Applied Mathematical Modelling 45 (2017) 748–767

Contents lists available at ScienceDirect

Applied Mathematical Modelling

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

Analytical variance based global sensitivity analysis for models with correlated variables

Kaichao Zhang, Zhenzhou Lu*, Danqing Wu, Yongli Zhang

P.O. Box 120, School of Aeronautics, Northwestern Polytechnical University, Xi'an 710072, Shaanxi, PR China

ARTICLE INFO

Article history:
Received 13 March 2015
Revised 19 April 2016
Accepted 14 December 2016
Available online 12 January 2017

Keywords:
Analytical method
Variance based GSA
Correlated variable
Subset decomposition
Orthogonal decorrelation
Kriging model

ABSTRACT

In order to quantitatively analyze the variance contributions by correlated input variables to the model output, variance based global sensitivity analysis (GSA) is analytically derived for models with correlated variables. The derivation is based on the input-output relationship of tensor product basis functions and the orthogonal decorrelation of the correlated variables. Since the tensor product basis function based simulator is widely used to approximate the input-output relationship of complicated structure, the analytical solution of the variance based global sensitivity is especially applicable to engineering practice problems. The polynomial regression model is employed as an example to derive the analytical GSA in detail. The accuracy and efficiency of the analytical solution of GSA are validated by three numerical examples, and engineering application of the derived solution is demonstrated by carrying out the GSA of the riveting and two dimension fracture problem.

1. Introduction

Sensitivity analysis aims at investigating the impact of input variations on the variation of a model output, which can be classified into two categories: local sensitivity analysis and global sensitivity analysis [1,2]. *Global sensitivity analysis* (GSA) is also called importance measure analysis [3]. The existing importance measures can be summarized to three categories: non-parameter techniques (correlation coefficient model) [4,5], variance based methods [1,6,7], and moment independent model [2,8]. Variance based methods can directly illustrate the variance contributions of the model output by inputs, and they have been widely used in engineering design. Variance based GSA was first employed by Cukier et al. in chemistry [9]. Then, Hora and Iman introduced the uncertainty importance, and Sacks et al. gave a visual inspection of sensitivity results by decomposition of the output [10]. Sobol was inspired by the formers' work and used *analysis of variance* (ANOVA) to define the variance based sensitivity indices [11,12].

There are abundant simulation-based methods for variance based GSA, such as Monte Carlo, SDP, FAST etc [12–16]. These simulation-based methods are easy to comprehend and program. Unfortunately, simulation-based method always needs a large number of samples, which results in huge computation burden in practice. For uncorrelated variables, an analytical variance based GSA method was proposed in Ref. [17] by the theory that multivariate integrals of *tensor product basis functions* can be translated to calculations of univariate integrals. For second order polynomial models with correlated variables, Refs. [18–20] derived the analytical variance based GSA.

* Corresponding author.
E-mail addresses: zhangkaichao123321@126.com (K. Zhang), zhenzhoulu@nwpu.edu.cn (Z. Lu), wudanqing86@163.com (D. Wu).

http://dx.doi.org/10.1016/j.apm.2016.12.036
0307-904X/

In this paper, we extend the analytical variance based GSA method for uncorrelated variables in Ref. [17] to models with correlated variables. Based on the input-output relationship constructed by tensor product basis functions, we derive a universal analytical solution of variance based GSA for models with correlated variables. Using orthogonal decorrelation of the correlated variables, we achieve a simplified and easy way to realize the analytical derivation for variance based GSA. The analytical method proposed in this paper is especially applicable in engineering practice because the tensor product basis functions are usually used to create an input-output relationship in engineering. Metamodels commonly used in engineering, such as polynomial regression model, Kriging model, Gaussian radial basis model, MARS model etc., can be translated into the form expressed by the tensor product basis functions [21]. If the metamodel has been constructed, we can conveniently and efficiently obtain the results using the analytical solution of variance based GSA, which needs little computation cost.

The definition of variance based global sensitivity indices, subset decomposition and the concept of subset sensitivity indices are shortly introduced in Section 2. In Section 3, based on the tensor product basis functions, the universal analytical solution of the variance based GSA is derived for both uncorrelated and correlated variables. In Section 4, after the orthogonal decorrelation of the correlated variables, the analytical variance based GSA for models with correlated variables is presented. In Section 5, some numerical examples are used to validate the method proposed in this paper and engineering practice problems are analyzed by the proposed method. The last section evaluates the methods proposed in this paper and draws some conclusions to GSA.

2. Variance based GSA

2.1. The definition of global sensitivity indices

Suppose $y=f(\mathbf{x})$ is a square integrable function, in which $\mathbf{x}$ is a M-dimension input vector, i.e., $\mathbf{x}=(x_1, x_2,..., x_M)$. The *probability density function* (PDF) of x_i is expressed by $p_i(x_i)$ and $p(\mathbf{x})$ is the joint PDF of $\mathbf{x}$. For models with uncorrelated variables, $p(\mathbf{x}) = \prod_{i=1}^{M} p_i(x_i)$. Using *high dimension model representation* (HDMR), $f(\mathbf{x})$ can be decomposited as [11]

$$f(\mathbf{x}) = f_0 + \sum_{i=1}^{M} f_i(x_i) + \sum_{i_1=1}^{M}\sum_{i_2=i_1+1}^{M} f_{i_1 i_2}(x_{i_1}, x_{i_2}) + \cdots + f_{12\cdots M}(x_1, x_2, \ldots, x_M), \tag{1}$$

where f_0 is the mean of $f(\mathbf{x})$, i.e.

$$f_0 = \int f(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} = E[f(\mathbf{x})] \tag{2}$$

in which $E[\cdot]$ is the expectation operator. $f_i(x_i)$ is called *main effect* which is only related to x_i and can be obtained by

$$f_i(x_i) = \int f(\mathbf{x})p(\mathbf{x}_{-i}|x_i)\mathrm{d}\mathbf{x}_{-i} - f_0 = E[f(\mathbf{x})|x_i] - f_0, \tag{3}$$

where $\mathbf{x}_{-i}=(x_1,..., x_{i-1}, x_{i+1},..., x_M)$, and $p(\mathbf{x}_{-i}|x_i)=p(\mathbf{x})/p(x_i)$ is the conditional PDF of $\mathbf{x}_{-i}$ on x_i. For uncorrelated variables, $p(\mathbf{x}_{-i}|x_i) = \prod_{j\neq i} p_j(x_j)$.

$f_{i_1 i_2}(x_{i_1}, x_{i_2})$ is called *second order interaction effect* which is related to two variables x_{i_1} and x_{i_2} and can be obtained by

$$\begin{aligned} f_{i_1 i_2}(x_{i_1}, x_{i_2}) &= \int f(\mathbf{x})p(\mathbf{x}_{-(i_1,i_2)}|x_{i_1}, x_{i_2})\mathrm{d}\mathbf{x}_{-(i_1,i_2)} - f_{i_1}(x_{i_1}) - f_{i_2}(x_{i_2}) - f_0 \\ &= E[f(\mathbf{x})|x_{i_1}, x_{i_2}] - f_{i_1}(x_{i_1}) - f_{i_2}(x_{i_2}) - f_0, \end{aligned} \tag{4}$$

where $p(\mathbf{x}_{-(i_1,i_2)}|x_{i_1}, x_{i_2}) = p(\mathbf{x})/p(x_{i_1}, x_{i_2})$ is the conditional PDF of $\mathbf{x}_{-(i_1,i_2)}$ on x_{i_1} and x_{i_2}. For uncorrelated variables $p(\mathbf{x}_{-(i_1,i_2)}|x_{i_1}, x_{i_2}) = \prod_{j\neq i_1,i_2} p_j(x_j)$.

In general, $f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s})$ is called sth *order interaction effect* which is related to s variables $x_{i_1}, \ldots, x_{i_s}$ and can be obtained by

$$\begin{aligned} f_{i_1\cdots i_s}(x_{i_1}, \ldots, x_{i_s}) &= \int f(\mathbf{x})p(\mathbf{x}_{-(i_1,\ldots,i_s)}|x_{i_1}, \ldots, x_{i_s})\mathrm{d}\mathbf{x}_{-(i_1,\ldots,i_s)} - \sum_{k=1}^{s-1}\sum_{j_1,\ldots,j_k\in(i_1,\ldots,i_s)} f_{j_1\ldots j_k}(x_{j_1}, \ldots, x_{j_k}) - f_0 \\ &= E[f(\mathbf{x})|x_{i_1}, \ldots, x_{i_s}] - \sum_{k=1}^{s-1}\sum_{j_1,\ldots,j_k\in(i_1,\ldots,i_s)} f_{j_1\ldots j_k}(x_{j_1}, \ldots, x_{j_k}) - f_0, \end{aligned} \tag{5}$$

where $j_1 < j_2 < \ldots < j_k$ and $p(\mathbf{x}_{-(i_1,\ldots,i_s)}|x_{i_1}, \ldots, x_{i_s}) = p(\mathbf{x})/p(x_{i_1}, \ldots, x_{i_s})$ is the conditional PDF of $\mathbf{x}_{-(i_1,\ldots,i_s)}$ on $x_{i_1}, \ldots, x_{i_s}$. For uncorrelated variables $p(\mathbf{x}_{-(i_1,\ldots,i_s)}|x_{i_1}, \ldots, x_{i_s}) = \prod_{j\neq i_1,\ldots,i_s} p_j(x_j)$.

When all the variables are uncorrelated, the variance V of $f(\mathbf{x})$ can be expressed as the summation of variances $V_{i_1\ldots i_s}$, i.e.,

$$V = \sum_{i=1}^{M} V_i + \sum_{i_1=1}^{M}\sum_{i_2=i_1+1}^{M} V_{i_1 i_2} + \cdots + V_{1\cdots M}. \tag{6}$$

Eq. (6) can be viewed as a decomposition of variance V, in which

$$V = V[f(\mathbf{x})] = \int f^2(\mathbf{x})p(\mathbf{x})\mathrm{d}\mathbf{x} - f_0^2, \tag{7}$$

$$\begin{aligned} V_{i_1\cdots i_s} &= V[f_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s})] = \int f^2_{i_1\cdots i_s}(x_{i_1},\ldots,x_{i_s})p(x_{i_1},\ldots,x_{i_s})\mathrm{d}\mathbf{x}_{(i_1,\ldots,i_s)} \\ &= V\{E[f(\mathbf{x})|x_{i_1},\ldots,x_{i_s}]\} - \sum_{k=1}^{s-1}\sum_{j_1,\ldots,j_k\in(i_1,\ldots,i_s)} V_{j_1\ldots j_k}, \end{aligned} \tag{8}$$

where $V_{i_1\ldots i_s}$ is named as *partial variance*, $V[\cdot]$ is the variance operator, $\mathbf{x}_{(i_1,\ldots,i_s)} = (x_{i_1},\ldots,x_{i_s})$, $p(x_{i_1},\ldots,x_{i_s})$, is the joint PDF of $\mathbf{x}_{(i_1,\ldots,i_s)}$, and $p(x_{i_1},\ldots,x_{i_s}) = \prod_{j=i_1}^{i_s} p_j(x_j)$ when the inputs are uncorrelated.

When there are correlated variables, we cannot directly obtain the variance decomposition Eq. (6) by squaring and integrating Eq. (1), but we can similarly define the partial variance for correlated variables, i.e.,

$$\begin{aligned} V_i &= V\{E[f(\mathbf{x})|x_i]\} \\ V_{ij} &= V\{E[f(\mathbf{x})|x_i,x_j]\} - V_i - V_j \\ V_{i_1\cdots i_s} &= V\{E[f(\mathbf{x})|x_{i_1},\ldots,x_{i_s}]\} - \sum_{k=1}^{s-1}\sum_{j_1,\ldots,j_k\in(i_1,\ldots,i_s)} V_{j_1\ldots j_k}. \end{aligned} \tag{9}$$

It is easy to validate that Eq. (9) is an exact decomposition of variance V, i.e., the variance V can also be expressed as the summation of partial variances $V_{i_1\ldots i_s}$ for models with correlated inputs.

