How Additive Are the Fourier Series in the Sense of High Dimensional Model Representation?

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Abstract: The focus of this work is to investigate the quality of High Dimensional Model Representation (HDMR) to Fourier series. Towards this end, we experimantate with various Fourier series which are constructed for known univariate functions. Although the investigations are kept univariate, the extension that we obtain here to multivariate cases seems to be straightforward. This is because we use the additivity measurers whose conceptual structures do not change from one multivariance to another. The additiviy measurers are certain well–ordered functionals mapping from a Hilbert space of multi or univariate functions to the interval $[0, 1]$ and their close–to–one values mean certain level of additivity and therefore higher qualities of truncated HDMR approximants. Hence, those entities are evaluated for certain known cases.

Key–Words: Multivariate Functions, Fourier Series, High Dimensional Model Representation, Additivity Measurers

1 Introduction

There are two important entities in this work; first Fourier series and second High Dimensional Model Representation. The first one is encountered almost everywhere periodic or oscillatory behaviors arise. Fourier series are in fact orthogonal function series whose convergence were well investigated and a sufficently strong theoretical and practical background exists to illuminate those who attempt to use them. Although they are mostly univariate, the extension of their theory to multivariate cases does not bring any remarkable conceptual difficulty and does not increase the computational expenses except for the well known dimension based expenses.

The second one is perhaps the most optimial way of representing a multivariate function[1]. It is a finite linear combination of less variate terms starting from a constant term which is followed by univariate terms, then, bivariate terms and so on. Despite the finiteness of the number of linearly combined terms, that number is 2^N for N independent variables and therefore the number of components rapidly grows as the number of the independent variables increases. In practical sense the case of $N = 10$ corresponds to 1024 components while $N = 100$ case produces 1048576 HDMR components. This urges those dealing with HDMR to truncate it at less variate terms like constant, univariate, or perhaps, bivariate components. The univariate terms requires $N + 1$ components while the bivariate truncation involves $N(N+1)/2$ HDMR components. The qualities of these truncation approximations depend on how additive the function to be expanded to HDMR is. This nature is measured by the functionals mapping from the Hilbert space the target function of HDMR belongs to, to the closed interval between 0 and 1. These entities are called "Additivity Measurers"and stand perhaps as the most powerful agents to estimate the truncation errors.

This paper is organised as follows. The second and third sections contain a brief presentation of HDMR and the definitions and certain important properties of the additivity measurers. The fourth section is about Fourier series and the fifth section covers the main goal of this paper, experimentation about the additivity of the various Fourier series. The sixth section finalizes the paper via concluding remarks.

2 High Dimensional Model Representation

High Dimensional Model Representation (HDMR) is defined for a given function $f(x_1, x_2, ..., x_N)$ as follows

$$f\left(x_1, x_2, ..., x_N\right) = f_0 +$$

$$+\sum_{i=1}^{N} f_i(x_i) + \sum_{\substack{i,j=1 \\ i<j}}^{N} f_{ij}(x_i, x_j) + \cdots + f_{12\ldots N}(x_1, \ldots, x_N) \qquad (1)$$

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 interaction 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 precision by choosing the appropriate truncation of HDMR. HDMR, its components and properties was first mentioned in 1993 by I. M. Sobol[2]. He used unit weight and $[0, 1]$ interval without considering the possibility of extension of these items since these entities were sufficient for his purpose.

H. Rabitz generalized Sobol's work by introducing the idea of weight functions [3, 4] and orthogonal hyperprisms. M. Demiralp defined and utilized various versions of HDMR and brought the addivity measurer concept to the theory, which is very useful for the estimation of truncation errors[1].

Demiralp's group continues their work developing new HDMR versions whose univariate truncation quality is higher or they can be optimised to get higher qualities. The HDMR components fulfill the condition

$$\int_{a_j}^{b_j} dx_j W_j(x_j) f_{i_1,\ldots,i_k}(x_{i_1}, \ldots, x_{i_k}) = 0, \quad x_j \in \{x_{i_1}, \ldots, x_{i_k}\}, \qquad 1 \le j, k \le N. \qquad (2)$$

which was imposed by Sobol to get unique HDMR components. We call these impositions "vanishing conditions". It can be used to calculate HDMR terms as follows

$$f_0 = \int_{a_1}^{b_1} dx_1 W_1(x_1) \ldots \times \int_{a_N}^{b_N} dx_N W_N(x_N) f(x_1, \ldots, x_N) \qquad (3)$$

