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Logarithmic High Dimensional Model Representation

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Abstract: - This paper presents a new version of the High Dimensional Model Representation (HDMR) which attempts to approximate a given multivariate function by an expansion starting from a constant term and continuing by adding univariate components and then the terms whose multivariances increase via bivariance, trivariance and so on. HDMR works well as long as the function under consideration behaves, more or less, additive. Factorized High Dimensional Model Representation (FHDMR) was considered as a powerful approach working well when the multivariate function under consideration is mostly multiplicative. The additivity of the function was defined through its HDMR components by introducing additivitiy measurers. FHDMR, unfortunately, disabled us to define efficient multiplicativity measurers. Hence, we develope Logarithmic High Dimensional Model Representation (LHDMR) to this end. It removes several unpleasent incapabilities of FHDMR.

Key-Words: - Multivariate Approximation, High Dimensional Model Representation, Factorized High Dimensional Model Representation, Additivity Measurers, Multiplicativity Measurers

1 Introduction

The direct evaluation of multivariate functions whose explicit structures are given through an evaluation rule or via some data generally becomes a nightmare when the dimensionality increases to high values because of the limitations in memory and computation speed of today's computers. Despite the dazzling development in the computer technology these limitations seem always to be existing for certain degree of dimensonality. Same thing is also correct and even worse for the indirect evaluation of the multivariate functions via differential or some other kind of equations. This reality urged mathematicians to develop certain divide–and–conquer type methods since all conventional tools like series expansions or discretizations becomes devastating when the dimensionality exceeds a certain criticial value. The first attempt to this end came from Sobol[1] although his work finds its roots in some studies of Kolmogorov. Sobol was offering a formula whose terms' multivariances gradually increase as we proceed to higher terms of the expansion. A little bit later Rabitz group [2-5] intensely focused on the topic and extended the issue by introducing a product type weight function to the definition of the expansion coefficients. The weight function was considered not mandatorily continuous but also discrete involving distribution–like functions (for example, Dirac's delta function). The weight function ought to be product type to avoid certain inconsistencies in the determination of the expansion coefficients. The geometry of the region where the expansion is developed was considered to be an orthogonal structure like an hyperprism or a multidimensional ball. The expansion was called "High Dimensional Model Representation". It was used in several applications in applied sciences.

Although HDMR was a finite representation the number of its components was becoming quite high (2^N if the number of independent variables, dimensionality, is N) when the dimensionality is sufficiently high. Even the value 10 which can be considered a moderate value for dimensionality was enforcing us to use 1024 terms in HDMR. Hence, the truncating HDMR at low multivariances like univariate or bivariate terms was standing as a good approximating facility. Although HDMR is finite, people does not generally intend to use HDMR's itself as a whole but its truncation, and wants to suffice to use only constant and univariate components and perhaps in certain cases at most bivariate terms. Today we use the "HDMR approximation" statement to this end.

Soon or later, it was noticed that the HDMR was working well when the function under consideration is mostly additive and it was turning out to be insufficient when the multiplicativity level of the multivariate function under consideration increases, and, at the purely multiplicative limit, it was presenting worst quality of approximation if one truncates it at low level multivariances like univariance or bivariance. This urged the scientists to develop a new version of HDMR to work well for the dominantly multiplicative functions. Demiralp's group developed the "Factorized High Dimensional Model Representation and published works for its certain applications [6-10].

Demiralp's group studied some other possibilities to extend HDMR to more general cases to increase its power and efficiency. Amongst these we can mention about the Hybrid High Dimensional Model Representation (HHDMR) which combines HDMR and FHDMR via a flexible combination parameter (hybridity). This type of HDMR works well up to some level of quality for both additive and multiplicative functions. This still requires orthogonal geometry and product type weight functions (product of univariate functions each of which depends on a different independent variable). To remove this requirement, Demiralp's group introduced a new version of HDMR where the weight function was more general (no requirement for product type). It was using an auxiliary product type weight function and the HDMR of the method's weight function. Method was called "Generalized High Dimensional Model Representation (GHDMR)". Although it was removing basic limitations leading to inconsistencies in HDMR, it was necessitating the solution of the multivariate integral equations to determine the expansion terms. This was obviously making the method expensive. However, in the case where the weight function is the linear combination of the Dirac's delta functions located at different positions in the space of the independent variables, the integral equations were turning out to be linear algebraic equations. Method was applied to certain interesting problems with success. One other HDMR variety developed by Demiralp's team was "Interval High Dimensional Model Representation (IHDMR)". Its basic aim was to reflect the uncertainties in the data given for a multivariate function to HDMR, FHDMR, or GHDMR. Not a unique structure for the function under consideration but a couple of upper and lower bounds were sought there.

