J Math Chem (2012) 50:2023–2042
DOI 10.1007/s10910-012-0018-6

ORIGINAL PAPER

Combined small scale high dimensional model representation

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Received: 5 March 2012 / Accepted: 6 April 2012 / Published online: 26 May 2012

Abstract Nowadays the utilization of High Dimensional Model Representation (HDMR), which is an algorithm for approximating multivariate functions, is becoming more pervasive in the applications of approximation theory. This extensive usage motivates new works on HDMR, to get better solutions while approximating to the multivariate functions. One of them is recently developed "Combined Small Scale High Dimensional Model Representation (CSSHDMR)". This new scheme not only optimises HDMR results but also provides good approximation with less terms than HDMR does. This paper presents the theory and the numerical results of the new method and shows that it is possible to apply approximation to multivariate functions by keeping only constant term of HDMR. From this aspect CSSHDMR can be used in any scientific problem which includes multivariate functions, from chemistry to statistics.

Keywords Multivariate analysis · Small scale high dimensional model representation · Approximation · Perturbation expansion

1 Introduction

Two important class of problems in scientific and engineering applications are focused on the decomposition two mathematical entities: (1) functions and (2) arrays. The latter which is related to ordinary linear algebra and multilinear algebra is outside the scope of this work which is devoted to the function decompositions. The function decomposition aims to express a given function in terms of certain well-known functions,

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linearly or nonlinearly. The linear representations are the ones using linear combinations involving finite or (mostly) infinite number of terms. Taylor or Maclaurin series, orthogonal function series, integral representations are among st such representations. The most important issue for these representations is the utilization of linearly independent functions in the linear combinations. Whereas the nonlinear representations focuses on the employment of functionally independent term sequences. Rational Approximants, more specifically Padé and Hermite–Padé approximants are good examples to this end.

In the linear decompositions a basis set which spans a linear vector space where the target function resides is used and linear combinations are constructed over the elements of this basis set. The orthogonality is perhaps the most desired feature since it facilitates the manipulations very much. The decomposition may become awkward when the target function depends on many independent variables and certain specific methods may be required to get efficient representations including terms ordered in ascending multivariance. To this end, High Dimensional Model Representation (HDMR) and its varieties can be mentioned even though a new efficient extension of HDMR has been proposed by Demiralp's group and called "Enhanced Multivariance Product Representation". As there have been various developments for HDMR from Demiralp's group, this work is devoted to the presentation of a finite-element-like method in certain details.

Paper is organised as follows. The second section covers the revisiting of HDMR by focusing on necessary details. The third section contains the details of so-called Small Scale HDMR (SSHDMR) which becomes very efficient when the size of the HDMR geometry diminishes to zero. The fourth section involves the basic issues of the combination of SSHDMRs over certain subgeometries of the considered HDMR problem to create a piecewise approximant structure, somehow a multidimensional spline structure. The fifth section is devoted to some illustrative implementations by presenting a table and some figures. The sixth section finalizes the paper with the concluding remarks. Certain subsections are also constructed when it is conside red necessary to emphasize on certain important details.

2 Recalling HDMR

High Dimensional Model Representation (HDMR) methods are based on a divide-and-conquer philosophy, enabling us to express a multivariate function by some other functions having less number of variables through an orthogonal decomposition. HDMR was first proposed by Sobol [1] and basically developed by Rabitz's [2–4] and also Demiralp's and his group's works [5,6] even though there have been a lot of new contributions [7–16] recently. It also finds its roots in one of the Kolmogorov's work [17]. HDMR of a given multivariate function is explicitly defined as follows

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

where the right hand side of the equality includes, a constant term (f_0), N univariate terms ($f_i(x_i), i = 1, \ldots N$), $N(N-1)/2$ bivariate terms $\left(f_{i_1,i_2}\left(x_{i_1}, x_{i_2}\right), 1 \le i_1 \le i_2 \le N\right)$ and so on. This equation includes 2^N unknown functions, hence urges us to impose certain conditions on the right hand side components. These impositions are due to Sobol and state that each right hand side component's integral (except the constant term) over its one of arguments along a prescribed interval and under a given weight function vanishes. The interval used by Sobol was [0, 1] and he employed unit const ant function as weight. The introduction of nonunit intervals and weight functions varying in the given interval is due to Rabitz. This generalization extended the utilization of HDMR on semi-infinite and infinite geometries and raised the possibility to give different importances to the function values at different points. However this never removed the requirement for the employment of orthogonal geometries since the Sobol's vanishing conditions create inconsistencies to determine the components in the case of nonorthogonal geometries. Even though there have been various new attempts to overcome this difficulty especially by Demiralp's and his colleagues' works like GHDMR [18] and new impositions [19], today's most widely used approaches are basically plain HDMR (Sobol's), Cut and Multicut HDMR [20,21] and FHDMR [22], EMPR [23] and GEMPR [24].

To determine the explicit structure of the HDMR components we need it to use the vanishing conditions. To this end one of the systematic ways is to use certain operators projecting to the subspaces spanned by functions with multivariance one less than the target function's, from the space where the target function lies

$$\widehat{I} f(x_1, \ldots, x_N) \equiv f(x_1, \ldots, x_N) \tag{2}$$

$$\widehat{P}_i f(x_1, \ldots, x_N) \equiv \int_{a_i}^{b_i} dx_i W_i(x_i) f(x_1, \ldots, x_N), \quad i = 1, \ldots, N \tag{3}$$

where we have assumed that the integral of $W_i(x_i)$ a long the interval $[a, b]$ is 1 to provide the idem potency to $\widehat{P}_i$. This apparently gives vanishing property to the products of $\widehat{P}_i$ and its complementary companion $\left[\widehat{I} - \widehat{P}_i\right]$ without regarding the order in the multiplication.

