# Fluctuationlessness Approximation Towards Orthogonal Hyperprismatic Grid Construction

BURCU TUNGA İstanbul Technical University Informatics Institute Maslak, 34469, İstanbul Turkey (TÜRKİYE) METIN DEMIRALP İstanbul Technical University Informatics Institute Maslak, 34469, İstanbul Turkey (TÜRKİYE)

Abstract: The main purpose of this work is to construct transformations which map the nodes created by the individual matrix representations N independent variables to the hypegrid nodes where the values of an N variate functions are given. Recent works of the Demiralp's group show that the matrix representation of a multivariate function can be approximated by the image of its independent variable matrix representations under that function at the fluctuationlessness limit. This brings the possibility of using only N dimensional cartesian space points which are characterized by N-tuples whose elements are the eigenvalues of the matrix representations of those independent variable. However, these points may not match the points where the values of the function under consideration are given. Hence, N-dimensional shifts of the eigenvalue based points to data given points is required. This can be done by using certain polynomial interpolations. This work aims at the evaluation of those polynomials.

*Key–Words:* Multivariate Functions, High Dimensional Model Representation, Approximation, Fluctuationless-ness Approximation.

### 1 Introduction

High dimensional model representation (HDMR) [1-6] was proposed to approximate the multivariate functions by the functions having less number of independent variables. The equation of the High Dimensional Model Representation for a given multivariate function  $f(x_1, \dots, x_N)$  is as follows

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

The sum of the right hand side terms of HDMR expansion represents the given multivariate function exactly. The HDMR components of the given multivariate function are the right hand side terms of this expansion. These terms are the constant term, univariate terms, bivariate terms and the other high-variate terms. The following vanishing conditions are used to obtain the right hand side components of the expansion.

$$\int_{a_1}^{b_1} dx_1 \cdots \int_{a_N}^{b_N} dx_N W(x_1, ..., x_N) f_i(x_i) = 0,$$

Here, the weight function is assumed as a product of given univariate functions each of which depends on a different independent variable.

$$W(x_1, \dots, x_N) \equiv \prod_{j=1}^N W_i(x_i),$$
  
$$x_i \in [a_i, b_i], \qquad 1 \le i \le N$$
(3)

 $1 \le i \le N$  (2)

The abovementioned vanishing conditions correspond to the following orthogonality conditions over HDMR components through an inner product as can be proven without any remarkable difficulty.

$$(f_{i_1...i_k}, f_{i_1...i_l}) = 0, \qquad 1 \le k, l \le N$$
  
$$\{i_1, \dots, i_k\} \not\equiv \{i_1, \dots, i_l\}$$
(4)

If we assume that  $u(x_1, \ldots, x_N)$  and  $v(x_1, \ldots, x_N)$ are two arbitrary square integrable multivariate functions in the space of square integrable functions over the hyperprism defined by the intervals  $a_i \leq x_i \leq b_i$ then the orthogonality conditions' inner product can be explicitly defined as follows

$$(u,v) \equiv \int_{a_1}^{b_1} dx_1 W_1(x_1) \dots \int_{a_N}^{b_N} dx_N W_N(x_N) \\ \times u(x_1, \dots, x_N) v(x_1, \dots, x_N)$$
(5)

The orthogonality condition and the vanishing condition help us to calculate HDMR terms. The constant term  $f_0$  and univariate terms  $f_i(x_i)$  are given as follows.

$$f_{0} = \int_{a_{1}}^{b_{1}} dx_{1} W_{1}(x_{1}) \dots \int_{a_{N}}^{b_{N}} dx_{N} W_{N}(x_{N}) \\ \times f(x_{1}, \dots, x_{N})$$
(6)

$$f_{i}(x_{i}) = \int_{a_{1}}^{b_{1}} dx_{1}W_{1}(x_{1})\dots\int_{a_{i-1}}^{b_{i-1}} dx_{i-1}$$

$$\times W_{i-1}(x_{i-1})\int_{a_{i+1}}^{b_{i+1}} dx_{i+1}W_{i+1}(x_{i+1})$$

$$\dots \int_{a_{N}}^{b_{N}} dx_{N}W_{N}(x_{N})f(x_{1},\dots,x_{N}) - f_{0}$$

$$1 \le i \le N$$
(7)