$$\begin{aligned} f_i(x_i) = & \int_{a_1}^{b_1} dx_1 W_1(x_1) \ldots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} W_{i-1}(x_{i-1}) \\ & \times \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} W_{i+1}(x_{i+1}) \ldots \\ & \times \int_{a_N}^{b_N} dx_N W_N(x_N) f(x_1, \ldots, x_N) - f_0 \\ & 1 \le i \le N \end{aligned} \qquad (4)$$

$$\begin{aligned} f_{ij}(x_i, x_j) = & \int_{a_1}^{b_1} dx_1 W_1(x_1) \ldots \int_{a_{i-1}}^{b_{i-1}} dx_{i-1} W_{i-1}(x_{i-1}) \\ & \times \int_{a_{i+1}}^{b_{i+1}} dx_{i+1} W_{i+1}(x_{i+1}) \ldots \\ & \times \int_{a_{j-1}}^{b_{j-1}} dx_{j-1} W_{j-1}(x_{j-1}) \\ & \times \int_{a_{j+1}}^{b_{j+1}} dx_{j+1} W_{j+1}(x_{j+1}) \ldots \\ & \times \int_{a_N}^{b_N} dx_N W_N(x_N) \\ & \times f(x_1, \ldots, x_N) - f_i(x_i) - f(x_j) - f_0 \\ & 1 \le i < j \le N \end{aligned} \qquad (5)$$

Other components can be calculated similarly. For a practical point of view the truncations containing at most the bivariate components are used. Zeroth, first and k-th order truncations are as follows [1, 2, 3, 4, 5].

$$\begin{aligned} s_0 &\equiv f_0, \\ s_1 &\equiv s_0 + \sum_{j=1}^{N} f_j(x_j), \\ &\vdots \\ s_k &\equiv s_{k-1} + \sum_{\substack{j_1,\ldots,j_k=1 \\ j_1<\cdots<j_k}} f_{j_1\ldots j_k}(x_{j_1}, \ldots, x_{j_k}). \end{aligned} \qquad (6)$$

The vanishing conditions mentioned above in fact correspond to orthogonality between HDMR components as it was first shown by Demiralp. This is due to the fact that each vanishing condition can in fact be interpreted as the inner product of the relevant component with the constant component, and the inner product of any two variate components will contain at least one integral which vanishes because of Sobol's vanishing conditions. The inner product under consideration here is defined as the N-fold integral of two functions over the region which is the cartesian product of individual intervals of the independent variables and under the product of the univariate weight functions of HDMR.

The mutual orthogonalities of HDMR components is a very important issue since it enables us to construct certain norm related equalities which can be used to measure the norm square contribution of each component to the norm square of the function whose

HDMR is under consideration. However this is valid only for the norm definition induced from the inner product definition used in the HDMR construction and the orthogonality conditions are established. Otherwise orthogonality amongst the HDMR components disappears and the formulation of relations towards the truncation error analysis becomes quite complicated.

3 Addivity Measurers

Let $f(x_1, ..., x_N)$ be a square integrable function, with the aid of the orthogonality conditions and the inner product mentioned above, we can get

$$\|f\|^2 = \|f_0\|^2 + \sum_{i=1}^{N} \|f_i\|^2 + \sum_{\substack{i,j=1 \\ i<j}} \|f_{i,j}\|^2 + \cdots + \|f_{12\ldots N}\|^2 \quad (7)$$

If we now divide both sides of this equation by $\|f\|^2$ we get

$$\frac{\|f_0\|^2}{\|f\|^2} + \frac{\sum\limits_{i=1}^{N} \|f_i\|^2}{\|f\|^2} + \frac{\sum\limits_{\substack{i,j=1 \\ i<j}} \|f_{i,j}\|^2}{\|f\|^2} + \cdots + \frac{\|f_{12\ldots N}\|^2}{\|f\|^2} = 1 \quad (8)$$

This urges us to define

$$\sigma_0 \equiv \frac{\|f_0\|^2}{\|f\|^2}, \quad \sigma_1 \equiv \frac{\sum\limits_{i=1}^{N} \|f_i\|^2}{\|f\|^2}, \quad \sigma_2 \equiv \frac{\sum\limits_{\substack{i,j=1 \\ i<j}} \|f_{i,j}\|^2}{\|f\|^2} \quad (9)$$

The σ_i's above (first three of them are given only) are called "Additivity Measurer of Order i". It is not hard to show that these entities vary between 0 and 1 inclusive and they are well ordered with respect to index i. That is,

$$0 \le \sigma_0 < \cdots < \sigma_N = 1 \quad (10)$$

which means that these measurers form a monotonously increasing sequence with respect to growing values of the index. The closer the σ_i is to 1, the better the quality of the i–th variate HDMR truncation.

