

Riemannian Manifold Hamiltonian Monte Carlo based subset simulation for reliability analysis in non-Gaussian space

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Abstract

This paper proposes a Riemannian Manifold Hamiltonian Monte Carlo based subset simulation (RMHMC-SS) method to overcome limitations of existing Monte Carlo approaches in solving reliability problems defined in highly-curved non-Gaussian spaces. RMHMC is based on the second-order geometric information of a probability space. Specifically, it generates an optimized path for Markov chain evolutions in a Hamiltonian constructed on the Riemannian manifold. Compared with the recently proposed Hamiltonian Monte Carlo based subset simulation (HMC-SS) approach, the RMHMC-SS approach shows better performance in handling highly-curved probability distributions. After a brief review of HMC-SS, the theory and implementation details of RMHMC-SS are presented. Finally, various reliability examples are studied to test and verify the proposed RMHMC-SS method.

Keywords: Riemannian manifold, Hamiltonian Monte Carlo, high-dimensional reliability, non-Gaussian space, subset simulation

1. Introduction

In reliability analysis, the main computational goal is to estimate the failure probability expressed as

$$P_f = \int_{\mathbb{R}^n} \mathbb{1}(\mathbf{q} \in \mathcal{F}) \pi(\mathbf{q}) d\mathbf{q}, \quad (1)$$

where $\mathbf{q}$ is an n -dimensional vector to quantify the uncertainties of interest, $\pi(\mathbf{q})$ is the joint probability density function (PDF) of $\mathbf{q}$, and $\mathbb{1}(\cdot)$ is a binary indicator function for the event $\mathbf{q} \in \mathcal{F}$. For non-trivial problems, Eq.(1) is typically evaluated by numerical methods. An incomplete list includes Monte Carlo simulation methods (MCS) [1–4], surrogate modelling [5, 6], and asymptotic methods [7–9].

One powerful variance reduction MCS approach to estimate Eq.(1) is the subset simulation [1]. The original algorithm uses a modified Metropolis-Hastings (M-H) algorithm, namely the component-wise M-H, as the sampler to generate Markov chains in each intermediate step (subset). Even in high-dimensional probability spaces, the component-wise M-H sampler shows acceptable mixing behavior with relatively high acceptance rates. However, the Markov chains generated by the component-wise M-H sampler may exhibit intense “random walk behavior”, which may cause high coefficient of variations in the final probability estimates. Here the phrase “random walk behavior” is only a qualitative description on the behavior of traditional M-H sampler when a random walk proposal distribution is used. The main feature of random walk behavior is that the Markov chain trajectories are highly irregular, and they do not explore the probability space in a consistent manner. Note that if a sufficiently large set of samples is generated, whether intense random walk occurs or not may not make a huge difference. However, in reliability analysis, for computational efficiency it is ideal to use as few samples as possible. This motivates the employment of non-random-walk based methods, so that the (small set of) samples could explore the full range of the probability space in a consistent and efficient manner. In fact, the random walk behavior is a natural

property of conventional M-H and Gibbs sampling methods. To alleviate the random walk behavior of Markov chains in subset simulation, a non-random-walk based subset simulation method, the Hamiltonian Monte Carlo based subset simulation (HMC-SS) [10], was recently proposed. Prior to [10], the method proposed in [11] also alleviates the random walk behavior. In fact, in [10] it was shown that the method of [11] is a special case of the Hamiltonian Monte Carlo in a Gaussian space.

Inspired by the Hamiltonian dynamics for conservative systems, the HMC [12, 13] method employs a deterministic mechanism for Markov chain evolutions. The mechanism uses the first-order geometric information to achieve an effective exploration of the probability space. However, with an increase in the curvature of the probability space, the exploration proposed by HMC becomes increasingly difficult, and it no longer provides an ideal path for Markov chain evolutions. Note that in the context of HMC method, the curvature of the probability space is related to the Hessian matrix of the potential energy (the negative log-likelihood function). To overcome the aforementioned limitation of HMC-SS, this paper proposes an important extension of HMC-SS that implements the Riemannian Manifold Hamiltonian Monte Carlo (RMHMC) [14] method.

The RMHMC method was originally developed by Girolami and Calderhead [14] in 2011. In the original RMHMC approach, the Fisher information matrix is used as the Riemannian metric tensor. The use of the Fisher information matrix requires that the target probability distribution possesses natural/obvious conditional variables. To expand RMHMC for more general distribution models and to further improve the performance, several variants (in terms of the Riemannian metric tensor constructions) are developed in the literature [15–18]. In general, RMHMC fully employs the geometric properties of the probability space via constructing a Hamiltonian on the Riemannian manifold with the metric tensor related to the PDF. The new mechanism of proposing samples contains the second-order geometric information, and it can lead to effective exploration of the probability spaces with large curvature and high dimensionality. In reliability engineering practice, especially when a Bayesian posterior distribution is involved, the limit-state function as well as the probability space of interest may exhibit high nonlinearity and large curvature. Therefore, it is of theoretical and practical interest to study RMHMC in the context of reliability analysis.

The structure of this paper is as follows. Section 2 briefly reviews the general concepts of HMC-SS. Section 3 elaborates the necessity of introducing RMHMC into the framework of subset simulation. Section 4 introduces principles and implementation details of RMHMC-SS. Section 5 presents a series of numerical investigations to test RMHMC-SS. Section 6 discusses some limitations and future directions. Finally, Section 7 summarizes the paper.

2. A review of Hamiltonian Monte Carlo based subset simulation

The central idea of subset simulation is to express the failure domain as an intersection of a sequence of nested intermediate domains $\mathcal{F}_j$, $j = 1, 2, \dots, M$, i.e.,

$$\mathcal{F} = \bigcap_{j=1}^M \mathcal{F}_j, \quad (2)$$

where $\mathcal{F}_1 \supset \mathcal{F}_2 \supset \dots \supset \mathcal{F}_M$, and $\mathcal{F}_M = \mathcal{F}$. Using Eq.(2) and the multiplication rule of probability, the failure probability can be written as a product of conditional probabilities,

$$P_f = \mathbb{P}(\mathbf{q} \in \mathcal{F}) = \prod_{j=1}^M \mathbb{P}(\mathbf{q} \in \mathcal{F}_j | \mathbf{q} \in \mathcal{F}_{j-1}), \quad (3)$$

where $\mathcal{F}_0 = \mathbb{R}^n$ so that $\mathbb{P}(\mathbf{q} \in \mathcal{F}_0) = 1$. The estimation of failure probability $\mathbb{P}(\mathbf{q} \in \mathcal{F})$ is now transformed into estimations of conditional probabilities $\mathbb{P}(\mathbf{q} \in \mathcal{F}_j | \mathbf{q} \in \mathcal{F}_{j-1})$, $j = 1, 2, \dots, M$. The conditional probabilities $\mathbb{P}(\mathbf{q} \in \mathcal{F}_j | \mathbf{q} \in \mathcal{F}_{j-1})$ can be constructed to be relatively large such that they can be estimated using a small number of random samples. To estimate $\mathbb{P}(\mathbf{q} \in \mathcal{F}_j | \mathbf{q} \in \mathcal{F}_{j-1})$, the Markov Chain Monte Carlo

(MCMC) technique is used to sample from the conditional distributions $\pi(\mathbf{q}|\mathcal{F}_{j-1})$. In practical implementations of subset simulation, the nested intermediate domains can be constructed adaptively such that $\mathbb{P}(\mathbf{q} \in \mathcal{F}_j | \mathbf{q} \in \mathcal{F}_{j-1})$, $j = 1, 2, \dots, M-1$, are approximately equal to a pre-specified percentile p_0 , and then the failure probability can be estimated by

$$P_f \cong \hat{P}_f = \frac{p_0^{M-1}}{N} \sum_{i=1}^N \mathbb{1}(\mathbf{q}_i \in \mathcal{F}_M), \quad (4)$$

where $\mathbf{q}_i$ are random samples drawn from the conditional distribution $\pi(\mathbf{q}|\mathcal{F}_{M-1})$. Au & Beck [1] recommended $p_0 = 0.1$, and Zuev et al. [19] found that the choice of $p_0 \in [0.1, 0.3]$ achieves similar efficiency. In this paper, p_0 is uniquely set to 0.1 unless stated the otherwise.

