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ARTICLE *in* STRUCTURAL SAFETY · JULY 2015

Impact Factor: 1.68 · DOI: 10.1016/j.strusafe.2014.12.005

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A new framework of variance based global sensitivity analysis for models with correlated inputs



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ARTICLE INFO

Article history:

Received 4 August 2014

Received in revised form 23 December 2014

Accepted 28 December 2014

Keywords:

Variance based global sensitivity analysis

Correlated variable

Variance contribution

Analytical test

ABSTRACT

In the past few decades, variance based global sensitivity analysis for models with only uncorrelated inputs has been well developed. It aims at investigating the impact of variations in uncorrelated inputs on the variation of a model output and ranking the importance of the inputs. However, for models with correlated inputs, only a few researches have been done and the existing theory of variance based global sensitivity is not so consummate. In this article, a new framework of variance based global sensitivity analysis is presented, which is suitable for models with both uncorrelated and correlated inputs. With this new framework, the variance based global sensitivity analysis for models with correlated variables can be conducted conveniently and the variance contributions of a correlated variable to the variance of model output can be identified and interpreted distinctly.

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1. Introduction

Global sensitivity analysis (GSA), also called importance measure analysis [1,2], aims at investigating the impact of variations in input variables on the variation of a model output and ranking the importance of the inputs. It can identify contributions of different inputs to the uncertainty of model output in full distribution domain of the inputs and comprehensively consider the average effect of the inputs on the output. GSA can also provide the importance sequence of the model inputs, which can help designers define the unknown parameters better to reduce the uncertainty scope of response and get an acceptable uncertain response range [3–5]. Over the past few decades, many GSA techniques have been developed, which can be summarized to three categories: non-parametric methods (e.g., correlation coefficient) [6–9], variance based methods [10–15], and moment-independent methods [16–19]. For models with only uncorrelated inputs, the variance based GSA can directly illustrate the variance contributions to the model output by inputs [20], and it has been widely used in engineering design.

Nowadays, many complex models have been developed in physics, chemistry, environmental sciences, risk analysis, etc. and these models usually involve correlated inputs. The significance

of GSA in engineering design cannot be over-emphasized. However, most of the above presented techniques for importance analysis are performed under the hypothesis of input independence. Only a few researches have focused on the importance analysis of models with correlated inputs [21–24], and most of them cannot explain the variance contribution clearly. Xu et al. proposed to decompose the variance contribution of an individual correlated input to model output into two parts: the uncorrelated variance contribution (contributed by the uncorrelated variations of the variable, i.e., variations unique to the variable) and the correlated variance contribution (contributed by the correlated variations of the variable, i.e., variations correlated with other parameters) [5]. This decomposition benefits the engineering design a lot and it can help designers decide whether they should focus on the correlated variations among specific variables (if the correlated contribution dominates) or the variable itself (if the uncorrelated contribution dominates). Moreover, it provides a thought to conduct the importance analysis of models with correlated inputs. Similarly, Li decomposed the variance contribution of a correlated input or a subset of inputs into a correlative contribution and a structural one [25], and Mara et al. made use of the orthogonal decorrelation of the correlated variables to compute partial variances [26], both of which give a bit more distinct interpretation of the variance contribution of a correlated variable. By analytically deriving the variances contributions of correlated variables to quadratic polynomial model, Hao gave more detail about variance contributions of correlated variables [27].

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In recent years, some works have been done to deal with the importance analysis problem for models with correlated inputs. However, most of the researchers just tried to compute and interpret the variance based global sensitivity indices defined by Sobol [12]. But, the analysis of variance (ANOVA) decomposition proposed by Sobol which is the foundation of variance based GSA is only available for independent variables. Extending this to correlated case will increase the complexity of variance based GSA. In this article, a novel framework of variance based GSA is proposed, by which the importance measure analysis for the correlated inputs can be conducted easily and it degenerates into ANOVA decomposition for models with only uncorrelated inputs. The total variance is decomposed into orders of partial variance contributions and each of them (except first order contributions) is further decomposed to uncorrelated interaction contribution and correlated contribution. With this framework, the variance contributions of correlated inputs to the variance of a model output can be identified clearly. Its rationality and correctness are illuminated by both theoretical derivation and analytical examples.

The remainder of this article is organized as follows. Section 2 reviews ANOVA decomposition and the classical variance based global sensitivity indices for model with only uncorrelated inputs. Section 3 is the core of the new detailed framework. The variance based GSA for models with correlated inputs is introduced and a further decomposition is conducted to have a more explicit cognition about the variance contributions of correlated variables. In addition, a general set of variance based global sensitivity indices are introduced and interpreted. Section 4 first applies the proposed theory to three simple polynomial models and presents their analytical results to interpret the theory introduced in Section 3, then applies the theory to numerical examples and Ishigami function. Section 5 concludes this article.

2. Review of the variance based GSA for uncorrelated variables

2.1. ANOVA

Suppose the computational model under investigation is represented by an input–output function $y = f(\mathbf{x})$, where $\mathbf{x} = (x_1, x_2, \dots, x_n)$ is a n -dimensional input vector, and the function $y = f(\mathbf{x})$ is square integrable to \mathbf{x} , which is generally true in practical application. Sobol considered a decomposition of $f(\mathbf{x})$ into terms of increasing dimensions [12], i.e.,

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{i=1}^n \sum_{j=i+1}^n f_{ij}(x_i, x_j) + \dots + f_{12\dots n}(x_1, x_2, \dots, x_n) \quad (1)$$

where

$$\begin{aligned} f_0 &= E(Y) \\ f_i(x_i) &= E(Y|x_i) - E(Y) \\ f_{ij}(x_i, x_j) &= E(Y|x_i, x_j) - f_i - f_j - f_0 \\ &\dots \end{aligned} \quad (2)$$

where $E(\bullet)$ is the expectation operator. For uncorrelated input variables, all the component functions are mutually orthogonal. Eq. (1) is called high dimensional model representation (HDMR) decomposition, which is the rationale for the variance based GSA.