A global sensitivity index is defined as the ratio of the partial variance and the total variance V, i.e.,

$$S_{i_1\ldots i_s} = V_{i_1\ldots i_s}/V \tag{10}$$

A sensitivity index S_i only corresponding to a single variable x_i is called *main sensitivity index*, and a sensitivity index $S_{i_1\ldots i_s}(s \geq 2)$ corresponding to two or more variables $\mathbf{x}_{(i_1\ldots i_s)}$ is called *interaction sensitivity index*. From Eq. (6), it is easy to know that all the sensitivity indices sum to 1, i.e.,

$$\sum_{i=1}^{M} S_i + \sum_{i_1=1}^{M}\sum_{i_2=i_1+1}^{M} S_{i_1 i_2} + \cdots + S_{1\ldots M} = 1. \tag{11}$$

The *total sensitivity index* S_i^t for variable x_i is given by

$$S_i^t = S_i + S_{i,-i} = 1 - S_{-i}, \tag{12}$$

where $S_{i,-i}$ is the sum of interactions between x_i and all the other inputs, and S_{-i} is the sum of all $S_{i_1\ldots i_s}$terms that do not involve the index i (i.e., the sum of sensitivity indices of all the inputs except x_i). For instance, for a model with three variables (x_1, x_2, x_3), S_1^t for variable x_1 is

$$S_1^t = S_1 + S_{1,2} + S_{1,3} + S_{1,2,3} = 1 - S_{-1} = 1 - (S_2 + S_3 + S_{2,3}). \tag{13}$$

2.2. Subset decomposition and subset sensitivity indices

For subset decomposition, all the sensitivity indices can be evaluated by two most fundamental quantities: noncentered subset main effect (or called conditional mean) and subset main variance [17,21]. In addition, by subset decomposition, input variables are divided into several subsets $\mathbf{x}_{U_1}\ldots\mathbf{x}_{U_T}$, and similar to variable based analysis of variance, we have the subset based analysis of variance. $f(\mathbf{x})$ can be decomposited as (the superscript $\hat{}$ means that the item is corresponding to subset)

$$f(\mathbf{x}) = f_0 + \sum \hat{f}_{U_i}(\mathbf{x}_{U_i}) + \sum_{i_1=1}^{T}\sum_{i_2=i_1+1}^{T} \hat{f}_{U_{i_1}U_{i_2}}(\mathbf{x}_{U_{i_1}},\mathbf{x}_{U_{i_2}}) + \cdots + \hat{f}_{U_1\cdots U_T}(\mathbf{x}_{U_{i_1}},\ldots,\mathbf{x}_{U_{i_T}}). \tag{14}$$

The definition of the decomposition item $\hat{f}_{U_{i_1}\ldots U_{i_s}}$is similar to $f_{i_1\ldots i_s}$ in Eq. (1). The variance of $f(\mathbf{x})$ can be decomposed into the sum of a set of subset variances, i.e.,

$$V = \sum \hat{V}_{U_i} + \sum_{i_1=1}^{T}\sum_{i_2=i_1+1}^{T} \hat{V}_{U_{i_1}U_{i_2}} + \cdots + \hat{V}_{U_1\cdots U_T}. \tag{15}$$

The *subset sensitivity indices* are defined as the subset variance normalized by the total variance V, i.e.,

$$\hat{S}_{U_{i_1}\ldots U_{i_s}} = \hat{V}_{U_{i_1}\ldots U_{i_s}}/V. \tag{16}$$

Similarly, a sensitivity index corresponding to one subset is called *subset main sensitivity index* (SMSI) and a sensitivity index corresponding to two or more subsets is called *subset interaction sensitivity index* (SISI). For instance, supposing there are three input variables in total, they are divided into two groups: $\mathbf{x}_{U_1} = \{x_1, x_2\}$ and $\mathbf{x}_{U_2} = \{x_3\}$, then,

$$\begin{aligned}\hat{S}_{U_1} &= S_1 + S_2 + S_{1,2},\ \hat{S}_{U_2} = S_3,\ \hat{S}_{U_1U_2} = S_{1,3} + S_{2,3} + S_{1,2,3}\\ \hat{S}^t_{U_1} &= S_1 + S_2 + S_{1,2} + S_{1,3} + S_{2,3} + S_{1,2,3} = 1 - S_3\\ \hat{S}^t_{U_2} &= S_3 + S_{1,3} + S_{2,3} + S_{1,2,3} = 1 - S_1 - S_2 - S_{1,2}.\end{aligned} \tag{17}$$

Subset decomposition is very significant. By subset decomposition, all the sensitivity indices can be evaluated by two most fundamental quantities: noncentered subset main effect (or called conditional mean) and subset main variance, which will be further discussed in the following section. In addition, it is meaningful to engineering to investigate subset sensitivity indices. Sometimes we can divide the input factors into different groups according to different demands in engineering practice, and by subset decomposition we can discuss how each group of factors influences the uncertainty of output. From the computational results of Eq. (17), it is easy to know a subset main sensitivity index is the sum of main sensitivity indices of the variables in the subset and their interaction sensitivity indices.

3. Analytical solution of the variance based GSA

3.1. Tensor product basis functions

A multivariate tensor product basis function $B_i(\mathbf{x})$ is defined as a product of M univariate basis functions $h_{il}(x_l)$, i.e.,

$$B_i(\mathbf{x}) = \prod_{l=1}^{M} h_{il}(x_l), \qquad (i = 1, 2, \ldots, N_b). \tag{18}$$

For instance, $B_i(\mathbf{x})=x_1x_2$ can be rewritten as $B_i(\mathbf{x})=h_{i1}(x_1)h_{i2}(x_2)$, in which $h_{i1}(x_1)=x_1$ and $h_{i2}(x_2)=x_2$. Note here $h_{il}(x_l)$ can be equal to 1 to represent a constant. Then a special category of functions, defined as tensor product basis function, can be represented as a linear expansion of these multivariate basis functions, i.e.,

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} \left[a_i \prod_{l=1}^{M} h_{il}(x_l) \right], \tag{19}$$

where $a_i (i=0,\ 1,\ldots,\ N_b)$ are constant coefficients. For instance, in $f(\mathbf{x}) = x_1^2 + x_1 \sin x_2$ there are two multivariate basis functions $B_1(\mathbf{x}) = x_1^2$ and $B_2(\mathbf{x})=x_1 \sin x_2$, including four univariate basis functions $h_{11}(x_1) = x_1^2$, $h_{12}(x_2)=1$, $h_{21}(x_1)=x_1$, $h_{22}(x_2)=\sin x_2$, respectively. Many commonly used metamodels, such as polynomial regression model, Kriging model, Gaussian radial basis model, MARS model all can be expressed as tensor product basis functions.

3.2. Universal analytical solution of the variance based GSA

With subset decomposition, all the sensitivity indices can be evaluated by two most fundamental quantities: noncentered subset main effect and subset main variance. The noncentered subset main effect of $\mathbf{x}_U$ is

$$\hat{f}_U(\mathbf{x}_U) = \int f(\mathbf{x}) p(\mathbf{x}_{-U} | \mathbf{x}_U) \mathrm{d}\mathbf{x}_{-U}, \tag{20}$$

where $p(\mathbf{x}_{-U}|\mathbf{x}_U)=p(\mathbf{x})/p(\mathbf{x}_U)$. The subset main variance of $\mathbf{x}_U$ is

$$\hat{V}_U = \int [\hat{f}_U(\mathbf{x}_U) - f_0]^2 p(\mathbf{x}_U) \mathrm{d}\mathbf{x}_U. \tag{21}$$

Substituting into Eq. (20) the expression of the tensor product basis function Eq. (19), we can rewrite the noncentered subset main effect of $\mathbf{x}_U$ as follows: ($l \in U$ means $x_l \in \mathbf{x}_U$)

$$\begin{aligned}\hat{f}_U(\mathbf{x}_U) &= \int \left\{ a_0 + \sum_{i=1}^{N_b} \left[a_i \prod_{l=1}^{M} h_{il}(x_l) \right] \right\} p(\mathbf{x}_{-U}) \mathrm{d}\mathbf{x}_{-U}\\ &= a_0 + \sum_{i=1}^{N_b} \left\{ a_i \left[\int \prod_{l \notin U} h_{il}(x_l) p(\mathbf{x}_{-U}) \mathrm{d}\mathbf{x}_{-U} \right] \prod_{l \in U} h_{il}(x_l) \right\}\\ &= a_0 + \sum_{i=1}^{N_b} \left[a_i C_{1,il}^{-U} \prod_{l \in U} h_{il}(x_l) \right],\end{aligned} \tag{22}$$

where

$$C_{1,il}^{-U} = \int \prod_{l \notin U} h_{il}(x_l) p(\mathbf{x}|\mathbf{x}_U) \mathrm{d}\mathbf{x}_{-U} = E\left[\prod_{l \notin U} h_{il}(x_l)|\mathbf{x}_U\right]. \tag{23}$$

Setting $\mathbf{x}_U$ empty (i.e., $U=\mathbf{\Phi}$), we can directly obtain the function mean f_0

$$f_0 = a_0 + \sum_{i=1}^{N_b}\left[a_i E\left[\prod_{l=1}^{M} h_{il}(x_l)\right]\right] = a_0 + \sum_{i=1}^{N_b}\left[a_i \widehat{C}_{1,il}\right], \tag{24}$$

where $\widehat{C}_{1,il} = \int \prod_{l=1}^{M} h_{il}(x_l) p(\mathbf{x}) \mathrm{d}\mathbf{x} = E[\prod_{l=1}^{M} h_{il}(x_l)]$.

Substitute Eqs. (22) and (24) into Eq. (21), we can rewrite the subset main variance of $\mathbf{x}_U$ as follows:

$$\begin{aligned}
\hat{V}_U &= \int \left\{\sum_{i=1}^{N_b}\left[a_i C_{1,il}^{-U} \prod_{l \in U} h_{il}(x_l)\right] - \sum_{i=1}^{N_b}[a_i \widehat{C}_{1,il}]\right\}^2 p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U \\
&= \int \left\{\sum_{i=1}^{N_b}\left[a_i C_{1,il}^{-U} \prod_{l \in U} h_{il}(x_l)\right]\right\}^2 p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U \\
&\quad -2\sum_{i=1}^{N_b}\left[a_i \int C_{1,il}^{-U} \prod_{l \in U} h_{il}(x_l) p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U\right]\sum_{i=1}^{N_b}[a_i \widehat{C}_{1,il}] + \left[\sum_{i=1}^{N_b}[a_i \widehat{C}_{1,il}]\right]^2 \\
&= \int \left\{\sum_{i=1}^{N_b}\left[a_i C_{1,il}^{-U} \prod_{l \in U} h_{il}(x_l)\right]\right\}^2 p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U - \left[\sum_{i=1}^{N_b}[a_i \widehat{C}_{1,il}]\right]^2 \\
&= \sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}\left\{a_{i_1}a_{i_2}\int C_{1,i_1 l}^{-U} C_{1,i_2 l}^{-U} \prod_{l \in U} h_{i_1 l}(x_l) h_{i_2 l}(x_l) p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U\right\} - \sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}\{a_{i_1}a_{i_2}\widehat{C}_{1,i_1 l}\widehat{C}_{1,i_2 l}\} \\
&= \sum_{i_1=1}^{N_b}\sum_{i_2=1}^{N_b}\{a_{i_1}a_{i_2}[C_{2,i_1 i_2 l}^{U} - \widehat{C}_{1,i_1 l}\widehat{C}_{1,i_2 l}]\},
\end{aligned} \tag{25}$$

where

$$C_{2,i_1 i_2 l}^{U} = \int C_{1,i_1 l}^{-U} C_{1,i_2 l}^{-U} \prod_{l \in U} h_{i_1 l}(x_l) h_{i_2 l}(x_l) p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U = E\left[C_{1,i_1 l}^{-U} C_{1,i_2 l}^{-U} \prod_{l \in U} h_{i_1 l}(x_l) h_{i_2 l}(x_l)\right]. \tag{26}$$

Denote $\mathbf{x}_U=\mathbf{x}$, we can directly obtain the variance of $f(\mathbf{x})$

$$V = \sum_{i_1}^{N_b}\sum_{i_2}^{N_b}\{a_{i_1}a_{i_2}[\widehat{C}_{2,i_1 i_2 l} - \widehat{C}_{1,i_1 l}\widehat{C}_{1,i_2 l}]\}, \tag{27}$$

where $\widehat{C}_{2,i_1 i_2 l} = \int \prod_{l=1}^{M} h_{i_1 l}(x_l) h_{i_2 l}(x_l) p(\mathbf{x})\mathrm{d}\mathbf{x} = E[\prod_{l=1}^{M} h_{i_1 l}(x_l) h_{i_2 l}(x_l)]$.

