Far East Journal of Mathematical Sciences (FJMS)
Volume 71, Number 2, 2012, Pages 417-442
Published Online: December 2012
Available online at http://pphmj.com/journals/fjms.htm
Published by Pushpa Publishing House, Allahabad, INDIA

A SURVEY ON SENSIBILITY AND UNCERTAINTY ANALYSES FOR MULTIDIMENSIONAL FUNCTIONS BY MEANS OF HIGH DIMENSIONAL MODEL REPRESENTATIONS (HDMR)

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Abstract

Sensibility and uncertainty analyses are essential for the study of mathematically modeled systems because they provide elements that help us match model and experimental results. In the case of complex systems, where a huge number of variables are involved, performing these analyses is extremely expensive. High Dimensional Model Representations (HDMR) are tools that help to improve mathematical modeling of physical systems in which many variables are involved. HDMR tools allow, in a fairly simple way, to discover the input variables that have great influence on the output and those with minimal influence. Making an analysis on the impact that each of the input variables has over the output by means of HDMR requires a much lower number of samples compared with traditional methods such as the Monte Carlo method. In addition, a correct result

2010 Mathematics Subject Classification: 41A63, 93A30.

Keywords and phrases: HDMR, sensibility analysis, uncertainty analysis, FEOM.

Received July 5, 2012

interpretation of complex systems becomes more complicated with traditional methods other than the HDMR method. This work is a compilation of what has been published related with HDMR sensibility and uncertainty analyses and it aims to be an incentive for applying these techniques in a wide range of applications.

1. Introduction

Sensibility analysis allows us to identify the effect of each of the input variables over the output of a system. The effect of each one of these variables is taken into account when they act in an independent way and the effects of these when they act in a combined way. *Uncertainty analysis* indicates the amount of uncertainty produced by each of the input variables over the total uncertainty of the output. The information provided in this kind of analysis indicates in which variable it is necessary to keep working in order to improve the quality of the model predictions [32]. In other words, uncertainty analysis gives one an idea of the model reliability and allows one to identify the input variables that could generate uncertainty over the output when their values are not precisely known.

Helton et al. [13] summarized what is necessary to do in order to carry out the sensibility analysis and the uncertainty analysis, in five steps: (i) Define the distributions $D_1, D_2, ..., D_n$ that characterize the uncertainty of each one of the elements $x_1, x_2, ..., x_n$ of the input $\mathbf{x}$, this is the most important step for sensibility and uncertainty analyses based on sampling. These distributions are commonly defined based on an expertly revised process which could imply the most expensive part of the analysis. (ii) Generation of a number s of samples $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, ..., \mathbf{x}^{(s)}$ of $\mathbf{x}$ according to the chosen distributions $D_1, D_2, ..., D_n$. There are many sampling strategies, random sampling, importance sampling, Latin hypercube [34] and so forth. This last kind of sampling is usually used in systems that demand a significant computational load because its stratification properties allow one to obtain enough information with only a small size sample. When numerous samples are required, the importance sampling can be used, even though

this kind of sampling complicates sensibility analysis because the sample elements do not have the same weight [13]. (iii) Obtain the system results of each sample $[x_i, y(x_i)]$, $i = 1, 2, ..., S$. This is frequently computationally intensive. (iv) Obtain the uncertainty analysis results, which are usually means, standard deviations, density functions, accumulative distribution functions, and box plots. The means and standard deviations alone have the disadvantage of losing significant amount of information. (v) Do sensibility analysis. The results will give the input **x** effects in the output **y** being $\mathbf{y} = f(\mathbf{x})$.

The work of [13] summarizes different sensibility analysis methods like: scatter plots, correlation, regression analysis, partial correlation, rank transformations, and non-parametric regression, among others, it even mentions the variance decomposition method, which is the basis of the HDMR sensibility analysis. They mentioned that there are a number of overwhelming calculations needed to obtain the component functions in an HDMR expansion. This inconvenience is reduced by using the orthogonal polynomials, explained in Section 3. As mentioned before, the sensibility analysis with HDMR has the advantage of requiring a reduced number of samples and easily interprets results even when the system contains high number of variables.

Carrying out sensibility and uncertainty analyses in models where great quantities of variables are involved (more than 20) is very expensive, computationally speaking. The Monte Carlo method for sensibility analysis [12] is very inconvenient in these cases, because it requires many samples and therefore a great quantity of model runs. Besides, when many variables are involved, there are many difficulties when results are being interpreted and presented [37]. The use of the HDMR expansions for sensibility and uncertainty analyses is relatively new and its development began since the first HDMR publications [1-3, 15-18, 28]. Using HDMR expansions to do sensibility analysis has proved to be a precise method when working with computationally intensive models, according to recent investigations

[4, 35-37]. This analysis provides valid results even for highly non-linear functions where the input variables interaction is important [35].

Section 2 is an overview of the HDMR expansions and the two variants: Cut-HDMR and RS-HDMR, it also describes the way in which its component functions are obtained; Section 3 presents the simplification of RS-HDMR expansions by using orthonormal polynomials and, finally, in Section 4, uncertainty and sensibility analyses with HDMR are explained. It is intended that with the provided elements in this work, the reader will understand how to carry out a sensibility analysis with HDMR, by using orthonormal polynomials and be able to develop ones' software system.