Other components can be calculated similarly. If we truncate the equation (1) at some level we obtain the HDMR approximants as given below

$$s_{0}(x_{1},...,x_{N}) = f_{0}$$

$$s_{1}(x_{1},...,x_{N}) = s_{0}(x_{1},...,x_{N}) + \sum_{i=1}^{N} f_{i}(x_{i})$$

$$\vdots$$

$$s_{k}(x_{1},...,x_{N}) = s_{k-1}(x_{1},...,x_{N})$$

$$+ \sum_{\substack{i_{1},...,i_{k}=1\\i_{1}<\cdots< i_{k}}}^{N} f_{i_{1}...i_{k}}(x_{i_{1}},...,x_{i_{k}})$$

$$1 \le k \le N$$
(8)

If we assume that  $f(x_1, \ldots, x_N)$  given in (1) is square integrable then we can write the following equation

$$||f||^{2} = ||f_{0}||^{2} + \sum_{i=1}^{N} ||f_{i}||^{2} + \sum_{\substack{i,j=1\\i < j}}^{N} ||f_{i,j}||^{2} + \cdots ||f_{12\cdots N}||^{2}$$
(9)

The last equation implies that the following relation is valid.

$$\frac{||f_0||^2}{||f||^2} + \frac{\sum_{i=1}^N ||f_i||^2}{||f||^2} + \frac{\sum_{\substack{i,j=1\\i< j}}^N ||f_{i,j}||^2}{||f||^2} + \frac{\cdots \frac{||f_{12\cdots N}||^2}{||f||^2}}{||f||^2} = 1$$
(10)

which us to make the definitions given below.

$$\sigma_0 \equiv \frac{1}{\|f\|^2} \|f_0\|^2$$

$$\sigma_{1} \equiv \frac{1}{\|f\|^{2}} \sum_{i=1}^{N} \|f_{i}\|^{2} + \sigma_{0}$$
  
$$\vdots$$
  
$$\sigma_{N} \equiv \frac{1}{\|f\|^{2}} \|f_{12...N}\|^{2} + \sigma_{N-1} \qquad (11)$$

These entities are called "Additivity Measurers" and they can hold a value between zero and one

$$0 \le \sigma_0 < \dots < \sigma_N = 1 \tag{12}$$

The best approximation quality for the  $i^{th}$  approximation is obtained as the  $\sigma_i$  value gets closer to 1.

The rest of the paper is organized as follows. The next section is about Fluctuationlessness Approximation. The third section presents the basic idea underlying grid construction. The fourth section contains simple illustrative applications for this new method and the fifth section finalizes the paper with concluding remarks.

### 2 Fluctuationlessness Approximation

In this section, a new method which is called Fluctuationlessness Approximation [6-9] and related theorem are given. We assume  $\mathcal{H}_n$  as finite dimensional subspace of Hilbert space  $\mathcal{H}$  spanned by  $w_1(x),...,w_n(x)$ . The difference between the unit matrix of  $\mathcal{H}$  and  $\mathcal{H}_n$  is called "Fluctuation Operator "in the proof of the following theorem whose proof was given in Demiralp's paper [9].

**Theorem :** The matrix representation of an algebraic multiplication operator multiplying its operand by f(x), a univariate function which is analytic on the interval [a, b], over  $H_n$  is the image of the matrix representation of the independent variable over  $H_n$  under the function f at the fluctuationlessness limit [9].

$$\mathbf{F}^{(n)} \approx f\left(\mathbf{X}^{(n)}\right) \tag{13}$$

Here  $\mathbf{X}^{(n)}$  which is given as follows is the matrix representation of the multiplication operator which multiplies its operand by the independent variable, x

$$\mathbf{X}^{(n)} \equiv \begin{bmatrix} X_{11}^{(n)} & \cdots & X_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ X_{n1}^{(n)} & \cdots & X_{nn}^{(n)} \end{bmatrix},$$
$$X_{jk}^{(n)} \equiv (w_j, \hat{x}w_k), \ 1 \le j, k \le n$$
(14)

and the matrix representation of the function f(x), denoted by  ${\bf F}^{(n)}$  here, can be given as follows

$$\mathbf{F}^{(n)} \equiv \begin{bmatrix} F_{11}^{(n)} & \cdots & F_{1n}^{(n)} \\ \vdots & \ddots & \vdots \\ F_{n1}^{(n)} & \cdots & F_{nn}^{(n)} \end{bmatrix},$$
$$F_{jk}^{(n)} \equiv \left( w_j, \hat{f} w_k \right), \ 1 \le j, k \le n$$
(15)

Here  $\hat{f}$  stands for the algebraic multiplication operator which multiplies its operand by the function f(x).

