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An effective approximation for variance-based global sensitivity analysis

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ABSTRACT

The paper presents a fairly efficient approximation for the computation of variance-based sensitivity measures associated with a general, n-dimensional function of random variables. The proposed approach is based on a multiplicative version of the dimensional reduction method (M-DRM), in which a given complex function is approximated by a product of low dimensional functions. Together with the Gaussian quadrature, the use of M-DRM significantly reduces the computation effort associated with global sensitivity analysis. An important and practical benefit of the M-DRM is the algebraic simplicity and closed-form nature of sensitivity coefficient formulas. Several examples are presented to show that the M-DRM method is as accurate as results obtained from simulations and other approximations reported in the literature.

1. Introduction

1.1. Motivation

In the context of a probabilistic analysis, the system response is typically represented by a function of random variables. The sensitivity of the response to input random variables can be quantified by the contribution of a random variable to the total variance of the response. This is the essence of the variance-based global sensitivity analysis in the literature [1]. The analytical basis for the global sensitivity analysis comes from ANOVA (Analysis of Variance) decomposition of the response variance [2]. Although ANOVA decomposition is conceptually simple, the computation of variance components of a general response function is rather a challenging task. The reason is that it involves a series of high-dimensional integrations for each global sensitivity coefficient. Therefore, the minimization of computational efforts is a primary area of research in the variance-based global sensitivity analysis, and several studies have already been presented in the literature.

The Monte Carlo simulation is the most effective method for global sensitivity analysis of a general response function. Smart simulation algorithms have been developed to evaluate high-dimensional integrals [3,4]. In case of a complex model however, the simulation method can be so time consuming that it can deter applications of sensitivity analysis in day to day engineering practice. This has motivated the development of simple approximations for the sensitivity analysis.

The most popular approach is based on the concept of high dimensional model representation (HDMR) [5], in which a complex function is decomposed into a hierarchy of low dimensional functions in an additive expansion. The HDMR basically creates a surrogate model, which simplifies the computation [6]. Tarantola et al. [7] proposed the random balance design (RBD) for sensitivity analysis of a nuclear waste disposal system. Sudret [8] reviewed polynomial chaos expansion on surrogate model construction, in which computation of global sensitivity coefficients is directly related to expansion coefficients of a PCE model [9]. Given the vast literature related to sensitivity analysis, the readers are referred to monographs for a detailed review of methods of sensitivity analysis [10,11].

1.2. Objective

The main objective of this paper is to simplify the variance-based global sensitivity analysis using the multiplicative dimensional reduction method (M-DRM), which is an alternative to a more commonly used additive DRM method. The univariate M-DRM approximates a complex function of random variables by a product of one-dimensional functions. This approach significantly

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reduces the computational efforts associated with the variance-based global sensitivity analysis. Another advantage of M-DRM is that simple algebraic expressions can be derived for primary, joint-variate and total sensitivity coefficients, which are easy to use in practice.

1.3. Organization

The paper is organized as follows. Section 2 summarizes the background of the sensitivity analysis and introduces key definitions and notations. Section 3 presents a multiplicative dimensional reduction method (M-DRM) to approximate high-dimensional integrals associated with the variance analysis. Six examples taken from the literature are analyzed using M-DRM in Section 4, which confirm comparable accuracy of M-DRM solutions. Section 5 presents the conclusions, and computational details are given in Appendices.

2. Background

2.1. Definitions

The random response of a system, Y, depends on a vector of n independent random variables, $\mathbf{X}=[X_1, X_2, \ldots, X_n]^{\mathrm{T}}$, via a functional relationship: $Y=h(\mathbf{X})$. The joint density of $\mathbf{X}$ is denoted as $f_{\mathbf{X}}(\mathbf{x})$. The expectation operation is denoted as $E[\cdot]$. Occasionally, a subscript is used to denote the random variable (or a vector) with respect to which the expectation operation is carried out. The mean and variance of Y are defined in the usual ways as

$$\begin{cases} \mu_Y = E_{\mathbf{X}}[Y] = \int_{\mathbf{X}} h(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x})\, d\mathbf{x} \\ V_Y = E_{\mathbf{X}}[(Y-\mu_Y)^2] = E_{\mathbf{X}}\{[h(\mathbf{X})]^2\} - \mu_Y^2 = \mu_{2Y} - \mu_Y^2 \end{cases} \tag{1}$$

Note that μ_{2Y} is the second moment of the response Y.

We define a sub-vector $\mathbf{X}_{-i}$ of $(n-1)$ elements, which contains all the elements of $\mathbf{X}$ except X_i. Similarly, $\mathbf{X}_{-ij}$ is a vector of $(n-2)$ elements without X_i and X_j. Since the mathematical formulation extensively utilizes the concept of conditional expectation, it is defined in a more compact way. We define two conditional expectations: Y given $X_i{=}x_i$ and Y given $X_i=x_i, X_j=x_j$ as

$$\begin{cases} \alpha_i(x_i) = E_{-i}[Y|X_i] = \int_{\mathbf{X}_{-i}} h(\mathbf{x}_{-i}, x_i) f_{\mathbf{X}_{-i}}(\mathbf{x}_{-i})\, d\mathbf{x}_{-i} \\ \alpha_{ij}(x_i, x_j) = E_{-ij}[Y|X_i, X_j] = \int_{\mathbf{X}_{-ij}} h(\mathbf{x}_{-ij}, x_i, x_j) f_{\mathbf{X}_{-ij}}(\mathbf{x}_{-ij})\, d\mathbf{x}_{-ij} \end{cases} \tag{2}$$

by which one can define other high-order conditional expectations. It should be noted that expectations of, i.e., α_i and α_{ij}, etc., are equal to the expected value of Y itself:

$$E_i[\alpha_i(X_i)] = \mu_Y, \quad E_{ij}[\alpha_{ij}(X_i, X_j)] = \mu_Y, \quad \ldots \tag{3}$$

We can also define the zero mean version of these conditional expectations as

$$\begin{cases} \beta_i(x_i) = E_{-i}[Y|X_i] - \mu_Y = \alpha_i(x_i) - \mu_Y \\ \beta_{ij}(x_i, x_j) = E_{-ij}[Y|X_i, X_j] - \beta_i(x_i) - \beta_j(x_j) - \mu_Y \\ \qquad\qquad = \alpha_{ij}(x_i, x_j) - \alpha_i(x_i) - \alpha_j(x_j) + \mu_Y \qquad (\forall j > i) \\ \ldots \end{cases} \tag{4}$$

In addition to zero mean, these functions are orthogonal if X_i are independent, i.e., $E[\beta_{\mathbf{p}_1} \cdot \beta_{\mathbf{p}_2}] = 0$ (for $\mathbf{p}_1 \neq \mathbf{p}_2$) [5]. Based on these two properties, the function, $Y=h(\mathbf{X})$, can be decomposed into a sum of functions of increasing dimensions:

$$h(\mathbf{X}) = \mu_Y + \sum_{k=1}^{n} \beta_i(X_i) + \sum_{i<j} \beta_{ij}(X_i, X_j) + \sum_{i<j<k} \beta_{ijk}(X_i, X_j, X_k) + \cdots + \beta_{12\cdots n}(\mathbf{X}) \tag{5}$$

In the literature, this decomposition is referred to as high-dimensional model reduction (HDMR) [5] or ANOVA decomposition [2]. In general, a satisfying approximation of $Y=h(\mathbf{X})$ can be achieved by this expansion limited to univariate terms only, i.e., $\beta_i(X_i)$, or at most to bivariate terms $\beta_{ij}(X_i, X_j)$.