2. High Dimensional Model Representations

There are systems in different areas of science that have a large number of input variables, each of these variables affects the output behavior differently. One of the most frequent targets is to identify relationships between the inputs and the outputs of a physical system. A finite sampling of input variables is used to find a function which can predict the output values having been given a starting point and input parameters. Construction of a full space to analyze the model input-output relationships without any a priori physical assumption on the nature of these relationships would be NP-complete with computational complexity scaling exponentially [2]. The computational load grows exponentially as the number of system variables increases, so working with n-variable systems, where $n \gg 10$ has a problem called the *course of dimensionality*. High Dimensional Model Representations (HDMR) is a mathematical technique introduced to improve the efficiency of deducing high dimensional input-output systems behavior [16]. It consists in expanding a multidimensional function in a set of hierarchically correlated functions that separate the influence of variables acting independently, two by two, and so on [2, 15, 16, 20]. This expansion is a generalization of Sobol's proposal [29], see equation (1):

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1\le i<j\le n} f_{ij}(x_i, x_j) + \sum_{1\le i<j<k\le n} f_{ijk}(x_i, x_j, x_k) + \cdots + f_{12\ldots n}(x_1, x_2, ..., x_n), \quad (1)$$

where f_0 represents the average value of $f(\mathbf{x})$ over the entire domain Ω of $\mathbf{x}$, and $\Omega \subset R^n$. The domain Ω of $\mathbf{x}$ is bounded according to the bounds of the input variables $x_1, x_2, ..., x_n$.

The first order cooperativity function $(l = 1)$ $f_i(x_i)$ represents the input variables x_i effect acting independently from the others. In general, the x_i variables which act independently over the output $f(\mathbf{x})$ perform in a non-linear way. When there is no interaction between the input variables of a system, only f_0 and the component functions $f_i(x_i)$ are necessary in order to represent it.

The second order cooperativity functions $(l = 2)$ $f_{ij}(x_i, x_j)$ describe the effect over the output function $f(\mathbf{x})$ when the input variables x_i and x_j act together. The terms of higher cooperativity order reflect the effects of an increasing number of variables all acting together to influence the output function $f(\mathbf{x})$. The last term represents all the input variables acting together to influence the output $f(\mathbf{x})$.

There is a fundamental HDMR ansatz that says that "for physical systems, the order of cooperativity amongst the input variables upon the output does not significantly increase as the number of inputs goes up" [2]. In practice, there does not seem to exist a high order of cooperativity between input variables, so the significant terms of HDMR expansions are expected to satisfy the relationship: $1 \ll n$ [2].

The experience has shown that the second order of cooperativity HDMR expression, as expressed in equation (2), frequently provides a

satisfactory description of $f(\mathbf{x})$ for many physical system models where multidimensional functions are involved [2]:

$$f(\mathbf{x}) \approx f_0 + \sum_{i=1}^{n} f_i(x_i) + \sum_{1 \le i < j \le n} f_{ij}(x_i, x_j). \tag{2}$$

This is a conjecture verified with many physical phenomena to which this technique has been applied, i.e., the theoretical results have been compared with HDMR expansions of cooperativity $l = 2$ [3, 7, 8, 15, 20, 21, 27, 28].

"An important point is that HDMR is designed for treating suitable physical problems and it is not claimed to be practical for arbitrary *n*-dimensional functions" [2].

There are two fundamental applications of the HDMR tools:

The representation of a system using a model called *FEOM* (*Fully Equivalent Operational Model*) which is an expansion of functions of low cooperativity order, usually up to second order, as in equation (2). When a mathematical model of the system cannot be constructed, FEOM plays the role of a mathematical model. Where the execution of the mathematical model is too time consuming; FEOM saves a significant amount of time in obtaining the outputs [18].

The identification of variables which have more influence on the output of a model is achieved through *sensibility and uncertainty analyses*.

There is a variety of areas where HDMR techniques are useful, they have specific applications in chemical kinetics [10, 28, 30-32], in radiation transport [27] in discovery and properties of materials [21, 23, 26] and in statistical analysis [4, 5, 14, 18, 32, 35-37]. It has also been applied to biology [5, 6].

There are two types of HDMR expansions commonly used:

Cut-HDMR - Depends on the value of $f(\mathbf{x})$ on a specific reference point $\hat{\mathbf{x}}$. It is used when an ordered sample of the output $f(\mathbf{x})$ at selected points $\mathbf{x}^{(i)}$ can be done.

RS-HDMR - Depends on the average value of $f(\mathbf{x})$ over the whole domain Ω. It is used when the sampling is randomly done. The component functions are determined by obtaining averages in a group of sample points selected at random over the Ω domain.

The component functions f_0, $f_i(x_i)$, $f_{ij}(x_i, x_j)$, ... are tabular. To obtain an output for a specific input, an interpolation must be done. The HDMR expansion choice depends on the type and amount of input data available. Cut-HDMR is used for ordered points of **x**, and RS-HDMR for randomly generated. When the number of input variables is large, it is more practical to work with the RS-HDMR expansion, although an ordered sampling can be done.