We can identically express a given multivariate function as follows by using (2) and (3)

$$f(x_1, \ldots, x_N) = \left(\prod_{i=1}^{N} \left(\widehat{P}_i + \left[\widehat{I} - \widehat{P}_i\right]\right)\right) f(x_1, \ldots, x_N) \tag{4}$$

The right hand side operator product can be expanded as follows

$$\prod_{i=1}^{N} \left(\widehat{P}_i + \left[\widehat{I} - \widehat{P}_i\right]\right) = \prod_{i=1}^{N} \widehat{P}_i + \sum_{i_1=1}^{N} \left(\prod_{i=1}^{i_1-1} \widehat{P}_i\right) \left[\widehat{I} - \widehat{P}_{i_1}\right] \left(\prod_{i=i_1+1}^{N} \widehat{P}_i\right)$$

$$+\sum_{\substack{i_1,i_2=1\\ i_1<i_2}}^{N}\left(\prod_{i=1}^{i_1-1}\widehat{P}_i\right)[\widehat{I}-\widehat{P}_{i_1}]\left(\prod_{i=i_1+1}^{i_2-1}\widehat{P}_i\right)[\widehat{I}-\widehat{P}_{i_2}]$$
$$\times\left(\prod_{i=i_2+1}^{N}\widehat{P}_i\right)+\cdots \tag{5}$$

whose action on the target multivariate function allows us to deter mine the HDMR components after using the orthogonality based annihilations as follows

Constant Term:

$$f_0=\left(\prod_{i=1}^{N}\widehat{P}_i\right)f\left(x_1,\ldots,x_N\right) \tag{6}$$

Univariate Terms:

$$f_{i_1}\left(x_{i_1}\right)=\left(\prod_{i=1}^{i_1-1}\widehat{P}_i\right)[\widehat{I}-\widehat{P}_{i_1}]\left(\prod_{i=i_1+1}^{N}\widehat{P}_i\right)f\left(x_1,\ldots,x_N\right) \tag{7}$$

Here we find it sufficient to give only constant and univariate components. However bivariate and higher variate terms can be defined within the same philosophy.

Equations (6) and (7) can be rewritten as follows by using explicity in projection operators there.

Constant Term:

$$f_0=\int_{a_1}^{b_1}dx_1\cdots\int_{a_N}^{b_N}dx_N W\left(x_1,\ldots,x_N\right)f\left(x_1,\ldots,x_N\right) \tag{8}$$

Univariate Terms:

$$f_i\left(x_i\right)=\int_{a_1}^{b_1}dx_1\ldots\int_{a_{i-1}}^{b_{i-1}}dx_{i-1}\int_{a_{i+1}}^{b_{i+1}}dx_{i+1}\cdots\int_{a_N}^{b_N}dx_N\prod_{\substack{j=1\\ j\neq i}}^{N}W_j\left(x_j\right)f\left(x_1,\ldots,x_N\right)$$
$$-f_0,\ 1\leq i\leq N \tag{9}$$

As we mentioned above we do not intend to go beyond the univariance. This is because HDMR is a finite term exact decomposition over 2^N components and the number of the terms may become too big for practical purposes when N tends to grow. This growth urges us to truncate the decomposition at lower multivariances. For practical purposes the level of truncation is desired to be kept at univariance and at most bivariance for certain specific cases. Hence we deal with only constant and univariate components here. This level of approximation fits also our small scale HDMR approach here as we will show through our progress.

Equation (8) shows that the constant HDMR component is in fact the weighed mean value of the multivariate target function over the orthogonal geometry and under the given product type weight function whose univariate factors are $W_i\ (x_i)$s. Similarly, (9) dictates us that the univariate components are means of the target multivariate function's unidirectional deviations from its overall average over the same geometry and under the product type weight function. In the statistical interpretation the univariate functions are corresponding to the directional variances we call directional fluctuations in the sense of mathematical theory of fluctuations [25–27].

The N dimensional integrals appearing in the HDMR component determination can be used for defining inner products. The inner product of any given two functions, which are square integrable over the rectangular hyperprismatic domain in the space spanned by x independent variables and under the product type weight functions, is defined as the integral of their products under the above mentioned geometry and weight functions. The norm of a function residing in the above mentioned space is defined as the inner product square root of the function with itself.

Apparently the constant term and all univariate terms above are mutually orthogonal over the rectangular hyperprismatic geometry and under the product weight. Even though Rabitz and Demiralp take the attention on this orthogonality there has been a lot of published works from Demiralp and his colleagues about the utilization of orthogonality. The quality (or additivity) measurer definitions based on this orthogonality by Demiralp have been extensively used by him and his group in their studies [28]. The orthogonality is defined through an appropriate inner product amongst the members of a li near vector space. Hence we use Hilbert space tools to this end. All these imply that HDMR is a finite number term including orthogonal decomposition. It somehow decomposes a function of an appropriately defined Hilbert space to finitely many orthogonal components. Each component spans a different one dimensional subspace depending on the target function. Hence the subspaces are not universal un less the target functions are assumed to be confined in a finite dimensional subspace where a universal set of functions can be constructed to be used in the HDMR although we do not intend to go beyond this point here since it is out of the scope of this work.

The case where the target function is approximated by the constant HDMR term only can be called "Constant HDMR Approximation" while the cases where constant and univariate terms are used to approximate the target function can be called "Univariate HDMR Approximation" despite univariance may not be considered cumulatively together with the constancy. The other approximations use the truncation approximants which can be defined accordingly. We give them through the following equalities

$$
\begin{aligned}
s_0\left(x_1,\ldots,x_N\right) &= f_0 \\
s_1\left(x_1,\ldots,x_N\right) &= s_0\left(x_1,\ldots,x_N\right) + \sum_{i_1=1}^{N} f_{i_1}\left(x_{i_1}\right) \\
&\vdots
\end{aligned}
$$

$$s_k(x_1,\ldots,x_N) = s_{k-1}(x_1,\ldots,x_N) + \sum_{\substack{i_1\ldots i_k=1 \\ i_1<\cdots<i_k}}^{N} f_{i_1\ldots i_k}\left(x_{i_1},\ldots,x_{i_k}\right), \quad 1 \le k \le N \tag{10}$$

