A Global Sensitivity Index Based on Fréchet Derivative and Its Efficient Numerical Analysis

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Abstract: Sensitivity analysis plays an important role in reliability evaluation, structural optimization and structural design, etc. The local sensitivity, i.e., the partial derivative of the quantity of interest in terms of parameters or basic variables, is inadequate when the basic variables are random in nature. Therefore, global sensitivity such as the Sobol' indices based on the decomposition of variance and the moment-independent importance measure, among others, have been extensively studied. However, these indices are usually computationally expensive, and the information provided by them has some limitations for decision making. Specifically, all these indices are positive, and therefore they cannot reveal whether the effects of a basic variable on the quantity of interest are positive or adverse. In the present paper, a novel global sensitivity index is proposed when randomness is involved in structural parameters. Specifically, a functional perspective is firstly advocated, where the probability density function (PDF) of the output quantity of interest is regarded as the output of an operator on the PDF of the source basic random variables. The Fréchet derivative is then naturally taken as a measure for the global sensitivity. In some sense such functional perspective provides a unified perspective on the concepts of global sensitivity and local sensitivity. In the case the change of the PDF of a basic random variable is due to the change of parameters of the PDF of the basic random variable, the computation of the Fréchet-derivative-based global sensitivity index can be implemented with high efficiency by incorporating the probability density evolution method (PDEM) and change of probability measure (COM). The numerical algorithms are elaborated. Several examples are illustrated, demonstrating the effectiveness of the proposed method.

Keywords: uncertainty quantification; global sensitivity index; probability density evolution method; change of probability measure; Fréchet derivative

1 Introduction

A sensitivity index measures, qualitatively or quantitatively, how strong the property of an output quantity of interest (QoI) will change against the change of property of input basic variable(s). Naturally, as the input basic variable(s) are deterministic, the partial derivative of the output QoI in terms of the input basic variable(s) can be naturally adopted as the sensitivity index [1,2], which plays an important role in, e.g., the reliability evaluation [3-8], structural optimization and structural design [9-12], etc. Such sensitivity index, however, is essentially a local sensitivity index and is inadequate if the basic random parameters are random in nature rather than deterministic. In this scenario, some local sensitivity indices may still work well, but a global sensitivity index (GSI) that characterizes global information is also needed, and considerably more informative. In particular, the effects of probability distributions of the input random basic variables should be taken into account.

To this end, extensive efforts have been devoted in the past two decades, yielding different formulations for GSI, including the Sobol' index [2,13,14] and the moment-independent importance measure [15-17], among others. The Sobol' index is based on the contribution of a basic variable or basic variable sets to the variance of the output QoI. An orthogonal decomposition of the response surface involving different input basic variables leads to the elegant definition of the Sobol' index [13]. In the past decade, great improvements in the computational efficiency of Sobol' index have been made [18,19]. However, in the Sobol' index, only the variance, i.e., the second-order statistics of the output QoI are involved. This is not sufficiently sensitive, and may even result in a misleading judgment in some cases, e.g., when the probability density function (PDF) of the output QoI has multiple modes [17]. Therefore, it is necessary to develop some kind of GSIs involving the PDF of output QoI. To this kind of GSI belongs the moment-independent importance measure [16], which is defined according to the absolute value of the difference between two different PDFs. Again, computational efficiency becomes an important issue and has been studied in amounts of researches [20].

Both the Sobol' type index and the moment-independent index produce positive values. Different from the local sensitivity, they cannot identify the positive or adverse direction, which is an important feature for the selection of direction in structural optimization and decision-making. Actually, an ideal and informative GSI can provide insights or information for the following issues: (1) The order of the importance of source random variables, which can be used to determine whether the uncertainty of some source random variables can be ignored in the detailed model so that the problem can be reduced or simplified; (2) The understanding of global properties of a complex system involving randomness; and (3) The information for the direction and step of iteration in structural design or optimization involving uncertainties. For these purposes, the global sensitivity should provide the magnitude as well as the direction (sign) in a distributed area in the space of the QoI. From the above point of view, the Sobol' index and moment-independent index satisfy the above Issue (1) and partly Issue (2), but not Issue (3). On the other hand, the partial derivative-based sensitivity, i.e., the one related to failure probability in terms of parameters of input random variables, satisfies Issue (3) but does not well satisfy Issues (1) and (2).

For this purpose, a novel global sensitivity index is proposed in the present paper. For clarity, a functional perspective to uncertainty propagation is firstly introduced. Then the Fréchet derivative, as a measure of the change of the PDF of the output QoI in terms of the change of the PDF of the input basic variables, is proposed and justified to be an appropriate GSI. Such a functional perspective provides a unified perspective for global and local sensitivity. In the scenario when the change of the PDF of the input source random variables is due to the change of parameters of the distribution, e.g., the mean value or standard deviation, the computational algorithm of GSI is elaborated. In this case, the probability density evolution method (PDEM) is incorporated with the change of probability measure (COM) to provide a highly efficient approach. Several examples are illustrated, demonstrating the effectiveness of the proposed method.

2 Global Sensitivity Index Based on Fréchet Derivative

2.1. A Functional Perspective to Uncertainty Propagation in Stochastic System Analysis

Without loss of generality, consider a system, of which the output QoI is denoted by X, and the input basic variables are denoted by $\boldsymbol{\Theta}$ of dimension n. Generally, solving the underlying physical equation will yield the solution, which means that X is a function of $\boldsymbol{\Theta}$, and can be denoted by the following general form

$$X = g(\boldsymbol{\Theta}). \tag{1}$$

In the present paper, the input basic parameters $\boldsymbol{\Theta}$ are regarded as random variables. Denote the known joint PDF of $\boldsymbol{\Theta}$ by $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$. The question arises that how we can capture the sensitivity of the QoI in terms of the input basic random variable(s).

To this end, a functional perspective is firstly advocated. In probability theory, it is well known that if the PDF of $\boldsymbol{\Theta}$ is given, and a function (change of random variable) is determined by Eq. (1), then the PDF of X can be determined by the rule of change of random variable(s) [21]. This fact can be expressed in an operator formula

$$p_X(x) = \psi\left(p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}); x\right) = \psi \circ p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}) \tag{2}$$

where ψ is an operator determined by $g(\cdot)$, and $\circ$ means the action of an operator on a function.

Note that ψ is essentially the Frobenius-Perron operator [22]. In fact, the operator between the output and input PDFs is essentially determined by the underlying physics via the function $g(\cdot)$. In other words, the operator can be regarded as a reflection of the underlying physics in the ensemble sense.

2.2. Fréchet-Derivative-Based Global Sensitivity Index

It is instructive to compare Eqs. (1) and (2). In Eq. (1), a transformation relation is established via a function between the input variables and the output QoI, whereas in Eq. (2), a transformation relation is established via an operator between the PDF of the input variable(s) and the PDF of the output QoI(s). A natural sensitivity index defined in the context of Eq. (1) (in particular when the input variable(s) are deterministic) is the partial derivative of the output QoI in terms of the input basic variable(s). Similarly, in the context of Eq. (2), the sensitivity index can be defined as an extension of the "partial derivative" of a function in the context of an operator. The Fréchet derivative provides such an opportunity. In this sense, the functional perspective provides a unified perspective on the concepts of global sensitivity and local sensitivity.

Consider a small perturbation on the joint PDF of input variables, i.e., $p_{\Theta}(\boldsymbol{\theta}) \mapsto p_{\Theta}(\boldsymbol{\theta}) + \delta p_{\Theta}$, where δp_{Θ} is an arbitrary function but satisfying $\int \delta p_{\Theta}(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta} = 0$ and $\delta p_{\Theta} > -p_{\Theta}(\boldsymbol{\theta})$ for $\forall \boldsymbol{\theta}$ to ensure the consistency and non-negativity of PDF . If a linear bounded operator $\mathsf{F}_{\psi} \in \mathsf{L}(V, W)$ exists such that [23]

$$\lim_{\|\delta p_{\Theta}\|_V \to 0} \frac{\left\| \psi\left(p_{\Theta}(\boldsymbol{\theta}) + \delta p_{\Theta}; x\right) - \psi\left(p_{\Theta}(\boldsymbol{\theta}); x\right) - \mathsf{F}_{\psi} \delta p_{\Theta} \right\|_W}{\left\| \delta p_{\Theta} \right\|_V} = 0 \tag{3}$$

or equivalently such that

$$\psi\left(p_{\Theta}(\boldsymbol{\theta}) + \delta p_{\Theta}; x\right) = \psi\left(p_{\Theta}(\boldsymbol{\theta}); x\right) + \mathsf{F}_{\psi} \delta p_{\Theta} + o\left(\left\| \delta p_{\Theta} \right\|_V\right), \quad \left\| \delta p_{\Theta} \right\|_V \to 0 \tag{4}$$

where $\|\cdot\|_W$ and $\|\cdot\|_V$ are the appropriately equipped norms with respect to p_X and p_{Θ} that are on the Banach spaces W and V , respectively, then F_{ψ} is the so-called Fréchet derivative of ψ. In the remaining content, all norms are simplified by $\|\cdot\|$ without inducing confusion.

The Fréchet derivative of ψ has a straightforward meaning: when the joint PDF of input random variables has a tiny perturbation, the PDF of the output QoI will be affected correspondingly with a certain quantity and direction specified by the Fréchet derivative. Obviously, this is exactly the natural “sensitivity” of the output QoI in terms of the input variable(s).

Remark 1.1: Further, let the probability of failure P_f be

$$P_f = \Pr\{X < 0\} = \int_{-\infty}^{0} p_X(x)\mathrm{d}x = \varphi \circ p_X(x), \tag{5}$$

then it is seen that P_f can be regarded as a functional of $p_X(x)$ with the integral operator φ. Similarly, following the rule of change of random variable(s) and Eq. (2), there is

$$P_f = \varphi \circ p_X(x) = \varphi \circ \psi\left(p_{\Theta}(\boldsymbol{\theta}); x\right) = \phi\left(p_{\Theta}(\boldsymbol{\theta})\right) = \phi \circ p_{\Theta}(\boldsymbol{\theta}) \tag{6}$$

and the Fréchet derivative is correspondingly given by

$$\lim_{\|\delta p_{\Theta}\| \to 0} \frac{\left\| \phi\left(p_{\Theta}(\boldsymbol{\theta}) + \delta p_{\Theta}\right) - \phi\left(p_{\Theta}(\boldsymbol{\theta})\right) - \mathsf{F}_{\phi}\delta p_{\Theta} \right\|}{\|\delta p_{\Theta}\|} = 0 \tag{7}$$

where F_{ϕ} is a linear operator. It is indicated that the sensitivity of the failure probability can also be characterized by F_{ϕ}, i.e., the Fréchet derivative with respect to basic distributions of input variables.

Remark 1.2: Aside from Eq. (7), we can also define the sensitivity of statistical moments of QoI. For instance, define the second-order moment of QoI by

$$D_X = \int_{-\infty}^{+\infty} x^2 p_X(x)\mathrm{d}x = \mathsf{D} \circ p_X(x) = \mathsf{D} \circ \psi\left(p_{\Theta}(\boldsymbol{\theta})\right) = D \circ p_{\Theta}(\boldsymbol{\theta}) \tag{8}$$

then the Fréchet derivative is defined by the linear operator F_D if there exists

$$\lim_{\|\delta p_{\Theta}\|\to 0}\frac{\left\|D\left(p_{\Theta}(\boldsymbol{\theta})+\delta p_{\Theta}\right)-D\left(p_{\Theta}(\boldsymbol{\theta})\right)-\mathsf{F}_{D}\delta p_{\Theta}\right\|}{\left\|\delta p_{\Theta}\right\|}=0. \tag{9}$$

Remark 1.3: In the context of Eq. (1), the sensitivity is defined as the partial derivative of output QoI in terms of the input basic variable(s). Clearly, the PDF of input basic variables is not involved, and the sensitivity is defined at a specified value. In this sense, it is essentially a local sensitivity index. In contrast, in the context of Eq. (2), the sensitivity is defined as the Fréchet derivative, which is the "ratio" of the perturbation of PDF or the perturbation of functional of PDF of the output QoI in terms of the perturbation of PDF of the input variables. Thus, it is defined not on a specified value, but on the whole support of the input variables in terms of the distribution. In this sense, it is a global sensitivity index. The counterparts of local and global sensitivity can be exposed in Table 1.

Table 1

Corresponding relationships between the local and global sensitivity

Quantities in the context of local sensitivity	Quantities in the context of global sensitivity
Input deterministic variable(s)	PDF of input random variable(s)
Output QoI	PDF of output QoI as a random variable
Output QoI = function of Input deterministic variable(s)	PDF of output QoI = Operator on/functional of PDF of input random variable(s)
Local sensitivity = the perturbation of output QoI divided by the perturbation of input variable(s)	Global sensitivity = the perturbation of PDF or statistics/failure probability of output QoI divided by the perturbation of PDF of input random variable(s)
Local sensitivity = partial derivative of the function	Global sensitivity = Fréchet derivative of the operator or functional

In this sense, the global sensitivity index based on the Fréchet derivative can be regarded as the extension of the local sensitivity. In other words, the above functional perspectives provide in a sense a unified perspective on the concept of global sensitivity and local sensitivity.

3 The Underlying Meaning and Mathematical Expression of the Fréchet-Derivative-based GSI for Stochastic Systems

3.1. The Expressions of GSI based on the Fréchet Derivative and Gâteaux Derivative

The Fréchet derivative can be related to the Gâteaux derivative, which is a generalization of the classical directional derivative, defined by [24]

$$\lim_{|\varepsilon|\to 0}\frac{\psi\left(p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})+\varepsilon\delta p_{\boldsymbol{\Theta}};x\right)-\psi\left(p_{\boldsymbol{\Theta}}(\boldsymbol{\theta});x\right)}{\varepsilon}=\mathsf{G}_{\psi}\delta p_{\boldsymbol{\Theta}},\ \forall\delta p_{\boldsymbol{\Theta}}\in V, \tag{10}$$

if there exists such an operator $\mathsf{G}_{\psi}\in\mathsf{L}\left(V,W\right)$, where the operator $\psi:K\subset V\to W$ is defined between two Banach spaces. Specifically, the Gâteaux derivative at $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$ is identical to the Fréchet derivative, if the limit in Eq. (10) is uniform with respect to $\delta p_{\boldsymbol{\Theta}}$ with $\left\|\delta p_{\boldsymbol{\Theta}}\right\|=1$ or if the Gâteaux derivative is continuous at $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$. This property makes it possible to compute the Fréchet derivative according to the definition of the Gâteaux derivative [24,25]. Thus, the proposed GSI in Eqs. (3) and (4) can be redefined by Eq. (10) with a well-defined norm, e.g.,

$$\left\|p\right\|_V=\frac{1}{2}\left\|p\right\|_{\mathsf{L}^1(\Omega_{\Theta})} \tag{11}$$

where the norm $\left\|\cdot\right\|_V$ is defined by the half of L^1-norm, i.e.,

$$\left\|p\right\|_V=\frac{1}{2}\int_{\Omega_{\Theta}}\left|p\right|\mathrm{d}\boldsymbol{\theta} \tag{12}$$

which is exactly the so-called *total variation distance* [28].

To provide more insight into the physical/geometrical meaning and to provide a pragmatic computational approach, the expression of the Fréchet-derivative-based GSI will then be elaborated in the following subsections for different cases.

3.2. *Case of Discrete Distributions*

The meaning of Fréchet-derivative-based GSI can be seen much more clearly when the input distributions are of the discrete type. For clarity, let us first consider the case when the input variable in Eq. (1) is a random variable Θ, i.e.,

$$X = g\left(\Theta\right). \tag{13}$$

Let the sample space be a finite and countable set $\{\theta_i\}_{i=1}^{N}$ on □, such that

$$\mathsf{P}\left\{\Theta = \theta_i\right\} = \mathsf{P}_{\Theta}^{(i)} \geq 0 \text{ and } \sum_{i=1}^{N} \mathsf{P}_{\Theta}^{(i)} = 1 \tag{14}$$

where $\mathsf{P}(\cdot)$ denotes the probability of an random event.

The physical relation in Eq. (13) gives the following mapping

$$x_k = g\left(\theta_{\{i\}_k}\right),\ k = 1, 2, \cdots, M \text{ with } \{i\}_k \subseteq \{1, 2, \cdots, N\} \tag{15}$$

where $\{i\}_p \cap \{i\}_q = \varnothing$ for $\forall p \neq q$ and $\cup_{k=1}^{M} \{i\}_k = \{1, 2, \cdots, N\}$. This means that for all $j \in \{i\}_k$, there is $x_k = g\left(\theta_j\right)$ yielding the same value x_k. In other words, for all the input values in the subset $\left\{\theta_j\right\}_{j \in \{i\}_k}$, the output values are identical. Denote the cardinal number of the subset $\{i\}_k$ by n_k, i.e., $n_k = \mathrm{card}\left(\{i\}_k\right) \geq 1$. Obviously, there is $M \leq N$ and $\sum_{k=1}^{M} n_k = N$ due to the many-to-one mapping.

