A Novel Hybrid High Dimensional Model Representation (HHDMR) Based on the Combination of Plain and Logarithmic High Dimensional Model Representations

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Abstract: This paper focuses on a new version of Hybrid High Dimensional Model Representation for multivariate functions. High Dimensional Model Representation (HDMR) was proposed to approximate the multivariate functions by the functions having less number of independent variables. Towards this end, HDMR disintegrates a multivariate function to components which are respectively constant, univariate, bivariate and so on in an ascending ordering of multivariance. HDMR method is a scheme truncating the representation at a prescribed multivariance. If the given multivariate function is purely additive then HDMR method spontaneously truncates at univariance, otherwise the highly multivariant terms are required. On the other hand, if the given function is dominantly multiplicative then the Logarithmic HDMR method which truncates the scheme at a prescribed multivariance of the HDMR of the logarithm of the given function is taken into consideration. In most cases the given multivariate function has both additive and multiplicative natures. If so then a new method is needed. Hybrid High Dimensional Model Representation method is used for these types of problems. This new representation method joins both plain High Dimensional Model Representation and Logarithmic High Dimensional Model Representation components via an hybridity parameter. This work focuses on the construction and certain details of this novel method.

Key–Words: Multivariate Approximation, High Dimensional Model Representation, Logarithmic HDMR

1 Introduction

High dimensional model representation (HDMR) was first designed by Sobol in 1993 [1]. It is based on the divide–and–conquer philosophy such that the original function is additively represented by a constant term followed by univariate terms, bivariate terms and so on. So, an N dimensional multivariate function under consideration can be represented by a constant term, N number of univariate terms, $N(N-1)/2$ bivariate terms, $N(N-1)(N-2)/6$ number of trivariate terms and so on. Hence, the total number of HDMR components for a given N–variate function is 2^N. Although this number is finite it may climb to very high number as N increases. For example, it contains 2^{100}, approximately one million additive components to have an exact representation for the case of hundred independent variables. This urges us to truncate HDMR at rather small multivariances as long as the truncation has a good representation quality. The general tendency is to truncate, at most, bivariance.

The most important advantage of HDMR method is to deal with less variate functions instead of highly multivariate functions as we have mentioned above. In spite of today's advanced computer technology, the direct evaluation of multivariate functions in computers is still fairly difficult especially when the function's dimensionality increases to high values due to the physical limitations on memory and processors. This reality stimulates the mathematicians to develope certain methods based on divide–and–conquer philosophy. One of most recently developed methods in this direction is called High Dimensional Model Representation(HDMR). HDMR and some other related algorithms were developed in a more comprehensive form by Rabitz and his group [2-5] after Sobol's revolutionary work. Sobols suggestion was generalized by Rabitz group such that the integration limits are assumed to be any two real numbers and a weight function which is product of univariate factors each of which depends on a different independent variable is inserted to the integrand as a multiplicative factor. Later, product type weight function is generalized beyond the Rabitz group's case by using a nonproduct type of weight function under another auxiliary product type weight function by Demiralp's group. Demiralp and his group developed some other related HDMR methods at the same time period.

Demiralp's group tried to extend HDMR to more general cases to increase its power and efficiency. Amongst the products of these efforts we can mention Hybrid HDMR(HHDMR) [8, 9] which combines HDMR and Factorized HDMR [6, 7]via a flexible combination parameter. This type of HDMR method works well when the original function has an intermediate nature which corresponds to neither an exactly additive nor an exactly multiplicative nature. In this work, a new HHDMR expansion including Logarithmic HDMR instead of Factorized HDMR again under a hybridity parameter, is proposed. The main idea here is to get rid of the main disadvantage of the FHDMR structure, which is about the definition of the multiplicativity measurers. The structure developed in Logarithmic HDMR method allows us to define new truncation quality measurers which are monotonously increasing from 0 to 1 in ascending multivariance. This feature furnishes us for better understanding of the behaviors and qualities of the HHDMR approximants.

The rest of the paper is organized as follows. The second section is about HDMR to recall the construction details of the method. The third section presents the basic idea underlying Logarithmic HDMR(LHDMR). Fourth section presents the core of this paper, "A New Hybrid Approach in High Dimensional Model Representations (HHDMR)". The fifth section contains simple illustrative applications for this new hybrid approach in HDMR and the sixth section finalizes the paper with concluding remarks.

