The Influence of the Peak Location on the Additivity of the High Dimensional Model Representation

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Abstract: Mathematical modeling of physical systems are commonly faced situations. Solution depends on the quality of the modeling directly. Among the many techniques, High Dimensional Model Representation (HDMR) is a new method that brings great efficiency to the modeling of a system. Although Interpolation, Splines, Finite differences etc. are useful methods, they do not often give as good results as HDMR does. These methods need more reference points or nodes and higher order polynomials for better results, and this means higher cost calculations. However, HDMR offers new expansions, truncation of intended order, needed for less sample points etc.. Since HDMR is a modeling method based on optimization and projection operator theory, solving problems with differential equations, input - output systems require less calculations with high effectiveness. In addition, HDMR contains analysis of variance calculations. Hence, HDMR is also an effective method for statistics.

Key–Words: Multivariate functions, Normalized linear exponential function, High Dimensional Model Representation, Additivity measurers

1 Introduction

In this work, normalized linear exponential function

$$G\left(x_1,x_2,x_3,x_4\right) \equiv \prod_{j=1}^{4} \mathrm{e}^{\alpha_j\left(x_j-c_j\right)^2}, \quad \alpha_i, c_i \in R \tag{1}$$

$$f\left(x_1,x_2,x_3,x_4\right) \equiv \frac{G\left(x_1,x_2,x_3,x_4\right)}{\|G\|}, \tag{2}$$

is taken into consideration. Structurewise, this function shows the properties of Gaussian Distribution. When α_i goes to infinity, each exponential factor of the function will approach the Dirac – Delta function with a support at c_i. It is not really feasible to consider Interpolation or Splines to model the above function for approximation, however a new approach called High Dimensional Model Representation (HDMR), expresses a multivariable function as a sum of a constant, univariate, bivariate functions etc.. In other words, HDMR uses a divide and conquer technique for problems having multivariate functions. The computational complexity of multivariate calculations are generally very high. However HDMR, as being a divide and conquer approach, attempts to diminish these complexities.

2 High Dimensional Model Representation

High Dimensional Model Representation (HDMR) renders to write a multivariate function symbolized by $f(x_1, x_2, ..., x_n)$ as a sum of a constant, univariate, bivariate etc. N variate functions[1, 2, 3, 4].

$$\begin{aligned} f\left(x_1,...,x_N\right) &= f_0 + \sum_{j=1}^{N} f_j\left(x_j\right) \\ &+ \sum_{\substack{i,j=1 \\ i<j}}^{N} f_{ij}\left(x_i,x_j\right) + \cdots \\ &+ f_{12...N}\left(x_1,x_2,...,x_N\right) \end{aligned} \tag{3}$$

There are 2^N terms at the right hand side of the expression (1.1). These terms are, a constant term f_0, univariate terms $f_i(x_i)$, bivariate terms $f_{ij}(x_i, x_j)$ and so on, respectively. All the univariate terms above indicate the contribution alone of each independent variable dependence on the original function without any mutual interactions. Multivariate terms bring the double, triple, ..., higher tuple mutual interactions' contributions. For example, if a zeroth order truncation is made, ignoring the terms following f_0, the mean value of the investigated function is obtained. Therefore, one of the advantages of HDMR is that there is no need to calculate every HDMR component to get the approximate value of a function within a predetermined sensitivity by choosing the appropriate version of HDMR. HDMR, its components and properties was first mentioned in 1993 by I. M. Sobol in his article "Sensitivity Estimates for Nonlinear Mathematical Models". Sobol used unit weight and $[0,1]$ interval in his article Later, H. Rabitz generalized Sobol's work by introducing the idea of weight functions [3, 4]. M. Demiralp defined and utilized various versions of HDMR and generalized the interval into $[a_i, b_i]$. Demiralp's group continues their work in suggesting new HDMR versions. The HDMR components fulfill the condition

$$\int_{a_j}^{b_j} dx_j W_j(x_j) f_{i_1,\dots,i_k}(x_{i_1},\dots,x_{i_k}) = 0 \tag{4}$$

for $x_j \in \{x_{i_1},\dots,x_{i_k}\}$, $1 \le j,k \le N$ This condition is known as vanishing under integration. It helps us to calculate HDMR terms as follows

$$\begin{aligned} f_0 &= \int_{a_1}^{b_1} dx_1 W_1(x_1) \dots \int_{a_N}^{b_N} dx_N W_N(x_N) \\ &\quad \times f(x_1,\dots,x_N) \end{aligned} \tag{5}$$