Denote the probability mass function of output by

$$\mathsf{P}\left\{x = x_k = g\left(\theta_{\{i\}_k}\right)\right\} = \mathsf{P}_X^{(k)} \geq 0,\ k = 1, 2, \cdots, M \text{ with } \{i\}_k \subseteq \{1, 2, \cdots, N\}. \tag{16}$$

Then according to Eq. (15) we have

$$\mathsf{P}_X^{(k)} = \sum_{j \in \{i\}_k} \mathsf{P}_{\Theta}^{(j)},\ k = 1, 2, \cdots, M. \tag{17}$$

For convenience, denote the probability measure of Θ be a vector $\mathsf{P}_\Theta = \left(\mathsf{P}_\Theta^{(1)}, \mathsf{P}_\Theta^{(2)}, \cdots, \mathsf{P}_\Theta^{(N)}\right)^{\bullet}$ and that of X by a vector $\mathsf{P}_X = \left(\mathsf{P}_X^{(1)}, \mathsf{P}_X^{(2)}, \cdots, \mathsf{P}_X^{(M)}\right)^{\bullet}$. Then, Eq. (17) can be rewritten in a matrix form by

$$\mathsf{P}_X = \mathbf{F}_{M\times N}\mathsf{P}_\Theta \tag{18}$$

where the matrix $\mathbf{F}_{M\times N}$ is a Boolean matrix whose element is either 1 or 0. According to Eq. (16), it is easy to determine the value of the components F_{kj} of the matrix $\mathbf{F}_{M\times N}$,

$$F_{kj} = I\left(j \in \{i\}_k\right) \tag{19}$$

for $k = 1, 2, \cdots, M;\ j = 1, 2, \cdots, N$, where $I(\cdot)$ is the indicator with the value being one if the event is true and otherwise zero. It is seen clearly that, for the case of many-to-one mapping, in each column only one element is valued 1 and all the other elements are valued zero, but in each row, there are at least one and possibly more elements valued 1. Actually, in the *k*-th row of $\mathbf{F}_{M\times N}$, the number of elements valued 1 is $n_k = \mathrm{card}\left(\{i\}_k\right) \geq 1$.

By doing so, Eq. (18) can be rewritten in a component form more explicitly

$$\mathsf{P}_X^{(k)} = \sum_{j=1}^{N} F_{kj}\mathsf{P}_\Theta^{(j)} = \sum_{j=1}^{N} I\left(j \in \{i\}_k\right)\mathsf{P}_\Theta^{(j)},\ k = 1, 2, \cdots, M\ . \tag{20}$$

Further, denoting $\mathsf{P}_X = \mathbf{F}_{M\times N}\mathsf{P}_\Theta = \mathsf{G}\left(\mathsf{P}_\Theta\right)$, it is easy to find that

$$\mathsf{G}\left(\mathsf{P}_\Theta + \delta\mathsf{P}_\Theta\right) = \mathbf{F}_{M\times N}\left(\mathsf{P}_\Theta + \delta\mathsf{P}_\Theta\right) = \mathbf{F}_{M\times N}\mathsf{P}_\Theta + \mathbf{F}_{M\times N}\delta\mathsf{P}_\Theta = \mathsf{G}\left(\mathsf{P}_\Theta\right) + \mathbf{F}_{M\times N}\delta\mathsf{P}_\Theta \tag{21}$$

where $\delta\mathsf{P}_\Theta$ is a variation of the vector P_Θ, or alternatively

$$\lim_{\varepsilon\to 0}\frac{\mathsf{G}\left(\mathsf{P}_\Theta + \varepsilon\delta\mathsf{P}_\Theta\right) - \mathsf{G}\left(\mathsf{P}_\Theta\right)}{\varepsilon} = \lim_{\varepsilon\to 0}\frac{\mathbf{F}_{M\times N}\left(\mathsf{P}_\Theta + \varepsilon\delta\mathsf{P}_\Theta\right) - \mathbf{F}_{M\times N}\mathsf{P}_\Theta}{\varepsilon} = \mathbf{F}_{M\times N}\delta\mathsf{P}_\Theta \tag{22}$$

which means that according to the definition in Eqs. (4) or (10), the Boolean matrix $\mathbf{F}_{M\times N}$ is nothing but the Fréchet derivative in the case of discrete distributions.

Further, by denoting the variation of the vector P_X by

$\delta \mathsf{P}_X = \delta \mathsf{G}(\mathsf{P}_\Theta) = \mathsf{G}(\mathsf{P}_\Theta + \delta \mathsf{P}_\Theta) - \mathsf{G}(\mathsf{P}_\Theta)$, then there is

$$\delta \mathsf{P}_X = \mathbf{F}_{M \times N} \delta \mathsf{P}_\Theta . \tag{23}$$

This means that once the Fréchet derivative is known, then the variation of the output probability mass function can be obtained directly from the variation of input probability mass function. Actually, this is consistent with the discussion of global sensitivity in Table 1. Also, from this expression, it is clear to see that the Fréchet derivative for the case of discrete distribution is a linear operator.

Now the underlying meaning of the Fréchet-derivative-based GSI becomes apparent: every element of value 1 in the Boolean matrix $\mathbf{F}_{M \times N}$ means the physical relation in Eq. (15) holds, and thus the probability measure can be propagated from the input distribution P_Θ to the distribution P_X of output QoI X. The sensitivity of the stochastic system strictly follows the physical pathway! Also, it is seen clearly that Eq. (23) is an extended version of the differentiation of a function.

To be more intuitive, consider a simple example. Let $X = \Theta^2$ and $\Theta \in \{-1, 0, 1\}$ with $\mathsf{P}_\Theta = (1/6,\ 1/3,\ 1/2)^{\bullet}$. It is easy to know that $X \in \{0, 1\}$ with $\mathsf{P}_X = (1/3,\ 2/3)^{\bullet}$ by admitting $\mathsf{P}_X = \mathbf{F}_{2\times 3} \mathsf{P}_\Theta$ where

$$\mathbf{F}_{2\times 3} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \tag{24}$$

is the Fréchet derivative. Clearly, it is a Boolean matrix that follows Eq. (19). Further, if there is a variation in P_Θ, e.g., $\delta \mathsf{P}_\Theta = (-1/12,\ -1/12,\ 1/6)^{\bullet}$, by substituting Eq. (24) in Eq. (23) we have $\delta \mathsf{P}_X = \mathbf{F}_{2\times 3} \delta \mathsf{P}_\Theta = (-1/12,\ 1/12)^{\bullet}$, and therefore the updated probability mass vector is $\mathsf{P}'_X = \mathsf{P}_X + \delta \mathsf{P}_X = (1/4,\ 3/4)^{\bullet}$. This result is, of course, consistent with the result of Eqs. (18) and (21) such that $\mathsf{P}'_X = \mathbf{F}_{2\times 3} \mathsf{P}'_\Theta$ where $\mathsf{P}'_\Theta = \mathsf{P}_\Theta + \delta \mathsf{P}_\Theta = (1/12,\ 1/4,\ 2/3)^{\bullet}$.

In the case the input in Eq. (1) is a random vector $\boldsymbol{\Theta} = (\Theta_1, \Theta_2, \cdots, \Theta_n)^{\bullet}$, if the sampling space is still a discrete set, e.g., $\left\{(\theta_{i_1}, \theta_{i_2}, \cdots, \theta_{i_n})^{\bullet}\right\}_{i_1=1,2,\cdots,N_1;\ \cdots,\ i_n=1,2,\cdots,N_n}$, where N_j denotes the number of realizable values of Θ_j, then a one-dimensional array can be adopted to store the values in the sampling space. For instance, we may denote $\boldsymbol{\theta}_k = (\theta_{i_1}, \theta_{i_2}, \cdots, \theta_{i_n})^{\bullet}$, where a one to one map between k and the array $(i_1, i_2, \cdots, i_n)$ can be established, e.g., by

$$k = (i_1 - 1) N_2 \cdots N_n + (i_2 - 1) N_3 \cdots N_n + (i_{s-1} - 1) N_n + i_n = \sum_{j=1}^{n-1} (i_j - 1) \prod_{m=j+1}^{n} N_m + i_n . \tag{25}$$

Then a vector can be used to denote the probability mass function, and thus the ideas in the present section for a random variable input can be adopted and similar deductions can be carried out. This will not be detailed here to avoid lengthiness of the paper.

3.3. Case of Continuous Distributions

3.3.1. General Expression

When the input distributions of discrete type tend to be continuous, things are getting much more interesting but also much more involved. Denote the input PDF of $\boldsymbol{\Theta}$ by $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$ and the output PDF of X by $p_X(x)$, then Eq. (18) should be extended to

$$p_X(x) = \int_{\Omega_{\boldsymbol{\Theta}}} \delta_{\mathrm{D}}\left(x - g(\boldsymbol{\theta})\right) p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta} \tag{26}$$

where $\delta_{\mathrm{D}}(\cdot)$ denotes the Dirac function to avoid possible confusion between the variation of a function and the Dirac function. By the definition of Fréchet derivative, if there is a variation in the input PDF $\delta p_{\boldsymbol{\Theta}}$, one can easily notice that

$$\begin{aligned}\psi\left(p_\Theta+\delta p_\Theta\right)&=\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)\left(p_\Theta+\delta p_\Theta\right)\mathrm{d}\boldsymbol{\theta}\\&=\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)p_\Theta\mathrm{d}\boldsymbol{\theta}+\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)\delta p_\Theta\mathrm{d}\boldsymbol{\theta}\\&=\psi\left(p_\Theta\right)+\mathsf{F}_\psi\circ\delta p_\Theta\end{aligned}\tag{27}$$

where ψ is the integral operator defined in Eq. (26) and F_ψ is the Fréchet derivative of ψ. Since ψ is a linear operator, the Fréchet derivative of ψ is nothing but itself [24]. This is consistent with the case involving discrete distributions.

Moreover, by the definition of Gâteaux derivative, it can be easily proved that

$$\begin{aligned}&\lim_{\varepsilon\to 0}\frac{\psi\left(p_\Theta+\varepsilon\delta p_\Theta\right)-\psi\left(p_\Theta\right)}{\varepsilon}\\&=\lim_{\varepsilon\to 0}\frac{\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)\left(p_\Theta+\varepsilon\delta p_\Theta\right)\mathrm{d}\boldsymbol{\theta}-\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)p_\Theta\mathrm{d}\boldsymbol{\theta}}{\varepsilon}\\&=\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)\delta p_\Theta\mathrm{d}\boldsymbol{\theta}\ \text{ for }\forall\delta p_\Theta\in V\end{aligned}\tag{28}$$

where one can see that the Boolean matrix in Eq . (21) or (22), i.e., the Fréchet derivative for the discrete case, turns to be the integral operator in terms of the Dirac function $\delta_{\mathrm{D}}(\cdot)$ as presented in Eq. (27) or (28), which is apparently reasonable: the selection property of the Dirac function works exactly the same as the logic calculation of the Boolean element (1 or 0), and the summation calculation evolves into the integral calculation when the system becomes continuous.

Further, if we denote $\delta p_X=\delta\psi\left(p_\Theta\right)=\psi\left(p_\Theta+\delta p_\Theta\right)-\psi\left(p_\Theta\right)$, then from Eq. (26) there is

$$\delta p_X=\int_{\Omega_\Theta}\delta_{\mathrm{D}}\left(x-g(\boldsymbol{\theta})\right)\delta p_\Theta\mathrm{d}\boldsymbol{\theta}=\mathsf{F}_\psi\circ\delta p_\Theta.\tag{29}$$

Similar to the cases involving discrete distributions, this expression means that once the Fréchet derivative is known, then the variation of the output PDF can be obtained directly from the variation of the input PDF. Again, this justifies the appropriation of taking the Fréchet derivative as a global sensitivity index, as shown in Table 1.

A more explicit expression for Eq. (28) by integrating in terms of the Dirac function yields

$$\begin{aligned} \delta p_X &= \int_{\Omega_\Theta} \delta_{\mathrm{D}}\left(x - g(\boldsymbol{\theta})\right) \delta p_\Theta \mathrm{d}\boldsymbol{\theta} \\ &= \int_{\Omega_{\Theta_{\sim 1}}} \sum_{j=1}^{R} \left(\left| \frac{\partial g(\theta_1; \boldsymbol{\theta}_{\sim 1})}{\partial \theta_1} \right|^{-1} \delta p_\Theta \right)_{\theta_1 = g_j^{-1}(x; \boldsymbol{\theta}_{\sim 1})} \mathrm{d}\boldsymbol{\theta}_{\sim 1} \\ &= \mathsf{F}_\psi \circ \delta p_\Theta \end{aligned} \tag{30}$$

where $\boldsymbol{\theta}_{\sim 1} = (\theta_2, \theta_3, \cdots, \theta_n)$, $\theta_1 = g_j^{-1}(x; \boldsymbol{\theta}_{\sim 1})$ is the j-th inverse function of g for fixed $\boldsymbol{\theta}_{\sim 1}$, R is the number of inverse function when the function of g for fixed $\boldsymbol{\theta}_{\sim 1}$ is non-monotonic. This expression, though usually unfeasible for practical computation, is theoretically important. It again shows that the Fréchet derivative is a linear operator, connects the variation of input PDF and the variation of output PDF, and can thus be in principle an appropriate global sensitivity index.

3.3.2. Parametric Expression

Generally, in many practical engineering cases, the distribution type is determined while the distribution parameters, e.g., the mean value μ and standard deviation σ in Gaussian or lognormal distributions, or the shape and shift parameters in Weibull distribution, may vary due to data sparsity, information updating, etc. For simplicity of writing, denote the distribution parameters by a vector $\boldsymbol{\xi} = \left(\xi_1, \cdots, \xi_m\right)^{\bullet}$, where m is the total number of distribution parameters, then the Fréchet derivative defined by Eq. (3) becomes

$$\mathsf{F}_\psi\left(x\right) = \frac{\partial F\left(x; \boldsymbol{\xi}\right) / \partial \boldsymbol{\xi}}{\left\| \partial p_\Theta(\boldsymbol{\theta}; \boldsymbol{\xi}) / \partial \boldsymbol{\xi} \right\|} = \left(\frac{\partial p_X\left(x; \boldsymbol{\xi}\right) / \partial \xi_1}{\left\| \partial p_\Theta(\boldsymbol{\theta}; \boldsymbol{\xi}) / \partial \xi_1 \right\|_V}, \cdots, \frac{\partial p_X\left(x; \boldsymbol{\xi}\right) / \partial \xi_m}{\left\| \partial p_\Theta(\boldsymbol{\theta}; \boldsymbol{\xi}) / \partial \xi_m \right\|_V} \right)^{\bullet} \tag{31}$$

where

$$F(x; \boldsymbol{\xi}) = \psi\left(p_\Theta(\boldsymbol{\theta}; \boldsymbol{\xi})\right) = \psi \circ p_\Theta(\boldsymbol{\theta}; \boldsymbol{\xi}) . \tag{32}$$

According to the consistency between the Fréchet derivative and the Gâteaux derivative in

Eq. (10), we have

$$\mathsf{F}_{\psi}\tilde{\delta} p_{\Theta}=\lim_{\varepsilon \to 0}\frac{\psi\left(p_{\Theta}+\varepsilon\tilde{\delta} p_{\Theta}\right)-\psi\left(p_{\Theta}\right)}{\varepsilon} \tag{33}$$

where $\left\|\tilde{\delta} p_{\Theta}\right\|_{V}=1$, $\delta p_{\Theta}=\tilde{\delta} p_{\Theta}/\varepsilon$ is a standardized variation for $\varepsilon>0$, and δp_{Θ} is the variation of input PDF satisfying $\int \delta p_{\Theta} \mathrm{d}\theta=0$ and $\delta p_{\Theta}>-p_{\Theta}(\theta)$. Noticing that the variation of input PDF is

$$\delta p_{\Theta}\left(\boldsymbol{\theta};\xi_1,\cdots,\xi_m\right)=p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right)-p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)=\sum_{j=1}^{m}\frac{\partial p_{\Theta}\left(\boldsymbol{\theta};\xi_1,\cdots,\xi_m\right)}{\partial \xi_j}\delta\xi_j \, . \tag{34}$$

There is

$$\left\|\tilde{\delta} p_{\Theta}\right\|_{V}=\left\|\left(p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right)-p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)\right)/\varepsilon\right\|_{V}=1, \tag{35}$$

or alternatively,

$$\varepsilon=\left\|p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right)-p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)\right\|_{V} . \tag{36}$$

Therefore,

$$\begin{aligned}
&\lim_{|\varepsilon|\to 0}\frac{\psi\left(p_{\Theta}(\boldsymbol{\theta})+\varepsilon\tilde{\delta} p_{\Theta};x\right)-\psi\left(p_{\Theta}(\boldsymbol{\theta});x\right)}{\varepsilon}\\
&=\lim_{|\delta\boldsymbol{\xi}|\to \mathbf{0}}\frac{\psi\left(p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right);x\right)-\psi\left(p_{\Theta}(\boldsymbol{\theta});x\right)}{\left\|p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right)-p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)\right\|_{V}}\\
&=\lim_{|\delta\boldsymbol{\xi}|\to \mathbf{0}}\sum_{j=1}^{m}\left(\frac{\partial p_X\left(x;\boldsymbol{\xi}\right)}{\partial \xi_j}\right)\delta\xi_j \Bigg/ \left\|\sum_{j=1}^{m}\left(\frac{\partial p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)}{\partial \xi_j}\right)\delta\xi_j\right\|_{V} .
\end{aligned} \tag{37}$$

Notice that if, without loss of generality, we further consider the situation $\delta\xi_j$'s are independent variation, and any component of the Fréchet derivative can be obtain from the above equation by letting $\delta\xi_j \neq 0$ whereas all the other variations are zero, i.e.,

$$\mathsf{F}_{\psi,j}=\frac{\partial p_X\left(x;\boldsymbol{\xi}\right)/\partial\xi_j}{\left\|\partial p_{\Theta}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)/\partial\xi_j\right\|_{V}},\quad j=1,2,\cdots,m \tag{38}$$

which is nothing but the result in Eq. (31).