4 Fourier Series

The generalized Fourier series [6] of a square integrable function $f : [a, b] \to C$ with respect to Φ, is

$$f(x) = \sum_{k=0}^{\infty} c_k \phi_k(x) \quad (11)$$

where c_k's are given by

$$c_k = \frac{< f, \phi_k >}{< \phi_k, \phi_k >} \quad (12)$$

The c_k coefficients above are called Fourier Coefficients and $\phi_k(x)$s form an orthogonal basis set. The inner product is defined by

$$< \phi_k, \phi_l >= \int_a^b dx \phi_k(x) \overline{\phi}_l(x) w(x) \quad (13)$$

where $w(x)$ is a weight function and $\overline{\phi}_l(x)$ stands for the complex conjugate of $\phi_l(x)$. In multi-dimensional space, we define the inner product as follows;

$$< \phi_k, \phi_l >= \int_{[a,b]^N} dx \phi_k(x) \overline{\phi}_l(x) w(x) \quad (14)$$

where $dx = dx_1 ... dx_N$. We use $\phi_k(x) = e^{ikx} = e^{i(k_1 x_1 + \cdots + k_N x_N)}$ for all possible integer values of k_is in this paper. The inner product definition above allows us to define a weighted norm

$$< \phi_k, \phi_k >= \int_{[a,b]^N} dx \phi_k(x) \overline{\phi}_k(x) w(x) \quad (15)$$

so

$$\|\phi_k\|_w^2 = \int_{[a,b]^N} dx \phi_k(x) \overline{\phi}_k(x) w(x) \quad (16)$$

This definition is the same as the norm definition used to calculate the additivity measurers of HDMR components if we assume $\phi_k(x)$ to be a real function. Hence we obtain

$$< \phi_k, \phi_k >= \int_{[a,b]^N} dx \phi_k^2(x) w(x)$$

In this work, we take $w(x) = 1$ as the weight function and $\phi_k(x) = e^{ikx} = e^{i(k_1 x_1 + \cdots + k_N x_N)}$ as the basis functions and the region is the $[0, 2\pi]^N$ hypercube. These functions, $\phi_k(x)$s form an orthogonal basis set since the inner product

$$< \phi_k, \phi_l > = \int_{[0,2\pi]^N} dx e^{i(k-l)x} \quad (17)$$

becomes equal to $(2\pi)^N$ when k and l match otherwise it vanishes. Thereby we can obtain an orthonormal basis set by dividing e^{ikx} by its norm. Under these circumstances the Fourier expansion of $f(x)$ is as follows

$$f(x)=\sum_{k=0}^{\infty}c_k\phi_k(x)=\sum_{k=0}^{\infty}c_k e^{ikx} \tag{18}$$

where

$$c_k=\frac{1}{(2\pi)^N}\int_{[0,2\pi]^N}dxf(x)e^{-ikx}. \tag{19}$$

We can use the limiting form of the Parseval inequalities to calculate the norms of the function $f(x_1,...,x_N)$ and its HDMR components. So we can write

$$\|f\|^2=\sum_{k_1=-\infty}^{\infty}\cdots\sum_{k_N=-\infty}^{\infty}\left|c^f_{k_1\ldots k_N}\right|^2 \tag{20}$$

where $c^f_{k_1\ldots k_N}$s are the Fourier coefficients of the function $f(x_1,...,x_N)$.

Proceeding in the same manner, HDMR component norms can be calculated by using their Fourier coefficients. If we represent the Fourier coefficients of f_0 with $c^{f_0}_{k_1k_2\ldots k_N}$ then

$$\|f_0\|^2=\sum_{k_1=-\infty}^{\infty}\cdots\sum_{k_N=-\infty}^{\infty}\left|c^{f_0}_{k_1\ldots k_N}\right|^2 \tag{21}$$

Similar relations can be written for other HDMR components. The only change in those formulae will be the replacement of the superscript of the Fourier coefficients with the appropriate strings like f_i for univariance $f_{i_1i_2}$ for bivariance and so on. We do not give them, instead, emphasize on certain reductive properties of the HDMR component Fourier coefficients. They are given below for the case of constancy, univariance, and bivariance respectively.

