Computer Physics Communications 184 (2013) 2540–2551

Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

A new variance-based global sensitivity analysis technique

Pengfei Wei, Zhenzhou Lu *, Jingwen Song

Northwestern Polytechnical University, Xi'an, Shaanxi, 710072, China

ARTICLE INFO

Article history:
Received 18 December 2012
Received in revised form
14 May 2013
Accepted 9 July 2013
Available online 16 July 2013

Keywords:
Variance-based sensitivity analysis
Sobol's indices
Variance ratio function
W-indices
Monte Carlo simulation
Model emulation

ABSTRACT

A new set of variance-based sensitivity indices, called W-indices, is proposed. Similar to the Sobol's indices, both main and total effect indices are defined. The W-main effect indices measure the average reduction of model output variance when the ranges of a set of inputs are reduced, and the total effect indices quantify the average residual variance when the ranges of the remaining inputs are reduced. Geometrical interpretations show that the W-indices gather the full information of the variance ratio function, whereas, Sobol's indices only reflect the marginal information. Then the double-loop-repeated-set Monte Carlo (MC) (denoted as DLRS MC) procedure, the double-loop-single-set MC (denoted as DLSS MC) procedure and the model emulation procedure are introduced for estimating the W-indices. It is shown that the DLRS MC procedure is suitable for computing all the W-indices despite its highly computational cost. The DLSS MC procedure is computationally efficient, however, it is only applicable for computing low order indices. The model emulation is able to estimate all the W-indices with low computational cost as long as the model behavior is correctly captured by the emulator. The Ishigami function, a modified Sobol's function and two engineering models are utilized for comparing the W- and Sobol's indices and verifying the efficiency and convergence of the three numerical methods. Results show that, for even an additive model, the W-total effect index of one input may be significantly larger than its W-main effect index. This indicates that there may exist interaction effects among the inputs of an additive model when their distribution ranges are reduced.

1. Introduction

Sensitivity analysis (SA) is a technique for investigating how the uncertainty in the model output of interest can be attributed to an individual or a set of inputs. It has been extensively applied for developing scientific computational models in many fields such as risk analysis [1,2], computational physics and chemistry [3,4], environmental science [5] and reliability engineering [6]. Generally, according to different analysis purposes, the available SA techniques can be divided into two groups: local SA and global SA.

The local SA index is usually defined as the partial derivative of model output with respect to a model input. It is computationally efficient, thus has been widely used in early study. However, the local SA index only reflects the effect of input on the model output at one given point, but cannot tell the global sensitivity information [7].

The global SA aims at quantifying the effect of an individual or a set of inputs to the uncertainty of model output by fixing the inputs over their full distribution ranges. Over the past few decades, many global SA techniques have been developed by researchers. Morris developed the elementary effect (EE) method for effectively screening the few important inputs in a model that involves a huge number of inputs, with a relatively small number of samples designed by properly distributing the input space [8]. This method was later improved by Campolongo et al. [9]. In Refs. [10,11], Borgonovo developed the density-based global SA index for measuring the average shift of the probability density function (PDF) of the model output when one input is fixed over its full distribution range. Sobol et al. presented the derivative-based global SA indices by averaging the derivatives of model output with respect to the inputs through the full distribution ranges of these inputs [12,13]. Another group of global SA indices, and also the most popular, is the variance-based one developed by Sobol [14], Homma and Saltelli [15].

The classical variance-based sensitivity indices, also called Sobol's indices, as pointed out by Saltelli [1], satisfy the requirement of "global, quantitative and model free", thus have attracted extensive attention of researchers and analysts, and many numerical methods have been developed for computing them [16–26]. Generally, for an individual or a set of inputs, the main and total effect indices gain specific attention of analysts.

Sobol's main effect index of an individual input quantifies the average reduction of model output variance when this input is fixed over its full distribution range. The higher it is, the greater reduction of variance of model output can be obtained while reducing the uncertainty of this input. Sobol's total effect index of an

* Correspondence to: School of Aeronautics, Mail Box 120, China. Tel.: +86 29 88460480; fax: +86 29 88460480.

E-mail address: zhenzhoulu@nwpu.edu.cn (Z. Lu).

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http://dx.doi.org/10.1016/j.cpc.2013.07.006

individual input reveals the mean residual variance of model output while the remaining inputs are fixed over their full distribution ranges. The lower it is, the less this input contributes to the variance of model output. For the inputs with total effect indices close to zero, one can fix them anywhere in their distribution ranges without affecting the variance of model output [27].

In this paper, a new framework of variance-based global SA indices, called W-indices, is presented for measuring the contribution of one or a set of inputs to the variance of model output. The W-main effect index of one input quantifies the average reduction of the variance of model output when the distribution range of this input is reduced over its full range. Thus the higher the main effect index is, the greater the reduction of model output variance one can obtain while reducing the range of this input. The W-total effect index of one input measures the average residual variance of model output when the distribution ranges of all the remaining inputs are reduced over their full ranges. If the total effect index of one input is close to zero, then one can reduce its range arbitrarily without affecting the variance of model output obviously.