2.1. Obtaining the component functions through Cut-HDMR

A Cut-HDMR expansion can be built when it is possible to use an *ordered sampling* of the output $f(\mathbf{x})$ in selected points of **x** that are distributed in a regular grid, for example, in the case of laboratory data with controlled values of **x**.

For the Cut-HDMR, it is necessary to first establish a reference point $\bar{\mathbf{x}} = (\bar{x}_1, \bar{x}_2, ..., \bar{x}_n)$ selected inside the domain Ω. The Cut-HDMR component functions $f_i(x_i)$, $f_{ij}(x_i, x_j)$, ... are defined along some cut lines, plans, sub-volumes, and so forth, across the reference point $\bar{\mathbf{x}}$ in the Ω domain, hence the name is Cut-HDMR [15]. The optimal component functions in Cut-HDMR have the structure given by [2]:

$$f_0 = f(\bar{\mathbf{x}}), \tag{3}$$

$$f_i(x_i) = f(x_i, \bar{\mathbf{x}}^i) - f_0, \tag{4}$$

$$f_{ij}(x_i, x_j) = f(x_i, x_j, \bar{\mathbf{x}}^{ij}) - f_i(x_i) - f_j(x_j) - f_0, \tag{5}$$

…

where:

$$(x_i, \bar{\mathbf{x}}^i) = (\bar{x}_1, ..., \bar{x}_{i-1}, x_i, \bar{x}_{i+1}, ..., \bar{x}_n),$$

$$(x_i, x_j, \bar{\mathbf{x}}^{ij}) = (\bar{x}_1, ..., \bar{x}_{i-1}, x_i, \bar{x}_{i+1}, ..., \bar{x}_{j-1}, x_j, \bar{x}_{j+1}, ..., \bar{x}_n).$$

The last component function, $f_{12...n}(x_1, x_2, ..., x_n)$, is determined by the difference $f(\mathbf{x})$ minus the rest of the component functions in equation (1).

To find the approximated value of $f(\mathbf{x})$ at any point $x \in \Omega$, it is necessary to interpolate values with component function data tables.

Since $f_i(x_i)$, $f_{ij}(x_i, x_j)$, ... are unknown, one way to approximate these component functions is building a table containing some samples of their actual values and then use interpolation to obtain other values. Then the value of an $f_i(x_i)$ for a given x_i is obtained by an interpolation in one dimension, in a similar way, the $f_{ij}(x_i, x_j)$ for a given pair (x_i, x_j) is an interpolation in two dimensions and so on.

To construct the component function tables, the original function $f(\mathbf{x})$ must be evaluated in repeated occasions fixing some variables and varying others. For example, each component function $f_i(x_i)$ represents the contribution to the total output of one variable. If the number of input variables is *n*, then the table for each $f_i(x_i)$ is obtained by fixing the $n-1$ values of the other variables to the value of the reference point $\bar{\mathbf{x}}$ and varying only x_i with *s* different values, as it is shown in Table 1. The contribution of x_i to the output is then $f_i(x_i) = f(x_i, \bar{\mathbf{x}}^i) - f_0$.

Table 1. Tabular function $f_i(x_i)$

$x_i^{(k)}$	$f_i(x_i^{(k)})$
$x_i^{(1)}$	$f(x_i^{(1)}, \bar{\mathbf{x}}^i) - f_0$
$x_i^{(2)}$	$f(x_i^{(2)}, \bar{\mathbf{x}}^i) - f_0$
...	
$x_i^{(s)}$	$f(x_i^{(s)}, \bar{\mathbf{x}}^i) - f_0$

For the $l = 1$ component functions, there are n different tables. Tables for $f_{ij}(x_i, x_j)$ are of $s_1 \times s_2$ size, where s_1 is the number of values that variable x_i can have, and s_2 is the number of values that variable x_j can have. The values of $f_{ij}(x_i, x_j)$ are obtained by evaluating the function in $f(x_i, x_j, \bar{\mathbf{x}}^{ij})$ and from the tabular functions f_i, f_j previously obtained.

For cooperativity order $l = 2$, one can build $\binom{n}{2} = \frac{n!}{2!(n-2)!}$ different tables, one for each pair of variables. If each input variable takes the same amount of different values s, in other words, if $s_1 = s_2 = s$, then the required number of evaluations of $f(\mathbf{x})$ to construct the tables of all the component functions $f_i(x_i)$, $f_{ij}(x_i, x_j)$, … is

$$1 + ns + \frac{n(n-1)}{2} s^2 + \frac{n(n-1)(n-2)}{3!} s^3 + \cdots + s^n,$$

where n is the number of input variables [9]. It may be noted that the number of function evaluations $f(\mathbf{x})$ is of polynomial complexity with respect to the number of samples n, but it is exponential with regard to the number of variables n, i.e., the *computational cost* grows exponentially with the number of function variables. The computational cost is the number of experiments required to construct the approximate function. However, based on the

fundamental conjecture of the HDMR expansions, it is sufficient to approximate the function $f(\mathbf{x})$ using an order of cooperativity $l = 2$, or in rare cases of order $l = 3$, thus significantly reducing the number of evaluations $f(\mathbf{x})$. This reduces the elaboration of tabular functions from exponential complexity to polynomial complexity. In this case, the *computational cost* grows quadratically. The number of samples required to build the tables $f_{ij}(x_i, x_j)$ is $O(s^2n^2)$, where n is the number of function variables and s is the number of samples of each variable [9].