$$\begin{aligned}
c^{f_0}_{k_1\ldots k_N} &= \delta_{k_10}\ldots\delta_{k_N0}c^{f_0}_{0\ldots0},\\
c^{f_i}_{k_1\ldots k_N} &= \delta_{k_10}\ldots\delta_{k_{i-1}0}\delta_{k_{i+1}0}\ldots\delta_{k_N0}c^{f_0}_{0\ldots0k_i0\ldots0},\\
&\quad 1\le i\le N,\qquad -\infty<k_i<\infty\\
c^{f_{i_1i_2}}_{k_1\ldots k_N} &= \delta_{k_10}\ldots\delta_{k_{i_1-1}0}\delta_{k_{i_1+1}0}\ldots\delta_{k_{i_2-1}0}\\
&\quad\times\delta_{k_{i_2+1}0}\ldots\delta_{k_N0}c^{f_0}_{0\ldots0k_{i_1}0\ldots0k_{i_2}0\ldots0},\\
&\quad 1\le i_1<i_2\le N,\\
&\quad -\infty<k_{i_1},k_{i_2}<\infty
\end{aligned} \tag{22}$$

These properties remove a lot of infinite sums in the formulae above and therefore facilitate numerical calculations. The first of these properties means that the HDMR's constant term corresponds to the the weighted average of the function $f(x_1,...,x_N)$ Hence, the oscillations around this average value determines how constant HDMR is. In other words, smaller the Fourier coefficients except the one constant basis function better quality is the HDMR truncated at constant component. Similar considerations are valid for other HDMR components.

5 Computational Experimentation

We illustrate three functions as examples in this work. First the additivity measurers of normalized exponential function with second degree multinomial argument are computed over $[0,1]^4$ hypercube

$$F_1(x) = \frac{\prod_{i=1}^{4} e^{-\alpha_i(x_i-c_i)^2}}{\prod_{i=1}^{4}\left\|e^{-\alpha_i(x_i-c_i)^2}\right\|},\qquad \alpha_i,\ c_i\in R,\quad 1\le i\le 4 \tag{23}$$

and then purely additive

$$F_2(x)=\frac{Sinx_1}{x_1}+\frac{Sinx_2}{x_2}+\frac{Sinx_3}{x_3}+\frac{Sinx_4}{x_4} \tag{24}$$

and purely multiplicative

$$F_3(x)=\frac{Sinx_1}{x_1}\frac{Sinx_2}{x_2}\frac{Sinx_3}{x_3}\frac{Sinx_4}{x_4} \tag{25}$$

functions are examined.

In the first example, the function's HDMR components are computed by using weight function $W(x_1,x_2,x_3,x_4)=1$ over $[0,1]^4$ hypercube. In Gülpınar's thesis[7], it is illustrated that the HDMR approximation gives the best results for the $\alpha_i=0.001$ and $c_i=0.5$ values. In this paper we specifically choose $c_i=0.5$ and HDMR approximation calculated for 5 different α_i values. In the first instance, all of the terms except the first five are neglected from the infinite series, then first 10 and first 15 terms are retained in the computation while calculating additive measurers.

First, computations were realised at $\alpha_i=0.001$ and $c_i=0.5$ values which provided the best approximation previously. We obtain $\sigma_0=0.99997630$ and $\sigma_1=\sigma_2=\sigma_3=\sigma_4=0.99997634$ by using the first five terms of the infinite sums in computations. The last 4 additivity measurers are same within 10^{-30} digit precision. σ_4 is smaller than one, because of the five term truncation and round off errors.

As the results of a previous work[8] show, the additivity measurers tend to 1 as α_i decreases to zero.

Greater the α_is smaller the additivity measurers. For example, when c_is are all 0.5 and α_is are 0.001 all σ_i values except σ_0 which is 0.9999999778 are equal to 1 within ten decimal digit accuracy. For the case where α_i are 0.01 the situation is almost same except the change in σ_0 whose value is now 0.9999977788. When α_is become 0.1 beside σ_0, σ_1 starts to deviate from 1. In the case where α_is become quite big like 10.0, only σ_4 preserves a value 1. The deviations become so great that σ_0 takes the value 0.3235044841 while σ_1 becomes 0.7553005983[8].

Table shows the results obtained using Fourier coefficients to calculate sensitivity indices.

If we take first ten of the Fourier coefficients, we observed that the results are distinctly closer to one. If we examine the table below, the results obtained are similar to the results at the[7].