In many practical applications, one generally cannot fix the inputs at given points, but only be able to reduce the distribution ranges of the inputs. Thus the W-indices can provide more reasonable global sensitivity information of model output variance with respect to model inputs than the Sobol's indices. We also provide geometrical interpretations for the W- and Sobol's indices. As will be seen, the W-indices include the full regional sensitivity information [28,29], whereas the Sobol's indices only reflect the marginal information.

Three methods, including the double-loop-repeated-set Monte Carlo (DLRS MC) procedure, the double-loop-single-set MC (DLSS MC) procedure and the model emulation, are introduced for computing the W-indices. The DLRS MC method is suitable for computing all the W-indices, but its computational cost is demanding. The DLSS MC needs only one set of samples of model inputs and output for implementing it, thus it is computationally efficient. However, it is only applicable for computing the lower order indices. The model emulation can be used for computing all the W-indices with low cost as long as the model behavior can be correctly captured by the emulator.

The rest of this paper is organized as follows. Section 2 reviews the Sobol's indices. Section 3 proposes the W-indices, and compares it with the Sobol's indices geometrically. Section 4 develops the DLRS MC, DLSS MC and model emulation methods for numerically computing the W-indices. Section 5 introduces the Ishigami function and a modified Sobol's function for comparing the W- and Sobol's indices and for demonstrating the convergence and efficiency of the three numerical methods. Section 6 applies the W- and Sobol's indices to a roof structure and a flap structure. Section 7 gives conclusions and discussions.

2. Review of Sobol's indices

Suppose the computational model under investigation is represented by an input–output function $Y = g(\boldsymbol{X})$, where $\boldsymbol{X} = (X_1, X_2, \ldots, X_n)$ denotes the n-dimensional input vector and Y is the scalar model output of interest. Let $f_{\boldsymbol{X}}(\boldsymbol{x})$ denote the joint PDF of all inputs, then the marginal PDF $f_i(x_i)$ of the model input X_i ($i = 1, 2, \ldots, n$) can be derived as

$$f_i(x_i) = \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} f_{\boldsymbol{X}}(\boldsymbol{x}) \prod_{j=1, j\neq i}^{n} \mathrm{d}x_j. \tag{1}$$

For a set of model inputs $\boldsymbol{X_R} = \left(X_{i_1}, X_{i_2}, \ldots, X_{i_r}\right)$ ($r = 1, 2, \ldots, n$), Sobol's main effect index $S_{\boldsymbol{R}}$ is defined as [14]

$$S_{\boldsymbol{R}} = \frac{V_{\boldsymbol{R}}\left(E_{\sim\boldsymbol{R}}\left(Y \mid \boldsymbol{X_R}\right)\right)}{V(Y)} \tag{2}$$

where $V(Y)$ is the total variance of model output, the subscript $\boldsymbol{R}$ indicates that the variance is computed with respect to $\boldsymbol{X_R}$ and the subscript $\sim \boldsymbol{R}$ indicates that the expectation is taken with respect to all input but $\boldsymbol{X_R}$, i.e., $\boldsymbol{X_{\sim R}}$.

The total effect index $S_{T\boldsymbol{R}}$ for $\boldsymbol{X_R}$ is defined as [15]

$$S_{T\boldsymbol{R}} = \frac{V(Y) - V_{\sim\boldsymbol{R}}\left(E_{\boldsymbol{R}}\left(Y \mid \boldsymbol{X_{\sim R}}\right)\right)}{V(Y)} = \frac{E_{\sim\boldsymbol{R}}\left(V_{\boldsymbol{R}}\left(Y \mid \boldsymbol{X_{\sim R}}\right)\right)}{V(Y)}. \tag{3}$$

By the total variance law [30], $V_{\boldsymbol{R}}\left(E_{\sim\boldsymbol{R}}\left(Y \mid \boldsymbol{X_R}\right)\right) = V(Y) - E_{\boldsymbol{R}}\left(V_{\sim\boldsymbol{R}}\left(Y \mid \boldsymbol{X_R}\right)\right)$. $E_{\boldsymbol{R}}\left(V_{\sim\boldsymbol{R}}\left(Y \mid \boldsymbol{X_R}\right)\right)$ can be interpreted as the mean residual variance when $\boldsymbol{X_R}$ is fixed over their full distribution ranges. Further, $V_{\boldsymbol{R}}\left(E_{\sim\boldsymbol{R}}\left(Y \mid \boldsymbol{X_R}\right)\right)$ measures the average reduction of the variance of model output. The higher $S_{\boldsymbol{R}}$ is, the more influential $\boldsymbol{X_R}$ is on the variance of model output. Similarly, $E_{\sim\boldsymbol{R}}\left(V_{\boldsymbol{R}}\left(Y \mid \boldsymbol{X_{\sim R}}\right)\right)$ can be explained as the mean residual variance of model output when all the inputs but $\boldsymbol{X_R}$ are fixed over their full distribution ranges. The lower $S_{T\boldsymbol{R}}$ is, the less $\boldsymbol{X_R}$ contributes to the variance of model output.