By squaring and integrating Eq. (1), and employing the orthogonality of the component functions for uncorrelated inputs, the variance V of $f(\mathbf{x})$ can be obtained as

$$V = \sum_{i=1}^n V_i + \sum_{i=1}^n \sum_{j=i+1}^n V_{ij} + \dots + V_{12\dots n} \quad (3)$$

where

$$\begin{aligned} V_i &= V[f_i(x_i)] = V[E(Y|x_i)] \\ V_{ij} &= V[f_{ij}(x_i, x_j)] = V[E(Y|x_i, x_j)] - V_i - V_j \\ &\dots \end{aligned} \quad (4)$$

where $V(\bullet)$ is the variance operator, $V_i, V_{ij}, \dots, V_{12\dots n}$ are referred to as partial variances. With Eq. (3) the total variance V of $f(\mathbf{x})$ is decomposed into separated portions attributable to each input and interaction. V_i is the main or marginal variance contribution of x_i , and $V_{ij}, \dots, V_{12\dots n}$ are the interaction variance contributions. The total variance contribution V_i^T to the output variation due to factor x_i is its main variance contribution plus all higher order interaction variance contributions related to x_i . For a three-factor model $y = f(x_1, x_2, x_3)$, for example, the total variance contribution of x_1 is

$$V_1^T = V_1 + V_{12} + V_{13} + V_{123} \quad (5)$$

Another way to obtain the total variance contribution V_i^T is

$$V_i^T = E[V(Y|\mathbf{x}_{-i})] = V(Y) - V[E(Y|\mathbf{x}_{-i})] \quad (6)$$

where \mathbf{x}_{-i} indicates all inputs except x_i . V_i^T is the average remaining variance of Y when all inputs except x_i are fixed.

2.2. Variance based global sensitivity indices

A variance based global sensitivity index is defined as the ratio of the partial variance $V_{i_1\dots i_s}$ to the total variance V , i.e.,

$$S_{i_1\dots i_s} = V_{i_1\dots i_s} / V \quad (7)$$

A sensitivity index S_i only corresponding to a single variable x_i is called main sensitivity index, and a sensitivity index $S_{i_1\dots i_s}$ ($s \geq 2$) corresponding to two or more variables (x_{i_1}, \dots, x_{i_s}) is called interaction sensitivity index. In practical application, two kinds of sensitivity indices are more used. The first one is the main sensitivity index (also termed as first order Sobol index) defined as [12],

$$S_i = V_i / V \quad (8)$$

The second one is the total sensitivity index, which is defined as,

$$S_i^T = V_i^T / V \quad (9)$$

The main sensitivity index considers the main variance contribution for the variance of the model output due to the corresponding input. The total sensitivity index accounts for the total variance contributions to the output variance due to the corresponding input, which include both first order and higher order indices due to the interactions among inputs. Hence, the difference between the main and total sensitivity indices can show the contributions of interactions between inputs. If the objective of the research is to fix the factors which are not important in the models, the total sensitivity indices should be used. In contrast, if the purpose is to prioritize the inputs importance, the main sensitivity indices are a better choice.

3. Variance based GSA for correlated variables

For models with correlated inputs, we can obtain partial variances using Eq. (4), but as discussed in many papers [27–30], the physical meaning of the partial variance is difficult to interpret clearly. In this section, a new framework of variance based GSA for model with correlated inputs is presented. With this novel framework, the variance contributions of correlated inputs to the variance of a model output can be interpreted clearly and it degenerates into ANOVA decomposition for model with only uncorrelated inputs. To further investigate the variance contribution of a correlated variable, we decompose the partial

variances to uncorrelated and correlated parts. In the last part of this section, a general set of variance based global sensitivity indices is presented.

3.1. Partial variance contributions and global sensitivity indices

The HDMR in Eq. (1) presents the function relationship between the input variables \mathbf{x} and model output Y . For uncorrelated variable, the physical meaning of this relationship is clear, for instance, conditional expectation $E(Y|x_i)$ presents the relationship between x_i and Y . This relationship is mainly related to the construction of function $y = f(\mathbf{x})$. For correlated variable the relationship is not so clear due to the correlation, which leads to the complex variance contributions defined by Eq. (4). This complexity includes two aspects. First, the variance contributions are difficult to identify clearly. Second, some additional variance contributions are introduced, which are not parts of the total variance. For example, $y = x_1 + x_2$, where $x_1 \sim N(\mu_1, \sigma_1^2)$, $x_2 \sim N(\mu_2, \sigma_2^2)$, the correlation coefficient between x_1 and x_2 is ρ_{12} . For this simple example, using Eq. (4) directly, we have the following results

$$\begin{aligned} V_1 &= \sigma_1^2 + 2\rho_{12}\sigma_1\sigma_2 + \rho_{12}^2\sigma_2^2 \\ V_2 &= \sigma_2^2 + 2\rho_{12}\sigma_1\sigma_2 + \rho_{12}^2\sigma_1^2 \\ V_{12} &= -2\rho_{12}\sigma_1\sigma_2 - \rho_{12}^2\sigma_2^2 - \rho_{12}^2\sigma_1^2 \end{aligned} \quad (10)$$

The total variance is

$$V(Y) = \sigma_1^2 + 2\rho_{12}\sigma_1\sigma_2 + \sigma_2^2 \quad (11)$$

We can see that $\rho_{12}^2\sigma_2^2$ and $\rho_{12}^2\sigma_1^2$ in V_1 , V_2 and V_{12} respectively are additional variance contributions and the results are difficult to interpret properly.

The function relationship between the input variables \mathbf{x} and model output Y is very useful for GSA rather than the conditional expectation $E(Y|x_i)$ itself. Inspired by this, we have a similar HDMR to Eq. (1) for models with correlated variables, i.e.,

$$\begin{aligned} f(\mathbf{x}) &= f_0 + \sum_{i=1}^n f_i(x_i) + \sum_{i=1}^n \sum_{j=i+1}^n f_{ij}(x_i, x_j) + \dots \\ &\quad + f_{12\dots n}(x_1, x_2, \dots, x_n) \end{aligned} \quad (12)$$

where

$$\begin{aligned} f_0 &= E^U(Y) \\ f_i(x_i) &= E^U(Y|x_i) - E^U(Y) \\ f_{ij}(x_i, x_j) &= E^U(Y|x_i, x_j) - f_i - f_j - f_0 \\ &\dots \end{aligned} \quad (13)$$

where $E^U(\bullet)$ is the expectation operator ignoring the correlations among input variables \mathbf{x} . This HDMR defines the function relationship between \mathbf{x} and output Y without taking into account the correlations among the input variables. It can be used for GSA with correlated variables. The variance V of $f(\mathbf{x})$ in Eq. (12) can be decomposed as

$$V = \sum_{i=1}^n V_i + \sum_{i=1}^n \sum_{j=i+1}^n V_{ij} + \dots + V_{12\dots n} \quad (14)$$

where

$$\begin{aligned} V_i &= V[E^U(Y|x_i)] \\ V_{ij} &= V[E^U(Y|x_i, x_j)] - V_i - V_j \\ &\dots \end{aligned} \quad (15)$$

Though the connection between Eqs. (12) and (14) is not so explicit, Eq. (14) is a reasonable decomposition of the total variance V and the partial variances V_i , V_{ij} , \dots , $V_{12\dots n}$ are easy to explain.