Since the additivity and multiplicativity properties were approximation quality determining agents certain entities to measure the additivity were defined and called "Additivity Measurers" in general. These were the elements of a set of scalars and composed of the terms called "Constancy Measurer", "First Order Addivity Measurer", "Second Order Additivity Measurer" and so on.

HDMR is an additive representation versus to the product type representation of FHDMR whose factors are produced from HDMR components. One was expecting that the truncations of the finite term product of FHDMR would give better quality of approximation when the multivariate function under consideration has an overdominating multiplicativity against its additivity. All observations were confirming this idea. We tried to define "Multiplicativity Measurers" for this case and soon noticed that the defined entities were not good agents to get insight about the multiplicativity since there was no warranty about the monotonicity of them as we proceed to higher multivariance measurers. This unpleasent situation remained as a "Butterfly in Stomach" issue until now. At this moment we know that the problem was in the structuring of FHDMR and we slightly modified FHDMR in a conceptually important way. This paper contains the presentation of this modification and the definition of the "Multiplicativity Measurers".

This section has been an oral introduction to the presentation of the subject. Hence, the formulae to make the presentation more readable mathematically will be given in the coming sections.

Paper is organized as follows. The second section presents the recalling of HDMR and Additivity Measurers while the third section is about FHDMR recalling. Fourth section presents the new method, "Logarithmic High Dimensional Model Representation (LHDMR)" and the definition of "Multiplicativity Measurers". The fifth section contains simple illustrative applications of LHDMR and concluding remarks.

2 HDMR and Additivity Measurers

The high dimensional model representation of a multivariate function $f(x_1, ..., x_N)$ where N is the dimension of the Euclidean space spanned by the independent variables is given as

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

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

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

where the weight function $W(x_1, ..., x_N)$ is a product type function, that is,

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

and we assume that $W_i(x_i)$ is given and its integral between a_i and b_i is equal to 1 (normalization). These factors can be chosen continuos or discontinuous as we mentioned before. Even their basic weight function property, preserving sign, can be relaxed formally. However this may lead to certain anomalies and incompletenesses in vector space related issues. Hence we do not intend to remove sign conserving rule.

The orthogonality amongst the HDMR components given in the right hand side of (1) suffices to determine those components uniquely. The multivariances of those components are self–explained, that is, the number of their arguments defines the multivariance. In this sense, f_0 is a constant and $f_{i_1}(x_{i_1})$s stand for univariate functions each of which depends on a unique and different independent variable. To simplify the explanation of the determination of HDMR components we can define the following integral operator via an arbitrary function $g(x_1, ..., x_N)$

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

The orthogonality of all higher than zero order multivariant components to f_0 dictates us that the integrals of those components over one of independent variables over the related interval under the corresponding univariate weight function given above vanish (vanishing property). Now the action of $\mathcal{P}_0$ on both sides of (1) and then the utilization of the vanishing properties of the higher than zero variate terms, and the normalized nature of the weight function factors lead us to write

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

We need to define another integral operator $\mathcal{P}_i$ such that it is equivalent to $\mathcal{P}_0$'s form obtained after discarding the integration over x_i and the univariate weight function factor $W_i(x_i)$. Its action on a multivariate function produces a univariate function depending on x_i in contrast to constant producing nature of $\mathcal{P}_0$. The action of this operator on both sides of (1) and the use of vanishing properties of all HDMR terms except the constant one and the normalization in univariate weight function factors enable us to write

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

As can be noticed immediately, the entities, $\mathcal{P}_0$, $\mathcal{P}_1$, ..., $\mathcal{P}_N$, are in fact certain kind of projection operators and we use them in the determination of the constant and univariate components of HDMR. The bivariate and the higher multivariate HDMR components can be determined in similar ways although we do not intend to give them explicitly here. However, we can state that we need to define further projection operators for brevity in the resulting formulae. To this end, in general, we need to use the operator $\mathcal{P}_{i_1,...,i_k}$ $(1 \le k \le N)$ which is obtained from $\mathcal{P}_0$ by discarding the integration over the variables x_{i_1},...,x_{i_k} and the univariate weight factors $W_{i_1}(x_{i_1})$,...,$W_{i_k}(x_{i_k})$ from the definition of $\mathcal{P}_0$.

