not work and the approximation will be handled only by plain HDMR terms. These effects can be easily seen in the four tables given in this section such that when α is zero q_{00} and q_{10} become equal and in the other case, when α is one, q_{00} and q_{01} are equal.

Table 1: Quality measurers of hybrid HDMR approximants for $f(x) = \mathrm{e}^x$ and $n = 5$

α	q_{00}	q_{10}	q_{01}	q_{11}
0.0	0.0757656853	0.0757656853	0.0000000000	0.0
0.2	0.0757656853	0.0484900391	0.0030306274	0.0
0.4	0.0757656853	0.0272756472	0.0121225097	0.0
0.6	0.0757656853	0.0121225097	0.0272756472	0.0
0.8	0.0757656853	0.0030306274	0.0484900391	0.0
1.0	0.0757656853	0.0000000000	0.0757656853	0.0

The tables given in this section are constructed to give the values of the quality measurers q_{00}, q_{10}, q_{01}, and q_{11} for certain values of hybridity parameter α and for the three functions mentioned above.

The first and second tables are for the functions e^x and $\sin(x)$ respectively. The quality measurer values are given at six different hybridity parameter values, 0.0, 0.2, 0.4, 0.6, 0.8, and 1.0.

Table 2: Quality measurers of hybrid HDMR approximants for $f(x) = sin(x)$ and $n = 5$

α	q_{00}	q_{10}	q_{01}	q_{11}
0.0	0.2250060642	0.2250060642	0.0000000000	0.0
0.2	0.2250060642	0.1440038810	0.0090002425	0.0
0.4	0.2250060642	0.0810021831	0.0360009702	0.0
0.6	0.2250060642	0.0360009702	0.0810021831	0.0
0.8	0.2250060642	0.0090002425	0.1440038810	0.0
1.0	0.2250060642	0.0000000000	0.2250060642	0.0

The functions of these two tables do not have any singularity in the finite regions of the complex plane for their arguments. Therefore they are analytic everwhere in finite regions of that complex plane and fulfill the basic requirement of the fluctuation free matrix representation approximation. Beyond this, the analyticity is reflected to the approximation qualities and makes the results highly accurate even in the five dimensional subspace case.

The third and fourth tables are constructed for the function $\sqrt{1-x^2}$ for the five and ten dimensional subspaces respectively.

The function in these tables has two branch points located at the -1 and 1 values of its argument in the complex plane of its independent variable. These branch points affect the quality of the approximants negatively because one of the branch points matches one of the end points of the integration interval.

We have deliberately chosen the abovementioned functions since their integrals analytically available for comparison purposes. The comparison of Table 3 and 4 implies that increasing subspace dimension

Table 3: Quality measurers of hybrid HDMR approximants for $f(x) = \sqrt{1-x^2}$ and $n = 5$

α	q_{00}	q_{10}	q_{01}	q_{11}
0.0	0.0747257950	0.0747257950	0.0000000000	0.0
0.2	0.0747257950	0.0478245090	0.0029890317	0.0
0.4	0.0747257950	0.0269012860	0.0119561271	0.0
0.6	0.0747257950	0.0119561271	0.0269012860	0.0
0.8	0.0747257950	0.0029890317	0.0478245090	0.0
1.0	0.0747257950	0.0000000000	0.0747257950	0.0

Table 4: Quality measurers of hybrid HDMR approximants for $f(x) = \sqrt{1-x^2}$ and $n = 10$

α	q_{00}	q_{10}	q_{01}	q_{11}
0.0	0.0747246110	0.0747246110	0.0000000000	0.0
0.2	0.0747246110	0.0478237520	0.0029889844	0.0
0.4	0.0747246110	0.0269008600	0.1195593780	0.0
0.6	0.0747246110	0.0119559378	0.2690086000	0.0
0.8	0.0747246110	0.0029889844	0.0478237520	0.0
1.0	0.0747246110	0.0000000000	0.0747246110	0.0

(the order) in fluctuation free matrix representation decreases the quality measurer values and therefore the better approximation is obtained.

We performed the numerical evaluations by an Intel Centrino 1.6 Ghz processor under Windows XP OS by using MATLAB R2006a [10]. All computations were realized within ten digit precision.

7 Conclusion

In this work, we have used fluctuationlessness theorem for univariate functions, to approximate the univariate integrals. With the help of these integrals, we tried to represent certain elementary functions whose integrals can be analytically evaluated under HHDMR algorithm. The results have been given through the tables where the approximation quality versus hybridity parameter is given and the change in approximation qualities with the value of chosen hybridity parameter α is shown. Also we have noted that the increasing fluctuationlessness order increases the quality of approximation. Beyond these we want to comment on the last columns of all tables. Since we choose univariate functions in our work for simplicity and deeper understanding, the hybridity approximant h_{11} will give the exact structure of the target function. So the error in this approximant, q_{11}, will be equal to zero. Although we used univariate functions, same processes can be realized for multivariate functions using multivariate fluctuationlessness theorem. This study is left as future work.

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