On Quartic Transformational High Dimensional Model Representation

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Abstract. This work focuses on the development of a multivariate function approximating method by using quartic Transformational High Dimensional Model Representation (THDMR). The method uses the target function's image under a quartic transformation for High Dimensional Model Representation(HDMR) instead of the function's itself.

Keywords: Quartic Equation, Transformational High Dimensional Model Reprsentation, Multivariate Functions
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INTRODUCTION

Various HDMR versions were suggested in order to tackle with different problem types encountered. Factorized HDMR is one of them. The main problem with FHDMR is that unlike additivity measures of HDMR, multiplicativity measures of FHDMR is not well ordered. This led to the idea of logarithmic HDMR. The main idea behind Logarithmic HDMR was to initially transform what is basically a function of multiplicative nature to one that is of additive nature. This would enable us to expand the transformed problem using plain HDMR and then transform back the individual terms. Previous works were focused on the HDMR constancy optimization under an affine transformation[1, 2] and a conic transformation[3]. We shall consider in this work a quartic transformation and attempt to find optimal parameters for such a transformation leading to a new approximation.

TRANSFORMATIONAL HIGH DIMENSIONAL MODEL REPRESENTATION

Let us consider a function $f(x_1,...,x_N)$ of N independent variables $x_1,x_2,...,x_N$ which has a non-additive structure. A transformation T can be chosen which yields a new multivariate function $\varphi_j(x_1,...,x_N)$.

$$Tf(x_1,...,x_N)=\varphi(x_1,...,x_N) \tag{1}$$

If we apply the HDMR expansion to φ we will get $\varphi(x_1,...,x_N)=\varphi_0+\sum_{\beta=1}^{N}\varphi_\beta(x_\beta)+\cdots+\varphi_{1...N}(x_1,...,x_N)$. Additivity measurers $\sigma_1(\varphi)$s can be defined for this expansion in the usual HDMR manner.

$$\sigma_0(\varphi)=\frac{\|\varphi_0\|^2}{\|\varphi\|^2},\qquad \sigma_1(\varphi)=\sigma_0(\varphi)+\sum_{\beta_1=1}^{N}\frac{\|\varphi_{\beta_1}\|^2}{\|\varphi\|^2},\qquad \sigma_2(\varphi)=\sigma_1(\varphi)+\sum_{\substack{\beta_1,\beta_2=1\\ \beta_1<\beta_2}}^{N}\frac{\|\varphi_{\beta_1,\beta_2}\|^2}{\|\varphi\|^2},\ \cdots \tag{2}$$

These measures will be different from those obtained by applying HDMR expansion to the original function f. Obviously the difference will be dependent on the specific choice of the transformation T . Since the basic philosophy of HDMR is to be able to represent the function with as few and as less variate terms as possible, we would prefer σ_0 and σ_1 to be as close to 1 as possible. In this study we choose to deal only with σ_0 and attempt to maximize it.

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QUARTIC TRANSFORMATIONAL HIGH DIMENSIONAL MODEL REPRESENTATION

A polynomial can be used as THDMRâĂŹs operator for choosing the transformation suggested in (1). Here the degree of the polynomial will be taken to be four. The linear combination coefficients of the quartic will be assumed to vary with independent variables. They will be regarded as operators dependent on the algebraic operators each of which multiplies its operand with a different independent variable. This gives flexibility to the relevant transformation and they can be selected so as to approximate the HDMR expansion optimally. Since only $\sigma_0(\varphi)$ will be under consideration, φ will be approximated by the constant component φ_0

$$Tf(x_1,...,x_N) = \varphi(x_1,...,x_N) = a_0(x_1,...,x_N) + a_1(x_1,...,x_N) f + \cdots + a_4(x_1,...,x_N) f^4 = \varphi_0$$

