Small Scale High Dimensional Model Representation

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Abstract: HDMR, High Dimensional Model Representation is one of the recently developed tool in the approximation of multivariate functions. It is based on multivariate integration over orthogonal geometries under product type weight functions and uses a divide–and–conquer algorithm such that the target function is separated into components in ascending multivariance. In almost all applications HDMR is desired to be truncated at constant, univariate, or at most, bivariate components as approximations. The approximating quality of these components increases as the target functions additive nature dominates. Here, our purpose is to investigate the role of the geometric scale of HDMR be anticipating to get efficiency in the small scale geometries. The ultimate goal of this approach is to develop a new HDMR like finite elements.

Key–Words: Multivariate functions, High Dimensional Model Representation, Maclaurin series, Perturbation expansion.

1 Introduction

Evaluation difficulties of multivariate functions can be handled by using High Dimensional Model Representation (HDMR)[1-4] which was developed by Sobol’s, Rabitz’s and Demiralp’s works although it finds its roots in one of Kolmogorov’s work. According to High Dimensional Model Representation a given multivariate function is denoted by \( f(x_1, ..., x_N) \) is represented as below

\[
f(x_1, ..., x_N) = f_0 + \sum_{i_1}^N f_{i_1}(x_{i_1}) + \sum_{i_1, i_2=1}^N f_{i_1i_2}(x_{i_1}, x_{i_2}) + ... + f_{12...N}(x_1, ..., x_N)
\]

where the right hand side contains \( 2^N \) unknown terms. \( f_0 \) is called constant term, \( f_i(x_i) \) s and \( f_{i_1i_2}(x_{i_1}, x_{i_2}) \) s are respectively univariate and bivariate terms, and so on. We can approximate the given multivariate function by truncating the right hand side of above equation. To do so some rules were imposed for unique determination of the HDMR components.

\[
\int_{a_j}^{b_j} dx_j W_j(x_j) f_{i_1...i_k}(x_{i_1}, ..., x_{i_k}) = 0
\]

\( x_j \in \{ x_{i_1}, x_{i_2}, ..., x_{i_N} \} \) \( 1 \leq j, k \leq N \) (2)

The overall weight function for HDMR is defined as follows

\[
W(x_1, ..., x_N) = \prod_{i=1}^N W_i(x_i)
\]

where the right hand side univariate factors are given entities. By using these conditions we can obtain the following expressions for constant, univariate HDMR components uniquely as follows

\[
f_i(x_i) = \int_{a_1}^{b_1} dx_1 \cdots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} \cdots \int_{a_N}^{b_N} dx_N W(x_1, ..., x_N) f(x_1, ..., x_N)
\]

\[
f_i(x_i) = \int_{a_1}^{b_1} dx_1 \cdots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} \cdots \int_{a_N}^{b_N} dx_N W(x_1, ..., x_N) f(x_1, ..., x_N)
\]

Other terms of HDMR can be found within the same consideration. We can see orthogonality which was first noticed by Demiralp from the vanishing-under-integration condition imposed by Sobol and definition
of inner product as follows

\[
\int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} W(x_1, \ldots, x_N) 
\times f_{i_1 \ldots i_k}(x_{i_1}, \ldots, x_{i_k}) 
\times f_{j_1 \ldots j_l}(x_{j_1}, \ldots, x_{j_l}) = 0 
\]

\[
\{i_1, \ldots, i_k\} \neq \{j_1, \ldots, j_l\} 
1 \leq i_1 < \cdots < i_k \leq N 
1 \leq j_1 < \cdots < j_l \leq N 
1 \leq k, l \leq N 
(6)
\]

Then norm definition can be written as follows

\[
||f_{i_1 \ldots i_k}||^2 = (f_{i_1 \ldots i_k}, f_{j_1 \ldots j_l}) 
\]

(8)

With this norm definition and the orthogonality features of the HDMR components we can obtain the following equation by taking the norm of both sides of the equation (1).

\[
||f||^2 = ||f_0||^2 + \sum_{i=1}^{N} ||f_i||^2 + \sum_{\begin{subarray}{c}i_1 \leq i_2 \\ i_1 < i_2 \end{subarray}} ||f_{i_1 \ldots i_2}||^2 
+ \cdots + ||f_{1 \ldots N}||^2 
\]

(9)