2.2. Variance-based sensitivity measures

Following the decomposition in Eq. (5), the total variance of Y can also be decomposed as

$$V_Y = \sum_{i=1}^{n} V_i + \sum_{i<j} V_{ij} + \cdots \tag{6}$$

where

$$V_i = E_i[\beta_i^2(X_i)], \quad V_{ij} = E_{ij}[\beta_{ij}^2(X_i, X_j)], \ldots \tag{7}$$

V_i can be interpreted as the expected reduction in the variance V_Y obtained as a result of fixing X_i. It is also referred to as primary (or main) effect. Similarly, V_{ij} is the effect of interaction between X_i and X_j on V_Y.

Computation of the primary variance, V_i, for example, can be formulated as

$$V_i = E_i[\beta_i^2(X_i)] = \int_{X_i} [\alpha_i(x_i) - \mu_Y]^2 f_i(x_i)\, dx_i = E_i[\alpha_i^2(X_i)] - \mu_Y^2 \tag{8}$$

in which

$$E_i[\alpha_i^2(X_i)] = \int_{X_i} \left(\int_{\mathbf{X}_{-i}} h(\mathbf{x}) f_{\mathbf{X}_{-i}}(\mathbf{x}_{-i})\, d\mathbf{x}_{-i} \right)^2 f_i(x_i)\, dx_i \tag{9}$$

For a general setting about high-order variance components, one can refer to Appendix A for details.

In a compact form, the primary sensitivity coefficient, S_i, can be expressed as [12–14]

$$S_i = \frac{V_i[E_{-i}(Y|X_i)]}{V_Y} = \frac{E_i[\beta_i^2(X_i)]}{V_Y} = \frac{E_i[\alpha_i^2(X_i)] - \mu_Y^2}{V_Y}, \quad 0 \le S_i \le 1 \tag{10}$$

With this definition, all sensitivity indices can be derived, and added up to one:

$$\sum_{i=1}^{n} S_i + \sum_{i<j} S_{ij} + \sum_{i<j<k} S_{ijk} + \cdots + S_{12\cdots n} = 1 \tag{11}$$

The concept of the total sensitivity index was first proposed by Homma and Saltelli [15], which focuses on the reduction in variance should all input variables but X_i be fixed. This reduction in variance is defined as $V_{-i}[E_i(Y|\mathbf{X}_{-i})]$. Thus, remaining variance of Y after fixing X_i is given as

$$V_{Ti} = V_Y - V_{-i}[E_i(Y|\mathbf{X}_{-i})] \tag{12}$$

Together with the identity of total variance, $V_Y = V_{-i}[E_i(Y|\mathbf{X}_{-i})] + E_{-i}[V_i(Y|\mathbf{X}_{-i})]$, the total sensitivity index can be derived as

$$S_{Ti} = \frac{V_Y - V_{-i}[E_i(Y|\mathbf{X}_{-i})]}{V_Y} = \frac{E_{-i}[V_i(Y|\mathbf{X}_{-i})]}{V_Y} \tag{13}$$

3. Computation of sensitivity coefficients

Although ANOVA decomposition of Y is conceptually simple, its computation in a general setting is a challenging task as it involves two-layer high-dimensional integrations for each of the sensitivity coefficient. For example, computation of V_i involves first the computation of an $(n-1)$ dimensional integration for $\alpha_i(x_i) = E_{-i}[Y|X_i]$ in Eq. (2), and then another integration associated with $E_i[\beta_i^2(X_i)]$ as shown in Eq. (7). The complexity of integration increases with number of interaction terms in the sensitivity coefficients, e.g., S_{ij}, as shown in Appendix A.

Monte Carlo simulation is the most effective method to evaluate such high-dimensional integrals, and various smart schemes have been developed in the literature for this purpose

[3,4]. Nevertheless, it is recognized that simulation method can be computationally expensive and time consuming in case of a complex model. This is motivated by the development of simple approximations to substitute or simplify the evaluation of ANOVA functions.

The most popular approximation is called cut-HDMR, in which the corresponding deterministic model, $y=h(\mathbf{x})$, is written with reference to a fixed input point, i.e., $\mathbf{x}=\mathbf{c}$, referred to as the cut point with coordinates $\mathbf{c}$. For example, an ith univariate function is defined by fixing all input variables, but x_i, to their respective cut point coordinates such that

$$h_i(x_i)=h(c_1,\ldots,c_{i-1},x_i,c_{i+1},\ldots,c_n) \tag{14}$$

Based on the univariate cut functions, the following additive approximation for Y is most commonly used in the literature:

$$h(\mathbf{x})\approx\sum_{i=1}^{n}h_i(x_i)-(n-1)h_0 \tag{15}$$

where $h_0=h(c_1,c_2,\ldots,c_n)$ is a constant.

3.1. Multiplicative dimensional reduction method

Instead of the conventional DRM (C-DRM), we propose to utilize a multiplicative form of dimensional reduction method for sensitivity analysis, referred to as M-DRM [16]. Appendix B summarized the details of M-DRM involving only univariate cut functions. It approximates the original function $y=h(\mathbf{x})$ as

$$h(\mathbf{x})\approx h_0^{1-n}\cdot\prod_{i=1}^{n}h(x_i,\mathbf{c}_{-i}) \tag{16}$$

In order to write compact mathematical expressions in subsequent sections, we denote the mean and mean square of a kth one dimensional function as ρ_k and θ_k, respectively, which are defined as

$$\begin{cases}\rho_k=E_k[h_k(X_k)]=\int_{X_k}h(c_1,\ldots,c_{k-1},x_k,c_{k+1},\ldots,c_n)f_k(x_k)\,\mathrm{d}x_k\\ \theta_k=E_k\{[h_k(X_k)]^2\}=\int_{X_k}[h(c_1,\ldots,c_{k-1},x_k,c_{k+1},\ldots,c_n)]^2f_k(x_k)\,\mathrm{d}x_k\end{cases} \tag{17}$$

A nice thing about M-DRM is that any expectation operation can be neatly separated in univariate integrals. The mean of Y can be approximated as

$$\mu_Y\approx\hat{\mu}_Y=E_{\mathbf{X}}\left[h_0^{1-n}\cdot\prod_{k=1}^{n}h_k(X_k)\right]=h_0^{1-n}\cdot\prod_{k=1}^{n}E_k[h_k(X_k)]=h_0^{1-n}\cdot\prod_{k=1}^{n}\rho_k \tag{18}$$

Similarly, the mean square of Y can be approximated as

$$E[Y^2]=\mu_{2Y}\approx E_{\mathbf{X}}\left[\left(h_0^{1-n}\cdot\prod_{k=1}^{n}h_k(X_k)\right)^2\right]=h_0^{2-2n}\cdot\prod_{k=1}^{n}\theta_k \tag{19}$$

Thus, the variance of Y can be obtained as

$$V_Y=\mu_{2Y}-\mu_Y^2\approx h_0^{2-2n}\cdot\left(\prod_{k=1}^{n}\theta_k-\prod_{k=1}^{n}\rho_k^2\right)=\hat{\mu}_Y^2\cdot\left[\left(\prod_{k=1}^{n}\theta_k/\rho_k^2\right)-1\right] \tag{20}$$

3.2. Primary sensitivity coefficients

Under the M-DRM approximation, an ith conditional expectation function, $\alpha_i(x_i)$, can be easily evaluated as

$$\alpha_i(x_i)=E_{-i}[h(\mathbf{X})]\approx E_{-i}\left[h_0^{1-n}\cdot\prod_{k=1}^{n}h_k(x_k)\right]=h_0^{1-n}\cdot h_i(x_i)\cdot\prod_{k=1,k\neq i}^{n}\rho_k$$