The HMC-SS uses the Hamiltonian Monte Carlo method to generate samples from the conditional distribution $\pi(\mathbf{q}|\mathcal{F}_j)$. In the physical interpretation of HMC, the negative log-likelihood of $\pi(\mathbf{q}|\mathcal{F}_j)$ is interpreted as the potential energy of a Hamiltonian system. Next, an auxiliary random momentum vector, $\mathbf{p}$, is used to introduce a fictitious (Newtonian) kinetic energy. For convenience, $\mathbf{p} \sim \mathcal{N}(\mathbf{p}|\mathbf{0}, \mathbf{\Sigma})$, where $\mathcal{N}(\cdot|\mathbf{0}, \mathbf{\Sigma})$ denotes a Gaussian distribution with mean $\mathbf{0}$ and covariance matrix $\mathbf{\Sigma}$. Similar to the potential energy, the negative log-likelihood of $\mathcal{N}(\mathbf{p}|\mathbf{0}, \mathbf{\Sigma})$ is interpreted as the kinetic energy. The Hamiltonian, as a sum of the potential and kinetic energy, is written as

$$H(\mathbf{q}, \mathbf{p}) = V(\mathbf{q}|\mathcal{F}_j) + K(\mathbf{p}) = -\log \pi(\mathbf{q}|\mathcal{F}_j) + \frac{1}{2} \log(2\pi)^n |\mathbf{\Sigma}| + \frac{1}{2} \mathbf{p}^\top \mathbf{\Sigma}^{-1} \mathbf{p}, \quad (5)$$

where $V(\mathbf{q}|\mathcal{F}_j)$ denotes the potential energy function, $K(\mathbf{p})$ denotes the kinetic energy function, and the term $\frac{1}{2} \log(2\pi)^n |\mathbf{\Sigma}|$ corresponds to the normalizing constant of $\mathcal{N}(\mathbf{p}|\mathbf{0}, \mathbf{\Sigma})$. In the implementation of HMC-SS, $\mathbf{\Sigma}$ is typically set to the identity matrix. Note that the constraint $\mathcal{F}_j$ introduces a “potential barrier” to Eq.(5), i.e., the region outside $\mathcal{F}_j$ has infinite potential energy and therefore cannot be reached by the Hamiltonian system.

Depending on how to handle the potential barrier, HMC-SS is classified into rejection sampling based HMC-SS and barrier-bouncing based HMC-SS. For the sake of simplicity and efficient implementations, this paper only considers the rejection sampling based HMC, but it can be easily extended to the other cases. The rejection sampling based HMC is essentially a MCMC method to generate samples from $\pi(\mathbf{q})$, and it is the final Metropolis accept-reject step that selects samples from $\pi(\mathbf{q}|\mathcal{F}_j)$. Therefore, in the rejection sampling based HMC, it is sufficient to only consider the Hamiltonian without the constraint $\mathcal{F}_j$, i.e.,

$$H(\mathbf{q}, \mathbf{p}) = V(\mathbf{q}) + K(\mathbf{p}) = -\log \pi(\mathbf{q}) + \frac{1}{2} \log(2\pi)^n |\mathbf{\Sigma}| + \frac{1}{2} \mathbf{p}^\top \mathbf{\Sigma}^{-1} \mathbf{p}. \quad (6)$$

The Hamiltonian equations, which governs the evolutions of the state vector $(\mathbf{q}, \mathbf{p})$, are expressed as

$$\begin{aligned} \frac{d\mathbf{q}}{dt} &= \frac{\partial H}{\partial \mathbf{p}}, \\ \frac{d\mathbf{p}}{dt} &= -\frac{\partial H}{\partial \mathbf{q}}. \end{aligned} \quad (7)$$

The trajectories of $(\mathbf{q}, \mathbf{p})$ determined by Eq.(7) define an equi-Hamiltonian surface. Using Eq.(7), the rejection sampling based HMC algorithm works as follows: i) generate a random $\mathbf{p}$ from $\mathcal{N}(\mathbf{p}|\mathbf{0}, \mathbf{\Sigma})$, select an initial $\mathbf{q}$, $\mathbf{q} \in \mathcal{F}_j$; ii) start from the initial state $(\mathbf{q}, \mathbf{p})$, propose a new state, $(\mathbf{q}^*, \mathbf{p}^*)$, as the solution of Eq.(7) for a specified time point; iii) if $\mathbf{q}^* \in \mathcal{F}_j$, $\mathbf{q}^*$ is accepted with probability 1, otherwise (i.e., $\mathbf{q}^* \notin \mathcal{F}_j$), $\mathbf{q}^*$ is rejected.

In the Gaussian Space (i.e., $\pi(\mathbf{q})$ is Gaussian), the solution of the Hamiltonian equations is analytical,

*The constant term $\frac{1}{2} \log(2\pi)^n |\mathbf{\Sigma}|$ does not have any influence on HMC algorithms, we highlight it here because it cannot be neglected in the following RMHMC extension.

making HMC method very efficient. Conversely, when the spaces are not Gaussians and probability transformations are not convenient, the Hamiltonian equations are solved numerically by symplectic integrators (e.g., the leapfrog method [20]).

The numerical integrators may introduce numerical errors that destroy the conservation of the Hamiltonian and consequently the detail balance. To maintain the detail balance condition, a Metropolis accept-reject rule is introduced, i.e.,

$$\text{Accept } (\mathbf{q}^*, \mathbf{p}^*) \text{ with the probability: } \min\{1, \exp[-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}, \mathbf{p})]\}. \quad (8)$$

Trivially, one could notice that if the Hamiltonian equations are solved analytically, $-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}, \mathbf{p}) = 0$ and the acceptance probability is 1. Also note that in the context of HMC-SS, Eq.(8) is used on the premise of $\mathbf{q}^* \in \mathcal{F}_j$. Specifically, the last step of the HMC algorithm is: If $\mathbf{q}^* \in \mathcal{F}_j$, $\mathbf{q}^*$ is accepted with probability $\min\{1, \exp[-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}, \mathbf{p})]\}$; $\mathbf{q}^*$ is rejected the otherwise.

3. Needs for introducing the Riemannian Manifold Hamiltonian Monte Carlo

In the HMC method, a constant mass matrix Σ is used to define the kinetic energy. The limitation of using a fixed Σ lies in two folds. First, the χ^2 distributed variable $\mathbf{p}^\top \Sigma^{-1} \mathbf{p}$ becomes increasingly concentrated around n (recall that n is the dimension of $\mathbf{p}$) as n increases [21–23]. Consequently, for a relatively large n the magnitude of a randomly drawn kinetic energy $\mathbf{p}^\top \Sigma^{-1} \mathbf{p}/2$ is always close to $n/2$. For a distribution $\pi(\mathbf{q})$ with large local curvature, there is no guarantee that such a (approximately) constant kinetic energy is large enough to “drive” the Hamiltonian system to effectively explore the typical set of $\pi(\mathbf{q})$, i.e., the potential energy $V(\mathbf{q})$ may span a larger gap than $n/2$. Second, in the practical implementations of HMC, it is challenging to specify an integration step (whether adaptive or not) that optimally addresses the trade-off between efficiency and the ability to explore regions with large curvature.

