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RELATIVE ENTROPY BASED METHOD FOR PROBABILISTIC SENSITIVITY ANALYSIS IN ENGINEERING DESIGN

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ABSTRACT

In this paper, a new Probabilistic Sensitivity Analysis (PSA) approach based on the concept of relative entropy is proposed for design under uncertainty. The relative entropy based method evaluates the impact of a random variable on a design performance by measuring the divergence between two probability density functions of a performance response, obtained before and after the variance reduction of the random variable. The method can be applied both over the whole distribution of a performance response (called global response probabilistic sensitivity analysis-GRPSA) and in any interested partial range of a response distribution (called regional response probabilistic sensitivity analysis-RRPSA). Such flexibility of our approach facilitates its use under various scenarios of design under uncertainty, for instance in robust design, reliability-based design, and utility optimization. The proposed method is applicable to both the prior-design stage for variable screening when a design solution is yet identified and the post-design stage for uncertainty reduction after an optimal design has been determined. The saddlepoint approximation approach is introduced for improving the computational efficiency of applying our proposed method. The proposed method is illustrated and verified by numerical examples and industrial design cases.

Key words: probabilistic sensitivity analysis, robust design, reliability based design, relative entropy, saddle point approximation

ACRONYMS

PSA	Probabilistic Sensitivity Analysis
GRPSA	Global Response Probabilistic Sensitivity Analysis
RRPSA	Regional Response Probabilistic Sensitivity Analysis
MSI	Main (Effect) Sensitivity Index
TSI	Total (Effect) Sensitivity Index
RSM	Response Surface Methodology
KDE	Kernel Density Estimation
SAP	Saddlepoint Approximation

1 INTRODUCTION

In deterministic design, sensitivity analysis has been used to find the *rate of change* in a model output by varying input variables *one at a time* near a given central point, which involves partial derivatives and is often called *local sensitivity analysis*. When uncertainty is considered in design decision making, sensitivity analysis has different meanings [1]. It is usually performed on the probabilistic characteristics, such as moments, probability, probability density function, etc., of a model response with respect to the probabilistic characteristics of model inputs. In general, *the* ***probabilistic sensitivity analysis (PSA)*** *studies the impact of uncertainties in random inputs on uncertainties in model outputs*. Results from the PSA can be used to assist engineering design from various aspects, such as to help reduce the dimension of a design problem by identifying insignificant factors, including both controllable and uncontrollable factors; to obtain insights about the probabilistic behavior of a model response; and to investigate potential improvement on a probabilistic response by reducing the uncertainty in random inputs.

Among the existing PSA methods, a popular category is the so-called variance-based methods [2-6], also called global sensitivity analysis methods. Based on the decomposition of the total variance of a model response (design performance) into items contributed by various sources of model input variations, variance-based methods provide global measures of the variability of a response over the entire distribution range of an input variable. Obviously, the variance-based PSA methods can be applied directly to robust design problems [7-10] where a part of the design objective is to reduce a performance *variance*, assessed based on the *whole distribution* of a response. However, variance-based methods cannot evaluate the effect of an input variable over a *partial range* of a performance distribution, such as at the tail of a distribution related to the probability of failure. Furthermore, all variance-based methods share the same assumption that the second moment (variance) is sufficient to describe the uncertainty in a performance. Such assumption may not always be valid, especially in the case where the performance distribution is highly skewed and the design objective involves more than just the mean and variance of a performance, such as in utility optimization [11-12] and reliability-based design [9, 13-15].

Different from the variance-based methods for PSA, another category of the existing PSA methods investigates the contribution of a random variable to a probability (reliability) of a performance that deals with a partial range of a response distribution. Wu [16] proposed normalized sensitivity coefficients of a failure probability with respect to a random variable as expectations of partial derivatives of a performance probability density function, evaluated over the failure region. Mavris et al. [17], extended Wu's method to evaluate the sensitivity of any probabilistic characteristics of a performance. Another sensitivity measure related to reliability is the Most Probable Point (MPP) based sensitivity coefficients [18], defined as the gradient of a limit state function at the MPP in the standard normal space, normalized by the reliability index. Contrary to the variance-based method, no method under this category can be used to evaluate the effect of a random variable over the entire range of a performance distribution. Their applicability is restricted to a failure region of a random performance.

In this paper, we propose a relative entropy based PSA method that can be adapted to seanalys de variei9 named as global response probabilistic sensitivity analysis (GRPSA) and regional response probabilistic sensitivity analysis (RRPSA), respectively. We adopt the Kullback-Leibler (K-L) (relative) entropy [19] to capture the impact of an input variable by measuring the change of a performance distribution due to the uncertainty elimination in that input. The major advantage of the proposed method is that it can capture more complete probabilistic sensitivity information by studying the impact of an input variable on the probabilistic distribution rather than on low-order moments such as on performance variance with the variance-based methods. Moreover, the proposed method is flexible to be used in various scenarios for design under uncertainty, such as in robust design, reliability-based design, and utility optimization, as it can be used to study the variable impact on either the whole or a partial distribution range of a response.

We start our discussion by investigating the principles and limitations of variance-based methods in Section 2. Based on different scenarios and formulations for design under uncertainty, we put forward our classification of the PSA methods. The concept of K-L entropy is also reviewed. In Section 3, we describe the proposed K-L entropy based PSA approach and discuss its usages in various situations of design under uncertainty. Computational issues of the proposed method are investigated in Section 4. Using both numerical and engineering examples, in Section 5, we demonstrate the applicability of our proposed method and compare the results with those from other methods. Section 6 is the summary of this paper.

2 TECHNICAL BACKGROUND

2.1 Variance-Based Methods for PSA

We briefly review here the variance-based methods to introduce the concepts of main effect and total effect in the PSA. In the later examples, our proposed method will be compared against the variance-based PSA. With variance-based methods, the total variance of an output Y=$h(\mathbf{X})$ is decomposed into items contributed by various sources of input variations $\mathbf{X}=[X_1,X_2,\ldots,X_n]$ in an ANOVA-like way [6]:

$$V = \sum_i V_i + \sum_{i<j} V_{ij} + \ldots + V_{1,2,3,\ldots,n}\,, \tag{1}$$

where V is the total variance of the model output. The first order term V_i represents the partial variance in Y due to the individual (main) effect of a random variable X_i, while higher order terms indicate interaction effects between two or more random inputs. For example, V_{ij} is the partial variance in Y due to the interaction between X_i and X_j.

A sensitivity index of a random variable X_i is defined by the ratio of the partial variance contributed by the randomness of X_i over the total variance in Y. The *main sensitivity index* (MSI) of X_i is obtained by the ratio of the main-effect variance over the total variance as shown in Eq. (2).

$$S_i = V_i / V\,, \quad 1 \le i \le n. \tag{2}$$

A general sensitivity index is given in Eq. (3).

$$S_{i,\, i+1,\ldots,n} = V_{i,\, i+1,\ldots,n} / V\,, \quad 1 \le i \le n\,, \tag{3}$$

where $S_{i,i+1,\ldots,n}$ indicates the interaction effect among random variables X_i, …, X_n.