Now, the second moment of $\alpha_i(x_i)$ can be derived as

$$E_i[\alpha_i^2(X_i)]\approx\int_{X_i}\left(h_0^{1-n}\cdot h_i(x_i)\cdot\prod_{k=1,k\neq i}^{n}\rho_k\right)^2f_i(x_i)\,\mathrm{d}x_i \tag{21}$$

The final result is

$$E_i[\alpha_i^2(X_i)]\approx h_0^{2-2n}\cdot\theta_i\cdot\prod_{k=1;k\neq i}^{n}\rho_k^2=\hat{\mu}_Y^2\cdot\theta_i/\rho_i^2 \tag{22}$$

Using Eq. (18), the primary variance component, V_i, can be expressed as

$$V_i=E_i[\alpha_i^2(X_i)]-\mu_Y^2\approx\hat{\mu}_Y^2\cdot(\theta_i/\rho_i^2-1) \tag{23}$$

Using Eq. (20), the primary sensitivity index can be approximated as

$$S_i=\frac{V_i}{V_Y}\approx\frac{\theta_i/\rho_i^2-1}{(\prod_{k=1}^{n}\theta_k/\rho_k^2)-1} \tag{24}$$

On the computation of other high-order sensitivity coefficients, i.e., S_{ij}, S_{ijk}, etc., one can refer to Appendix C for details.

3.3. Total sensitivity coefficients

To evaluate the total sensitivity index, S_{Ti}, first we need to compute the following conditional variance:

$$V_i[Y|\mathbf{X}_{-i}]=E_i[Y^2|\mathbf{X}_{-i}]-[E_i(Y|\mathbf{X}_{-i})]^2 \tag{25}$$

Using the M-DRM, the expectations in the right hand side of Eq. (25) can be approximated as

$$E_i[Y^2|\mathbf{X}_{-i}]\approx h_0^{2-2n}\cdot\left(\prod_{k=1,k\neq i}^{n}[h_k(x_k)]^2\right)\cdot\theta_i \tag{26}$$

and

$$[E_i(Y|\mathbf{X}_{-i})]^2\approx h_0^{2-2n}\cdot\left(\prod_{k=1,k\neq i}^{n}[h_k(x_k)]^2\right)\cdot\rho_i^2 \tag{27}$$

Finally, the conditional variance is obtained as

$$V_i[Y|\mathbf{X}_{-i}]\approx h_0^{2-2n}\cdot\left(\prod_{k=1,k\neq i}^{n}\theta_k\right)\cdot(\theta_i-\rho_i^2) \tag{28}$$

Subsequently, the expectation of conditional variance is obtained as

$$E_{-i}[V_i(Y|\mathbf{X}_{-i})]\approx h_0^{2-2n}\cdot\left(\prod_{k=1,k\neq i}^{n}\theta_k\right)\cdot(\theta_i-\rho_i^2) \tag{29}$$

Using Eq. (13), the total sensitivity index of X_i can be evaluated as

$$S_{Ti}=\frac{E_{-i}[V_i(Y|\mathbf{X}_{-i})]}{V_Y}\approx\frac{1-\rho_i^2/\theta_i}{1-(\prod_{k=1}^{n}\rho_k^2/\theta_k)} \tag{30}$$

In original setting, the global sensitivity analysis requires to evaluate a series of two-layer high-dimensional integrations as shown in Eq. (9). With the proposed M-DRM approximation, the corresponding simple algebraic formulas on the primary sensitivity coefficient in Eq. (24), the joint sensitivity coefficient in Appendix C, as well the total sensitivity coefficient in Eq. (30), are derived, which only need to compute n one-dimensional integrations about a physical model with n input variables. This approximation will significantly reduce the total number of model evaluations.

3.4. Integration of univariate functions

The Gaussian quadrature is quite efficient for computing one-dimensional integrals as summarized in Appendix D:

$$\begin{cases} \rho_k \approx \sum_{l=1}^{N} w_{kl} h(c_1, \ldots, c_{k-1}, x_{kl}, c_{k+1}, \ldots, c_n) \\ \theta_k \approx \sum_{l=1}^{N} w_{kl} [h(c_1, \ldots, c_{k-1}, x_{kl}, c_{k+1}, \ldots, c_n)]^2 \end{cases} \tag{31}$$

An lth Gaussian Abscissa, x_{kl}, and its weight, w_{kl}, can be determined according to the probability distribution of X_k. Note that no additional function evaluations are required for computing θ_k.

In an N-point Gauss quadrature, the total number of functional evaluations about $y=h(\mathbf{x})$ for complete sensitivity analysis is merely nN. Thus M-DRM approximation requires substantially less computational efforts than simulation-based and quadrature-based methods.

4. Numerical examples

Seven examples, taken from the literature, are reanalyzed to illustrate the proposed method.

4.1. Polynomial function

The first example considers a polynomial function:

$$h(\mathbf{X}) = \frac{1}{2^n} \prod_{k=1}^{n} (3X_k^2 + 1) \tag{32}$$

where X_i are independently and identically distributed (i.i.d.) uniform random variable over [0,1]. This example was proposed by Sobol' [17], and later studied by Sudret [8] to examine the performance of polynomial chaos expansion (PCE) method for global sensitivity analysis.

The mean and variance of the function are exactly given as

$\mu_Y = 1;\quad$ and $\quad V_Y = (6/5)^n - 1.$

A generic sensitivity coefficient can be analytically derived as

$$S_{i_1 i_2 \cdots i_s} = \frac{5^{-s}}{(6/5)^n - 1} \quad (1 \le i_1 < \cdots < i_s \le n)$$

Table 1 compares exact numerical results for $n=3$ against those obtained by M-DRM and other two methods reported in the literature. Using the third-point Gauss Legendre quadrature ($N=3$) and 10 functional evaluations, the proposed M-DRM is able to reproduce exact results for all sensitivity indices, since the function can be perfectly fitted by M-DRM. The polynomial chaos expansion [8] and polynomial decomposition method [6] are also able to reproduce exact results, albeit at a higher computational cost.

4.2. Ishigami function

Consider the following function proposed by Ishigami and Homma [4]:

$$h(\mathbf{X}) = \sin(X_1) + a[\sin(X_2)]^2 + b \sin(X_1) X_3^2 \tag{33}$$

where X_i are i.d.d. uniform random variables over $[-\pi, \pi]$.

The variance of Y is

$$V_Y = \frac{1}{2} + \frac{a^2}{8} + \frac{b\pi^4}{5} + \frac{b^2\pi^8}{18}$$

The sensitivity coefficients are analytically derived as

$$S_1 = \frac{b\pi^4/5 + b^2\pi^8/50 + 1/2}{V_Y}; \quad S_2 = \frac{a^2/8}{V_Y}; \quad S_{13} = \frac{8b^2\pi^8/225}{V_Y} \tag{34}$$

as well as the total sensitivity coefficients

$$S_{T1} = \frac{b\pi^4/5 + b^2\pi^8/18 + 1/2}{V_Y}; \quad S_{T2} = \frac{a^2/8}{V_Y}; \quad S_{T3} = \frac{8b^2\pi^8/225}{V_Y} \tag{35}$$

The remaining sensitivity indices are zero.

In Table 2, numerical results are presented for $a=0.1$ and $b=0.7$. M-DRM results were obtained using the Gauss–Legnedre quadrature of increasing order N from 3 to 5. It is clear that M-DRM based three-point ($N=3$) quadrature is not adequate, as it results in large error. However, numerical accuracy of M-DRM results is remarkably improved with fifth-order ($N=5$) Gaussian quadrature. In a sense, the M-DRM results seem to converge to the right answer as the order of quadrature rule is increased.