As a result of the aforementioned limitations, for probability spaces with high dimensionality and large (local) curvature, the overall mixing behavior of HMC may not be ideal. A numerical illustration of this phenomenon will be provided in Section 5.1 using *Neal’s funnel distribution* [24]. A remedy to the limitations is to introduce a position dependent mass matrix Σ , denoted by $\Sigma(\mathbf{q})$. Since $\Sigma(\mathbf{q})$ is related to the Riemannian metric tensor of the probability space of $\pi(\mathbf{q})$, the corresponding HMC method is known as Riemannian Manifold HMC method. In RMHMC, the Hamiltonian dynamics involves the second-order geometric information of the probability space and it provides an effective path for Markov chain evolutions in highly curved probability space. As it is mentioned in the Introduction, the ability to handle highly curved probability space makes RMHMC attractive in reliability analysis.

It is important to mention that the HMC-SS approach in the standard Gaussian space does not suffer from the aforementioned issues of HMC, since in this circumstance the potential and kinetic energy are in the same magnitude. Moreover, it can be shown that the RMHMC in the standard Gaussian space is equivalent to the original HMC. This is because the Hessian matrix corresponding to the standard Gaussian distribution is constant. Therefore, this paper only considers non-Gaussian space applications, while Gaussian space problems can be effectively handled by the original HMC-SS. The RMHMC-SS is particularly useful for problems where the transformation to standard Gaussian space is difficult/infeasible, typically because the distribution is known only up to a proportionality constant, e.g., Bayesian reliability problems.

4. Details of the Riemannian Manifold Hamiltonian Monte Carlo based subset simulation

4.1. Hamiltonian and Hamilton’s equations

A series of studies [25–28] have shown that many statistical models have a natural Riemannian geometry with the Riemannian metric tensor $\Sigma(\mathbf{q})$ for PDF $\pi(\mathbf{q})$. The RMHMC exploits this manifold structure by adopting $\Sigma(\mathbf{q})$ as the mass tensor. The momentum vector $\mathbf{p}$ is distributed according to a position-dependent Gaussian distribution, i.e., $\mathbf{p} \sim \mathcal{N}(\mathbf{p}|\mathbf{0}, \Sigma(\mathbf{q}))$. The Hamiltonian can be written as [14]

$$H(\mathbf{q}, \mathbf{p}) = V(\mathbf{q}) + K(\mathbf{p}) = -\log \pi(\mathbf{q}) + \frac{1}{2} \log(2\pi)^n |\Sigma(\mathbf{q})| + \frac{1}{2} \mathbf{p}^\top \Sigma(\mathbf{q})^{-1} \mathbf{p}. \quad (9)$$

Eq.(9) indicates that the Hamiltonian is defined on the Riemannian manifold with Riemannian metric tensor $\Sigma(\mathbf{q})$. The Hamiltonian equations for each component can be explicitly expressed as [14]

$$\begin{aligned}\frac{dq_i}{dt} &= \frac{\partial H}{\partial p_i} = \{\Sigma(\mathbf{q})^{-1}\mathbf{p}\}_i, \\ \frac{dp_i}{dt} &= -\frac{\partial H}{\partial q_i} = \frac{\partial \log \pi(\mathbf{q})}{\partial q_i} - \frac{1}{2}\text{tr}\left\{\Sigma(\mathbf{q})^{-1}\frac{\partial \Sigma(\mathbf{q})}{\partial q_i}\right\} + \frac{1}{2}\mathbf{p}^T \Sigma(\mathbf{q})^{-1} \frac{\partial \Sigma(\mathbf{q})}{\partial q_i} \Sigma(\mathbf{q})^{-1} \mathbf{p},\end{aligned}\tag{10}$$

where $\{\Sigma(\mathbf{q})^{-1}\mathbf{p}\}_i$ denotes the i -th component of vector $\Sigma(\mathbf{q})^{-1}\mathbf{p}$, and $\text{tr}\{\cdot\}$ denotes the matrix trace. The trajectories generated by Eq.(10) satisfy the *Liouville's Theorem* of volume preservation. However, in contrast with the constant mass matrix case, the Hamiltonian in RMHMC cannot be factorized into independent contributions from $\mathbf{q}$ and $\mathbf{p}$. A consequence of this feature is that a naive application of the leapfrog integrator will no longer lead to reversible and volume preserving chains. To address this issue, Girolami and Calderhead [14] proposed a second-order semi-explicit symmetric integrator, the *generalized leapfrog integrator*, to solve Eq.(10). The generalized leapfrog integrator reads as follows,

$$\begin{aligned}\mathbf{p}(t + \Delta t/2) &= \mathbf{p}(t) - \frac{\Delta t}{2} \nabla_{\mathbf{q}} H(\mathbf{q}(t), \mathbf{p}(t + \Delta t/2)), \\ \mathbf{q}(t + \Delta t) &= \mathbf{q}(t) + \frac{\Delta t}{2} [\nabla_{\mathbf{p}} H(\mathbf{q}(t), \mathbf{p}(t + \Delta t/2)) + \nabla_{\mathbf{p}} H(\mathbf{q}(t + \Delta t), \mathbf{p}(t + \Delta t/2))], \\ \mathbf{p}(t + \Delta t) &= \mathbf{p}(t + \Delta t/2) - \frac{\Delta t}{2} \nabla_{\mathbf{q}} H(\mathbf{q}(t + \Delta t), \mathbf{p}(t + \Delta t/2)).\end{aligned}\tag{11}$$

Unfortunately, the first two lines of Eq.(11) are implicit equations of $\mathbf{p}(t + \Delta t/2)$ and $\mathbf{q}(t + \Delta t)$, respectively, and thus iterative methods, (e.g., direct fixed point iteration and quasi-Newton methods) are needed. Consequently, the computational cost of RMHMC is larger than that of HMC. Similar to the conventional leapfrog integrator, the generalized leapfrog integrator will also introduce numerical errors, and thus the Metropolis accept-reject rule in Eq.(8) is also needed for RMHMC.

In this study, the Δt in the generalized leapfrog integrator is typically set to 0.01. In the current context, Δt is not a critical parameter that requires meticulously tuning. This is because as long as Δt is relatively small, the leapfrog integrator would be accurate, and consequently the conservation of Hamiltonian or the acceptance rate of proposal samples would be acceptable. Also note that only the last step of the leapfrog integrator requires evaluation of the limit-state function.

4.2. Riemannian metric tensor

So far, the issue of how to construct $\Sigma(\mathbf{q})$ for a specified distribution has not been fully addressed. In fact, the construction of $\Sigma(\mathbf{q})$ is not trivial and not even unique [14–18]. A natural choice of $\Sigma(\mathbf{q})$ is to use the Hessian of the potential energy $V(\mathbf{q})$,

$$\mathcal{H}_{i,j} = \frac{\partial^2 V(\mathbf{q})}{\partial q_i \partial q_j} = -\frac{\partial^2 \log \pi(\mathbf{q})}{\partial q_i \partial q_j},\tag{12}$$

where $i, j = 1, 2, \dots, n$. To intuitively understand the use of the Hessian matrix Eq.(12), consider the case where $\pi(\mathbf{q})$ is Gaussian, the Hessian matrix will be the inverse of the covariance matrix of $\pi(\mathbf{q})$. Setting $\Sigma = \mathcal{H}$ indicates that the momentum $\mathbf{p}$ follows a Gaussian distribution with the covariance matrix equals to the inverse of the covariance matrix of the position $\mathbf{q}$. Due to the dual property of the momentum and position spaces, such a selection on covariance matrix leads to the optimal performance of HMC [13]. However, for general distributions of $\mathbf{q}$ the Hessian matrix Eq.(12) can be indefinite. Therefore, more general alternative approaches are needed to construct $\Sigma(\mathbf{q})$.