2 HDMR

The high dimensional model representation[1-10] of a multivariate function $f(x_1,...,x_N)$ is given as

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

where N stands for the number of the independent variables and the right hand side components are orthogonal in an Hilbert space over the hyperprism defined by the intervals $a_i \le x_i \le b_i$, (where $1 \le i \le N$ and a_i, b_i are assumed to be given). The inner product in Hilbert space is defined as follows for two arbitrary square integrable multivariate functions $g\left(x_1,...,x_N\right)$ and $h\left(x_1,...,x_N\right)$

$$
\begin{aligned}
(g,h) \quad &\equiv \int_{a_1}^{b_1} dx_1 ... \int_{a_N}^{b_N} dx_N W\left(x_1,...,x_N\right) \\
&\quad \times g\left(x_1,...,x_N\right) h\left(x_1,...,x_N\right) \qquad (2)
\end{aligned}
$$

where $W\left(x_1,...,x_N\right)$ stands for a product type function and it can be given as follows,

$$
W\left(x_1,...,x_N\right) \equiv \prod_{i=1}^{N} W_i(x_i) \qquad (3)
$$

Here we assume that $W_i(x_i)$ ($1 \le i \le N$), the components of $W\left(x_1,...,x_N\right)$, are given and the integral of these components between a_i and b_i are equal to 1. These weight factors must be chosen to fulfill the requirement for being true weight functions (they should be either always positive everywhere or always negative everywhere except at certain finite number of points where they may vanish). Otherwise the monotonic increasing nature in truncation quality measurers for ascending multivariance may disappear.

The HDMR components in the right hand side of (1) can be determined uniquely by imposing mutual orthogonality amongst these components. This feature allows us to determine constant term f_0 by using the following projection operator.

$$
\begin{aligned}
&\mathcal{P}_0 g\left(x_1,...,x_N\right) \equiv \\
&\qquad \int_{a_1}^{b_1} dx_1 ... \int_{a_N}^{b_N} dx_N W\left(x_1,...,x_N\right) \\
&\qquad \times g\left(x_1,...,x_N\right) \qquad (4)
\end{aligned}
$$

The orthogonality of all higher than zero order multivariate components to f_0 implies that the integrals of those components over one of their independent variables over the related interval under the corresponding univariate weight function vanish (vanishing property proposed by Sobol). Now if we apply the projection operator $\mathcal{P}_0$ on both sides of (1) and then utilize the vanishing properties of the higher than zero variate terms, and the normalized nature of the weight function factors then we can write

$$
f_0 = \mathcal{P}_0 f\left(x_1,...,x_N\right) \qquad (5)
$$

To determine the univariate terms, $f_i(x_i)$s, by using the orthogonality feature we have to define another projection operators $\mathcal{P}_i$ ($1 \le i \le N$). They are equivalent to $\mathcal{P}_0$'s new forms obtained after removing the integration over x_i and discarding the univariate weight function factor $W_i(x_i)$. If we apply the action of $\mathcal{P}_i$ on both sides of (1) then the employment of the vanishing properties of all HDMR terms except the constant one and the normalization in univariate weight factors enable us to write

$$f_i(x_i) = \mathcal{P}_i f(x_1, ..., x_N) - f_0, \quad 1 \le i \le N \quad (6)$$

As can be easily seen the determination of bivariate and higher multivariate HDMR components can be realised by defining other projection operators $\mathcal{P}_{i_1,...,i_k}$ ($1 \le i \le N$). We do not intend to explicitly give them here. By using these operators the higher order HDMR terms can be obtained in a similar manner.

It is not hard to see from the HDMR equation given in (1) that the schemes based on HDMR truncations are finite step methods. However, working with all HDMR components becomes nightmare when the dimensionality increases to high values as we have aforementioned. This is because of the exponential growth, 2^N, with respect to N in the number of HDMR terms. To avoid this problem HDMR equation (1) can be truncated at some level of multivariance (preference is at most to keep bivariate terms). These truncations are called HDMR approximants and are given below

$$\begin{aligned}
s_0(x_1, ..., x_N) &= f_0 \\
s_1(x_1, ..., x_N) &= s_0(x_1, ..., x_N) + \sum_{i=1}^{N} f_i(x_i) \\
&\vdots \\
s_k(x_1, ..., x_N) &= s_{k-1}(x_1, ..., x_N) \\
&\quad + \sum_{\substack{i_1,...,i_k=1 \\ i_1<\cdots<i_k}}^{N} f_{i_1 \ldots i_k}(x_{i_1}, ..., x_{i_k}) \\
&\qquad 1 \le k \le N
\end{aligned} \quad (7)$$

Next question is to measure the quality of these approximants for the characterisation of the original function within a desired numerical precision. The following entities which are called "Additivity Measurers" are defined for this purpose

$$\begin{aligned}
\sigma_0 &\equiv \frac{1}{\|f\|^2} \|f_0\|^2 \\
\sigma_1 &\equiv \frac{1}{\|f\|^2} \sum_{i=1}^{N} \|f_i\|^2 + \sigma_0 \\
&\vdots \\
\sigma_N &\equiv \frac{1}{\|f\|^2} \|f_{12\ldots N}\|^2 + \sigma_{N-1}
\end{aligned} \quad (8)$$

Here, σ_0 is called "Constancy Measurer"and it defines the contribution percentage of the constant term to the HDMR expansion's norm square. σ_1 is called as "First Order Additivty Measurer" and it defines the contribution percentage of the constant term and univariate terms to the HDMR expansion's norm square. As a generalization σ_k called "k-th Order Additivity Measurer"and it defines the contribution percentage of the all terms from constant term to k-th order term inclusive to the HDMR expansion's norm.