It is very easy to show that all HDMR components except the constant one vanish if the target function is a constant function. A similar situation raises when the target function is sum of some univariate functions and a constant function. One can prove that all HDMR components except the constant and univariate ones vanish. These are not peculiar to constancy and univariance only. The case where the target function is a sum of constant, univariate and multivariate terms whose multivariance level is at most k results in an HDMR whose nonvanishing components' multivariance level is at most k. All these imply that the univariate HDMR truncations show up in better qualities as the target function's additive univariance dominates. Therefore we can expect good quality for univariate truncation approximant when the target function has a dominating additive univariance. Univariate truncation of plain HDMR tends to fail as the target function goes far away from the additive univariance. An important example is the case where the target function is purely multiplicative, in other words, the product of univariate functions. Univariate truncation becomes very poor for these cases. To cure the negativity of these cases new HDMR types are constructed. Factorized HDMR (FHDMR) proposed by Demiralp group is for this purpose [29]. The cases where the target function is neither purely additive (the sum of univariate functions) nor purely multiplicative a linear combination of plain HDMR and FHDMR is constructed for applications. We call them Hybrid HDMR (HHDMR) [30–32].

Another possibility to overcome the failure of univariate truncations in plain HDMR is to partition the geometry to appropriate subgeometries and then try to use univariate truncations. The heart of this work is focused on this attempt.

3 Small scale high dimensional model representation (SSHDMR)

The mainlines of this work are arisen when the question "How are the HDMR components and its truncation approximants affected when the size of the HDMR geometry tends to vanish?". Roots of this question based on different studies [33–35], however this work is the first which expands theory with perturbation expansion and analysis on different examples. It has been seen that the univariance dominancy increases when the HDMR geometry is contracted then the division of the entire HDMR geometry to appropriate subgeometries will facilitate it to get higher approximation qualities in each subgeometry. The final step than is to combine these small scale HDMRs appropriately.

3.1 Formulation

Let us focus on the HDMR whose geometry is given by the intervals $[\,a_i, b_i\,]$ $(i = 1,\ldots,N)$. We can convert this rectangular hyperprismatic geometry to unit hypercube whose ith edge is the interval $[\,0, 1\,]$ by using the following coordinate changes

$$x_i = (b_i - a_i)\left(y_i - \frac{1}{2}\right) + \frac{b_i + a_i}{2}, \qquad dx_i = (b_i - a_i)\, dy_i, \qquad y_i \in [0, 1], \quad 1 \le i \le N \tag{11}$$

which permits us to rewrite the constant HDMR component of a given multivariate function $f(x_1, \ldots, x_N)$ as follows

$$f_0 = \int_0^1 dy_1 \ldots \int_0^1 dy_N \left\{ \prod_{i=1}^{N} (b_i - a_i)\, W_i \left((b_i - a_i)\left(y_i - \frac{1}{2}\right) + \frac{b_i + a_i}{2} \right) \right\} \times f\left((b_1 - a_1)\left(y_1 - \frac{1}{2}\right) + \frac{b_1 + a_1}{2}, \ldots, (b_N - a_N)\left(y_N - \frac{1}{2}\right) + \frac{b_N + a_N}{2} \right) \tag{12}$$

which means

$$\{f_0\}_{\mathbf{b}\to\mathbf{a}} \approx \left\{ \prod_{i=1}^{N} (b_i - a_i)\, W_i \left(\frac{b_i + a_i}{2} \right) \right\} f\left(\frac{b_1 + a_1}{2}, \ldots, \frac{b_N + a_N}{2} \right) \tag{13}$$

This is apparently a constant value implying that the zero size limiting enables us to deal with integration free expressions.

The above formulae is such that the y variable's interval midpoints are matching the midpoints of the original corresponding intervals. To proceed more efficiently we define

$$\alpha_i \equiv \frac{b_i + a_i}{2}, \qquad u_i \equiv b_i - a_i, \qquad i = 1, \ldots, N \tag{14}$$

where u parameters are responsible for the behaviors of the multivariate expression at the zero size limit. Any function depending on x variables can be expressed in terms of y variables and the relation between x and y variables dictates us that the differentiation with respect to any y variable of that function scales the derivative of the same function with respect to the corresponding x variable by the length of that x variable's interval length. This scaling property urges us to use this scaling factors, that is, us as the perturbation parameters in our HDMR relations. To deal with multi variate Taylor expansion more efficiently we define

$$\mathscr{D}_\alpha = \left[u_1 \left(y_1 - \frac{1}{2} \right) \frac{\partial}{\partial \alpha_1} + \cdots + u_N \left(y_N - \frac{1}{2} \right) \frac{\partial}{\partial \alpha_N} \right] \tag{15}$$

which enables us to write the following multivariate Taylor expansion in powers of us

$$f(\mathbf{x}) = \sum_{k=0}^{\infty} \frac{1}{k!} \mathscr{D}_\alpha^k f(\alpha) \tag{16}$$

where $\mathbf{x}$ and $\boldsymbol{\alpha}$ stand for the set of xs and αs respectively. Equivalent expansions can be given for the weight functions although we do not present them explicitly. In these expansions we have inserted a common factor (somehow perturbation parameter) to each u_i first and then expanded the resulted expression in that factor's natural number powers and finally set that factor equal to 1 at its every appearence.

