Application of MCMC samplers with replica exchange and Russian Roulette in estimating structural reliability via importance sampling

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ABSTRACT: Sharp changes in performance function values near regions of failure, the presence of multiple failure regions of importance, and disconnected failure regions separated can pose substantial difficulties in accurately estimating structural reliability. This study proposes an importance sampling (IS) scheme that utilizes the replica exchange strategy in Markov chain Monte Carlo sampling. This strategy improves the chances of detecting all significant failure regions even when the difficulties mentioned above are present. This study also uses the Russian Roulette technique to reduce sampling variance further. The methodology is applied to performance functions that exhibit the mentioned difficulties and is shown to identify all important failure regions and produce accurate estimates of failure probability. The results are compared with existing state-of-the-art IS schemes which are not guaranteed to provide acceptable estimates of failure probability when such complications arise in performance functions.

1. INTRODUCTION

The problem of computational reliability modeling involves the estimation of the probability of failure of a structure written as the multifold integral, $P_F = \int_{\mathbb{R}^n} I\{g(\mathbf{x}) \le 0\} p_X(\mathbf{x}) d\mathbf{x}$

, where I[.] is the indicator function, $p_X(x)$ is the joint pdf of the $n \times 1$ vector of random variables associated with the structure (X), and g(.) is the performance function. The random vector X is often transformed through Rosenblatt or Nataf's transformation into the standard normal space, and the reliability integral is rewritten as $P_F = \int_{\mathbb{R}^n} I\{G(u) \le 0\} p_U(u) du$,

where G(.) is the transformed performance function and $p_U(\mathbf{u})$ is the *n*-dimensional standard normal pdf. The present study focuses on the estimation of P_F using the importance sampling (IS) technique, wherein P_F is expressed

as,
$$P_F = \int_{\mathbb{R}^n} \frac{\mathrm{I}\{G(\boldsymbol{u}) \le 0\} p_U(\boldsymbol{u})}{q(\boldsymbol{u})} q(\boldsymbol{u}) d\boldsymbol{u}$$
, where

 $q(\mathbf{u})$ the importance sampling pdf (ISpdf). The Monte Carlo estimator of this integral is, $\hat{P}_{F}^{IS} = \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} \frac{I\{G(\mathbf{u}_{i}) \leq 0\} p_{U}(\mathbf{u}_{i})}{q(\mathbf{u}_{i})}$, where

 $u_i, i = 1, 2, ..., N_{IS}$ are iid samples from q(u). Although numerous methods to choose suitable ISpdfs have been developed in the structural reliability literature (Au and Beck 1999; Cheng et al. 2023; Dubourg et al. 2013; Kurtz and Song 2013; Papaioannou et al. 2016, 2019), accurate estimation of reliability still remains a challenge when the performance function exhibits one or more of the following features: (a) sharp changes in performance function values, (b) existence of disconnected regions of failure, (c) presence of multiple failure regions that contribute to the failure probability. If any reliability estimation algorithm fails to take these features into account, it leads to an omission of one or more important

failure regions, which, in turn, results in an underestimation of failure probability. Thus, the first objective of this study is to develop an algorithm that chooses an ISpdf capable of handling the difficulties mentioned above in performance functions. The proposed procedure for selecting the ISpdf closely follows the algorithm proposed by Au and Beck (1999), wherein a Markov Chain Monte Carlo (MCMC) sampler is initiated in the failure region with the target pdf $p_{U}(\boldsymbol{u}|\mathbf{F})$. The ISpdf is then selected by using the kernel density estimation method on the obtained samples. In this procedure, the difficulties mentioned above manifest as a difficulty in drawing samples from a multimodal pdf using MCMC samplers. This study introduces a replica exchange-based MCMC algorithm that enhances the capacity of the sampler to generate samples from possibly multimodal pdfs and hence deals with the difficulties as mentioned earlier more effectively. The second objective of this study is to use the Russian Roulette (RR) technique to probabilistically kill/disregard the summands in the estimator that contribute insignificantly to the estimator, thus avoiding the need to call the performance function for those samples. The preserved computational effort is used towards generating samples that contribute more substantially to the estimator. This strategy serves to further reduce the sampling variance. Although RR has previously been used for computation of time-variant reliability, it seems to have remained unexplored in the context of timeinvariant reliability estimation. The proposed method is applied to several numerical examples with performance functions containing the difficulties mentioned above to demonstrate the method's ability to effectively deal with them. It is also demonstrated that these difficulties arise naturally in reliability estimation of vibrating structures and structures that are prone to loss of stability. Results obtained from the method are compared with current state-of-the-art IS algorithms.