As we aforementioned, it is very hard to construct truncation quality measurers monotonically increasing as the multivariance ascends in the case of FHDMR although it is possible to truncate the finite term product at certain level of multivariance. As a matter of fact such measurers could have not been constructed yet. To avoid this difficulty the Logarithmic HDMR (LHDMR) has been developed.

3 Logarithmic HDMR

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

$$\begin{aligned}
&ln\left[f(x_1, ..., x_N) - \phi(x_1, ..., x_N)\right] = \\
&\qquad \varphi_0 + \sum_{i_1=1}^{N} \varphi_{i_1}(x_{i_1}) \\
&\qquad + \sum_{\substack{i_1,i_2=1 \\ i_1<i_2}}^{N} \varphi_{i_1,i_2}(x_{i_1}, x_{i_2}) + \cdots
\end{aligned} \quad (9)$$

where $\phi(x_1, ..., x_N)$ is a minorant function to the given function, $f(x_1, ..., x_N)$ 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. The right hand side components of (9) are mutualy orthogonal and can be determined by tracing the basic rule of the HDMR method.

If the equation given in (9) is reorganized the following representation formula for LHDMR is obtained.

$$\begin{aligned}
&f(x_1, ..., x_N) = \phi(x_1, ..., x_N) + \\
&\quad \mathrm{e}^{\varphi_0} \left[\prod_{\mathrm{i}_1=1}^{\mathrm{N}} \mathrm{e}^{\varphi_{\mathrm{i}_1}(\mathrm{x}_{\mathrm{i}_1})}\right] \left[\prod_{\substack{\mathrm{i}_1,\mathrm{i}_2=1 \\ \mathrm{i}_1<\mathrm{i}_2}}^{\mathrm{N}} \mathrm{e}^{\varphi_{\mathrm{i}_1,\mathrm{i}_2}(\mathrm{x}_{\mathrm{i}_1},\mathrm{x}_{\mathrm{i}_2})}\right] \\
&\quad \times \cdots
\end{aligned} \quad (10)$$

The explicit expressions of LHDMR approximants can be written as follows when the minorant function is assumed to be vanishing for simplicity (otherwise they will be more complicated although a recursive structure can be constructed)

$$\begin{aligned}
\lambda_0(x_1,...,x_N) &= \mathrm{e}^{\varphi_0} \\
\lambda_1(x_1,...,x_N) &= \lambda_0(x_1,...,x_N)\prod_{i_1=1}^{N}\mathrm{e}^{\varphi_{\mathrm{i}_1}(\mathrm{x}_{\mathrm{i}_1})} \\
&\vdots \\
\lambda_k(x_1,...,x_N) &= \lambda_{k-1}(x_1,...,x_N) \\
&\quad\times\prod_{\substack{i_1,\cdots,i_k=1\\ i_1<\cdots<i_k}}^{N}\mathrm{e}^{\varphi_{\mathrm{i}_1,\cdots,\mathrm{i}_k}(\mathrm{x}_{\mathrm{i}_1},\cdots,\mathrm{i}_k)} \\
&\qquad 1\le k\le N
\end{aligned} \tag{11}$$

LHDMR method allows us to define the following truncation quality measurers

$$\begin{aligned}
\nu_0 &\equiv \frac{\|\varphi_0\|^2}{\|ln\,(f-\phi)\|^2} \\
\nu_1 &\equiv \frac{\|\varphi_0\|^2+\sum\limits_{i_1=1}^{N}\|\varphi_{i_1}\|^2}{|ln\,(f-\phi)\|^2} \\
\nu_2 &\equiv \frac{\|\varphi_0\|^2+\sum\limits_{i_1=1}^{N}\|\varphi_{i_1}\|^2+\sum\limits_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\|\varphi_{i_1,i_2}\|^2}{\|ln\,(f-\phi)\|^2} \\
&\vdots
\end{aligned} \tag{12}$$

The following inequality holds for these measurers

$$0\le\nu_0\le\nu_1\le\cdots\le\nu_N\le 1 \tag{13}$$

Until this point we have presented some preliminary information about HDMR methods appearing in the new version of the HHDMR. Now we have been sufficiently equipped to present the novel version of HHDMR.