Now we are sufficiently equipped to deal with the addivity measurers. Towards this goal we need to define a norm in the Hilbert space used for the formulation of HDMR. We can use the norm induced by the inner product given above. We can write the following identicality

$$\|g\| \equiv (g, g)^{\frac{1}{2}} \qquad (7)$$

where g denotes, $g(x_1, ..., x_N)$, any multivariate function in the Hilbert space under consideration.

By taking norm squares of the both sides of (1) and considering the orthogonalities of the HDMR components we arrive at the following identicality

$$\|f\|^2 \equiv \|f_0\|^2 + \sum_{i_1=1}^{N} \left\|f_{i_1}\right\|^2 + \sum_{\substack{i_1,i_2=1 \\ i_1<i_2}}^{N} \left\|f_{i_1 i_2}\right\|^2 + \cdots \qquad (8)$$

The first norm square at the right hand side of this formula measures the contribution of the constant term to the whole norm. Similarly the first sum at the right hand side measures the contribution of the univariate components to the total norm whereas the sum of first norm square and the first sum at the right hand side measures the contribution of the purely additive terms to entire norm. This interpretation is equivalently applicable to all terms in fact and urges us to define the following entities

$$\begin{aligned}
\sigma_0 &\equiv \frac{\|f_0\|^2}{\|f\|^2} \\
\sigma_1 &\equiv \frac{\|f_0\|^2 + \sum\limits_{i_1=1}^{N} \left\|f_{i_1}\right\|^2}{\|f\|^2} \\
\sigma_2 &\equiv \frac{\|f_0\|^2 + \sum\limits_{i_1=1}^{N} \left\|f_{i_1}\right\|^2 + \sum_{\substack{i_1,i_2=1 \\ i_1<i_2}}^{N} \left\|f_{i_1 i_2}\right\|^2}{\|f\|^2} \\
... &\equiv ...
\end{aligned} \qquad (9)$$

We call σ_0 "Constancy Measurer" since it defines the contribution percentage of the constant term in total norm. σ_1 is called "First Order Additivity Measurer" since it becomes 1 when the multivariate function under consideration is purely additive, that is, when it is exactly sum of univariate functions. If the HDMR of the function under consideration spontaneously truncates at bivariate terms we can still interprete the function additive but not purely. To distinguish these additivities we call σ_2 "Second Order Additivity Measurer". This naming philosophy can be generalized by calling σ_k "k–th Order Additivity Measurer". These measurers satisfy the following inequalities

$$0 \le \sigma_0 \le \sigma_1 \le ... \le \sigma_N \le 1 \tag{10}$$

Hence they form a finite sequence of monotonicaly increasing bounded from above elements. These terms also define the relative norm of the truncation errors. Indeed, $(1 - \sigma_k)$ is the norm of the error arising when HDMR is truncated by discarding its all components with multivariances higher than k. This explains why low level HDMR truncations work well when the multivariate function under consideration is dominantly additive and fails if the function is dominantly multiplicative. As a matter of fact, in the case of dominantly multiplicative functions all terms of the HDMR are generally required by making the truncation approximation impossible. This urges us to define another type of representation which can be truncated at low level variant terms without apparently affecting the approximation quality. We deal with this approach in the next section.

3 FHDMR

The factorized high dimensional model representation (FHDMR) of a function $f(x_1, ..., x_N)$ is defined through the following formula

$$\begin{aligned} f(x_1, ..., x_N) = r_0 & \left[\prod_{i_1}^{N} \left(1 + r_{i_1}(x_{i_1})\right) \right] \\ \times & \left[\prod_{\substack{i_1, i_2 = 1 \\ i_1 < i_2}}^{N} \left(1 + r_{i_1 i_2}(x_{i_1}, x_{i_2})\right) \right] \cdots \end{aligned} \tag{11}$$

where r_0, $r_{i_1}(x_{i_1})$, $r_{i_1 i_2}(x_{i_1}, x_{i_2})$,... stand for the FHDMR components and are undetermined yet. For their determination we define a commutative set of idempotent operators by denoting its general element by $\mathcal{I}_k$ where k varies between 1 and N inclusive. That is, they satisfy the following relations

$$\begin{aligned} \mathcal{I}_j^2 &\equiv \mathcal{I}_k, \qquad 1 \le k \le N \\ \mathcal{I}_j \mathcal{I}_k &\equiv \mathcal{I}_k \mathcal{I}_j, \qquad 1 \le j, k \le N \end{aligned} \tag{12}$$