It is interesting that the difference between the Fréchet derivative and the usual partial derivative in the parametric case is that there is a normalization factor. This is important, because this naturally occurred normalization factor eliminates the effect of dimensionality of different parameters.

In this case, the propagation of uncertainty as exhibited by the effects of variation of input probabilistic information on the output probabilistic information becomes

$$\begin{aligned}\delta p_X\left(x;\boldsymbol{\xi}\right) &= p_X\left(x;\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right)-p_X\left(x;\boldsymbol{\xi}\right)\\ &= \mathsf{F}_{\psi}\circ\delta\tilde{\boldsymbol{\xi}}\end{aligned} \tag{39}$$

where $\delta\tilde{\boldsymbol{\xi}}$ is the normalized or dimensionless variation of parametric vector

$$\delta\tilde{\boldsymbol{\xi}}=\left(\frac{\delta\xi_1}{\left\|\partial p_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)/\partial\xi_1\right\|_V},\frac{\delta\xi_2}{\left\|\partial p_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)/\partial\xi_2\right\|_V},\cdots,\frac{\delta\xi_m}{\left\|\partial p_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)/\partial\xi_m\right\|_V}\right)^T. \tag{40}$$

It is easy to prove Eq. (39) as follows

$$\begin{aligned}\delta p_X\left(x;\boldsymbol{\xi}\right) &= p_X\left(x;\boldsymbol{\xi}+\delta\boldsymbol{\xi}\right)-p_X\left(x;\boldsymbol{\xi}\right)\\ &=\int_{\Omega_{\boldsymbol{\Theta}}}\delta_{\mathrm{D}}\left(x-g\left(\boldsymbol{\theta}\right)\right)\left(\sum_{j=1}^{m}\frac{\partial p_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta};\xi_1,\cdots,\xi_m\right)}{\partial\xi_j}\delta\xi_j\right)\mathrm{d}\boldsymbol{\theta}\\ &=\sum_{j=1}^{m}\left(\frac{\partial}{\partial\xi_j}\int_{\Omega_{\boldsymbol{\Theta}}}\delta_{\mathrm{D}}\left(x-g\left(\boldsymbol{\theta}\right)\right)p_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta};\xi_1,\cdots,\xi_m\right)\mathrm{d}\boldsymbol{\theta}\right)\delta\xi_j\\ &=\sum_{j=1}^{m}\left(\frac{\partial p_X\left(x;\xi_1,\cdots,\xi_m\right)/\partial\xi_j}{\left\|\partial p_{\boldsymbol{\Theta}}\left(\boldsymbol{\theta};\boldsymbol{\xi}\right)/\partial\xi_j\right\|_V}\right)\delta\tilde{\xi}_j\\ &=\mathsf{F}_{\psi}\circ\delta\tilde{\boldsymbol{\xi}}.\end{aligned} \tag{41}$$

On this condition, the Fréchet derivative reduces to a normalized version of "ordinary derivative". For instance, if the change of PDF of input basic random variables is due to change of the mean of input basic random variables, then Eq. (31) further reduces to

$$\mathsf{F}_{\psi}\left(x\right)=\frac{\partial F\left(x;\boldsymbol{\mu}\right)/\partial\boldsymbol{\mu}}{\left\|\partial p_{\boldsymbol{\Theta}}(\boldsymbol{\theta};\boldsymbol{\mu})/\partial\boldsymbol{\mu}\right\|_V} \tag{42}$$

where $\boldsymbol{\mu}$ is the vector of mean value of the input random variables, and it is easy to verify that

$$\int_{-\infty}^{\infty} \mathsf{F}_{\psi}(x)\,\mathrm{d}\,x = 0 \tag{43}$$

which means that, if the Fréchet derivative in Eq. (42) is not always be zero at all *x*, then it cannot be always positive nor always negative, but must be positive in some areas and negative in the rest areas in terms of *x*. In other words, the curve of the Fréchet derivative must have at least one additional point crossing the abscissa besides the left and right end points. This property can be adopted as a qualitative property for the verification of analytical or numerical results.

Note that the sensitivity index in Eq. (42) is computed for the whole PDF of X, even for a specified value of $\boldsymbol{\mu}$. In this sense, even the sensitivity in Eq. (42) reduces to a normalized "usual" partial derivative, it is a global sensitivity index.

Generally, the calculation of the norm term in Eqs. (31) and (42) is quite simple, since there exist analytical results (available in Appendix B for some common distributions), but the computation of the partial term defined in Eq. (31) or (42) requires multiple rounds of stochastic response analysis (or reliability evaluation), and in each round of stochastic analysis multiple, say, for different problems in the order of magnitude of 10^3 to 10^8 in Monte Carlo simulation, deterministic function evaluations are needed. This leads to prohibitively large computational efforts. Incorporating the probability density evolution method (PDEM) and the change of probability measure (COM) [26], a highly efficient algorithm can be implemented and will be elaborated in the following sections.

4 Numerical Algorithm for Fréchet-Derivative-based GSI

In order to evaluate the proposed GSI in Eq. (31), the numerical algorithm is discussed in terms of Gâteaux derivative presented in Section 4.1. Besides, the probability density evolution method (PDEM) and the change of probability measure (COM) are incorporated. To be clear, the pivotal theories and numerical algorithms for PDEM and COM are firstly summarized in Section 4.2 and 4.3, respectively. Then, the complete numerical algorithm for the Fréchet-derivative-based GSI is elaborated in Section 4.4.

4.1. The Basic Idea of Numerical Algorithm in terms of Gâteaux Derivative

In numerical implementation, the Gâteaux derivative usually takes advantage in computation over the Fréchet derivative. Therefore, the basic idea of numerical algorithm to generate the Fréchet derivative is to take advantage of the evaluation of Gâteaux derivative, which requires the following two assumptions [25]: (1) the Gâteaux derivative is continuous at $p_\Theta(\boldsymbol{\theta})$, and (2) the variation of input PDF is unit, i.e., $\left\|\tilde{\delta} p_\Theta\right\|_V = 1$.

Moreover, by denoting the variation of input PDF as

$$\tilde{p}_\Theta(\boldsymbol{\theta}) = p_\Theta(\boldsymbol{\theta}) + \varepsilon\tilde{\delta} p_\Theta, \tag{44}$$

we immediately have

$$\left\|\tilde{p}_\Theta(\boldsymbol{\theta}) - p_\Theta(\boldsymbol{\theta})\right\|_V = \left\|\varepsilon\tilde{\delta} p_\Theta\right\|_V = \varepsilon \tag{45}$$

where ε is an infinitesimal number defined in Eq. (10). In practical computation, ε can be taken as a small value, e.g., $\varepsilon = 0.01$, and then the Gâteaux derivative can be approximated by

$$\mathsf{G}_\psi \approx \frac{\psi\left(\tilde{p}_\Theta(\boldsymbol{\theta}); x\right) - \psi\left(p_\Theta(\boldsymbol{\theta}); x\right)}{\varepsilon} \tag{46}$$

where $\tilde{p}_\Theta(\boldsymbol{\theta})$ is an arbitrary PDF satisfying Eq. (45). The basic idea of numerical algorithm for the evaluation of Gâteaux derivative is then summarized as below:

Step 0.1. Set ε to be a small value, e.g., $\varepsilon = 0.01$;

Step 0.2. Find one proper PDF $\tilde{p}_\Theta(\boldsymbol{\theta})$ satisfying Eq. (45).

Step 0.3. Calculate Eq. (46).

In **Step 0.3** required is the evaluation of $\psi\left(\tilde{p}_{\mathbf{\Theta}}(\boldsymbol{\theta});x\right)$ and $\psi\left(p_{\mathbf{\Theta}}(\boldsymbol{\theta});x\right)$, which is usually time-consuming. To efficiently and accurately compute these two quantities, the probability density evolution method (PDEM) combined with the change of probability measure (COM) [26] (PDEM-COM) is adopted hereafter, where PDEM (introduced in Sections 4.2) is utilized to evaluate $\psi\left(p_{\mathbf{\Theta}}(\boldsymbol{\theta});x\right)$ while COM (summarized in Sections 4.3) is adopted to compute $\psi\left(\tilde{p}_{\mathbf{\Theta}}(\boldsymbol{\theta});x\right)$. The PDF found in **Step 0.2** is not numerically unique, therefore the parametric form in Section 3.3.2 is taken into account. It should be emphasized that introducing parametric distributions will not change the properties of the proposed Fréchet-derivative-based GSI, according to the **Proposition** in Appendix A.

4.2. Uncertainty Propagation via Probability Density Evolution Method (PDEM)

For clarity, consider a one-dimensional stochastic dynamical system:

$$\dot{X} = G(X,\mathbf{\Theta},t),\ X\left(t_0\right) = X_0 \tag{47}$$

where $\mathbf{\Theta}$ is a random vector with joint PDF $p_{\mathbf{\Theta}}(\boldsymbol{\theta})$ characterizing the source of randomness involved in the system, and X_0 is the initial value. Obviously, for a well-posed system, the solution of Eq. (47) uniquely exists, and is continuously dependent on $\mathbf{\Theta}$ and X_0. Without loss of generality, the solution is assumed to take the form

$$X = H\left(X_0,\mathbf{\Theta},t\right). \tag{48}$$

Moreover, the derivative of X with respect to time t can be written as

$$\dot{X} = h\left(X_0,\mathbf{\Theta},t\right) \tag{49}$$

where $h(\cdot) = \partial H(\cdot)/\partial t$, and $\dot{X}$ is the generalized velocity. In [27], it is elaborated that, if there is no existent random factors disappear, nor new random factors arise, the system will be probability preserved. Accordingly, a generalized density evolution equation (GDEE) can be derived as [28]

$$\frac{\partial p_{X\boldsymbol{\Theta}}(x,\boldsymbol{\theta},t)}{\partial t}+h(\boldsymbol{\theta},t)\frac{\partial p_{X\boldsymbol{\Theta}}(x,\boldsymbol{\theta},t)}{\partial x}=0 \tag{50}$$

where the initial value X_0 in Eq. (50) is omitted without inducing confusion. The corresponding initial condition is

$$p_{X\boldsymbol{\Theta}}\left(x,\boldsymbol{\theta},t_0\right)=\delta_{\mathrm{D}}\left(x-H\left(\boldsymbol{\theta},t_0\right)\right)\cdot p_{\boldsymbol{\Theta}}(\boldsymbol{\theta}) \tag{51}$$

where $\delta_{\mathrm{D}}(\cdot)$ is the Dirac function.

The PDEM is adopted herein due to its efficiency and flexibility in the analysis of uncertainty propagation, which has been validated in [29]. In general, the solution procedure of PDEM includes the following four steps:

Step 1.1. Partition the probability space by a set of optimally selected points, of which the GF-discrepancy of point set is minimized [30,31]. Denote the optimal point set by $M=\left\{\boldsymbol{\theta}_q,P_q\right\}_{q=1}^{n_{\mathrm{sel}}}$, where $\boldsymbol{\theta}_q$ is the q-th representative points with corresponding assigned probability $P_q=\int_{\Omega_q}p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}$, n_{sel} is the total number of the representative points. Here Ω_q stands for the representative domain specified by the Voronoi cell [32]. Note that if $\boldsymbol{\Theta}$ is a high-dimensional vector, some appropriate dimension-reduction strategies should be utilized, e.g., the mapping method [33] and the active subspace method [34], etc.

Step 1.2. For each $\boldsymbol{\Theta}=\boldsymbol{\theta}_q$, solve Eq. (47) to yield the corresponding $\dot{X}_q$ or $h\left(\boldsymbol{\theta}_q,t\right)$.

Step 1.3. For each $\boldsymbol{\Theta}=\boldsymbol{\theta}_q$, solve Eq. (50) and get $p_{X\boldsymbol{\Theta}}^{(q)}$ for $q=1,\cdots,n_{\mathrm{sel}}$. Notice that the initial condition of Eq. (51) now becomes $p_{X\boldsymbol{\Theta}}^{(q)}\left(x,\boldsymbol{\theta},t_0\right)=\delta_{\mathrm{D}}\left(x-x_0\right)P_q$. Since Eq. (50) is a typical hyperbolic partial differential equation, the finite difference method (FDM) is adopted.

Moreover, in order to tradeoff the dissipation and dispersion in numerical computation, the TVD (Total Variation Diminishing) scheme is suggested [35].

Step 1.4. Assemble all the solutions in **Step 1.3** to yield the PDF of X, i.e.,

$$p_X(x,t) = \int_{\Omega_{\boldsymbol{\Theta}}} p_{X\boldsymbol{\Theta}}(x,\boldsymbol{\theta},t)\mathrm{d}\boldsymbol{\theta} \approx \sum_{q=1}^{n_{\mathrm{sel}}} p_{X\boldsymbol{\Theta}}^{(q)}\left(x,\boldsymbol{\theta}_q,t\right) \quad \text{where} \quad \Omega_{\boldsymbol{\Theta}} = \cup_{q=1}^{n_{\mathrm{sel}}} \Omega_q .$$

4.3. *Change of Probability Measure (COM) and Radon-Nikodym Derivative*

After performing one round of PDEM analysis for a specified joint PDF of source basic random variables, if it is found that the joint PDF of source basic random variables should be changed to some other joint PDF, say, due to the epistemic uncertainty [26], then a completely new round of PDEM analysis is needed. The new round of PDEM analysis will of course make the previous round of PDEM analysis totally invalid. Most recently, the change of probability measure (COM) by the Radon-Nikodym derivative was incorporated with PDEM to expedite the procedure of uncertainty propagation in the case the joint PDF of source basic random variables is changed. In the PDEM-COM, the most time-consumed underlying deterministic analyses in PDEM in **Step 1.2** [26] are re-used. The basic idea is as follows:

Consider two close but different distributions of $\boldsymbol{\Theta}$, denoted as $p_{\boldsymbol{\Theta}}^{(1)}(\boldsymbol{\theta})$ and $p_{\boldsymbol{\Theta}}^{(2)}(\boldsymbol{\theta})$, respectively. If Eq. (47) holds, the corresponding PDF for the response X can be firstly calculated by one round of PDEM analysis in terms of $p_{\boldsymbol{\Theta}}^{(1)}(\boldsymbol{\theta})$, and thus $p_X^{(1)}(x)$ is obtained. For the case of $p_X^{(2)}(x)$ with respect to $p_{\boldsymbol{\Theta}}^{(2)}(\boldsymbol{\theta})$, instead of doing another complete round of PDEM analysis, the Radon-Nikodym operator [21], denoted as $\mathsf{T}_{2,1}$, is advocated such that

$$p_X^{(2)}(x) = \mathsf{T}_{2,1} p_X^{(1)}(x) . \tag{52}$$

The approach presented in [26] is then summarized as the following three steps:

Step 2.1. For a certain $p_{\boldsymbol{\Theta}}^{(1)}(\boldsymbol{\theta})$, accomplish one round of PDEM analysis, as shown in Section 4.2. Denote the point set as $M^{(1)} = \left\{\boldsymbol{\theta}_q^{(1)}, P_q^{(1)}\right\}_{q=1}^{n_{\mathrm{sel}}}$, where the superscript "(1)" is corresponding to $p_{\boldsymbol{\Theta}}^{(1)}(\boldsymbol{\theta})$. Besides, the values of $h\left(\boldsymbol{\theta}_q^{(1)}, t\right)$ and $p_X^{(1)}(x)$ for $q = 1, \cdots, n_{\mathrm{sel}}$ are stored.