In Eq. (14), V_i is the first order variance contribution or main variance contribution of x_i to the variance of model output, which relates to the uncertainty or variance of x_i alone. Since only x_i is considered in $V[E^U(Y|x_i)]$, no correlation is included in V_i and it is the uncorrelated variance contribution of x_i . We also call it uncorrelated main variance contribution definitely.

V_{ij} is the second order variance contribution of x_i and x_j . Both x_i and x_j are considered in $V[E^U(Y|x_i, x_j)]$ and it measures the joint effect of x_i and x_j . Therefore, V_{ij} is the variance contribution that attributes to the interaction and correlation between x_i and x_j . Similarly, higher order variance contributions can be explained.

For the simple model $y = x_1 + x_2$ discussed above, with the new framework we have the following results of the variance decomposition

$$V_1 = \sigma_1^2, \quad V_2 = \sigma_2^2, \quad V_{12} = 2\rho_{12}\sigma_1\sigma_2 \quad (16)$$

The results are very clear and easy to interpret. V_1 and V_2 are the main variance contributions of x_1 and x_2 , and they are only related to the variance of x_1 and x_2 , respectively. V_{12} is the second order variance contribution of x_1 and x_2 . Because there is no interaction in this example, V_{12} is the variance contribution that attributes to the correlation between x_1 and x_2 .

The summation of all the terms in Eq. (15) where the x_i is related (with i included in the subscripts) is the total variance contribution V_i^T of x_i . Another way to obtain the total variance contribution V_i^T is

$$V_i^T = V(Y) - V[E^U(Y|\mathbf{x}_{-i})] \quad (17)$$

Eq. (17) can be derived from Eq. (15). For example, for a three-factor model $y = f(x_1, x_2, x_3)$ we have

$$\begin{aligned} V(Y) - V[E^U(Y|\mathbf{x}_{-1})] &= V(Y) - V[E^U(Y|x_2, x_3)] \\ &= V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} \\ &\quad + V_{123} - (V_2 + V_3 + V_{23}) \\ &= V_1 + V_{12} + V_{13} + V_{123} = V_1^T \end{aligned} \quad (18)$$

V_i^T measures the total variance contributions to the output variance due to x_i , which include both first order and higher order indices due to the interactions among inputs.

3.2. Further decomposition of the partial variance contributions

To explore the variance contributions of correlated inputs more comprehensively, we give a more detailed decomposition of the partial variance contributions in this subsection. The partial variance contributions are decomposed into uncorrelated and correlated sorts, and the uncorrelated parts are further decomposed into main and interaction contributions as ANOVA does. Total uncorrelated and total correlated variance contributions are defined, which can be helpful to the engineering application. Fig. 1 helps to make sense of these variance contributions.

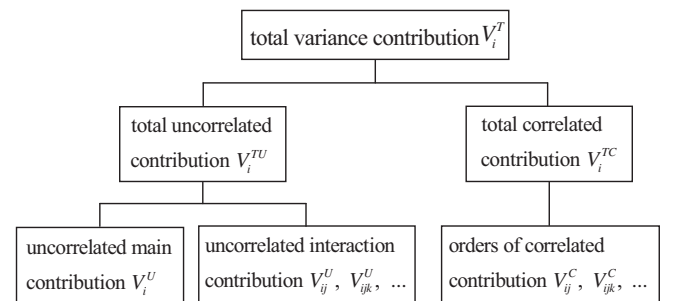


Fig. 1. The components of the variance contributions of x_i .

- Uncorrelated main contribution

The uncorrelated main variance contribution V_i^U is only related to the uncertainty of a single variable x_i . It is the uncorrelated variance contribution of a unique input x_i to the variance of model output Y and it can be calculated by

$$V_i^U = V^U[E^U(Y|x_i)] \quad (19)$$

where $V^U[\bullet]$ is the variance operator taking no account of the correlations among \mathbf{x} . Actually, the uncorrelated main variance contribution V_i^U is the same as the first order variance contribution V_i .

- Uncorrelated interaction contribution

The uncorrelated interaction variance contributions are the variance contributions caused by the uncorrelated interactions of input variables and they can be computed by

$$\begin{aligned} V_{ij}^U &= V^U[E^U(Y|x_i, x_j)] - V_i^U - V_j^U \\ V_{ijk}^U &= V^U[E^U(Y|x_i, x_j, x_k)] - V_{ij}^U - V_{ik}^U - V_{jk}^U - V_i^U - V_j^U - V_k^U \\ &\dots \end{aligned} \quad (20)$$

V_{ij}^U is the variance contribution contributed by the interaction of x_i and x_j ignoring the correlation of x_i and x_j , i.e., V_{ij}^U is the variance contribution only related to the uncorrelated interaction between x_i and x_j . V_{ijk}^U is the variance contribution that attributes to the uncorrelated interactions of x_i , x_j and x_k .

- Correlated contribution

The correlated contributions are the variance contributions caused by the correlations among input variables and they can be computed by

$$\begin{aligned} V_{ij}^C &= V_{ij} - V_{ij}^U \\ V_{ijk}^C &= V_{ijk} - V_{ijk}^U \\ &\dots \end{aligned} \quad (21)$$

V_{ij}^C is second order correlated variance contribution contributed by the correlation between x_i and x_j , V_{ijk}^C is third order correlated variance contribution that attributes to the correlations of x_i , x_j and x_k and so on.

- Total uncorrelated contribution

The total uncorrelated contribution V_i^{TU} of x_i is defined as the summation of uncorrelated variance contributions which include the uncorrelated main contribution of x_i and all the uncorrelated interaction contributions that relate to x_i . V_i^{TU} can also be obtained by

$$V_i^{TU} = V^U(Y) - V^U[E^U(Y|\mathbf{x}_{-i})] \quad (22)$$

The total uncorrelated contribution is similar to the total variance contribution of ANOVA introduced in Section 2.

- Total correlated contribution

The total correlated contribution V_i^{TC} of x_i is defined as the summation of all orders of correlated contributions that relate to x_i and it can also be obtained by

$$V_i^{TC} = V_i^T - V_i^{TU} \quad (23)$$

Eq. (23) is not difficult to understand since the variance contribution is very clear with the knowledge introduced above.

Obviously, the variance contributions related to the correlation vanish as the correlations among the input variables disappear. Then, it degenerates to ANOVA proposed by Sobol.

3.3. Variance based global sensitivity indices

In this subsection, we present a general set of variance based global sensitivity indices, which is adaptive for both correlated and uncorrelated variables. As introduced in Section 2, a variance based global sensitivity index is defined as the ratio of the partial variance and total variance V . According to this definition, many sensitivity indices can be defined. They can be classified into four categories: the main sensitivity indices, the total sensitivity indices, the uncorrelated interaction sensitivity indices and correlated sensitivity indices. For correlated variables, the total sensitivity indices can be further decomposed to uncorrelated and correlated ones.