From the derivation of Eqs. (22)–(27), the evaluations of all the sensitivity indices are simplified as the computations of $C_{1,il}^{-U}$ and $C_{2,i_1 i_2 l}^{U}$ in Eqs. (23) and (26), respectively, i.e., the computations of conditional expectation and expectation of the corresponding input variables. For models with uncorrelated variables, the computations of $C_{1,il}^{-U}$ and $C_{2,i_1 i_2 l}^{U}$ can be further simplified to the computations of expectations of univariate basis functions and two univariate basis functions' products.

Actually, the analytical derivation from Eq. (20) to Eq. (27) presents a universal analytical solution which is applicable to the GSA of uncorrelated variables as well as correlated variables. However, generally the computations of $C_{1,il}^{-U}$ and $C_{2,i_1 i_2 l}^{U}$ are difficult to conduct for model with the correlated variables, and it is not easy to achieve the universal programming for computations of $C_{1,il}^{-U}$ and $C_{2,i_1 i_2 l}^{U}$ due to the diversity of the product items. In Section 4, we take orthogonal decorrelation of the correlated variables into account. For decorrelated variables, the computations of $C_{1,il}^{-U}$ and $C_{2,i_1 i_2 l}^{U}$ can be simplified to the computations of decorrelated variables' means, variances and high order moments. We achieve an analytical solution which is simple and easy to program for variance based GSA of the correlated input variables in Section 4.

3.3. Verification and numerical examples

In this subsection, a simple linear model and a second order polynomial model with correlated variables are presented to prove the analytical solution is universal for uncorrelated variables as well as correlated variables.

(1) Consider a linear function $y=a_1x_1+a_2x_2$, where x_1 and x_2 follow the normal distribution $N(\mu_i,\sigma_i^2)(i=1,2)$, the correlation coefficient between x_1 and x_2 is ρ_{12}, a_1 and a_2 are constants. First, we define the univariate basis functions as

$$h_{il}=\begin{cases}1 & i\neq l\\ x_l & i=l\end{cases}. \tag{28}$$

Then, multivariate tensor product basis functions are

$$B_i(\mathbf{x})=\prod_{l=1}^{2}h_{il}(x_l)=x_i. \tag{29}$$

We can rewrite the linear model as

$$f(\mathbf{x})=a_0+\sum_{i=1}^{N_b}a_iB_i(\mathbf{x})=a_1x_1+a_2x_2. \tag{30}$$

The computations of S_1 and S_2: we define $\mathbf{x}_{U_1}=\{x_1\}$ and $\mathbf{x}_{U_2}=\{x_2\}$. With Eq. (22) we can obtain,

$$\hat{f}_{U_1}(x_{U_1})=a_1x_1+a_2E(x_2|x_1), \tag{31}$$

$$\hat{f}_{U_2}(x_{U_2})=a_1E(x_1|x_2)+a_2x_2, \tag{32}$$

where $E(x_2|x_1)=\mu_2+\rho_{12}(x_1-\mu_1)\frac{\sigma_2}{\sigma_1}$, $E(x_1|x_2)=\mu_1+\rho_{12}(x_2-\mu_2)\frac{\sigma_1}{\sigma_2}$. Using Eq. (25) we can obtain partial variances as

$$\hat{V}_{U_1}=a_1^2\sigma_1^2+2a_1a_2\rho_{12}\sigma_1\sigma_2+a_2^2\rho_{12}^2\sigma_2^2, \tag{33}$$

$$\hat{V}_{U_2}=a_1^2\rho_{12}^2\sigma_1^2+2a_1a_2\rho_{12}\sigma_1\sigma_2+a_2^2\sigma_2^2. \tag{34}$$

With Eq. (27) we can obtain total variance

$$V(y)=a_1^2\sigma_1^2+2a_1a_2\rho_{12}\sigma_1\sigma_2+a_2^2\sigma_2^2. \tag{35}$$

According to the definition of global sensitivity index, we can obtain S_1 and S_2 easily.

(2) Consider a second order polynomial model $y=a_1x_1^2+a_2x_2$, where x_1 and x_2 follow the normal distribution, i.e., $x_i\sim N(\mu_i,\sigma_i^2)(i=1,2)$, the correlation coefficient between x_1 and x_2 is ρ_{12}, a_1 and a_2 are constants. For the sake of simplicity, we define the univariate basis functions as $h_{11}(x_1)=x_1^2$, $h_{12}(x_2)=1$, $h_{21}(x_1)=1$ and $h_{22}(x_2)=x_2$ (the general univariate basis functions for second order polynomial model are $h_{(i,j)l}=\{\begin{smallmatrix}1 & \text{none of } (i,j)=l\\ x_l & \text{only one of } (i,j)=l\\ x_l^2 & \text{both of } (i,j)=l\end{smallmatrix}$). Then, multivariate tensor product basis functions are $B_1(\mathbf{x})=x_1^2$ and $B_2(\mathbf{x})=x_2$. The second order polynomial model can be rewritten as

$$f(\mathbf{x})=a_0+\sum_{i=1}^{N_b}a_iB_i(\mathbf{x})=a_1x_1^2+a_2x_2. \tag{36}$$

Denote $\mathbf{x}_{U_1}=\{x_1\}$ and $\mathbf{x}_{U_2}=\{x_2\}$ and use Eq. (25), we can obtain partial variances $\hat{V}_{U_1}$ and $\hat{V}_{U_2}$ as follows:

$$\hat{V}_{U_1}=a_1^2[Ex_1^4-(Ex_1^2)^2]+2a_1a_2\{E[E(x_2|x_1)\cdot x_1^2]-Ex_1^2\cdot Ex_2\}+a_2^2\{E[E(x_2|x_1)\cdot E(x_2|x_1)]-(Ex_2)^2\}, \tag{37}$$

$$\begin{aligned}\hat{V}_{U_2}=&a_1^2\{E[E(x_1^2|x_2)\cdot E(x_1^2|x_2)]-(Ex_1^2)^2\}\\&+2a_1a_2\{E[E(x_1^2|x_2)\cdot x_2]-Ex_1^2\cdot Ex_2\}+a_2^2[Ex_2^2-(Ex_2)^2].\end{aligned} \tag{38}$$

The total variance can be obtained by use of Eq. (27)

$$V(y)=a_1^2[Ex_1^4-(Ex_1^2)^2]+2a_1a_2[E(x_1^2\cdot x_2)-Ex_1^2\cdot Ex_2]+a_2^2[Ex_2^2-(Ex_2)^2], \tag{39}$$

where (Ref. [18])

$$Ex_1^4=3\sigma_1^4+6\mu_1^2\sigma_1^2+\mu_1^4, \tag{40}$$

$$E(x_1^2|x_2)=\sigma_1^2(1-\rho_{12}^2)+\mu_1^2+2\mu_1\rho_{12}(x_2-\mu_2)\frac{\sigma_1}{\sigma_2}+\rho_{12}^2(x_2-\mu_2)^2\frac{\sigma_1^2}{\sigma_2^2}. \tag{41}$$

The two examples in this subsection validate the universality of the analytical method obtained in Section 3.2. In addition, from the computations of these two examples we can observe that as the models become more complicated the computations of $C_{1,il}^{-U}$ and $C_{2,i_1i_2l}^{U}$ in Eqs. (23) and (26) turn to be more and more difficult. For the computational formula' diversity, this method is not easy to program. That is to say, it is not a practical method for engineering application. In Section 4, we will present an analytical method which is simple and easy to program for variance based GSA.

4. Analytical method for variance based GSA with correlated variables

4.1. Orthogonal decorrelation of correlated variables

A procedure to derive a set of orthogonal decorrelation variables from a set of correlated random variables **x** is given in Ref. [22], i.e.,

$$\begin{cases} \bar{x}_1 = x_1 \\ \bar{x}_2 = x_2 - E[x_2|\bar{x}_1] \\ \quad \vdots \\ \bar{x}_i = x_i - E[x_i|\bar{x}_1, \ldots, \bar{x}_{i-1}], \quad \forall i = 2, \ldots, M \end{cases}. \tag{42}$$

Under the assumption that only the first-order conditional moment characterizes the dependences between the inputs (x_1, x_2,..., x_M), the new variables $\bar{x}_i (i = 2, \ldots, M)$ are orthogonal and independent. To simplify the derivation in the sequel, we change the first item $\bar{x}_1$ a little, i.e.,

$$\begin{cases} \bar{x}_1 = x_1 - E[x_1] \\ \bar{x}_2 = x_2 - E[x_2|\bar{x}_1] \\ \quad \vdots \\ \bar{x}_i = x_i - E[x_i|\bar{x}_1, \ldots, \bar{x}_{i-1}], \quad \forall i = 2, \ldots, M \end{cases}. \tag{43}$$

It is obvious that to minus the first item by $E[x_1]$ (a constant) does not change the orthogonality and independence of the new variables. Compared to Eq. (42), the structure form of Eq. (43) is more unified, and Eq. (43) can simplify the formula derivation in the sequel and facilitate programming.

The new sensitivity indices $\bar{S}_{i_1 \cdots i_s}$ evaluated by the new variables are interpreted as follows [22]

- $\bar{S}_1 = V[E[f(\mathbf{x})|\bar{x}_1]]/V[f(\mathbf{x})] = S_1$ is the full marginal contribution of x_1 to the variance $V[f(\mathbf{x})]$.
- $\bar{S}_2 = V[E[f(\mathbf{x})|\bar{x}_2]]/V[f(\mathbf{x})] = S_{2-1}$ is the marginal contribution of x_2 to the variance $V[f(\mathbf{x})]$ without its correlative contribution with x_1, since $\bar{x}_2$ is uncorrelated with x_1.
- $\bar{S}_3 = V[E[f(\mathbf{x})|\bar{x}_3]]/V[f(\mathbf{x})] = S_{3-12}$ is the marginal contribution of x_3 to the variance $V[f(\mathbf{x})]$ without its correlative contribution with {x_1, x_2}.
- $\cdots$
- $\bar{S}_M = V[E[f(\mathbf{x})|\bar{x}_M]]/V[f(\mathbf{x})] = S_M^u$ is the uncorrelated marginal contribution of x_M to the variance $V[f(\mathbf{x})]$.
- $\cdots$
- $\bar{S}_M^{tu} = 1 - V[E[f(\mathbf{x})|\bar{\mathbf{x}}_{-M}]]/V[f(\mathbf{x})] = S_M^{tu}$ is the uncorrelated total contribution of x_M to the variance $V[f(\mathbf{x})]$.

The interpretations of correlated variables' sensitivity indices are complicated [23]. In this paper, we focus on three sensitivity indices $\bar{S}_1$, $\bar{S}_M$ and $\bar{S}_M^{tu}$, i.e., the full marginal contribution S_i (correlated total contribution, SI), the uncorrelated marginal contribution S_i^u (SIU) and the uncorrelated total contribution S_i^{tu} (SITU) of x_i, due to their explicit physical meanings.