The *total sensitivity* index (TSI) is a useful measure of the importance of a random input that includes its main effect as well as all interaction effects involving the random input of interest. When there are a large number of interaction terms, to simplify the computation, the whole input variable set can be partitioned into a subset of interest and its complementary [3, 5-6], i.e., X_i and $\mathbf{X}_{\sim i}$, and the TSI is given by

$$S_{Ti} = 1 - S_{\sim i}, \tag{4}$$

where, $S_{\sim i} = S_{1,\ldots,i-1,i+1,\ldots,n}$ is the index for the combined effect of all random inputs except X_i. Existing variance-based PSA methods follow the above definitions, with certain computational variations [2-6, 20]. In particular, Sobol [2] proposed an ANOVA-like decomposition of a function with an increasing dimensionality for evaluations of sensitivity indices. To further ease the computational burden, based on Sobol's 'freezing unessential variables' concept [2], Homma and Saltelli [3], Sobol [5], and Jansen [21] proposed efficient Monte Carlo methods for TSI and MSI evaluations by re-sampling the random variable of interest and its complementary set, respectively. In Chen et al. [6], analytical formulations are derived via the commonly used metamodels such as polynomial functions and Kriging models. As pointed out in Section 1, all variance-based methods study the variable impact on the second moment (variance) of a performance. It is not sufficient to use them for describing the variable impact on a complete probabilistic distribution. In this paper, we compare the results from our proposed method to those from Sobol's method [5].

2.3 Global versus Regional Interests in Performance Distribution

In the context of design under uncertainty, the role that the PSA is expected to play varies under different probabilistic design scenarios (Fig. 1). For instance, in robust design, the PSA is to identify those random variables which contribute the most to the variation (e.g., variance) of a response. For reliability-based design, the interest is on the impacts of different uncertainty sources on the performance reliability.

Robust Design	**Reliability-Based Design**
Find $\mathbf{d}, \boldsymbol{\mu}_{\mathbf{X}}$	Find $\mathbf{d}, \boldsymbol{\mu}_{\mathbf{X}}$
min. $f = f\left(\mu_y, \sigma_y\right)$	min. $Y = h\left(\mathbf{d}, \mathbf{X}, \mathbf{P}\right)$
s.t. $\mu_{g_j} + k_j \sigma_{g_j} \geq 0,$	s.t. $P\left\{g_j\left(\mathbf{d}, \mathbf{X}, \mathbf{P}\right) \geq 0\right\} \geq R_j,$
$\mathbf{d}^{\mathrm{L}} \leq \mathbf{d} \leq \mathbf{d}^{\mathrm{U}},$	$\mathbf{d}^{\mathrm{L}} \leq \mathbf{d} \leq \mathbf{d}^{\mathrm{U}},$
$\boldsymbol{\mu}_{\mathbf{X}}^{\mathrm{L}} \leq \boldsymbol{\mu}_{\mathbf{X}} \leq \boldsymbol{\mu}_{\mathbf{X}}^{\mathrm{U}},$	$\boldsymbol{\mu}_{\mathbf{X}}^{\mathrm{L}} \leq \boldsymbol{\mu}_{\mathbf{X}} \leq \boldsymbol{\mu}_{\mathbf{X}}^{\mathrm{L}},$
$j = 1, 2, \ldots, m.$	$j = 1, 2, \ldots, m.$

Figure 1 Examples of probabilistic design formulations

In the examples of probabilistic design formulations shown in Fig. 1, **d** and **X** are vectors of deterministic and random design variables (i.e., control factors), respectively. **P** is a vector of random uncontrollable variables (i.e., noise factors). μ and σ represent the mean and the standard deviation of a performance quantity. In reliability-based design formulation, R_j is the desired probability of constraint satisfaction (also called reliability) corresponding to g_j. Even though our formulation shows that multiple reliability constraints can be set for design performances, in some cases, a single constraint that captures the system reliability or the primary failure mode can be used.

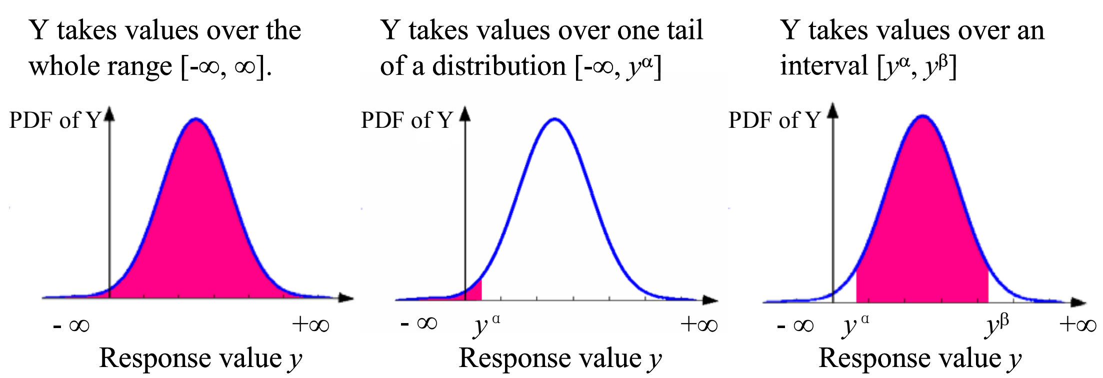

Figure 2 Whole vs. partial range of a response distribution

It is shown in Fig. 2 that the different design scenarios lead to the different ranges of interest in a performance distribution. In robust design, because the design objective is to reduce the response variation, the variable impact on the full range distribution of a response Y, i.e., [-∞,+∞] is of interest. On the other hand, in reliability-based design, the interest is on preventing the failure in a partial region, say [-∞, y^{α}] or [y^{α}, y^{β}], where y^{α} and y^{β} are response values at α and β quantiles, respectively. Accordingly, we define two types of PSA methods:

- **Global response probabilistic sensitivity analysis (GRPSA)** — PSA for the case that the interest is among the variable impact on the entire distribution of a response;
- **Regional response probabilistic sensitivity analysis (RRPSA)** — PSA for the case that the interest is among the variable impact on a partial range of a response distribution.

It should be noted that the word "global" in the term "global sensitivity analysis" from literature [3-6, 20] refers to the interest in studying the impact on a performance across a *global range of input variables*. On the other hand, the terms "global" and "regional" in our defined GRPSA and RRPSA have different meanings. They are used to differentiate the *interested range of a response*, covering either a whole or a partial range of a performance distribution based on the design scenario. Depending on whether the PSA is applied to the prior-design or the post-design stage, the distribution of response Y in Fig. 2 will be generated for a range of design variables or at a specific design setting, respectively. More details will be provided in Section 3.2. In the following discussion, we introduce the use of the relative entropy as a unified measure to deal with both GRSPA and RRSPA.

2.4 Kullback-Leibler Entropy

Emerged from the information theory [22], entropy is a measure for the information content in a random variable. Various information (uncertainty) measures in the literature can all be expressed or interpreted as divergence measures for the information (uncertainty) changes in a random quantity. The Kullback-Leibler (K-L) entropy [19] was derived in statistics as an average information measure in a random quantity Y for the discrimination between its two distributions, p_1 and p_0. It does not require the evaluation of the joint probability density function (PDF) or the conditional PDFs as needed for the mutual entropy [23]. The K-L entropy, also called the relative entropy, is defined as

$$D_{KL}(p_1 \mid p_0) = \int_{-\infty}^{\infty} p_1(y) \cdot log \frac{p_1(y)}{p_0(y)} dy = E_{p_1}\left[log \frac{p_1(y)}{p_0(y)} \right]. \quad (5)$$

The Kullback-Leibler entropy has the following mathematical properties [24]:

- It is nonnegative. It is zero if and only if p_1 and p_0 are exactly the same.
- It is not a true metric because the measure is not symmetric and it does not satisfy triangle inequality.