Now we can write the following formula for the constant HDMR component by using the Cauchy product with respect to above mentioned dummy perturbation parameter

$$f_0(\mathbf{u},\alpha)=\int_0^1 dy_1\cdots\int_0^1 dy_N\sum_{j=0}^{\infty}\frac{1}{j!}\sum_{k=0}^{j}\binom{j}{k}\left[\mathscr{D}_{\alpha}^{k}W(\mathbf{u},\alpha)\right]\left[\mathscr{D}_{\alpha}^{j-k}f(\alpha)\right] \quad (17)$$

where

$$W(\mathbf{u},\alpha)=\prod_{i=1}^{N}u_i W_i(\alpha_i) \quad (18)$$

Following expressions can be obtained for the univariate components

$$f_\ell(\mathbf{u},\alpha)=\int_0^1 dy_1\ldots\int_0^1 dy_{\ell-1}\int_0^1 dy_{\ell+1}\ldots\int_0^1 dy_N\sum_{j=0}^{\infty}\frac{1}{j!}\sum_{k=0}^{j}\binom{j}{k}$$
$$\times\left[\mathscr{D}_{\alpha}^{k}W^{(\ell)}(\mathbf{u},\alpha)\right]\left[\mathscr{D}_{\alpha}^{j-k}f(\alpha)\right]-f_0,\qquad \ell=1,\ldots,N \quad (19)$$

where we have used the following shorthand notation despite it does not contain α_ℓ

$$W^{(\ell)}(\mathbf{u},\alpha)\equiv\left[\prod_{\substack{i=1\\ i\neq\ell}}^{N}u_i W(\alpha_i)\right] \quad (20)$$

3.2 Truncations for constant and univariate components

Even though these are exact expansions as long as the convergence exists we may prefer the following truncations for numerical applications

$$f_0(\mathbf{u},\alpha)=\int_0^1 dy_1\cdots\int_0^1 dy_N\sum_{j=0}^{n}\frac{1}{j!}\sum_{k=0}^{j}\binom{j}{k}\left[\mathscr{D}_{\alpha}^{k}W(\mathbf{u},\alpha)\right]\left[\mathscr{D}_{\alpha}^{j-k}f(\alpha)\right] \quad (21)$$

$$f_\ell(\mathbf{u},\alpha)=\int_0^1 dy_1\ldots\int_0^1 dy_{\ell-1}\int_0^1 dy_{\ell+1}\ldots\int_0^1 dy_N\sum_{j=0}^{n}\frac{1}{j!}\sum_{k=0}^{j}\binom{j}{k}$$

$$\times \left[\mathscr{D}_{\alpha}^{k} W^{(\ell)} (\mathbf{u}, \alpha) \right] \left[\mathscr{D}_{\alpha}^{j-k} f (\alpha) \right] - f_0, \qquad \ell = 1, \ldots, N \tag{22}$$

The higher multivariate terms can be expanded by using the above approach. However our basic tendency is to accomplish to catch high quality truncations without climbing to the terms beyond the univariate components. Hence we find this information sufficient to this end.

Formulation given in (21) and (22) for the constant and univariate HDMR components can be called "Small Scale HDMR (SSHDMR)" when it is used for lower number of terms. The basic tendency is to use the leading terms although it is possible to keep the higher powers of us as the size of geometry is not sufficiently small.

3.3 Constancy behavior at zero geometry limit

The inner product of two arbitrary functions, $f(\mathbf{x})$ and $g(\mathbf{x})$ in the Hilbert space where the target function and its HDMR component lie is defined as follows

$$(f, g) \equiv \int_{a_1}^{b_1} dx_1 \ldots \int_{a_N}^{b_N} dx_N W(\mathbf{x}) f(\mathbf{x}) g(\mathbf{x}) \tag{23}$$

which permits us to define the norm of a function in the above mentioned Hilbert space as follows

$$\|f\| \equiv (f, g)^{\frac{1}{2}} \tag{24}$$

The mutual orthogonality of the HDMR components for a target function $f(x_1, \ldots, x_N)$ urges us to define the following parameters

$$\begin{aligned}
\sigma_0 &\equiv \frac{\|f_0\|^2}{\|f\|^2} \\
\sigma_1 &\equiv \sigma_0 + \sum_{i=1}^{N} \frac{\|f_i\|^2}{\|f\|^2} \\
\sigma_2 &\equiv \sigma_1 + \sum_{\substack{i_1, i_2 = 1 \\ i_1 < i_2}}^{N} \frac{\|f_{i_1, i_2}\|^2}{\|f\|^2} \\
&\vdots
\end{aligned} \tag{25}$$

where we have not explicitly shown the arguments of components, as we did in the definitions of inner product and norm, since those are dummy integration variables of the integrals in the norms. We call σ parameters which are in fact functionals "Additivity Measurers" or equivalently "Quality Measurers". We use the word "Additivity" since

they measure the cumulative percentages of relevant terms' norm squares in an additive decomposition. We prefer to use "measurer" instead of "measure" to emphasize on their verbal actions, not the values they produce. These entities are well-ordered and satisfy the following inequalities

$$0 \leq \sigma_0 \leq \sigma_1 \leq \cdots \leq \sigma_N = 1. \tag{26}$$

We call σ_0 "Constancy Measurer" or sometimes more briefly just "Constancy". Similarly, σ_1 can be called "Univariance Measurer" or more briefly just "Univariance" as long as it does not lead some misunderstandings or confusions.

Well-orderedness of the quality measurers implies that all higher indexed σs will be much closer to 1 as the constancy approaches 1. Hence, it is an important issue to investigate first the behavior of constancy to estimate the HDMR's truncation approximant qualities. Especially it will be a good action to get the behavior of the constancy at the zero geometry limit. To this end we need it to evaluate the norm square of the target function. We can write

$$\begin{aligned} \|f(\mathbf{u},\alpha)\|^2 = & \int_0^1 dy_1 \cdots \int_0^1 dy_N \sum_{j=0}^{\infty} \frac{1}{j!} \sum_{k=0}^{j} \binom{j}{k} \\ & \times \left[\mathscr{D}_{\alpha}^{k} W(\mathbf{u},\alpha) \right] \left[\mathscr{D}_{\alpha}^{j-k} \left(f(\alpha)^2 \right) \right] \end{aligned} \tag{27}$$

where the dependence of f on y variables is not explicitly shown. This equality implies that

$$\left\{ \|f(\mathbf{u},\alpha)\|^2 \right\}_{\mathbf{u}\to\mathbf{0}} = \{W(\mathbf{u},\alpha)\}_{\mathbf{u}\to\mathbf{0}} f(\alpha)^2 = f(\alpha)^2 \tag{28}$$

where we have used the following equality

$$\int_{a_i}^{b_i} dx_i W_i(x_i) = 1 \implies \int_0^1 dy_i u_i W_i(u_i y_i + \alpha_i) = 1 \implies \{u_i W_i(\alpha_i)\}_{u_i \to 0} = 1 \tag{29}$$

which means

$$\{W(\mathbf{u},\alpha)\}_{\mathbf{u}\to\mathbf{0}} = 1 \tag{30}$$

whose utilization in (17) gives

$$\{f_0(\mathbf{u},\alpha)\}_{\mathbf{u}\to\mathbf{0}} = f(\boldsymbol{\alpha}). \tag{31}$$

