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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

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

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

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

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

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

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:

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

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

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

in which

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

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:

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

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