Step 2.2. If a perturbation of the source PDF is introduced, then $p_{\boldsymbol{\Theta}}^{(1)}(\boldsymbol{\theta})$ will be correspondingly changed to $p_{\boldsymbol{\Theta}}^{(2)}(\boldsymbol{\theta})$. Instead of conducting another complete round of PDEM analysis, the procedure of change of probability measure is implemented [26]. Accordingly, the new point set $M^{(2)} = \left\{\boldsymbol{\theta}_q^{(1)}, P_q^{(2)}\right\}_{q=1}^{n_{\mathrm{sel}}}$ is generated, where the point $\boldsymbol{\theta}_q^{(1)}$ is unchanged, but the assigned probability is updated by $P_q^{(2)} = \int_{\Omega_q^{(1)}} p_{\boldsymbol{\Theta}}^{(2)}(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}$, in which $\Omega_q^{(1)}$'s are the Voronoi cells.

Step 2.3. With the stored $h\left(\boldsymbol{\theta}_q^{(1)}, t\right)$ and the updated assigned probability $P_q^{(2)}$, re-conduct **Steps 1.3** and **1.4** to obtain the updated PDF of output, $p_X^{(2)}(x)$.

Notice that the efficiency is improved by a factor of $O\left(10^2\right) \sim O\left(10^5\right)$ [26], which is mainly due to the reuse of the underlying deterministic analysis results in **Step 1.2**. It is noteworthy that, some similar but implied ideas can also be found, e.g., in [36] in the context of Bayesian updated PDEM, and in [37,38] in the context of Monte Carlo simulation, etc.

4.4. Approximation of Fréchet-Derivative-based GSI via PDEM-COM

By combining the PDEM and COM, the Fréchet-derivative-based GSI in Eq. (31) in a parametric form, can be evaluated by the following three steps:

Step 3.1. Estimate the original PDF $p_X(x)$. Notice that $p_X(x)$ is corresponding to $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$, where the embedded physical mechanism $X = g(\boldsymbol{\Theta})$ holds. From $p_{\boldsymbol{\Theta}}(\boldsymbol{\theta})$ to $p_X(x)$, an uncertainty quantification method is needed. Traditionally, this part can be completed by, e.g., the analytical method (for some simple cases) [35,39], the kernel density estimation (KDE) [40], or PDEM [28], etc. In the present paper, the PDEM outlined in Section 4.2 is adopted for its high accuracy and efficiency.

Step 3.2. Estimate the perturbed PDF $p_X^{(i)}(x)$ for $i=1,\cdots,n$. For the *i*-the input variable Θ_i, let a small perturbation be added on the PDF of Θ_i, i.e., p_{Θ_i} is changed to p'_{Θ_i}, and then the joint PDF becomes $p'_{\Theta}(\boldsymbol{\theta})=\prod_{j=1,j\neq i}^{n} p_{\Theta_j}\left(\theta_j\right)\cdot p'_{\Theta_i}\left(\theta_i\right)$. Here the independence of basic random variables is assumed just for the sake of simplicity. If the input PDFs do not follow a specific model, but rather given by estimated histograms (data), the fourth-moment method could be an alternative, see Ref. [41] for details.

Further, assume this perturbation is only due to the change of distribution parameters of the input variables. For instance, if p_{Θ_i} can be uniquely determined by its first two moments, i.e., the mean value and standard deviation, denoted as $p_{\Theta_i}\left(\theta_i \mid \mu_i, \sigma_i\right)$, then this perturbation can be divided into two parts, namely, small variations of μ_i and σ_i, respectively. Then we have

$$p'_{\Theta_i}=\begin{cases} p'_{\Theta_i|\mu_i}\left(\theta_i \mid \mu_i+\Delta\mu_i\right), \\ p'_{\Theta_i|\sigma_i}\left(\theta_i \mid \sigma_i+\Delta\sigma_i\right). \end{cases} \tag{53}$$

More generally, Eq. (53) can be written as [42]

$$p_{\boldsymbol{\Theta}|\Theta_i}^{(l)}=p_{\boldsymbol{\Theta}|\Theta_i}^{(l)}\left(\boldsymbol{\theta} \mid \boldsymbol{\xi}+\boldsymbol{e}_{i,l}\Delta\xi_{i,l}\right),\ i=1,\cdots,n;\ l=1,\cdots,n_i \tag{54}$$

where $\boldsymbol{e}_{i,l}$ is a selection vector whose entries are zeros except its *l*-th location for the *i*-th variable being equal to one. The distribution parameters, denoted as $\boldsymbol{\xi}$, are perturbed by $\Delta\xi_{i,l}$ and n_i is the total number of distribution parameters for the *i*-th random variable.

With the perturbed PDF $p_{\boldsymbol{\Theta}|\Theta_i}^{(l)}$ in hand, the corresponding PDF of the response, see $p_X^{(i,l)}(x)$, should be computed. As discussed in Section 4.3, in a recent paper by Chen & Wan [26], this time-consuming procedure can be greatly expedited by advocating the change of probability measure.

Step 3.3. Approximate the Fréchet derivative by the numerical difference scheme. From Eq. (31), the Fréchet derivative can be approximated by a forward difference scheme:

$$\mathsf{F}_{\psi}^{(i,l)} \approx \frac{p_X^{(i,l)}(x) - p_X(x)}{\Delta\xi_{i,l}} \Big/ \left\| \partial p_{\boldsymbol{\Theta}} / \partial \xi_{i,l} \right\|_V, i = 1,\cdots,n; l = 1,\cdots,n_i \tag{55}$$

where the norm term is analytically calculated, see Appendix B in details.

Here the central difference scheme is suggested. To this end, a pair of perturbed PDF is in need, i.e., Eq. (54) is revised to

$$\begin{cases} p_{\boldsymbol{\Theta}|\Theta_i}^{(l)+} = p_{\boldsymbol{\Theta}|\Theta_i}^{(l)+}\left(\boldsymbol{\theta} \,|\, \boldsymbol{\xi} + \boldsymbol{e}_{i,l}\Delta\xi_{i,l}\right), \\ p_{\boldsymbol{\Theta}|\Theta_i}^{(l)-} = p_{\boldsymbol{\Theta}|\Theta_i}^{(l)-}\left(\boldsymbol{\theta} \,|\, \boldsymbol{\xi} - \boldsymbol{e}_{i,l}\Delta\xi_{i,l}\right), \ i = 1,\cdots,n, \ l = 1,\cdots,n_i. \end{cases} \tag{56}$$

Besides, $p_X^{(i,l)+}$ and $p_X^{(i,l)-}$ are simultaneously generated by the PDEM-COM algorithm, respectively. Hence, Eq. (55) is modified by

$$\mathsf{F}_{\psi}^{(i,l)} \approx \frac{1}{2}\frac{p_X^{(i,l)+}(x) - p_X^{(i,l)-}(x)}{\Delta\xi_{i,l}} \Big/ \left\| \partial p_{\boldsymbol{\Theta}} / \partial \xi_{i,l} \right\|_V, \ i = 1,\cdots,n, \ l = 1,\cdots,n_i. \tag{57}$$

Now we discuss the efficiency of the above algorithm. Denote the computational cost of evaluation of p_X for a certain $p_{\boldsymbol{\Theta}}$ be C_0. Let the total number of distribution parameters be $m = \sum_{i=1}^{n} n_i$ where n_i stands for the number of distribution parameters of the i-th random variable, then it is clear to see that, by the double-loop scheme, the total computational cost of sensitivity analysis would be $C_{\text{D-L}} = 2mC_0$ where the number 2 is due to the utilization of the central difference scheme. However, by the PDEM-COM algorithm the computational cost is $C_{\text{PDEM-COM}} = C_0 + 2mC_{\text{COM}}$, where C_{COM} is the computational cost for the calculation of change of probability measure in **Step 2.2**. Since $C_{\text{COM}} \ll C_0$, we have $C_{\text{PDEM-COM}} \approx C_0$. Therefore, $\dfrac{C_{\text{D-L}}}{C_{\text{PDEM-COM}}} \approx 2m$, which indicates the high efficiency of the proposed PDEM-COM scheme on evaluating the Fréchet-derivative-based GSI compared to the direct PDEM. Note that compared to MCS and other methods, the efficiency of PDEM is again much higher by a factor of 10～100 or more. Therefore, the efficiency of evaluating the Fréchet-derivative-based GSI by the PDEM-COM is higher than that of MCS by a factor of 20*m*～200*m* or more.

5 Numerical Applications

To illustrate the Fréchet-derivative-based GSI and its numerical algorithm, five cases are studied. Firstly, two analytical cases are investigated as benchmark tests. Then, three engineering applications are exemplified.

5.1. Example 1: The Riccati Equation

We start with a simple case where only one random parameter is involved. A Riccati equation with a random parameter is written as

$$\dot{X}(t) + \Theta X^2(t) - X(t) = 0,\ \dot{X} = \mathrm{d}X/\mathrm{d}t,\ X(0) = 1 \tag{58}$$

where Θ is a random variable with the following log-normal PDF

$$p_\Theta(\theta) = \frac{1}{\sqrt{2\pi}\sigma\theta}\exp\left\{-\frac{(\ln\theta - \mu)^2}{2\sigma^2}\right\} \tag{59}$$

where μ and σ are the distribution parameters. The analytical solution of Eq. (58) is [39]

$$X = g(\Theta, t) = \frac{e^t}{\Theta e^t - \Theta + 1}. \tag{60}$$

Combining Eqs. (59) and (60), and according to the rule of change of random variable, it is easy to obtain the PDF of X

$$p_X(x,t) = \mathrm{J} \cdot p_\Theta\left(\theta = g^{-1}(x)\right) \tag{61}$$

where $\mathrm{J} = e^t / x^2\left(e^t - 1\right)$ is the Jacobian. Expanding Eq. (61) yields

$$p_X(x,t) = \frac{1}{\sqrt{2\pi}\,x\left(e^t - x\right)\sigma}\exp\left\{t - \frac{1}{2\sigma^2}\left\{\ln\left(\frac{e^t - x}{xe^t - x}\right) - \mu\right\}^2\right\}. \tag{62}$$

Notice that, all the known information characterizing the uncertainty, i.e., the PDF of Θ in Eq. (59), driven by the physical evolution mechanism by Eq. (60), is completely propagated into the PDF of QoI X, $p_X(x,t)$ in Eq. (62). Obviously, $p_X(x,t)$ is a functional of $p_\Theta(\theta)$, as explained in Eq. (2). Because $p_\Theta(\theta)$ is uniquely determined by μ and σ; $p_X(x,t)$ becomes a function of μ and σ, which is clearly exhibited in Eq. (62).

5.1.1. *Analytical Solutions*

Then, the Fréchet-derivative-based GSI can be obtained analytically by

$$\frac{\partial p_X}{\partial \mu} = \frac{1}{\sqrt{2\pi}\left(e^t - x\right)x\sigma^3}\exp\left\{t - \frac{1}{2\sigma^2}\left(\ln\left\{\frac{e^t - x}{xe^t - x}\right\} - \mu\right)^2\right\}\left\{\ln\left(\frac{e^t - x}{xe^t - x}\right) - \mu\right\} \tag{63}$$

and

$$\begin{aligned}\frac{\partial p_X}{\partial \sigma} = & \frac{1}{\sqrt{2\pi}\left(e^t - x\right)x\sigma^4}\exp\left\{t - \frac{1}{2\sigma^2}\left(\ln\left\{\frac{e^t - x}{xe^t - x}\right\} - \mu\right)^2\right\}\left\{\ln\left(\frac{e^t - x}{xe^t - x}\right) - \mu\right\}^2 \\ & - \frac{1}{\sqrt{2\pi}\left(e^t - x\right)x\sigma^2}\exp\left\{t - \frac{1}{2\sigma^2}\left(\ln\left\{\frac{e^t - x}{xe^t - x}\right\} - \mu\right)^2\right\}\end{aligned}. \tag{64}$$

Here the norm terms with respect to the mean parameter is 0.3989 and the standard deviation parameter is 0.4839 (see Appendix B), and they are both omitted for simplicity without inducing confusion in Section 5.1.

For clarity, we firstly study some properties of the Fréchet-derivative-based GSI from the analytical solutions. The numerical solutions by the PDEM-COM algorithm will be illustrated later in Section 5.1.2. At a certain time instant $t=1$, the conditional Fréchet derivative of Eq. (63) in terms of μ with fixed $\sigma=1$ is shown in Fig. 1, while the conditional Fréchet derivative of Eq. (64) in terms of σ when μ is fixed to 0 is shown in Fig. 2. Several observations can be made from these figures: (1) The Fréchet-derivative-based GSIs in terms of the distribution parameters of basic random variables are curves rather than a single value, which characterize the effects of change of the distribution parameters on the global, rather than local properties of output QoI. (2) The Fréchet-derivative-based GSIs in terms of the distribution parameters of basic random variables at different nominal values of the parameters are quite different. For instance, from Fig. 2 it is seen that the Fréchet-derivative-based GSI at $\sigma=1.4$ is much flatter than that at $\sigma=0.6$, which implies that if the standard deviation of source random variable is relatively small, then a slight perturbation of the input standard deviation will induce relatively large perturbation on the PDF of output QoI. This is intuitively reasonable; and (3) The surface of the Fréchet-derivative-based GSI in terms of σ looks more complex than that in terms of μ. This means that generally the rule of influence of the standard deviation of the basic random variable on QoI is more complex than that of the mean of the basic random variable. Note that the change of mean of the basic random variable with fixed standard deviation will make the source PDF shifted without shape changed, whereas the change of standard deviation of the basic random variable with fixed mean value will make the shape of source PDF changed. In other words, the complexity of change of source PDF induced by the change of standard deviation is greater than that induced by the change of mean value of the basic random variable. Therefore, the surface in Fig. 2 being more complex than that in Fig. 1 implies that if the change of source PDF is more complex, then the change of output PDF is also more complex.

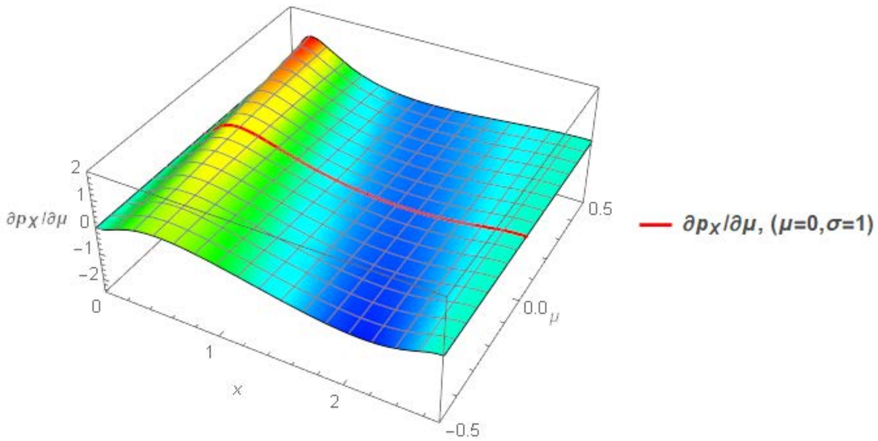


Fig. 1. Conditional Fréchet-derivative-based GSI with the change of μ ($\sigma=1$).