We are going to use these operators as the ordering agents and rewrite (11) as follows by inserting these terms to appropriate places

$$\begin{aligned} f(x_1, ..., x_N) = r_0 & \left[\prod_{i_1}^{N} \left(\mathcal{I} + r_{i_1}(x_{i_1}) \mathcal{I}_{i_1}\right) \right] \\ \times & \left[\prod_{\substack{i_1, i_2 = 1 \\ i_1 < i_2}}^{N} \left(\mathcal{I} + r_{i_1 i_2}(x_{i_1}, x_{i_2}) \mathcal{I}_{i_1} \mathcal{I}_{i_2}\right) \right] \cdots \end{aligned} \tag{13}$$

The special form of this formula when all appearences of $\mathcal{I}_j$s are replaced by the unit operator $\mathcal{I}$ matches (11). We can do the same thing we have done to (11) to (1) and obtain the following extended form of HDMR

$$\begin{aligned} f(x_1, ..., x_N) &= f_0 \mathcal{I} + \sum_{i_1=1}^{N} f_{i_1}(x_{i_1}) \mathcal{I}_{i_1} \\ &+ \sum_{\substack{i_1, i_2 = 1 \\ i_1 < i_2}}^{N} f_{i_1, i_2}(x_{i_1}, x_{i_2}) \mathcal{I}_{i_1} \mathcal{I}_{i_2} + \cdots \end{aligned} \tag{14}$$

Now to construct the equations for the determination of the FHDMR components we can expand all products in (13) to a sum and then use the commutativity and the idempotency of the indexed $\mathcal{I}$ operators above and then we compare the coefficients of the all products of indexed $\mathcal{I}$ operators above. This produces the following equations

$$\begin{aligned} r_0 &= f_0 \\ r_{i_1}(x_{i_1}) &= \frac{f_{i_1}(x_{i_1})}{f_0} \\ r_{i_1 i_2}(x_{i_1}) &= \frac{1}{f_0} f_{i_1 i_2}(x_{i_1}, x_{i_2}) - \frac{1}{f_0^2} f_{i_1}(x_{i_1})(x_{i_2}) \\ ... &= ... \end{aligned} \tag{15}$$

whose solutions can be obtained uniquely because of the structure of the equations. We are not going to give them explicitly but we state that all FHDMR components are obtained in terms of the HDMR components and, as can be shown easily via mathematical induction, they are mutually orthogonal.

It is of course possible to truncate the product of FHDMR at low level multivariate terms to get an approximation and to expect high quality approximations for at least dominantly multiplicative functions. However, despite all our efforts, we could not be able to define certain entities to measure the multiplicativity over truncation products as we defined additivity measurers in HDMR. This was the perhaps most inconvenient aspect of FHDMR although many applications were verifying its effectivity for dominantly multiplicative functions. As our prediction the inconvenience was coming from the definition of FHDMR and certain aspects of the representation ought to be modified. After several attempts we arrive at a new representation which has the same roots of FHDMR philosophically but a new simple structure enabling us to define multiplicativity measurers. This will be the main focus of the next section.

4 LHDMR

The basic idea of LHDMR, Logarithmic High Dimensional Model Representation, is to expand the natural logarithm of a nonnegative multivariate function to HDMR. Since nonnegativity is not a universally countered property we subtract a rather simple structured function from the multivariate function under consideration to get nonnegativity. Then the resulting function's natural logarithm is expanded to HDMR.

If $\phi\left(x_1,...,x_N\right)$ denotes the minorant function of $f\left(x_1,...,x_N\right)$, that is, the function which remains always equal to or less than $f\left(x_1,...,x_N\right)$ in the integration domain of HDMR then we can write

$$\begin{aligned}&ln\left[\, f\left(x_1,...,x_N\right)-\phi\left(x_1,...,x_N\right)\right]=\\&\quad\varphi_0+\sum_{i_1=1}^{N}\varphi_{i_1}\left(x_{i_1}\right)+\sum_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\varphi_{i_1,i_2}\left(x_{i_1},x_{i_2}\right)+\cdots\end{aligned} \tag{16}$$

where the right hand side components are mutually orthogonal and can be determined by tracing the route presented in the construction of the HDMR components in the second section. We call these terms LHDMR components within an analogy to HDMR. The minorant function $\phi\left(x_1,...,x_N\right)$ is determined by imitating the asymptotic nature of $f\left(x_1,...,x_N\right)$ at its singularities in the hyperprismatic integration domain of HDMR. If $f\left(x_1,...,x_N\right)$ does not have any singularity in the integration domain of HDMR then $\phi\left(x_1,...,x_N\right)$ turns out to be a constant. We have to emphasize on one important point that the singularities which disable integrability under certain weight functions may lead integrability under some other weight functions. Hence, the selection of the weight function in HDMR, FHDMR, or LHDMR is an important issue. We call $\phi\left(x_1,...,x_N\right)$ "Reference Function" since it takes somehow the role of the origin in the space of the functions.