4.3. Non-smooth function

Consider the following non-smooth function proposed by Sobol' [3]:

$$h(\mathbf{X}) = \prod_{k=1}^{n} \frac{|4X_k - 2 + a_k|}{a_k + 1} \tag{36}$$

where X_k ($k=1, \ldots, n$) are i.i.d. and [0, 1] uniform random variables. The following analytical results are available:

$$\begin{cases} \text{Variance}: & V_Y = -1 + \prod_{k=1}^{n} \left[\frac{1}{3(a_k+1)^2} + 1 \right] \\ \text{Sensitivity}: & S_{i_1 \cdots i_s} = \frac{1}{V_Y} \prod_{k=1}^{s} \frac{1}{3(a_{i_k}+1)^2} \quad (1 \le i_1 < \cdots i_s \le n) \end{cases}$$

Table 1
Sensitivity coefficients: polynomial function.

Sensitivity	Exact	M-DRM		PCE		PDD	
		$N=2$	$N=3$	$p=3$	$p=6$	$m=1$	$m=2$
S_1	0.2747	0.2780	0.2747	0.2879	0.2747	0.2780	0.2747
S_2	0.2747	0.2780	0.2747	0.2773	0.2747	0.2780	0.2747
S_3	0.2747	0.2780	0.2747	0.2773	0.2747	0.2780	0.2747
S_{12}	0.0549	0.0521	0.0549	0.0506	0.0549	0.0521	0.0549
S_{13}	0.0549	0.0521	0.0549	0.0506	0.0549	0.0521	0.0549
S_{23}	0.0549	0.0521	0.0549	0.0481	0.0549	0.0521	0.0549
S_{123}	0.0110	0.0098	0.0110	0.0081	0.0110	0.0098	0.0110
Number of FEs	–	6	9	29	116	8	27

PCE, polynomial chaos expansion [8]; PDD, polynomial dimensional decomposition [6]; M-DRM, multiplicative dimensional reduction method; FEs, functional evaluations.

We consider the following parameter values: $n=8$, $a_1=0.001$, $a_2=1$, $a_3=4.5$, $a_4=9$ and $a_5=\cdots=a_8=99$ [17].

In Table 3, numerical results obtained by M-DRM and other three methods reported in the literature are compared. They are trivariate polynomial dimensional decomposition (T-PDD) [6], random balance design (RBD) and state-dependent parameter method (SDP) [18].

In this case, ninth order ($N=9$) quadrature has to be used to achieve high numerical accuracy of the sensitivity coefficients. Nevertheless, M-DRM requires a considerably small number of function evaluations, only 72, as compared to the other three methods which require several thousands of function evaluations to achieve comparable accuracy.

4.4. Corner peak function

This example analyzes a corner peak function proposed by Genz [19]:

$$h(\mathbf{X})=\left(1+\sum_{i=1}^{n}a_iX_i\right)^{-(n+1)} \tag{37}$$

where X_i are i.i.d. and [0, 1] uniform random variables.

In Table 4, numerical results are presented for a trivariate case ($n=3$) with the following parameters $a_1=0.02$, $a_2=0.05$, $a_3=0.08$. M-DRM results obtained using the three order quadrature method are fairly close to those obtained from numerical integration.

The second case considers a ten-dimensional problem ($n=10$) and the parameter values are assumed as $a_1=0.01, a_2=0.02, \ldots, a_{10}=0.10$. Here, the Monte Carlo simulations with $10^4\times10^3$ samples are used to compute benchmark results against which the performance of M-DRM is compared. As shown in Fig. 1, results of M-DRM with third order Gaussian quadrature totally involved 30 function evaluations that are in excellent agreement with those obtained from simulations.

4.5. Discontinuous function

The example further considers Genz's discontinuous function [19]:

$$h(\mathbf{X})=\begin{cases}0 & \text{if } X_1\in[0,u_1] \text{ OR } X_2\in[u_2,1.0]\\ \exp\left(\sum_{i=1}^{n}a_iX_i\right) & \text{otherwise}\end{cases} \tag{38}$$

where X_i are i.i.d. and [0, 1] uniform variables, u_i are characteristic constants on discontinuity of the function, and weighting constants $[a_1,a_2,\ldots,a_{10}]^{\mathrm{T}}=[0.1,0.2,\ldots,1.0]^{\mathrm{T}}$.

Assume that $u_1=0$ and $u_2=1.0$, the function is degenerated as a continuous function. The corresponding sensitivity coefficients are computed as shown in Fig. 2. M-DRM with 40 functional evaluations determines accurate estimates of primary and total sensitivity indices. Since the weighting constants, a_i, are linearly increased from 0.1 to 1.0, X_1 and X_2 are the two most insignificant input variables.

Second case of the example further considers $u_1=0.3$, $u_2=0.8$ to declare discontinuity of Eq. (38). M-DRM with various orders of Gauss–Legendre scheme (i.e., $N=4$, $N=6$ and $N=14$, respectively) is employed to compute the sensitivity coefficients, which are depicted in Fig. 3.

Four- and six-point Gaussian quadratures ($N=4$ and $N=6$) are not adequate for accurate estimates of sensitivity indices. Until increasing to $N=14$, the high-order quadrature scheme can generate reliable results compared to those from simulations. The M-DRM procedure totally requires 140 ($=14\times10$) functional evaluations.

4.6. Thermally induced stress intensity factor

This example is taken from the literature by Mohamed et al. [20]. The thermally induced stress intensity factor (SIF) in a rectangular plate with a crack of size a is given by the following analytical

Table 2
Sensitivity coefficients: Ishigami function.

Sensitivity	Exact	M-DRM		
		$N=3$	$N=4$	$N=5$
S_1	0.3932	0.5876	0.4111	0.3907
S_2	4.59×10^{-6}	4.72×10^{-11}	2.47×10^{-11}	7.65×10^{-11}
S_{13}	0.6068	0.4124	0.5889	0.6093
S_{T1}	1.0	1.0	1.0	1.0
S_{T2}	4.59×10^{-6}	2.00×10^{-6}	3.58×10^{-6}	1.02×10^{-5}
S_{T3}	0.6068	0.4124	0.5889	0.6093
No. FEs	–	9	12	15

M-DRM, multiplicative dimensional reduction method.

Table 4
Sensitivity coefficients: corner peak function ($n=3$).

Sensitivity	Primary sensitivity			Total sensitivity		
	S_1	S_2	S_3	S_{T1}	S_{T2}	S_{T3}
Exact	0.0429	0.2681	0.6851	0.0441	0.2736	0.6886
M-DRM	0.0430	0.2685	0.6860	0.0443	0.2726	0.6855

M-DRM, multiplicative dimensional reduction method; Exact, result determined by analytic integration.

Table 3
Sensitivity coefficients: non-smooth function.