3. The *W*-indices

3.1. Definition and interpretation

Before the proposition of the W-indices, it is necessary to introduce some notations. Let

$$\begin{aligned} \boldsymbol{Q} &= \begin{bmatrix} q_{1(1)} & q_{2(1)} & \cdots & q_{n(1)} \\ q_{1(2)} & q_{2(2)} & \cdots & q_{n(2)} \end{bmatrix}^T, \\ \boldsymbol{Q_R} &= \begin{bmatrix} q_{i_1(1)} & q_{i_2(1)} & \cdots & q_{i_r(1)} \\ q_{i_1(2)} & q_{i_2(2)} & \cdots & q_{i_r(2)} \end{bmatrix}^T \end{aligned} \tag{4}$$

where each element is a quantile value, and they satisfy $0 < q_{k(1)} < q_{k(2)} < 1$ for $k = 1, 2, \ldots, n$, and $0 < q_{i_k(1)} < q_{i_k(2)} < 1$ for $k = 1, 2, \ldots, r$, and $r \leq n$. $q_{k(1)}$ and $q_{k(2)}$ are correlated and uniformly distributed variables, $q_{k(1)} \sim U(0, 1)$ and $q_{k(2)} \sim U\left(q_{k(1)}, 1\right)$. $q_{k(1)}$ and $q_{l(1)}$ ($l \neq k$) are independent. Further, we define:

$$\begin{aligned} \boldsymbol{U} &= \begin{bmatrix} u_{1(1)} & u_{2(1)} & \cdots & u_{n(1)} \\ u_{1(2)} & u_{2(2)} & \cdots & u_{n(2)} \end{bmatrix}^T, \\ \boldsymbol{U_R} &= \begin{bmatrix} u_{i_1(1)} & u_{i_2(1)} & \cdots & u_{i_r(1)} \\ u_{i_1(2)} & u_{i_2(2)} & \cdots & u_{i_r(2)} \end{bmatrix}^T \end{aligned} \tag{5}$$

where $u_{k(1)} = F_k^{-1}\left(q_{k(1)}\right)$, $u_{k(2)} = F_k^{-1}\left(q_{k(2)}\right)$, $u_{i_k(1)} = F_{i_k}^{-1}\left(q_{i_k(1)}\right)$ and $u_{i_k(2)} = F_{i_k}^{-1}\left(q_{i_k(2)}\right)$. $F_k^{-1}(\cdot)$ and $F_{i_k}^{-1}(\cdot)$ denote the inverse cumulative distribution functions (CDFs) of the input X_k and X_{i_k}, respectively. $\boldsymbol{X_R} \in \boldsymbol{U_R}$ indicates that $X_{i_k} \in \left[u_{i_k(1)}, u_{i_k(2)}\right]$ for $k = 1, 2, \ldots, r$. Similarly, we can define the notations $\boldsymbol{Q_{\sim R}}$ and $\boldsymbol{U_{\sim R}}$.

For a set of model inputs $\boldsymbol{X_R}$, the W-main effect index $W_{\boldsymbol{R}}$ is defined as

$$\begin{aligned} W_{\boldsymbol{R}} &= \frac{E_{\boldsymbol{Q_R}}\left(V(Y) - V_{\boldsymbol{X}}\left(Y \mid \boldsymbol{X_R} \in \boldsymbol{U_R}\right)\right)}{V(Y)} \\ &= 1 - \frac{E_{\boldsymbol{Q_R}}\left(V_{\boldsymbol{X}}\left(Y \mid \boldsymbol{X_R} \in \boldsymbol{U_R}\right)\right)}{V(Y)} \end{aligned} \tag{6}$$

where the conditional variance $V_{\boldsymbol{X}}\left(Y \mid \boldsymbol{X_R} \in \boldsymbol{U_R}\right)$ is computed with respect to $\boldsymbol{X_R}$ over the reduced ranges $\boldsymbol{U_R}$ and with respect to $\boldsymbol{X_{\sim R}}$ over their full ranges. Thus $V_{\boldsymbol{X}}\left(Y \mid \boldsymbol{X_R} \in \boldsymbol{U_R}\right)$ is a function of all elements of $\boldsymbol{Q_R}$. The subscript $\boldsymbol{Q_R}$ in Eq. (6) indicates that the expectation is taken with respect to all elements of $\boldsymbol{Q_R}$.

The total effect index $W_{T\boldsymbol{R}}$ for $\boldsymbol{X_R}$ is defined as

$$W_{T\boldsymbol{R}} = \frac{E_{\boldsymbol{Q_{\sim R}}}\left(V_{\boldsymbol{X}}\left(Y \mid \boldsymbol{X_{\sim R}} \in \boldsymbol{U_{\sim R}}\right)\right)}{V(Y)} \tag{7}$$