2. ANALYSIS

2.1. MCMC using replica exchange and formulation of ISpdf

Replica exchange-based MCMC sampling (Geyer 1991) aims to alleviate the difficulty of drawing samples from a multidimensional and multimodal pdf. This sampler has been explored in the context of reliability estimation and details of its implementation can be found in (Sharma and Manohar 2023). Firstly, a separate "explorer pdf" is defined. Two chains are run in parallel: one that draws samples from the target pdf and another that draws samples from the explorer pdf. Each chain is propagated using any of the available MCMC samplers. After propagation of the chain at each time step (called "forward step"), an exchange of the states is attempted between these two chains (called "exchange step"). This mechanism of exchanging states assists the chain that samples from the target pdf to be transported to regions of the state space that it would not have been able to reach unassisted. If such regions contain important modes, then the chain must visit these regions of the state space. Therefore, the replica exchange strategy allows the sampler to draw samples more effectively from multimodal pdfs. Clearly, this algorithm's success depends on the explorer pdf's choice. The explorer pdf must adequately contain all regions of interest from which we wish to draw samples, and the chain should freely be able to traverse these regions.

In this study, the explorer pdf is chosen as follows. Firstly, M samples are simulated from $p_U(u; \mu = 0, \Sigma = \sigma^2 \mathbf{I})$ (here we take $\sigma = 3$), say $u^i, i = 1, 2, ..., M$. The performance function values of these samples are computed, and the samples that lie in the failure region $F = \{ u \in \mathbb{R}^n : G(u) \le 0 \}$ are selected. Let the number of such samples be \tilde{M} . Then, the failure region F is repopulated with additional samples using MCMC sampling to retain the total of samples in F as M. These samples are now renamed as $u^i, i = 1, 2, ..., M$. Then, the orthants (a generalization of quadrants for higher

dimensions) in which these M samples lie are recorded by taking the component-wise signum function of these vectors. Let the set of the recorded orthants be \mathbb{O} . For each i, the Euclidean distance from the origin, $\|\boldsymbol{u}^i\|_2 = \sqrt{\boldsymbol{u}^{iT}\boldsymbol{u}^i}$ is computed, and the sample with the minimum value of $\|\boldsymbol{u}_i\|_2$ is recorded. Let the sample be denoted as \boldsymbol{u}_{\min} . Let $r_{\min} = \sqrt{\boldsymbol{u}_{\min}^T \boldsymbol{u}_{\min}}$. set is now defined. following The $\mathbf{C} = \left\{ \boldsymbol{u} \in \mathbb{O} : \sqrt{\boldsymbol{u}^T \boldsymbol{u}} \ge r_{\min} \right\}$. The explorer pdf is finally defined as $p_U(\boldsymbol{u}|\mathbf{C})$. Figure 1 shows region F for the performance function defined in Section 3.1 and region C obtained from this algorithm. The explorer pdf $p_U(\boldsymbol{u}|\mathbf{C})$ defined this way allows for drawing of iid samples from the pdf. Finally, having defined the explorer pdf, two chains can now be initiated, which draw samples from the target pdf and the explorer pdf. respectively. Propagation of the chain that draws from the target pdf here is done using the modified Metropolis algorithm (Au and Beck 2001). It is noted that propagating the chain that draws from the explorer pdf does not require performance function evaluation. Following this forward step, the exchange step of the replica exchange based MCMC algorithm is executed where the states of the two chains are exchanged probabilistically. Treatment of the burn-in phase for this MCMC sampler is done as follows. From the previously obtained samples $u^i, i = 1, 2, ..., M$ and their computed performance function values, a quadratic response surface for the limit surface is obtained. Instead of the original performance function, this inexpensive function is called during the burn-in phase of the MCMC sampler. The end of burn-in phase can be detected using the Gelman-Rubin diagnostic test. After the end of burn-in has been detected, the replica exchange MCMC algorithm is run, and a total of Msamples drawn according to $p_{u}(\boldsymbol{u}|\mathbf{F})$ are obtained. Finally, the adaptive kernel density