As can be noticed easily σ_0 depends on both $\mathbf{u}$ and α. Its definition enables us to get the following limiting relation

$$\{\sigma_0(\mathbf{u},\alpha)\}_{\mathbf{u}\to\mathbf{0}} = 1. \tag{32}$$

This is the mathematical expression of the following statement: "The constancy dominancy in norm square approaches hundred percent at the zero size geometry limit". In other words, the constancy in the target function's HDMR expansion dominates. This is, of course, a pleasent fact facilitating the simple utilization of HDMR expansion; truncating at constancy level allows us to get high approximation quality at sufficiently small scale HDMRs.

4 Combined small scale high dimensional model representation (CSSHDMR)

Small Scale HDMR (SSHDMR) alone may not be so practical since almost all of the applications are relevant to geometries whose sizes are beyond the zero value. However, this does not mean that the utilization of SSHDMR is completely impractical. We can divide the entire HDMR geometry to sufficiently large number of subgeometries and then apply the SSHDMR to the target function for each individual sub geometry. Of course, the size of each geometry will not be zero since we prefer to use finite number of subgeometries. This means that the unit constancy may not be obtained in each subgeometry if we use just constant truncations. However, it is possible to go beyond the constancy in some or all subgeometries depending on the nature of the target function. The univariate or higher variate terms will contain integrals over the multinomials of y variables and there fore be performed analytically even though the number of the terms will increase. So the choosing optimum number of subgeometries with optimum sizes is based on good experience and insights about the target function. We prefer to use sufficiently small geometries enabling us to use only constancy. However this creates a multidimensional spline structure in the resulting piecewise expression for the HDMR truncation such that the constant values result in discontinuities at the border hypersurfaces of the subgeometries. This discontinuities can be softened by using univariance and higher variances even though we do not intend to get into the details of these issues.

4.1 Formulation

To formulate the HDMR approximants mentioned above we can define the following subintervals

$$[\,a_i, b_i\,] = \bigcup_{j_i=1}^{n_i} \mathscr{I}_{i,j_i}, \qquad \mathscr{I}_{i,j_i} \equiv \left[\,\alpha_{i,j_i-1}, \alpha_{i,j_i}\,\right], \qquad j_i = 1, 2, \ldots, n_i,$$
$$i = 1, 2, \ldots, N; \qquad \alpha_{i,0} = a_i, \qquad \alpha_{i,n_i} = b_i, \qquad i = 1, 2, \ldots, N \tag{33}$$

We can denote a truncated SSHDMR of a given multivariate function $f\,(x_1, \ldots, x_N)$ on the following rectangular hyperprismatic region

$$\mathscr{V}_{j_1,\ldots,j_N} \equiv \mathscr{I}_{1,j_1} \times \cdots \times \mathscr{I}_{N,j_N}, \qquad j_i = 1, 2, \ldots, n_i, \;\; i = 1, 2, \ldots, N. \tag{34}$$

by $f^{(approx)}_{j_1,\ldots,j_N}$ and then the combined approximant which is defined on the union of $\mathscr{V}$s can be expressed as follows

$$\begin{aligned} &f\left(x_1,\ldots,x_N\right) \approx f_{app}\left(x_1,\ldots,x_N\right); \\ &f_{app}\left(x_1,\ldots,x_N\right) = f^{(approx)}_{j_1,\ldots,j_N}, \qquad \mathbf{x} \in \mathscr{V}_{j_1,\ldots,j_N}, \qquad j_i = 1,\ldots,n_i, \;\; i = 1,\ldots,n \end{aligned} \tag{35}$$

which is apparently a piecewise approximant such that it remains continuous inside each subgeometry. Discontinuity can appear only at the borders of the relevant subgeometry. It is expected to be highest level when SSHDMR kept at the constant level. To soften the discontinuity one way is to increase the multivariance in the truncations while the other uses the size reduction in the SSHDMRs by highly populating them.

The geometry partitioning mentioned above somehow recalls the widely used "Finite Element Method" which partitions the integration domain into integrals over subgeometries of the entire integration domain. It combines various SSHDMRs to get the total representation of the target function. Hence we call this approach "Combined SSHDMR (CSSHDMR)". Finite element methods are used at most over three dimensional geometries despite there have been certain at tempts to use it in higher dimensions. This is because practical applications in engineering are in this way. However various branches of sciences like quantum dynamics involve more than three dimensional geometries. This work focuses on basics of the issue only.

5 Illustrative numerical implementations

In this section we present some illustrative CSSHDMR implementations on certain test functions to support our ideas. Although we have previously taken attention to the implications for using above mentioned additivity or quality measurers to estimate the errors in norm square, combined nature of the CSSHDMR algorithm urges us to use well-known standard error definitions instead of quality measurers. One way to this end is to use Euclidean distance between the true function and its approximation in the relevant Hilbert space of functions where the target multivariate function resides. We define

$$E \equiv \left\| f\left(\mathbf{u},\boldsymbol{\alpha}\right) - f_{app}\left(\mathbf{u},\boldsymbol{\alpha}\right) \right\|^2 \tag{36}$$

which can be additively disintegrated to the norm squares on individual subgeometries. These individual norm squares are proportional to the deviation of constancy from 1. Hence the Euclidean distance based error definition is not so different from the constancy measurer utilization. In fact if we would use the relative error defined as the ratio of the above mentioned Euclidean distance to the square of the target function at the midpoint of the subgeometry, then the result would be the cumulative constancy measurer deviations from 1 as long as the constant truncations are used.