$$\begin{aligned} f_i(x_i) &= \int_{a_1}^{b_1} dx_1 W_1(x_1) \dots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} \\ &\quad \times W_{i-1}(x_{i-1}) \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} W_{i+1}(x_{i+1}) \\ &\quad \dots \int_{a_N}^{b_N} dx_N W_N(x_N) f(x_1,\dots,x_N) \\ &\quad -f_0 \qquad 1 \le i \le N \end{aligned} \tag{6}$$

$$\begin{aligned} f_{ij}(x_i,x_j) &= \int_{a_1}^{b_1} dx_1 W_1(x_1) \dots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} \\ &\quad \times W_{i-1}(x_{i-1}) \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} \\ &\quad \times W_{i+1}(x_{i+1}) \dots \int_{a_{j-1}}^{b_{j-1}} dx_{j-1} \\ &\quad \times W_{j-1}(x_{j-1}) \int_{a_{j+1}}^{b_{j+1}} dx_{j+1} \dots \\ &\quad \times W_{j+1}(x_{j+1}) \int_{a_N}^{b_N} dx_N \\ &\quad \times W_N(x_N) f(x_1,\dots,x_N) \\ &\quad -f_0 - f_i(x_i) - f_j(x_j), \\ &\quad 1 \le i < j \le N \end{aligned} \tag{7}$$

Other components can be calculated similarly. Truncations can be done by using the components above. Zeroth,first and k-th order truncations are as follows [1, 2, 3, 4],

$$\begin{aligned} s_0 &\equiv f_0, \\ s_1 &\equiv s_0 + \sum_{j=1}^{N} f_j(x_j), \\ &\vdots \\ s_k &\equiv s_{k-1} + \sum_{\substack{j_1,\dots,j_k=1 \\ j_1<\dots<j_k}}^{N} f_{j_1\dots j_k}(x_{j_1},\dots,x_{j_k}) \end{aligned} \tag{8}$$

We can define an orthogonality condition among the HDMR terms as,

$$\begin{aligned} &(f_{i_1,\dots,i_k}, f_{j_1,\dots,j_\ell}) = 0, \\ &\quad 1 \le i_1 < i_2 < \dots < i_k \le N, \\ &\quad 1 \le j_1 < j_2 < \dots < j_\ell \le N, \\ &\quad\quad 1 \le k < \ell \le N \end{aligned} \tag{9}$$

where the inner product is defined through the following equation

$$\begin{aligned} &(f_{i_1,\dots,i_k}, f_{j_1,\dots,j_\ell}) \equiv \int_{a_1}^{b_1} dx_1 W_1(x_1) \dots \\ &\times \int_{a_N}^{b_N} dx_N W_N(x_N) f_{i_1,\dots,i_k}(x_{i_1},\dots,x_{i_k}) \\ &f_{j_1,\dots,j_\ell}(x_{j_1},\dots,x_{j_\ell}), \end{aligned} \tag{10}$$

where $1 \le i_1 < \dots < i_k \le N$, $1 \le j_1 < \dots < j_\ell \le N$, $1 \le k,\ell \le N$. We can now define a norm as;

$$\| f_{i_1\dots i_k} \| = (f_{i_1\dots i_k}, f_{i_1\dots i_k}) \tag{11}$$

Let $f(x_1,\dots,x_N)$ be a square integrable function, with the help of the orthogonality condition and the scalar product defined above, we can get

$$\begin{aligned} \|f\|^2 &= \|f_0\|^2 + \sum_{i=1}^{N} \|f_i\|^2 + \sum_{\substack{i,j=1 \\ i<j}}^{N} \|f_{i,j}\|^2 \\ &\quad + \dots + \|f_{12\dots N}\|^2 \end{aligned} \tag{12}$$

if now we divide both sides of equation (1.8) by $\|f\|^2$

$$\frac{\|f_0\|^2}{\|f\|^2}+\frac{\sum\limits_{i=1}^{N}\|f_i\|^2}{\|f\|^2}+\frac{\sum\limits_{\substack{i,j=1\\i<j}}^{N}\|f_{i,j}\|^2}{\|f\|^2}+\cdots+\frac{\|f_{12\ldots N}\|^2}{\|f\|^2}=1 \tag{13}$$

This equation helps us to make the following definitions;

$$\sigma_0 \equiv \frac{\|f_0\|^2}{\|f\|^2}, \tag{14}$$

$$\sigma_1 \equiv \frac{\sum\limits_{i=1}^{N}\|f_i\|^2}{\|f\|^2}+\sigma_0, \tag{15}$$

$$\sigma_2 \equiv \frac{\sum\limits_{\substack{i,j=1\\i<j}}^{N}\|f_{i,j}\|^2}{\|f\|^2}+\sigma_1 \tag{16}$$

The σ_is above (first three of them are given only) are called "Additivity measurers of order i". It can be clearly observed that these additivity measurers can hold a value between zero and one

$$0 \le \sigma_0 < ... < \sigma_N = 1 \tag{17}$$

This means it is a monotonously increasing sequence. The closer the σ_i is to one, the better the quality of the i-th approximation.