For the simple linear example in Section 3.3, by using the transformation $(1)\{ {}^{\bar{x}_1 = x_1 - E[x_1]}_{\bar{x}_2 = x_2 - E[x_2|\bar{x}_1]}$, the function $y = a_1x_1 + a_2x_2$ can be rewritten as

$$y^{(1)} = \left(a_1 + a_2\rho_{12}\frac{\sigma_2}{\sigma_1}\right)\bar{x}_1 + a_2\bar{x}_2 + a_1\mu_1 + a_2\mu_2 \tag{44}$$

and by using transformation $(2)\{ {}^{\bar{x}_2 = x_2 - E[x_2]}_{\bar{x}_1 = x_1 - E[x_1|\bar{x}_2]}$, the function $y = a_1x_1 + a_2x_2$ can be rewritten as

$$y^{(2)} = a_1\bar{x}_1 + \left(a_2 + a_1\rho_{12}\frac{\sigma_1}{\sigma_2}\right)\bar{x}_2 + a_1\mu_1 + a_2\mu_2. \tag{45}$$

We use superscript (1) and (2) to stand for the results of transformations (1) and (2), respectively. In transformation (1), we have $V(\bar{x}_1) = \sigma_1^2$ and $V(\bar{x}_2) = \sigma_2^2(1 - \rho_{12}^2)$ (the detailed derivation is presented in the following Section 4.3). Denote $\mathbf{x}_{U_1} = \{\bar{x}_1\}$ and $\mathbf{x}_{U_2} = \{\bar{x}_2\}$, and use Eq. (25), we can obtain partial variance

$$\hat{V}_{U_1}^{(1)} = V_1 = \left(a_1 + a_2\rho_{12}\frac{\sigma_2}{\sigma_1}\right)^2 \cdot \sigma_1^2. \tag{46}$$

Similarly, in conversion (2) we have $V(\bar{x}_2) = \sigma_2^2$ and $V(\bar{x}_1) = \sigma_1^2(1 - \rho_{12}^2)$. Setting $\mathbf{x}_{U_1} = \{\bar{x}_1\}$ and $\mathbf{x}_{U_2} = \{\bar{x}_2\}$, and using Eq. (25) we can obtain partial variance

$$\hat{V}_{U_2}^{(2)} = V_2 = \left(a_1\rho_{12}\frac{\sigma_1}{\sigma_2} + a_2\right)^2 \cdot \sigma_2^2. \tag{47}$$

With Eq. (27) we can obtain total variance

$$V(y) = V(y^{(1)}) = V(y^{(2)}) = a_1^2\sigma_1^2 + 2a_1a_2\rho_{12}\sigma_1\sigma_2 + a_2^2\sigma_2^2. \tag{48}$$

The above computation results of partial and total variances are exactly the same as those obtained in Section 3.3.

4.2. Analytical variance based GSA for decorrelated variables

As mentioned in Section 3, for models with uncorrelated variables the computations of $C_{1,il}^{-U}$ and $C_{2,i_1i_2l}^{U}$ in Eqs. (23) and (26) can be further simplified to the computations of expectations of univariate basis functions and two univariate basis functions' products, respectively, i.e.,

$$C_{1,il}^{-U} = \int \prod_{l\notin U} h_{il}(x_l)p(\mathbf{x}_{-U})\mathrm{d}\mathbf{x}_{-U} = \prod_{l\notin U}\int h_{il}(x_l)p(x_l)\mathrm{d}x_l = \prod_{l\notin U} D_{1,il}, \tag{49}$$

$$\begin{aligned} C_{2,i_1i_2l}^{U} &= \int C_{1,i_1l}^{-U}C_{1,i_2l}^{-U}\prod_{l\in U} h_{i_1l}(x_l)h_{i_2l}(x_l)p(\mathbf{x}_U)\mathrm{d}\mathbf{x}_U \\ &= C_{1,i_1l}^{-U}C_{1,i_2l}^{-U}\prod_{l\in U}\int h_{i_1l}(x_l)h_{i_2l}(x_l)p(x_l)\mathrm{d}x_l = C_{1,i_1l}^{-U}C_{1,i_2l}^{-U}\prod_{l\in U} D_{2,i_1i_2l}, \end{aligned} \tag{50}$$

where

$$D_{1,il} = \int h_{il}(x_l)p(x_l)\mathrm{d}x_l = E[h_{il}(x_l)], \tag{51}$$

$$D_{2,i_1i_2l} = \int h_{i_1l}(x_l)h_{i_2l}(x_l)p(x_l)\mathrm{d}x_l = E[h_{i_1l}(x_l)h_{i_2l}(x_l)]. \tag{52}$$

Here, we take polynomial regression model as an example to illustrate how to conduct analytical variance based GSA for correlated variables. Consider the most widely used second order regression model,

$$f(\mathbf{x}) = \beta_0 + \sum_{i=1}^{M}\beta_i x_i + \sum_{i=1}^{M}\beta_{ii}x_i^2 + \sum_{i=1}^{M}\sum_{j=i+1}^{M}\beta_{ij}x_ix_j, \tag{53}$$

where $0 \le i, j \le M$, $j \neq 0$. Define multivariate tensor product basis functions as

$$B_{(i,j)} = \begin{cases} x_j & i = 0 \\ x_j^2 & i = j \\ x_ix_j & i < j \end{cases}. \tag{54}$$

The univariate basis functions corresponding to variable x_l are

$$h_{(i,j)l} = \begin{cases} 1 & \text{none of } (i,j) = l \\ x_l & \text{only one of } (i,j) = l \\ x_l^2 & \text{both of } (i,j) = l \end{cases}. \tag{55}$$

Then, the second order regression model can be rewritten as

$$f(\mathbf{x}) = \beta_0 + \sum_{0\le i,j\le M, j\ne 0}\beta_{ij}B_{(i,j)} = \beta_0 + \sum_{0\le i,j\le M, j\ne 0}\beta_{ij}\prod_{l=1}^{M} h_{(i,j)l}, \tag{56}$$

where $\beta_{0j} = \beta_j$. D_1 and D_2 can be computed by

$$D_{1,(i,j)l} = \begin{cases} 1 & \text{none of } (i,j) = l \\ \int x_l p_l(x_l)\mathrm{d}x_l = \mu_l & \text{only one of } (i,j) = l \\ \int x_l^2 p_l(x_l)\mathrm{d}x_l = \mu_l^2 + \sigma_l^2 & \text{both of } (i,j) = l \end{cases}, \tag{57}$$

$$D_{2,(i_1,j_1)(i_2,j_2)l} = \begin{cases} 1 & \text{none of } (i_1,j_1,i_2,j_2) = l \\ \int x_l p_l(x_l)\mathrm{d}x_l = \mu_l & \text{only one of } (i_1,j_1,i_2,j_2) = l \\ \int x_l^2 p_l(x_l)\mathrm{d}x_l = \mu_l^2 + \sigma_l^2 & \text{only two of } (i_1,j_1,i_2,j_2) = l \\ \int x_l^3 p_l(x_l)\mathrm{d}x_l = \mu_{l,3} + 3\mu_l\sigma_l^2 + \mu_l^3 = \alpha_{l,3} & \text{only three of } (i_1,j_1,i_2,j_2) = l \\ \int x_l^4 p_l(x_l)\mathrm{d}x_l = \mu_{l,4} + 4\mu_l\mu_{l,3} + 6\mu_l^2\sigma_l^2 + \mu_l^4 & \\ \qquad = \alpha_{l,4} & \text{all of } (i_1,j_1,i_2,j_2) = l \end{cases}, \tag{58}$$

respectively, where μ_l and σ_l^2 are the mean and variance of input variable x_l, $\mu_{l,k}$ (k is a positive integer) is the kth centered moment of x_l, i.e., $\mu_{l,k} = \int (x_l - \mu_l)^k p(x_l)\mathrm{d}x_l$, $\alpha_{l,k}$ is the kth origin moment of x_l, i.e., $\alpha_{l,k} = \int {x_l}^k p(x_l)\mathrm{d}x_l$. For second order model, the input variables in Eqs. (57) and (58) are the new variables from the orthogonal decorrelation of correlated variables. Thus, we have to compute the means, variances and high order moments (centered or origin moments) of the variables $\bar{x}_i$ in Eq. (43), and the highest order required is $2\times 2 = 4$.

For nth order polynomial model, we can define the univariate basis functions corresponding to variable x_l as

$$h_{(i^{(1)},\ldots,i^{(n)})l} = \begin{cases} 1 & \text{none of } (i^{(1)},\ldots,i^{(n)}) = l \\ x_l & \text{only one of } (i^{(1)},\ldots,i^{(n)}) = l \\ x_l^2 & \text{both of } (i^{(1)},\ldots,i^{(n)}) = l \\ \vdots & \vdots \\ x_l^n & \text{all of } (i^{(1)},\ldots,i^{(n)}) = l \end{cases}, \tag{59}$$

where $0 \le i^{(1)},\ldots, i^{(n)} \le M$. Then, the nth order polynomial model can be rewritten as

$$f(\mathbf{x}) = \beta_0 + \sum_{0\le i^{(1)},\ldots,i^{(n)}\le M,(i^{(1)},\ldots,i^{(n)})\neq 0} \beta_{ij} \prod_{l=1}^{M} h_{(i^{(1)},\ldots,i^{(n)})l} \tag{60}$$

and D_1 and D_2 can be computed by

$$D_{1,(i^{(1)},\ldots,i^{(n)})l} = \begin{cases} 1 & \text{none of } (i^{(1)},\ldots,i^{(n)}) = l \\ \int x_l p_l(x_l)\mathrm{d}x_l = \mu_l & \text{only one of } (i^{(1)},\ldots,i^{(n)}) = l \\ \int x_l^2 p_l(x_l)\mathrm{d}x_l = \mu_l^2+\sigma_l^2 & \text{both of } (i^{(1)},\ldots,i^{(n)}) = l \\ \vdots & \vdots \\ \int x_l^n p_l(x_l)\mathrm{d}x_l = \alpha_{l,n} & \text{all of } (i^{(1)},\ldots,i^{(n)}) = l \end{cases}, \tag{61}$$

$$D_{2,(i_1^{(1)},\ldots,i_1^{(n)})(i_2^{(1)},\ldots,i_2^{(n)})l} = \begin{cases} 1 & \text{none of } (i_1^{(1)},\ldots,i_1^{(n)},i_2^{(1)},\ldots,i_2^{(n)}) = l \\ \int x_l p_l(x_l)\mathrm{d}x_l = \mu_l & \text{only one of } (i_1^{(1)},\ldots,i_1^{(n)},i_2^{(1)},\ldots,i_2^{(n)}) = l \\ \int x_l^2 p_l(x_l)\mathrm{d}x_l = \mu_l^2+\sigma_l^2 & \text{only two of } (i_1^{(1)},\ldots,i_1^{(n)},i_2^{(1)},\ldots,i_2^{(n)}) = l \\ \vdots & \vdots \\ \int x_l^{2n} p_l(x_l)\mathrm{d}x_l = \alpha_{l,2n} & \text{all of } (i_1^{(1)},\ldots,i_1^{(n)},i_2^{(1)},\ldots,i_2^{(n)}) = l \end{cases}. \tag{62}$$

Similarly, for nth order polynomial model the input variables are the new variables from the orthogonal decorrelation of correlated variables, either. We have to compute the means, variances and high order origin moments of the variables $\bar{x}_i$ in Eq. (43), and the highest order required is $2n$.

4.3. Derivation of mean, variance, high order moments of $\bar{x}_i$

To develop the derivation, we first define a new matrix operation "*", Z^* means square each element of the matrix Z. If $Z = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$, then $Z^* = \begin{pmatrix} a_{11}^2 & a_{12}^2 \\ a_{21}^2 & a_{22}^2 \end{pmatrix}$.

Assuming that all the input variables follow normal distribution, i.e., $x_i \sim N(\mu_i, \sigma_i^2)$, the means and variances of the variables $\bar{x}_i (i = 1, 2, \ldots, M)$ in Eq. (43) can be obtained

$$E\bar{x}_i = Ex_i - E[E(x_i|\bar{x}_1,\ldots,\bar{x}_{i-1})] = 0, \tag{63}$$

$$V\bar{x}_i = \sigma_i^2 - \left(\sum_{i(i-1)} \sum_{(i-1)(i-1)}^{-1} \right)^* \sum_{(i-1)}^{\mathrm{T}}, \tag{64}$$

where $\sum_{i(i-1)} = (\mathrm{cov}(x_i,\bar{x}_1),\ldots,\mathrm{cov}(x_i,\bar{x}_{i-1}))$, $\sum_{(i-1)(i-1)} = \begin{pmatrix} V\bar{x}_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & V\bar{x}_{i-1} \end{pmatrix}$ and $\sum_{(i-1)} = (V\bar{x}_1,\ldots,V\bar{x}_{i-1})$.