which gives the approximate equality

$$f_1 = \frac{a_3}{4a_4} - \frac{1}{2}\sqrt{\frac{a_3^2}{4a_4^2} - \frac{2a_2}{3a_4} + \frac{2^{\frac{1}{3}}p}{3a_4\left\{q+\sqrt{-4p^3+q^2}\right\}^{\frac{1}{3}}} + \frac{\left\{q+\sqrt{-4p^3+q^2}\right\}^{\frac{1}{3}}}{2^{\frac{1}{3}}3a_4}}$$
$$-\frac{1}{2}\sqrt{\left(\frac{a_3^2}{2a_4^2} - \frac{4a_2}{3a_4} - \frac{2^{\frac{1}{3}}p}{3a_4\left\{q+\sqrt{-4p^3+q^2}\right\}^{\frac{1}{3}}} - \frac{\left\{q+\sqrt{-4p^3+q^2}\right\}^{\frac{1}{3}}}{2^{\frac{1}{3}}3a_4} - \right.}$$
$$\left.\left(-\frac{a_3^3}{a_4^3} + \frac{4a_3a_2}{a_4^2} - \frac{8a_1}{a_4}\right) \Big/ \left(4\sqrt{\frac{a_3^2}{4a_4^2} - \frac{2a_2}{3a_4} + \frac{2^{\frac{1}{3}}p}{3a_4\left\{q+\sqrt{-4p^3+q^2}\right\}^{\frac{1}{3}}} + \frac{\left\{q+\sqrt{-4p^3+q^2}\right\}^{\frac{1}{3}}}{2^{\frac{1}{3}}3a_4}}\right)\right) \quad (3)$$

where

$$p = a_2^2 - 3a_3a_1 + 12a_4(a_0 - \varphi_0),$$
$$q = 2a_2^3 - 9a_3a_2a_1 + 27a_4a_1^2 + 27a_3^2(a_0 - \varphi_0) - 72a_4a_2(a_0 - \varphi_0).$$

In this work we will consider only f_1. The other roots may be considered analogically. The aim here is to find convenient forms for a_0, a_1, a_2, a_3 and a_4 that maximize σ_0 in (3). To this end a_0, a_1, a_2, a_3 and a_4 will be taken in L^2 class. Hence orthonormal basis of the Hilbert space $H^{(N)}$ will be taken into consideration. Orthonormality will be defined $(u_j,u_k) = \int_V dVW(x_1,...,x_N)u_j(x_1,...,x_N)u_k(x_1,...,x_N) = \delta_{jk}$, $1 \le j,k \le \infty$; where $V = [a_1,b_1]\times\cdots\times[a_N,b_N]$ represents the hyperprism which is the HDMR construction domain and $W(x_1,...,x_N)$ the multiplicative weight function used in HDMR. The individual weight functions will be chosen as constants, normalized over the corresponding domain and dV is the product of individual differentials $dx_1...dx_N$.

Although the basis mentioned above has an infinite number of elements, in practice a finite number of elements will be taken into consideration. Therefore φ can be expressed as

$$\varphi(x_1,...,x_N) = \sum_{j=2}^{m} a_j^{(0)}u_j\left(\sum_{k=1}^{n} a_k^{(1)}u_k\right)f + \left(\sum_{l=1}^{p} a_l^{(2)}u_l\right)f^2 + \left(\sum_{s=1}^{t} a_s^{(3)}u_s\right)f^3 + \left(\sum_{v=1}^{z} a_v^{(4)}u_v\right)f^4 \quad (4)$$

To obtain the constant HDMR term φ_0 both sides of (4) are to be integrated with respect to x_1,...,x_N over V under the weight function W. We define vectors η and μ. The elements of vector μ are defined as

$$\mu_j^{(0)} = \int_V dV\left(\prod_{\beta=1}^{N} W_\beta(x_\beta)\right)u_j = (u_j,h), \quad \mu_k^{(1)} = \int_V dV\left(\prod_{\beta=1}^{N} W_\beta(x_\beta)\right)u_j = (u_j,h)...\text{etc}$$