estimation algorithm is used as proposed by Au and Beck (1999) to obtain the ISpdf. The complete procedure of obtaining the kernel density estimate and sampling from this pdf is outlined therein.



Figure 1: (a) Failure region (F) shaded in red, (b) Region C shaded in green

2.2. Russian Roulette technique

Application of the Russian Roulette and splitting algorithm is well known in the computation of time-variant structural reliability (Melnik-Melnikov et al. 1997; Pradlwarter and Schuëller 1997). The idea is to probabilistically kill/stop simulating response trajectories which are less likely to reach the failure region. This helps conserve computational effort, which is instead employed in simulating response trajectories that are more likely to reach failure. However, in the context of time-invariant reliability estimation, the implementation of RR is somewhat different (Pegoraro 2016). Recall, the IS estimator given is

by,
$$\hat{P}_{F}^{IS} = \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} \frac{I\{G(\boldsymbol{u}_{i}) \leq 0\} p_{U}(\boldsymbol{u}_{i})}{q(\boldsymbol{u}_{i})}$$
. This estimator is modified as,

estimator is modified

$$\hat{P}_{F}^{IS} = \frac{1}{N_{IS}} \sum_{i=1}^{N_{IS}} \alpha\left(\boldsymbol{u}_{i}\right) \text{ where,}$$

$$\alpha\left(\boldsymbol{u}_{i}\right) = \begin{cases} \frac{1}{s\left(\boldsymbol{u}_{i}\right)} \left[\frac{I\left\{G\left(\boldsymbol{u}_{i}\right) \le 0\right\} p_{U}\left(\boldsymbol{u}_{i}\right)}{q\left(\boldsymbol{u}_{i}\right)}\right], & \text{w.p. } s(\boldsymbol{u}_{i}) \\ 0, & \text{w.p. } 1 - s(\boldsymbol{u}_{i}) \end{cases}$$

Here $\boldsymbol{u}_i, i = 1, 2, ..., N_{IS}$ are iid samples from $q(\mathbf{u})$. The quantity $s(\mathbf{u}_i)$ is called the "survival probability" of the sample. Therefore, with probability $1-s(u_i)$, the contribution of the

sample in the estimator is set to 0. This eliminates the need to call the performance function for that sample which saves computational effort. It is desirable to set the values of those terms to 0 whose contribution to the estimator is negligible so that the preserved computational effort can be directed towards samples that contribute substantially to the estimator. $s(u_i)$ should be small for samples that contribute minimally and large for samples that contribute significantly to the estimate. It is defined as follows. Firstly, a "reference contribution" is defined as $c^* = \frac{p_U(\boldsymbol{u}_{\min})}{q(\boldsymbol{u}_{\min})}$. Then, for a sample \boldsymbol{u}_i simulated from the ISpdf $q(\mathbf{u})$, the "sample contribution"