The main sensitivity index or first order sensitivity index S_i of an individual input x_i is

$$S_i = \frac{V[E^U(Y|x_i)]}{V(Y)} \quad (24)$$

It can also be called the uncorrelated main sensitivity index since $V[E^U(Y|x_i)] = V^U[E^U(Y|x_i)]$. S_i measures the main variance contribution of a single variable x_i to the variance of output Y .

The total sensitivity index S_i^T of x_i is the ratio of the total variance contribution V_i^T and the variance of output Y , i.e.,

$$S_i^T = \frac{V_i^T}{V(Y)} = \frac{V(Y) - V[E^U(Y|\mathbf{x}_{-i})]}{V(Y)} \quad (25)$$

S_i^T measures the total variance contribution of x_i to $V(Y)$, including main contribution, uncorrelated interaction contributions and correlated contributions related to x_i . The total sensitivity index S_i^T can be further decomposed to total uncorrelated sensitivity index S_i^{TU} and total correlated sensitivity index S_i^{TC} and they can be obtained by

$$S_i^{TU} = \frac{V_i^{TU}}{V(Y)} = \frac{V^U(Y) - V^U[E^U(Y|\mathbf{x}_{-i})]}{V(Y)} \quad (26)$$

$$S_i^{TC} = \frac{V_i^T - V_i^{TU}}{V(Y)} = S_i^T - S_i^{TU} \quad (27)$$

S_i^{TU} measures the total uncorrelated variance contribution of x_i to $V(Y)$, including main contribution and uncorrelated interaction contributions related to x_i ; S_i^{TC} measures the total correlated variance contribution of x_i to $V(Y)$, which includes all orders of correlated contributions related to x_i .

The second order sensitivity index S_{ij} can be computed by

$$S_{ij} = \frac{V_{ij}}{V(Y)} = \frac{V[E^U(Y|x_i, x_j)] - V_i - V_j}{V(Y)} \quad (28)$$

It measures the variance contribution that attributes to the relation of x_i and x_j , including uncorrelated interaction and correlation. The second order uncorrelated interaction sensitivity index (or second order uncorrelated sensitivity index) S_{ij}^U is

$$S_{ij}^U = \frac{V_{ij}^U}{V(Y)} = \frac{V^U[E^U(Y|x_i, x_j)] - V_i^U - V_j^U}{V(Y)} \quad (29)$$

S_{ij}^U measures the uncorrelated interaction variance contribution between x_i and x_j to the variance of output Y . The second order correlated sensitivity index S_{ij}^C can be evaluated by

$$S_{ij}^C = \frac{V_{ij}^C}{V(Y)} = \frac{V_{ij} - V_{ij}^U}{V(Y)} = S_{ij} - S_{ij}^U \quad (30)$$

S_{ij}^C measures the correlated variance contribution between x_i and x_j to the total variance $V(Y)$. Higher order sensitivity indices can be computed and interpreted in a similar way.

4. Examples

4.1. Analytical test examples

In this subsection, we take three simple polynomial models with correlated variables as examples. By deriving their analytical GSA results using the formulae of variance and the properties of covariance [31] the novel GSA framework introduced in Section 3 is interpreted. Some useful formulae derived by the integral of probability density function of a normally distributed variable in Ref. [28] are given in Appendix A. In addition, another two essential formulae are derived in the same way in Appendix A, too.

4.1.1. Test case 1

The model we discuss in the first case is

$$y = x_1 + x_2^2 \quad (31)$$

where $(x_1, x_2) \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, mean vector $\boldsymbol{\mu} = (\mu_1, \mu_2)$ and covariance matrix $\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$.

With the formulae in Appendix A, the total variance $V(y)$ can be obtained as

$$V(y) = \sigma_1^2 + 4\mu_2\rho_{12}\sigma_1\sigma_2 + (2\sigma_2^4 + 4\mu_2^2\sigma_2^2) \quad (32)$$

and the partial variance contributions are listed in Table 1.

From the results listed in Table 1, it is clear that $V_i = V_i^U (i = 1, 2)$. In this case, there is no interaction between x_1 and x_2 , thus the uncorrelated interaction variance contribution V_{12}^U is equal to 0. The correlated variance contribution V_{12}^C is related to the correlation between x_1 and x_2 , which is represented by the correlation coefficient ρ_{12} . The partial variance contributions all can be figured out from the total variance $V(y)$. It is a reasonable decomposition of the total variance.

4.1.2. Test case 2

Consider a computational model represented by

$$y = x_1 + x_2 + x_1x_2 \quad (33)$$

where $(x_1, x_2) \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, mean vector $\boldsymbol{\mu} = (\mu_1, \mu_2)$ and covariance matrix $\boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$.

The total variance $V(y)$ can be obtained with the formulae in Appendix A

$$\begin{aligned} V(y) &= V[x_1 + x_2] + V[x_1x_2] + 2Cov(x_1 + x_2, x_1x_2) \\ &= (\sigma_1^2 + 2\rho_{12}\sigma_1\sigma_2 + \sigma_2^2) + (\mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2 \\ &\quad + 2\mu_1\mu_2\rho_{12}\sigma_1\sigma_2 + \rho_{12}^2\sigma_1^2\sigma_2^2 + \sigma_1^2\sigma_2^2) + 2(\mu_2\sigma_1^2 \\ &\quad + \mu_1\rho_{12}\sigma_1\sigma_2 + \mu_1\sigma_2^2 + \mu_2\rho_{12}\sigma_1\sigma_2) \end{aligned} \quad (34)$$

Table 1

Analytical results of partial variance contributions in test case 1.

Item	V_1	V_2	V_{12}	V_1^U	V_2^U	V_{12}^U	V_{12}^C
Result	σ_1^2	$2\sigma_2^4 + 4\mu_2^2\sigma_2^2$	$4\mu_2\rho_{12}\sigma_1\sigma_2$	σ_1^2	$2\sigma_2^4 + 4\mu_2^2\sigma_2^2$	0	$4\mu_2\rho_{12}\sigma_1\sigma_2$

Table 2

Analytical results of partial variance contributions in test case 2.