$h(x_1,...,x_N)$ appearing in the first inner product is a function which has the constant value 1 for all x_β in the first inner product is a function which has the constant value 1 for all x_βs in the hyperprism domain $[a_1,b_1]\times\cdots\times[a_N,b_N]$. φ_0

can now be written as inner product $\varphi_0 = \eta^T \mu$. Since φ_0 has a constant value, the square of its norm will be equal to the square of the function φ_0. $\|\varphi_0\|^2 = |\eta\mu|^2 = \eta^T \mu\mu^T \eta$. $\|\varphi\|^2$ on the other hand can be expressed in terms of the above defined vector η and a square matrix $\mathbf{A}$ which can be expressed in terms of its blocks as

$$\mathbf{A} \equiv \begin{bmatrix} \mathbf{K} & \mathbf{L} & \mathbf{N} & \mathbf{S} & \mathbf{B} \\ \mathbf{L}^T & \mathbf{M} & \mathbf{P} & \mathbf{T} & \mathbf{C} \\ \mathbf{N}^T & \mathbf{P}^T & \mathbf{R} & \mathbf{Y} & \mathbf{D} \\ \mathbf{S}^T & \mathbf{T}^T & \mathbf{Y}^T & \mathbf{Z} & \mathbf{F} \\ \mathbf{B}^T & \mathbf{C}^T & \mathbf{D}^T & \mathbf{F}^T & \mathbf{G} \end{bmatrix}$$

$K_{jk} \equiv (u_j, u_k),\ 2 \le j,k \le m,\ L_{jk} \equiv (u_j, f u_k),\ 2 \le j \le m,\ 1 \le k \le n,\ M_{jk} \equiv \left(u_j, f^2 u_k\right),\ 1 \le j,k \le n,$
$N_{jk} \equiv \left(u_j, f^2 u_k\right),\ 2 \le j \le m,\ 1 \le k \le p,\ P_{jk} \equiv \left(u_j, f^3 u_k\right),\ 1 \le j \le n,\ 1 \le k \le p,$
$R_{jk} \equiv \left(u_j, f^4 u_k\right),\ 1 \le j,k \le p,\ S_{jk} \equiv \left(u_j, f^3 u_k\right),\ 2 \le j \le m,\ 1 \le k \le t,$
$T_{jk} \equiv \left(u_j, f^4 u_k\right),\ 1 \le j \le n,\ 1 \le k \le t,\ Y_{jk} \equiv \left(u_j, f^5 u_k\right),\ 1 \le j \le p,\ 1 \le k \le t,\ Z_{jk} \equiv \left(u_j, f^6 u_k\right),\ 1 \le j,k \le t,$
$B_{jk} \equiv \left(u_j, f^4 u_k\right),\ 2 \le j \le m, 1 \le k \le z,\ C_{jk} \equiv \left(u_j, f^5 u_k\right),\ 1 \le j \le n,\ 1 \le k \le z,$
$D_{jk} \equiv \left(u_j, f^6 u_k\right),\ 1 \le j \le p,\ 1 \le k \le z,\ F_{jk} \equiv \left(u_j, f^7 u_k\right),\ 1 \le j \le t,\ 1 \le k \le z,\ G_{jk} \equiv \left(u_j, f^8 u_k\right),\ 1 \le j,k \le z,$

