Reliability sensitivity analysis with subset simulation: application to a carbon dioxide storage problem

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Abstract. Reliability sensitivity analysis (RSA) is a sensitivity analysis to measure the effect of modelling parameters on the predicted reliability of a system. It can be used for reliability-based design, safety management, etc. The output-classification-based version of RSA compares the failure-conditional probability density function (PDF) of model parameters with their unconditional PDF to measure sensitivity. The main challenge is to estimate failure-conditional PDFs. Usually, these PDFs can be estimated through the failure samples obtained by Monte Carlo simulation. However, practical systems usually have a small failure probability. For such cases, the brute-force Monte Carlo simulation requires a larger number of samples to obtain enough failure samples. Therefore, the computational cost is very high. In this paper, we propose to use subset simulation to estimate the output-classification-based reliability sensitivity index. Subset simulation introduces a series of intermediate failure events which are easier to sample from, and then iteratively samples in each constrained failure region until the target failure event is reached. Compared to brute-force Monte Carlo simulation, subset simulation samples in a direction towards the target failure domain. Therefore, the failure samples can be obtained more efficiently. We apply subset simulation to perform RSA for a carbon dioxide storage benchmark problem. We show that subset simulation can estimate the output-classification-based reliability sensitivity index more efficiently compared to brute-force Monte Carlo simulation.

1. Introduction

In practice, uncertainty often exists in computational models of engineering systems, and it will lead to uncertain performance of models [1–3]. Then, the model may not provide a perfect prediction. To evaluate the degree of confidence of model predictions and perform risk assessment, uncertainty analysis has been widely used in practice [4, 5]. To better control and reduce the uncertainty of model output, one usually wants to know “how uncertainty in the output of a model (numerical or otherwise) can be apportioned to different sources of uncertainty in the model input” [6]. Then, more resources can be allocated to the more importance parameters so as to reduce the uncertainty of output most effectively [7]. Sensitivity analysis can be used to answer this question. Generally, sensitivity analysis can be divided into local sensitivity analysis (LSA) and global sensitivity analysis (GSA). LSA is usually based on partial derivatives and measures the effect of one parameter on the output when other parameters are fixed at nominal values [8]. Thus, LSA can only provide useful information around the nominal point where the derivative is computed. On the other hand, GSA can measure the effect of parameters on the output on average over their entire distribution ranges while all other parameters are varying as well [8–
10], and identify what are the most critical and essential contributors to output uncertainty and risk [11]. During the last several decades, a wide range of GSA methods has been proposed. For instance, the screening method [12–14] was proposed for the cases where there are a lot of input variables and few model assumptions. Variance-based methods [15, 16] were proposed to quantitatively measure the variance contribution of input parameters to the model output. Later, the moment-independent method [17–19] was proposed to measure the effect of input variables on the whole distribution of model output.

In reliability analysis, what one cares most is whether a system fails or not [20]. Then, model output can be considered as a binary variable. The GSA methods mentioned above focus mainly on real-valued continuous model output and could not be used in reliability analysis directly [21]. To perform GSA in reliability analysis, an output-classification-based RSA method was recently proposed [22]. The corresponding reliability sensitivity index in this method is defined as the difference between failure-conditional PDFs of modelling parameters and their unconditional PDFs. It can also reflect the average effect of input parameters on system’s failure probability.

In order to estimate this sensitivity index, one needs to estimate the failure-conditional PDFs of input parameters. The direct approach is performing a brute-force Monte Carlo simulation and using the failure samples to estimate the failure-conditional PDFs. However, for problems with small failure probabilities, it requires a large number of samples to obtain enough failure samples, and the computational cost will be very high. Subset simulation is an advanced method for reliability analysis [23]. Through introducing a series of intermediate failure events which approach the target failure event gradually, subset simulation iteratively samples in each constrained failure region until the target failure event is reached. Since subset simulation samples in a direction towards the target failure domain, it can get the failure samples more efficiently. Therefore, subset simulation is used in this paper to estimate the output-classification-based reliability sensitivity index.

The rest of the paper is organized as follows. Section 2 gives a brief review of the output-classification-based RSA method and shows how to estimate the sensitivity index with subset simulation. In Section 3, RSA through subset simulation is applied to a carbon dioxide storage benchmark problem. Section 4 gives the conclusion.