Item	V_1	V_2	V_{12}
Result	$(1 + \mu_2)^2\sigma_1^2$	$(1 + \mu_1)^2\sigma_2^2$	$2(\rho_{12}\sigma_1\sigma_2 + \mu_1\rho_{12}\sigma_1\sigma_2 + \mu_2\rho_{12}\sigma_1\sigma_2 + \mu_1\mu_2\rho_{12}\sigma_1\sigma_2) + \rho_{12}^2\sigma_1^2\sigma_2^2 + \sigma_1^2\sigma_2^2$
Item	V_1^U	V_2^U	V_{12}^U
Result	$(1 + \mu_2)^2\sigma_1^2$	$(1 + \mu_1)^2\sigma_2^2$	$\sigma_1^2\sigma_2^2$
Item	V_1^C	V_2^C	V_{12}^C
Result	$2(\rho_{12}\sigma_1\sigma_2 + \mu_1\rho_{12}\sigma_1\sigma_2 + \mu_2\rho_{12}\sigma_1\sigma_2 + \mu_1\mu_2\rho_{12}\sigma_1\sigma_2) + \rho_{12}^2\sigma_1^2\sigma_2^2$		

The partial variance contributions are listed in Table 2.

In this case, the interaction between x_1 and x_2 exists, thus the uncorrelated interaction variance contribution V_{12}^U appears. From the results, we can also have the conclusion $V_i = V_i^U (i = 1, 2)$ and the correlated variance contribution V_{12}^C includes the correlation coefficient ρ_{12} . Each of the partial variance contributions is a part of the total variance $V(y)$. The second order contribution V_{12} includes two parts of variance contributions, the uncorrelated interaction contribution V_{12}^U and the correlated contribution V_{12}^C .

4.1.3. Test case 3

In this case, we consider a model with three input variables

$$y = x_1x_2 + x_2x_3 \quad (35)$$

where $(x_1, x_2, x_3) \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, mean vector $\boldsymbol{\mu} = (\mu_1, \mu_2, \mu_3)$ and covariance

$$\text{matrix } \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \rho_{12}\sigma_1\sigma_2 & \rho_{13}\sigma_1\sigma_3 \\ \rho_{12}\sigma_1\sigma_2 & \sigma_2^2 & \rho_{23}\sigma_2\sigma_3 \\ \rho_{13}\sigma_1\sigma_3 & \rho_{23}\sigma_2\sigma_3 & \sigma_3^2 \end{pmatrix}.$$

The total variance $V(y)$ can be obtained as

$$\begin{aligned} V(y) &= V[x_1x_2 + x_2x_3] \\ &= (\mu_1^2\sigma_2^2 + \mu_2^2\sigma_1^2 + 2\mu_1\mu_2\rho_{12}\sigma_1\sigma_2 + \rho_{12}^2\sigma_1^2\sigma_2^2 + \sigma_1^2\sigma_2^2) \\ &\quad + (\mu_2^2\sigma_3^2 + \mu_3^2\sigma_2^2 + 2\mu_2\mu_3\rho_{23}\sigma_2\sigma_3 + \rho_{23}^2\sigma_2^2\sigma_3^2 + \sigma_2^2\sigma_3^2) \\ &\quad + 2 \cdot (\mu_1\mu_2\rho_{23}\sigma_2\sigma_3 + \mu_2^2\rho_{13}\sigma_1\sigma_3 + \mu_1\mu_3\sigma_2^2 + \mu_2\mu_3\rho_{12}\sigma_1\sigma_2 \\ &\quad + \rho_{12}\rho_{23}\sigma_1\sigma_2\sigma_3 + \rho_{13}\sigma_1\sigma_2\sigma_3) \end{aligned} \quad (36)$$

The first order partial variance contributions are listed in Table 3.1.

It is clear that $V_i = V_i^U$, which has been interpreted in Section 3. In this case, we can easily figure out the origin of the variance contributions from the results. The first order variance contribution V_i only relates to the variance of a unique input variable x_i . The second order partial variance contributions are listed in Table 3.2.

From the expression of Eq. (35), there is no interaction between x_1 and x_3 , thus the uncorrelated interaction contribution V_{13}^U equals 0. The second order variance contribution V_{ij} relates to the variances of x_i and x_j . Thus, both V_{ij}^U and V_{ij}^C relates to the variances of x_i and x_j , and V_{ij}^C also relates to the correlation coefficient ρ_{ij} . The third order partial variance contribution are listed in Table 3.3.

Since there is no third order interaction, V_{123}^U equals 0. From the results listed in Table 3.3, the third order variance contribution

Table 3.1

Analytical results of first order partial variance contributions in test case 3.

Item	V_1	V_2	V_3	V_1^U	V_2^U	V_3^U
Result	$\mu_2^2\sigma_1^2$	$(\mu_1 + \mu_3)^2\sigma_2^2$	$\mu_2^2\sigma_3^2$	$\mu_2^2\sigma_1^2$	$(\mu_1 + \mu_3)^2\sigma_2^2$	$\mu_2^2\sigma_3^2$

Table 3.2

Analytical results of second order partial variance contributions in test case 3.

Item	V_{12}				V_{13}	V_{23}
Result	$2\mu_1\mu_2\rho_{12}\sigma_1\sigma_2 + 2\mu_2\mu_3\rho_{12}\sigma_1\sigma_2 + \rho_{12}^2\sigma_1^2\sigma_2^2 + \sigma_1^2\sigma_2^2$				$2\mu_2^2\rho_{13}\sigma_1\sigma_3$	$2\mu_2\mu_3\rho_{23}\sigma_2\sigma_3 + 2\mu_1\mu_2\rho_{23}\sigma_2\sigma_3 + \rho_{23}^2\sigma_2^2\sigma_3^2 + \sigma_2^2\sigma_3^2$
Item	V_{12}^U	V_{13}^U	V_{23}^U	V_{12}^C	V_{13}^C	V_{23}^C
Result	$\sigma_1^2\sigma_2^2$	0	$\sigma_2^2\sigma_3^2$	$2\mu_1\mu_2\rho_{12}\sigma_1\sigma_2 + \rho_{12}^2\sigma_1^2\sigma_2^2 + 2\mu_2\mu_3\rho_{12}\sigma_1\sigma_2$	$2\mu_2^2\rho_{13}\sigma_1\sigma_3$	$2\mu_2\mu_3\rho_{23}\sigma_2\sigma_3 + \rho_{23}^2\sigma_2^2\sigma_3^2 + 2\mu_1\mu_2\rho_{23}\sigma_2\sigma_3$

Table 3.3

Analytical results of third order partial variance contributions in test case 3.

Item	V_{123}	V_{123}^U	V_{123}^C
Result	$2\rho_{12}\rho_{23}\sigma_1\sigma_2\sigma_3 + 2\rho_{13}\sigma_1\sigma_2^2\sigma_3$	0	$2\rho_{12}\rho_{23}\sigma_1\sigma_2\sigma_3 + 2\rho_{13}\sigma_1\sigma_2^2\sigma_3$

V_{123} is not equal to 0, because there is third order correlated contribution V_{123}^C . V_{123}^C relates to the variances of x_1 , x_2 and x_3 , and it relates to the correlation among x_1 , x_2 and x_3 which is reflected by the correlation coefficients ρ_{12} , ρ_{23} and ρ_{13} .

