Cubic Transformational High Dimensional Model Representation

Erdoğan Şen [†,◊] and Kamil Oruçoğlu [†]

[†] Istanbul Technical University Mathematics Engineering Department, Maslak, 34469, Istanbul, TURKEY
senerdogan@itu.edu.tr, koruc@itu.edu.tr

[◊] Namik Kemal University Mathematics Department, 59030, Tekirdag, TURKEY
esen@nku.edu.tr

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

Keywords: Cubic Equation, Transformational High Dimensional Model Representation, Multivariate Functions, Approximation

Introduction

When a natural event is analyzed, the number of factors affecting the event is higher than calculated. General way to overcome this is to eliminate or ignore some of factors which will be less effective. However as the investigated event complicates, the number of affecting factors increases. Nowaday computer technology cannot be suitable to the calculation limitations on this type of problems. High Dimensional Model Representation (HDMR) is perhaps the most fruitful solution to those multidimensional problems. Various HDMR versions were suggested in order to tackl 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 unfortunately not well ordered. This led to the 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 was focused on the HDMR constancy optimization under an affine transformation (Yaman, 2008 and Yaman, Demiralp, 2009), conic transformation (Gündoğar, Baykara, Demiralp, 2010 and Gündoğar, Baykara, Demiralp, 2011) and quartic transformation (Şen, 2011). We shall consider in this work a cubic transformation and attempt to find optimal parameters for such a transformation leading to a new approximation.

Transformational hıgh dımensıonal model representatıon

Let us consider a function $f\left(x_1,x_2,...,x_N\right)$ 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 $\varphi\left(x_1,...,x_N\right)$

$$Tf\left(x_1,x_2,...x_N\right)\equiv\varphi\left(x_1,x_2,...x_N\right) \tag{1}$$

If we apply the HDMR expansion to φ we will get

$$\varphi\left(x_1,...,x_N\right)=\varphi_0+\sum_{\beta=1}^{N}\varphi_\beta\left(x_\beta\right)+...+\varphi_{1...N}\left(x_1,...,x_N\right).$$

Addititivity measures $\sigma_i\left(\varphi\right)$s can be defined for this expansion in the usual HDMR manner.

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

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.

Cubic Transformational hıgh dımensıonal model representatıon

A polynomial can be used as THDMR's operator for choosing the transformation suggested in (1). Here the degree of the polynomial will be taken to be three. The linear combination coefficients of the cubic 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.

$$Tf\left(x_1,...,x_N\right)=\varphi\left(x_1,...,x_N\right)=a_0\left(x_1,...,x_N\right)+a_1\left(x_1,...,x_N\right)f+a_2\left(x_1,...,x_N\right)f^2+a_3\left(x_1,...,x_N\right)f^3.$$

Since only $\sigma_0\left(\varphi\right)$ will be under consideration, φ will be approximated by the constant component φ_0

$$\varphi=a_0+a_1 f+a_2 f^2+a_3 f^3\approx\varphi_0$$

which gives the approximate equality

$$\begin{aligned} f_1 &\approx \sqrt[3]{-A+\sqrt{A^2+B^3}}+\sqrt[3]{-A-\sqrt{A^2+B^3}} \\ f_2 &\approx \left(-\frac{1}{2}+i\frac{\sqrt{3}}{2}\right)\sqrt[3]{-A+\sqrt{A^2+B^3}}+\left(-\frac{1}{2}+i\frac{\sqrt{3}}{2}\right)^2\sqrt[3]{-A-\sqrt{A^2+B^3}} \\ f_3 &\approx \left(-\frac{1}{2}+i\frac{\sqrt{3}}{2}\right)^2\sqrt[3]{-A+\sqrt{A^2+B^3}}+\left(-\frac{1}{2}+i\frac{\sqrt{3}}{2}\right)\sqrt[3]{-A-\sqrt{A^2+B^3}}, \end{aligned} \tag{3}$$

where

$$i^2=-1,\ A=\frac{1}{2}\left(\frac{a_0-\varphi_0}{a_3}-\frac{a_2 a_1}{a_3^2}+\frac{2a_2^3}{27a_3^3}\right)\ \text{and}\ B=\frac{1}{3}\left(\frac{a_1}{a_3}-\frac{a_2^2}{3a_3^2}\right).$$

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 and a_3 that maximize σ_0 in (2). To this end a_0, a_1, a_2 and a_3 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 in terms of the inner product as

$$\left(u_j,u_k\right)=\int_V dVW\left(x_1,...x_N\right)u_j\left(x_1,...x_N\right)u_k\left(x_1,...x_N\right)=\delta_{jk},\quad 1\le j,k\le\infty$$

where $V=\left[a_1,b_1\right]\times...\times\left[a_N,b_N\right]$ represents the hyperprism which is the HDMR construction domain and $W\left(x_1,...x_N\right)$ 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 $dx_1...dx_N$.