2. Methodology

Let \( X = [X_1, X_2, ..., X_d] \) be the \( d \)-dimensional vector of random input parameters for the model \( Y = g(X) \). \( Y \) represents the output variable. The joint PDF of \( X \) is denoted as \( f_X(x) \). For convenience, we assume all the input parameters are independent to each other. Then the joint PDF of \( X \) can be represented as \( f_X(x) = \prod_{i=1}^{d} f_{X_i}(x_i) \), where \( f_{X_i}(x_i) \) is the marginal PDF of \( X_i \). The failure probability can be defined as the probability when output \( Y = g(X) \) is greater than a threshold \( u \), i.e. \( P(F) = P(g(X) > u) \). The corresponding failure domain can be represented as \( F = \{ X: g(X) > u \} \).

2.1. Review of the output-classification-based reliability sensitivity analysis method

To measure the effect of input parameter \( X_i \) on the failure of the system, the difference between the failure-conditional PDF \( f_{X_i}(x_i | F) \) and the unconditional PDF \( f_{X_i}(x_i) \) is used. The sensitivity index proposed in [22] is defined as

\[
S_i = \frac{1}{2} \int_{x_i} \left| f_{X_i}(x_i) - f_{X_i}(x_i | F) \right| \, dx_i
\] (1)

The sensitivity index \( S_i \) uses the area closed by \( f_{X_i}(x_i) \) and \( f_{X_i}(x_i | F) \) to measure their difference and hence the effect of input parameter \( X_i \) on system failure. The constant \( 1/2 \) is used to make sure \( S_i \in [0, 1] \). If there is significant difference between \( f_{X_i}(x_i) \) and \( f_{X_i}(x_i | F) \), input parameter \( X_i \) has significant effect on system failure. The idea behind this sensitivity index \( S_i \) can date back to [24], which performs a generalized sensitivity analysis by classifying the model output based on manifesting a certain behavior or not. More properties and explanation of this sensitivity index can be found in [22].
Based on the definition in equation (1), in order to estimate $S_i$, one needs to estimate $f_{X_i}(x_i | F)$ at first. A direct approach is performing a brute-force Monte Carlo simulation and then analyzing the failure samples to estimate $f_{X_i}(x_i | F)$. When the failure probability is small, this approach requires a large number of samples to obtain enough failure samples and the computational cost is very high. More details about this approach also can be found in [22]. Subset simulation is an advanced Monte Carlo simulation method and it can obtain enough failure samples with a lower computational cost. In the next subsection we will introduce subset simulation and use it to estimate the failure-conditional PDF $f_{X_i}(x_i | F)$.

### 2.2. Estimating the sensitivity index with subset simulation

Subset simulation was initially proposed by Au and Beck [23] to estimate small failure probabilities. The idea behind subset simulation is to introduce a series of intermediate failure events and convert a small failure probability into a product of a series of larger conditional probabilities. Since the larger probabilities are easier to be estimated, the original small failure probability can be estimated efficiently.

Let $u_0 = -\infty < u_1 < u_2 < \cdots < u_m = u$ be a sequence of increasing failure thresholds, then one can obtain a corresponding sequence of nested failure domains $F_0 \supseteq F_1 \supseteq F_2 \supseteq \cdots \supseteq F_m = F$, where $F_t = \{ \mathbf{x}: g(\mathbf{x}) > u_t \}, t = 0, 1, ..., m$. According to the nested properties of failure domains $F_t$, it is straightforward that $F_t = \bigcap_{i=0}^{t} F_i$. Then, using the nested properties of failure domains and the definition of conditional probability, one can obtain

$$P(F_{t+1}) = P(F_{t+1} \cap F_t) = P(F_t) P(F_{t+1} | F_t), \quad \forall t = 0, 1, ..., m-1. \quad (2)$$

Noting that $P(F_0) = 1$, the failure probability can be rewritten as

$$P(F_t) = P(F_m) = \prod_{i=0}^{m-1} P(F_{i+1} | F_i) \quad (3)$$

Therefore, subset simulation covert the problem of estimating a small failure probability into the problem of estimating a series of higher conditional probabilities. It requires choosing $m$ and $F_t$, $t = 1, 2, ..., m-1$ appropriately so that the conditional probabilities are large enough to be estimated efficiently through Monte Carlo simulation.