In this subsection, we present the analytical results of partial variances rather than sensitivity indices. It helps make sense of the variance contributions clearly. From the results, we can observe that with the new GSA framework introduced in this article the variance contributions can be interpreted clearly. It is shown that the correlated variance contributions become zero as the correlations among inputs disappear, and it degenerates into the Sobol's variance based GSA for uncorrelated variables, thus, the proposed variance based GSA can be readily employed for both correlated and uncorrelated inputs.

4.2. Numerical examples and application

4.2.1. Example 1

Consider a computational model represented by

$$y = 5 + x_1 + 2x_2 + 3x_3 + 2x_1^2 + 3x_1x_2 + x_1x_3 + 4x_2^2 + 3x_2x_3 + 2x_3^2 \quad (37)$$

in which $x_1 \sim N(1, 2^2)$, $x_2 \sim N(2, 1^2)$, $x_3 \sim N(2, 2^2)$, the correlation coefficients are $\rho_{12} = 0.3$, $\rho_{13} = 0.4$, $\rho_{23} = 0.2$, respectively.

Using Monte Carlo Simulation (MCS), we can conveniently obtain the GSA results. However, as we know the MCS is time consuming and the correctness of the results needs to be given a judgement. For this example, the first order and second order

Table 4.1

Accurate variance contribution results of example 1.

Item	V_1	V_2	V_3	V_{12}^U	V_{13}^U	V_{23}^U
Result	804	761	1424	36	16	36

Table 4.2

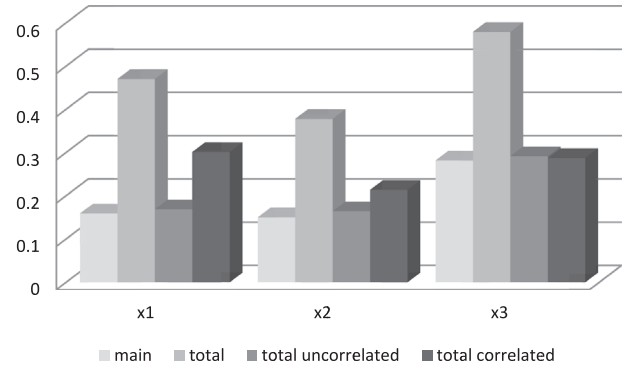
Estimate variance contribution results of example 1.

Item	V_1	V_2	V_3	V_{12}^U	V_{13}^U	V_{23}^U
Result	803.9856	760.9905	1424.0511	33.8143	14.4941	33.6093

Table 4.3

The main and total sensitivity indices of example 1.

SI	S_1				S_2	S_3			
Result	0.1590				0.1505	0.2817			
SI	S_1^T	S_2^T	S_3^T	S_1^{TU}	S_2^{TU}	S_3^{TU}	S_1^{TC}	S_2^{TC}	S_3^{TC}
Result	0.4704	0.3781	0.5793	0.1690	0.1643	0.2917	0.3014	0.2138	0.2876

**Fig. 2.** Histogram of the main and total sensitivity indices of example 1.

uncorrelated variance contributions can be analytically derived and their accurate results are listed in Table 4.1.

The accurate results listed in Table 4.1 can be a judgement or reference of the results computed by MCS.

The first order and second order uncorrelated variance contributions evaluated by MCS are listed in Table 4.2.

Comparing the results listed in Table 4.2 to Table 4.1, the first order variance contributions estimated by MCS are very close to the accurate results, while the second order uncorrelated variance contributions estimated by MCS are not so good, but the results are acceptable since they are much smaller than the first order variance contributions and the results give the exact magnitude relationship. It costs too much to compute the second order uncorrelated variance contributions exactly. The results of sensitivity indices are presented as follows:

GSA mainly concerns with the main and total sensitivity indices, and they are listed in Table 4.3. To view the magnitude relationship more clearly, we draw the histogram of the results listed in Table 4.3 as Fig. 2.

From the results, we can draw the following conclusions. The main sensitivity index of x_3 is the biggest, then is that of x_1 , the last is x_2 , which means that the magnitude relationship of the single variable variance contributions is $x_3 > x_1 > x_2$. The total sensitivity index of x_3 is much bigger than that of x_1 and x_2 , which tells us that among the total variance contributions x_3 contributes the most and the magnitude relationship is the same as that of the single variable variance contributions. Among the total uncorrelated sensitivity indices, x_3 is the biggest, i.e., the total uncorrelated variance contribution of x_3 contributes most. The total correlated sensitivity index of x_1 is bigger than that of x_3 and x_3 is bigger than that of x_2 , which reflects that the total correlated variance contribution of x_1 is bigger than the other two variables. The magnitude relationship

of the total correlated sensitivity indices can reflect the strength of the correlation between an individual variable and other variables in a certain extent.

To further explore the variance contributions of the relations among sets of inputs, second order and higher order sensitivity indices are needed. The second order and third order sensitivity indices are listed in Table 4.3. Fig. 3 is the histogram of the second order sensitivity indices listed in Table 4.4.

From Fig. 3, it is clear that the second order sensitivity index of x_1 and x_3 is much bigger than that of the other two. It means that

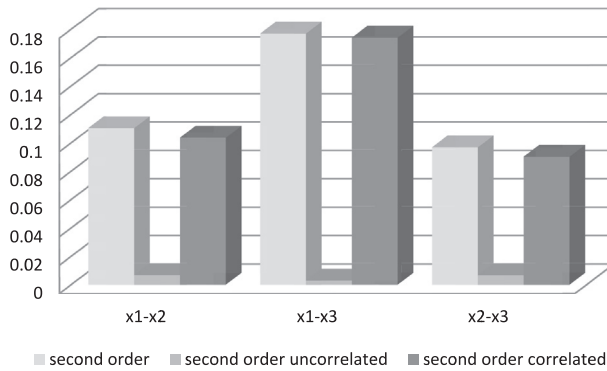


Fig. 3. Histogram of the second order sensitivity indices of example 1.

the variance contribution which attributes to the relation between x_1 and x_3 is much bigger than that of the other two. The second order uncorrelated sensitivity indices are much smaller, i.e., the variance contributions that attribute to the second order uncorrelated interactions are much fewer. The second order correlated sensitivity index of x_1 and x_3 is the biggest, then is that of x_1 and x_2 . It tells us that the magnitude relationship of the variance contributions which attribute to the correlations is: $(x_1 \text{ and } x_3) > (x_1 \text{ and } x_2) > (x_2 \text{ and } x_3)$. From the results of the third order sensitivity indices listed in Table 4.4, the third order uncorrelated sensitivity index is close to zero, which means the third order uncorrelated variance contribution is zero. It is clear because there is no third order interaction in Eq. (37). The third order correlated sensitivity index is very small, so does the third order sensitivity index.