$$W\left(x_1,...x_N\right)=\prod_{\beta=1}^{N}W_\beta\left(x_\beta\right)=\prod_{\beta=1}^{N}\frac{1}{b_\beta-a_\beta}$$

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

$$a_0\left(x_1,...x_N\right)=\sum_{j=2}^{m}a_j^{(0)}u_j,\ a_1\left(x_1,...x_N\right)=\sum_{k=1}^{n}a_k^{(1)}u_k,\ a_2\left(x_1,...x_N\right)=\sum_{l=1}^{p}a_l^{(2)}u_l,\ a_3\left(x_1,...x_N\right)=\sum_{s=1}^{t}a_s^{(3)}u_s. \tag{4}$$

With these expressions in hand, the constancy measurer $\sigma_0\left(\varphi\right)$ will be a function of the parameters $a_j^{(0)},a_k^{(1)},\ a_l^{(2)},a_s^{(3)}$ where

$$2\le j\le m,\ 1\le k\le n, 1\le l\le p,\ 1\le s\le t.$$

Thus

$$\sigma_0\left(\varphi\right)=\sigma_0\left(\varphi,a_2^{(0)},...,a_m^{(0)},a_1^{(1)},...,a_n^{(1)},a_1^{(2)}...,a_p^{(2)},a_1^{(3)},...,a_t^{(3)}\right).$$

Using (4) φ can be expressed as

$$\varphi(x_1,...x_N)=\sum_{j=2}^{m}a_j^{(0)}u_j+\left(\sum_{k=1}^{n}a_k^{(1)}u_k\right)f+\left(\sum_{l=1}^{p}a_l^{(2)}u_l\right)f^2+\left(\sum_{s=1}^{t}a_s^{(3)}u_s\right)f^3 \quad (5)$$

To obtain the constant HDMR term φ_0 both sides of (5) are to be integrated with respect to $x_1,...x_N$ over V under the weight function W .

$$\varphi_0=\sum_{j=2}^{m}a_j^{(0)}\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_j+\sum_{k=1}^{n}a_k^{(1)}\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_k f+$$
$$\sum_{l=1}^{p}a_l^{(2)}\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_l f^2+\sum_{s=1}^{t}a_s^{(3)}\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_s f^3$$

Defining vectors η and

$$\eta=\left(a_2^{(0)},...,a_m^{(0)},a_1^{(1)},...,a_n^{(1)},a_1^{(2)}...,a_p^{(2)},a_1^{(3)},...,a_t^{(3)}\right),\ \tau=\left(\tau_2^{(0)},...,\tau_m^{(0)},\tau_1^{(1)},...,\tau_n^{(1)},\tau_1^{(2)}...,\tau_p^{(2)},\tau_1^{(3)},...,\tau_t^{(3)}\right)^T$$

With the elements of vector τ defined as

$$\begin{aligned}\tau_j^{(0)}&=\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_j=(u_j,h),\ \tau_k^{(1)}=\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_k f=(u_k,f),\\ \tau_l^{(2)}&=\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_l f^2=(u_l,f^2),\ \tau_s^{(3)}=\int_V dV\left(\prod_{\beta=1}^{N}W_\beta(x_\beta)\right)u_s f^3=(u_s,f^3),\end{aligned} \quad (6)$$

where

$$2\le j\le m,\ 1\le k\le n, 1\le l\le p,\ 1\le s\le t.$$

$h(x_1,...x_N)$ appearing in the first inner product in (6) is a function which has the constant value 1 for all x_β in the hyperprism domain $[a_1,b_1]\times\ ...\times[a_N,b_N]$. φ_0 can now be written as an inner product $\varphi_0=\eta\tau$. Since φ_0 has a constant value, the square of its norm will be equal to the square of the function φ_0 .