The multivariate counterpart of this theorem is also existing and proven but not published yet. There we can replace the single independent variable x by N number of indpendent variables,  $x_1,...,x_N$  and the function f(x) should be replaced by its N-variate counterpart,  $f(x_1,...,x_N)$ . Then, we can write

$$\mathbf{F}^{(n)} \approx f\left(\mathbf{X}_{1}^{(n_{1})}, ..., \mathbf{X}_{N}^{(n_{N})}\right)$$
(16)

which is based on certain ideas and manipulations using matrix theoretical direct products.

## 3 Grid Construction At No Fluctuation Limit

HDMR can be used over a data located at he nodes of a finite orthogonal prismatic grid in N dimension if the values of function under consideration are given all nodes by using either Dirac's delta function. Quite recently a new opportunity has been borne after recent stages of HDMR works in Demiralp's group. This is a new method to deal with the functions given by finite number of data without using Dirac's delta functions as the pointwise value picking agents. There, the integrals of HDMR are approximated by the multivariate Fluctuationless theorem such that only the values of the function under consideration in HDMR at the points belonging to the cartesian product of the spectra of independent variable matrix representations. This cartesian product is composed of N-tuples which are certainly depend only on the universal quantities, matrix representations of independent variables, not on the HDMR's target function. This universality is very good in one hand since reduced the number of the calculations enormously; is not so good in the other hand since the grid created through this theorem may not contain whole or any data given coordinates. This means that certain transformations must be used to indirectly use this grid not itself but its somehow shifted form. This can be accomplished in a tricky way. Not the function  $f(x_1, ..., x_N)$ 's itself but the function  $f(g_1(x_1, ..., x_N), ..., g_N(x_1, ..., x_N))$  with the g

functions unknown yet can be taken into consideration. Then, g functions are determined in such a way that each of them produces only the values of the data given grid nodes from the eigenvalue based grid. This is of course an interpolation problem whose solution is straightforward. Here we use Lagrange's method by accepting all pitfalls of the interpolation. As long as the grid-to-grid mapping is smooth the interpolatory problems remain far away. However, the decrease in smoothness and therefore increase in curvature may result in unpleasent polynomials highly oscillating. Even in those cases, they can be again used for our purposes since we would not need the values at the values which are not interpolation points. whe

### 4 Implementations

In this section a numerical implementation is given to discuss the usage of this method. The multivariate data is constructed through the analytically known multivariate functions to test the performance of this new method. In this example the problem has six independent variables. The points for each independent variable will be given as follows

$$D_{1} = \{0.2, 0.3, 0.4, 0.5\}$$

$$D_{2} = \{0.6, 0.7, 0.8, 0.9, 1.0\}$$

$$D_{3} = \{0.1, 0.2, 0.3, 0.4\}$$

$$D_{4} = \{0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0\}$$

$$D_{5} = \{0.7, 0.8, 0.9, 1.0, 1.1\}$$

$$D_{6} = \{1.2, 1.3\}$$
(17)

and a cartesian product set having 6400 nodes is constructed by using these points.

When the method given in the previous section is applied to this interpolation problem, the following six polynomials are obtained. These polynomials provide a transformation for shifting the given points onto the eigenvalues of each  $\mathbf{X}^{(n)}$  matrix corresponding to each independent variable. In other words, the transformation rule,  $g_1$  polynomial, is determined to shift the points given on the  $x_1$ -axis onto the eigenvalues of the  $\mathbf{X}_1^{(n)}$  matrix. As this process is applied for each independent variable six different polynomials are obtained.

$$g_{1} = - 0.34661707965617775044 * x_{1}^{3} + 0.51992561948426662566 * x_{1}^{2} - 0.54408073937000812415 * x_{1} + 0.53538609977095962446 (18)$$

$$g_2 = -0.0000000000000000001 * x_2^4$$



Figure 2:

### 5 Conclusion

In this work we have found the way of using the grids constructed via multivariate fluctuationlessness theorem. The basic idea has been to transform the grid constructed as the cartesian product of spectra of individual matrix represantations of independent variables, each of which may be in a different but finite dimension, to the grid whose each nodal point is accompanied by a given value of the multivariate function under consideration. Grid-to-grid transformations are provided by using certain degree polynomials each of which depends on a different independent variable. What we have obtained is that this idea seems to be working as expected as long as sufficiently smooth transformations are under consideration, although the other where curvature is higher seem not to be creating so much numerical problems. This work can be considered as a baby theory yet leaving the very enthusiastic expectations to future works. Our group is getting concentrated on this issue nowadays.