According to the HDMR fundamental ansatz, there are only tables for variables acting independently, two by two or at most three acting on the output, thus savings on sampling for large values of n are significant compared with traditional sampling s^n. Finally, the problem of evaluating the function $f(\mathbf{x})$ at any arbitrary point $\mathbf{x}$, comes down to constructing tables for component functions with cooperativity order $l = 1$, $l = 2$ (or $l = 3$ in rare cases) and interpolating in 1, 2 (or 3) dimensions.

2.2. Obtaining the component functions through RS-HDMR

The RS-HDMR component functions are mutually orthogonal, i.e., the inner product between any two of them is zero, and they are determined by obtaining the averages on a set of points *randomly sampled* over the domain Ω.

It is necessary to normalize the variables x_i so that $0 \le x_i \le 1$ for $i = 1, 2, ..., n$. The output function $f(\mathbf{x})$ is defined in the unit hypercube

$$K^n = \{(x_1, x_2, ..., x_n) | 0 \le x_i \le 1, i = 1, 2, ..., n\}.$$

The RS-HDMR component functions are defined as follows:

$$f_0 = \int_{k^n} f(\mathbf{x}) d\mathbf{x}, \tag{6}$$

$$f_i(x_i) = \int_{k^{n-1}} f(x_i, \mathbf{x}^i) d\mathbf{x}^i - f_0 \text{ with (a)}, \tag{7}$$

$$f_{ij}(x_i, x_j) = \int_{k^{n-2}} f(x_i, x_j, \mathbf{x}^{ij}) d\mathbf{x}^{ij} - f_i(x_i) - f_j(x_j) - f_0 \text{ with (b),} \quad (8)$$

...

where:

(a) $d\mathbf{x}^i = \prod_{k \neq i} dx_k$,

(b) $d\mathbf{x}^{ij} = \prod_{k \neq i, j} dx_k$.

In a similar way to the Cut-HDMR, the last component function, $f_{12...n}(x_1, x_2, ..., x_n)$, is determined by the difference $f(\mathbf{x})$ minus the rest of the component functions.

It should be noticed that in the RS-HDMR, the domain Ω is a unit hypercube, and f_0 is actually the average value of $f(\mathbf{x})$ over the entire domain, while in the Cut-HDMR, f_0 is the value of $f(\mathbf{x})$ in only one reference point $\bar{\mathbf{x}}$.

The name RS-HDMR comes from *random sampling*. The evaluation of multidimensional integrals in the RS-HDMR expansion can be done by the Monte Carlo method for *integration by random sampling* [19, 25].

Random points in an n-dimensional space $\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N$ are necessary to calculate the integral of a multidimensional function, where the N samples are uniformly distributed. The basic theorem of the Monte Carlo integration over an n-dimensional space is:

$$\int_V f(x_1, x_2, ..., x_n) dv = \int_V dv \cdot \bar{f}(\mathbf{x}) \approx V \cdot \left(\frac{1}{N} \sum_{s=1}^{N} f(\mathbf{x}_s) \right), \quad (9)$$

where V is the n-dimensional space volume.

To build the data tables for the component functions of RS-HDMR, it is necessary to evaluate the integrals:

$$\int_{k^n} f(\mathbf{x})dx, \int_{k^{n-1}} f(\mathbf{x})dx^i, \int_{k^{n-2}} f(\mathbf{x})dx^{ij}, \ldots.$$

For example, N samples of a vector of dimension n, $\mathbf{x}^{(s)} = (x_1^{(s)}, x_2^{(s)}, ..., x_n^{(s)})$, $(s = 1, 2, ..., N)$ in the n-dimension hypercube space K^n are randomly and uniformly generated.

f_0 is the average value of $f(\mathbf{x})$ for all samples $\mathbf{x}^{(s)}$, keeping in mind that one is working within a unit hypercube $(V = 1)$, we can express (3) using (9):

$$f_0 = \int_{k^n} f(\mathbf{x})dx \approx \frac{1}{N}\sum_{s=1}^{N} f(\mathbf{x}^{(s)}). \tag{10}$$

As usual, the integrals of the Monte Carlo method converge very fast; a relatively small value of N gives a very good result. Very often, the approximation of the integral by the Monte Carlo method does not significantly depend on the dimension n of the vector $\mathbf{x}$. This is very useful when working with multidimensional systems, i.e., models with a large number of input variables [17]. However, the direct determination of all component functions of RS-HDMR expansion involves integrating each $f(\mathbf{x})dx^i$, $f(\mathbf{x})dx^{ij}$, … with N samples for each integral, this means that it requires a lot of random samples. For example, for functions with cooperativity order $l = 1$, it is necessary to make N samples of $f(x_i, \mathbf{x}^i)$ in the points $(x_i, \mathbf{x}^i)^{(s)} = (x_1^{(s)}, x_2^{(s)}, ..., x_{i-1}^{(s)}, x_i, x_{i+1}^{(s)}, ..., x_n^{(s)})$ for different grid fixed values of x_i [29], in this way, we can express (4) using (9) as follows:

$$f_i(x_i) = \int_{k^{n-1}} f(\mathbf{x})d\mathbf{x}^i - f_0 \approx \frac{1}{N}\sum_{s=1}^{N} f((x_i, \mathbf{x}^i)^{(s)}) - \frac{1}{N}\sum_{s=1}^{N} f(\mathbf{x}^{(s)}). \tag{11}$$