3 HDMR Investigation for the Gauss Type Exponential Function

In this work, the normalized linear exponential function was chosen because of its structure. Since the function shows the properties of Gaussian Distribution, it is commonly used in statistics. Let us focus on an inhomogenous N-dimensional hyperprism $\mathcal{V}$. Our aim is to find its center of gravity. Since it is nonhomogenous its mass and center of gravity can be found by statistical formulas. As $\mu(\mathbf{x})$ (where boldfaced x means the set of independent variables) is the density function, the body's mass is given by,

$$M \equiv \int_{\mathcal{V}} d\mathcal{V}\mu(\mathbf{x}) \tag{18}$$

where the integration is N-fold. If we define the center of gravity as $G=(\overline{\mathbf{x}})$ the averaged coordinates are defined as

$$\overline{\mathbf{x}} \equiv \frac{1}{M}\int_{\mathcal{V}} d\mathcal{V}\mathbf{x}\mu(\mathbf{x}) \tag{19}$$

If we choose the HDMR terms for approximation, the calculated closest approximation results gives us the center of gravity of the body. Furthermore, normalized linear exponential function was chosen because plots of the function make peaks. Plots of the function for specific values of α_i and c_i values are enough to determine the peak location.

In this work, the unit weight $W(x_1,x_2,x_3,x_4)=1$ is utilized on the hyperprism $[0,1]^4$and investigations are made on how well various levels of HDMR approximate the original function for various α_i and c_i values. All calculations were made and the integrals taken by using MAPLE. Although we chose real α_i and c_i values, they can in general be complex numbers. Additivity measurers for various approximation levels for different values of α_i and c_i are calculated and results are compared. In this comparison, additivity measurers obtained by 9 different α_i and 5 different c_i values are tabulated. Sensitivity of calculations were made using 50 digit arithmetic. In addition to these comparisons, plots are also used for the same purpose. In the preparation stage of the tables, $-1, 0, 0.5, 1,\ 1.5$ values were chosen for c_i and $0.001, 0.01, 0.1, 0.5, 1, 2, 5,\ 10, 40$ values were chosen for α_i values, respectively. The table for $c_i=-1$ and for all α_i values is as follows;

α	$(1-\sigma_0)$	$(1-\sigma_1)$	$(1-\sigma_2)$	$(1-\sigma_3)$
0.001	3×10^{-6}	0.0	0.0	0.0
0.010	3×10^{-4}	3×10^{-8}	0.0	0.0
0.100	3×10^{-2}	3×10^{-4}	2×10^{-6}	3×10^{-9}
0.500	5×10^{-1}	1×10^{-1}	1×10^{-2}	4×10^{-4}
1.000	8×10^{-1}	5×10^{-1}	1×10^{-1}	2×10^{-2}
5.000	1.0	1.0	1.0	5×10^{-2}
10.000	1.0	1.0	1.0	1.0

It was observed that the function $G(x_1,x_2,x_3,x_4)$'s norm becomes small when the values of α_i get large. For α_i values greater than 14.805002501 the value of the function is less than10^{-50} and MAPLE calculations accept this number as zero. Hence, for the values $\alpha_i >$ 14.805002501 the value of the normalized linear exponential function converges to infinity. Therefore, in the above table,$\alpha_i = 40$ is ignored. As it is observed in the table, first order additivity measurer tells us that it is enough to calculate first order HDMR approximation when $\alpha_i = 0,001$. When the α_i values become large, the quality of approximations become lower. The best result was reached when c_i is 0.5 and α_i is 0.001. For example, for the values $c_i = 0.5$ and $\alpha_i = 0.001$ it is enough to calculate first order HDMR components to get exact results.

In the table below, results are given for $c_i = 0.5$ As is observed from the table, even zeroth order truncation of HDMR is sufficient for specific purposes. Results are satisfactory for up to $\alpha_i = 5$. $\alpha_i = 40$ is also included in the above table since in this case such a value makes sense. The main point in this table is, $c_i = 0.5$ acts as symmetry axis. Therefore, this value is also the center of gravity. Results are also compared using plots. Since the normalized linear exponential function is a 4-variable function, the variables x_3 and x_4 are taken as constants in calculations and plots are drawn in 3-dimension. Since the best results were reached at $c_i = 0, 5$, this point works as a symmetry axis, this value is taken in all plots.