Table 1 shows the cumulative errors (Es) in the constant and univariate CSSHDMR for the function $f\left(x_1,x_2,x_3\right) = \left(x_1+x_2+x_3\right)^{10}$. This is just one example from a set of multivariate functions whose general term can be given as

$$f(x_1, \ldots, x_N) = (x_1 + \cdots + x_N)^m \tag{37}$$

where the numbers N and m are considered as positive integers. Hence this is the general term of multinomials. For $m = 1$ this function is purely additive, that is, the sum of univariate functions. When m is taken equal to 2, it involves not only univariate but also bivariate terms. The case where $m = 3$ adds the trivariate components and as m increases much higher multivariances are added to the expansion of the multinomial. N and m parameters take the values 3 and 10 respectively, in Table 1. The increasing m values cause growing curvature values and the steepness in the ascending (or descending) values of the function especially around the point where all x variables take the value of 1.

In Table 1 we use the equally distributed nodal points over the unit intervals [0, 1] for each independent variable. This might be increasing the errors because of the steep climbing (or steep fall) of the function when the corner (1, 1, 1) is approached from the interior region encapsulated by the unit cube. Hence one can use variable length subintervals to increase the efficiency of CSSHDMR. We do not report anything over inequal subintervals here.

As can be noticed immediately the cumulative errors diminish in Table 1 as the number of the subcubes increases. This shows the success of the CSSHDMR for this chosen function.

Error tabulation is not the only way to show how precise the HDMR truncations are. Even though it results in a deeper understanding of the quality of the approximants, the plotting of the true functions and the approximants gives the chance of rather rough but easily realizable comparisons. However the latter case is more restricted since the envisualization of functions containing more than two variables via plotting may become inefficient because even the three dimensional figures can describe at most bivariate functions. This restriction is not impossibility and somehow projecting the variations of the multivariate functions over their domains onto a real line via an ordering index can make it possible to have planar figures.

Indexing we mention here is in fact a correspondence rule. We exemplify this approach for the case of three independent variables. Our purpose is to construct a

Table 1 Euclidean distance squares errors at different number of sub-regions for $f(x_1, x_2, x_3) = (x_1 + x_2 + x_3)^{10}$

Sub-regions	Constant approximant	Univariate approximant
2^3	5.3×10^6	2.1×10^6
10^3	4.5×10^4	7.6×102
50^3	8.1×10^1	5.3×10^{-2}
100^3	5.1	8.3×10^{-4}
500^3	8.1×10^{-3}	5.3×10^{-8}
$1{,}000^3$	5.1×10^{-4}	8.2×10^{-10}
$2{,}000^3$	3.0×10^{-5}	3.7×10^{-10}
$3{,}000^3$	6.0×10^{-6}	6.7×10^{-13}

relation between finite sets. This urges us to discretize the intervals of independent variables. This means that the evaluations are not performed for all points of the intervals. Only finite number of selected points (nodes) are used to this end. So each node in each interval is accompanied by an index which takes finitely many integer values. Hence, each nodal point in the three dimensional space is specified by a triple of integers. Then to project these triples onto a line is just a matter of ordering of the triples. This should be done in a one-to-one correspondence. If we consider the case where each interval contains just three nodes then the number of the triples is 27. We can use the following correspondence to be able to use just a single index

$$
\begin{array}{lll}
1 \to (0,0,0) & 2 \to (0,1,0) & 3 \to (0,2,0) \\
4 \to (1,0,0) & 5 \to (1,1,0) & 6 \to (1,2,0) \\
7 \to (2,0,0) & 8 \to (2,1,0) & 9 \to (2,2,0) \\
10 \to (0,0,1) & 11 \to (0,1,1) & 12 \to (0,2,1) \\
13 \to (1,0,1) & 14 \to (1,1,1) & 15 \to (1,2,1) \\
16 \to (2,0,1) & 17 \to (2,1,1) & 18 \to (2,2,1) \\
19 \to (0,0,2) & 20 \to (0,1,2) & 21 \to (0,2,2) \\
22 \to (1,0,2) & 23 \to (1,1,2) & 24 \to (1,2,2) \\
25 \to (2,0,2) & 26 \to (2,1,2) & 27 \to (2,2,2)
\end{array}
$$

If the single numbers in the correspondence on this table, from 1 to 27 are indicated by i then there will be different node values for different i's. One can plot the f values on the nodes of above table versus corresponding i values. In this plotting i values are ordered on the horizontal axis while the f values at the corresponding nodes are ordered on the vertical axis. Then the above correspondences in the table produces 27 points in the plotting plane. Then by joining neighbor planar points by straight line segments we can obtain broken line plots. The increasing number of planar points (that is, the number of nodes) results in better quality graphics.

This scheme is quite appropriate for the CSSHDMR when constant truncations are used since only the function values at the center of the subgeometries are needed. The following figures are prepared in this way. Figure 1 is designed for the application of CSSHDMR on the function in (37) when $m = 10$ and $N = 3$. This function is far beyond being additive because of the high exponentiation. It can be considered as rather simple but close to multiplicative functions. Hence it may be a good focus to be investigated for better under standing the efficiency of CSSHDMR on multiplicative functions. Figure 1 contains Zeroth Order Approximant (SSHDMR constant compo nents) and First Order Approximant (SSHDMR univariate component) of CSSHDMR at 10^3 subgeometries. These approximants are compared with First Order (Univariate) Approximant of HDMR and also original test function. According to the results it seems to be insufficient to divide every interval into 10 subintervals for this test function not only in the Constant Approximant but also First Order Approximant utilization. In such problematic cases there are different possibilities for maximizing approximation quality. Increasing truncation level of perturbation expansion, increasing components of CSSHDMR are optional ways. However they also raise the algebraic complexity. So it is reasonable increasing number of subgeometries, because in this way even if the number of calculations increase we do the same calculations for each subregion