The detailed derivation is presented as follows:

(1) For $\bar{x}_1$, it is easy to prove that $E\bar{x}_1 = E(x_1 - \mu_1) = 0$ and $V\bar{x}_1 = V(x_1 - \mu_1) = \sigma_1^2$.
(2) For $\bar{x}_2$, we can obtain that $E\bar{x}_2 = Ex_2 - E[E[x_2|\bar{x}_1]] = 0$ and $V\bar{x}_2 = \sigma_2^2(1-\rho_{12}^2)$.
Firstly, we have a result about covariance which is

$$\mathrm{cov}(x_k,\bar{x}_1) = E[x_k(x_1-\mu_1)] = \mathrm{cov}(x_k,x_1). \tag{65}$$

According to Eq. (65), it is easy to find that the correlation coefficient between x_k and $\bar{x}_1$ is equal to that between x_k and x_1 which is ρ_{1k}.
The computation of $V\bar{x}_2$ is shown as

$$V\bar{x}_2 = V[x_2 - E(x_2|\bar{x}_1)] = Vx_2 + V[E(x_2|\bar{x}_1)] - 2\mathrm{cov}(x_2, E(x_2|\bar{x}_1)). \tag{66}$$

From the knowledge of probability, we know that

$$E(x_2|\bar{x}_1) = \mu_2 + \rho_{12}(\bar{x}_1 - \bar{\mu}_1)\frac{\sigma_2}{\sigma_1}. \tag{67}$$

Then,

$$V[E(x_2|\bar{x}_1)] = \rho_{12}^2\sigma_2^2 \tag{68}$$

$$\begin{aligned}\mathrm{cov}(x_2, E(x_2|\bar{x}_1)) &= E[x_2E(x_2|\bar{x}_1)] - Ex_2Ex_2 \\ &= E\left[\mu_2x_2 + \rho_{12}(\bar{x}_1x_2 - \bar{\mu}_1x_2)\frac{\sigma_2}{\sigma_1}\right] - \mu_2^2 = \rho_{12}^2\sigma_2^2.\end{aligned} \tag{69}$$

(3) For $\bar{x}_i$, we have $E\bar{x}_i = Ex_i - E[E(x_i|\bar{x}_1,\dots,\bar{x}_{i-1})] = 0$ and $V\bar{x}_i = \sigma_i^2 - (\sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1})^*\sum_{(i-1)}^{\mathrm{T}}$.

The derivation of $V\bar{x}_i$ is presented as

$$V\bar{x}_i = V[x_i - E(x_i|\bar{x}_1,\dots,\bar{x}_{i-1})] = Vx_i + V[E(x_i|\bar{x}_1,\dots,\bar{x}_{i-1})] - 2\mathrm{cov}(x_i, E(x_i|\bar{x}_1,\dots,\bar{x}_{i-1})). \tag{70}$$

For convenience, we denote $\bar{\mathbf{x}}_{(i-1)} = (\bar{x}_1,\dots,\bar{x}_{i-1})^{\mathrm{T}}$.
We know that

$$E(x_i|\bar{\mathbf{x}}_{(i-1)}) = \mu_i + \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)}), \tag{71}$$

$$V(x_i|\bar{\mathbf{x}}_{(i-1)}) = \sigma_i^2 - \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}\sum_{(i-1)i}^{\mathrm{T}}, \tag{72}$$

where $\bar{\mu}_{(i-1)} = E(\bar{\mathbf{x}}_{(i-1)}) = (E(\bar{x}_1),\dots,E(\bar{x}_{i-1}))^{\mathrm{T}} = 0$ and $\sum_{(i-1)i} = (\mathrm{cov}(x_i,\bar{x}_1),\dots,\mathrm{cov}(x_i,\bar{x}_{i-1}))$.
Thus,

$$\begin{aligned}V[E(x_i|\bar{\mathbf{x}}_{(i-1)})] &= V\left[\mu_i + \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})\right] \\ &= \left(\sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}\right)^*\sum_{(i-1)}^{\mathrm{T}},\end{aligned} \tag{73}$$

$$\begin{aligned}\mathrm{cov}[x_i, E(x_i|\bar{\mathbf{x}}_{(i-1)})] &= E\left\{x_i\left[\mu_i + \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})\right]\right\} - \mu_i^2 \\ &= \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}E[x_i(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})].\end{aligned} \tag{74}$$

Since $x_i = \bar{x}_i + E[x_i|\bar{x}_1,\dots,\bar{x}_{i-1}]$, we can obtain that

$$\begin{aligned}E[x_i(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})] &= E[\bar{x}_i(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)}) + E(x_i|\bar{\mathbf{x}}_{(i-1)})(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})] \\ &= E\left[\mu_i(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)}) + \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})\right] \\ &= E\left[\sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})\right].\end{aligned} \tag{75}$$

It can be proved that $\mathrm{cov}[x_i, E(x_i|\bar{\mathbf{x}}_{(i-1)})] = (\sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1})^*\sum_{(i-1)}^{\mathrm{T}}$ (the detailed derivation is shown in Appendix A.1).

The calculation of covariance $\mathrm{cov}(x_k,\bar{x}_i)$ is a recursive process as

$$\mathrm{cov}(x_k,\bar{x}_i) = E(x_k\bar{x}_i) = \mathrm{cov}(x_k,x_i) - \sum_{i(i-1)}\sum_{(i-1)(i-1)}^{-1}E[x_k(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})]. \tag{76}$$

In conclusion, we can obtain that

$$V\bar{x}_i = \sigma_i^2 - \left(\sum_{i(i-1)} \sum_{(i-1)(i-1)}^{-1} \right)^* \sum_{(i-1)}^{\mathrm{T}} . \tag{77}$$

Up to now we have gained the mean and variance of $\bar{x}_i$, and the kth centered moments can be calculated by (the detailed derivation is shown in Appendix A.2)

$$\mu_{i,k} = \begin{cases} (\sqrt{V\bar{x}_i})^k (k-1)(k-3)\ldots 3 \times 1, & k \text{ is even number} \\ 0, & k \text{ is odd number} \end{cases} . \tag{78}$$

Because the mean of $\bar{x}_i$ is equal to zero, the kth centered moment is equal to the kth origin moment of $\bar{x}_i$, i.e.,

$$\alpha_{i,k} = \mu_{i,k}. \tag{79}$$

4.4. GSA analytical results of commonly used metamodels

The Kriging model [24,25] can be rewritten in the form of tensor product function, i.e.,

$$f(\mathbf{x}) = \beta + \sum_{i=1}^{N} \kappa_i \prod_{l=1}^{M} h_{il}(x_l), \tag{80}$$

where $h_{il}(x_l) = \exp[-\theta_l (x_l - x_{il})^2]$ and is called Gaussian correlation function, θ_l is the correlation coefficient. For variables following normal distribution, we have [21]

$$D_{1,il} = \frac{1}{\sqrt{2\sigma_l^2 \theta_l + 1}} \exp\left[-\frac{\theta_l}{2\sigma_l^2 \theta_l + 1} (\mu_l - x_{il})^2 \right], \tag{81}$$

$$D_{2,i_1 i_2 l} = \frac{1}{\sqrt{4\sigma_l^2 \theta_l + 1}} \exp\left\{ -\frac{\theta_l}{4\sigma_l^2 \theta_l + 1} \left[(\mu_l - x_{i_1 l})^2 + (\mu_l - x_{i_2 l})^2 \right] + 2\sigma_l^2 \theta_l (x_{i_1 l} - x_{i_2 l})^2 \right\}. \tag{82}$$

The Gaussian radial basis model [26] can be transformed into the form of tensor product function [17], i.e.,

$$f(\mathbf{x}) = \beta + \sum_{i=1}^{N_\phi} \left[\lambda_i \prod_{l=1}^{M} h_{il}(x_l) \right], \tag{83}$$

where $h_{il}(x_l) = \exp[-(x_l - t_{il})^2 / 2\tau_i^2]$ in which τ_i is width (also called radius) of a radial based function and t_i is the center of the radial basis function and has elements t_{il}. For normal distribution, we derive that [17]

$$D_{1,il} = \frac{1}{\sqrt{\sigma_l^2/\tau_l^2 + 1}} \exp[-(\mu_l - t_{il})^2 / (2\tau_i^2 + 2\sigma_l^2)], \tag{84}$$

$$D_{2,i_1 i_2 l} = \frac{\tau_{i_1} \tau_{i_2}}{\sqrt{b_{i_1 i_2 l}}} \exp\left\{ -\frac{1}{2b_{i_1 i_2 l}} \left[\tau_{i_2}^2 (\mu_j - t_{i_1 j})^2 + \tau_{i_1}^2 (\mu_j - t_{i_2 j})^2 + \sigma_j^2 (t_{i_1 j} - t_{i_2 j})^2 \right] \right\}, \tag{85}$$

where $b_{i_1 i_2 l} = \sigma_l^2 (\tau_{i_1}^2 + \tau_{i_2}^2) + \tau_{i_1}^2 \tau_{i_2}^2$.

The MARS model [27] can be viewed as a weighted sum of tensor spline basis functions, i.e.,

$$f(\mathbf{x}) = a_0 + \sum_{i=1}^{N_b} a_i B_i(\mathbf{x}). \tag{86}$$

Similarly, we can transform it into the form of tensor product function, either. For normal distribution, it is proved that [17]

$$D_{1,il} = s_{il} \left\{ \frac{\mu_l - t_{il}}{\sigma_l} \Phi\left(\frac{x_l - \mu_l}{\sigma_l} \right) - \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{(x_l - \mu_l)^2}{2\sigma_l^2} \right] \right\} \Big|_{lb_1}^{ub_1} \quad (l \in \mathbf{K}_i), \tag{87}$$

$$\begin{aligned} D_{2,i_1 i_2 l} = s_{i_1 l} s_{i_2 l} \Bigg\{ & \left[\frac{(\mu_l - t_{i_1 l})(\mu_l - t_{i_2 l})}{\sigma_l} + \sigma_l \right] \Phi\left(\frac{x_l - \mu_l}{\sigma_l} \right) \\ & - \frac{x_l + \mu_l - t_{i_1 l} - t_{i_2 l}}{\sqrt{2\pi}} \exp\left[-\frac{(x_l - \mu_l)^2}{2\sigma_l^2} \right] \Bigg\} \Big|_{lb_2}^{ub_2} \quad (l \in \mathbf{K}_{i_1}, l \in \mathbf{K}_{i_2}). \end{aligned} \tag{88}$$

The detailed derivations of these models can be found in Refs. [17] and [21].

Table 1
Sensitivity indices of a linear model.

Input		x_1	x_2	x_3
Mara's results	S_i	0.9446	0.4018	0.5786
	S_i^u	0.0196	0.0546	0.0262
Hao's results	S_i	0.9446	0.4018	0.5786
	S_i^u	0.0196	0.0546	0.0262
	S_i^{tu}	0.0196	0.0546	0.0262
Results in this paper	S_i	0.9446	0.4018	0.5786
	S_i^u	0.0196	0.0546	0.0262
	S_i^{tu}	0.0196	0.0546	0.0262

Table 2
Sensitivity indices of a second order polynomial model (1).

Input		x_1	x_2
Hao's results	S_i	0.8375	0.6000
	S_i^u	0.4000	0.1375
	S_i^{tu}	0.4000	0.1625
Results in this paper	S_i	0.8375	0.6000
	S_i^u	0.4000	0.1375
	S_i^{tu}	0.4000	0.1625

Table 3
Variance results of a second order polynomial model.

$V(y)$	V_1	V_2	V_3	V_1^u	V_2^u	V_3^u
5056.0	2730.9	1901.1	3006.8	613.6	683.9	1168.3

Table 4
Sensitivity indices of a second order polynomial model (2).

Input		x_1	x_2	x_3
Hao's results	S_i	0.5401	0.3760	0.5947
	S_i^u	0.1214	0.1353	0.2311
Results in this paper	S_i	0.5401	0.3760	0.5947
	S_i^u	0.1214	0.1353	0.2311
	S_i^{tu}	0.1564	0.1629	0.2638

5. Numerical tests and engineering applications

5.1. Numerical test: a linear model

In the first test, a linear model $y=x_1+x_2+x_3$ is considered, in which $x_i(i=1, 2, 3)$ follows standard normal distribution and the correlation coefficients are $\rho_{12}=0.5$, $\rho_{13}=0.8$ and $\rho_{23}=0$, respectively. For this model, the sensitivity indices results given by Refs. [22] and [19] and this paper is shown in Table 1.

From Table 1, it is obvious that the sensitivity indices computed by these three methods is identical. S_i is the full marginal contribution of x_i to the total variance $V[y]$, including the uncorrelated marginal contribution and marginal contribution caused by correlativity of x_i. S_i^u is the uncorrelated marginal contribution of x_i to the total variance $V[y]$. S_i^{tu} is the uncorrelated total contribution of x_i to the total variance $V[y]$. We can observe that in this example $S_i^u = S_i^{tu}$. It is not difficult to make sense. Since there is no cross item, the uncorrelated marginal contribution of a variable is equal to its uncorrelated total contribution.