Comparing the first order sensitivity indices in Table 4.3 and the second order sensitivity indices in Table 4.4, the second order uncorrelated sensitivity indices are much smaller, while the second order correlated sensitivity indices are not so small. For models with correlated variables, the higher variance contributions are considerable and they should not be ignored.

4.2.2. Example 2

Now, let us consider the Ishigami function from Ref. [30]

$$y = \sin(x_1) + 7 \sin^2(x_2) + 0.1x_3^4 \sin(x_1) \quad (38)$$

Table 4.4

The second order and third order sensitivity indices of example 1.

SI	S_{12}	S_{13}	S_{23}	S_{12}^U	S_{13}^U	S_{23}^U	S_{12}^C	S_{13}^C	S_{23}^C
Result	0.1103	0.1770	0.0968	0.0067	0.0029	0.0066	0.1036	0.1741	0.0902
SI	S_{123}			S_{123}^U			S_{123}^C		
Result	0.0214			0.0004			0.0210		

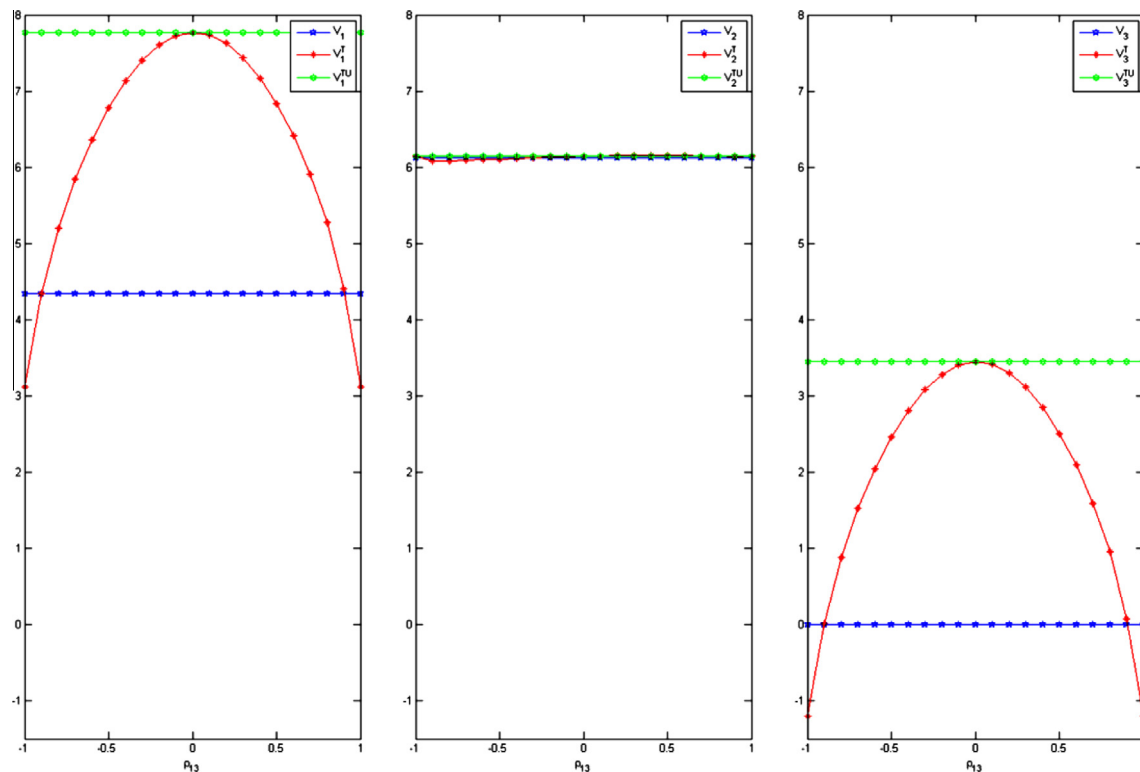


Fig. 4. The first order and total variance contributions at different values of ρ_{13} .

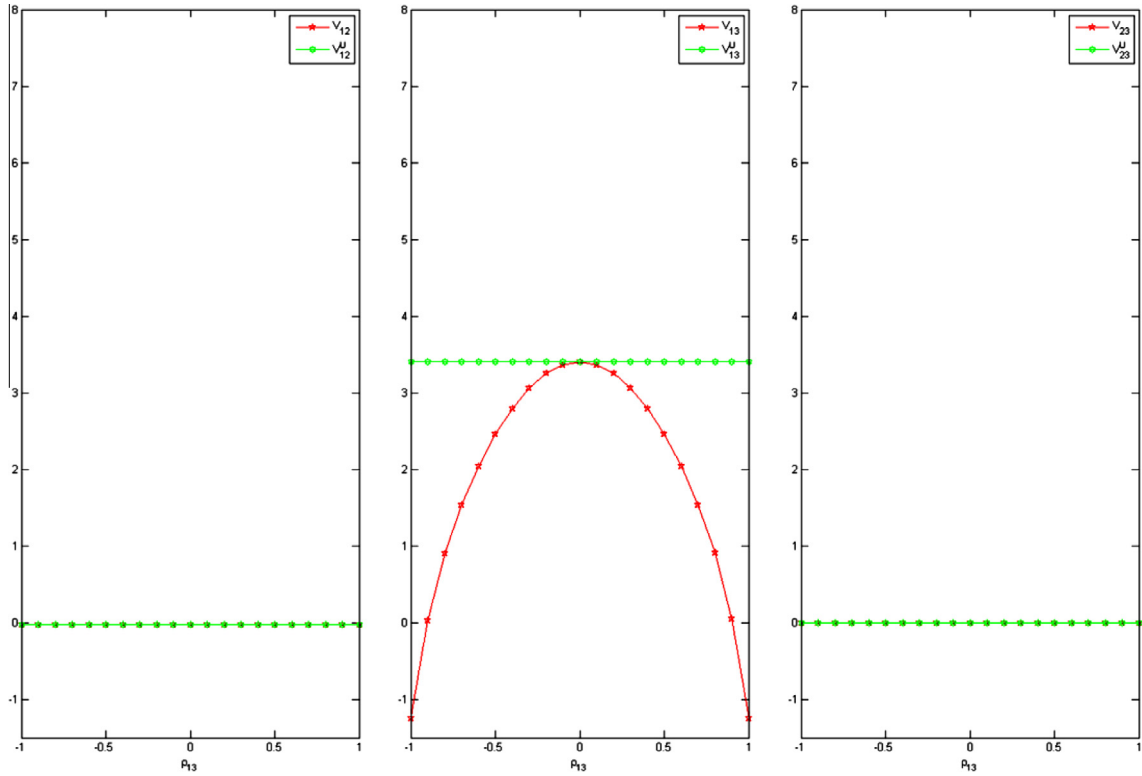


Fig. 5. The second order variance contributions at different values of ρ_{13} .

where the input variables x_1, x_2, x_3 are uniformly distributed over $[-\pi, \pi]$, x_1 and x_3 are correlated and the correlation coefficient is ρ_{13} .