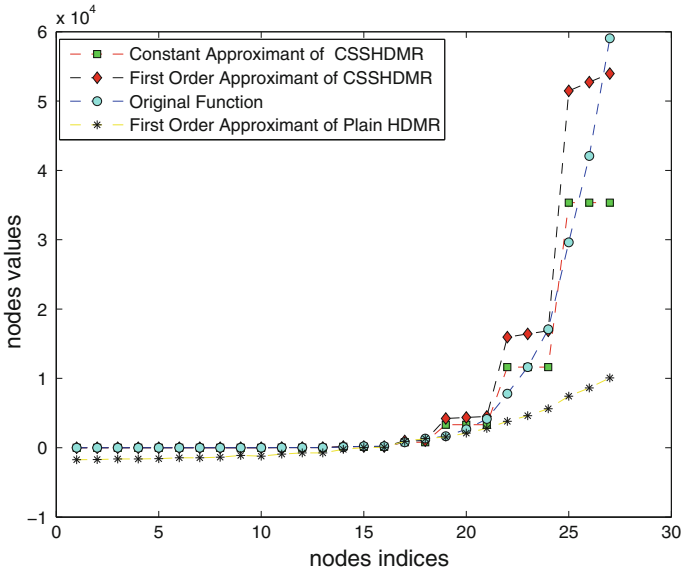

Fig. 1 HDMR versus CSSHDMR at 10^3 for $f(x_1, x_2, x_3) = (x_1 + x_2 + x_3)^{10}$

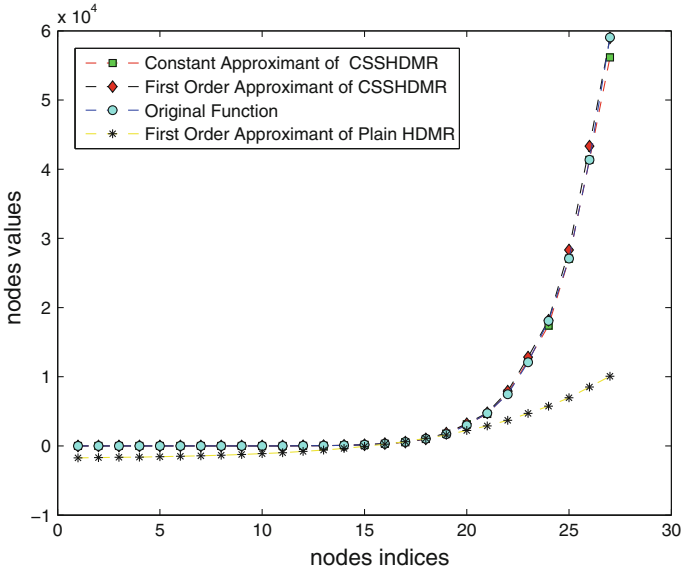

Fig. 2 HDMR versus CSSHDMR at 100^3 for $f(x_1, x_2, x_3) = (x_1 + x_2 + x_3)^{10}$

within same simplicity, so it is a good way to avoid complicated forms which come from the calculation of higher variate terms of CSSHDMR.

Figure 2 shows the results of 100^3 subregions. Both Constant and First Order Approximants are successful at approximation, so the values of the results are

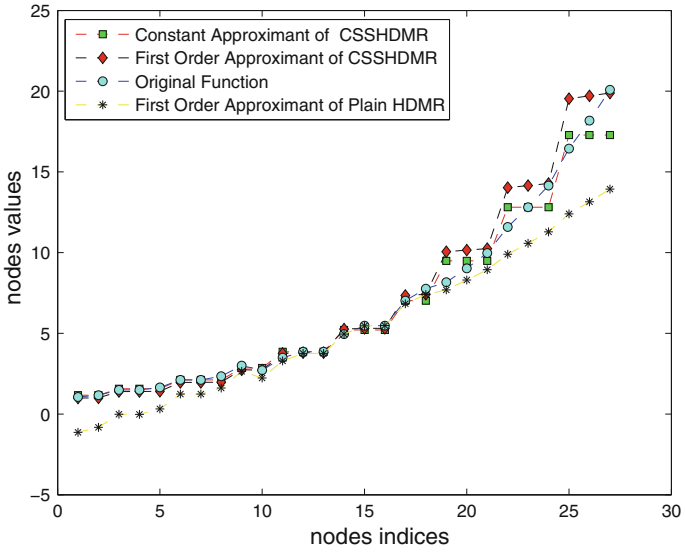

Fig. 3 HDMR versus CSSHDMR at 10^3 subgeometries for $f\,(x_1, x_2, x_3) = \mathrm{e}^{(x_1+x_2+x_3)}$

appearing overlapped, but plain HDMR gives results under the average and can't represent the function.

The above test function has a hybrid structure having both additive and multiplicative characters, so we chose exponential function to see the effectiveness of the present method on completely multiplicative functions.

$$f\,(x_1, x_2, x_3) = \mathrm{e}^{(x_1+x_2+x_3)} \tag{38}$$

Number of subregions are same as previous examples, 10^3 and 100^3. Unlike the previous example for 100^3 the original function and CSSHDMR approximants are overlapping because curvature of the previous test function much higher than this exponential function. Although Fig. 3 shows a weak quality approximation, Fig. 4 with 100^3 subregions shows a successful representation.

Another test function we take into account is a periodic function

$$f\,(x_1, x_2, x_3) = \sin 10\,(x_1 + x_2 + x_3) \tag{39}$$

which is defined at $[\,0, 1\,] \times [\,0, 1\,] \times [\,0, 1\,]$. To have a high periodic structure we get frequency multiplier as 10. As expected 10^3 subregions does not suffice for a successful approximation. Figure 5 displays the results of 27 chosen nodes for 10^3 subgeometries. Accord ing to the results Constant Approximant of CSSHDMR is weaker than First Order Approximant. The use of more subregions provides us accurate results, though second try on this test function is for 100^3 and gives more accurate results as shown in Fig. 6.