At first, subset simulation generates $n$ samples $\{\mathbf{x}_0^{(k)} \}, k = 1, 2, ..., n$ from the prior PDF $f_{\mathbf{x}}(\mathbf{x})$. The subscript in $\mathbf{x}_0^{(k)}$ denotes the iteration number and superscript denotes the sample number. These samples are propagated through the performance function to get the corresponding output samples $y_0^{(k)} \in \mathbb{R}$, $k = 1, 2, ..., n$. Then, the first threshold $u_1$ is approximated through making the conditional probability $P(F_1 | F_0)$ equal to a given value $p_0 \in [0, 1]$. These samples in the first failure domain $F_1$ are a representation of $F_1$, and $u_1$ can be defined as the largest output sample without in $F_1$. For the next iteration, one uses those samples in $F_1$ as seeds to simulate more samples from the new prior PDF $f_{\mathbf{y}}(\mathbf{y}|F_1)$ (the new samples should also satisfy $y > u_1$). To get more samples, a Markov chain Monte Carlo method is used in [23] to obtain $(1 - p_0) \times n$ samples that satisfy $y > u_1$. Thus, the total number of samples satisfying $y > u_1$ is equal to $n$ again. The second threshold is approximated using the same conditional probability $p_0$ and the iteration continues until the real threshold $u$ is reached.

Compared to brute-force Monte Carlo simulation, subset simulation samples in the direction towards the failure domain. Therefore, it can get failure samples more efficiently. The failure samples in the last step fall into the real failure domain $F$ and they can be used to estimate the failure-conditional PDF $f_{X_i}(x_i | F)$. The main task in subset simulation is to get new samples in each iteration. Au and Beck [23] proposed a modified Metropolis algorithm for Markov chain Monte Carlo simulation to generate these samples and it is shown as follows.

For every $j = 1, 2, ..., d$, let $q_j(\xi | x)$ be a one-dimensional proposal PDF for $\xi$ centred at $x$ with symmetry property $q_j(\xi | x) = q_j(x | \xi)$. This proposal PDF can be, e.g., the uniform or normal distribution. Then, generate a sequence of samples $\{\mathbf{x}_1^{(1)}, \mathbf{x}_2^{(1)}, \ldots \}$ from an initial sample $\mathbf{x}_1^{(1)}$. The next
sample $\mathbf{x}^{(k+1)}$ is generated based on the current sample $\mathbf{x}^{(k)} = \{x_1^{(k)}, x_2^{(k)}, \ldots, x_d^{(k)}\} (k = 1, 2, \ldots)$ as follows:

1. Generate a candidate state $\tilde{\mathbf{x}} = [\tilde{x}_1, \tilde{x}_2, \ldots, \tilde{x}_d]$: For each component $j = 1, 2, \ldots, d$, simulate $\xi_j$ from $q_j(\xi_j | x_j^{(k)})$. Compute the ratio $r_j = f_{\mathbf{x}}(\xi_j) / f_{\tilde{\mathbf{x}}}(\xi_j^{(k)})$. Set $\tilde{x}_j = \xi_j$ with probability $\min\{1, r_j\}$ and set $\tilde{x}_j = x_j^{(k)}$ with the remaining probability $1 - \min\{1, r_j\}$.

2. Accept or reject $\tilde{\mathbf{x}}$: Check the location of $\tilde{\mathbf{x}}$. If $\tilde{\mathbf{x}} \in F$, accept it as the next sample, i.e. $\mathbf{x}^{(k+1)} = \tilde{\mathbf{x}}$; otherwise reject it and take the current sample as the next sample, i.e. $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)}$.

After getting the failure samples in the last iteration, we can estimate the failure-conditional PDF $f_{\mathbf{x}}(x_i | F)$ based on these failure samples. It can be easily estimated through a histogram of the failure samples. Then the integration in equation (1) can be estimated with numerical quadrature rules such as the composite trapezoidal rule. Given a set of discrete values of $x_i$: $x_i^{(1)} < \cdots < x_i^{(l)} < \cdots < x_i^{(p)}$, the sensitivity index can be estimated as

$$\hat{S}_i = \frac{1}{2} \sum_{i=1}^{p-1} \left( x_i^{(l(i))} - x_i^{(l(i-1))} \right) \frac{Q_{l(i)} + Q_{l(i-1)}}{2} dx_i,$$

where $Q_I = \left| f_{\mathbf{x}}(x_i^{(l)}) - f_{\mathbf{x}}(x_i^{(l)} | F) \right|$.  