$$\|\varphi_0\|^2=(\eta\tau)(\eta\tau)^T=\eta\tau\tau^T\eta.\ \|\varphi\|^2$$

On the other hand can be expressed in terms of the above defined vector η and a square matrix C which can be expressed in terms of its blocks as

$$C=\begin{pmatrix}K & L & N & S\\ L^T & M & P & T\\ N^T & P^T & R & Y\\ S^T & T^T & Y^T & Z\end{pmatrix}$$

where

$$\begin{aligned}&K_{jk}=(u_j,u_k),\ 2\le j,k\le m,\ L_{jk}=(u_j,fu_k),\ 2\le j\le m, 1\le k\le n,\\ &M_{jk}=(u_j,f^2u_k),\ 1\le j,k\le n,\ N_{jk}=(u_j,f^2u_k),\ 2\le j\le m, 1\le k\le p,\\ &R_{jk}=(u_j,f^4u_k),\ 1\le j,k\le p,\ P_{jk}=(u_j,f^3u_k),\ 1\le j\le n, 1\le k\le p,\\ &S_{jk}=(u_j,f^3u_k),\ 2\le j\le m, 1\le k\le t,\ T_{jk}=(u_j,f^4u_k),\ 1\le j\le n, 1\le k\le t,\\ &Y_{jk}=(u_j,f^5u_k),\ 1\le j\le p, 1\le k\le t,\ Z_{jk}=(u_j,f^6u_k),\ 1\le j,k\le t.\end{aligned}$$

C is a symmetric, positive definite matrix. Norm square of φ can be expressed in terms of C and η as

$$\|\varphi\|^2 = \eta C \eta^T .$$

So the constancy measurer σ_0 becomes

$$\sigma_0 = \frac{\|\varphi_0\|^2}{\|\varphi\|^2} = \frac{\eta\mu\mu^T\eta^T}{\eta C\eta^T} . \quad (7)$$

Our aim is to maximize σ_0 which can be written as a Rayleigh quotient as

$$\sigma_0 = \frac{y^T C^{-1/2}\tau\tau^T C^{-1/2} y}{y^T y}$$

where $y = C^{1/2}\eta^T$. However, a Rayleigh quotient takes its maximum value at the maximum eigenvalue of its kernel, in this case $C^{-1/2}\tau\tau^T C^{-1/2}$. Similarly 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,

$$\sigma_0 = \tau^T C^{-1}\tau, \quad y = C^{-1/2}\tau .$$

The equation for y gives us the vector η^T in (7) that maximizes σ_0 as

$$\eta^T = C^{-1/2} y = C^{-1}\tau.$$

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 and a_3 in terms of matrix algebraic entities. φ_0 can be written in compact form as

$$\varphi_0 = \eta\tau = \tau^T C^{-1}\tau .$$

We define a vector ξ with $(m+n+p+t-1)$ elements $\xi = \left[\xi_2,\ldots,\xi_m,\xi_1,\ldots,\xi_n,\xi_1,\ldots,\xi_p,\xi_1,\ldots,\xi_t\right]^T$ and express a_0, a_1, a_2 and a_3 more compactly as

$$a_0 = \eta^{(0)}\xi^{(0)},\ a_1 = \eta^{(1)}\xi^{(1)},\ a_2 = \eta^{(2)}\xi^{(2)},\ a_3 = \eta^{(3)}\xi^{(3)}.$$

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

$$\eta^{(0)} = \left[a_2^{(0)},\ldots,a_m^{(0)}\right],\ \eta^{(1)} = \left[a_1^{(1)},\ldots,a_n^{(1)}\right],\ \eta^{(2)} = \left[a_1^{(2)},\ldots,a_p^{(2)}\right],\ \eta^{(3)} = \left[a_1^{(3)},\ldots,a_t^{(3)}\right],$$
$$\xi^{(0)} = \left[\xi_2,\ldots,\xi_m\right]^T,\ \xi^{(1)} = \left[\xi_1,\ldots,\xi_n\right]^T,\ \xi^{(2)} = \left[\xi_1,\ldots,\xi_p\right]^T,\ \xi^{(3)} = \left[\xi_1,\ldots,\xi_t\right]^T.$$

To proceed we define $(m+n+p+t-1)\times(m+n+p+t-1)$ projection matrices P_1, P_2 and P_3 as

$$P_1 = \sum_{\beta=1}^{m-1} e_\beta e_\beta^{\,T},\ P_2 = \sum_{\beta=m}^{m+n-1} e_\beta e_\beta^{\,T},\ P_3 = \sum_{\beta=m+n}^{m+n+p-1} e_\beta e_\beta^{\,T}$$