If we truncate the right hand side of (9) at certain level multivariances we obtain the additivity measurers which were defined by Demiralp. These measurers are defined as the quality of a truncated HDMR. Hence they can be used efficiently in the error estimation

\[
\sigma_0 = \frac{1}{||f||^2} ||f_0||^2 
\]

\[
\sigma_1 = \frac{1}{||f||^2} \sum_{i=1}^{N} ||f_i||^2 + \sigma_0 
\]

\[
\vdots 
\]

\[
\sigma_N = \frac{1}{||f||^2} \sum_{i=1}^{N} ||f_{1 \ldots N}||^2 + \sigma_{N-1} 
\]

(10)

where \(\sigma_0\) is called “Constancy Measurer”, \(\sigma_1\) is “Univariance Measurer” and as generalization \(\sigma_k\) is called “\(k\)-th Order Additivity Measurer” and these form a well-ordered sequence as shown below

\[
0 \leq \sigma_0 \leq \sigma_1 \cdots \leq \sigma_N = 1 
\]

(11)

The main purpose of this research to develop a new vantage point for the method we have summarized above, by considering the cases where the interval sizes diminish to zero. So we focus on these cases, that is,

\[
b_i - a_i \rightarrow 0, \quad 1 \leq i \leq N 
\]

(12)

and then try to investigate how HDMR components will be affected. To reply this question we can convert each interval to \([0,1]\) with the following variable transformation and work on this standard interval which was first used by Sobol

\[
x_i = (b_i - a_i)y_i + a_i, \quad dx_i = (b_i - a_i)dy_i 
\]

\[
y_i \in [0,1], \quad 1 \leq i \leq N 
\]

(13)

Hence, with these considerations, we will construct a new divide-and-conquer algorithm based on HDMR and this limiting structure we call “Small Scale High Dimensional Model Representation (SSHDMR)”.

### 2 SSHDMR’s Constant Component and Constancy Measurer

For a given multivariate function \(f(x_1, \ldots, x_N)\) we can rewrite constant term of HDMR after the variable transformation in (13) as below

\[
f_0 = \prod_{k=1}^{N} (b_k - a_k) \int_{0}^{1} dy_1 \cdots \int_{0}^{1} dy_N 
\]

\[
\times W(u_1y_1 + a_1, \ldots, u_Ny_N + a_N) 
\times f(u_1y_1 + a_1, \ldots, u_Ny_N + a_N) 
\]

(14)

where we have used the shorthand notations \(u_k = b_k - a_k, k = 1\ldots N\) to facilitate the typography.

By expanding the target multivariate and weight functions in ascending natural number powers of \(u\) we can facilitate the further analysis. However, it is better again to use somehow shorthand notation to avoid typographical difficulties.

\[
D_a \equiv \left( u_1y_1 \frac{\partial}{\partial a_1} + \cdots + u_Ny_N \frac{\partial}{\partial a_N} \right) 
\]

(15)

where the symbol \(a\) in the subscript is and will be used to recall all \(a\) values. This definition enables us to
express the constant term of SSHDMR as follows

$$f_0(u) = \left[ \prod_{i=1}^{N} u_i \right] \int_0^1 dy_1 \cdots \int_0^1 dy_N \sum_{j=0}^{\infty} \frac{1}{j!} D_a^j W(a)$$

$$\times \sum_{k=0}^{\infty} \frac{1}{k!} D_a^k f(a)$$

(16)

where $u$ stands for the ensemble of $u$s. This equation permits us to express $f_0$ as a power series of $u$'s. We can define the following finite truncations of this series to facilitate the further analysis by using a Cauchy product type expression.

$$f_0^{(n)}(u) = \left[ \prod_{i=1}^{N} u_i \right] \int_0^1 dy_1 \cdots \int_0^1 dy_N \sum_{j=0}^{n} \frac{1}{j!} D_a^j W(a)$$

$$\times \sum_{k=0}^{j} \frac{1}{k!} D_a^k f(a)$$

(17)

First of these multinomials in $u$s is given below

$$f_0^{(0)}(u) = u_1 \cdots u_N W(a) f(a)$$

(18)

The norm square of the target function of SSHDMR can also be expanded into a similar infinite sum where the only change is the replacement of $f$ by its square. If we denote the $n$-th degree truncation of this series in $u$s by $\|f\|_n^2$, these truncations which are multinomials in $u$s can be used to approximate the norm square of the SSHDMR's target function. The first one of them is explicitly given below

$$\|f\|_0^2 = u_1 \cdots u_N W(a) f(a)^2$$

(19)