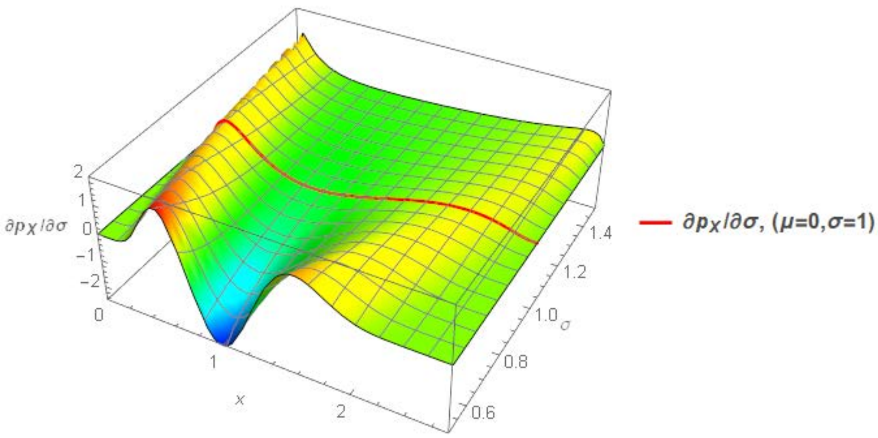


Fig. 2. Conditional Fréchet-derivative-based GSI with the change of σ ($\mu=0$).

To be clearer, consider the PDF of response $p_X(x,t)$ at $t=1$ and its Fréchet-derivative-based GSIs at $\mu=0$ and $\sigma=1$. Then, the three curves by Eqs. (62) to (64) can be plotted in Fig. 3, respectively. A more vivid description of Fig. 3 is present in Fig. 4 in a vector form, where both the direction and rate of change of the value of PDF of output QoI due to the perturbation of input distribution parameters are shown. From these figures, it can be observed that:

Firstly, it is noticed from Fig. 3 that the curves of Fréchet-derivative-based GSIs are not always positive or negative, nor are they monotonic functions. Actually, by inspection it is seen that there is at least one intermediate point crossing the abscissa besides the left and right ends of the curve, and the area between the curves of Fréchet-derivative-based GSIs and the abscissa is zero, which is consistent with Eq. (43). It is seen that at the left and right tails of PDF of the output QoI, the values of Fréchet-derivative-based GSIs are close to zero. Besides, there is one single intermediate point at the curve of Fréchet-derivative-based GSI in terms of the mean of source random variable crossing the abscissa, whereas there are two intermediate points at the curve of Fréchet-derivative-based GSI in terms of the standard deviation of source random variable crossing the abscissa. This is also noticed in the preceding paragraph that the surface in Fig. 2 is more complex than that in Fig. 1.

Secondly, in Fig. 4 it is shown how the PDF of the output QoI will change if there is perturbation in the distribution parameters of the source random variable. It is seen that, if the mean of the source random variable increases, then the left part of PDF of the output QoI will increase (according to the direction of the arrows) and the right part will decrease, resulting in a PDF of the output QoI with centroid (the mean value of output QoI) shifted to left. On the other hand, if the standard deviation of the source random variable increases, then the left and right part of the PDF of output QoI will increase and the middle part will decrease, which means that the PDF of output QoI will become flatter. This also implies that the standard deviation of the output QoI will increase. Quantitatively, the change of PDF of the output QoI due to the perturbation of mean of the source random variable in the neighborhoods of 0.4 and 1.6 (in the response space) is much greater than that in other areas (see Fig. 3), whereas the change of PDF of the output QoI due to the perturbation of standard deviation of the source random variable in the neighborhoods of 0.2, 0.9 and 2.2 (the extrema of the curve in Fig. 3) is much greater than that in other areas. This information is of course useful for decision-making for practical engineering problems, because the quantitative effects on the possible subset in the response space due to perturbation of mean and standard deviation of source random variable are captured.

The above discussions demonstrate that, different from most existent GSI indices, the Fréchet-derivative-based GSI can not only reflect how much the sensitivity is in a global sense via the change of PDF of output QoI, but also point out the certain direction of such change.

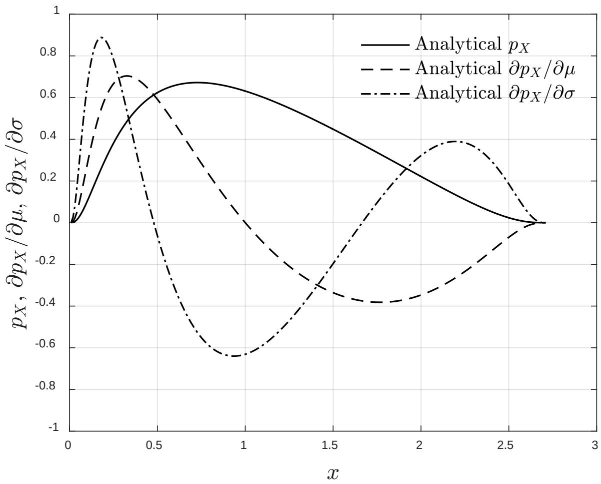


Fig. 3. PDF of QoI at $t=1$ and its Fréchet-derivative-based GSI ($\mu=0$ and $\sigma=1$).

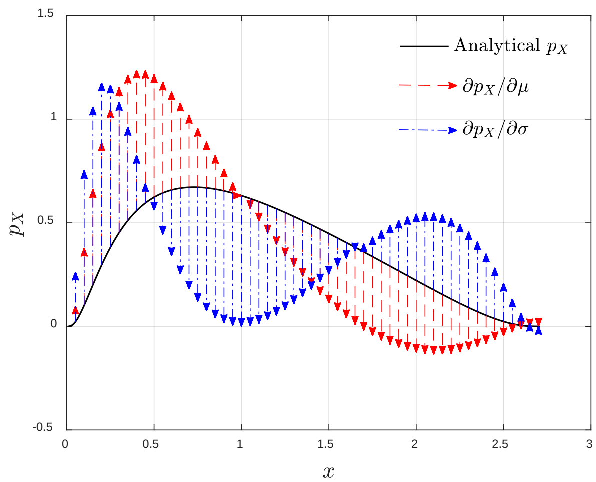


Fig. 4. PDF of QoI at $t=1$ and its Fréchet-derivative-based GSI in vector form ($\mu=0$ and $\sigma=1$).

Remark 2.1: Specifically, if the failure domain is defined as $\Omega_f : X < x_{\lim}$, by integrating Eqs. (63) and (64) we have

$$\int_{\Omega_f} \frac{\partial p_X}{\partial \mu} \mathrm{d}x = \left. \frac{\partial P_f}{\partial \mu} \right|_{x=x_{\lim}}, \int_{\Omega_f} \frac{\partial p_X}{\partial \sigma} \mathrm{d}x = \left. \frac{\partial P_f}{\partial \sigma} \right|_{x=x_{\lim}}. \tag{65}$$

Eq. (65) is exactly the sensitivity of failure probability with respect to the distribution parameters of input random variables, see also related researches in [4,42-43].

The analytical expressions of Eq. (65) is

$$\frac{\partial P_f}{\partial \mu} = -\frac{1}{\sqrt{2\pi}\sigma} \exp\left\{ -\frac{1}{2\sigma^2} \left(\ln\left\{ \frac{e^t - x}{xe^t - x} \right\} - \mu \right)^2 \right\} \Bigg|_{x=x_{\lim}} \tag{66}$$

and

$$\frac{\partial P_f}{\partial \sigma} = -\frac{1}{\sqrt{2\pi}\sigma^2} \exp\left\{ -\frac{1}{2\sigma^2} \left(\ln\left\{ \frac{e^t - x}{xe^t - x} \right\} - \mu \right)^2 \right\} \cdot \left(\mu - \ln\left\{ \frac{e^t - x}{xe^t - x} \right\} \right) \Bigg|_{x=x_{\lim}}. \tag{67}$$

Meanwhile, the analytical expression of failure probability P_f is given by

$$P_f = \int_{-\infty}^{x_{\lim}} p_X \mathrm{d}x = 1 - \frac{1}{2} \mathrm{erf}\left\{ \frac{1}{\sqrt{2}\sigma} \left(\mu - \ln\left\{ \frac{e^t - x}{xe^t - x} \right\} \right) \right\} \Bigg|_{-\infty}^{x_{\lim}} \tag{68}$$

where $\mathrm{erf}(\cdot)$ is the Gaussian error function.

It should be emphasized that, similar but unlike the researches in [4,42], the present paper aims to propose a new GSI with respect to the PDF of output QoI, rather than the failure probability of QoI. But the sensitivity of failure probability of QoI can be a byproduct of the proposed GSI, as shown in Eqs. (6) and (65). Moreover, the proposed GSI in the present paper can be evaluated efficiently by the PDEM-COM method, which makes it more applicable for practical applications.

Remark 2.2: Similarly, Eqs. (66) to (68) are plotted in Figs. 5 and 6 to gain a more straightforward and intuitive understanding on how P_f is sensitive to the input variable. At first glance it is noticed that the sensitivity of P_f at the end points of $x_{\lim}$ is zero. This is reasonable because $\lim_{x_{\lim} \to -\infty} P_f = 1$ and $\lim_{x_{\lim} \to \infty} P_f = 0$, i.e., the failure probability will not change against the change of mean and standard deviation of source random variable at these two extreme points. In addition, different from the sensitivity curves in Fig. 3, the sensitivity curves in Fig. 5 can be always positive or always negative, or partly positive but partly negative. Interestingly, it is shown that a positive perturbation of μ will always reduce P_f of QoI, see the direction of the arrows in Fig. 6, and compare the curves with and without perturbation of the mean of source random variable in Fig. 7. On the other hand, as σ increases, there are different situations in two intervals: for $x_{\lim} \in (-\infty, 1)$, P_f will decrease; while for $x_{\lim} \in (1, +\infty)$, P_f will increase, see the direction of the arrows in Fig. 6, and compare the curves with and without perturbation of the standard deviation of source random variable in Fig. 8. Therefore, there is a crucial point, i.e., $x_{\lim} = 1$, which makes P_f of QoI stays insensitive to the input variable, at least for the distribution parameter of σ. Again, here it is noticed that the effect of perturbation of the standard deviation of source random variable on the failure probability is more complex than that of the mean of source random variable. Evidently, for engineering purposes, the above analytical results will provide valuably qualitative and quantitative information for designers and decision-makers.

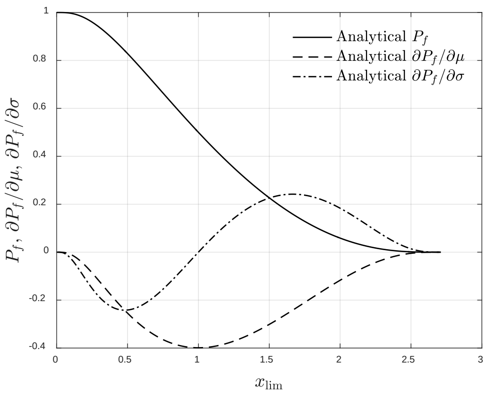


Fig. 5. Failure probability of QoI and its Fréchet-derivative-based GSI ($\mu = 0$, $\sigma = 1$ and $t = 1$).

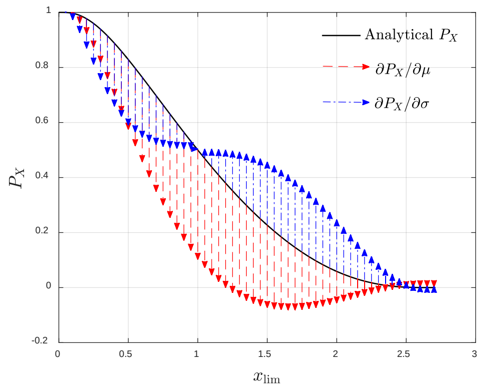


Fig. 6. Failure probability of QoI and its Fréchet-derivative-based GSI in vector form ($\mu=0$, $\sigma=1$ and $t=1$).

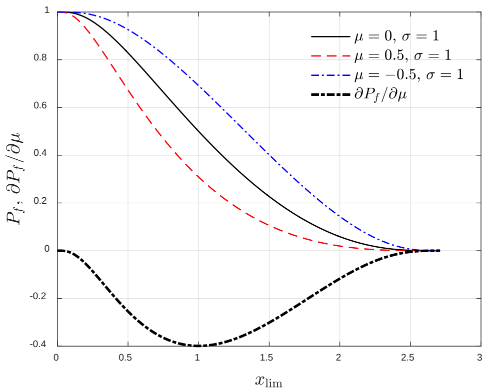


Fig. 7. The influence of μ on failure probability ($\sigma=1$ and $t=1$).

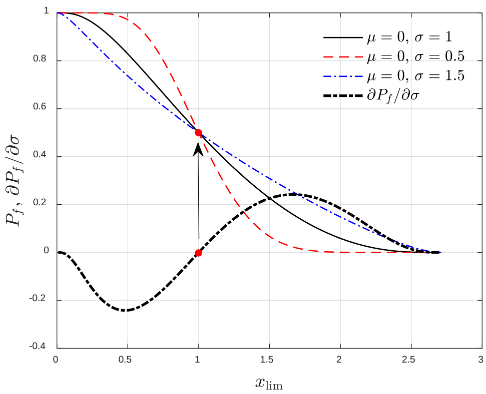
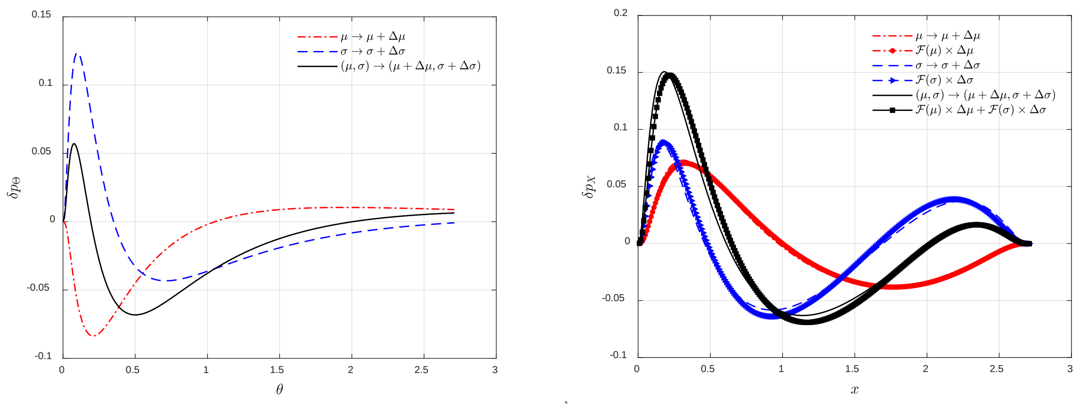


Fig. 8. The influence of σ on failure probability ($\mu=0$ and $t=1$).

Remark 2.3: The proposed Fréchet-derivative-based GSI can be naturally utilized to observe the variation of the output PDF of QoI, when the input PDF gives some variations. In

Fig.9, assume the input PDF is perturbed in three ways: (1) the parameter μ is changed from 0 to 0.1, (2) the parameter σ is set from 1 to 1.1 and (3) the parameters (μ,σ) are chosen from (0,1) to (0.1,1.1), i.e., to be changed simultaneously. Then the proposed GSI presented in Eqs. (63) and (64) are taken into calculation, where one can see that a good linear approximation is achieved, compared with analytical results. It should be emphasized again that though the proposed GSI is under a framework of parametric distributions, it serves well to observe the variation of output PDF when the input PDF is changed, see the third case in Fig. 9 when both parameters are perturbed.



(a) The variation of input PDF (b) The variation of output PDF via analysis and proposed GSI

Fig. 9. A direct function of the proposed Fréchet-derivative-based GSI.