is defined as $c(\boldsymbol{u}_i) = \frac{p_U(\boldsymbol{u}_i)}{q(\boldsymbol{u}_i)}$. The sample is likely to make an insignificant contribution to the estimator either if: (a) $c(\boldsymbol{u}_i)$ is much smaller than c^* , or if (b) $c(u_i)$ is much larger than c^* . In case (a), the ratio $c(\boldsymbol{u}_i) = \frac{p_U(\boldsymbol{u}_i)}{q(\boldsymbol{u}_i)}$ would be very small and therefore contribute minimally to the estimator. In case (b), even though the ratio $c(\boldsymbol{u}_i) = \frac{p_U(\boldsymbol{u}_i)}{q(\boldsymbol{u}_i)}$ would be very large, the sample

is much more likely to lie in the safe region, thereby not contributing to the estimator at all. The survival probability is therefore defined as

$$s(\boldsymbol{u}_i) = \left[\min\left(\frac{c(\boldsymbol{u}_i)}{c^*}, \frac{c^*}{c(\boldsymbol{u}_i)}\right)\right]^{\psi} \quad (\quad \psi = 2 \quad \text{was}$$

found to be a suitable value for a wide range of numerical examples). Then, with probability $s(\boldsymbol{u}_i)$ the term

$$\alpha(\boldsymbol{u}_{i}) = \frac{1}{s(\boldsymbol{u}_{i})} \left[\frac{\mathrm{I}\{G(\boldsymbol{u}_{i}) \leq 0\} p_{U}(\boldsymbol{u}_{i})}{q(\boldsymbol{u}_{i})} \right] \qquad \text{is}$$

computed and with probability $1-s(u_i)$, $\alpha(u_i) = 0$. If a sample survives for which

 $c(\boldsymbol{u}_i) > c^*$ and $G(\boldsymbol{u}_i) \le 0$ hold, then the reference contribution c^* is updated to the new value $c(\mathbf{u}_i)$. Samples are continued to be generated until the performance function has been called N_{calls} times, which needs to be specified beforehand (here, we use $N_{calls} = 500$). Let \overline{N}_{IS} be the number of samples generated. The failure probability estimate is then computed as,

$$\hat{P}_{F}^{IS} = \frac{1}{\overline{N}_{IS}} \sum_{i=1}^{N_{IS}} \alpha(\boldsymbol{u}_{i}).$$

3. NUMERICAL ILLUSTRATIONS

Four illustrative examples with performance containing aforementioned function the difficulties are considered. Results of the following IS schemes are compared:

- (a) M1: Proposed algorithm. Here, the number of samples for constructing ISpdf is taken as M = 500 and $N_{calls} = 500$.
- (b) M2: Sequential directional importance sampling. This is implemented via the MATLAB package available at https://github.com/KaiChengDM/SDIS. Number of importance directions per level = 500, length of Markov chains = 5, and initial $\sigma = 3$ (Cheng et al. 2023).
- (c) M3: Improved cross entropy method von Mises-Fisher-Nakagami mixture. This is implemented via MATLAB package available at https://www.cee.ed.tum.de/en/era/softwar e/reliability/cross-entropy-method-andimproved-cross-entropy-method. Number of samples per level = 500, the initial number of distributions in the mixture = 5and maximum number of iterations = 20(Papaioannou et al. 2019).

Results from these algorithms are compared with the direct Monte Carlo method. The following quantities are reported for each illustrative example: (a) number of samples drawn from the ISpdf (N_{IS}) (in case of method M1, N_{IS} is the number of survived samples), (b) mean probability of failure from 100 independent runs of the reliability algorithm (\hat{P}_{F}^{mean}), (c) coefficient of variation ($\hat{\delta}$) obtained from 100 independent runs of the algorithm, (d) the total number of performance function calls for each run (N_{FC}). Before executing the reliability estimation algorithms, all performance functions have been transformed into the standard normal space.

3.1. Example 1

Consider the following performance function in the standard normal space (Breitung 2019):

$$G(U) = \min\left(5 - U_1, \frac{1}{1 + \exp(-2(U_2 + 6))} - 0.5\right).$$
(1)

Here, the performance function value displays a sharp change near the most important failure region. Figure 2(a) shows the failure region shaded in orange. As seen from samples in Figure 2(b) and 2(c), the proposed method M1 and M2 succeed in sampling from the important failure regions. However, method M3 fails to detect any failure region in this case (Figure 2(d) shows the failure samples drawn using this method). Table 1 shows details of the numerical results obtained using these algorithms.