$\mathbf{A}$ is a symmetric, positive definite matrix. Norm square of φ can be expressed in terms of $\mathbf{A}$ and η as $\|\varphi\|^2 = \eta^T \mathbf{A} \eta$. So the constancy measurer σ_0 becomes $\sigma_0 = \eta^T \mu\mu^T \eta / \eta \mathbf{A} \eta$. Our aim is to maximize σ_0 which can be written as a Rayleigh quotient as $\left(\mathbf{y}^T \mathbf{A}^{-1/2} \mu\mu^T \mathbf{A}^{-1/2} \mathbf{y}\right) / (\mathbf{y} T \mathbf{y})$ where $\mathbf{y} \equiv \mathbf{A}^{1/2} \eta$. However, a Rayleigh quotient takes its maximum value at the maximum eigenvalue of its kernel, in this case $\mathbf{A}^{-1/2} \mu\mu^T \mathbf{A}^{-1/2}$. Similarly $\mathbf{y}$ is the eigenvector corresponding to the maximum eigenvalue. An analysis of the kernel will give the maximum eigenvalue and the corresponding eigenvector of it. They are respectively, $\sigma_0 = \mu^T \mathbf{A}^{-1} \mu$, $\mathbf{y} = \mathbf{A}^{-1/2} \mu$. The equation for $\mathbf{y}$ gives us the vector η that maximizes σ_0 as $\eta = \mathbf{A}^{-1/2} \mathbf{y} = \mathbf{A}^{-1} \mu$. Utilizing these equalities we can construct a function for φ_0. To complete this we can express φ_0, a_0, a_1, a_2, a_3, and a_4 in terms of matrix algebraic entities. φ_0 can be written in compact form as $\varphi_0 = \eta^T \mu = \mu^T \mathbf{A}^{-1} \mu$. We define a vector ξ with $\xi = [\xi_2 \ldots \xi_m\ \xi_1 \ldots \xi_p\ \xi_1 \ldots \xi_t\ \xi_1 \ldots \xi_z]^T$ and express a_0, a_1, a_2, a_3, and a_4 more compactly as $a_0 = \eta^{(0)^T} \xi^{(0)}$, $a_1 = \eta^{(1)^T} \xi^{(1)}$, $a_2 = \eta^{(2)^T} \xi^{(2)}$, $a_3 = \eta^{(3)^T} \xi^{(3)}$, $a_4 = \eta^{(3)^T} \xi^{(4)}$.

Here the vectors $\eta^{(0)}$, $\eta^{(1)}$, $\eta^{(2)}$, $\eta^{(3)}$, $\eta^{(4)}$ and $\xi^{(0)}$, $\xi^{(1)}$, $\xi^{(2)}$, $\xi^{(3)}$, $\xi^{(4)}$ are explicitly defined as

$$\eta^{(0)} = \left[a_2^{(0)} \ldots a_m^{(0)}\right]^T, \ldots, \eta^{(4)} = \left[a_1^{(4)} \ldots a_z^{(4)}\right]^T;\ \ \xi^{(0)} = [\xi_2 \ldots \xi_m]^T, \ldots, \xi^{(4)} = [\xi_1 \ldots \xi_z]^T;$$

To proceed we define $(m+n+p+t+z-1) \times (m+n+p+t+z-1)$ projection matrices $\mathbf{P}_1$, $\mathbf{P}_2$, $\mathbf{P}_3$ and $\mathbf{P}_4$ as

$$\mathbf{P}_1 = \sum_{\beta=1}^{m-1} \mathbf{e}_\beta \mathbf{e}_\beta^T, \qquad \mathbf{P}_2 = \sum_{\beta=1}^{m+n-1} \mathbf{e}_\beta \mathbf{e}_\beta^T, \qquad \mathbf{P}_3 = \sum_{\beta=1}^{m+n+p-1} \mathbf{e}_\beta \mathbf{e}_\beta^T, \qquad \mathbf{P}_4 = \sum_{\beta=1}^{m+n+p+t-1} \mathbf{e}_\beta \mathbf{e}_\beta^T.$$

Now these substitutions may be introduced into (3) to obtain

$$f_1 \approx -\frac{\sqrt{\chi}}{4} - \frac{1}{2}\sqrt{\frac{\chi}{4} - \gamma + \psi + \kappa} - \frac{1}{2}\sqrt{\frac{\chi}{2} - 2\gamma - \psi - \kappa + \frac{\chi^{3/2} - \frac{4a_2\sqrt{\chi} - 8\mu^T \mathbf{A}^{-1} P_2 \xi}{\left[\mu^T \mathbf{A}^{-1} (\mathbf{I} - \mathbf{P}_1 - \mathbf{P}_2 - \mathbf{P}_3 - \mathbf{P}_4) \xi\right]}}{4\sqrt{\frac{\chi}{4} - \gamma + \psi + \kappa}}}$$