α	$(1-\sigma_0)$	$(1-\sigma_1)$	$(1-\sigma_2)$	$(1-\sigma_3)$
0.001	2×10^{-8}	0.0	0.0	0.0
0.010	2×10^{-6}	0.0	0.0	0.0
0.100	2×10^{-4}	2×10^{-8}	0.0	0.0
0.500	5×10^{-3}	1×10^{-5}	1×10^{-8}	0.0
1.000	2×10^{-2}	2×10^{-4}	6×10^{-7}	0.0
5.000	3×10^{-1}	5×10^{-2}	3×10^{-3}	9×10^{-5}
10.000	7×10^{-1}	3×10^{-1}	5×10^{-2}	4×10^{-3}
40.000	1.0	8×10^{-1}	5×10^{-1}	2×10^{-1}

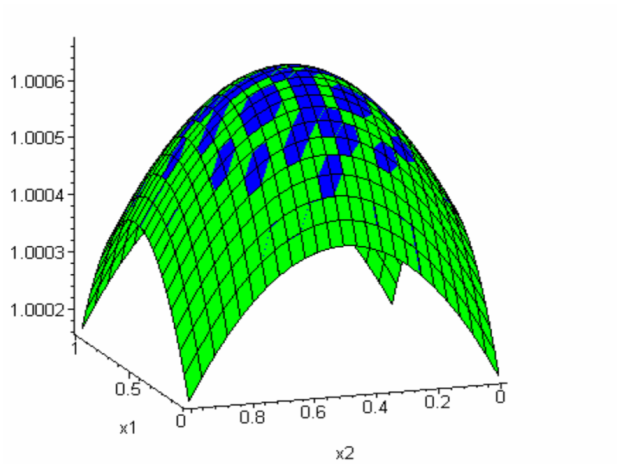

Figure 1: *Comparison of the normalized exponential function for $c_i = 0.5$ and $\alpha_i = 0.001$ with first order HDMR truncation s_1. Dark color (blue) denotes the original function whereas the light one (green) corresponds to first order HDMR truncation.*

We also attempted to compare various HDMR approximation levels for various α_is. c_i value was kept at 0.5 which turned up to yield the best resultys in additivity measurer analysis. As is seen in Figure 1, the function and the approximation coincide quite well. This is because we choose very small α_i. Only first order HDMR approximation is sufficient.

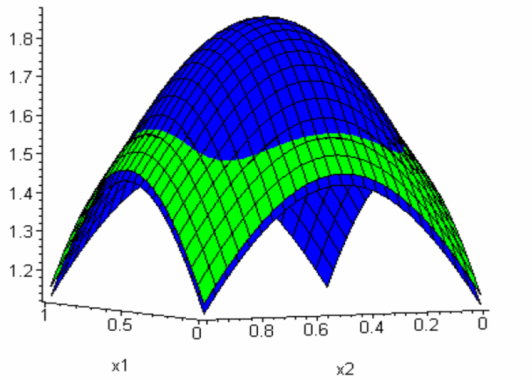

Figure 2: *Comparison of the normalized exponential function for $c_i = 0.5$ and $\alpha_i = 1.0$ with first order HDMR truncation s_1. Dark color (blue) denotes the original function whereas the light one (green) corresponds to first order HDMR truncation.*

In Figure 2 it is observed that the function function and the first order HDMR truncation do not coincide as well as that observed in Figure 1. This obviously happens because the α_i value relatively much higher. Deviation between the function and the approximation at the ends of the plot is observed.

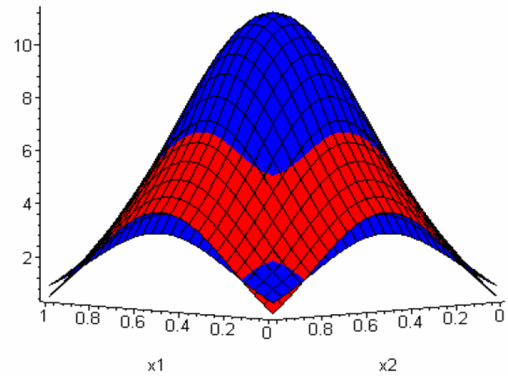

Figure 3: *Comparison of the normalized exponential function for $c_i = 0.5$ and $\alpha_i = 5.0$ with second order HDMR truncation s_2. Dark color (blue) denotes the original function whereas the light one (red) corresponds to first order HDMR truncation.*

It is observed that for the higher α_i value of 5.0 the first order truncation s_1 is rather insufficient. In Figure 3, we compare the original function with the second order HDMR truncation s_2. When α_i grows, function tends to tighter form.