Two extreme cases of the integrand in Eq. (5) are defined as $p \cdot log\left(p/0\right) = \infty$ and $0 \cdot log\left(0/p\right) = 0$.

The Kullback-Leibler entropy is traditionally used to measure the divergence from the true distribution p_1 to its estimation p_0. The K-L entropy can be interpreted as the expectation of the log likelihood of a random quantity (Y) following a PDF of $p_1(y)$. Shannon entropy or the differential entropy could be viewed as a special case of Eq. (5), when p_0 is a uniform probability mass (density) function. In other words, Shannon entropy measures the divergence from a PDF to a uniform distribution. In this work, based on the concept of the K-L entropy, we propose a PSA method that measures the importance of a random variable by studying the divergence between two PDFs, corresponding to before and after uncertainty reduction of the random variable of interest, respectively. As more details will be disclosed later, the K-L entropy based measure offers the flexibility for both GRPSA and RRPSA by only changing the integration range of a response distribution.

3 RELATIVE ENTROPY BASED PSA METHOD

3.1 Relative Entropy Based Method for GRPSA and RRPSA

In this work, we propose an entropy-based PSA approach that suits both the GRPSA and the RRPSA. The key concept is to measure the importance of a random input variable based on the change of a response distribution, either in the whole or a partial range of the response, before and after the uncertainty elimination in that input variable.

Suppose a random response $Y = h(\mathbf{X})$ has a PDF of p_0, where $\mathbf{X}$ denotes a vector of random inputs, i.e., $\mathbf{X} = [X_1,X_2,\ldots,X_n]$. Based on the concept of "omission sensitivity" [25, page 101] (removing all uncertainty in a random input, i.e., replacing it with a deterministic value, say, its nominal value), if a random input X_i is fixed to its mean value, or it is perfectly known (i.e., X_i is a constant), the PDF of Y becomes p_1. Since all uncertainty in X_i is eliminated, including both the main effect of X_i and its interactions with other random inputs, the relative entropy provides the total effect of X_i on the variability of Y. As shown in Eq. (6), an K-L entropy based measure is used to assess the total sensitivity of a random variable X_i in GRPSA.

$$D_{KLx_i}(p_1 \mid p_0) = \int_{-\infty}^{\infty} p_1(y(x_1,...,\bar{x}_i,...,x_n)) \cdot log \frac{p_1(y(x_1,...,\bar{x}_i,...,x_n))}{p_0(y(x_1,...,x_i,...,x_n))} dy, \quad (6)$$

where $\bar{x}_i$ stands that X_i is fixed at a value, usually at its mean, μ_{x_i}. Over the entire distribution range of Y from -∞ to +∞, Eq. (6) measures how much the PDF of Y changes after eliminating the variability in X_i. $D_{KLx_i}(p_1 \mid p_0)$ is considered as the total sensitivity index of X_i. The larger the $D_{KLx_i}(p_1 \mid p_0)$, the more important X_i is.

Similarly, the combined effect of all random variables except X_i can be obtained by fixing the complementary set of X_i to get p_1, as shown in Eq. (7).

$$D_{KL\sim x_i}(p_1 \mid p_0) = \int_{-\infty}^{\infty} p_1(y(\bar{x}_1,...,x_i,...,\bar{x}_n)) \cdot log \frac{p_1(y(\bar{x}_1,...,x_i,...,\bar{x}_n))}{p_0(y(x_1,...,x_i,...,x_n))} dy. \quad (7)$$

$D_{KL\sim x_i}(p_1 \mid p_0)$ in Eq. (7) can be viewed as the reverse of the main effect of X_i. Since the K-L entropy is only a relative measure and its value (ranging from 0 to +∞) cannot be normalized, we define the main effect of X_i as,

Main Effect of $X_i = -D_{KL\sim x_i}(p_1 \mid p_0)$. (8)

The obtained main effect by Eq. (8) is negative, which ensures that the larger the value of a main effect, the more important X_i is.

One advantage of our proposed K-L entropy approach is that the proposed method can be extended fairly easily for the RRPSA by simply changing the integration range of y from [-∞, +∞] to the partial region of interest [y_L, y_U]. The total effect of X_i for the RRPSA is defined as

$$D_{KLx_i}(p_1 \mid p_0) = \int_{y_L}^{y_U} p_0(y(x_1,...,\bar{x}_i,...,x_n)) \cdot \left| log \frac{p_1(y(x_1,...,\bar{x}_i,...,x_n))}{p_0(y(x_1,...,x_i,...,x_n))} \right| dy, \quad (9)$$

where y_L and y_U stand for the lower and upper bounds of a partial range of Y. Similarly, the main effect of X_i for the RRPSA is defined as the negative of the combined effect of the complementary set $\mathbf{X}_{\sim i}$, i.e.,

Main Effect of X_i =

$$-D_{KL\sim x_i}\left(p_1 \mid p_0\right) = -\int_{y_L}^{y_U} p_0\left(y\left(\bar{x}_1,\ldots,x_i,\ldots,\bar{x}_n\right)\right)\cdot\left|log\frac{p_1\left(y\left(\bar{x}_1,\ldots,x_i,\ldots,\bar{x}_n\right)\right)}{p_0\left(y\left(x_1,\ldots,x_i,\ldots,x_n\right)\right)}\right|dy\,. \tag{10}$$

Different from Eqs. (6) and (8), Eqs. (9) and (10) measure the *absolute* divergence between two distributions over a region of interest. The absolute value is used for the RRPSA because in a partial region of Y, the log-likelihood can take both positive and negative values, shown illustratively as the shaded areas of A and B in Fig. 3. For the integral calculation, without taking the absolute values, the positive and negative log-likelihood values may cancel with each other. In that case, the relative entropy value could be very small, although there is actually large difference between p_0 and p_1, as the case shown in Fig. 3. Integration of the absolute values better reflects the actual difference between two distributions (p_0 and p_1) in a specified region. In addition, in Eqs. (9) and (10), p_0 is used as a weighting factor applied in front of the log-likelihood, instead of p_1. The reason is that in a partial region, such as the extreme tail of a distribution, compared to p_0, the value of p_1 may be very small or even approaching to zero because p_1 stands for the distribution of Y after eliminating the uncertainty of input variables. In such a case, small values of p_1 may diminish the actual divergence from p_1 to p_0. As illustratively shown in Fig. 4, the value of p_0 (distribution before uncertainty is eliminated) is larger at the tail and better suited to be used as the weighting factor.

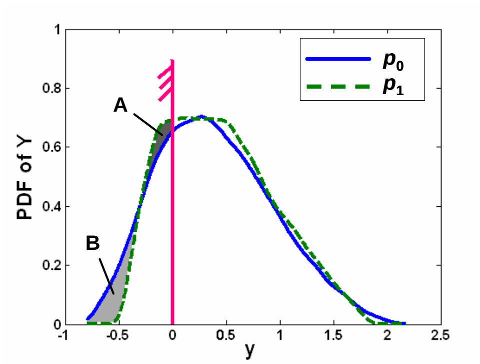

Figure 3 Absolute divergence in RRPSA

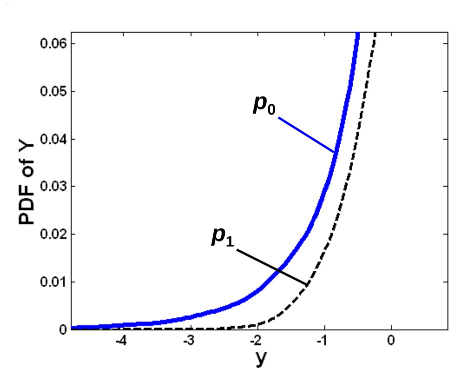

Figure 4 p_0 as weighting factor in RRPSA

For reliability-based design, the sensitivity of the probability of failure (P_f) or its complementary – the probability of success (i.e., reliability) (1-P_f) is of particular interest. For a given design setting, the system has two possible outcomes: safe or unsafe, with probability of 1-P_f and P_f respectively. If we view the system safety as a discrete event [26], a relative entropy based PSA for reliability can be calculated based on contributions of random variables to both the success and failure conditions, denoted as $D_{KLx_i}^{P_f}\left(\hat{P}_f \mid P_f\right)$, as follows:

$$D_{KLx_i}^{P_f}\left(\hat{P}_f \mid P_f\right) = \hat{P}_f \, log \frac{\hat{P}_f}{P_f} + \left(1-\hat{P}_f\right) log \frac{1-\hat{P}_f}{1-P_f}, \tag{11}$$

where P_f is the original probability of failure of a performance. $\hat{P}_f$ is the probability of failure when fixing X$_i$ at a specific value. Eq. (11) is the total sensitivity (effect) index of X$_i$ on the reliability. We view the formulation in Eq. (11) as an alternative approach to that in Eq. (9). Similarly, by fixing all random variables except X$_i$ in $\hat{P}_f$, $-D_{KL\sim x_i}^{P_f}\left(\hat{P}_f \mid P_f\right)$ provides an equivalent measure of the main effect of X$_i$.

3.2 GRPSA and RRPSA in Design under Uncertainty

In the context of design under uncertainty, the proposed PSA methods can be performed at different stages in a design process. At the prior-design stage, the PSA can provide valuable information for dimension reduction of a large scale probabilistic design problem by screening out those variables (controllable or uncontrollable) that have low impacts on the distribution of a response. For the purpose of screening, since a design solution is yet determined, no matter whether a design variable is deterministic or random, it will be treated as a random variable that follows a *uniform* distribution within the lower and upper bounds of its allowable design range in PSA. In fact, applying our proposed GRPSA in a prior-design stage is identical to the usage of the global sensitivity analysis in literature [3-6], except the metric for assessing the importance is different.

It should be noted that using our proposed PSA for variable screening is different from the traditional variable screening based on design of experiments (DOE), which are only capable of identifying the main effects and factor interactions separately. Group screening design is a fractional factorial design of resolution IV [27], which can get unbiased estimation of main effects. Sequential bifurcation design developed by Kleijnen [28] is under the assumption that higher-order effects are small and difficult to interpret. Existing screening designs based on DOEs cannot capture the total effect of a random variable as a combination of both the main effect and interaction effects in the way that the proposed PSA methods do. As DOEs only set factors at a finite number of levels with equal chance of occurrence, existing screening designs cannot take into account the probabilistic distributions of random variables (e.g., uncontrollable noise variables).

The concept of "omission sensitivity" [25, page 101] used in our approach has been used by other screening methods in literature, but with different scopes of applicability. For example, the backwards screening in [29] determines the total impact of an input based on the change in metamodel prediction errors due to omitting that factor out of the metamodel. The backwards screening method requires the construction of a metamodel, and the validity will depend on the accuracy of the metamodel. Besides, the method cannot capture the probabilistic descriptions of random noise variables. It treats the noise variables and design variables in the same way in screening. Our proposed entropy-based method does not have the restriction of using metamodels. It can also capture the randomness of a noise variable based on the given probabilistic description.

At the post-design stage once the optimal solution is determined, for a particular setting of design variables, our proposed PSA can be applied to prioritize available resources for further uncertainty reduction by studying the impact of remaining uncertainties in a response. Here, the randomness of input variables is associated with either the local variability of design variables or the randomness of noise variables. Although the post-design PSA cannot tell directly whether it is cost effective to spend extra resources, it does prioritize uncertainty reduction in model inputs from the aspect of improving a probabilistic performance behavior.

The choice of using either the GRPSA or the RRPSA in prior- or post- design stages will depend on whether the probabilistic design scenario is associated with a whole or a partial range of a performance distribution, as illustrated in Fig.2. For example, if robustness or expected utility is used as the design criterion for a particular probabilistic performance, the interest is on the whole distribution of a performance response, therefore the GRPSA formulations in Eqs. (6) and (8) will be used. On the other hand, if reliability is the major concern for a probabilistic performance, the interest is focused on the partial range of a performance distribution, in that case, the RRPSA formulations in Eqs. (9) and (10) or in Eq. (11) will be considered.

4 COMPUTATIONAL ISSUES

Existing PSA methods are mostly evaluated numerically due to the difficulty in obtaining analytical solutions, hence computational cost is a key factor to the applicability and affordability of PSA methods. Evaluations of the proposed K-L entropy measures (Eqs. (6-11)) involve the estimation of two PDFs (p_0 and p_1) of a given response: one before and one after variation reduction in inputs. For low-cost models, Monte Carlo simulations can be employed. However, for design using expensive simulation models, the PDF estimation via Monte Carlo simulation is impractical or even impossible.

In this paper, we discuss several alternatives but not exclusive approximation approaches to ease the computational burden. One approach is to use the metamodeling techniques [6], when affordable, to build surrogate models as approximations to computationally expensive models. Sampling techniques are then applied to the easy-to-compute metamodels. Based on samples, the PDF of a random response can be obtained by the kernel density estimation (KDE) at any value of y defined as

$$\hat{f}(y) = \frac{1}{n\delta}\sum_{i=1}^{n} K\left(\frac{y_i - y}{\delta}\right) \tag{12}$$

where K is a symmetric probability density function, called a kernel function; δ is the window width or called bandwidth; and n is the total number of samples [30].

Although the metamodeling approach can improve the efficiency of using the proposed PSA methods, its accuracy will largely depend on the accuracy of a metamodel, which may be expensive to build. Building an accurate metamodel is even more challenging for predicting probabilistic behaviors that may involve local variability. In those cases, methods that are efficient enough to directly work with the original simulation models without building metamodels could be more effective. One approach is to use reliability analysis based approaches such as the most probable point based uncertainty analysis (MPPUA) method [31]. The other alternative is to use the Saddlepoint Approximation [32]. These approaches are especially effective for assessing the tail performance of a distribution. The concept of the most probable point (*MPP*) can be utilized to generate the cumulative distribution function (*CDF*) of a system output by evaluating probability estimations at a serial of discretized limit states across a range of output performance. The PDF can then be derived as the derivative of the CDF [31]. As demonstrated by Du and Sudjianto [33], the saddlepoint approximation approach appears to be more accurate and more efficient for the distribution estimation compared to the MPP-based method. Du and Sujianto' work provides a detailed description of the method, which is not repeated here. In brief, the PDF of a random variable is obtained by the inverse Fourier transformation of its cumulant generating function (CGF), as shown in Eq. (13).

$$f(y) = \frac{1}{2\pi} \int_{-i\infty}^{i\infty} e^{[K(t) - ty]} dt , \tag{13}$$

where, $K(y)$ is the cumulant generating function of y. A saddlepoint, t_s, is the solution to the following equation:

$$K'(t) = y\,, \tag{14}$$

where, $K'(y)$ is the first order derivative of $K(y)$. After obtaining the saddlepoint, the PDF of a random variable can be obtained by Eq. (15).

$$\hat{f}(y) = \left(\frac{1}{2\pi K''(t_s)}\right)^{\frac{1}{2}} e^{\left[K(t_s) - t_s y\right]}. \tag{15}$$

CDF can be obtained at the same computational expense. In Du and Sudjianto's implementation [33], the CGF and its derivatives are obtained by the estimation of cumulants based on efficient sampling methods, such as optimized Latin Hypercube sampling and uniform design. In this paper, an example is used to verify the advantage of using saddlepoint approximation approach for the PSA. In real applications, the choice of a computational approach to the PSA is situation dependent. Since the purpose of PSA is to rank order the importance of input variables, less-than-accurate but approximate approaches can still provide valuable information.