Method	<i>M1</i>	M2	М3		
N _{IS}	500	500	500		
\hat{P}_{F}	2.89×10^{-7}	2.88×10^{-7}	Failed		
δ	0.05	0.08	-		
N _{FC}	2394	9688	-		
Direct Monte Carlo estimate with 10 ⁹ samples					
$= 3.05 \times 10^{-7}$					

Table 1: Numerical results of example 1

3.2. Example 2

Consider in the standard normal space the following performance function:

$$G(U) = \left(\sqrt{U_1^2 + U_2^2} - 4.00\right) \left(\sqrt{U_1^2 + U_2^2} - 4.25\right)$$

$$\left(\sqrt{U_1^2 + U_2^2} - 4.50\right) \left(\sqrt{U_1^2 + U_2^2} - 4.75\right).$$
(2)



Figure 2: Example 1: (a) Shaded failure region; Samples generated in a run of (b) M1, (c) M2, and (d)M3

In this case, the failure region comprises two disconnected failure regions separated by a region of safety (see Figure 3(a)). Since the failure regions are in the form of two annuli, multiple directions contribute equally to the failure probability. The IS scheme must be able to adequately sample from all directions. Here as well, the proposed method M1 successfully samples from both failure regions. The replica exchange algorithm allows the MCMC sampler to adequately explore both important failure regions in all directions (shown in Figure 3(b)). Method M3 can also capture the failure region adequately. as seen by the failure samples in Figure 3(d). Method M2 requires very high computational effort (the samples drawn are shown in Figure 3(c)). Table 2 contains the numerical results obtained for this example. This problem has an exact solution which can be written in terms of the chi CDF with 2 degrees of freedom, $\chi_2(.)$ as follows:

$$P_F = \chi_2(4.25) - \chi_2(4) + \chi_2(4.75) - \chi_2(4.5)$$

= 2.43×10⁻⁴.

Tuete 2. Tranciteur results of example 2					
Method	M1	M2	M3		
N _{IS}	500	500	500		
$\hat{P}_{_F}$	2.43×10^{-4}	2.70×10^{-4}	2.47×10^{-4}		
δ	0.06	0.06	0.18		
N _{FC}	2392	31284	10000		
Direct Monte Carlo estimate with 10 ⁶ samples					
$= 2.55 \times 10^{-4}$.					

 Table 2: Numerical results of example 2



Figure 3: Example 2: (a) Shaded failure region; Samples generated in a run of (b) M1, (c) M2, and (d)M3

3.3. Example 3

This example pertains to a structural system whose failure occurs through loss of stability. Consider a rigid bar of length L=1 m with a torsional spring at its base subject to a vertical downward load (see Figure 4). The random variables considered are the torsional spring constant

 $K_{T} \sim \text{Lognormal} \left(\mu = 2.5 \times 10^{9} \text{ Nm/rad, CoV} = 0.1 \right)$ and the vertical load

 $P \sim \text{Lognormal}(\mu = 1.0 \times 10^9 \text{ N}, \text{ CoV} = 0.1)$

which are assumed to be independent.



Figure 4: Example 3: Rigid bar with torsional spring

Here, failure is defined as the vertical downward displacement exceeding 1×10^{-3} m. Thus, the performance function is written as $g(K_{\tau}, P) = 1 \times 10^{-3} - \Delta$, where Δ is the downward displacement. The details of computation of Δ can be found in (Thompson and Hunt 1973). The failure region has been indicated in Figure 5(a). The difficulty in the performance function lies in the fact that if the structure is in the safe zone, the performance function value is a positive constant, 1×10^{-3} m, and when it fails, the performance function value suddenly starts declining. Hence, reliability estimation methods that rely on an adaptive search of failure regions would fail to identify any such regions. The intermediate samples would give no indication of the location of the failure zone due to the constant nature of the performance function. Indeed, it is seen that method M3, due to its adaptive nature, fails to detect the failure region for the majority of the runs (see Figure 5(d)). This leads to an underestimation of the failure probability in Table 3. It is also observed that method M2 could detect the failure region (see Figure 5(c)). Again, the proposed methodology, detects the failure region and correctly computes the probability of failure (see Figure 5(b)).