Acknowledgements: Both authors and second author are grateful to WSEAS and Turkish Academy of Sciences respectively for their support and motivation.

$$g_{3} = - 0.34661707965617775043 * x_{2}^{2} \\ - 0.519925619482034820315997 (19)$$

$$g_{3} = - 0.34661707965617775043 * x_{3}^{3} \\ + 0.51992561948426662565 * x_{3}^{2} \\ - 0.54408073937000812414 * x_{3} \\ + 0.43538609977095962446 (20)$$

$$g_{4} = - 15.368362545388038606 * x_{4}^{7} \\ + 53.789268908858135121 * x_{4}^{6} \\ - 78.449849358485813221 * x_{4}^{5} \\ + 61.65145112406919525 * x_{4}^{4} \\ - 28.546718069803941045 * x_{4}^{3} \\ + 8.0632604350657838778 * x_{4}^{2} \\ - 1.9089249220845798656 * x_{4} \\ + 1.0349372138846292443 (21)$$

$$g_{5} = - 0.52702255124972718971 * x_{5}^{3} \\ + 0.79053382687459078458 * x_{2}^{2}$$

 $0.52702255124972718956 * x_2^3$ 

$$-$$
 0.7284876825889267942 \*  $x_5$ 

$$+ 1.1324882034820315997 \tag{22}$$

$$g_6 = - 0.17320508075688772935 * x_6 + 1.3366025403784438647$$
(23)

To examine these polynomials carefully a number of additional plots are given here. Although each polynomial is dependent to one independent variable such as  $g_1$  depends on  $x_1$ , to show the characteristics of these polynomials we assume that all depend on the variable x and we use only one plot for the purpose. However, the reason for drawing a seperate plot for  $g_4$  is to bypass the scaling problem. Otherwise, the characteristics of the other polynomials cannot be observed as the value of the function  $g_4$  increases fastly. The reason is the number of given points for the corresponding independent variable. As the number of given points for an independent variable increases the fluctuation of the q polynomial increases.

In this part all the computations are done by using MuPAD[10] Computer Algebra System with 20-digit precision. The program codes are run under Linux (Ubuntu 7.10) Operating System.

#### References:

- I.M. Sobol, Sensitivity Estimates for Nonlinear Mathematical Models, Mathematical Modeling and Computational Experiments, 1993, VOL. 1, pp 407-414.
- [2] J.A. Shorter, P.C. Ip, and H. Rabitz, An Efficient Chemical Kinetics Solver Using High Dimensional Model Representation, txitext J. Phys. Chem. A, 1999, VOL 103, pp 7192-7198.
- [3] Ö. Alış and H. Rabitz, Efficient Implementation of High Dimensional Model Representations, Journal of Mathematical Chemistry, 2001, VOL 29, pp 127-142.
- [4] G. Li, S. W. Wang, H. Rabitz, S. Wang and P. Jaffe, Global uncertainty assessments by high dimensional model representation (HDMR), Chemical Engineering Science, 2002, VOL 57, pp 4445-4460.
- [5] M. Demiralp and M.A. Tunga, High Dimensional Model Representation of Multivariate Interpolation via Hypergrids, The Sixteenth International Symposium on Computer and Informa-

tion Sciences (ISCIS XVI), 416-423, (2001).

- [6] M. Demiralp, High Dimensional Model Representation and its application varieties, Tools for Mathematical Methods, Mathematical Research, 2003, VOL 9, pp 146-159.
- [7] M. Demiralp, A New Fluctuation Expansion Based Method for the Univariate Numerical Integration Under Gaussian Weights, WSEAS-2005 Proceedings, WSEAS 8-th International Conference on Applied Mathematics, 16-18 December, 2005, Tenerife, Spain, 68-73.
- [8] M. Demiralp, Convergence Issues in the Gaussian Weighted Multidimensional Fluctuation Expansion for the Univariate Numerical Integration, WSEAS Tracsaction on Mathematics, 4, 486-492.
- [9] M. Demiralp, Fluctuationlessness Theorem to Approximate Univariate Functions Matrix Representations, Applied Mathematics and Computation (submitted).
- [10] W. Oevel, F. Postel, S. Wehmeier and J. Gerhard, The MuPAD Tutorial, Springer, (2000).