Sensitivity	Exact	M-DRM		T-PDD		RBD		SDP	
		$N=5$	$N=9$	$m=4$	$m=8$	Small size	Large size	Small size	Large size
S_1	0.7162	0.7046	0.7122	0.7140	0.7218	0.704	0.714	0.717	0.716
S_2	0.1791	0.1667	0.1751	0.1642	0.1723	0.173	0.181	0.179	0.179
S_3	0.0237	0.0213	0.0229	0.0193	0.0207	0.0314	0.0278	0.0235	0.0236
S_4	0.0072	0.0064	0.0069	0.0053	0.0057	0.0084	0.0073	0.0070	0.0071
S_5	7.2×10^{-5}	6.3×10^{-5}	6.9×10^{-5}	4.8×10^{-5}	5.2×10^{-5}	4.4×10^{-3}	3.0×10^{-4}	2.1×10^{-5}	6.1×10^{-5}
S_6	7.2×10^{-5}	6.3×10^{-5}	6.9×10^{-5}	4.8×10^{-5}	5.2×10^{-5}	3.8×10^{-3}	3.0×10^{-4}	2.3×10^{-5}	5.8×10^{-5}
S_7	7.2×10^{-5}	6.3×10^{-5}	6.9×10^{-5}	4.8×10^{-5}	5.2×10^{-5}	2.2×10^{-3}	4.0×10^{-4}	2.2×10^{-5}	5.8×10^{-5}
S_8	7.2×10^{-5}	6.3×10^{-5}	6.9×10^{-5}	4.8×10^{-5}	5.2×10^{-5}	1.7×10^{-3}	3.0×10^{-4}	2.0×10^{-5}	5.9×10^{-5}
No. FEs	–	40	72	4065	30,529	4096	32,768	4096	32,768

M-DRM, multiplicative dimensional reduction method; T-PDD, trivariate polynomial dimensional decomposition [6]; RBD, random balance design [18]; SDP, state dependent parameter modelling [18].

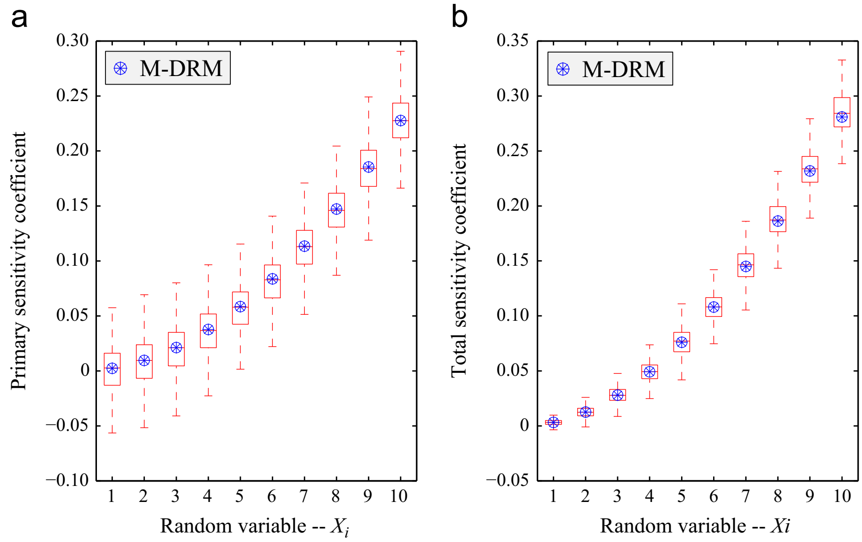

Fig. 1. Global sensitivity coefficients of the ten-dimensional corner peak function (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

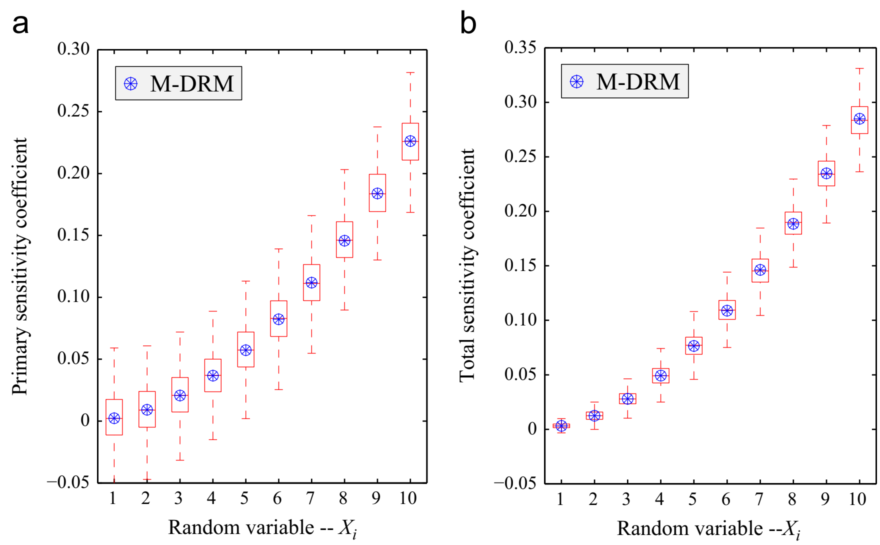

Fig. 2. Global sensitivity coefficients of Genz's discontinuous function: Continuous case (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

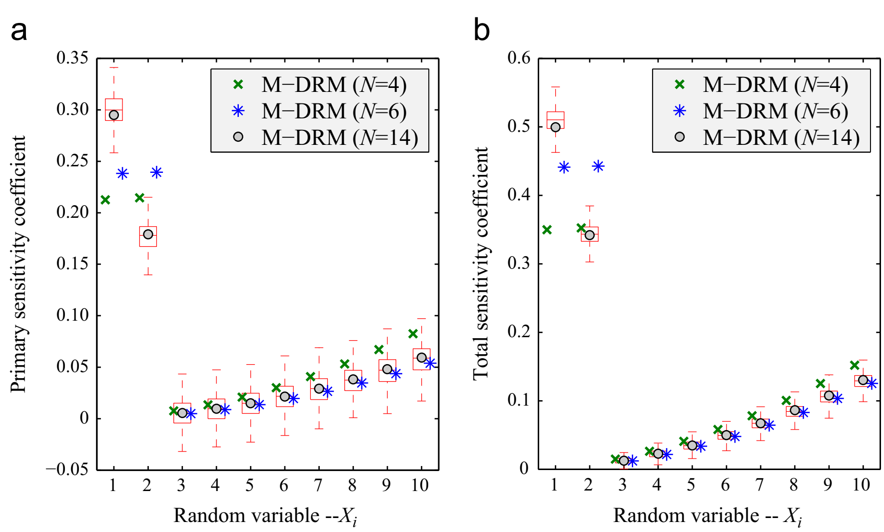

Fig. 3. Global sensitivity coefficients of Genz's discontinuous function: Discontinuous case (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each; N: the order of Gauss-Legendre quadrature): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

expression [21]:

$$K_{IC}(\mathbf{X}) = -\alpha E(T - T_0)\sqrt{\frac{\pi a}{\cos(\pi a/4B)}}\left[1 - 0.025\left(\frac{a}{2B}\right)^2 + 0.06\left(\frac{a}{2B}\right)^4\right] \quad (39)$$

All the variables of this formula are described in Table 5.

Table 5
Random variables in the example of thermal induced stress intensity factor.

Variable	Description	Distribution	Mean	COV
T_0	Initial hot temperature	Lognormal	100 °C	0.20
T	Amphibian cool temperature	Lognormal	20 °C	0.20
a	Crack size	Lognormal	10 mm	0.20
B	Width of plate	Lognormal	200 mm	0.20
E	Young's module	Lognormal	210 GPa	0.20
α	Thermal expansion coefficient	Deterministic	12.5×10^{-6} °C^{-1}	–

Results of M-DRM with five-point Gauss-Hermite quadrature are compared with the Monte Carlo simulation in Fig. 4. The primary and total sensitivity coefficients provided by M-DRM are in close agreement with simulation results.

4.7. Eigenvalue of a spring-mass system

The last example examines the accuracy of M-DRM for global sensitivity analysis by considering eigenvalue analysis of a linear spring-mass system [22].