Table 3: Numerical results of example 3

Method	M1	M2	M3
N_{IS}	500	500	500
$\hat{P}_{_F}$	3.62×10^{-5}	3.65×10^{-5}	1.28×10^{-5}





Figure 5: Example 3: (a) Shaded failure region; Samples generated in a run of (b) M1, (c) M2, and (d)M3

3.4. Example 4

This example considers reliability computation of reliability of a vibrating two-degree-of-freedom mass-spring-dashpot as seen in Figure 6. The random variables considered here are the stiffness parameters of the springs, $K_1, K_2 \sim \text{Lognormal}(\mu = 2.5 \times 10^5 \text{ N/m}, \text{ CoV} = 0.2)$ which are assumed to be independent. Values of the masses are $M_1 = M_2 = 2000 \text{ kg}$, and that of the modal damping ratios are $\eta_1 = \eta_2 = 0.02$. The mass M_2 is subjected to an excitation $P(t) = 2000 \sin(11t)$. The performance function is defined as follows:

$$g(K_1, K_2) = 0.024 - \max_{0 \le t \le 20} x_1(t)$$
(3)

Here, it is seen that the region of failure comprises of two disconnected regions which contribute significantly to the failure probability. Hence, for accurate estimation of failure probability, IS schemes must be able to correctly sample from both regions. From the numerical details presented in Table 4, it is seen that the proposed method M1 can accurately report the failure probability with much less computational effort than methods M2 and M3. Figure 7(a) shows the failure region, and Figure 7(b), 7(c), and 7(d) show the failure samples obtained from methods M1, M2 and M3, respectively.



Figure 6: Example 4: A two-degree-of-freedom massspring-dashpot system

1000	Tuble II I lunter teal results of example 1					
Method	M1	M2	<i>M3</i>			
N _{IS}	500	500	500			
\hat{P}_{F}	2.34×10 ⁻⁵	2.10×10^{-5}	1.30×10^{-5}			
δ	0.05	0.09	0.57			
N _{FC}	2368	9528	8200			
Direct Monte Carlo estimate with 10 ⁷ samples						
$= 2.28 \times 10^{-5}$.						

Table 4: Numerical results of example 4

4. DISCUSSION AND CLOSURE

The difficulties in performance functions described in previous sections are manifested in reliability estimation methods as challenges in sufficiently exploring the parameter space and detecting important regions of failure. The present study contributes to solving this problem by proposing a replica exchange-based MCMC sampler. This algorithm proves to be a powerful tool in effectively dealing with performance functions that exhibit difficulties that traditional reliability estimation methods cannot contend with. The numerical illustrations in the previous section show that the proposed methodology achieves enhanced parameter space exploration and accurately estimates failure probability. It achieves this exploration and accuracy while spending much less computational effort than other methods. A limitation of the proposed methodology arises in dealing with highdimensional problems. It is known that kernel density estimation requires a large number of samples to construct an estimate of the pdf in high dimensions accurately. In addition, the replica exchange method also faces difficulty in high dimensions since the number of orthants in n dimensional space is 2^n . When n is large and the difficulties of the kind mentioned earlier emerge,



Figure 7: Example 4: (a) Shaded failure region; Samples generated in a run of (b) M1, (c) M2, and (d)M3

important orthants are likely to remain unexplored. A possible solution to this is the utilization of machine learning techniques which would be feasible in high dimensions to characterize the failure region in conjunction with the replica exchange strategy. This approach is currently being explored by the authors.

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