5.2. Numerical test: second order polynomial models

(1) Consider a second order polynomial model $y = 5 + 8x_1 + x_2^2$, in which $x_i \sim N(2, 2^2)(i=1, 2)$ and the correlation coefficient between x_1 and x_2 is $\rho_{12}=0.5$. For this model, the sensitivity indices results given in Ref. [19] and this paper is shown in Table 2.
It is obvious that the results of sensitivity indices obtained by the polynomial model in this paper is the same as that given in Ref. [19]. This second order polynomial model does not have cross item. We can observe that $S_1^u = S_1^{tu}$ while $S_2^u < S_2^{tu}$, that is because the correlativity will lead cross effect in x_2^2 which is explained in Ref. [19] in detail.

Table 5
Sensitivity indices of a third order polynomial model.

Input		x_1	x_2
Polynomial model	S_i	0.6111	0.9424
	S_i^u	0.0285	0.2310
	S_i^{tu}	0.0576	0.3889
Kriging model	S_i	0.6067	0.9486
	S_i^u	0.0300	0.2393
	S_i^{tu}	0.0572	0.3913

Note: 1000 samples are used to construct Kriging model.

Table 6
Basic random variables and their distribution parameters.

Random variables	Mean value	Coefficient of variance	Distribution
d (mm)	5	0.002	Normal
h (mm)	20	0.015	Normal
D_0 (mm)	5.1	0.002	Normal
t (mm)	5	0.01	Normal
K (MPa)	547.2	0.01	Normal

Table 7
Sensitivity indices of a headless rivet model.

Input	d	h	D_0	t	K
S_i	0.2021	0.8016	0.0057	0.0271	0.1325
S_i^u	0.0355	0.6325	0.0036	0.0187	0.1280
S_i^{tu}	0.0401	0.6385	0.0037	0.0226	0.1316

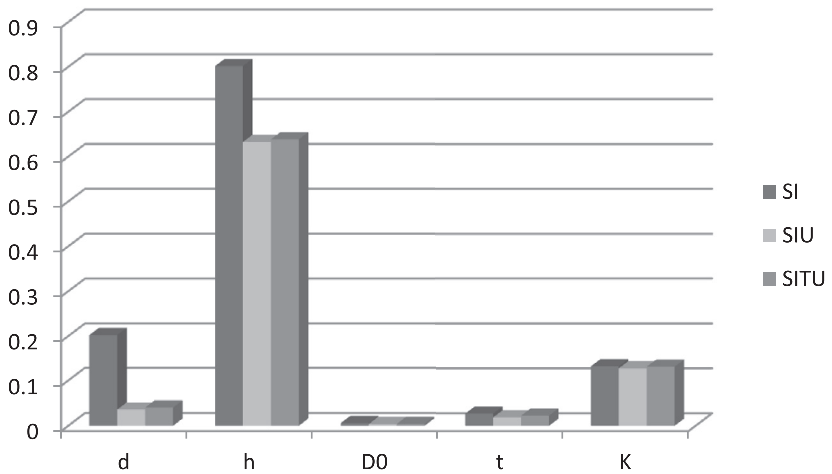

Fig. 1. Histogram of sensitivity indices of a headless rivet model.

(2) Consider $y = 5 + x_1 + 2x_2 + 3x_3 + 2x_1^2 + 3x_1x_2 + x_1x_3 + 4x_2^2 + 3x_2x_3 + 2x_3^2$, that is a second order polynomial model and 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 is $\rho_{12}=0.3$, $\rho_{13}=0.4$, $\rho_{23}=0.2$, respectively. Variance results are given in Ref. [20] and listed in Table 3.

Using the variance results in Table 3, we can obtain sensitivity indices S_i and S_i^u, and sensitivity indices S_i, S_i^u and S_i^{tu} can be obtained by the method in this paper. The results are listed in Table 4.

It is obvious that the results of S_i and S_i^u is the same.

The above two simple tests are to validate the method proposed in this paper, and the results are all compared to that of the exiting analytical methods. They are exactly fitted each other.

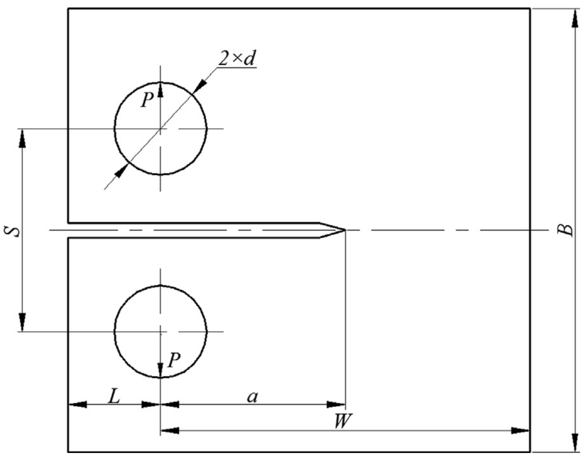

Fig. 2. A two dimension model of CSTE.

Table 8
Basic random variables and their distribution parameters.

Random variables	Mean value	Coefficient of variance	Distribution
a (mm)	50	0.04	Normal
W (mm)	100	0.04	Normal
B (mm)	120	0.04	Normal
L (mm)	25	0.04	Normal
S (mm)	55	0.04	Normal
d (mm)	25	0.1	Normal
P (MPa)	0.12	0.1	Normal
E (GPa)	220	0.1	Normal

Table 9
Sensitivity indices of a two dimension fracture model.

Input	a	W	B	L	S	d	P	E
S_i	0.1006	0.1557	0.0016	2×10^{-5}	2×10^{-5}	0.4065	0.4252	5×10^{-6}
S_i^u	0.1300	0.1857	0.0016	3×10^{-5}	3×10^{-5}	0.2707	0.2873	3×10^{-6}
S_i^{tu}	0.1385	0.1936	0.0027	0.0006	0.0005	0.2771	0.2936	0.0003

Note: 1000 samples are used to construct Kriging model.

5.3. Numerical test: a third order polynomial model

In this test, a third order polynomial model $y=3+x_1+5x_1x_2+x_1^2x_2+2x_2^3$ is considered, in which $x_i\sim N(2,\,2^2)(i=1,\,2)$ and the correlation coefficient between x_1 and x_2 is $\rho_{12}=0.7$. Using polynomial model in this paper, we can obtain the exact analytical result of sensitivity indices and an approximate analytical result of sensitivity indices can be obtained by Kriging model in this paper. The results are listed in Table 5.

The result of sensitivity indices by Kriging model is not exact but approximate because the Kriging model constructed is just an approximation of the original function. We can obtain an exact metamodel of the model in this test by polynomial model and its result is exact. From the result in Table 5, we can observe that Kriging model can achieve a well enough analytical approximate result with a few samples.

5.4. Engineering applications

(1) A headless rivet model
There are many thin cliff components in aeroplane, for instance, skin, stringer, lug etc. These components are mainly connected by rivets. Thus, riveting is significant to the safety and fatigue life. A headless rivet model is created in Ref. [16] to evaluate the maximum squeeze force needed in a certain riveting process, i.e.,

$$F_{\max}=\frac{\pi}{4}\frac{d^2h-D_0^2t}{2H}K\left(\ln\frac{d^2h-D_0^2t}{2Hd^2}\right)^{n_{SHE}},\tag{89}$$

where d and h are the initial diameter and length of the rivet, respectively, D_0 is the diameter of the rivet in the middle stage (the diameter of the rivet hole), t is the whole thickness of the two connection parts, H is the height of

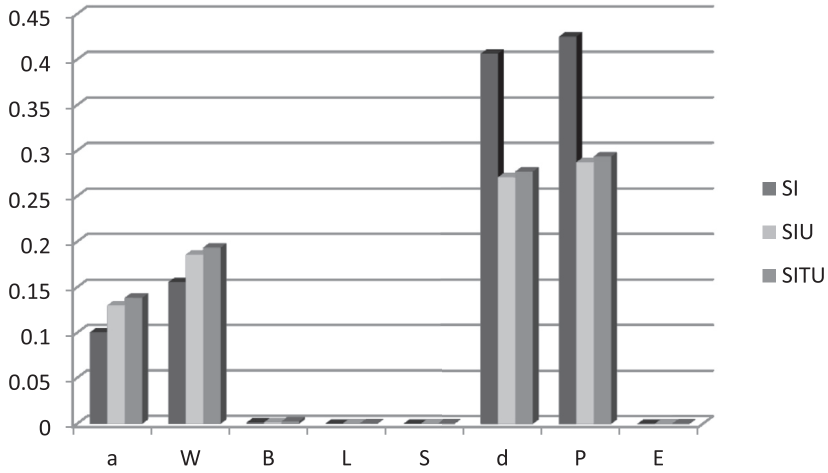

Fig. 3. Histogram of sensitivity indices of the two dimension fracture model.

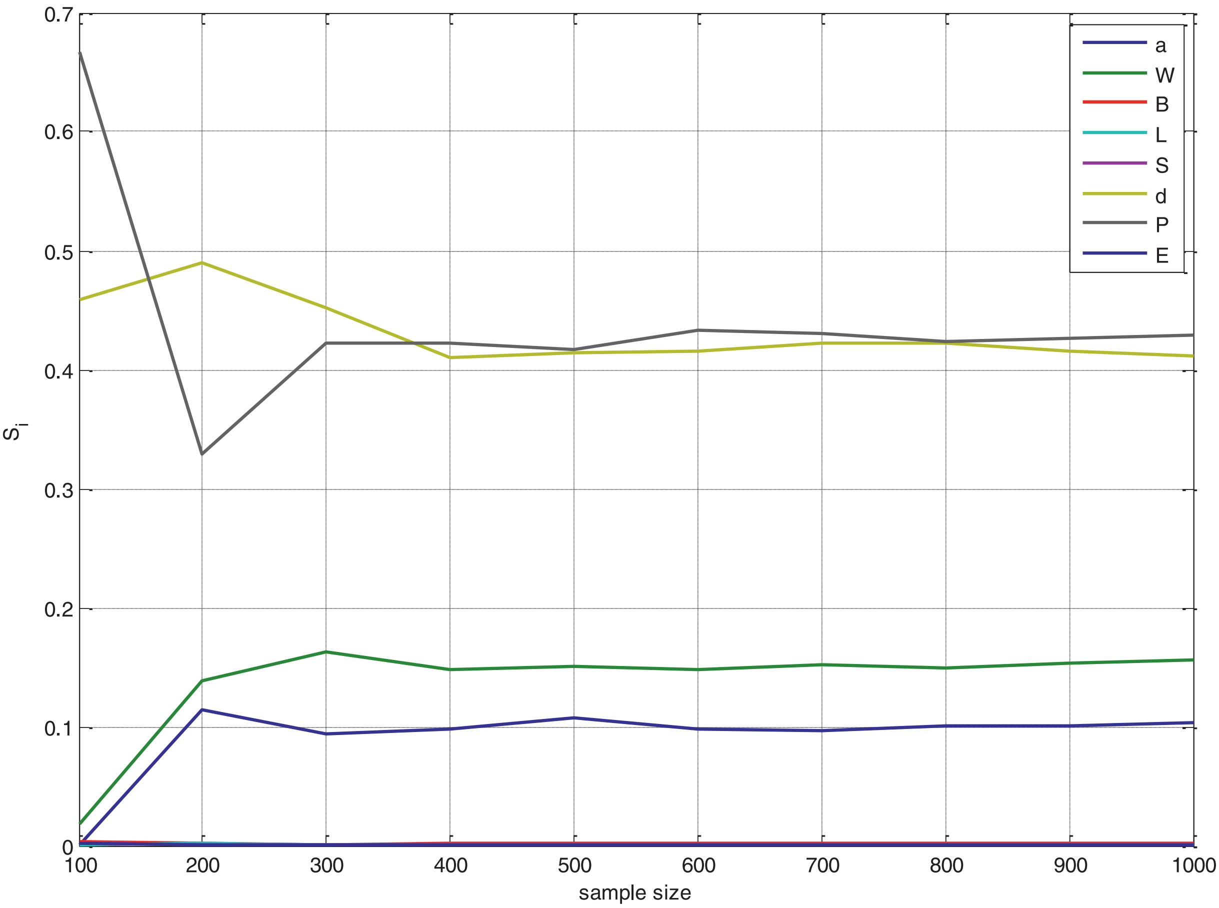

Fig. 4. The convergence of S_i.

the driven rivet head after riveting, K is the strength coefficient of the rivet material, n_{SHE} is the strain hardening exponent of the rivet material. If the material of the headless rivet is 2017-T4, the strain hardening exponent $n_{SHE}=0.15$. All the other variables follow normal distribution and their distribution parameters are listed in Table 6. Among these variables, d and h are correlated with correlation coefficient $\rho_{dh}=0.3$ and D_0 and t are also correlated with correlation coefficient $\rho_{D_0t} = 0.1$.