Denoting $[M]$ as the mass matrix, $[\ddot{Z}]$ as the 2nd time derivative of displacement $[Z]$, and $[K]$ as the stiffness matrix, the vibrational model analysis needs to consider the following motion of equation:

$$[M][\ddot{Z}] + [K][Z] = [0] \quad (40)$$

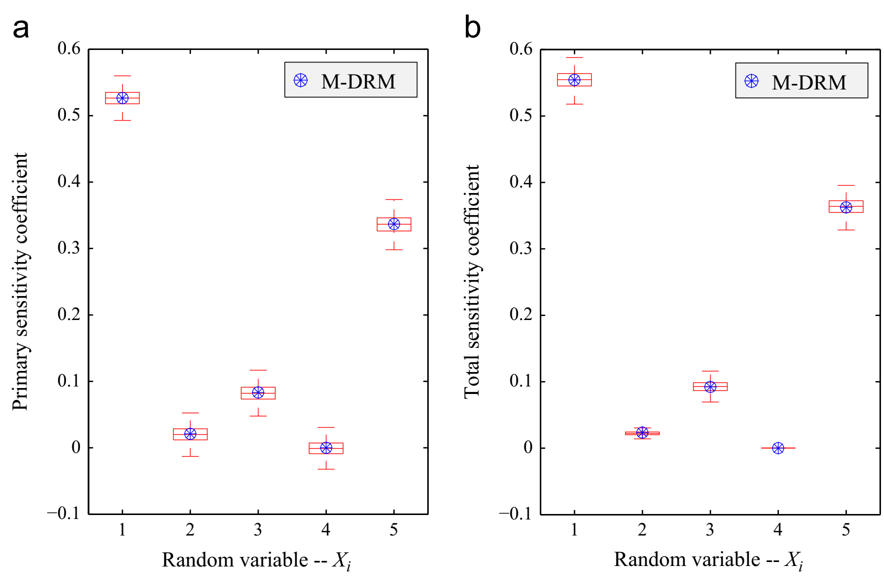

Fig. 4. Global sensitivity analysis about the thermally induced stress intensity factor (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

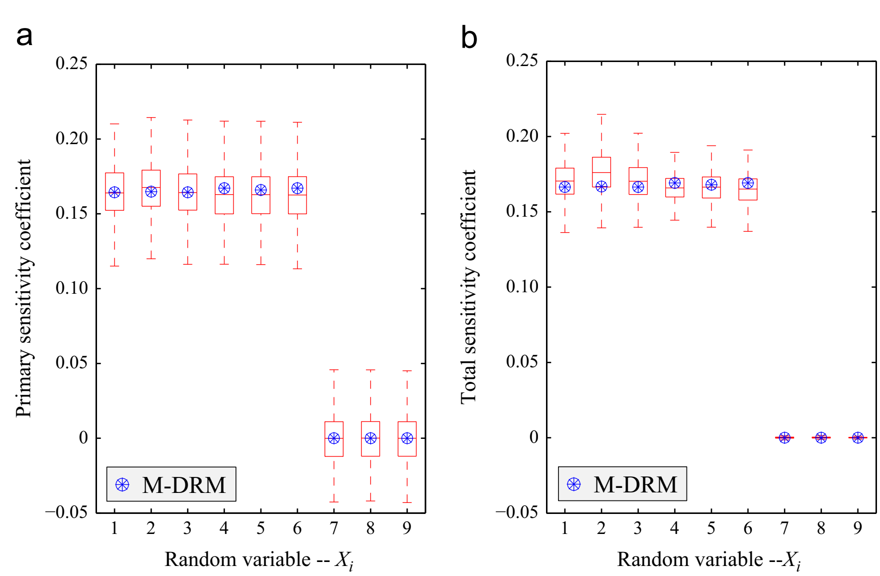

Fig. 5. Global sensitivity index about 1st eigenvalue of the system (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

This is a general eigensystem. One can determine each eigenvalue via the system characteristic equation:

$$\det\{[K]-\lambda[M]\}=0 \tag{41}$$

in which a jth eigenvalue of the system should be an implicit function about structural parameters $[M]$ and $[K]$.

Assume that structural mass matrix is

$$[M]=\begin{bmatrix} M_1 & 0 & 0 \\ 0 & M_2 & 0 \\ 0 & 0 & M_3 \end{bmatrix}$$

as well as the stiffness matrix:

$$[K]=\begin{bmatrix} K_1+K_4+K_6 & -K_4 & -K_6 \\ -K_4 & K_2+K_4+K_5 & -K_5 \\ -K_6 & -K_5 & K_3+K_5+K_6 \end{bmatrix}$$

Mean-values of mass and stiffness are assumed as $\mu_{M_i}=1$ kg (i=1,2,3), $\mu_{K_i}=1$ N/m for i=1,…,5, and $\mu_{K_6}=3$ N/m. All input random variables are Lognormally distributed with COV=15%.

With a five-point Gauss–Hermite quadrature, the primary and total sensitivity coefficients on input random variables are computed for each eigenvalue of the 3-DOF dynamic system. According to the box plot in Figs. 5–7, it is clear to see that the proposed method is fairly efficient, i.e., the number of functional evaluations is only limited to 45 (=5 × 9). Compared to the box plot provided by experiments of Monte Carlo simulation (10^3 rounds simulation with 10^4 samples in each), it has illustrated accuracy of the proposed method for eigenvalue sensitivity analysis of the dynamic system.

5. Conclusion

The paper presents an effective approximate method for the computation of variance-based sensitivity coefficients. The proposed method is based on multiplicative dimensional reduction method (M-DRM), in which the response function is approximated as a product of univariate functions.

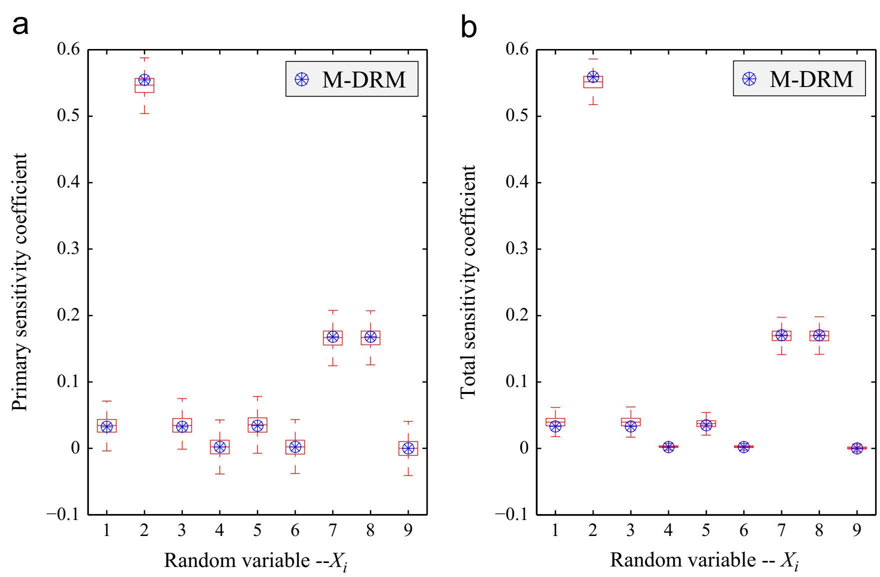

Fig. 6. Global sensitivity index about 2nd eigenvalue of the system (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