4 New Version of Hybrid HDMR

The multivariate functions which are neither dominantly additive nor dominantly multiplicative push us to develop an hybrid algorithm. Previously developed Hybrid HDMR joins plain HDMR and FHDMR methods under a hybridity parameter. In this work, Logarithmic HDMR takes the role of Factorized HDMR. Hence, Hybrid HDMR method to be presented here has a new expansion including both HDMR and LHDMR expansions via a hybridity parameter now.

$$\begin{aligned}
f(x_1,...,x_N) &= \alpha\left(f_0+\sum_{i_1=1}^{N}f_{i_1}(x_{i_1})+\cdots\right)+ \\
&(1-\alpha)\left(\phi\,(x_1,...,x_N)+\mathrm{e}_0^{\varphi}\left[\prod_{\mathrm{i}_1=1}^{\mathrm{N}}\mathrm{e}^{\varphi_{\mathrm{i}_1}(\mathrm{x}_{\mathrm{i}_1})}\right]\right. \\
&\left.\times\left[\prod_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\mathrm{e}^{\varphi_{\mathrm{i}_1,\mathrm{i}_2}(\mathrm{x}_{\mathrm{i}_1},\mathrm{x}_{\mathrm{i}_2})}\right]\cdots\right)
\end{aligned} \tag{14}$$

where α is the hybridity parameter. We can define the following approximants through this definition

$$\begin{aligned}
&f(x_1,...,x_N)\approx h_{jk}(x_1,...,x_N;\alpha) \\
&\equiv \alpha s_j(x_1,...,x_N)+(1-\alpha)\lambda_k(x_1,...,x_N), \\
&1\le j,k\le N
\end{aligned} \tag{15}$$

This approximant is called the (j,k)-th order hybrid HDMR approximant. An $(N+1)\times(N+1)$ table like Padé Ratios can be constructed and then used for approximating the original function.

$$\begin{array}{cccc}
h_{00} & h_{01} & \cdots & h_{0N} \\
h_{10} & h_{11} & \cdots & h_{1N} \\
\vdots & \vdots & \cdots & \vdots \\
h_{N0} & h_{N1} & \cdots & h_{NN}
\end{array} \tag{16}$$

The approximating capability of each HHDMR approximant can be defined as follows

$$q_{jk}=\frac{\|f-h_{jk}\|^2}{\|f\|^2} \tag{17}$$

which is somehow error bound. The best approximating capability is of course 0 for these approximants.

5 Implementations

To illustrate how HHDMR works we can choose a multivariate function whose additivity and multiplicativity can be controlled by a single integer parameter as follows

$$f\,(x_1,...,x_N)\equiv(x_1+\cdots+x_N)^m \tag{18}$$

where m is an integer varying between 0 and N inclusive. The function above starts from the constant value when $m=1$ and its multivariance increases through univariance, bivariance, and so on as m increases one by one as long as the HDMR's geometry is taken a hyperprism whose one corner is located in the origin of the Cartesian space spanned by the independent variables. Hence at the case of $m = 1$ it is purely additive and its multiplicativity increases as m grows although pure multiplicativity is never achieved.

If we use (15) in (17) then we obtain the following formula

$$\begin{aligned} q_{jk} &= \frac{\|f-\lambda_k\|^2}{\|f\|^2} + 2\alpha\frac{(f-\lambda_k,\lambda_k-s_j)}{\|f\|^2} \\ &\quad +\alpha^2\frac{\|\lambda_k-s_j\|^2}{\|f\|^2} \qquad 0 \le j,k \le N \end{aligned} \tag{19}$$

The optimisation of this entity with respect to α gives the following unique result for the optimum value of α

$$\alpha^{(opt)}_{j,k} = \frac{(f-\lambda_k, s_j-\lambda_k)}{\|\lambda_k-s_j\|^2}, \qquad 0 \le j,k \le N \tag{20}$$

As can be noticed easily this value turns out to be 1 when $j = 0$, $k = 0$, and f is a constant. However, it differs then one in the other cases. Although there is no warranty that it will stay between 0 and 1 one can investigate the situation and tries to find which kind of functions causes to get optimised α values in $[0, 1,]$. Our observations show that our test function behaves in this manner. However this may not be true for some other type multivariate functions which are neither purely additive nor purely multiplicative. We do not intend to get further details of this issue here. Also we do not report the details of our observations here due to space limitation.

6 Conclusion

This work is devoted to the construction of a more efficient version of HHDMR. This has been necessary to replace FHDMR which has no truncation quality measurers increasing parallel to the increase in multivariance with LHDMR which has such kind of measurers. LHDMR is based on the expansion of a multivariate function's logarithm to plain HDMR and is based on the fact that logarithm converts multiplicativity to additivity and this is the reason why it is used here.

The implementation results encourage us to use HHDMR in the approximation of the functions which are not dominantly additive or multiplicative.

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