176 The Fisher-Rao metric tensor

177 In 1945, Rao [29] showed that the expected Fisher information matrix is a natural Riemannian metric tensor.
 178 The expected Fisher information matrix is expressed by

$$\mathbb{E}_{\mathbf{v}|\mathbf{q}} \left[\frac{\partial^2 V(\mathbf{v}|\mathbf{q})}{\partial q_i \partial q_j} \right] = -\mathbb{E}_{\mathbf{v}|\mathbf{q}} \left[\frac{\partial^2 \log \pi(\mathbf{v}|\mathbf{q})}{\partial q_i \partial q_j} \right], \quad (13)$$

179 where $\mathbf{v}$ are conditional variables. The key idea of Eq.(13) is to make use of any conditional variables $\mathbf{v}$
 180 via marginalizing the Hessian over $\mathbf{v}$, and the resulting Fisher-Rao metric is *guaranteed* to be positive semi-
 181 definite. Clearly, the use of Eq.(13) resolves the theoretical issue of using the Hessian directly. However, due
 182 to the arbitrary nature of specifying $\mathbf{v}$, the resulting RMHMC may not be effective, and the marginalization
 183 step can be computationally demanding (even unfeasible). To extend the applicability of RMHMC and to
 184 further improve the performance, the *AbsSoft* map based modified Hessian matrix approach [15] provides
 185 an attractive alternative, and will be adopted to solve the numerical examples in this study.

186 The modified Hessian matrix

187 The modified Hessian matrix approach uses the *SoftAbs* map of the Hessian matrix, defined as [15]

$$\wr \mathcal{H} := [\exp(\alpha \mathcal{H}) + \exp(-\alpha \mathcal{H})] \cdot \mathcal{H} \cdot [\exp(\alpha \mathcal{H}) + \exp(-\alpha \mathcal{H})]^{-1}, \quad (14)$$

188 where α ($\alpha \neq 0$) is a specified parameter. The *SoftAbs* map approximates the absolute value of the eigen-
 189 spectrum with a smooth function. Matrix $\wr \mathcal{H}$ can be expressed in an eigen-decomposition form as [15]

$$\begin{aligned} \wr \mathcal{H} &= \mathbf{Q} \cdot \wr \boldsymbol{\lambda} \cdot \mathbf{Q}^T, \\ \wr \boldsymbol{\lambda} &= \text{Diag} \left(\lambda_i \frac{e^{\alpha \lambda_i} + e^{-\alpha \lambda_i}}{e^{\alpha \lambda_i} - e^{-\alpha \lambda_i}} \right) = \text{Diag}(\lambda_i \coth \alpha \lambda_i), \end{aligned} \quad (15)$$

190 where $\mathbf{Q}$ is the eigenvector matrix of $\mathcal{H}$ and λ_i are the corresponding eigenvalues. Figure 1 shows the relation
 191 between the original eigenvalues and the transformed eigenvalues.

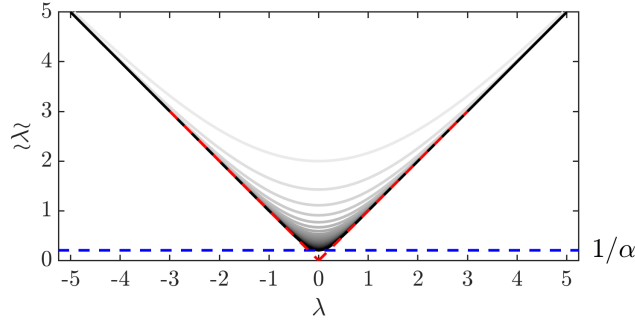


Figure 1: **The *SoftAbs* map of eigenvalues (after Betancourt [15]).** The lighter to darker curves are associated with an increasing sequence of α values. The inverse of α controls the “hardness” of the approximation. As $\alpha \rightarrow \infty$, the *SoftAbs* map approximates the exact absolute map.

192 Matrix $\wr \mathcal{H}$ is not only symmetric and positive-definite, but also it preserves the eigenspace properties of
 193 the Hessian matrix. Therefore, $\wr \mathcal{H}$ can be used as the Riemannian metric tensor $\boldsymbol{\Sigma}(\mathbf{q})$. To incorporate as
 194 much original features of the Hessian as possible, the parameter α should be set as large as possible, as long
 195 as the generalized leapfrog integrator is stable. In practice, this stability can be checked by monitoring the
 196 conservation of Hamiltonian. In our implementation, α is chosen adaptively starting from a value as large
 197 as 10^6 , and it is iteratively reduced to 90% if the acceptance rate of a trial chain is less than 0.7. Note that
 198 the trial chain is used to sample from $\pi(\mathbf{q})$, therefore no limit-state function calls are needed.

Given $\Sigma(\mathbf{q}) = \mathcal{H}$, the generalized leapfrog integrator requires knowledge of the gradient of $\mathbf{p}^\top \mathcal{H}^{-1} \mathbf{p}$ and the gradient of $\log |\mathcal{H}|$ (see Eq.(11) and Eq.(10)). According to [15], the gradient of $\mathbf{p}^\top \mathcal{H}^{-1} \mathbf{p}$ can be evaluated by

$$\partial(\mathbf{p}^\top \mathcal{H}^{-1} \mathbf{p}) = -\text{tr}\{\mathbf{Q} \cdot \mathbf{D} \cdot \mathbf{J} \cdot \mathbf{D} \cdot \mathbf{Q}^\top \cdot \partial \mathcal{H}\}, \quad (16)$$

where

$$\mathbf{D} = \text{Diag}[(\mathbf{Q}^\top \cdot \mathbf{p})_i / \lambda_i \coth(\alpha \lambda_i)], \quad (17)$$

and

$$\mathbf{J}_{ij} \equiv \frac{\lambda_i \coth(\alpha \lambda_i) - \lambda_j \coth(\alpha \lambda_j)}{\lambda_i - \lambda_j}. \quad (18)$$

Particularly, if $i = j$, $\mathbf{J}_{ij}$ becomes the derivative

$$\mathbf{J}_{ii} = \frac{\partial}{\partial \lambda_i} \lambda_i \coth(\alpha \lambda_i). \quad (19)$$

The gradient of $\log |\mathcal{H}|$ can be evaluated by

$$\log |\mathcal{H}| = \text{tr}\{\mathbf{Q} \cdot (\mathbf{R} \circ \mathbf{J}) \cdot \mathbf{Q}^\top \cdot \partial \mathcal{H}\}, \quad (20)$$

where

$$\mathbf{R} = \text{Diag}\left(\frac{1}{\lambda_i \coth(\alpha \lambda_i)}\right). \quad (21)$$

The symbol $\circ$ denotes Hadamard product [30]. To avoid repeatedly performing matrix multiplications in gradient computations, the matrices $\mathbf{Q} \cdot \mathbf{D} \cdot \mathbf{J} \cdot \mathbf{D} \cdot \mathbf{Q}^\top$ and $\mathbf{Q} \cdot (\mathbf{R} \circ \mathbf{J}) \cdot \mathbf{Q}^\top$ should be evaluated first and then recorded.

4.3. Implementation details of RMHMC-SS

Given a specified Riemannian metric tensor and the generalized leapfrog integrator to evaluate the Hamiltonian equations, the RMHMC algorithm to generate samples from $\pi(\mathbf{q}|\mathcal{F}_j)$ can be developed as follows.

Algorithm 1: Rejection sampling based RMHMC to sample from $\pi(\mathbf{q}|\mathcal{F}_j)$

Step 1 Random momentum generation

- For an initial $\mathbf{q}_{\text{init}}$, generate a random initial momentum $\mathbf{p}_{\text{init}}$ from the Gaussian distribution $\mathcal{N}(\mathbf{p}|\mathbf{0}, \Sigma(\mathbf{q}_{\text{init}}))$.

Step 2 Riemannian Hamiltonian dynamics evolution

- Propose a new state, $(\mathbf{q}^*, \mathbf{p}^*)$, via the generalized leapfrog integrator integrated for $L = t_f / \Delta t$ steps starting from the initial state $(\mathbf{q}_{\text{init}}, \mathbf{p}_{\text{init}})$.