Table 1: Sensivity Indices

	n_r	$\alpha_i = 0.001$	$\alpha_i = 10$
$1-\sigma_0$	5	3×10^{-5}	86106×10^{-5}
	10	6×10^{-5}	86499×10^{-5}
	15	8×10^{-5}	86499×10^{-5}
$1-\sigma_1$	5	2×10^{-5}	50707×10^{-5}
	10	2×10^{-5}	51655×10^{-5}
	15	0.8×10^{-5}	51438×10^{-5}
$1-\sigma_2$	5	2×10^{-5}	16885×10^{-5}
	10	6×10^{-5}	17465×10^{-5}
	15	0.8×10^{-5}	17293×10^{-5}
$1-\sigma_3$	5	2×10^{-5}	2523×10^{-5}
	10	6×10^{-5}	2598×10^{-5}
	15	0.8×10^{-5}	2514×10^{-5}
$1-\sigma_4$	5	2×10^{-5}	236×10^{-5}
	10	6×10^{-5}	174×10^{-5}
	15	0.8×10^{-5}	115×10^{-5}

To give an example of discontinuous functions we illustrated the purely additive

$$F_2(x) = \frac{Sinx_1}{x_1} + \frac{Sinx_2}{x_2} + \frac{Sinx_3}{x_3} + \frac{Sinx_4}{x_4}$$

and purely multiplicative

$$F_3(x) = \frac{Sinx_1}{x_1}.\frac{Sinx_2}{x_2}.\frac{Sinx_3}{x_3}.\frac{Sinx_4}{x_4}$$

functions over $[0,1]^4$ hyperprism. Both of these functions are discontinuous at the point $x = 0$. With this aim sensitivity indices are calculated as well as using norm definition at the HDMR definitions after $F_2(x) = \frac{Sinx_1}{x_1} + \frac{Sinx_2}{x_2} + \frac{Sinx_3}{x_3} + \frac{Sinx_4}{x_4}$ function's HDMR components computed. With reference to sensitivity indices for first 5 terms of Fourier coefficients the norm is

$$\sigma_0 = 0.99326$$

$$\sigma_1 = 0.99444$$

$$\sigma_2 = 0.99444$$

$$\sigma_3 = 0.99444$$

$$\sigma_4 = 0.99444$$

In here σ_1, σ_2, σ_3, σ_4 terms are equal to each other within 10^{-50}digit precision. The sensitivity indices calculated by using first 10 terms of Fourier coefficients are given below:

$$\sigma_0 = 0.99483$$

$$\sigma_1 = 0.99606$$

$$\sigma_2 = 0.99606$$

$$\sigma_3 = 0.99606$$

$$\sigma_4 = 0.99606$$

When first 15 terms were used are

$$\sigma_0 = 0.99573$$

$$\sigma_1 = 0.99697$$

$$\sigma_2 = 0.99697$$

$$\sigma_3 = 0.99697$$

$$\sigma_4 = 0.99697$$

Proceeding in the same manner σ_1, σ_2, σ_3, σ_4, terms are equal to each other with a precision of 10^{-50}. This gives us enough information about the approximation quality. We can say, how much closer to the real function our approximation is on the basis of the sensitivity indices σ_1, σ_2, σ_3, σ_4. When we computed the sensitivity indices by using the norm definition

$$\sigma_0 = 0.99937$$

$$\sigma_1 = 1.00000$$

$$\sigma_2 = 1.00000$$

$$\sigma_3 = 1.00000$$

$$\sigma_4 = 1.00000$$

are obtained.

By using similar calculations for obtaining sensitivity indices for the function $F_3(x) = \frac{Sinx_1}{x_1}.\frac{Sinx_2}{x_2}.\frac{Sinx_3}{x_3}.\frac{Sinx_4}{x_4}$ we obtain

$$\sigma_0 = 0.96642$$

$$\sigma_1 = 0.98486$$

$$\sigma_2 = 0.98499$$

$$\sigma_3 = 0.98499$$

$$\sigma_4 = 0.98499$$

when we include first 5 terms of Fourier coefficients. For the first 10 terms

$$\sigma_0 = 0.97161$$

$$\sigma_1 = 0.99096$$

$$\sigma_2 = 0.99110$$

$$\sigma_3 = 0.99110$$

$$\sigma_4 = 0.99111$$

are obtained. For the first 15 terms, we obtain

$$\sigma_0 = 0.97492$$

$$\sigma_1 = 0.99435$$

$$\sigma_2 = 0.99449$$

$$\sigma_3 = 0.99450$$

$$\sigma_4 = 0.99450$$

If we use the norm definition to compute the sensitivity indices instead of Fourier Coefficients norm, we obtain

$$\sigma_0 = 0.98994$$

$$\sigma_1 = 0.99992$$

$$\sigma_2 = 1.00000$$

$$\sigma_3 = 1.00000$$

$$\sigma_4 = 1.00000$$

6 Conclusion

Fourier series specificly used in investigating piecewise functions and functions which have points that cause discontinuity in their domains. Moreover, it is necessary to make calculations by means of generali- zed or numeric integration at the points where the function has discontinuity. On the other hand, the observation that the number of terms necessary to be considered grows exponentially as the dimension increases can be seen as a disadvantage in utilizing Fourier series in the calculation of sensitivity indices.

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