Equation (16) can be put into the following more amenable form

$$\begin{aligned}&f\left(x_1,...,x_N\right)=\phi\left(x_1,...,x_N\right)+\\&e^{\varphi_0}\left[\prod_{i_1=1}^{N}e^{\varphi_{i_1}\left(x_{i_1}\right)}\right]\left[\prod_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}e^{\varphi_{i_1,i_2}\left(x_{i_1},x_{i_2}\right)}\right]\cdots\end{aligned} \tag{17}$$

We call this formula "Logarithmic High Dimensional Model Representation (LHDMR)". It defines a product type representation relative to a multivariate reference function.

The structure in (16) urges us to define additivity measurers for the logarithm of the difference between the multivariate function under consideration and the reference function. Additivity with respect to a logarithm can be of course interpreted as the multiplicativity with respect to logarithm's argument. These measurers depend on the reference function beside the function under consideration. Their explicit definitions can be given through the following formula

$$\begin{aligned}\nu_0&\equiv\frac{\|\varphi_0\|^2}{\|\ln(f-\phi)\|^2}\\ \nu_1&\equiv\frac{\|\varphi_0\|^2+\sum\limits_{i_1=1}^{N}\left\|\varphi_{i_1}\right\|^2}{\|\ln(f-\phi)\|^2}\\ \nu_2&\equiv\frac{\|\varphi_0\|^2+\sum\limits_{i_1=1}^{N}\left\|\varphi_{i_1}\right\|^2+\sum_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\left\|\varphi_{i_1 i_2}\right\|^2}{\|\ln(f-\phi)\|^2}\\ ...&\equiv\;...\end{aligned} \tag{18}$$

We call these entities "Multiplicativity Measurers Relative to $\phi\left(x_1,...,x_N\right)$". They satisfy the following inequalities

$$0\le\nu_0\le\nu_1\le...\le\nu_N\le 1 \tag{19}$$

4 Simple Illustrative Applications and Conclusion

Consider the following purely multiplicative function and its HDMR over the hypercube $0\le x_j\le 1$ $(1\le j\le N)$ under the unit weight function (Sobol's case)

$$f(x_1,...,x_N) = F_1(x_1)\cdots F_N(x_N) \tag{20}$$

where the univariate functions $F_1(x_1)$,...,$F_N(x_N)$ are all assumed to be given. The reference function of LHDMR to this function can be taken zero everywhere in the integration domain of LHDMR. All LHDMR components except the constant and univariate ones of this case vanish. The constant and univariate components are determined as

$$\begin{aligned} \varphi_0 &= \sum_{i=1}^{N}\int_0^1 dx_i \ln(F_i(x_i)) \\ \varphi_i &= \ln(F_i(x_i)) - \int_0^1 dx_i \ln(F_i(x_i)), \\ &\qquad 1 \le i \le N \end{aligned} \tag{21}$$

which mean that $\nu_1 = \nu_2 = \cdots = \nu_N = 1$. That is, first order multiplicativity measurer explicitly shows that the given function is purely multiplicative with respect to zero function.

In the LHDMR of the function

$$\begin{aligned} f(x_1,...,x_N) &= F_1(x_1)\cdots F_N(x_N) F_{jk}\left(x_j,x_k\right), \\ &\quad 1 \le j,k \le N \end{aligned} \tag{22}$$

with the same geometry and weight of the previous case we can show that $\nu_2 = \nu_3 = \cdots = \nu_N = 1$ which means that the function under consideration is second order multiplicative. As we add more factors including higher order multivariance to the right hand side of (22) LHDMR (with the same geometry and the weight) exactly returns the function under consideration when it is truncated at the same level multivariance and the multiplicativity measurers predict the multiplicativity level at the same level multivariance.

These applications finalizes the paper. The conclusion is that the HDMR version (LHDMR) which works for dominantly multiplicative functions has now been developed. The monotonically increasing multiplicativity measurers are also available now. Hence the most important deficits of FHDMR are now removed. We will use LHDMR for various future applications.

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