Step 3 Accept-reject

- If $\mathbf{q}^* \in \mathcal{F}_j$, $\mathbf{q}^*$ is accepted with probability $\min\{1, \exp[-H(\mathbf{q}^*, \mathbf{p}^*) + H(\mathbf{q}_{\text{init}}, \mathbf{p}_{\text{init}})]\}$; else, set $\mathbf{q}^* \leftarrow \mathbf{q}_{\text{init}}$.
-

Similar to HMC-SS, the fundamental tuning parameter in Algorithm 1 is the stopping time t_f . If t_f is too large, the likelihood of $\mathbf{q}^* \in \mathcal{F}_j$ would be small and the acceptance rate would be low. If t_f is too small, the acceptance rate would be high but the correlation between states would be large. Therefore, an adaptive tuning technique is needed so that the acceptance rate would be neither too high nor too low. In the HMC-SS approach for non-Gaussian space [10], t_f is initially set to $\bar{T}_0/8$ ^{*}, and then t_f is adaptively

^{*} $\bar{T}_0$ represents the mean period of the Hamiltonian system, evaluated using random samples from $\pi(\mathbf{q}|\mathcal{F}_0)$.

tuned using the acceptance rate for sampling from $\pi(\mathbf{q}|\mathcal{F}_j), j = 1, 2, \dots, M$. In RMHMC-SS, we use a similar approach to tune t_f . However, it is found that in RMHMC an initial setting of $t_f \leftarrow \bar{T}_0/8$ may not be appropriate. This is because typically the mean period $\bar{T}_0$ in RMHMC is fairly long, and setting $t_f \leftarrow \bar{T}_0/8$ typically leads to a large proportion of rejected candidates in sampling from $\pi(\mathbf{q}|\mathcal{F}_1)$. To address this issue, we develop an approach to initialize t_f based on the traveling time from $\mathcal{F}_2$ to $\mathcal{F}_1$. Specifically, for the initial subset with N samples sorted according to ascending order of limit-state function values, the $N \cdot p_0^{\text{th}}$ sample is selected and the time to travel to the boundary of $\mathcal{F}_1$ is crudely estimated. The implementation detail is described in [Appendix A](#). With t_f initialized, in each intermediate step of RMHMC-SS the adaptive tuning technique is the same as in [10]. To make this paper self-contained, the adaptive tuning technique is listed in [Appendix B](#).

To conclude this section, the overall procedures of RMHMC-SS are given as follows.

Algorithm 2: Procedures of RMHMC-SS

Step 1 Initialization

- Set N , the number of samples in each subset.
- Set percentile p_0 .
- Set Δt , the incremental step in leapfrog integrator.

Step 2 Initial run

- Generate N random samples from $\pi(\mathbf{q})$, denoted by $\{\mathbf{q}_0^{(i)}, i = 1, 2, \dots, N\}$, via i.i.d. sampling (if feasible) or RMHMC sampling with thinning (if i.i.d. sampling is unfeasible).
- Sort $\{\mathbf{q}_0^{(i)}, i = 1, 2, \dots, N\}$ in ascending order of the limit-state function values $G(\mathbf{q}_0^{(i)})$.
- Set $j \leftarrow 1$
- Set g_j as the p_0 -percentile of $G(\mathbf{q}_0^{(i)})$, so that $\mathcal{F}_j = \{\mathbf{q} | G(\mathbf{q}) - g_j \leq 0\}$.

Step 3 Subsequent iterations

Repeat while $g_j > 0$

- **if** $j = 1$ **then**
 Initialize t_f using [Algorithm 3](#).
- **else**
 Initialize t_f as the value of t_f in the $j - 1$ step.
- **end**
- Randomly permute the first $N \cdot p_0$ samples in $\{\mathbf{q}_j^{(i)}\}$, and discard the rest.
- Using the permuted $N \cdot p_0$ samples as seeds, run [Algorithm 1](#) in conjunction with [Algorithm 4](#) until N samples from $\pi(\mathbf{q}|\mathcal{F}_j)$ are obtained, and label them as $\{\mathbf{q}_j^{(i)}\}$.
- Sort $\{\mathbf{q}_j^{(i)}, i = 1, 2, \dots, N\}$ in ascending order of the limit-state function values $G(\mathbf{q}_j^{(i)})$.
- Set $g_{(j+1)}$ as the p_0 -percentile of $\{G(\mathbf{q}_j^{(i)}), i = 1, 2, \dots, N\}$.
- Set $j \leftarrow j + 1$

Step 4 Evaluate the failure probability

- Estimate the failure probability using [Eq.\(4\)](#).

It is important to note from the algorithm that if independent sampling for the initial subset is impossible,

one could generate a long Markov chain with $k \cdot N$ samples and thin it into N to reduce the correlations. The effects of thinning are extensively discussed in [10]. Moreover, in Step 3 since the $N \cdot p_0$ chains are independent from each other, one could parallelize the computational codes of this step to facilitate efficient implementations.

5. Numerical investigations

5.1. Typical behavior of RMHMC method

To illustrate the typical behavior of the RMHMC method, we use HMC and RMHMC to sample from an $(n + 1)$ -dimensional Neal’s funnel distribution introduced in [24]

$$\pi(x_1, \dots, x_{n+1}) = \prod_{i=1}^n \mathcal{N}(x_i | 0, e^{x_{n+1}}) \cdot \mathcal{N}(x_{n+1} | 0, 1), \quad (22)$$

where $n = 100$. First, the HMC and RMHMC are used to generate two long Markov chains of 5000 samples starting from the tail region with the initial position $[0.1, 0.1, \dots, 0.1, -4]^\top$. The incremental time step Δt is set to 0.01 for both methods, and $\alpha = 1 \times 10^6$ is adopted for the SoftAbs map in RMHMC. The Markov chains obtained from the two methods, and the corresponding energy trajectories are shown in Figure 2.