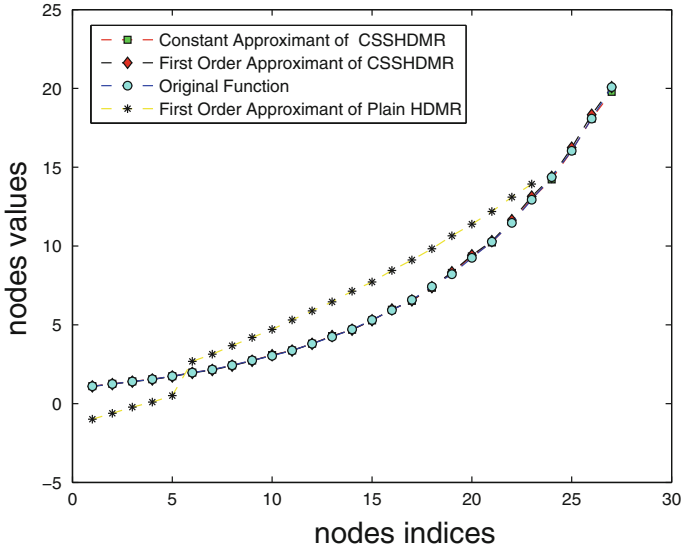

Fig. 4 HDMR versus CSSHDMR at 100^3 for $f\,(x_1, x_2, x_3) = \mathrm{e}^{(x_1+x_2+x_3)}$

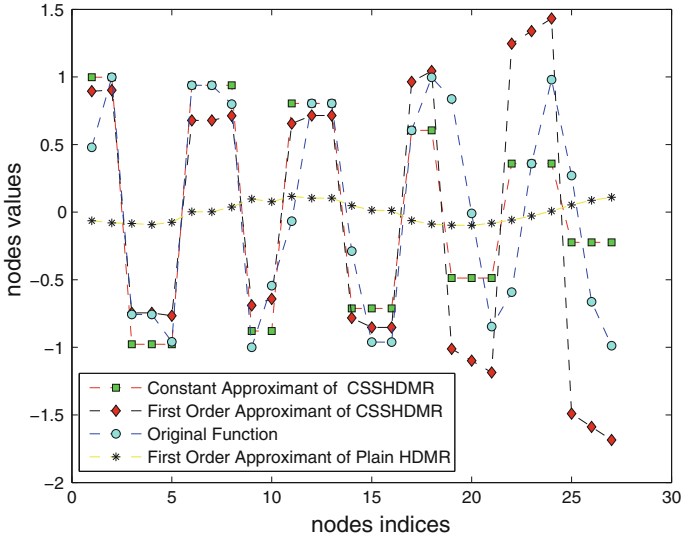

Fig. 5 HDMR versus CSSHDMR at 100^3 for $f\,(x_1, x_2, x_3) = \sin 10\,(x_1 + x_2 + x_3)$

6 Concluding remarks

The main purpose of this work has been to add another divide-and-conquer philosophy to HDMR to be able to get higher qualities in the utilization of "Constant" or at most "Univariate" truncations. To this end first we have observed the nature of the HDMR truncations when the size of the HDMR geometry tends to vanish. What we have found

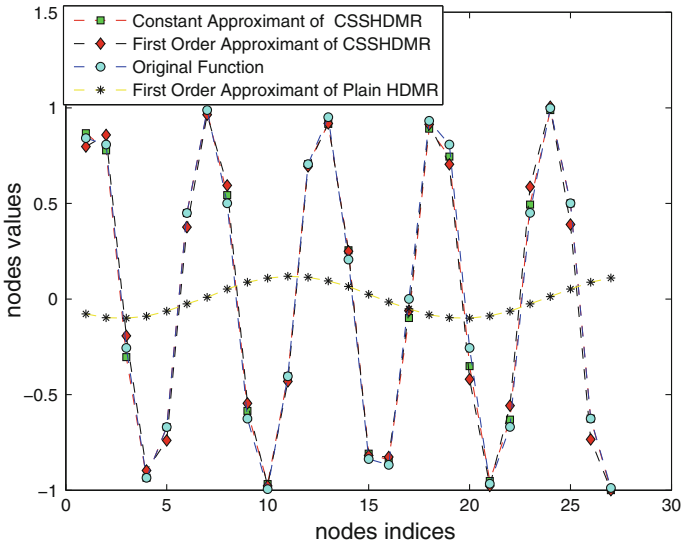

Fig. 6 HDMR versus CSSHDMR at 100^3 for $f\,(x_1, x_2, x_3) = \sin 10\,(x_1 + x_2 + x_3)$

interesting has been the limiting form of constancy. It approaches 1 when the size of the geometry vanishes. This has motivated to construct HDMRs over small geometries. We have divided the whole domain to sufficiently small subgeometries. Then the HDMRs constructed on each individual subgeometry are combined to a single piecewise representation, CSSHDMR. We enumerate the important aspects below:

1 Even though we have used at most univariate truncations it is possible to use higher variate terms at the expense of increasing computational complexity;
2 We have used the limiting forms of HDMR components which are in fact perturbation expansions in unidirectional size parameters, us;
3 The important issues are the selection of most efficient number of perturbative terms and the number of the subgeometries;
4 CSSHDMR may work on nonorthogonal geometries as long as the appropriate partitionings to orthogonal subgeometries can be constructed;
5 CSSHDMR may also be utilized on the nonproduct type weight functions as long as the sufficient care is paid to the individual SSHDMRs by preventing the negativities coming from the nonproduct character in the local behaviors of the weight functions;
6 There seem to be existing certain optimisation possibilities to suppress the deviations in the piecewise representations when passing through from a subgeometry to its closest neighbors.

Acknowledgments The second author is grateful to Turkish Academy of Sciences, where he is a principal member, for its support and motivation.

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