The ratio of the square of the constant SSHDMR component to the norm square of the target function is the constancy measurer $\sigma_0$ by definition and this measurer depends on all $u$ values. We can denote its approximants obtained by truncating both in numerator and denominator at the same degree, say $n$, by $\sigma_0^{(n)}(u)$. Then the crudest approximant which corresponds to zero volume orthogonal hyper prism, $\sigma_0^{(0)}(u)$ can be explicitly given as follows

$$\sigma_0^{(0)}(u_1, \ldots, u_N) = u_1 \cdots u_N W(a_1, \ldots, a_N)$$

(20)

However, the integral of the weight function over the originally given hyper prism must be equal to 1 by definition. If we use the above type expansions in powers of $u$s for this integral then we can show that the requirement to be 1 for this integral dictates the following equality in zero volume limit.

$$u_1 \cdots u_N W(a_1, \ldots, a_N) = 1$$

(21)

which means

$$\sigma_0^{(0)}(u_1, \ldots, u_N) = 1$$

(22)

Therefore we have proven that the constancy measurer of HDMR for zero volume limit is its uppermost value 1. This implies that zero volume HDMR can be truncated at constancy level without producing any error. This is a quite expected result and implies that the dominancy of the constancy and therefore the univariance of HDMR will increase as its orthogonal hyper prism’s volume decrease. Although we do not give here, the increasing nature of the constancy measurer as the volume decreases can be shown by approximating it with the aid of a hyperconical function and investigating its Hessian matrix.

The abovementioned facts inspires us to develop a new type of HDMR approximation by partitioning the HDMR geometries such that the each subgeometry permits to suffice univariance in HDMR within a prescribed precision. To control the errors we can use of course the univariance measurer. Then a piecewise function which is the sum of an appropriate constant with the appropriate univariate components evaluated on the relevant subgeometry. The size of the subgeometries can be diminished to get better qualities. Each HDMR on each subgeometry is called “SSHDMR” as we did before.

### 3 Recursive Integral Evaluations

The above discussions are for quite general structures. However, in the actual implementations more specific structures are under consideration and they may facilitate a lot of intermediate stages in the evaluation of the SSHDMR terms. Here we start to deal with the following function

$$f(x_1, \ldots, x_N) = (x_1 + \cdots + x_N)^m$$

(23)

where $m$ is a natural number. This function is purely additive when $m = 1$ and its additivity decreases at the expense of an increase in the multiplicativity as $m$ grows. We assume that the HDMR geometry is a hypercube whose closest corner to origin is located at $(a, \ldots, a)$ and the position of the farthest corner is $(b, \ldots, b)$. We concern with the cases where $(b-a)$ is small. We can first change the independent variables as follows

$$x_i = (b-a)y_i + a \quad 1 \leq i \leq N$$

(24)

which changes the function in (23) as follows

$$f((b-a)y_1 + a, \ldots, (b-a)y_N + a) = \left[ Na + (b-a)(y_1 + \cdots + y_N) \right]^m$$

(25)
If we use constant weight function, that is,
\[ W(x_1, ..., x_N) = \frac{1}{(b - a)^N} \tag{26} \]
here then we can write
\[
I_0 = \int_0^1 dy_1 \cdots \int_0^1 dy_N \\
\times ((b-a)y_1 + a + \cdots + (b-a)y_N + a)^m
\]
\[
= \int_0^1 dy_1 \cdots \int_0^1 dy_N
\]
\[
\times (Na + (b-a)(y_1 + \cdots + y_N))^m
\]
\[
= \int_0^1 dy_1 \cdots \int_0^1 dy_N \sum_{k=0}^m \binom{m}{k} (Na)^k (b-a)^{m-k}
\]
\[
\times (y_1 + \cdots + y_N)^{m-k}
\]
\[
= \sum_{k=0}^m \binom{m}{k} (Na)^k (b-a)^{m-k} I_{m-k,N} \tag{27}
\]
where
\[ I_{m,N} \equiv \int_0^1 dy_1 \cdots \int_0^1 dy_N (y_1 + \cdots + y_N)^m \tag{28} \]
This integral can be evaluated either through a multilinear expansion or a recursion. In the first case, after multilinear expansion, the integrations are needed although those integrals are all simple. This yields a multisummation algorithm which can be parallelised but its utilization is not as attractive as the second case, recursion. For the second case we can use the binomial expansion in the kernel of (28) as follows
\[
(y_1 + \cdots + y_N)^m = \sum_{i=0}^m \binom{m}{i} (y_1 + \cdots + y_{N-1})^i y_N^{m-i} \tag{29}
\]
which leads us to the following recursion
\[
I_{m,N} = \sum_{i=0}^m \binom{m}{i} \frac{1}{m-i+1} I_{i,N-1} \tag{30}
\]
This is a nonlocal recursion since the order of the recursion changes as \( m \) varies and is in fact nothing different than the abovementioned multivariate sum. We suffice this information here for this simple case of constant component evaluation.