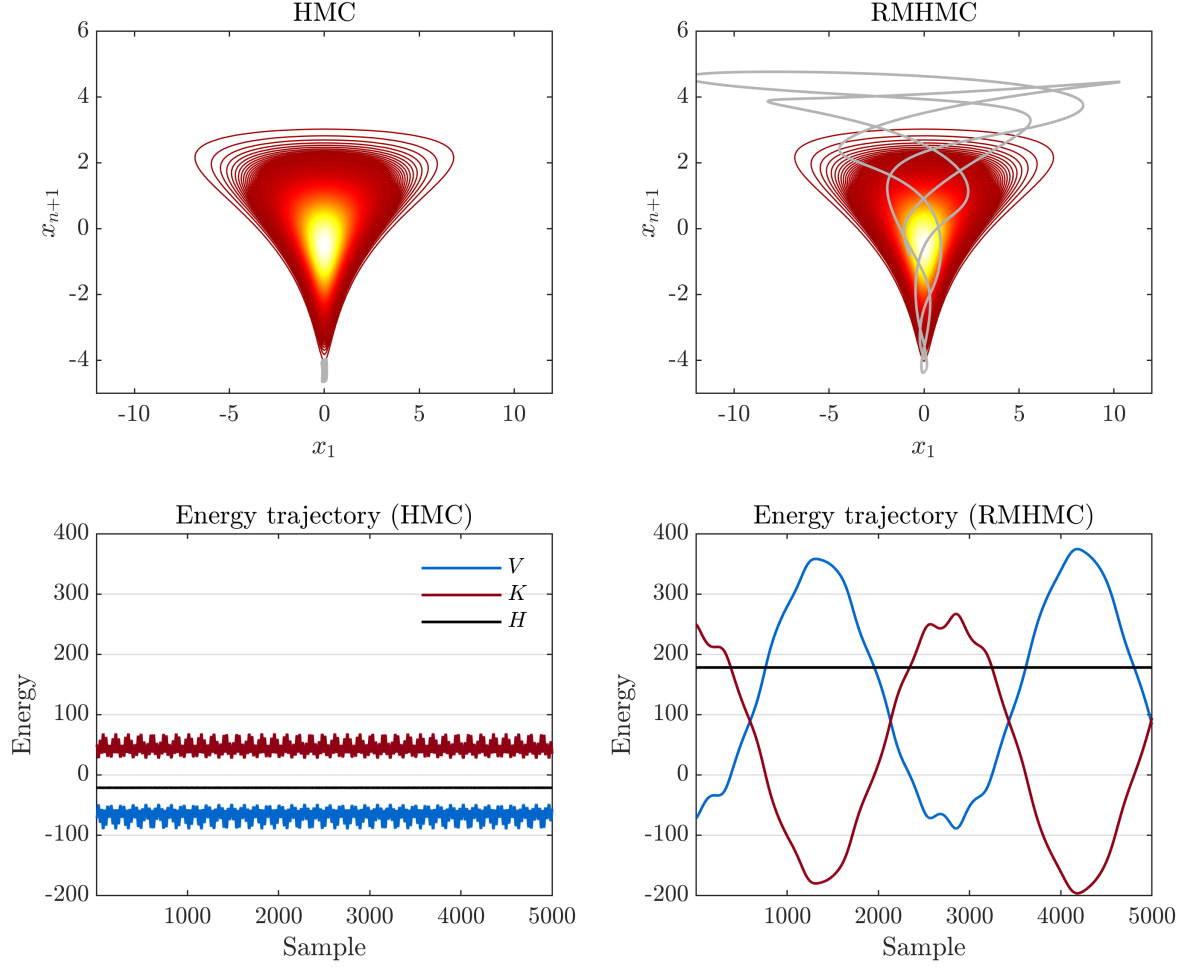


Figure 2: Markov Chain trajectories obtained from HMC and RMHMC methods projected to the x_1 - x_{n+1} plane, and the corresponding energy trajectories. Notice the grey cluster of the trajectory in the tail of the funnel distribution on the top left panel (HMC). On the contrary, the RMHMC trajectory on the top right panel explores effectively the distribution.

It is clearly illustrated that the HMC trajectories barely move (concentrated in the tail regions). This supports the statement in Section 3 that an approximately constant kinetic energy (red lines in Figure 2) may not be large enough to drive the Hamiltonian system to explore the typical set. The RMHMC trajectories exhibit more effective exploration of the probability space, and they collectively resemble the shape of the funnel distribution. Moreover, it is seen from the energy trajectories that the RMHMC spans much larger energy levels than the HMC, and the period of RMHMC is significantly longer (Figure 2, bottom panels).

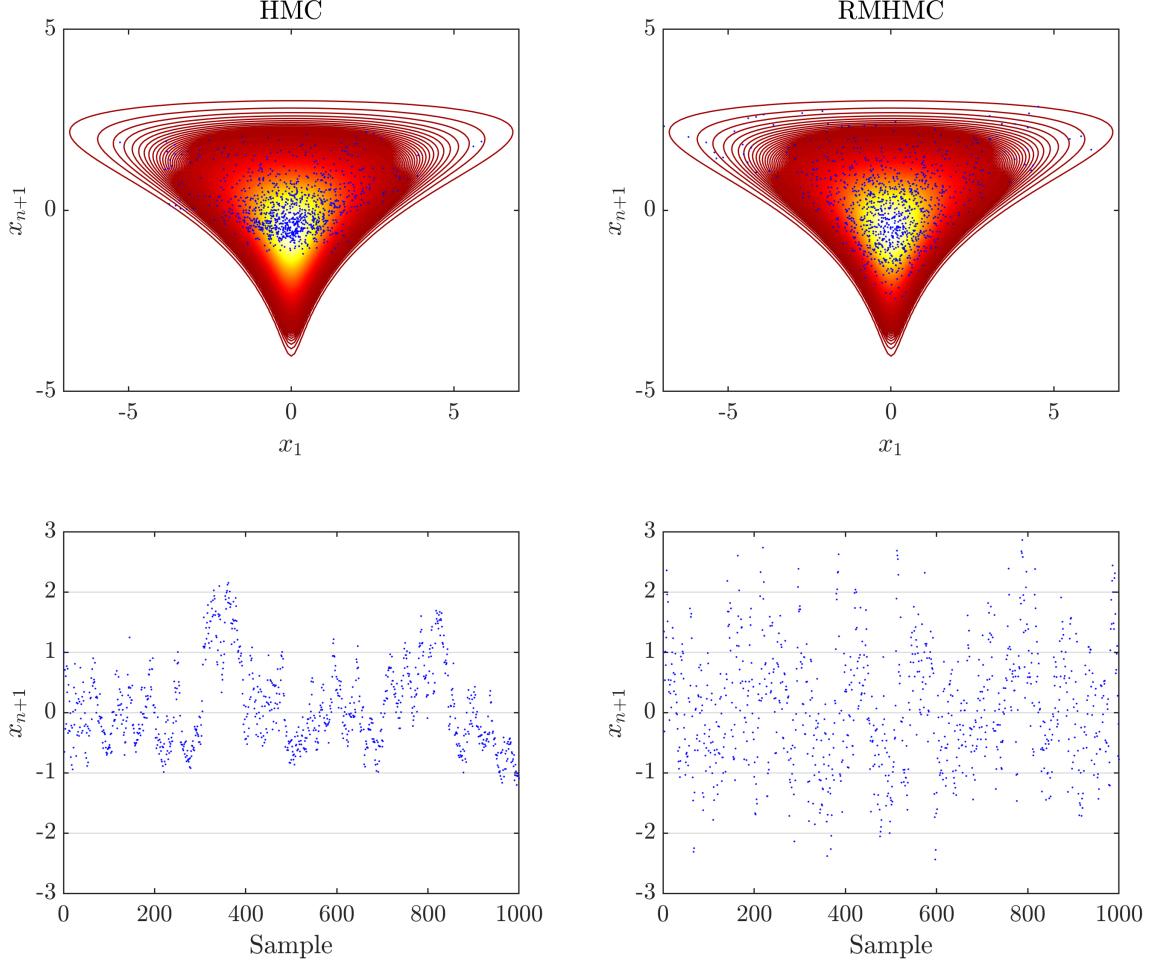


Figure 3: Samples obtained from long HMC and RMHMC chains in the x_1 - x_{n+1} plane, and the x_{n+1} coordinate values.

Next, we generate 1000 samples (Figure 3) started from the high density region with the initial position $[1, 1, \dots, 1]^\top$. The incremental time step Δt is set to 0.05 for both methods, and $\alpha = 1 \times 10^6$ is again used for the SoftAbs map in RMHMC. Figure 3 indicates that the correlation of RMHMC samples is noticeably weaker than that of the HMC samples. As aforementioned, for distribution models where independent and identically distributed (i.i.d) samples are difficult to generate, one needs to use MCMC algorithm to generate samples for the initial subset. For such cases, the low correlation feature of RMHMC makes it particularly attractive for subset simulation.

In subset simulation, several short Markov chains are generated at each intermediate subset level. To illustrate the collective behavior of multiple short chains, using the HMC and RMHMC we generate 100 short chains while each chain only contains 10 samples. The 100 seed samples for the short chains are obtained by the following two steps: i) we generate a chain of 10 samples starting from the initial position $[1, 1, \dots, 1]^\top$; ii) we choose the previous 10 samples as initial positions and generate 10 chains with 10 samples each chain. It is seen from Figure 4 that the correlation of RMHMC samples is noticeably weaker than that of the HMC samples. Therefore, even for the short Markov chains, the performance of the RMHMC is better than that of the HMC.