When n is large, it is not worth spending the time to obtain the RS-HDMR component functions because the sampling effort is very high. To

construct a tabular function, we need to define N_1 fixed values, for each x_i it is required a set of samples large enough to obtain a good accuracy. Let N_2 be the size of this set. Suppose there are N_1 fixed values for each variable and that there are *n* variables. The number of samples that are needed is then $N_1 \cdot x \cdot N_2 \cdot x \cdot n$. The number of random samples required grows exponentially with the RS-HDMR component functions cooperativity order: *l*. One way to reduce the large sampling effort is to *approximate the component functions with orthonormal polynomials*. The use of orthonormal polynomials can provide savings of around 10^3 in the sampling effort to represent a multivariable function compared with using a direct sampling technique [17].

3. Representation of RS-HDMR through Orthonormal Polynomials

When direct determination of the RS-HDMR component functions is done by sampling the output function $f(\mathbf{x})$ in a regular net to evaluate the integrals with the Monte Carlo approach, the sampling effort would become prohibitively expensive. The approximation of the component functions to an analytic function greatly reduces the sampling effort. Li et al. [17] proposed the approximation of component functions to an analytic function represented by orthonormal polynomials. A component function $f(x_i)$ can be approximated to a sum of *k* different functions of the same variable x_i called *basis functions*, each multiplied by a constant coefficient α_r^i, as follows:

$$f_i(x_i) \approx \sum_{r=1}^{k} \alpha_r^i \varphi_r(x_i), \tag{12}$$

and in the case of two variable functions:

$$f_{ij}(x_i, x_j) \approx \sum_{p=1}^{l} \sum_{q=1}^{l'} \beta_{pq}^{ij} \varphi_p(x_i) \varphi_q(x_j), \tag{13}$$

where k, l and l' represent the polynomial expansion order. With (12) and (13), equation (1) can be expressed as [17]:

$$f(\mathbf{x}) \approx f_0 + \sum_{i=1}^{n}\sum_{r=1}^{k} \alpha_r^i \varphi_r(x_i) + \sum_{1\le i<j\le n}\sum_{p=1}^{l}\sum_{q=1}^{l'} \beta_{pq}^{ij}\varphi_{pq}(x_i, x_j) + \cdots. \quad (14)$$

The constant coefficients α_r^i and β_{pq}^{ij} are determined by a minimization process and the Monte Carlo integration [15]. Each set of coefficients $\varepsilon \in \{\alpha_r^i, \beta_{pq}^{ij}, ...\}$ for the basis functions with the same variables can be obtained by solving the linear equation:

$$\mathbf{Ay} = \mathbf{b}, \quad (15)$$

where **A** is a non-singular matrix of constants, **y** is the vector of coefficients for the basis functions associated with the same variables and **b** is a vector whose elements are integrals on the product of $f(\mathbf{x})$ with the basis functions.

The matrix **A** and vector **b** terms are obtained with the technique described by [17]. They determined the constant coefficients α_r^i by:

$$\alpha_r^i = \int_{k^n} f(\mathbf{x})\varphi_r(x_i)dx \approx \frac{1}{N}\sum_{s=1}^{N} f(\mathbf{x}^{(s)})\varphi_r(x_i^{(s)}). \quad (16)$$

When we evaluate the polynomial $\varphi_r(x)$ in the value x_i of the sample "s", we obtain $\varphi_r(x_i^{(s)})$ of equation (16). With a sample of size N, cooperativity order $l = 1$ component functions: $f_i(x_i)$ were obtained.

Using orthonormal polynomials, the required number of uniformly distributed samples is N instead of $N_1 \cdot x \cdot N_2 \cdot x \cdot n$ required for RS-HDMR as explained at the end of Subsection 2.2. Although N still needs to be large enough to obtain good accuracy, [17] showed that this number is not very high. The main advantage of this method is the independency of n and N, which are normally non-low numbers.

The accuracy of an approximation using orthonormal polynomials depends on the polynomial order used. In many cases, the polynomials of first, second and third order: $\varphi_1(x)$, $\varphi_2(x)$, $\varphi_3(x)$ are enough to obtain adequate accuracy [17, 18, 30, 35, 36]. In equation (16), φ_r are the components of the orthonormal basis obtained. The basis shown in equations (17), (18) and (19) was obtained following the Gram-Schmidt orthonormalization process [9] up to order 3:

$$\varphi_1(x) = \sqrt{3}(2x - 1), \tag{17}$$

$$\varphi_2(x) = 6\sqrt{5}\left(x^2 - x + \frac{1}{6}\right), \tag{18}$$

$$\varphi_3(x) = 20\sqrt{7}\left(x^3 - \frac{3}{2}x^2 + \frac{3}{5}x + \frac{1}{20}\right). \tag{19}$$

The accuracy of the resulting HDMR functions depends on the size of the sample N, since the Monte Carlo integration error decreases approximately in $1/\sqrt{N}$ [19]. The number of samples N that provides the desired accuracy for a specific application must be found experimentally (variation of N until obtained the desired accuracy).