5 VERIFICATIONS AND APPLICATIONS

There are five objectives in our verification study. First, we want to verify whether our proposed entropy based approach for the GRPSA will provide consistent results compared with those from the Sobol' method. We need to bear in mind that we do not expect the ranking of variables from two methods are exactly the same because our proposed entropy based method shows the impact on the whole PDF of a response which includes all the higher order moment statistics, while the Sobol' method provides the impact on the response variance (i.e., the second order moment) only. The second objective is to gain some insight into situations where the two methods will provide distinctively different rankings of variables. The third objective is to verify whether two alternative methods proposed for the RRPSA (Eqs. (9) and (11)) indeed provide the consistent ranking of variables in terms of their impact on improving the performance reliability. We verify the RRPSA results by obtaining the improvement in the reliability due to uncertainty reduction in each random variable. The first three objectives are demonstrated by three numerical examples respectively. The fourth objective is to illustrate that our proposed method can truly benefit the process of design under uncertainty in two engineering design examples. Finally, in the last example that involves the RRPSA, we show the advantage of the saddlepoint approximation for the PDF estimation with an improved efficiency, compared with the KDE approach. For all other examples, we use the KDE for PDF estimations based on samples obtained through simulations. The Gaussian kernel is shown as *K* in Eq. (12).

5.1 PSA for Numerical Models

(1) GRPSA for A Nonlinear Model

We first consider a simple quadratic model $y = x_1 x_2 + x_3^2$ with three independent input factors, each in the range of [-1,1]. When using the GRPSA method to identify the variable importance, all variables are assumed to follow uniform distributions over the range of [-1,1]. We intend to compare the impacts of three inputs on the entire range of *y*. Both Eq. (6) of our proposed K-L entropy based method and the Sobol' method [5] are applied to determine the main and the total effects of each factor. The global sensitivity information obtained by the two methods is listed in Table 1. Again, the larger the main/total effect, the more important an input is.

Table 1 Comparison of GRPSA results

		X_1	X_2	X_3
K-L entropy based PSA	$-D_{KL\sim x_i}(p_1 \mid p_0)$ - Main	-4.0783	-3.9953	-0.2917
	$D_{KLx_i}(p_1 \mid p_0)$ - Total	0.3783	0.3783	0.3523
Sobol' $V = 0.2$	Main effect variance, V_i	0.0004	0.0003	0.0891
	Main sensitivity index, S_i	0.0019	0.0017	0.4455
	Total effect variance, V_{T_i}	0.1112	0.1113	0.0891
	Total sensitivity index, S_{T_i}	0.5560	0.5565	0.4455

From Table 1, it is noted that both methods provide the same importance ranking of three variables. X_1 and X_2 have almost the same main and total effects. We know from the explicit mathematical structure that X_1 and X_2 are symmetric and independent with identical distributions. Therefore, they should have the same effect on the response Y. This is verified in Fig. 5, where the PDF of Y by fixing X_1 at its mean value coincides exactly with the PDF by fixing X_2 at the mean. Another observation is that the ranking based on the main effect is different from that based on the total effect. In particular, the main effect of X_3 is larger than that of X_1 or X_2, while its total effect is slightly smaller than that of X_1 or X_2. These observations are consistent with the structure of the equation $y = x_1 x_2 + x_3^2$, where the interaction only occurs between X_1 and X_2. X_3 does not have any interaction effect. Finally, it should be noted that the K-L entropy based method can only provide the relative but not the absolute importance of random variables. It can not answer absolutely how much uncertainty in Y comes from a random variable X_i. On the other hand, the indices from the Sobol' method are absolute and normalized measures, also called quantitative measures [20].

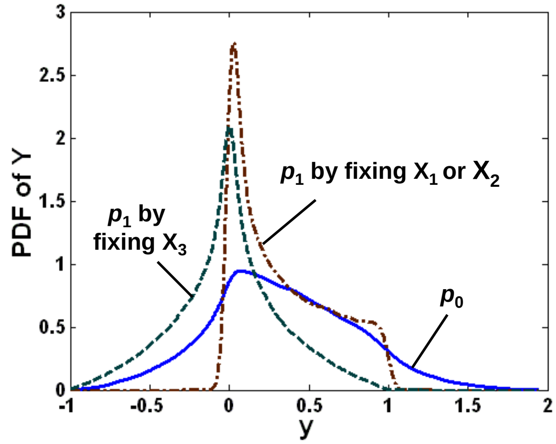

Figure 5 Comparison of impacts of uncertainty in inputs

(2) GRPSA on Highly-Skewed Distribution of Y

We consider here another simple nonlinear model $y = x_1/x_2$. X_1 and X_2 both follow χ^2 distributions with degrees of freedom as 10 and 13.978, respectively, shown in Fig. 6. From Fig. 7, the distribution of Y is positive-skewed with a heavy right tail (also known as fat tail or long tail), i.e., its right tail decaying slower than its left tail [34]. The impact of uncertainties in X_1 and X_2 on the distribution of the response is illustrated in Fig. 7. We compare the TSIs of two variables from our K-L entropy based method with indices from the Sobol' method in Table 2. Based on the relative entropy, X_1 is more important than X_2. However, the Sobol' method shows that X_1 and X_2 are equally important. The divergence of the PDF curves in Fig. 7 indicates that the effect of X_1 is higher, which means that the results from the relative entropy method are more trustworthy. This example shows that since the Sobol' method only evaluates the second moment of a distribution, it is no longer a good measure of dispersion for highly-skewed and heavily-tailed distributions.

Table 2 Comparison of the total sensitivity indices

	X_1	X_2

KL entropy based method	$D_{KLx_i}(p_1 \mid p_0)$, Total effect	0.1571	0.0791
Sobol' method	Total effect variance, V_{Ti}	0.1676	0.1677
	Total sensitivity index, S_{Ti}	0.5462	0.5465

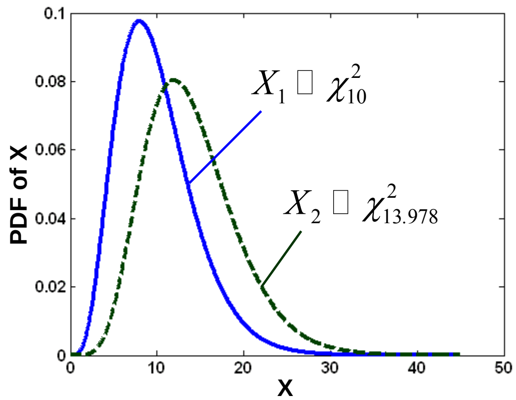

Figure 6 Distributions of random inputs

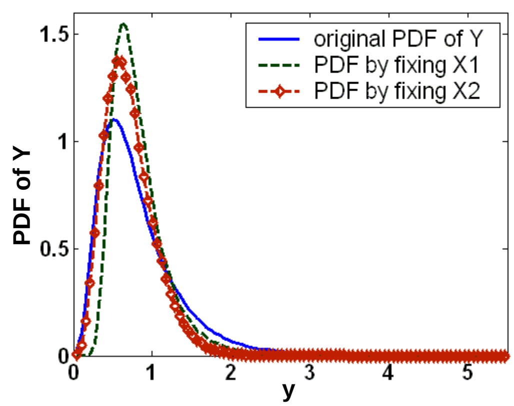

Figure 7 Comparison of impacts of inputs

(3) Verification of RRPSA Methods

For the same numerical model in the first example, we apply the RRPSA methods in Eqs. (9) and (11) for a reliability constraint $P\left\{Y = X_1X_2 + X_3^2 \geq 0\right\} \geq 90\%$. We assume that the three inputs are random, following the same normal distribution with mean and variance both as 1.0. For a desired reliability 90%, a critical failure mode is defined as $Y = X_1X_2 + X_3^2 \geq 0.068$. We apply both Eqs. (9) and (11) over the failure range of Y, [-∞, 0.068]. We expect that the reduction of uncertainty in the most critical variables would lead to the largest improvement on the reliability.