5.1.2. Numerical Solutions by the PDEM-COM Method

To numerically evaluate the Fréchet-derivative-based GSIs, one round of PDEM analysis is firstly required. To this end, 100 representative points are firstly generated by the GF-discrepancy minimized strategy [31], and then an ensemble evolution scheme of PDEM [44] is adopted to evaluate the PDF of output QoI, $p_X(x;\mu,\sigma)$. Next, without additional evaluations of the Riccati equation, the COM is implemented to estimate the four perturbed PDFs of QoI [26], namely $p_X(x;\mu+\Delta\mu,\sigma)$, $p_X(x;\mu-\Delta\mu,\sigma)$, $p_X(x;\mu,\sigma+\Delta\sigma)$ and

$p_X(x;\mu,\sigma-\Delta\sigma)$, respectively. By the central difference scheme, the Fréchet-derivative-based GSI are then approximated by

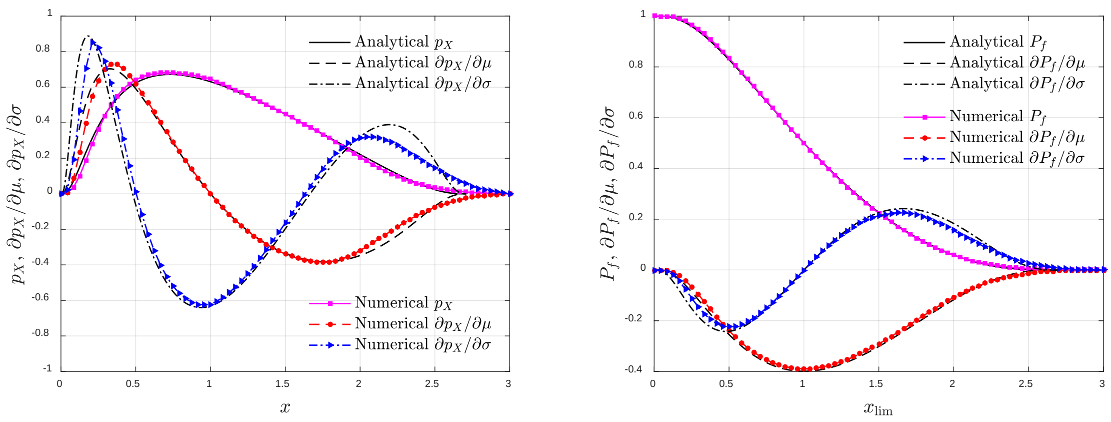
$$\frac{\partial p_X}{\partial \mu} \approx \frac{\Delta p_X}{\Delta \mu} = \frac{1}{2}\frac{p_X(x;\mu+\Delta\mu,\sigma) - p_X(x;\mu-\Delta\mu,\sigma)}{\Delta\mu} \tag{69}$$

and

$$\frac{\partial p_X}{\partial \sigma} \approx \frac{\Delta p_X}{\Delta \sigma} = \frac{1}{2}\frac{p_X(x;\mu,\sigma+\Delta\sigma) - p_X(x;\mu,\sigma-\Delta\sigma)}{\Delta\sigma} \tag{70}$$

respectively, where $\Delta\mu$ and $\Delta\sigma$ take small values, say 0.1 in this case.

Shown in Fig. 10 is the comparison between the analytical solutions and the numerical solutions by PDEM-COM, which demonstrates a good accuracy of the proposed method. In spite of some errors between analytical solutions and numerical ones in Fig. 10(a), the major shape and magnitude are consistent. Meanwhile, as for the sensitivity of failure probability of QoI in Fig. 10(b), the error is relatively small.



(a) Sensitivity of PDF of QoI (b) Sensitivity of CDF (failure probability) of QoI

Fig. 10. Comparison between analytical solutions and numerical solutions via PDEM-COM.

5.2. Example 2: Sum of Gaussian Random Variables

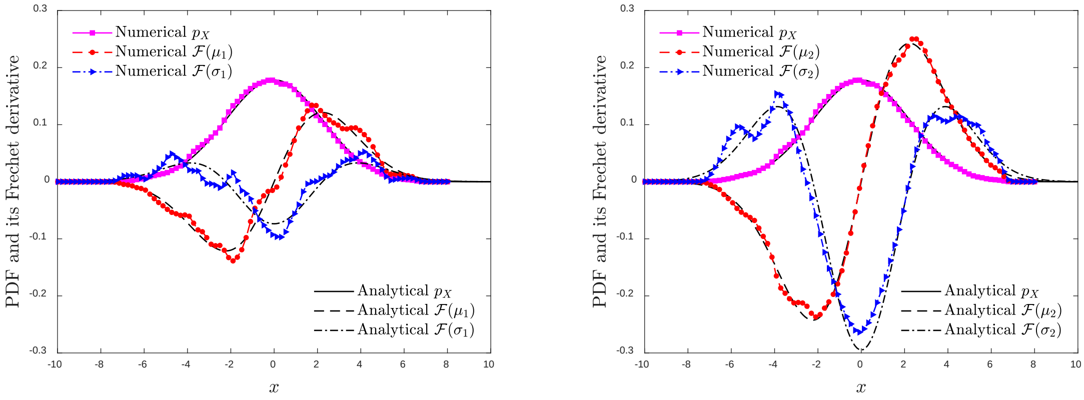
5.2.1. Subcase 1

Consider two independent random variables Θ_1 and Θ_2, and the QoI X is given by the following function:

$$X = \Theta_1 + 2\Theta_2 . \tag{71}$$

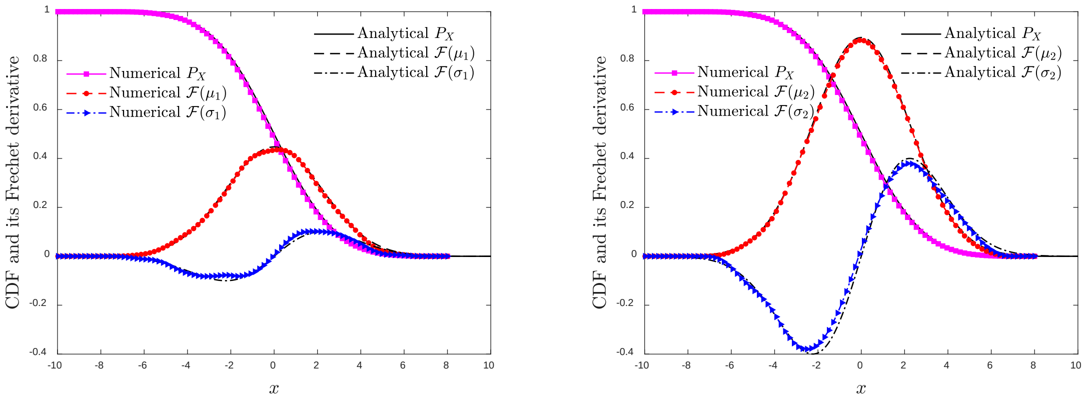
Assume both Θ_1 and Θ_2 are normally distributed random variables with mean values μ_1 and μ_2, and standard deviations σ_1 and σ_2, respectively. To avoid lengthiness here, the analytical expressions of the Fréchet-derivative-based GSI in terms of μ_1, μ_2, σ_1 and σ_2 are provided in Appendix C.

Without loss of generality, assume $\mu_1 = \mu_2 = 0$ and $\sigma_1 = \sigma_2 = 1$. The numerical results are shown in Figs. 11 and 12, compared with the analytical solutions in Appendix C. In this case, a fairly good approximation is achieved in Fig. 11, while a perfect agreement is observed in Fig. 12 as well. With all these informative results at hand, some valuable conclusions can be drawn here: (1) Obviously, it is easy to find that in this system the PDF of output QoI is more sensitive to Θ_2 than to Θ_1 because the maximum value of the GSIs in terms of parameters of Θ_2 in Fig. 11(b) are greater by twice than the corresponding ones of Θ_1 in Fig. 11(a), which is intuitively reasonable from Eq. (71); (2) Similar to Example 1, in each sensitivity curve in terms of the mean of source random variables only one single intermediate point crossing the abscissa exists in Fig. 11(a), whereas in each sensitivity curve in terms of the standard deviation of source random variables there are two intermediate points crossing the abscissa in Fig. 11(b); and (3) The failure probability will certainly always increase due to a small increment of the mean values as shown in Fig. 12, while for the standard deviations, the influence of increasing or reducing the failure probability is dependent on the threshold. Interestingly, similar to Example 1, there also exists a fixed point at $x_{\lim} = 0$.



(a) Sensitivity of PDF of QoI for Θ_1 (b) Sensitivity of PDF of QoI for Θ_2

Fig. 11. Fréchet-derivative-based GSIs of PDF in terms of Θ_1 and Θ_2.



(a) Sensitivity of failure probability of QoI for Θ_1 (b) Sensitivity of failure probability of QoI for Θ_2

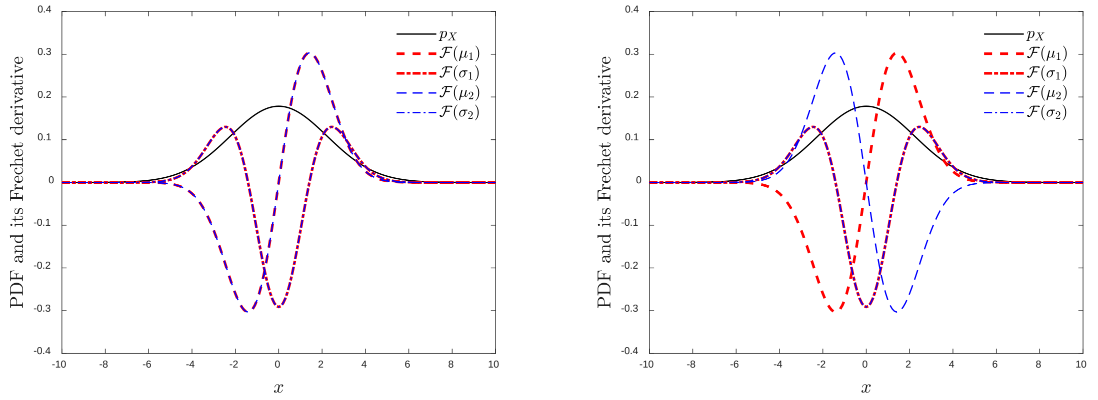
Fig. 12. Fréchet-derivative-based GSI of failure probability in terms of Θ_1 and Θ_2.

5.2.2. Subcase 2

Now we consider two similar but not identical functions:

$$\text{(a)} \quad X_a = \Theta_1 + \Theta_2 \quad \text{and (b)} \quad X_b = \Theta_1 - \Theta_2 \tag{72}$$

where the subscripts “*a*” and “*b*” denote the QoIs that generated by Eqs. (72)a and (72)b, or Subcase 2a and Subcase 2b, respectively. The information of Θ_1 and Θ_2 is identical to that in Subcase 1. Therefore, X_a and X_b are normally distributed as well. To avoid lengthiness here, the analytical expressions of Fréchet-derivative-based GSI of X_a and X_b are available in Appendix C. Again, let $\mu_1 = \mu_2 = 0$ and $\sigma_1 = \sigma_2 = 1$. The Fréchet-derivative-based GSIs for Subcase 2a and Subcase 2b are shown in Fig. 13.



(a) Fréchet-derivative-based GSIs for Subcase 2a (b) Fréchet-derivative-based GSIs for Subcase 2b

Fig. 13. Fréchet-derivative-based GSIs for two Subcases.

From Fig. 13, it is easy to observe how each input variable affects the QoI in terms of both magnitude and direction. It is clearly seen that the proposed GSIs in Subcase 2a are apparently different from those in Subcase 2b. Actually, from Fig. 13(a) it is seen that the sensitivity curves in terms of the means of both source variables are identical. Simultaneously, the sensitivity curves in terms of the standard deviations of both source variables are also identical. This is intuitively reasonable because from Eq. (72)a it is noticed that the QoI is symmetric in terms of Θ_1 and Θ_2. However, from Fig. 13(b) it is noticed that, though the sensitivity curves in terms of the standard deviations of both source variables are still identical, the sensitivity curves in terms of the means of the two source random variables are not identical any more. Actually, in this case, the amplitudes are still identical but the signs are opposite. Considering the QoI in Eq. (72)b is anti-symmetric in terms of Θ_1 and Θ_2, again the properties shown in Fig. 13(b) are intuitively understandable.

Unfortunately, the existent sensitivity indices, including the Sobol' indices [13] or moment-independent importance measures [16] as listed in Table 2, cannot distinguish the sensitivity of Θ_1 and Θ_2 in Eq. (72)b. It is seen from Table 2 that there is no difference between the sensitivity indices of Subcase 2a and Subcase 2b, which is somewhat misleading [17].

Table 2

Analytical results of Subcase 2a and Subcase 2b [17].

Subcases	Subcase 2a		Subcase 2b	
Input variables	Θ_1	Θ_2	Θ_1	Θ_2
Sobol' indices:	0.5	0.5	0.5	0.5
Moment-independent IMs:	0.306	0.306	0.306	0.306

5.3. *Example 3: A Cantilever Beam*

In this case, a cantilever beam subjected to two concentrated forces is studied [45], as shown in Fig. 14. The responses of the beam, i.e., the maximum displacement and stress, can be analytically obtained, thus we have the following two performance functions:

(a) displacement performance function

$$g_D = d_0 - \frac{4L^3}{Ewh}\sqrt{\left(\frac{Y}{h^2}\right)^2 + \left(\frac{X}{w^2}\right)^2}, \tag{73}$$

(b) stress performance function

$$g_S = R - \frac{6L}{wh^2}(X+Y) \tag{74}$$

where all the parameters in Eqs. (73) and (74) are listed in Table 3.

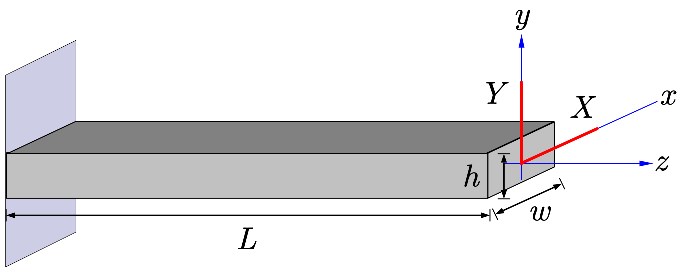


Fig. 14. A cantilever beam structure [45].

These two performance functions are obviously functions of the source random variables X, Y, E and R. Assume these four basic random variables are independent and normally distributed, while the corresponding distribution parameters of X, Y, E and R are denoted as (μ_X, σ_X), (μ_Y, σ_Y), (μ_E, σ_E) and (μ_R, σ_R), respectively, and listed in Table 3 for details.

Table 3

Model parameters in the cantilever beam structure.

Parameters	Value/Distribution	Mean	Std.D	Physical senses
L (in)	100	-	-	Beam length
w (in)	4	-	-	Beam width
h (in)	2	-	-	Beam thickness
d_0 (in)	5	-	-	Displacement threshold
X (lbf)	Normal	500	100	Horizontal force
Y (lbf)	Normal	1000	100	Vertical force
E (psi)	Normal	2.9×10^7	1.45×10^6	Modulus of elasticity
R (psi)	Normal	6.4×10^4	3.2×10^4	Yield stress

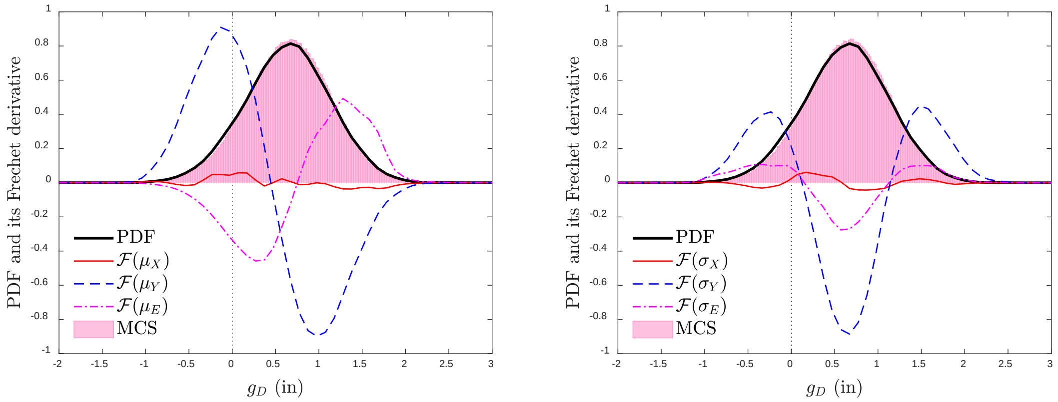
In this practical case, it is emphasized that since the unit of each parameter is different, thus the digital values of realizations of different random variables may differ for several orders of magnitude. For instance, the order of magnitude of vertical force is about $O\left(10^{3}\right)$ while the order of magnitude of the modulus of elasticity is around $O\left(10^{7}\right)$. This of course may induce numerical singularity. Therefore, in this aspect, the norm term in the proposed Fréchet-derivative-based GSI in Eq. (31) can be regarded as a non-dimensional-normalization factor, which is naturally defined in the definition of the Fréchet derivative, i.e.,

$$\begin{cases} \dfrac{\partial p/\partial \mu_X}{\left\|\partial p_\Theta/\partial \mu_X\right\|}, \dfrac{\partial p/\partial \mu_Y}{\left\|\partial p_\Theta/\partial \mu_Y\right\|}, \dfrac{\partial p/\partial \mu_E}{\left\|\partial p_\Theta/\partial \mu_E\right\|}, \dfrac{\partial p/\partial \mu_R}{\left\|\partial p_\Theta/\partial \mu_R\right\|}, \\ \dfrac{\partial p/\partial \sigma_X}{\left\|\partial p_\Theta/\partial \sigma_X\right\|}, \dfrac{\partial p/\partial \sigma_Y}{\left\|\partial p_\Theta/\partial \sigma_Y\right\|}, \dfrac{\partial p/\partial \sigma_E}{\left\|\partial p_\Theta/\partial \sigma_E\right\|}, \dfrac{\partial p/\partial \sigma_R}{\left\|\partial p_\Theta/\partial \sigma_R\right\|}. \end{cases} \tag{75}$$

where p stands for the PDF of QoI, i.e., the displacement performance function g_D, or the stress performance function g_S, while p_Θ denotes the PDF of inputs.