Li et al. [17] used equation (20) to obtain the cooperativity order $l = 2$ component functions $f_{ij}(x_i, x_j)$ with the same orthonormal basis $\varphi_1(x)$, $\varphi_2(x)$, $\varphi_3(x)$ in equations (17), (18) and (19):

$$\beta_{pq}^{ij} = \int_{k^n} f(\mathbf{x})\varphi_p(x_i)\varphi_q(x_j)dx \approx \frac{1}{N}\sum_{s=1}^{N} f(\mathbf{x}^{(s)})\varphi_p(x_i^{(s)})\varphi_q(x_j^{(s)}). \tag{20}$$

Using a third order polynomial expansion, the number of coefficients β_{pq}^{ij} which are necessary to calculate for an n input variable system is $3^2 n(n-1)/2$ and the number of calculated α_r^i is $3n$.

The system's model is a tabular function, then to find the value of function $f(\mathbf{x})$ at any given point $(x_1, x_2, ..., x_n)$, it is necessary to

interpolate. However, with the component function approximation using orthonormal polynomials, the fully equivalent operational model is given by equation (14).

So, to get the value of the function $f(\mathbf{x})$ at any point, it is not necessary to interpolate, but only to evaluate equation (14) at a given point $(x_1, x_2, ..., x_n)$.

4. Uncertainty and Sensibility Analyses by HDMR Expansions

4.1. Variance decomposition in the HDMR expansions and its relation with uncertainty analysis

In the HDMR approach, σ_i^2 is the contribution to the total variance $\sigma_{\bar{f}}^2$ of the acting single variables x_i and σ_{ij}^2 is the contribution to $\sigma_{\bar{f}}^2$ of the correlated variables x_i, x_j. Also, σ_i^2 is independent from σ_{ij}^2 [18]. Using the definition of variance and expressing $f(\mathbf{x})$ as the expansion of equation (1):

$$\sigma_{\bar{f}}^2 = \int_{k^n} [f(\mathbf{x}) - \bar{f}]^2 dx = \int_{k^n} [f(\mathbf{x}) - f_0]^2 dx$$

$$= \int_{k^n} \left[\sum_{i=1}^{n} f_i(x_i) + \sum_{1 \le i < j \le n} f_{ij}(x_i, x_j) + \cdots \right]^2 dx,$$

where $\bar{f}$ is the mean of $f(\mathbf{x})$ over the whole domain Ω.

The HDMR component functions are mutually orthogonal, in other words, any two component functions satisfy:

$$f_{i_1 i_2 \cdots i_l}(x_{i_1}, x_{i_2}, ..., x_{i_l}) f_{j_1 j_2 \cdots j_k}(x_{j_1}, x_{j_2}, ..., x_{j_k}) \big|_{x_s = \bar{x}_s} = 0,$$

$$s \in \{i_1, i_2, ..., i_l\} \cup \{j_1, j_2, ..., j_k\}.$$

So, if any of the $x_{i_1}, x_{i_2}, ..., x_{i_l}$ or the $x_{j_1}, x_{j_2}, ..., x_{j_l}$ is equal to the corresponding x of the reference vector $\bar{\mathbf{x}}$, then the product is zero [2]. Because of the HDMR component functions orthogonality, the products among them are zero, and then we have only the following terms (keeping in mind that K^n is a unit hypercube):

$$\sigma_f^2 = \sum_{i=1}^{n} \int_0^1 f_i^2(x_i)dx_i + \sum_{1\le i<j\le n} \int_0^1\int_0^1 f_{ij}^2(x_i, x_j)dx_i dx_j + \cdots$$

$$= \sum_{i=1}^{n} \sigma_i^2 + \sum_{1\le i<j\le n} \sigma_{ij}^2 + \cdots.$$

The total variance σ_f^2 of $f(\mathbf{x})$ caused by all the input variables can be decomposed into the sum of contributions of each of the input variables because component functions are independent and each one provides unique information about how it affects the relationship between the input variables to the output properties:

$$\sigma_f^2 = \sum_{i=1}^{n} \sigma_i^2 + \sum_{1\le i<j\le n} \sigma_{ij}^2 + \cdots. \tag{21}$$

The property (21) given by [18] is valid over the entire domain and is very useful for global sensibility and uncertainty analyses, since component functions variance can be interpreted directly as the importance of the input variables involved. Balakrishnan et al. [4] conducted a study which showed that uncertainty analysis results obtained with the Monte Carlo method were practically the same as the results obtained with HDMR uncertainty analysis, however, while with the Monte Carlo method 1000 samples were used, for the HDMR method, only 45 FEOM results were used. Li et al. [18] demonstrated that with HDMR, a few hundred random samples are enough to provide reliable uncertainty assessments over the input region.