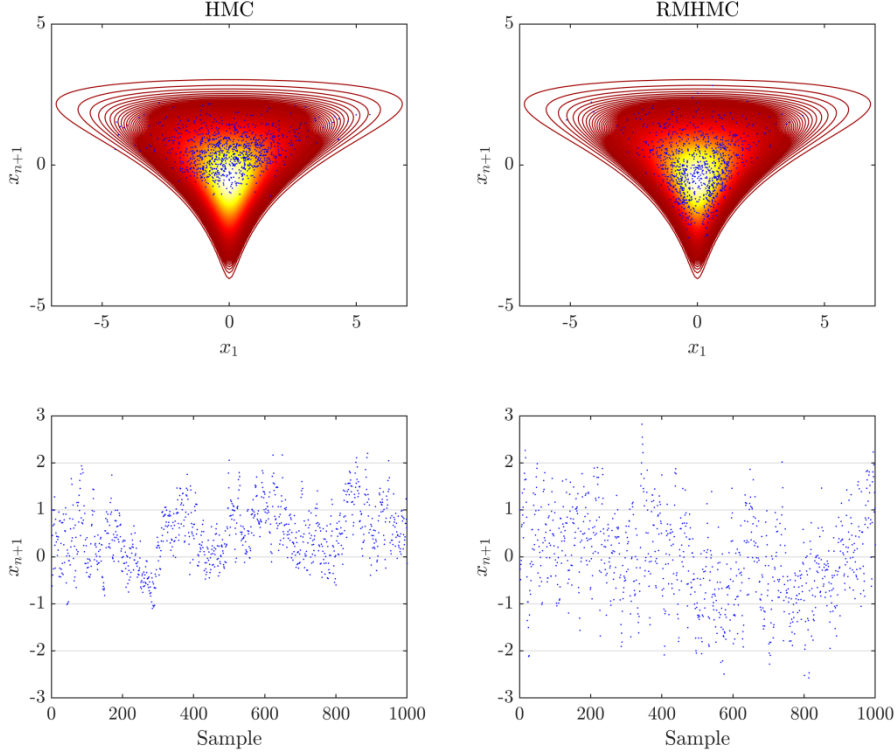


Figure 4: Samples obtained from short chains of HMC and RMHMC in the x_1 - x_{n+1} plane, and the x_{n+1} coordinate values.

5.2. Reliability analysis examples

In this section, RMHMC-SS will be tested and compared with HMC-SS for reliability examples with highly-curved probability spaces. In all the following examples, the parameters of subset simulation, N and p_0 are set as 1000 and 0.1, respectively. The incremental time step Δt is set to 0.01 for both methods, and α for the SoftAbs map in RMHMC is selected such that the leapfrog integrator is stable. The HMC-SS and RMHMC-SS will be run 100 times to obtain various statistics of the probability estimates.

5.2.1. Hyperspherical limit-state function with funnel distribution

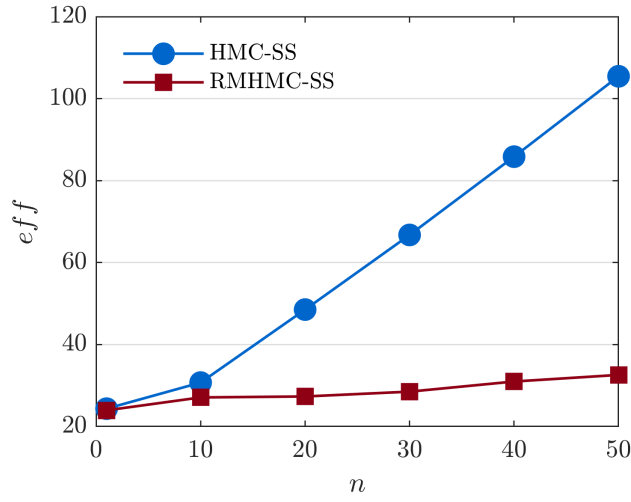
Consider a hyperspherical limit-state function defined by

$$G(\mathbf{x}, x_{n+1}) = \sum_{i=1}^n x_i^2 + (x_{n+1} + a)^2 - r^2, \quad (23)$$

where $a = 6$ and $(\mathbf{x}, x_{n+1})$ follows the $(n+1)$ -dimensional Neal's funnel distribution defined in Eq.(22). To study the influence of dimensionality, r is fixed to 2 and subset simulation is performed for a sequence of dimensions ranging from 2 to 51. The simulation results obtained from HMC-SS, RMHMC-SS and crude MCS with 10^7 runs are given in Table 1. In the table the mean number of limit-state function evaluations is denoted as NG . According to [31], we use $eff = \text{c.o.v} \times \sqrt{NG}$ to measure the efficiency of the sampling method. A low eff indicates high efficiency. The eff against the dimensionality n is plotted in Figure 5. It can be concluded that RMHMC-SS is particularly efficient for relatively high dimensions.

Table 1: Comparison between HMC-SS and RMHMC-SS for various dimensions

n	HMC			RMHMC			MCS	
	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v
1	3.13×10^{-5}	0.36	4600	3.11×10^{-5}	0.35	4761	3.12×10^{-5}	0.057
10	2.75×10^{-5}	0.45	4618	2.75×10^{-5}	0.39	4802	2.46×10^{-5}	0.064
20	2.37×10^{-5}	0.71	4685	2.33×10^{-5}	0.39	4859	2.20×10^{-5}	0.067
30	1.89×10^{-5}	0.95	4946	1.99×10^{-5}	0.41	4905	2.00×10^{-5}	0.071
40	1.98×10^{-5}	1.22	4951	1.57×10^{-5}	0.44	5071	1.68×10^{-5}	0.077
50	1.70×10^{-5}	1.48	5077	1.37×10^{-5}	0.45	5152	1.40×10^{-5}	0.085

Figure 5: The eff - n curves for various methods

Next, to study the influence of the level of failure probability, we fix the dimensionality to 51 and run subset simulation for a sequence of r values. Table 2 reports the results and Figure 6 illustrates the eff - β curve, where $\beta = -\Phi^{-1}(p_f)$ is the generalized reliability index ($\Phi^{-1}(\cdot)$ is the inverse CDF function of standard Gaussian distribution).

Table 2: Comparison between HMC-SS and RMHMC-SS for various probability levels

r	HMC			RMHMC			MCS	
	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v
5	3.28×10^{-2}	0.15	1900	3.33×10^{-2}	0.13	2220	3.28×10^{-2}	0.0017
4	5.80×10^{-3}	0.27	2791	5.90×10^{-3}	0.21	3117	5.80×10^{-3}	0.0041
3	4.80×10^{-4}	0.52	3646	4.74×10^{-4}	0.34	4009	4.61×10^{-4}	0.015
2	1.70×10^{-5}	1.48	5077	1.37×10^{-5}	0.45	5152	1.40×10^{-5}	0.085
1	1.26×10^{-7}	2.69	7174	1.36×10^{-7}	0.55	7065	-	-

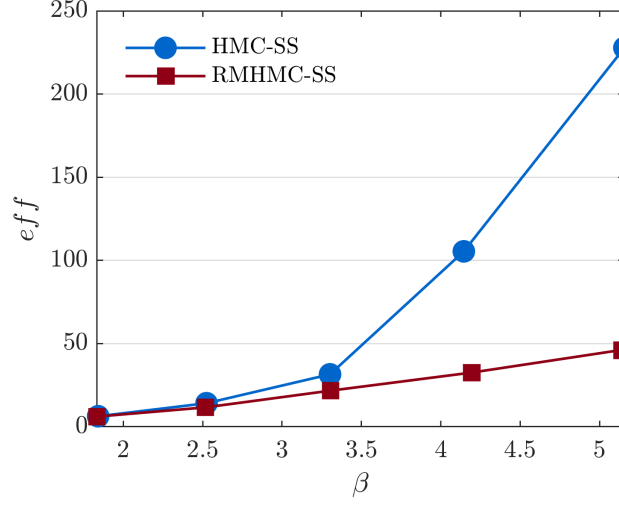


Figure 6: The eff - β curves for various methods

Note that for this example one can transform the distribution space to the standard Gaussian, and if a HMC-SS is run there one may expect different results compared from those in Table 1 and Table 2.