As observed from Fig. 8, in the failure range, fixing X_1 or X_2 will cause larger divergence in the distribution curve of Y than that by fixing X_3. Therefore, X_1 and X_2 are more important than X_3. This observation is confirmed by the sensitivity information obtained from two alternative formulations for RRPSA, Eqs. (9) and (11). Since the K-L entropy only provides a relative but not absolute measure of importance, the entropy values listed in Table 3 only indicate the importance ranking of different input variables, but do not illustrate how far they are apart. The obtained ranking is further verified by calculating the percentage of reliability improvement (last row in Table 3), before and after a random input is fixed at its mean. Although it is often not possible to eliminate completely the uncertainty in a random variable, the RRPSA results are good indications of where to put efforts to effectively improve the reliability.

Table 3 Effects of random variables in the failure range of the performance

	X_1	X_2	X_3
Eq. (9): $\int_{-\infty}^{0.068} p_0 \left\| \log \frac{p_1}{p_0} \right\| dy$	0.1320	0.1324	0.0478
Eq. (11): $D_{KLx_i}^{p_f}\left(\hat{p}_f \mid p_f\right)$	0.0128	0.0128	0.0074
Reliability improvement*	4.43%	4.43%	3.44%

*: The percentage increase of reliability by eliminating the uncertainty of a random variable

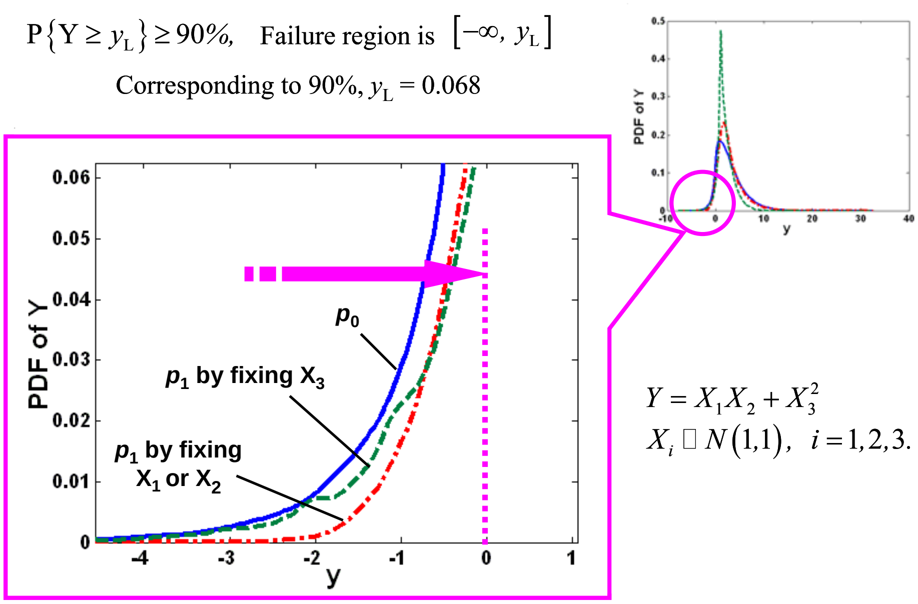

Figure 8 PDF of Y and the enlargement of the left tail (failure range)

5.2 Applications of PSA in Engineering Design Problems

(1) Robust Design for Engine Block and Head Joint Sealing Assembly

This example is used to illustrate the effectiveness of the proposed GRPSA method (Eq. (6)) to reduce the number of input variables in the prior-design stage. The dimensionality of the example problem is small compared to real engineering problems. The example problem is used here to demonstrate the principle and the potential benefits of using our proposed PSA methods.

Engine block and head joint sealing assembly is one of the most crucial structural designs in an automotive internal combustion engine. As shown in Table 4, there are six deterministic design variables (x_1-x_6), and two random noise factors (P_1 and P_2) following normal distributions. For reasons of confidentiality, the values of all variables and noise factors are normalized within [1, 3] and the exact model is not disclosed in this paper. The robust design objective is to minimize the *gap lift* of the assembly (x_1-x_6) as well as its sensitivity to manufacturing variations (P_1 and P_2). The design is very complex involving multiple components with complicated geometry. To reduce the computational cost, a Kriging model is created for the gap lift based on the data from computer experiments.

Table 4 Description of inputs to the assembly model

	Meaning	Lower limit	Upper limit	μ	σ
x_1	Gasket thickness	1	3	–	–
x_2	Number of contour zones	1	3	–	–
x_3	Zone-to-zone transition	1	3	–	–
x_4	Bead profile	1	3	–	–
x_5	Coining depth	1	3	–	–
x_6	Deck face surface flatness	1	3	–	–
P_1	Load/deflection variation	–	–	2	0.33
P_2	Head bolt force variation	–	–	2	0.33

In the prior-design stage, since the optimal solution is unknown, we assume that a design variable has equal chance in taking any value over its allowable range defined by the variable bounds. In GRPSA, we consider design variables (x_1-x_6) following uniform distributions within their allowable design ranges. The noise variables, P_1 and P_2, follow their pre-specified (normal) distributions. The sensitivity information obtained by our proposed GRPSA method and that by the Sobol' method is shown in Tables 5 and 6, respectively. The importance rankings of all input variables by two methods are compared in Fig. 9.

Table 5 Main and total effect indices by the KL-based method

	x_1	x_2	x_3	x_4	x_5	x_6	P_1	P_2
Main Effect $-D_{KL\sim x_i}$	-0.4589	-0.406	-6.523	-11.030	-3.300	-0.647	-9.589	-2.559
Total Effect D_{KLx_i}	0.3334	0.121	0.0	0.0	0.0	0.195	0.0	0.006

Table 6 Main and total effects by the Sobol' method

	x_1	x_2	x_3	x_4	x_5	x_6	P_1	P_2
Main Effect V_i	0.203	0.020	0.001	0.001	0.004	0.081	0.001	7.51e-5
Total Effect V_{Ti_i}	0.351	0.064	1.66e-6	2.03e-6	0.010	0.248	6.47e-7	0.007

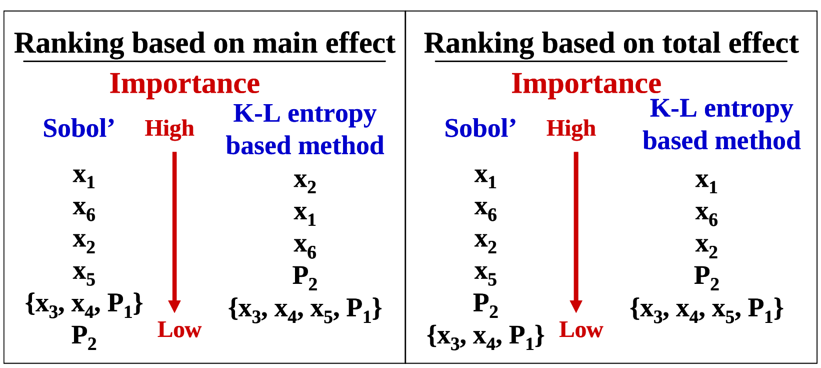

Figure 9 Importance rankings of engine design

Figure 9 indicates that the rankings of the total effects by two methods are generally consistent, except the relative importance of x_5 and P_2. Note that x_3, x_4, and P_1 are not important for both the main and the total effects. Therefore, we can fix x_3 and x_4 as constants ([2, 2]) and P_1 at its mean. The model for robust design is reduced to the one with four deterministic design variables (x_1, x_2, x_5, and x_6) and only one random noise parameter (P_2). The sensitivity information is verified by conducting robust design for both the original model and the reduced model with the formulation shown in Fig. 10.