When the height of the driven rivet head $H=2.5$ mm, we can obtain the sensitivity indices of the variables in Table 6 with the Kriging model in this paper and the results are listed in Table 7.

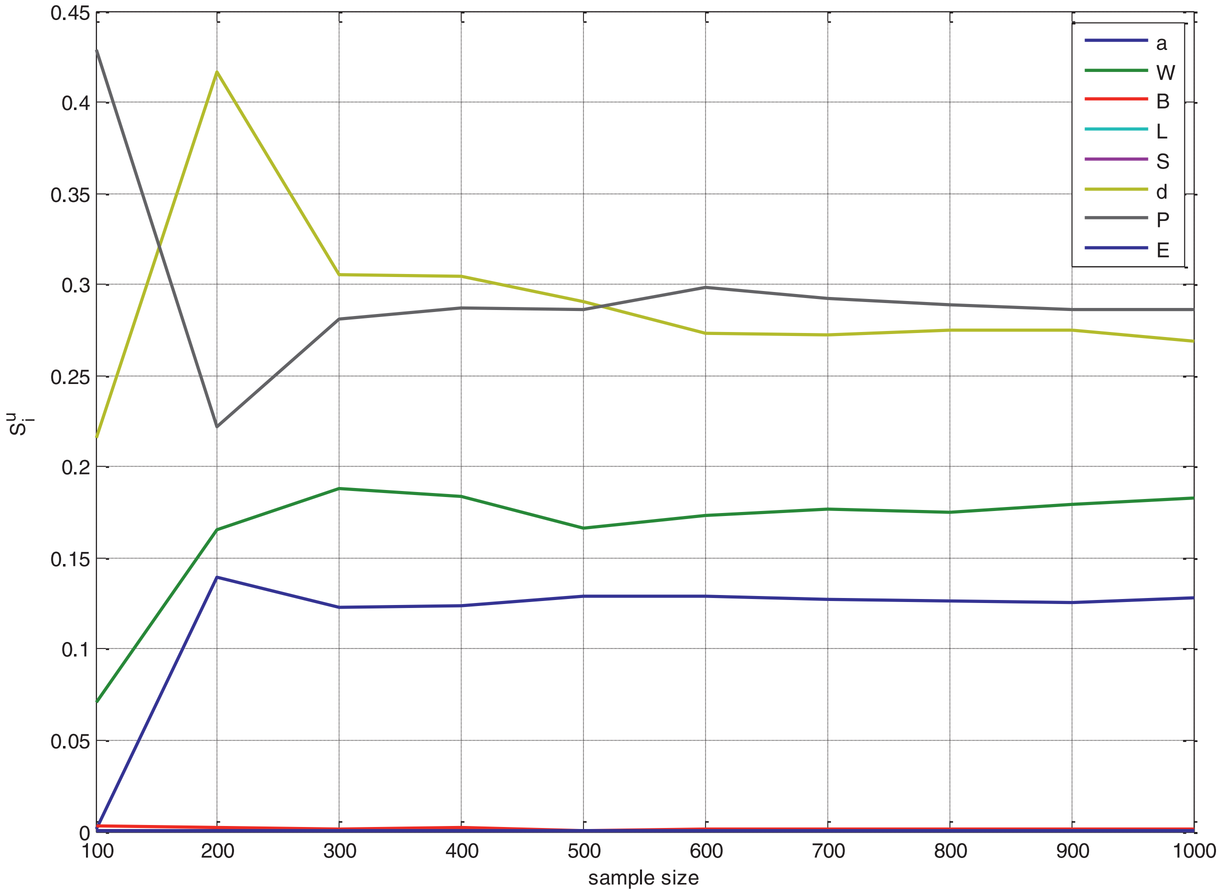

Fig. 5. The convergence of S_i^u.

Fig. 1 is the histogram of the results listed in Table 7.

From Fig. 1 we can clearly see the sensitivity indices of each parameter and can obtain the following conclusions. The initial length of the rivet h affects the uncertainty of the maximum squeeze force $F_{\max}$ most, then is the strength coefficient of the rivet material K. The indices S_i^u and S_i^{tu} of the initial diameter of the rivet d is more or less the same, while S_i is bigger, which indicates the correlativity of d affects the uncertainty of $F_{\max}$ more. The diameter of the rivet in the middle stage D_0 and the whole thickness of the two connection parts t affect the uncertainty of $F_{\max}$ less. With these conclusions, when evaluating the maximum squeeze force we can pay more attention to reducing the uncertainty of the parameter which affect more on the uncertainty of $F_{\max}$ to effectively reduce the uncertainty of the maximum squeeze force. From the results, to effectively reduce the uncertainty of $F_{\max}$, we can try to reduce the uncertainty of the initial length of the rivet h and the correlation betweend d and h, which can be achieved through improving the manufacture condition of the rivet, such as instrument, technics, process, environment, etc. Reducing the uncertainty of the strength coefficient of the rivet material K is also effective, and it can be realized by improving the material of the rivet.

(2) A two dimension fracture model—computation of the stress intensity factor

Fracture mechanics believes that there are macroscopical cracks in the components. It is a subject which investigates cracks in components in aspect of theory and experiment, using the approaches in linear elastic fracture mechanics and plastic fracture mechanics. Usually, we investigate the spread of cracks in structures carrying loads by calculating the fracture parameters (such as the stress intensity factor) in fracture areas. For *compact tension specimen* (CTS) shown as Fig. 2, using ANSYS (a finite elements analysis software) we can construct two dimension fracture models and figure out the stress intensity factors.

In experiment, the six size parameters (a, W, B, L, S, d) and load (P) always cannot be obtained accurately. They all have some errors, i.e., they are random variables, which will lead that the stress intensity factor calculated is not accurate. In order to acquire a more exact result, we can try to reduce the effects of these variables to the uncertainty of the stress intensity factor. Applying GSA, we can be informed which variables affect the uncertainty of the stress intensity factor more and efficiently reduce the uncertainty.

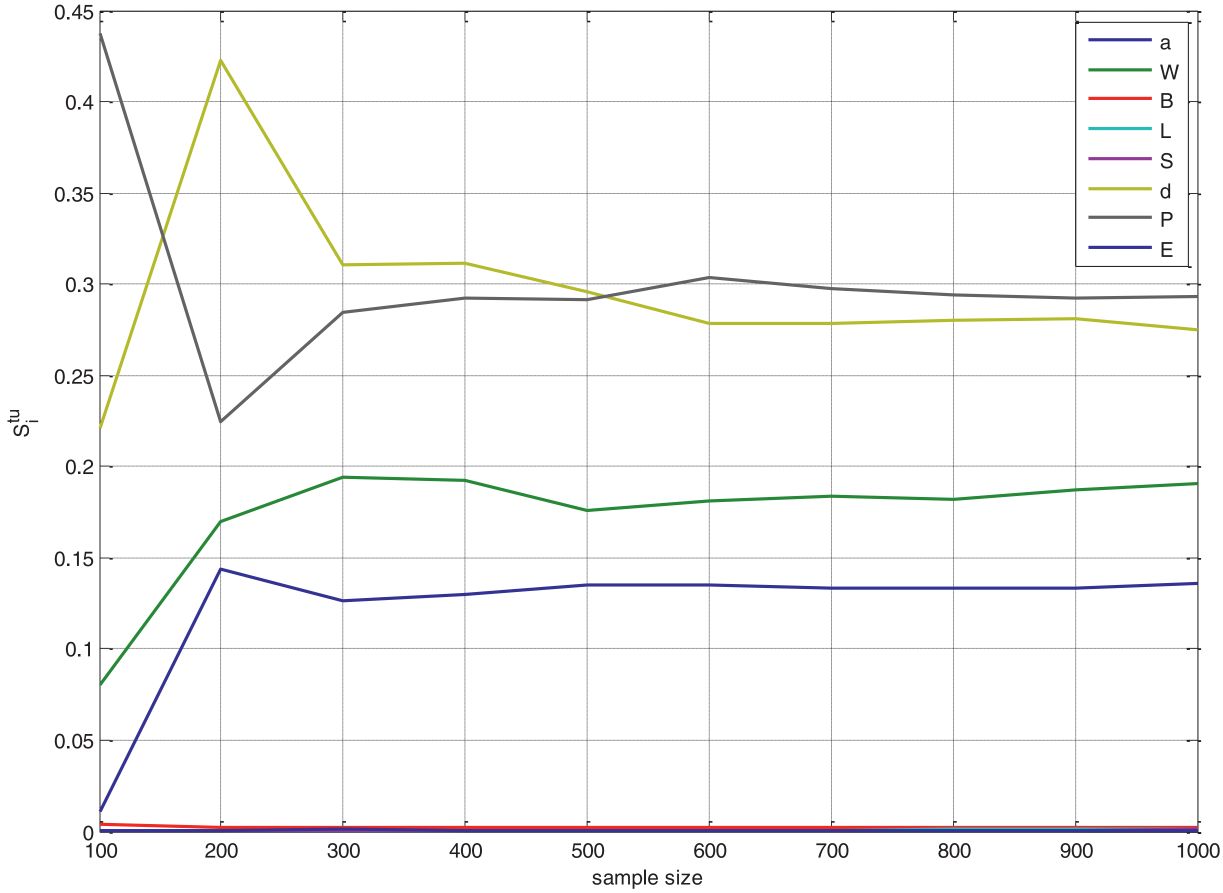

Fig. 6. The convergence of S_i^{tu}.

With some primary analysis, the variables listed in Table 8 may affect the calculation of the stress intensity factor, and their distribution parameters are shown in Table 8. Among these variables, a and W are correlated with correlation coefficient $\rho_{aW}=0.1$, P and E are correlated with correlation coefficient $\rho_{PE}=0.2$. Applying the method proposed in this paper with Kriging model to analyze the importance of these variables, we can achieve the results of sensitivity indices shown in Table 9.

Fig. 3 is the histogram of the results listed in Table 9.

From Fig. 3, it is clear that among the eight random variables, the three kinds sensitivity indices of d and P are bigger, then is that of a and W, sensitivity indices of other variables are close to zeros. Therefore, the uncertainties of d and P affect more the uncertainty of the stress intensity factor, then is that of a and W, the influences of other variables are very small. Basing on these sensitivity results, we should pay more attention on controlling the uncertainties of d, P, a and W to achieve a more exact stress intensity factor. In this example, the two dimension fracture model is constructed by ANSYS software and the computation efficiency is mainly affected by samples' calculation in sensitivity analysis. Simulation based methods always demand a large number of samples, which will lead to huge amount of computation. Only a few of samples are needed to construct metamodels and we can obtain analytical results of sensitivity indices by the method proposed in this paper. Figs. 4, 5 and 6 show the convergence of S_i, S_i^u and S_i^{tu}, respectively. We can see the results converge quickly as the sample size increases and hundreds of samples are adequate for this problem.

6. Conclusion

This paper aims at GSA for models with correlated variables and presents an analytical solution for variance based GSA. This solution relies on the tensor product basis function based metamodels and is especially applicable to complicated engineering structure, since the most commonly used metamodels, such as polynomial regression model, Kriging model, Gaussian radial basis model, MARS model, in the complicated engineering structure can be expressed as tensor product basis functions. Basing on these metamodels and using the solution presented in this paper, we can conveniently obtain the analytical results for GSA.