Using HDMR has two advantages: first: it requires a much smaller number of samples $\mathbf{x}^{(s)}$, and second, once we have the $f(\mathbf{x}^{(s)})$ one can build FEOM and get results faster which are very similar to the results obtained from the complete model [11, 24, 27, 28].

Using equation (21), one can determine which model variables are the most important and how they interact with each other. Analyzing the total variance $\sigma^2_{\bar{f}}$ components magnitudes: $\sigma^2_i, \sigma^2_{ij}, ...,$ one can find how much each of the input variables uncertainties influences the total output uncertainty, since each variable uncertainty is directly proportional to its variance.

The next section shows the usefulness of the property in equation (21) for the sensibility analysis of multidimensional functions.

4.2. Global sensibility analysis with HDMR

Sensibility analysis provides information of the effect of each variable in the model over its output, both when they act independently and when two or more act together. In other words, this analysis can identify which set of input variables affects the model outputs most.

The identification of key variables through a sensibility analysis, in a system modeled by a multidimensional function, allows us to eliminate the variables that are not important; considering them as system parameters. When those variables, whose variance is minimal, are considered as parameters, the number of variables involved in the model is reduced without reducing its quality [18]. This is very useful, since it decreases the computational load and sampling effort, x_i can be fixed and thus reducing the dimensionality of the model.

Another purpose of doing sensibility analysis is the validation of the model, i.e., to determine if its predictions are reasonable and if they correspond to the observed data. This indicates which variables are necessary to continue working to improve quality of the model predictions.

When we have small models, in most cases, it is possible to determine the influence of each of the variables in the results with an analysis of the model equations. However, when many variables are involved, these relationships are not so obvious. In these cases, performing a *sensibility analysis* is very useful. A *global sensibility analysis* explores the interactions between variables in the entire space of input variables, while the *local sensibility analysis* can only be applied when the uncertainties of the input space are small, as in the case where the input parameters are well known or when the model is not highly non-linear. When the uncertainties of the input space are large, the sensibilities obtained with local analysis are often not representative of all input space regions [35].

The global sensibility analysis methods usually treat the model as a black box; wide areas are explored within the space of input variables. But this approach has the disadvantage of requiring a large number of model runs, particularly, when the effects of these variables acting together are investigated. HDMR tools can efficiently perform global sensibility analysis for multidimensional models overcoming the complexity and the computational cost.

If we get σ_i^2, σ_{ij}^2, … with HDMR approach, then it is also possible to determine the kind of cooperativity that exists between input variables. If the second order variances: σ_{ij}^2 are negligible, the cooperativity order l of system is 1, on the contrary, if there are terms σ_{ij}^2 of considerable size, then the cooperativity order l is 2. In addition, one can set a threshold to eliminate component function whose contribution to output is negligible [36] and therefore is not important to include it in the HDMR expansion.

Li et al. [18] found that the effect of variables acting independently is much higher than the variables' effect with cooperativity order $l = 2$ and this has been confirmed in a considerable amount of research where HDMR has been applied: [4, 18, 30, 35, 36], among others. It has been observed that the contribution to the total variance of the partial variances with $l = 1$ is

much higher than that of the partial variances with $l = 2$ contributions, this is: $\sum \sigma_i^2 \gg \sum \sigma_{ij}^2$ and so on, i.e., $\sum \sigma_i^2 \gg \sum \sigma_{ij}^2 \gg \sum \sigma_{ijk}^2 \cdots$.

Therefore, based on the fundamental conjecture of the HDMR expansions [2], we will analyze only the σ_i^2 and σ_{ij}^2, in other words, we will assume a cooperativity order $l = 2$ to find the key model variables.

The Monte Carlo method is a good way to evaluate the integrals $\int f_i^2(x_i)dx_i$ and $\int\int f_{ij}^2(x_i, x_j)dx_i dx_j$, which are used to obtain each variance σ_i^2 and σ_{ij}^2 [18]. If N samples are randomly generated from an input vector of dimension n, then using the Monte Carlo method for calculating the f_0 component function (equation (10)), the total variance can be expressed as in equation (22):

$$\sigma_{\bar{f}}^2 = \int_{k^n} [f(\mathbf{x}) - f_0]^2 d\mathbf{x} \approx \frac{1}{N}\sum_{s=1}^{N} f^2(\mathbf{x}^{(s)}) - f_0^2. \tag{22}$$

When $N \to \infty$, accurate values of f_0 and $\sigma_{\bar{f}}$ are obtained. However, frequently f_0 and $\sigma_{\bar{f}}$ converge quite rapidly and a modest value of N can give very good results [18]. The effort to build the component function tables grows exponentially with the number of variables, so it is better to use orthonormal polynomials when calculating them.

An important finding of [18] is the fact that all input variables' variances obtained from different sized samples are basically the same. This provides the possibility of reducing the sampling effort without impairing the quality of results.

Sensibility analysis with HDMR has also proven to be useful even when the input variables cannot be determined very accurately due to nature of the studied system, i.e., when there are significant uncertainties [5].