5.3.1. The GSI of the Displacement Performance Function

Let the QoI firstly be g_D. Numerical results of the GSI by the PDEM-COM method are plotted in Fig. 15. By inspection some instructive properties are clear: (1) For the mean values of distribution parameters of the source random variables, μ_Y is of most influence, while the effect of μ_X is comparatively very small. Noting from Table 3 that *w* is twice *h* from Eq. (73) so it can be estimated roughly that the effect of *Y* should be at least greater than that of *X* by a factor of around $(2)^2 = 4$. This is consistent with the above observation. (2) Moreover, it is noted that the GSIs of QoI in terms of μ_Y and μ_E are almost completely opposite in Fig. 15(a), which is also reasonable since Y is related to the external load effect, while E stands for the intrinsic structural resistance. From a physical perspective, the effects of these two variables must be opposite. And (3) it is seen that, in terms of *Y* and *E*, the mean values of source random variables have greater effects on QoI than the standard deviations of source random variables by comparing Figs. 15(a) and 15(b).

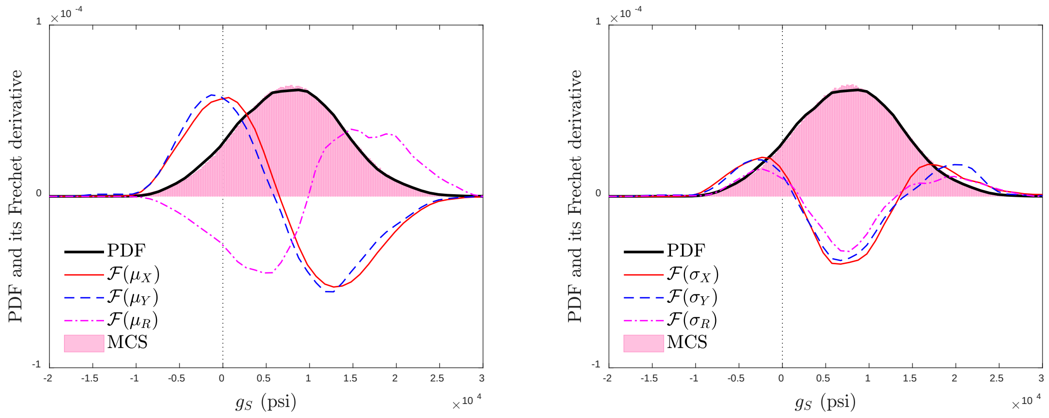


(a) GSI with respect to the mean value (b) GSI with respect to the standard deviation

Fig. 15. PDF of g_D and its Fréchet-derivative-based GSIs.

5.3.2. Stress Performance Function

Now we consider g_S. The GSIs are plotted in Fig. 16. It is clear to see that: (1) μ_X, μ_Y and μ_R are all of remarkable effect on QoI, in an order of $\mu_Y \approx \mu_X > \mu_R$ in terms of sensitivity, which is easily understandable from Eq. (74). In particular, in this case because *X* has the same factor -1 as that of *Y* from Eq. (74), it is roughly estimated that the sensitivity of *X* is close to that of *Y*, which is verified from Fig. 16(a). This is also true for the μ_R but because the factor of *R* becomes to 1 so the direction of GSI based on μ_R is opposite to those of μ_X and μ_Y. (2) Besides, σ_X, σ_Y and σ_R are of less and close effect, which is due to the coincidence that $\sigma_R = 3200\text{psi}$ while $\frac{6L}{wh^2}\sigma_X = \frac{6L}{wh^2}\sigma_Y = 3750\text{psi}$ from Eq. (74), but one can still see that the effects of σ_X, σ_Y and σ_R are in an order of $\sigma_Y \approx \sigma_X > \sigma_R$.



(a) GSI with respect to the mean value (b) GSI with respect to the standard deviation

Fig. 16. PDF of g_S and its Fréchet-derivative-based GSIs.

5.3.3. *Discussion and Verification*

Actually, since it is not always easy to obtain the analytical expressions of Example 3, the results by the Monte Carlo Simulation (MCS) are adopted as a reference. The kernel density estimation (KDE) [40], as an important method in sensitivity analysis, is employed to estimate the probability density function. One million times of evaluations are completed for one single loop of sensitivity analysis, and the results are shown in Fig. 17. Compared with the numerical results plotted in Fig. 15(a), the accuracy of the GSIs by PDEM-COM is again verified, but the efficiency of PDEM-COM is much higher since only 500 function evaluations are needed for the whole analysis.

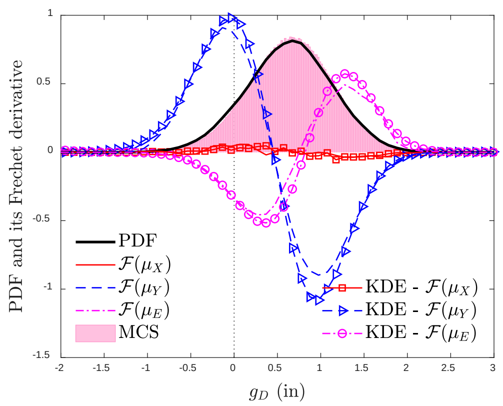


Fig. 17. Comparison between PDEM-COM and MCS-KDE.

5.4. *Example 4: The Short Column Function*

The short column function is commonly utilized as a benchmark in reliability-based structural optimization [45-47]. The limit state function is explicitly defined as

$$g\left(M_1, M_2, P, Y\right) = 1 - \frac{4M_1}{bh^2Y} - \frac{4M_2}{b^2hY} - \left(\frac{P}{bhY}\right)^2 \tag{76}$$

where Y stands for the yield stress, b and h are the width and depth of the rectangular cross section of the short column, which is subjected to bi-axial bending moments M_1 and M_2. According to [46], the geometrical parameters b and h are all set to the optimal values, e.g., 300mm and 600mm, respectively. The uncertainty is considered to be originated from M_1, M_2, P and Y with the probability distributions listed in Table 4. Here the statistically independency of M_1, M_2, P and Y is assumed for simplicity.

Table 4

Model parameters in the short column function [46].

Parameters	Distribution	Mean	C.O.V.	Physical senses
M_1 (kN · m)	Lognormal	250	0.30	Bending moment
M_2 (kN · m)	Lognormal	125	0.30	Bending moment
P (kN)	Weibull	2500	0.20	Axial force
Y (MPa)	Gamma	40	0.10	Yield stress

Note: C.O.V. is the abbreviation of coefficient of variation.

The first and second distribution parameters of M_1, M_2, P and Y are analytically calculated by the mean value and the standard deviation listed in Table 4, and are denoted by

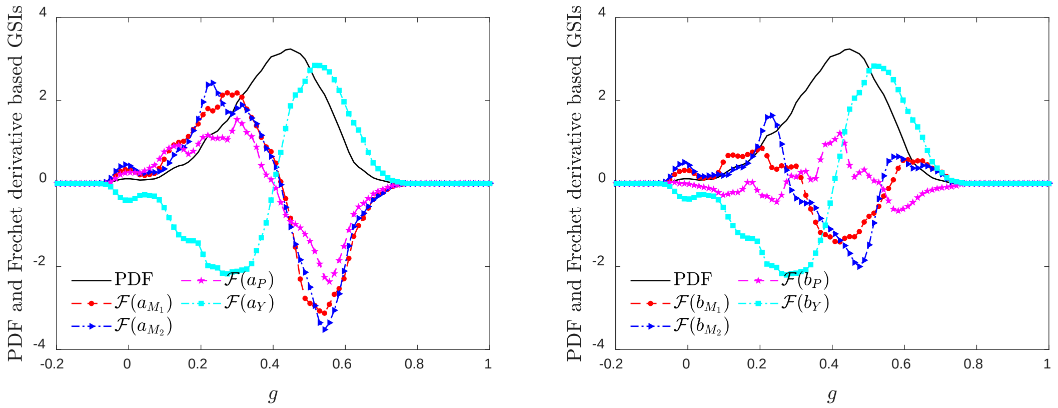
$\left(a_{M_1}, b_{M_1}\right)$, $\left(a_{M_2}, b_{M_2}\right)$, $\left(a_P, b_P\right)$ and $\left(a_Y, b_Y\right)$, respectively. Specifically, the PDFs of M_1, M_2, P and Y are correspondingly written by

$$\begin{cases} p_{M_1}\left(x; a_{M_1}, b_{M_1}\right) = \dfrac{1}{x\sqrt{2\pi}b_{M_1}} \exp\left\{-\dfrac{\left(\ln x - a_{M_1}\right)^2}{2b_{M_1}^2}\right\}, \\ p_{M_2}\left(x; a_{M_2}, b_{M_2}\right) = \dfrac{1}{x\sqrt{2\pi}b_{M_2}} \exp\left\{-\dfrac{\left(\ln x - a_{M_2}\right)^2}{2b_{M_2}^2}\right\}, \\ p_P\left(x; a_P, b_P\right) = \dfrac{b_P}{a_P}\left(\dfrac{x}{a_P}\right)^{b_P - 1} \exp\left\{-\left(\dfrac{x}{a_P}\right)^{b_P}\right\}, \\ p_Y\left(x; a_Y, b_Y\right) = \dfrac{1}{b_Y^{a_Y}\Gamma\left(a_Y\right)} x^{a_Y - 1} \exp\left(-\dfrac{x}{b_Y}\right) \end{cases} \tag{77}$$

where $\Gamma(\cdot)$ is the Gamma function.

The Fréchet-derivative-based GSIs evaluated by the PDEM-COM method are plotted in Fig. 18. It is seen from Fig. 18 that the GSIs in terms of the first and second parameters of M_1 are almost identical to those in terms of M_2, respectively. This is actually the reflection of the fact from Eq. (76) that the function is symmetric in terms of M_1 and M_2. Moreover, it can be seen clearly that the influence of the first parameter of Y on PDF of g is in an opposite way compared to the effects of the means of M_1, M_2 and P. This can be easily interpreted: according to Eq. (76), Y is in the dominator while M_1, M_2 and P are all in the numerator. In the reliability-based structural optimization, the direction (sign) of sensitivity in terms of basic input variables is of paramount significance [48]. A verification of the proposed PDEM-COM is also completed in Fig. 19 via the MCS-KDE as illustrated in Example 3. Here we arbitrarily verify some of the indices in Fig. 18, and the verified results in Fig. 19 indicate a high accuracy of the proposed method of calculating the proposed GSI.

In a sense, this kind of opposite or positive influences (direction) on the PDF of QoI, are natural sensitivities with certain directions due to the embedded physical mechanisms, which can be captured by the proposed Fréchet-derivative-based GSIs.



(a) GSI with respect to the first parameter (b) GSI with respect to the second parameter

Fig. 18. Fréchet-derivative-based GSIs in terms of the first and second parameters in Example 4.

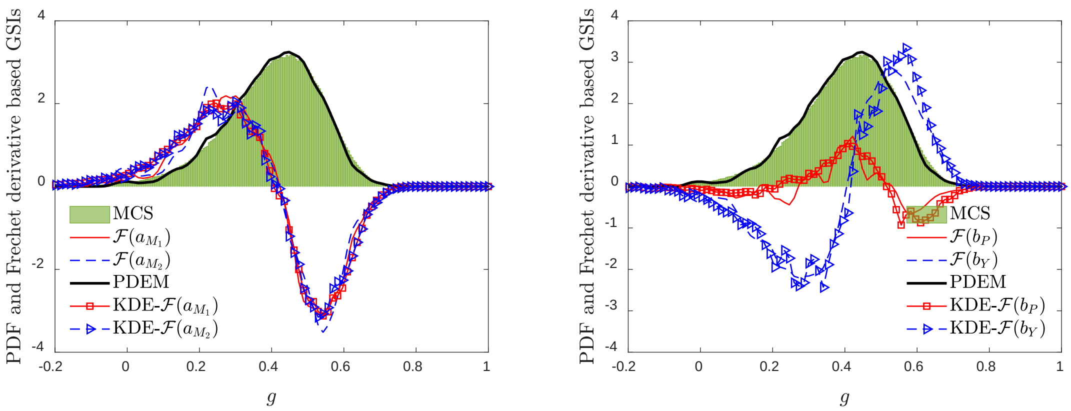


Fig. 19. Fréchet-derivative-based GSIs in terms of the first and second parameters in Example 4 via PDEM-COM and MCS-KDE.

5.5. Example 5: A Roof Truss Structure

A more complex case involving a roof truss structure [6] is studied hereinafter (Fig. 20). The structure is subjected to uniformly distributed load q, which could be equivalent to three nodal loads $F = ql/4$. The top four components and the two compressive bars are made from concrete materials, while the inner two elements and the bottom three tension bars are of steel materials. The displacement of point O can be analytically constructed by

$$d_o = \frac{ql^2}{2}\left(\frac{3.81}{A_c E_c} + \frac{1.13}{A_s E_s}\right) \tag{78}$$

where the model parameters in Eq. (78) are listed in Table 5.

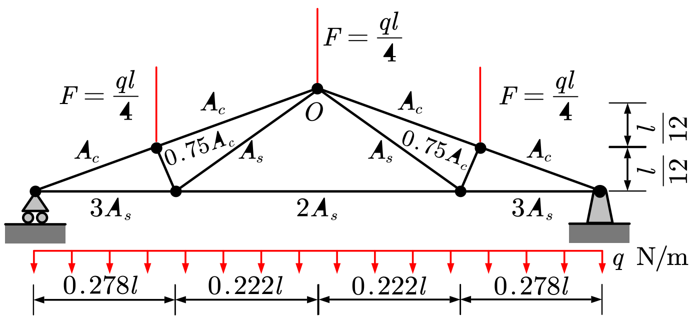


Fig. 20. A roof truss structure [6].

Table 5

Model parameters of the roof truss structure [6].

Parameters	Distribution	Mean	C.O.V.	Physical meanings
q (N/m)	Normal	20,000	0.07	Uniform load
l (m)	Normal	12	0.01	Length of component
A_c (m^2)	Normal	0.04	0.12	Sectional area of concrete
A_s (m^2)	Normal	9.82×10^{-4}	0.06	Sectional area of steel
E_c (N/m^2)	Normal	2×10^{10}	0.06	Modulus of elasticity of concrete
E_s (N/m^2)	Normal	1×10^{11}	0.06	Modulus of elasticity of steel

Note: C.O.V. is the abbreviation of coefficient of variation.

Though the normal distribution is not perfectly physically consistent with the above parameters, in the present case it is still appropriate because the standard deviation (calculated by C.O.V.) is relatively small, therefore it is almost impossible to generate negative values that have no physical sense.

Numerical results of the GSIs in terms of the mean values of source random variables are shown in Fig. 21 while pictured in Fig. 22 are the GSIs in terms of the standard deviations of source random variables. It is seen that in terms of the mean values of source random variables, the order of importance is $\mathsf{F}\left(\mu_q\right) > \mathsf{F}\left(A_c\right) \approx \mathsf{F}\left(\mu_{E_c}\right) \approx \mathsf{F}\left(\mu_{A_s}\right) \approx \mathsf{F}\left(\mu_{E_s}\right) > \mathsf{F}\left(\mu_l\right)$, where $\mathsf{F}\left(\mu_q\right)$ is the GSI in terms of μ_q and similar symbols apply to other GSIs. In terms of the standard deviations of source random variables, it is found that the rule of GSIs in terms of the standard deviations of source random variables are more complex compared to those in terms of the means of source random variables. This is consistent with the discussions in Example 1. It should be emphasized that these orders are qualitative, while the quantitative information shown in Figs. 21 and 22 can be adopted for more rational decision-making or employed in reliability-based structural optimization. For instance, it is seen from Fig. 22 that the GSIs in terms of σ_l and σ_{E_c} are much smaller compared to the GSIs in terms of the standard deviations of the other source random variables. This means that, if a decision-making is needed whether the epistemic uncertainty in the standard deviations of source random variables are needed, then it can be such decided that the effects of epistemic uncertainty in the standard deviations of l and E_c can be ignored, and thus the involved factors in terms of epistemic uncertainty in the problem can be reduced.