Where e_β is the unit vector in $(m+n+p+t-1)$ dimensional space. Utilizing these projection operators a_0, a_1, a_2 and a_3 can be approximated as

$$a_0 = \eta P_1\xi = \tau^T C^{-1} P_1\xi,\ a_1 = \eta P_2\xi = \tau^T C^{-1} P_2\xi,$$
$$a_2 = \eta P_3\xi = \tau^T C^{-1} P_3\xi,\ a_3 = \eta\left(I - P_1 - P_2 - P_3\right)\xi = \tau^T C^{-1}\left(I - P_1 - P_2 - P_3\right)\xi$$

where I identity matrix. If now these substitutions are introduced into (3) we obtain

$$f_1 \approx \sqrt[3]{-\frac{1}{2}\left(\frac{\tau^T C^{-1}P_1\xi-\tau^T C^{-1}\tau}{\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi}-\frac{\tau^T C^{-1}P_3\xi\tau^T C^{-1}P_2\xi}{\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^2}+\frac{2\left[\tau^T C^{-1}P_3\xi\right]^3}{27\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^3}\right)+\sqrt{\frac{1}{4}\left(\frac{\tau^T C^{-1}P_1\xi-\tau^T C^{-1}\tau}{\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi}-\frac{\tau^T C^{-1}P_3\xi\tau^T C^{-1}P_2\xi}{\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^2}+\frac{2\left[\tau^T C^{-1}P_3\xi\right]^3}{27\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^3}\right)^2+\frac{1}{27}\left(\frac{\tau^T C^{-1}P_2\xi}{\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi}-\frac{\left[\tau^T C^{-1}P_3\xi\right]^2}{3\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^2}\right)^3}}$$

$$+\sqrt[3]{-\frac{1}{2}\left(\frac{\tau^T C^{-1}P_1\xi-\tau^T C^{-1}\tau}{\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi}-\frac{\tau^T C^{-1}P_3\xi\tau^T C^{-1}P_2\xi}{\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^2}+\frac{2\left[\tau^T C^{-1}P_3\xi\right]^3}{27\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^3}\right)-\sqrt{\frac{1}{4}\left(\frac{\tau^T C^{-1}P_1\xi-\tau^T C^{-1}\tau}{\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi}-\frac{\tau^T C^{-1}P_3\xi\tau^T C^{-1}P_2\xi}{\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^2}+\frac{2\left[\tau^T C^{-1}P_3\xi\right]^3}{27\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^3}\right)^2+\frac{1}{27}\left(\frac{\tau^T C^{-1}P_2\xi}{\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi}-\frac{\left[\tau^T C^{-1}P_3\xi\right]^2}{3\left[\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi\right]^2}\right)^3}}$$

$$-\frac{\tau^T C^{-1}P_3\xi}{3\tau^T C^{-1}\left(I-P_1-P_2-P_3\right)\xi},$$

To simplify this expression we can use a spectral decomposition of C^{-1} as

$$C^{-1}=\sum_{\beta=1}^{m+n+p+t-1}\frac{1}{\lambda_\beta}\varphi_\beta{\varphi_\beta}^T$$

where λ_β is an eigenvalue of C and φ_β is an eigenvector corresponding to the eigenvalue λ_B. A good approximation will be to use the minimal eigenpairs of C as $C^{-1}=\lambda_{\min}^{-1}\varphi_{\min}{\varphi_{\min}}^T$.

Conclusıon

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 third 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.

References

Şen, E. (2011). On Quartic Transformational High Dimensional Model Representation. *Numerical Analysis and Applied Mathematics ICNAAM 2011 American Institute of Physics Conference Proceedings*, 1389 (pp.2044-2047). Halkidiki, Greece.

Yaman, İ., (2008). Construction of New Rational Approximation Based on Transformational High Dimensional Model Representation and Efficient Usage of Them by Fluctuation Approximation. Ph.D Thesis, İstanbul Technical University Informatics Institute.

Yaman, İ., Demiralp, M. (2009), A New Rational Approximation Technique Based on Transformational High Dimensional Model Representation. *Springer U.S.line* Volume 52, No. 3 (pp.385-407), ISSN: 1017-1398 (Print) 1572-9265 (Online).

Demiralp, M. (2003). High Dimensional Model Representation and its Applications. *Tools for Mathematical Modelling*, 9, (pp.146-159).

Demiralp, M. (2006). Transformational High Dimensional Model Representation. *ICCMSE (International Conference of Computational Methods in Engineering)*, Crete, Greece.

Gündoğar Z., Baykara, N.A., Demiralp, M. (2010). Basic Features of Conic Transformational High Dimensional Model Representation. *Int. Conf. on Numerical Analysis and Applied Mathematics*, Rhodes, Greece.

Gündoğar, Z., Baykara, N.A., Demiralp, M. (2011). Conic Transformational High Dimensional Model Representation in Comparison with Hermite-Padé Approximants, *Proceedings of the Int. Conf. on Applied Informatics and Computing Theory*, Prague, Czech Republic, (pp.45-51).