Find μ_{X_i}, $i = 1, 2, ..., n.$
Minimize $f = w\frac{\mu_Y}{\mu_{Y\_\min}} + (1-w)\frac{\sigma_Y}{\sigma_{Y\_\min}}$
subject to $\vec{x}_L \le \vec{x} \le \vec{x}_U$.

Figure 10 Robust design formulation for the engine assembly design

In the above formulation, μ_{Y_min} and σ_{Y_min} are ideal solutions obtained by setting the weighting factor w at 1 and 0, respectively. For both the original model and the reduced model, w is set to be 0.5. Various starting points are tried to reach the global optimum. When using the original robust design model, the optimum solution is f^*= 1.0872 with $\mu_Y = 2.0580$ and $\sigma_Y = 1.8e-3$. The optimum point is $\mathbf{x}^*$=[1.7774, 1.0, 1.9557, 3.0, 1.0317, 2.9387]. For the reduced model by fixing x_3, x_4, and P_1, the optimum point is $\mathbf{x}^*$=[1.7522, 1.0726, 2.0, 2.0, 2.0043, 2.9104]. Plugging the optimal point back into the original (unreduced) model, we get the confirmed design performance as f^*= 1.0919 with μ_Y = 2.1110 and σ_Y = 7.1408e-4. Using the reduced model, the robust design reaches almost the same solution as that by using the original model. It verifies that x_3, x_4, and P_1 are truly unimportant. Even though the dimensionality of this example problem is small, the problem illustrates the potential benefits of using our proposed GRPSA method for reducing the complexity of a large-scale robust design problem with little sacrifice on the design quality.

(2) Reliability-Based Design for the Vehicle Crashworthiness of Side Impact

This example shows the application of the proposed entropy-based RRPSA methods, Eqs. (9) and (11), for PSA in the post-design stage of a reliability-based design for vehicle crashworthiness of side impact. The design problem has 11 random variables, among which nine are design variables and the other two are noise factors. The objective is to minimize the weight of the structure being considered. Detailed descriptions of the reliability-based design problem can be found in [15, 35]. The required reliability is 99.865% for all ten probabilistic constraints. At the optimum point, f^*=28.4397 kg, and three probabilistic constraints are active, whose limit state functions are shown in Fig. 11. For the post-design PSA, the goal is to identify a (set of) variable(s) whose variation has the most impact on the reliability. If possible, by controlling the uncertainty in those critical variables, the largest possible improvement on reliabilities can be expected. The total effects based on $D_{KLx_i}(p_1 \mid p_0)$ and $D_{KLx_i}^{p_f}(\hat{p}_f \mid p_f)$ are shown in Table 7.

$$g_2 = 1.0 - \frac{46.36 - 9.9X_2 - 12.9X_1X_8 + 0.1107X_3P_1}{32},$$

$$g_8 = 1.0 - \frac{4.72 - 0.5X_4 - 0.19X_2X_3 - 0.0122X_4P_1 + 0.009325X_6P_1 + 0.000191P_2^2}{4.01},$$

$$g_{10} = 1.0 - \frac{16.45 - 0.489X_3X_7 - 0.843X_5X_6 + 0.0432X_9P_1 - 0.0556X_9P_2 - 0.000786P_2^2}{15.69}.$$

Figure 11 Limit state functions of active constraints

Table 7 Total effects by the RRPSA methods on three active constraints

	g_2		g_8		g_{10}	
	$D_{KLx_i}(p_1 \mid p_0)$	$D_{KLx_i}^{p_f}(\hat{p}_f \mid p_f)$	$D_{KLx_i}(p_1 \mid p_0)$	$D_{KLx_i}^{p_f}(\hat{p}_f \mid p_f)$	$D_{KLx_i}(p_1 \mid p_0)$	$D_{KLx_i}^{p_f}(\hat{p}_f \mid p_f)$
X_1	3.0e-4	5.34e-5	—	—	—	—
X_2	9.0e-4	1.61e-4	4.0e-5	1.57e-5	—	—
X_3	2.0e-4	3.83e-6	9.0e-5	7.41e-5	2.27e-5	3.36e-7
X_4	—	—	6.0e-5	3.16e-5	—	—
X_5	—	—	—	—	1.74e-3	4.887e-4
X_6	—	—	1.1e-4	1.08e-4	2.65e-4	2.904e-5

X_7	—	—	—	—	4.92e-5	1.849e-6
X_8	1.0e-4	1.49e-7	—	—	—	—
X_9	—	—	—	—	6.89e-5	1.492e-7
P_1	0.5752	1.34e-3	9.44e-3	1.34e-3	2.02e-2	1.351e-3
P_2	—	—	6.55e-3	1.34e-3	1.79e-4	5.506e-6

The importance rankings based on total effects in Table 7 are shown in Fig. 12. The rankings of random variables for three active constraints are verified by the improvement of reliabilities through uncertainty reduction in random inputs (shown in Figs. 13-15).