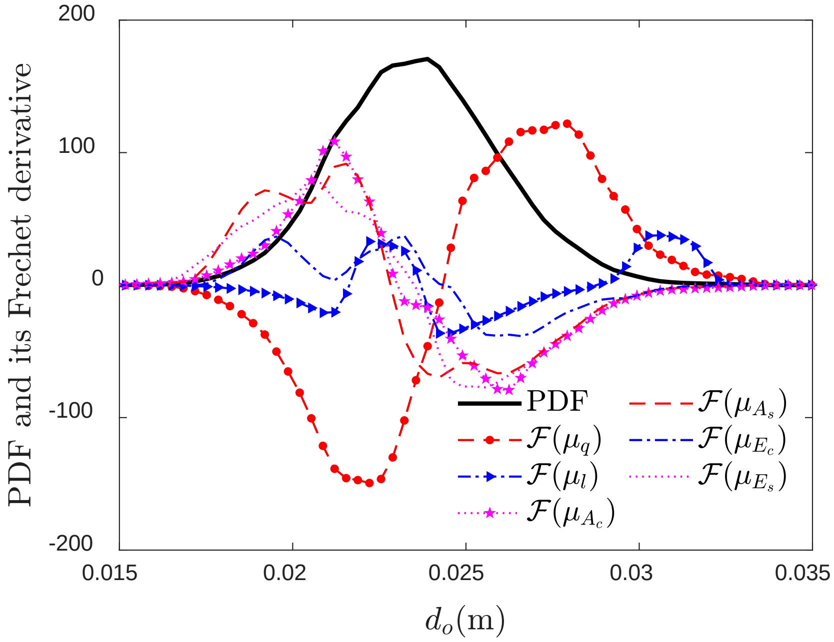


Fig. 21. Fréchet-derivative-based GSIs in terms of mean values for Example 5.

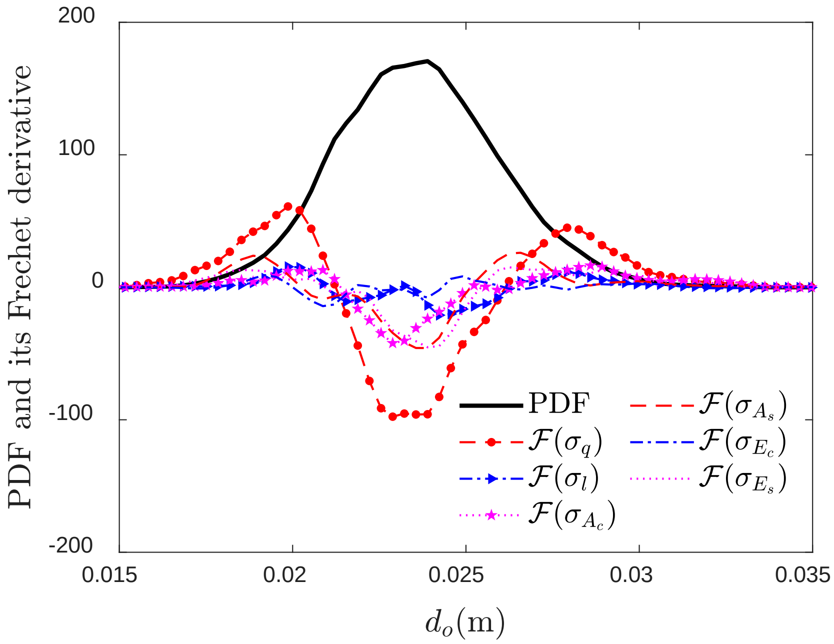


Fig. 22. Fréchet-derivative-based GSIs with respect to standard deviations for Example 5.

6 Concluding Remarks

In the present paper, for the systems involving random parameters, starting from a functional perspective, a Fréchet-derivative-based global sensitivity index is proposed. Highly efficient numerical algorithms are elaborated by incorporating the probability density evolution method and the change of probability measure (PDEM-COM algorithm). The main findings and conclusions are:

(1) The proposed sensitivity defined by the Fréchet derivative, i.e., the change of the PDF of the output QoI in terms of the change of the PDF of the input basic random variables is essentially a global sensitivity index. Compared to the traditional sensitivity indices, e.g., the Sobol' indices and the moment-independent IMs, the proposed GSI is more informative and flexible by providing not only the magnitude of change at the level of the PDF, but also the direction of effects being positive or adverse.

(2) The PDEM-COM algorithm by incorporating the probability density evolution method (PDEM) and the change of probability measure (COM) provides a highly efficient and fairly accurate tool for the evaluation of the proposed GSI in terms of the distribution parameters of input random variables.

(3) Numerical examples, including two analytical and three engineering cases, are extensively studied, demonstrating the accuracy and effectiveness of the proposed GSI as well as the PDEM-COM algorithm.

Some important and interesting issues for extension shall be studied further, including, e.g., how to apply the present GSI for dependent source random variables and subsets of variables, etc.

Acknowledgement

Financial supports from the National Natural Science Foundation of China (NSFC Grant Nos. 51725804, 51538010 and 11761131014), the DFG Grant No. 392113882, the NSFC-Guangdong Province Joint Project (Grant No. U1711264) are highly appreciated. The China Scholarship Council (CSC) is gratefully appreciated by the second author.

Appendix A. A Proposition on Fréchet-Derivative-based GSI

The following proposition in terms of the Fréchet-derivative-based GSI is stated and proved.

Proposition. *The definition in Eq.* (31) *in a parametric form allows that*

$$\left\|\delta\tilde{p}_X-\delta p_X\right\|\le\left\|\delta\tilde{p}_\Theta-\delta p_\Theta\right\|_V\cdot\sup_{0\le t\le 1}\left\|\mathsf{F}_\psi\left(p_\Theta+t\delta\tilde{p}_\Theta+(1-t)\delta p_\Theta\right)\right\| \tag{79}$$

holds, where $\delta\tilde{p}_X$ *is the variation of* $\tilde{p}_X$ *due to an arbitrary variation of* p_Θ *by* $\delta\tilde{p}_\Theta$, *while* δp_X *is the variation of* p_X *due to a parametric variation of* p_Θ *by* δp_Θ. *It indicates that the variation of the output PDF is a.e. the same no matter the input PDF is parametric or not, as long as the variation of the input PDF is sufficiently small.*

Proof. Denote

$$\begin{cases}\delta\tilde{p}_X=\psi\left(p_\Theta+\delta\tilde{p}_\Theta\right)-\psi\left(p_\Theta\right),\\ \delta p_X=\psi\left(p_\Theta+\delta p_\Theta\right)-\psi\left(p_\Theta\right),\end{cases} \tag{80}$$

and

$$\delta\tilde{p}_X-\delta p_X=\psi\left(p_\Theta+\delta\tilde{p}_\Theta\right)-\psi\left(p_\Theta+\delta p_\Theta\right). \tag{81}$$

According to the mean value theorem [24], we have

$$\begin{aligned}\left\|\delta\tilde{p}_X-\delta p_X\right\|&=\left\|\psi\left(p_\Theta+\delta\tilde{p}_\Theta\right)-\psi\left(p_\Theta+\delta p_\Theta\right)\right\|\\&\le\left\|\delta\tilde{p}_\Theta-\delta p_\Theta\right\|_V\cdot\sup_{0\le t\le 1}\left\|\mathsf{F}_\psi\left(p_\Theta+t\delta\tilde{p}_\Theta+(1-t)\delta p_\Theta\right)\right\|\end{aligned} \tag{82}$$

where F_ψ is the Fréchet derivative of ψ. ■

Appendix B. Analytical Expressions of the Norm Term of GSI for Some Common Distributions

The norm term in the proposed Fréchet-derivative-based GSI in Eq. (31) is defined as

$$\left\|\frac{\partial p_{\Theta}(\theta;\boldsymbol{\xi})}{\partial \xi_j}\right\|_V = \frac{1}{2}\int_{\Omega_\Theta}\left|\frac{\partial p_{\Theta}(\theta;\boldsymbol{\xi})}{\partial \xi_j}\right|\mathrm{d}\theta,\ j=1,2,\cdots,m \tag{83}$$

where $\boldsymbol{\xi}$ is the distribution parameter of the input PDF $p_{\Theta}(\theta;\boldsymbol{\xi})$. This defined norm can be exactly evaluated for some common distributions, and the results are summarized as follows.

(1) Normal distribution $p_{\Theta}(\theta;\mu,\sigma)=\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(\theta-\mu)^2}{2\sigma^2}}$ for $\theta\in\mathbb{R}$.

A normal distribution with the mean value μ and the standard deviation σ has the explicitly defined norms by

$$\begin{cases}\left\|\frac{\partial p_{\Theta}(\theta;\mu,\sigma)}{\partial \mu}\right\|_V = \frac{1}{2}\int_{-\infty}^{+\infty}\left|\frac{\theta-\mu}{\sigma^2}\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(\theta-\mu)^2}{2\sigma^2}}\right|\mathrm{d}\theta=\frac{1}{\sqrt{2\pi}\sigma}, \\ \left\|\frac{\partial p_{\Theta}(\theta;\mu,\sigma)}{\partial \sigma}\right\|_V = \frac{1}{2}\int_{-\infty}^{+\infty}\left|\frac{(\theta-\mu)^2-\sigma^2}{\sigma^3}\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(\theta-\mu)^2}{2\sigma^2}}\right|\mathrm{d}\theta=\frac{2}{\sqrt{2\pi}\sigma}e^{-1/2}.\end{cases} \tag{84}$$

(2) Log-normal distribution $p_{\Theta}(\theta;\alpha,\beta)=\frac{1}{\sqrt{2\pi}\beta\theta}e^{-\frac{(\ln\theta-\alpha)^2}{2\beta^2}}$ for $\theta>0$.

The derivatives of the function $p_{\Theta}(\theta;\alpha,\beta)$ in terms of the parameters α and β have explicit forms, therefore the norms are computed by

$$\begin{cases}\left\|\frac{\partial p_{\Theta}(\theta;\alpha,\beta)}{\partial \alpha}\right\|_V = \frac{1}{2}\int_{0}^{+\infty}\left|\frac{\ln\theta-\alpha}{\beta^2}\frac{1}{\sqrt{2\pi}\beta\theta}e^{-\frac{(\ln\theta-\alpha)^2}{2\beta^2}}\right|\mathrm{d}\theta=\frac{1}{\sqrt{2\pi}\beta}, \\ \left\|\frac{\partial p_{\Theta}(\theta;\alpha,\beta)}{\partial \beta}\right\|_V = \frac{1}{2}\int_{0}^{+\infty}\left|\frac{(\ln\theta-\alpha)^2-\beta^2}{\beta^3}\frac{1}{\sqrt{2\pi}\beta\theta}e^{-\frac{(\ln\theta-\alpha)^2}{2\beta^2}}\right|\mathrm{d}\theta=\frac{2}{\sqrt{2\pi}\beta}e^{-1/2}.\end{cases} \tag{85}$$

For the norm of some other distributions, the numerical computation on the derivative as well as the integral is recommended.

Appendix C. Analytical Expressions of GSI in Example 2

(1) Subcase 1

Theoretically, X is also normally distributed with the mean value $\mu = \mu_1 + 2\mu_2$ and the standard deviation $\sigma = \sqrt{\sigma_1^2 + 4\sigma_2^2}$, therefore the PDF of X is

$$p_X(x) = \frac{1}{\sqrt{2\pi\left(\sigma_1^2 + 4\sigma_2^2\right)}} \exp\left\{-\frac{\left(x - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\}. \tag{86}$$

Then, taking derivatives of Eq. (86) with respect to μ_1, μ_2, σ_1 and σ_2, we have

$$\frac{\partial p_X}{\partial \mu_1} = \frac{\left(x - \mu_1 - 2\mu_2\right)}{\sqrt{2\pi}\left(\sigma_1^2 + 4\sigma_2^2\right)^{3/2}} \exp\left\{-\frac{\left(x - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\}, \tag{87}$$

$$\frac{\partial p_X}{\partial \mu_2} = \frac{2\left(x - \mu_1 - 2\mu_2\right)}{\sqrt{2\pi}\left(\sigma_1^2 + 4\sigma_2^2\right)^{3/2}} \exp\left\{-\frac{\left(x - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\}, \tag{88}$$

$$\frac{\partial p_X}{\partial \sigma_1} = \frac{\sigma_1}{\sqrt{2\pi}} \exp\left\{-\frac{\left(x - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\} \cdot \frac{\left(x - \mu_1 - 2\mu_2\right)^2 - \left(\sigma_1^2 + 4\sigma_2^2\right)}{\left(\sigma_1^2 + 4\sigma_2^2\right)^{5/2}}, \tag{89}$$

and

$$\frac{\partial p_X}{\partial \sigma_2} = \frac{4\sigma_2}{\sqrt{2\pi}} \exp\left\{-\frac{\left(x - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\} \cdot \frac{\left(x - \mu_1 - 2\mu_2\right)^2 - \left(\sigma_1^2 + 4\sigma_2^2\right)}{\left(\sigma_1^2 + 4\sigma_2^2\right)^{5/2}}. \tag{90}$$

Integrating Eqs. (87) to (90) in the failure domain $\Omega_f : X < x_{\lim}$ leads to

$$\frac{\partial P_X}{\partial \mu_1} = \frac{1}{\sqrt{2\pi\left(\sigma_1^2 + 4\sigma_2^2\right)}} \exp\left\{-\frac{\left(x_{\lim} - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\}, \tag{91}$$

$$\frac{\partial P_X}{\partial \mu_2} = \frac{2}{\sqrt{2\pi\left(\sigma_1^2 + 4\sigma_2^2\right)}} \exp\left\{-\frac{\left(x_{\lim} - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\}, \tag{92}$$

$$\frac{\partial P_X}{\partial \sigma_1} = \frac{\sigma_1\left(x_{\lim} - \mu_1 - 2\mu_2\right)}{\sqrt{2\pi}\left(\sigma_1^2 + 4\sigma_2^2\right)^{3/2}} \exp\left\{-\frac{\left(x_{\lim} - \mu_1 - 2\mu_2\right)^2}{2\left(\sigma_1^2 + 4\sigma_2^2\right)}\right\}, \tag{93}$$

and

$$\frac{\partial P_X}{\partial \sigma_2}=\frac{4\sigma_2\left(x_{\lim}-\mu_1-2\mu_2\right)}{\sqrt{2\pi}\left(\sigma_1^2+4\sigma_2^2\right)^{3/2}}\exp\left\{-\frac{\left(x_{\lim}-\mu_1-2\mu_2\right)^2}{2\left(\sigma_1^2+4\sigma_2^2\right)}\right\}. \tag{94}$$

Eqs. (91) to (94) are exactly the Fréchet derivatives of failure probability in terms of the distribution parameters of input basic random variables, where the norm terms are omitted for simplicity but all are available in Appendix B.

(2) Subcase 2

For μ_1 and μ_2, there is:

$$\text{(a)}\ \frac{\partial p_{X_a}}{\partial \mu_1}=\frac{\partial p_{X_a}}{\partial \mu_2}=\frac{\left(x-\mu_1-\mu_2\right)}{\sqrt{2\pi}\left(\sigma_1^2+\sigma_2^2\right)^{3/2}}\exp\left\{-\frac{\left(x-\mu_1-\mu_2\right)^2}{2\left(\sigma_1^2+\sigma_2^2\right)}\right\},$$

$$\text{(b)}\ \frac{\partial p_{X_b}}{\partial \mu_1}=-\frac{\partial p_{X_b}}{\partial \mu_2}=\frac{\left(x-\mu_1+\mu_2\right)}{\sqrt{2\pi}\left(\sigma_1^2+\sigma_2^2\right)^{3/2}}\exp\left\{-\frac{\left(x-\mu_1+\mu_2\right)^2}{2\left(\sigma_1^2+\sigma_2^2\right)}\right\}. \tag{95}$$

For σ_1 and σ_2, there is:

$$\text{(a)}\ \frac{\partial p_{X_a}}{\partial \sigma_{1,2}}=\frac{\sigma_{1,2}}{\sqrt{2\pi}}\exp\left\{-\frac{\left(x-\mu_1-\mu_2\right)^2}{2\left(\sigma_1^2+\sigma_2^2\right)}\right\}\cdot\frac{\left(x-\mu_1-\mu_2\right)^2-\left(\sigma_1^2+\sigma_2^2\right)}{\left(\sigma_1^2+\sigma_2^2\right)^{5/2}},$$

$$\text{(b)}\ \frac{\partial p_{X_b}}{\partial \sigma_{1,2}}=\frac{\sigma_{1,2}}{\sqrt{2\pi}}\exp\left\{-\frac{\left(x-\mu_1+\mu_2\right)^2}{2\left(\sigma_1^2+\sigma_2^2\right)}\right\}\cdot\frac{\left(x-\mu_1+\mu_2\right)^2-\left(\sigma_1^2+\sigma_2^2\right)}{\left(\sigma_1^2+\sigma_2^2\right)^{5/2}}. \tag{96}$$

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