3. Example

In this section, we consider a multiphase flow problem in porous media, where CO$_2$ is injected into a deep aquifer and spreads within the aquifer. This technique is used to reduce anthropogenic CO$_2$ emissions into the atmosphere as an interior solution to mitigate climate change [25]. CO$_2$ injection leads to a pressure buildup and a CO$_2$ plume evolves. If the rock formation that should contain the CO$_2$ cracks due to excessive pressure or if the CO$_2$ can escape through a pre-existing leak, CO$_2$ can leak back to the atmosphere and the system fails. In the current paper, we consider a benchmark problem defined in [26] and developed in a benchmark study [27]. We assume that fluid properties such as density and viscosity of CO$_2$ are constant, all processes are isothermal, CO$_2$ and brine (i.e. the mineral-rich groundwater at that depth) are two separate and immiscible phases, mutual dissolution is neglected, the formation is isotropic rigid and chemically inert, and capillary pressure is negligible. This model requires solving some partial differential equations. The details of the models can be found in [27].

The quantity of interest in this example is the CO$_2$ saturation in the deep aquifer at a critical distance, which is a function of space and time. Particularly, we will consider the CO$_2$ saturation after 100 days at the distance of 100 meters away from the injection well. Here, an event with an exceedance probability of about 1% is considered as the failure event, and the corresponding critical value for saturation at that distance is set to 0.75.

In this study, three kinds of uncertainties are considered: uncertainty of boundary conditions, uncertainty of parameters in constitutive relations (within the multiphase flow equation) and uncertainty of material properties. For each kind of uncertainty, one random variable is identified. The uncertainty of boundary conditions is represented through uncertainty of the CO$_2$ injection rate $\theta_1$. The uncertainty of parameters in constitutive relations is introduced via uncertainty in the relative permeability degree $\theta_2$. The uncertainty of material properties is represented via uncertainty of aquifer porosity $\theta_3$. These three random variables all follow the beta distribution, i.e. $\theta_1 \sim B(4,2)$, $\theta_2 \sim B(1.25,1.25)$ and $\theta_3 \sim B(2.4,9)$ according to their physical behaviours. Details about the definition of these random variables can be found in [27].

We perform subset simulation by setting the conditional probability as $p_0 = 0.2$ and the sample size in each level as $n = 500$. Finally, subset simulation generates 4 intermediate failure events. figure 1 shows the samples obtained in each level. We can see that the samples are gradually approaching the
failure domain (under the shaded surface). In the last level, we get the samples falling into the failure domain, which can be used to estimate the failure-conditional PDF \( f_{X_i}(x_i | F) \). To estimate the sensitivity indices with the composite trapezoidal rule (equation (4)), the number of discrete values of random parameters is set as \( p = 30 \). Figure 2 shows the estimates of sensitivity indices based on brute-force Monte Carlo simulation and subset simulation. It shows that the result based on subset simulation is close to that based on Monte Carlo simulation. However, Monte Carlo simulation uses 10000 model runs while subset simulation only uses 1700 model runs. The coefficients of variation of the results obtained by Monte Carlo simulation and subset simulation are also estimated through bootstrapping based on their failure samples with 50 repetitions, and they are shown in table 1. We can see that the results obtained by subset have lower coefficients of variation. This shows that subset simulation not only has a lower computational cost but also has a high stability compared to Monte Carlo simulation. We can also see that parameter \( \theta_3 \), i.e. uncertainty of material properties, has the largest effect on the failure of system. The effect of \( \theta_1 \) and \( \theta_2 \) is almost neglectable. Therefore, more attention should be paid on \( \theta_3 \).

![Figure 1. Samples in different levels.](image1)

![Figure 2. Estimates of sensitivity indices.](image2)

**Table 1.** Coefficients of variation of the estimates.

|         | \( S_{\theta_1} \) | \( S_{\theta_2} \) | \( S_{\theta_3} \) |
|---------|---------------------|---------------------|---------------------|
| Monte Carlo | 0.1309              | 0.0921              | 0.0083              |
| Subset   | 0.1183              | 0.0895              | 0.0001              |

### 4. Conclusion

Reliability sensitivity analysis is useful to provide information of how random input parameters affect the failure of a system. The output-classification-based reliability sensitivity index can provide a quantitative measure of this effect and is useful for allocation of limited resources, simplification of reliability analysis, etc. In this paper, subset simulation is adopted to estimate the reliability sensitivity index. Then, it is applied to a carbon dioxide storage benchmark problem to measure the effect of random input parameters on the failure of the system. Through introducing a series of intermediate failure events, subset simulation samples in a direction towards the target failure domain. Therefore, subset simulation can get the failure samples more efficiently compared to brute force Monte Carlo simulation. Then the reliability sensitivity index can be estimated with a higher efficiency.
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