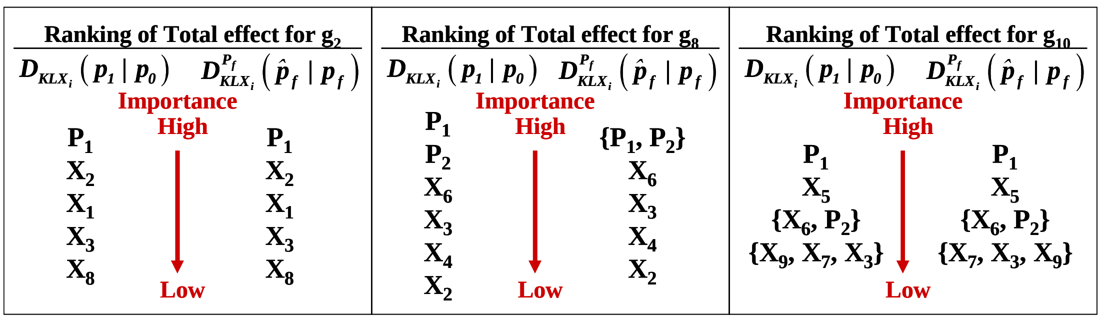

Figure 12 Importance rankings based on total effects

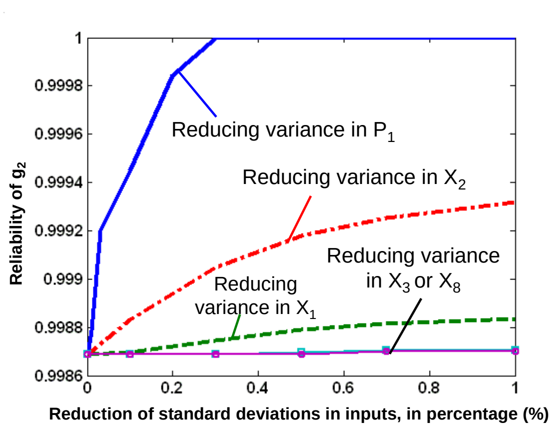

Figure 13 Reliability improvement by variation reduction in inputs – g_2

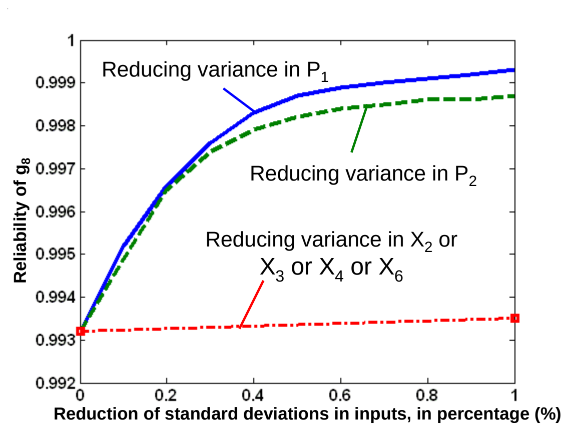

Figure 14 Reliability improvement by variation reduction in inputs – g_8

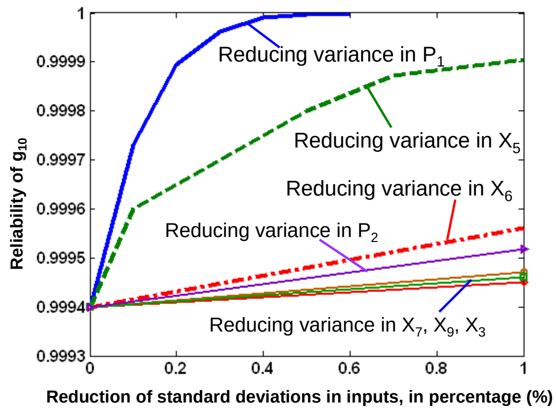

Figure 15 Reliability improvement by variation reduction in random inputs – g_{10}

Table 7 and Figure 12 show that P_1 is ranked as the most important variable for all three constraints. In Figs. 13 to 15, by reducing the same percentage of uncertainty, P_1 leads to the largest reliability increase than any other random variable. The inconsistent ranking of P_1 and P_2 from Eqs. (9) and (11) for g_8 is caused by the numerical error of using Eq. (11) for assessing the RRPSA at the extreme tail. It is noted in Table 7 that the values of $D_{KLx_i}^{p_f}\left(\hat{p}_f \mid p_f\right)$ are quite small. Considering the numerical errors introduced in the estimation of PDFs, $D_{KLx_i}^{p_f}\left(\hat{p}_f \mid p_f\right)$ may not be a good measure to discern the relative importance among random variables for a quite small p_f. The sensitivity information obtained is useful when the actual reliability of a failure mode does not meet the required level. For example, by reducing a partial variation in P_1, such as 30%, the reliability of g_2 and g_{10} would reach a level very close to 1. On the other hand, little improvement on the reliability is expected when even totally eliminating the uncertainties in insignificant random variables, such as X_3 and X_8 in g_2.

The total sensitivity indices in Table 7 are based on the kernel density estimation (KDE) in Eq. (12). To improve the efficiency of the PDF estimation, the saddlepoint approximation (SAP) approach [33] can be applied for the PSA, illustrated for g_2 and g_8. The total sensitivity indices are compared with those by the KDE approach in Table 8.

Table 8 Comparison of RRPSA results by KDE and SAP

	g_2				g_8			
	$D_{KLx_i}(p_1 \mid p_0)$		$D_{KLx_i}^{p_f}(\hat{p}_f \mid p_f)$		$D_{KLx_i}(p_1 \mid p_0)$		$D_{KLx_i}^{p_f}(\hat{p}_f \mid p_f)$	
	KDE	SAP	KDE	SAP	KDE	SAP	KDE	SAP
X_1	3.0e-4	5.3e-4	5.34e-5	7.44e-5	—	—	—	—
X_2	9.0e-4	1.13e-3	1.61e-4	2.59e-4	4.0e-5	6.2e-4	1.57e-5	2.95e-4
X_3	2.0e-4	4.8e-4	3.83e-6	6.35e-5	9.0e-5	6.0e-4	7.41e-5	2.73e-4
X_4	—	—	—	—	6.0e-5	5.8e-4	3.16e-5	2.57e-4

very close, almost overlap with each other. The example indicates that it may be reasonable to apply the saddle point approximation approach when the simulation time is in the magnitude of minutes rather than hours.

In this paper, we only compared our proposed approach with the Sobol' method for GRPSA. In our paper [36], a more comprehensive comparison is given, including more details on comparing our method with the Wu's sensitivity coefficients [16] and the MPP based sensitivity coefficients for RRPSA [18].

6 CONCLUSION

In this paper, we demonstrate that the probabilistic sensitivity analysis (PSA) is a useful tool in design under uncertainty that provides valuable information about the impact of variables on the probabilistic characteristics of a response. Based on whether the interest is on the whole range or the partial range of a performance distribution (e.g., in robust design or reliability based design), we classify the PSA into two categories: the global response probabilistic sensitivity analysis (GRPSA) and the regional response probabilistic sensitivity analysis (RRPSA). To capture more complete information on the impacts of random variables and to develop a PSA method applicable for both GRPSA and RRPSA, we propose in this article the Kullback-Leibler entropy based PSA method that can be easily adapted to evaluate the effects of random variables over either a whole or a partial distribution of a response.

Demonstrated by three numerical examples as well as two engineering design problems, we show that the proposed approach is effective and beneficial under various design scenarios and at different design stages. By comparing our proposed entropy based method with the Sobol' method for the GRPSA, we observe that our proposed method provides more complete information about the impact of a variable due to the incorporation of the PDF of a response, while the Sobol' method captures only the impact on the response variance (the second moment). In many cases, the rankings obtained from these two methods can be similar. However, for highly-skewed distributions, the rankings are most likely different. Our proposed entropy method provides a better measure of rankings in such cases.

Our study also shows that the two alternative formulations for the RRPSA are both valid. The RRPSA formulation that treats reliability satisfaction as a discrete event might be more sensitive to numerical errors when dealing with very small failure probabilities. To alleviate this problem, parametric distribution such as pareto distribution [37] may be employed to separately fit the tail distribution. This approach is subject to further research. Our examples demonstrate the potential of the RRPSA as an effective tool to quantify the variable impact of uncertainty reduction for reliability improvement.

One limitation of the relative entropy based PSA method is that they can only provide a ranking of relative importance. The sensitivity values do not have absolute physical meanings. While the proposed relative entropy based PSA method offers more information than the variance-based methods by examining the complete response distributions, its computational demand is higher. Our study shows that when a metamodel is not available, compared to the traditional sampling approach, the saddlepoint approximation approach is a viable approach to improving the computational efficiency of the proposed method while providing consistent rankings of the importance of variables in the PSA. In practical applications, the choice of an appropriate computational technique is situation dependent. Designers will face the tradeoff between getting more complete information of the probabilistic performance versus the additional computational effort. Our proposed PSA methods offer alternative approaches that the designers can choose from.

ACKNOWLEDGMENTS

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