where

$$p = \left[\mu^T \mathbf{A}^{-1} \mathbf{P}_3 \xi\right]^2 - 3\mu^T \mathbf{A}^{-1} \mathbf{P}_4 \xi \mu^T \mathbf{A}^{-1} \mathbf{P}_2 \xi + 12\mu^T (\mathbf{I} - \mathbf{P}_1 - \mathbf{P}_2 - \mathbf{P}_3 - \mathbf{P}_4) \xi \left(\mu^T \mathbf{A}^{-1} \mathbf{P}_1 \xi - \mu^T \mathbf{A}^{-1} \mu\right),$$
$$q = 2\left[\mu^T \mathbf{A}^{-1} \mathbf{P}_3 \xi\right]^3 - 9\mu^T \mathbf{A}^{-1} \mathbf{P}_4 \xi \mu^T \mathbf{A}^{-1} \mathbf{P}_3 \xi \mu^T \mathbf{A}^{-1} \mathbf{P}_2 \xi + 27\mu^T (\mathbf{I} - \mathbf{P}_1 - \mathbf{P}_2 - \mathbf{P}_3 - \mathbf{P}_4) \xi \left[\mu^T \mathbf{A}^{-1} \mathbf{P}_2 \xi\right]^2$$

$$+27\left[\mu^T\mathbf{A}^{-1}\mathbf{P}_4\xi\right]^2\left(\mu^T\mathbf{A}^{-1}\mathbf{P}_1\xi-\mu^T\mathbf{A}^{-1}\mu\right)-72\mu^T\left(\mathbf{I}-\mathbf{P}_1-\mathbf{P}_2-\mathbf{P}_3-\mathbf{P}_4\right)\xi\mu^T\mathbf{A}^{-1}\mathbf{P}_3\xi$$
$$\times\left(\mu^T\mathbf{A}^{-1}\mathbf{P}_1\xi-\mu^T\mathbf{A}^{-1}\mu\right)$$

$$\chi=\frac{\left[\mu^T\mathbf{A}^{-1}\mathbf{P}_3\xi\right]^2}{\left[\mu^T\left(\mathbf{I}-\mathbf{P}_1-\mathbf{P}_2-\mathbf{P}_3-\mathbf{P}_4\right)\xi\right]^2},\qquad \kappa=\frac{\left\{q+\sqrt{-4p^3+q^2}\right\}^{1/3}}{2^{1/3}\mu^T\left(\mathbf{I}-\mathbf{P}_1-\mathbf{P}_2-\mathbf{P}_3-\mathbf{P}_4\right)\xi}$$

$$\psi=\frac{2^{1/3}p}{3\mu^T\left(\mathbf{I}-\mathbf{P}_1-\mathbf{P}_2-\mathbf{P}_3-\mathbf{P}_4\right)\xi\left\{q+\sqrt{-4p^3+q^2}\right\}^{1/3}},\qquad \gamma=\frac{2\mu^T\mathbf{A}^{-1}\mathbf{P}_3\xi}{3\mu^T\left(\mathbf{I}-\mathbf{P}_1-\mathbf{P}_2-\mathbf{P}_3-\mathbf{P}_4\right)\xi}$$

To simplify expression we can use a spectral decomposition of $\mathbf{A}^{-1}$. A good approximation will be to use to minimal eigenpairs of $\mathbf{A}$ as $\mathbf{A}^{-1}=\lambda_{min}^{-1}\varphi_{min}\varphi_{min}^T$.

CONCLUSION

In this study we inserted certain flexibilities into the approximation. Because we want to improve its quality. Hence we applied HDMR on the image of the original function under a fourth degree transformation. The coefficients of the transformation are chosen to make the error of HDMR approximation as small as possible and this increases the efficiency of the method.

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