By having the constant term in hand we can evaluate the univariate terms. To this and all we have to do is the application of the same philosophy with one exemption. We discard the integration over one of the independent variable. Together with the corresponding univariate weight factor from the integrals.
\[
f_i(x_i) = \int_0^1 dy_1 \cdots \int_0^1 dy_{i-1} \int_0^1 dy_{i+1} \cdots \int_0^1 dy_N \\
\times [Na + (b-a)(y_1 + \cdots + y_N)]^m
\]
\[
\times (y_1 + \cdots + y_N)^{m-k} - f_0
\]
\[
\times \sum_{k=0}^m \binom{m}{k} (Na)^k (b-a)^{m-k}
\]
\[
\times (y_1 + \cdots + y_N)^{m-k} - f_0
\]
\[
\times \sum_{j=0}^{m-k} (y_1 + \cdots + y_{i-1} + y_{i+1} + \cdots + y_N)^j
\]
\[
\times y_i^{m-k-j} - f_0
\]
\[
= \sum_{k=0}^m \binom{m}{k} (Na)^k (b-a)^{m-k}
\]
\[
\times \sum_{j=0}^{m-k} \binom{m-k}{j} \frac{1}{m-k-j+1} I_{j,N-1}
\]
\[
- \sum_{k=0}^m \binom{m}{k} (Na)^k (b-a)^{m-k}
\]
\[
\times \sum_{j=0}^{m-k} \binom{m-k}{j} \frac{1}{m-k-j+1} I_{j,N-1}
\]
\[ \tag{31} \]
This special case gives some idea about how the SSHDMR integrals can be handled. In this case we have assumed that the closest corner of the HDMR cube has been located at \((a, \ldots, a)\) which was a very specific point and we will need some other points when we try to divide a given HDMR’s geometry into small subgeometries. Hence, we need to know how the above analysis can be modified to cover these cases. In fact, it is quite simple. We need just to replace every appearance of \(Na\) by its general form \((a_1 + \cdots + a_N)\).
The target HDMR function above was very specific one. However what we have done above gives the clues for the general case as we slightly mentioned before. The function will be expanded into an ascending natural number power series in $u$s. Then, the expansion will be integrated term by term without any difficulty since the integrands of these integrals will be just the product of certain powers of $y$s. The result will be of course a multivariate infinite series. However, they can be truncated to multinomials as long as the volume of the SSHDMR geometry is sufficiently small.

4 Conclusion

The main goal of this work has been to investigate the truncation quality of an HDMR expansion when the volume of its geometry is small. Our investigations show that it is possible to prove that the HDMR components’ contributions are focused on the constant component only when the geometry size diminishes to zero since the constancy measurer goes to 1 at that limit. The implication of this fact is to suffice univariate only for geometries whose sizes are smaller than a threshold value for a prescribed precision. We call this cases and the corresponding univariate truncation of the HDMR “Small Scale HDMR”. Since the threshold value mentioned above is exceeded in many given HDMR geometries we can not use univariate truncations unless the target function of HDMR has a very specific nature which very dominantly additive. If this is on the scene then the geometry of the HDMR can be divided into subgeometries in such a way that SSHDMR can be used on each of these geometries. This brings the possibility of constructing a new HDMR as the combination of sufficient number SSHDMRs on appropriately chosen subgeometries. This possibility illuminates the way of construction somehow constructing finite element like HDMR. Although it is not configured in all details yet we call this HDMR “Combined Small Scale High Dimensional Model Representation (CSSHDMR)”. It is under intense studies now.

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