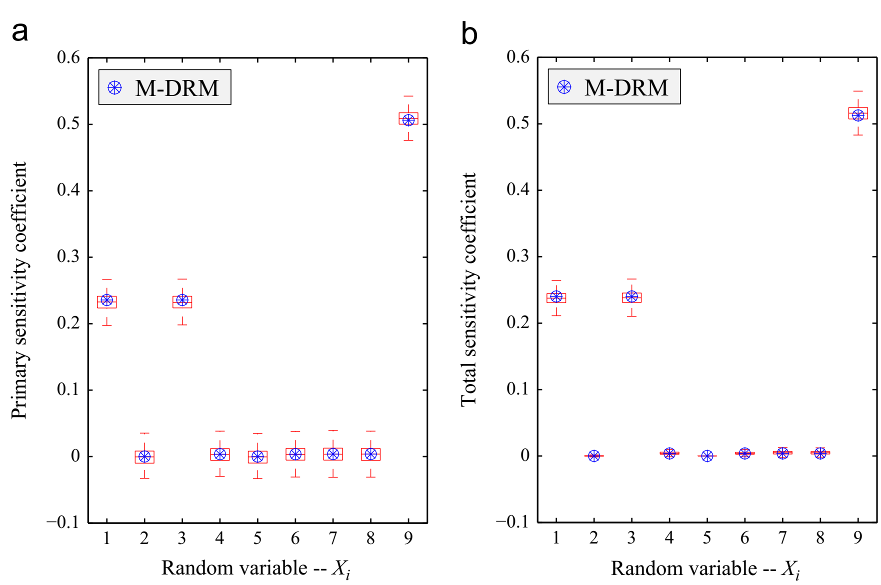

Fig. 7. Global sensitivity index about 3rd eigenvalue of the system (M-DRM, the multiplicative dimensional reduction method; Box plot, 10^3 rounds Monte Carlo simulation with 10^4 samples in each): (a) primary sensitivity coefficient and (b) total sensitivity coefficient.

The most notable aspect of the proposed M-DRM is that simple algebraic formulas can be derived for the primary, high-order (on joint effect) and the total sensitivity coefficients. Based on an N-point Gaussian quadrature, M-DRM requires nN function evaluations only in the sensitivity analysis of a function of n random variables, which implies that the proposed method significantly reduces the number of functional evaluations required for the sensitivity analysis.

The performance of M-DRM is evaluated by analyzing six examples taken from the literature. In all the cases, sensitivity coefficients obtained from M-DRM are in excellent agreement with analytical or simulation-based reference solutions.

In summary, the multiplicative dimensional reduction method provides a simple and efficient alternative for global sensitivity analysis in a practical setting.

Acknowledgments

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Appendix A. Bivariate and high-order sensitivity measures

The joint effect about X_i and X_j $(i<j)$ acting together can be evaluated by

$$S_{ij} = \frac{V_{ij}[E_{-ij}(Y|X_i, X_j)]}{V_Y} = \frac{E[\alpha_{ij}^2(X_i, X_j)] - E[\alpha_i^2(X_i)] - E[\alpha_j^2(X_j)] + \mu_Y^2}{V_Y} \tag{A.1}$$

Generally, for an arbitrary multivariate sensitivity index, $S_{\mathbf{p}}$, one needs to calibrate the joint variance about input random variables $\mathbf{X_p}$, given $\mathbf{p} = \{i_1, i_2, \ldots, i_s\}$ [12]. It can be defined by using second moments of s- and lower-variate conditional expectations:

$$S_{\mathbf{p}} = \frac{V_{\mathbf{p}}[E_{-\mathbf{p}}(Y|\mathbf{X_p})]}{V_Y} = \frac{E_{\mathbf{p}}[\alpha_{\mathbf{p}}^2(\mathbf{X_p})] - \sum_{\mathbf{q}\subset\mathbf{p}} E_{\mathbf{q}}[\alpha_{\mathbf{q}}^2(\mathbf{X_q})] + \mu_Y^2}{V_Y} \tag{A.2}$$

where the index vectors $\mathbf{q} = \{j_1, j_2, \ldots, j_k\}$ is a subset of $\mathbf{p}$, i.e., $k<s$. The expression implies that to compute all sensitivity indices up to order s, one has to evaluate 2^s-1 two-layer high-dimensional integrals:

$$E_{\mathbf{q}}[\alpha_{\mathbf{q}}^2(\mathbf{X_q})] = \int_{\mathbf{X_q}} \left(\int_{\mathbf{X_{-q}}} h(\mathbf{x}) f_{\mathbf{X_{-q}}}(\mathbf{x_{-q}})\, \mathrm{d}\mathbf{x_{-q}} \right)^2 f_{\mathbf{X_q}}(\mathbf{x_q})\, \mathrm{d}\mathbf{x_q} \tag{A.3}$$

Appendix B. Multiplicative dimensional reduction method

Consider a general response function, $y = h(\mathbf{x})$. By using the logarithmic transformation, one can obtain

$$\varphi(\mathbf{x}) = \log[\mathrm{abs}(y)] = \log\{\mathrm{abs}[h(\mathbf{x})]\} \tag{B.1}$$

Following the univariate C-DRM in literature [23], an approximation of $\varphi(\mathbf{x})$ can be written as

$$\varphi(\mathbf{x}) \approx \sum_{i=1}^{n} \varphi(x_i, \mathbf{c}_{-i}) - (n-1)\varphi_0 \tag{B.2}$$

where the functions can be related to those in the original space as follows:

$$\begin{cases} \varphi_0 = \log\ \{\mathrm{abs}[h(c_1, c_2, \ldots, c_n)]\} \\ \varphi(x_i, \mathbf{c}_{-i}) = \log\ \{\mathrm{abs}[h(c_1, \ldots, c_{i-1}, x_i, c_{i+1}, c_n)]\} \end{cases} \tag{B.3}$$

By inverting the transformation, the original function can be written as

$$\begin{aligned} \exp[\varphi(\mathbf{x})] &\approx \exp\left[\sum_{i=1}^{n} \varphi(c_1, \ldots, c_{i-1}, x_i, c_{i+1}, c_n) - (n-1)\varphi_0\right] \\ &= \exp[(1-n)\varphi_0] \times \exp\left[\sum_{i=1}^{n} \varphi(c_1, \ldots, c_{i-1}, x_i, c_{i+1}, c_n)\right] \end{aligned} \tag{B.4}$$

Substituting for the expressions from Eq. (B.3) into Eq. (B.4) leads to a multiplicative approximate of the response function:

$$h(\mathbf{x}) \approx [h(\mathbf{c})]^{1-n} \cdot \prod_{i=1}^{n} h(c_1, \ldots, c_{i-1}, x_i, c_{i+1}, \ldots, c_n) \tag{B.5}$$

This approximate model of original input–output relation is referred to as the univariate multiplicative dimensional reduction method (M-DRM) in this paper.