In example 1, we discuss and interpret the results of sensitivity indices in detail. While, in this example we will analyze the variation of the variance contributions at different values of correlation coefficient ranging from $\rho_{13} = -1$ to $\rho_{13} = 1$. We can obtain numerical results with MCS and the copula approach introduced in Ref. [30].

Fig. 4 shows the first order and total variance contributions of each input variable respectively at different values of ρ_{13} . It is clear that the ranging of ρ_{13} has no effects on the first order and total uncorrelated variance contributions. Uncorrelated variance contributions have no connection with the correlations among input variables. V_1^T and V_3^T change obviously with the ranging of ρ_{13} , while V_2^T does not change at all. For this example, only x_1 and x_3 are correlated, i.e., only V_{13}^C exists, V_{12}^C and V_{23}^C are equal to 0, which is presented clearly by Fig. 5. In addition, there is no uncorrelated interaction between x_2 and the other two input variables, thus $V_2 = V_2^{TU} = V_2^T$.

Fig. 5 shows the second order variance contributions at different values of ρ_{13} . We can obtain $V_{12} = V_{12}^U = 0$ and $V_{23} = V_{23}^U = 0$. From Figs. 4 and 5, we can also obtain the correlated variance contributions changing with the ranging of ρ_{13} conveniently. It is easy to see that the correlated variance contribution between x_1 and x_3 ($V_{13}^C = V_{13} - V_{13}^U$) is negative for this example, thus $V_1^T < V_1^{TU}$ and $V_3^T < V_3^{TU}$. When $\rho_{13} = \pm 1$ the negative correlated variance contribution V_{13}^C is so strong that in these two cases $V_1^T < V_1$ and $V_3^T < V_3$. Since $V_2 = 0$ and $V_{23} = V_{23}^U = 0$, we have $V_2^T = V_2$ and $V_2^{TU} = V_2^U$, which is shown clearly in Figs. 4 and 5.

5. Conclusion

In this article, a new framework of variance based global sensitivity analysis for models with correlated inputs is introduced.

It is adaptive for both uncorrelated and correlated variables. With the new framework the total variance is decomposed into orders of partial variance contributions, and in order to have a more explicit cognition about the variance contributions of correlated variables, the second order and higher orders of partial variance contributions are further decomposed into uncorrelated interaction contributions and correlated contributions. It is significant and rational to divide the correlated contributions to the second order and higher orders of partial variance contributions because they are a kind of interaction.

In addition, a general set of variance based global sensitivity indices is introduced, which is adaptive for both correlated and uncorrelated variables. Many sensitivity indices are defined and their physical meanings are interpreted in detail. Among the sensitivity indices, the main sensitivity indices and the total sensitivity indices are most commonly used and the total sensitivity indices can be further decomposed into total uncorrelated sensitivity indices and total correlated sensitivity indices. If we want to investigate the impact of two or a set of inputs on the variance of model output, we need the second order or higher order sensitivity indices including uncorrelated interaction sensitivity indices and correlated sensitivity indices.

From the results of analytical test examples, the new framework proposed in this article can clearly interpret and analyze the variance contributions of correlated variables to the variance of total variance. Though the new variance based global sensitivity analysis can be conveniently actualized by Monte Carlo method, it is very time consuming. Some efficient method should be developed for the variance based global sensitivity analysis of correlated variables.

Acknowledgment

This article was supported by the National Natural Science Foundation of China (Grant No. NSFC 51475370).

Appendix A.

Some useful formulae derived in Ref. [28] for normally distributed variables

$$\begin{aligned}
 E(x_i^2) &= \sigma_i^2 + \mu_i^2, \\
 E(x_i^3) &= 3\mu_i\sigma_i^2 + \mu_i^3, \\
 E(x_i^4) &= 3\sigma_i^4 + 6\mu_i^2\sigma_i^2 + \mu_i^4, \\
 E(x_i x_j) &= \mu_i\mu_j + \rho_{ij}\sigma_i\sigma_j, \\
 E(x_i x_j^2) &= \mu_i\mu_j^2 + (\mu_i\sigma_j + 2\rho_{ij}\mu_i\sigma_i)\sigma_j, \\
 E(x_i^2 x_j^2) &= \mu_i^2\mu_j^2 + \mu_j^2\sigma_i^2 + \mu_i^2\sigma_j^2 + 4\rho_{ij}\mu_i\mu_j\sigma_i\sigma_j + (2\rho_{ij}^2 + 1)\sigma_i^2\sigma_j^2,
 \end{aligned} \quad (39)$$

In this article, we need another two formulae which are derived in the same way as in Ref. [28]

$$E(x_i x_j x_l) = \mu_i\mu_j\mu_l + \mu_i\rho_{jl}\sigma_j\sigma_l + \mu_j\rho_{il}\sigma_i\sigma_l + \mu_l\rho_{ij}\sigma_i\sigma_j \quad (40)$$

$$\begin{aligned}
 E(x_i x_j x_l x_m) &= \mu_i\mu_j\mu_l\mu_m + \mu_i\mu_j\rho_{lm}\sigma_l\sigma_m + \mu_i\mu_l\rho_{jm}\sigma_j\sigma_m \\
 &\quad + \mu_j\mu_l\rho_{im}\sigma_i\sigma_m + \mu_i\mu_m\rho_{jl}\sigma_j\sigma_l + \mu_j\mu_m\rho_{il}\sigma_i\sigma_l \\
 &\quad + \mu_l\mu_m\rho_{ij}\sigma_i\sigma_j + \rho_{ij}\rho_{lm}\sigma_i\sigma_j\sigma_l\sigma_m + \rho_{il}\rho_{jm}\sigma_i\sigma_j\sigma_l\sigma_m \\
 &\quad + \rho_{im}\rho_{jl}\sigma_i\sigma_j\sigma_l\sigma_m
 \end{aligned} \quad (41)$$

Appendix B. Supplementary data

Supplementary data associated with this article can be found, in the online version, at <http://dx.doi.org/10.1016/j.strusafe.2014.12.005>.

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