4.3. Sensibility analysis by orthonormal polynomials

Determining the constant coefficients α_k^i and β_{pq}^{ij} according to

equations (16) and (20) of Section 3, σ_i^2 and σ_{ij}^2 can be obtained using the orthonormal property of the basis formed by $\varphi_k(x_i)$, with $k = 1, 2, 3$ as follows [18]:

$$\sigma_i^2 = \int_0^1 f_i^2(x_i)dx_i \approx \int_0^1 \left[\sum_{k=1}^{3} \alpha_k^i \varphi_k(x_i)\right]^2 dx_i$$

$$= (\alpha_1^i)^2 \int_0^1 \varphi_1^2(x_i)dx_i + (\alpha_2^i)^2 \int_0^1 \varphi_2^2(x_i)dx_i + (\alpha_3^i)^2 \int_0^1 \varphi_3^2(x_i)dx_i,$$

$$\sigma_i^2 \approx \sum_{k=1}^{3} (\alpha_k^i)^2, \tag{23}$$

similarly:

$$\sigma_{ij}^2 = \int_0^1 \int_0^1 f_{ij}^2(x_i, x_j)dx_i dx_j \approx \int_0^1 \int_0^1 \left[\sum_{p=1}^{3}\sum_{q=1}^{3} \beta_{pq}^{ij} \varphi_p(x_i)\varphi_q(x_j)\right]^2 dx_i dx_j$$

$$= \sigma_{ij}^2 \approx \sum_{p=1}^{3}\sum_{q=1}^{3} (\beta_{pq}^{ij})^2. \tag{24}$$

Only one reasonably sized set of random samples of $f(\mathbf{x})$ is necessary to determine f_0 and all the coefficients $\alpha_k^i, \beta_{pq}^{ij}, \ldots$ for the expansion $f_i(x_i), f_{ij}(x_i, x_j), ...,$ therefore only one set of random samples is needed to determine $\sigma_{\bar{f}}^2$, σ_i^2 and σ_{ij}^2 [18].

The system output total variance $\sigma_{\bar{f}}^2$ is obtained with equation (21). The total variance is approximated using $l = 2$, as in [18, 35]:

$$\sigma_{\bar{f}}^2 \approx \sum_{i=1}^{n} \sigma_i^2 + \sum_{1 \le i < j \le n} \sigma_{ij}^2. \tag{25}$$

The first order variances $\sum_{i=1}^{n} \sigma_i^2$ measure the contributions of the variables x_i to the output function total variance, and the second order variances $\sum_{1 \le i < j \le n} \sigma_{ij}^2$ measure how the output function is affected by the interaction between the variables x_i and x_j.

Once the total variance $\sigma_{\bar{f}}^2$ and the partial variances σ_i^2, σ_{ij}^2 are obtained, the sensibility indexes S_i and S_{ij} can be obtained normalizing the partial variances with the total variance as follows [14, 35]:

$$S_i = \frac{\sigma_i^2}{\sigma_{\bar{f}}^2}, \tag{26}$$

$$S_{ij} = \frac{\sigma_{ij}^2}{\sigma_{\bar{f}}^2}. \tag{27}$$

By equation (25), the sum of all sensibility indexes is not exactly one; however, this amount is very close to unity. This small discrepancy is due to the Monte Carlo error in the calculation of α_r^i and β_{pq}^{ij} (equations (16) and (20)) [35]:

$$\sum_{i=1}^{n} S_i + \sum_{1 \le i < j \le n} S_{ij} = \frac{1}{\sigma_{\bar{f}}^2} \left(\sum_{i=1}^{n} \sigma_i^2 + \sum_{1 \le i < j \le n} \sigma_{ij}^2 \right) \approx 1. \tag{28}$$

The Monte Carlo error can be reduced by increasing the sample size *N*. The relevance of each input variable for the model output can be determined classifying the variables according to their sensibility index: from highest to lowest. In summary, the first order sensibility index S_i measures the effect of

a single input variable x_i over the output and the second order sensibility index S_{ij} measures the effect of the interaction between variables x_i and x_j over the output.

5. Conclusions

Sensibility and uncertainty analyses help us identify where the efforts have to be focused in order to improve a model's quality and they are very useful when working with models where a large number of variables are involved, however, performing analyses such as these in multidimensional systems is extremely expensive and therefore the result may not be viable because of two significant aspects: (i) the interpretation of results is too complicated and (ii) obtaining results from the numerous samples that are required is computationally intensive.

When the HDMR expansions are used for sensibility and uncertainty analyses, the number of samples needed is much lower than the one required by other methods and the results' interpretation is simple even in models with many variables. With the results of these analyses, the number of involved variables can be reduced and the process for obtaining the system outputs can be accelerated.

On the other hand, once we have the HDMR component functions, an FEOM (fully equivalent operational model) can be built and produce faster results very close to those obtained with the complete model of the system. The reliability assessment of the mathematical-computational model of a physical system, which is normally done through the uncertainty and sensibility analyses, can be accomplished with the HDMR tools when working with systems in which the number of variables involved prohibit using other methods of analyses, the foregoing is helpful for researchers who work with multidimensional models in any area of engineering or physics.

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