As an example, consider the approximation of a trivariate function about a cut-point $\mathbf{c} = [c_1, c_2, c_3]^{\mathrm{T}}$ using the univariate C-DRM and M-DRM, respectively

$$\begin{cases} \text{C-DRM}: & h(x_1, x_2, x_3) \approx h(x_1, c_2, c_3) + h(c_1, x_2, c_3) + h(c_1, c_2, x_3) - 2h(c_1, c_2, c_3) \\ \text{M-DRM}: & h(x_1, x_2, x_3) \approx \dfrac{h(x_1, c_2, c_3) \times h(c_1, x_2, c_3) \times h(c_1, c_2, x_3)}{[h(c_1, c_2, c_3)]^2} \end{cases} \tag{B.6}$$

Appendix C. High-order sensitivity coefficients

In general, to compute an s-variate sensitivity index, $S_{\mathbf{p}}$, one needs to evaluate the high-order integrations as shown in Eq. (A.3). Substituting for the M-DRM approximation about $h(\mathbf{x})$, the two-layer multidimensional integration can be generally approximated as

$$\begin{aligned} E_{\mathbf{p}}[\alpha_{\mathbf{p}}^2(\mathbf{X_p})] \approx h_0^{2-2n} &\left(\prod_{k=1; k\neq i_1,\ldots,i_s}^{n} \{E_k[h(X_k, \mathbf{c}_{-k})]\}^2 \right) \\ &\times \left(\prod_{k=i_1,\cdots,i_s} E_k\{[h(X_k, \mathbf{c}_{-k})]^2\} \right) \end{aligned} \tag{C.1}$$

Using the notations ρ_i and θ_i defined in Eq. (17), it can be rewritten as

$$E_{\mathbf{p}}[\alpha_{\mathbf{p}}^2(\mathbf{X_p})] \approx \left(h_0^{2-2n} \cdot \prod_{k=1}^{n} \rho_k^2 \right) \cdot \left(\prod_{k=i_1,\ldots,i_s} \frac{\theta_k}{\rho_k^2} \right) \tag{C.2}$$

A special case starting from $s=2$, the second order moment of bivariate conditional expectation can be computed as

$$E_{ij}[\alpha_{ij}^2(X_i, X_j)] \approx \left(h_0^{2-2n} \cdot \prod_{k=1}^{n} \rho_k^2 \right) \cdot \frac{\theta_i \theta_j}{\rho_i^2 \rho_j^2} \tag{C.3}$$

Given the joint component variance

$$V_{ij} = E_{ij}[\alpha_{ij}^2(X_i, X_j)] - E_i[\alpha_i^2(X_i)] - E_j[\alpha_j^2(X_j)] + \mu_Y^2$$

the M-DRM can approximate it as

$$V_{ij} \approx \left(h_0^{2-2n} \cdot \prod_{k=1}^{n} \rho_k^2 \right) \cdot \left(\frac{\theta_i}{\rho_i^2} - 1 \right) \cdot \left(\frac{\theta_j}{\rho_j^2} - 1 \right) = \hat{\mu}_Y^2 \cdot (\theta_i/\rho_i^2 - 1) \cdot (\theta_j/\rho_j^2 - 1) \tag{C.4}$$

The bivariate Sobol' sensitivity index, hence, can be determined as

$$S_{ij} = \frac{V_{ij}}{V_Y} \approx \frac{(\theta_i/\rho_i^2 - 1)(\theta_j/\rho_j^2 - 1)}{\left(\prod_{k=1}^{n} \theta_k/\rho_k^2\right) - 1} \tag{C.5}$$

With this convention, if a vector with s-variate input random variables is considered, the corresponding sensitivity measure can be approximated by M-DRM as

$$S_{\mathbf{p}} = \frac{V_{i_1 i_2 \cdots i_s}}{V_Y} \approx \frac{\prod_{k=1}^{s}(\theta_{i_k}/\rho_{i_k}^2 - 1)}{(\prod_{k=1}^{n}\theta_k/\rho_k^2) - 1} \tag{C.6}$$

Appendix D. Issues on one-dimensional integration

The one-dimensional integral in M-DRM can be efficiently computed by the rules of Gaussian quadrature [24]. Using an Nth order Gaussian quadrature, mean-value and second moment of the one-dimensional function in Eqs. (17) can be numerically determined as

$$\begin{cases} \int_{X_i} h(X_i, \mathbf{c}_{-i}) f_i(x_i)\,\mathrm{d}x_i \approx \sum_{k=1}^{N} w_{ik} h(c_1, \ldots, c_{i-1}, x_{ik}, c_{i+1}, \ldots, c_n) \\ \int_{X_i} [h(X_i, \mathbf{c}_{-i})]^2 f_i(x_i)\,\mathrm{d}x_i \approx \sum_{k=1}^{N} w_{ik} [h(c_1, \ldots, c_{i-1}, x_{ik}, c_{i+1}, \ldots, c_n)]^2 \end{cases} \tag{D.1}$$

in which, the corresponding Gaussian point x_{ik} and weight w_{ik} are computed by orthogonal polynomial as follows.

Assume that X is a Uniform variable $X \in [a, b]$. A kth order moment of $h(X)$ can be defined as

$$M_Y^k = \int_a^b [h(x)]^k f_X(x)\,\mathrm{d}x \tag{D.2}$$

where $f_X(x) = 1/(b-a)$.

By changing variable,

$$X = \frac{a+b}{2} + \frac{b-a}{2} Z \tag{D.3}$$

the kth order moment of Y can be numerically estimated by Gaussian–Legendre quadrature as

$$M_Y^k = \int_a^b [h(x)]^k f_X(x)\,\mathrm{d}x \approx \frac{1}{2}\sum_{i=1}^{N} w_i \left[h\left(\frac{b-a}{2} z_i + \frac{a+b}{2}\right)\right]^k \tag{D.4}$$

where an ith Gaussian Legendre weight, w_i, and point z_i are listed as shown in Table D1.

Davis and Rabinowitz [25] give the expressions of each order Legendre polynomial. As an N-order Gaussian–Legendre quadrature is employed in numerical integration, an ith element of Gaussian nodes, z_i, can be determined as the ith root of the Nth order Legendre orthogonal polynomial, $p_N(z)$, as shown in Appendix E. The corresponding Gaussian weight, w_i, can be calculated by

$$w_i = \frac{2}{(1 - z_i^2)[p_N'(z_i)]^2} \tag{D.5}$$

Table D1
Gaussian point and weight about the Legendre quadrature.

Order of Gaussian quadrature (N)	Gaussian point (z_i)	Gaussian weight (w_i)
1	0	2
2	$\pm 1/\sqrt{3}$	1
3	0	8/9
	$\pm\sqrt{3/5}$	5/9
4	$\pm\sqrt{(3-2\sqrt{6/5})/7}$	$(18+\sqrt{30})/36$
	$\pm\sqrt{(3+2\sqrt{6/5})/7}$	$(18-\sqrt{30})/36$
5	0	128/225
	$\pm\frac{1}{3}\sqrt{5-2\sqrt{10/7}}$	$(322+13\sqrt{70})/900$
	$\pm\frac{1}{3}\sqrt{5+2\sqrt{10/7}}$	$(322-13\sqrt{70})/900$

Residual error associated with the numerical scheme is

$$\mathcal{R} = \frac{2^{2N+1}(N!)^4}{[(2N)!]^3(2N+1)} \frac{\mathrm{d}^{2N} h(\xi)}{\mathrm{d}x^{2N}} \quad \text{where} \quad \xi \in (a, b) \tag{D.6}$$

Therefore, as the degree of x in $h(x)$ is less than $2N-1$, the scheme should give exact result of the one-dimensional integration.

Appendix E. Legendre orthogonal polynomial

The Legendre orthogonal polynomials are the general solution to Legendre's differential equation:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(1+x^2)\frac{\mathrm{d}}{\mathrm{d}x} p_i(x)\right] + i(i+1)p_i(x) = 0 \quad (i = 0, 1, \ldots) \tag{E.1}$$

Given $p_0(x) = 1$ and $p_1(x) = x$, Bonnet's recursion formula of the polynomial can be given as

$$(i+1)p_{i+1}(x) = (2i+1)xp_i(x) - ip_{i-1}(x) \tag{E.2}$$

Orthogonality of the polynomials with respect to the $\mathbb{L}^2$ inner product on the interval $x \in [-1, 1]$ can be expressed as

$$\int_{-1}^{1} p_i(x) p_j(x) \mathrm{d}x = \frac{2}{2i+1}\delta_{ij} \tag{E.3}$$

where δ_{ij} denotes the Kronecker delta.

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