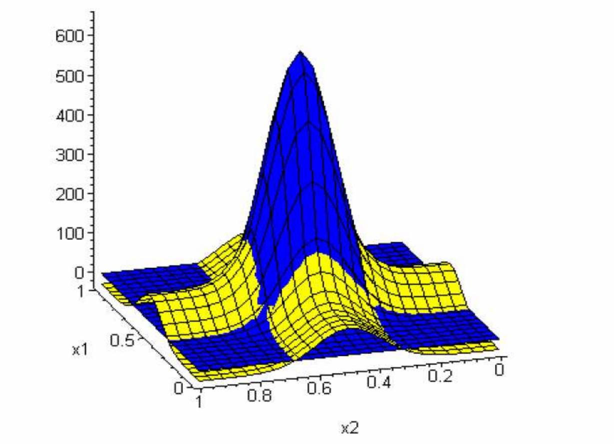

Figure 4: *Comparison of the normalized exponential function for $c_i = 0.5$ and $\alpha_i = 40.0$ with second order HDMR truncation s_3. Dark color (blue) denotes the original function whereas the light one (yellow) corresponds to first order HDMR truncation.*

Finally, as α_i attains larger values, truncation order of HDMR must be higher. For as high an α_i value 40.0 truncation levels of zeroth, first, and second order the agreement is quite poor. In Figure 4, the comparison is made for the third order HDMR truncation level. It is seen in the plot that the function gets quite a tight shape.

4 Conclusion

Calculations have shown us that HDMR is an efficient and low cost method for approximations. Truncations at intended order is another advantage. Even when the values were chosen without extra care, higher order HDMR truncations deal with this problem. Applicability to many field of study and easy handling makes HDMR a valuable approach.

All authors and the third author are grateful respectively to WSEAS and Turkish Academy of Sciences for their supports.

References:

[1] M. Demiralp, High Dimensional Model Representation and Its Application Varieties, *Proceedings of the Fourth International Conference on Tools for Mathematical Modelling*, St. Petersburg, Russia, 2003, pp. 146–159

[2] I.M. Sobol, Theorems and Examples on High Dimensional Model Representations, *Reliability Engineering Safety,* 79, 2003, pp. 187–193.

[3] H. Rabitz, Ö. Alış, General Foundations of High Dimensional Model Representations, *J. Math. Chem.* 25, 1999, pp. 197–233.

[4] G. Li, C. Rosenthal and H. Rabitz, High Dimensional Model Representations, *J. Math. Chem. A* 105-33, 2001, pp. 7765–7777.

[5] M. Demiralp, A. Kurşunlu, Additive and Factorized HDMR Applications to the Multivariate Diffusion Equation Under Vanishing Derivative Boundary Conditions, *Proceedings of the Fourth International Conference on Tools For Mathematical Modelling* St. Petersburg, Russia, 2003, pp. 315–327.

[6] N.A. Baykara and M. Demiralp, Hyperspherical or Hyperellipsoidal Coordinates in the Evaluation of HDMR Approximants*Proceedings of the Fourth International Conferance on Tools For Mathematical Modelling* St. Petersburg, Russia, 2003, pp. 48–62.

[7] M. Demiralp and T. Civelekoğlu, An HDMR Application to the Schrdinger's Equation for Free Particles Under an External Field with Dipole Polarization and Vanishing Flux Boundary Conditions, *Proceedings of the Fourth International Conferance on Tools For Mathematical Modelling*, St. Petersburg, Russia, 2003, pp. 110–121.

[8] H. Kaya, M. Kaplan, H. Saygın, A Recursive Algorithm for Finding HDMR terms for Sensitivity Analysis , *Computer Physics Communications* 158, 2004, pp. 106–112.

[9] I.M. Sobol, S.S. Kucherenko, Global Sensitivity Indices for Non-linear Mathematical Models, *Wilmott Magazine.* 2, 2005, pp. 2-7.

[10] H. Rabitz, Ö. Alış, Efficient Implementation of HDMR, *Journal of Mathematical Chemistry* 29-2, 2001, pp. 127–142

[11] C. Gülpınar, High Dimensional Model Representation and Domain Geometry, *M.Sc. Thesis, Marmara Univ., Math. Dept.* 2007 (in Turkish)