The universal analytical method for the variance based GSA presented in Section 3.2 is adaptive for both uncorrelated variables and correlated variables. A simple linear model and a second order polynomial model with correlated variables are analyzed for verification. In the implementation of the presented method, the computation of the conditional expectation on correlated variables is a key issue, and it is always difficult to achieve and program. In Section 4, we propose an analytical method which is easy to program for variance based GSA. By orthogonal decorrelation of correlated variables, this method can be realized easily. We take polynomial regression model as an example to illustrate how to achieve analytical variance based GSA for correlated variables in detail, and the analytical expressions of GSA for Kriging model, Gaussian radial basis model and MARS model are also presented. The universal method is suitable for the case that the variables don't follow the normal distribution, but the derived formulas in Section 4.3 are not applicable because Eqs. (63) and (64) are only available for normally distributed variables. In this case, an available and effective approach is to transform these variables into normal distributed variables and it is a commonly used method. If there are similar equations as Eqs. (63) and (64) for a specific distribution, a similar derivation can be conveniently obtained as these in Section 4.3.

Several academic simple examples is performed to validate the proposed method, the method is applied to the GSA of engineering examples. The results show if a metamodel of original model can be achieved with high precision, the analytical GSA results can be exactly obtained by the proposed method. In addition, using the method in this paper, we can obtain all orders of interaction sensitivity indices of the decorrelated variables, but their physical meaning need further analysis, which will be discussed in the future.

Acknowledgments

This article was supported by the National Natural Science Foundation of China (Grant No. NSFC 51475370) and the Key Laboratory for Fault Diagnosis and Maintenance of Spacecraft in Orbit (Grant No. SDML_OF 5015001).

Appendix A

A.1

The derivation of $V[E(x_i|\bar{\mathbf{x}}_{(i-1)})]$ and $\mathrm{cov}[x_i, E(x_i|\bar{\mathbf{x}}_{(i-1)})]$,

$$\begin{aligned}
V[E(x_i|\bar{\mathbf{x}}_{(i-1)})] &= \left(\sum_{i(i-1)} \sum_{(i-1)(i-1)}^{-1}\right)^{*} \sum_{(i-1)}^{\mathrm{T}} \\
&= \left[(\mathrm{cov}(x_i,\bar{x}_1),\dots,\mathrm{cov}(x_i,\bar{x}_{i-1}))\begin{pmatrix} V\bar{x}_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & V\bar{x}_{i-1}\end{pmatrix}^{-1}\right]^{*}\begin{pmatrix} V\bar{x}_1 \\ \vdots \\ V\bar{x}_{i-1}\end{pmatrix} \\
&= \{[\mathrm{cov}(x_i,\bar{x}_1)/V\bar{x}_1]^2,\dots,[\mathrm{cov}(x_i,\bar{x}_{i-1})/V\bar{x}_{i-1}]^2\}\begin{pmatrix} V\bar{x}_1 \\ \vdots \\ V\bar{x}_{i-1}\end{pmatrix} \\
&= \mathrm{cov}^2(x_i,\bar{x}_1)/(V\bar{x}_1) + \cdots + \mathrm{cov}^2(x_i,\bar{x}_{i-1})/(V\bar{x}_{i-1}),
\end{aligned} \tag{90}$$

$$\begin{aligned}
E[x_i(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})] &= E[\sum_{i(i-1)} \sum_{(i-1)(i-1)}^{-1} (\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})] \\
&= E[(\mathrm{cov}(x_i,\bar{x}_1),\dots,\mathrm{cov}(x_i,\bar{x}_{i-1}))\begin{pmatrix} V\bar{x}_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & V\bar{x}_{i-1}\end{pmatrix}^{-1}\begin{pmatrix} \bar{x}_1 - \bar{\mu}_1 \\ \vdots \\ \bar{x}_{i-1}\end{pmatrix}\begin{pmatrix} \bar{x}_1 - \bar{\mu}_1 \\ \vdots \\ \bar{x}_{i-1}\end{pmatrix}] \\
&= E\{[\mathrm{cov}(x_i,\bar{x}_1)(\bar{x}_1 - \bar{\mu}_1)/V\bar{x}_1 + \cdots + \mathrm{cov}(x_i,\bar{x}_{i-1})\bar{x}_{i-1}/V\bar{x}_{i-1}]\begin{pmatrix} \bar{x}_1 - \bar{\mu}_1 \\ \vdots \\ \bar{x}_{i-1}\end{pmatrix}\} \\
&= \begin{pmatrix} \mathrm{cov}(x_i,\bar{x}_1)E[(\bar{x}_1 - \bar{\mu}_1)^2]/V\bar{x}_1 \\ \vdots \\ \mathrm{cov}(x_i,\bar{x}_{i-1})E[\bar{x}_{i-1}^2]/V\bar{x}_{i-1}\end{pmatrix} = \begin{pmatrix} \mathrm{cov}(x_i,\bar{x}_1) \\ \vdots \\ \mathrm{cov}(x_i,\bar{x}_{i-1})\end{pmatrix},
\end{aligned} \tag{91}$$

$$\begin{aligned}
\mathrm{cov}[x_i, E(x_i|\bar{\mathbf{x}}_{(i-1)})] &= \sum_{i(i-1)} \sum_{(i-1)(i-1)}^{-1} E[x_i(\bar{\mathbf{x}}_{(i-1)} - \bar{\mu}_{(i-1)})] \\
&= [\mathrm{cov}(x_i, \bar{x}_1), \dots, \mathrm{cov}(x_i, \bar{x}_{i-1})] \begin{pmatrix} V\bar{x}_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & V\bar{x}_{i-1} \end{pmatrix}^{-1} \begin{pmatrix} \mathrm{cov}(x_i, \bar{x}_1) \\ \vdots \\ \mathrm{cov}(x_i, \bar{x}_{i-1}) \end{pmatrix} \\
&= [\mathrm{cov}(x_i, \bar{x}_1)/V\bar{x}_1, \dots, \mathrm{cov}(x_i, \bar{x}_{i-1})/V\bar{x}_{i-1}] \begin{pmatrix} \mathrm{cov}(x_i, \bar{x}_1) \\ \vdots \\ \mathrm{cov}(x_i, \bar{x}_{i-1}) \end{pmatrix} \\
&= \mathrm{cov}^2(x_i, \bar{x}_1)/(V\bar{x}_1) + \dots + \mathrm{cov}^2(x_i, \bar{x}_{i-1})/(V\bar{x}_{i-1}).
\end{aligned} \tag{92}$$

A.2

Suppose $X \sim N(\mu, \sigma^2)$, then the kth centered moment μ_k of X is

$$\mu_k = E(X - EX)^k = \int_{-\infty}^{+\infty} (x-\mu)^k \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \mathrm{d}x. \tag{93}$$

Let $\frac{x-\mu}{\sigma} = t$, then

$$\mu_k = \frac{\sigma^k}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} t^k \mathrm{e}^{-\frac{t^2}{2}} \mathrm{d}t. \tag{94}$$

The above integral is convergent for any positive integer k, and when k is odd, $\mu_k = 0$. If k is even number

$$\begin{aligned}
\mu_k &= -\frac{\sigma^k}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} t^{k-1} \mathrm{d}\mathrm{e}^{-\frac{t^2}{2}} = -\frac{\sigma^k}{\sqrt{2\pi}} t^{k-1} \mathrm{e}^{-\frac{t^2}{2}} |_{-\infty}^{+\infty} + \sigma^2(k-1)\frac{\sigma^{k-2}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} t^{k-2} \mathrm{e}^{-\frac{t^2}{2}} \mathrm{d}t \\
&= 0 + \sigma^2(k-1)\mu_{k-2} = \sigma^2(k-1)\mu_{k-2}.
\end{aligned} \tag{95}$$

Thus

$$\mu_k = \begin{cases} \sigma^k (k-1)(k-3)\dots 3\cdot 1, & k \text{ is even number} \\ 0, & k \text{ is odd number} \end{cases}. \tag{96}$$

References

[1] T. Homma, A. Saltelli, Importance measures in global sensitivity analysis of nonlinear models, Reliab. Eng. Syst. Saf. 51 (1996) 1–17.
[2] L.J. Cui, Z.Z. Lu, X.P. Zhao, Moment-independent importance measure of basic random variable and its probability density evolution solution, Sci. China Tech. Sci. 53 (2010) 1138–1145.
[3] J. Guo, X.P. Du, Sensitivity analysis with mixture of epistemic and aleatory uncertainties, AIAA J 45 (2007) 2337–2349.
[4] K. Doksum, A. Samarov, Nonparametric estimation of global functionals and a measure of the explanatory power of covariates in regression, Ann. Stat. 23 (1955) 1443–1473.
[5] A. Satelli, The role of sensitivity analysis in the corroboration of models and its link to model structural and parametric uncertainty, Reliab. Eng. Syst. Saf. 57 (1997) 1–4.
[6] I.M. Sobol', Theorems and examples on high dimensional model representations, Reliab. Eng. Syst. Saf. 79 (2003) 187–193.
[7] R.L. Iman, S.C. Hora, A robust measure of uncertainty importance for use in fault tree system analysis, Risk Anal. 10 (1990) 401–406.
[8] E. Borgonovo, A new uncertainty importance measure, Reliab. Eng. Syst. Saf. 92 (2007) 771–784.
[9] R.I. Cukier, C.M. Fortuin, K.E. Shuler, A.G. Petschek, J.H. Schaibly, Study of the sensitivity of coupled reaction systems to uncertainties in rate coefficients. I Theory, J. Chem. Phys. 59 (1973) 3873–3878.
[10] A. Saltelli, M. Ratto, T. Andres, et al., Global Sensitivity Analysis: The Primer, Wiley, Chichester, 2008.
[11] I.M. Sobol', Sensitivity analysis for non-linear mathematical models, Mat. Model. Comp. Exper. 1 (1993) 407–414 Translated from Russian: I.M. Sobol'. Sensitivity estimates for nonlinear mathematical models. Mat. Model. 2 (1990) 112-118.
[12] I.M. Sobol', Global sensitivity indices for nonlinear mathematical models and their Monte Carlo estimates, Math. Comput. Simulat. 55 (2001) 271–280.
[13] M. Ratto, A. Pagano, P.C. Young, State Dependent Parameter metamodelling and sensitivity analysis, Comput. Phys. Commun. 177 (2007) 863–876.
[14] M. Ratto, A. Pagano, P.C. Young, Non-parametric estimation of conditional moments for sensitivity analysis, Reliab. Eng. Syst. Saf. 94 (2009) 237–243.
[15] C. Xu, G. Gertner, Extending a global sensitivity analysis technique to models with correlated parameters, Comput. Stat. Data Anal. 51 (2007) 5579–5590.
[16] L.F. Tian, Z.Z. Lu, W.R. Hao, Moving Least Squares based sensitivity analysis for models with dependent variables, Appl. Math. Model. 37 (2013) 6097–6109.
[17] W. Chen, R.C. Jin, A. Sudjianto, Analytical variance-based global sensitivity analysis in simulation-based design under uncertainty, J. Mech. Design. 127 (2005) 875–886.
[18] W.R. Hao, Z.Z. Lu, L.F. Tian, Importance measure of correlated normal variables and its sensitivity analysis, Reliab. Eng. Syst. Saf. 99 (2012) 151–160.
[19] W.R. Hao, Z.Z. Lu, P.F. Wei, Uncertainty importance measure for models with correlated normal variables, Reliab. Eng. Syst. Saf. 112 (2013) 48–58.
[20] W.R. Hao, Z.Z. Lu, L.Y. Li., A new interpretation and validation of variance based importance measure analysis for model with correlated inputs, Comput. Phys. Commun. 184 (2013) 1401–1413.
[21] R.C. Jin, Enhancements of Metamodeling Techniques in Engineering Design, University of Illinois at Chicago, Chicago, IL, 2004 PhD dissertation.
[22] T.A. Mara, S. Tarantola, Variance-based sensitivity indices for models with dependent inputs, Reliab. Eng. Syst. Saf. 107 (2012) 115–121.

[23] C.G. Xu, G.Z. Gertner, Uncertainty and sensitivity analysis for model with correlated parameters, Reliab. Eng. Syst. Saf. 93 (2008) 1563–1573.
[24] S. Sakata, F. Ashida, M. Zako, Structural optimization using Kriging approximation, Comput. Method. Appl. M. 192 (2003) 923–939.
[25] I. Kaymaz, Application of Kriging method to structural reliability problems, Struct. Saf. 27 (2005) 133–151.
[26] R.L. Hardy, Multiquadratic equations of topography and other irregular surfaces, J. Geophys. Res. 76 (1971) 1905–1915.
[27] J.H. Friedman, Multivariate adaptive regression splines, Ann. Stat. 19 (1991) 1–67.