5.2.2. Ring-shaped conditional distribution in a Bayesian context

Consider a “ring-shaped” conditional distribution $\pi(\boldsymbol{\theta}|\mathbf{x}) = \pi(\theta_1, \theta_2, \dots, \theta_n|\mathbf{x})$. The parameter $\mathbf{x}$ can be regarded as observation data in Bayesian analysis. We let the components of $\boldsymbol{\theta}$ and $\mathbf{x}$ independently follow the Gaussian distributions

$$\theta_i \sim \mathcal{N}(0, 1), i = 1, 2, \dots, n, \quad (24)$$

and

$$x_j \sim \mathcal{N}(\mu_x, \sigma_x^2), j = 1, 2, \dots, 100, \quad (25)$$

where $\mu_x = 2$ and $\sigma_x = 4$.

The likelihood function $\mathcal{L}(\mathbf{x}|\boldsymbol{\theta})$ is defined as

$$\mathcal{L}(\mathbf{x}|\boldsymbol{\theta}) := \prod_{j=1}^{100} \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{(x_j - s_\theta)^2}{2\sigma_x^2} \right], \quad (26)$$

where

$$s_\theta := \sum_{i=1}^n \theta_i^2. \quad (27)$$

Using Bayes rule, the ring-shaped conditional distribution can be expressed as

$$\pi(\boldsymbol{\theta}|\mathbf{x}) \propto \pi(\boldsymbol{\theta})\mathcal{L}(\mathbf{x}|\boldsymbol{\theta}) \propto \exp \left[-\frac{s_\theta}{2} - \frac{1}{2\sigma_x^2} \sum_{j=1}^{100} (x_j - s_\theta)^2 \right]. \quad (28)$$

Using Eq.(25), we draw a random sample of $\mathbf{x}$, denoted by $\mathbf{x}_o$, and fix $\mathbf{x}_o$ hereafter. In the context of Bayesian analysis this suggests that an observation is made and recorded. Now the limit-state function is defined as

$$G(\boldsymbol{\theta}) = r^2 - (\theta_1 - 2)^2 - \sum_{i=2}^n \theta_i^2, \quad (29)$$

where $r = 3.6$. We are interested in the posterior failure probability $\mathbb{P}(G(\boldsymbol{\theta}) \leq 0)$, $\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta}|\mathbf{x}_o)$. The prior and posterior distributions of $\boldsymbol{\theta}$ (with a dimension of 2) and the limit-state surface are illustrated in Figure 7.

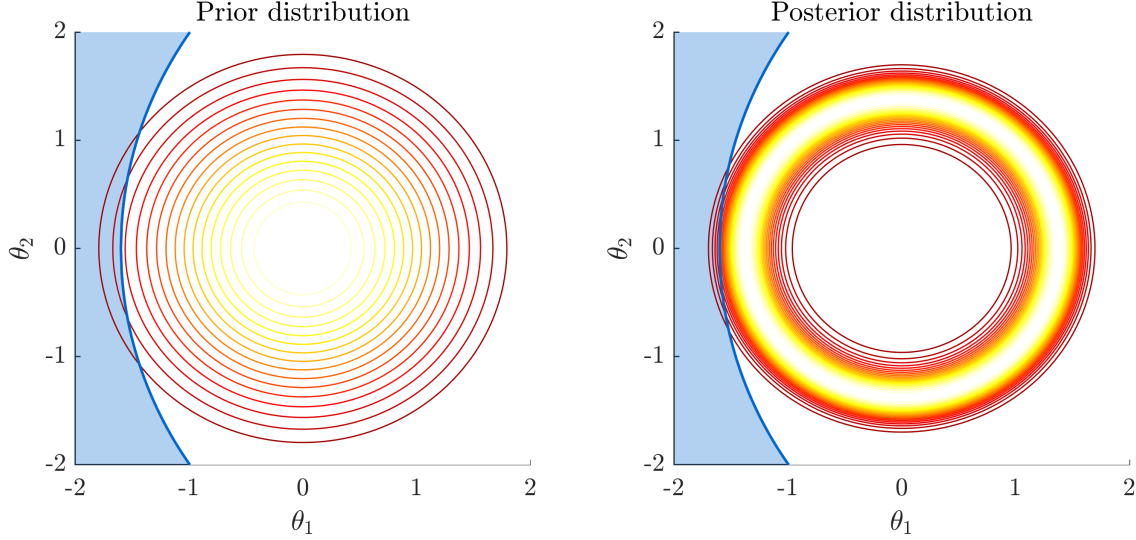


Figure 7: **The prior distribution $\pi(\boldsymbol{\theta})$ and the posterior distribution $\pi(\boldsymbol{\theta}|\mathbf{x}_o)$.** The blue line represents the limit-state surface, and the shaded area represents the failure domain.

To study the influence of dimensionality, subset simulation is performed for a sequence of dimensions ranging from 2 to 10. The performance of various methods are shown in Table 3. In contrast with the previous example, here a direct independent sampling from the posterior distribution is difficult, and thus the reference solution is obtained using 10^6 samples (for each run) drawn by an affine invariant MCMC sampler [32]. The MCMC is independently performed 50 times to obtain the mean and coefficient of variation for the probability estimate.

Table 3: Comparison between HMC-SS and RMHMC-SS for various dimensions

n	HMC-SS			RMHMC-SS			MCMC	
	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v
2	5.00×10^{-3}	0.42	2800	5.00×10^{-3}	0.23	2913	4.80×10^{-3}	0.018
4	6.47×10^{-4}	0.69	3529	7.56×10^{-4}	0.28	3647	7.37×10^{-4}	0.051
6	2.05×10^{-4}	1.14	3930	2.10×10^{-4}	0.41	3828	1.99×10^{-4}	0.13
8	7.65×10^{-5}	1.22	4438	6.32×10^{-5}	0.42	4594	6.53×10^{-5}	0.24
10	3.28×10^{-5}	1.48	4600	2.89×10^{-5}	0.50	4686	3.03×10^{-5}	0.33

Table 3 demonstrates the superior performance of RMHMC-SS over HMC-SS. Figure 8 illustrates the $eff-n$ curve.

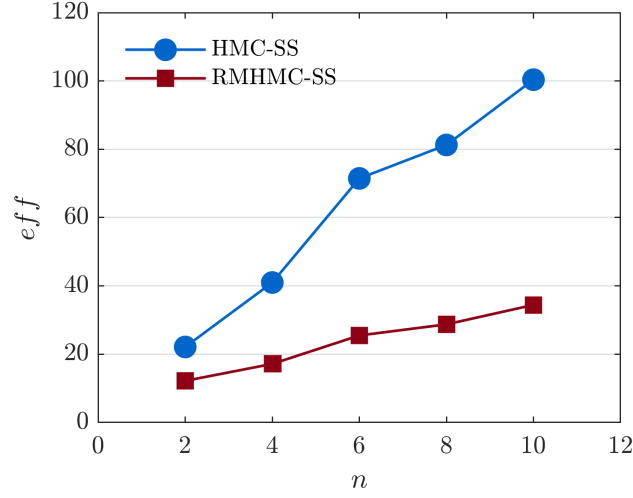


Figure 8: The eff - n curves for various methods.

309 Next, to study the influence of the level of the failure probability, we fix the dimensionality to 10 and
 310 run subset simulation for a sequence of r values. Table 4 reports the results, and Figure 9 illustrates the
 311 relation between eff and β .

Table 4: Comparison between HMC-SS and RMHMC-SS for various probability levels

r	HMC-SS			RMHMC-SS			MCMC	
	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v
3.40	1.50×10^{-3}	0.34	3016	1.40×10^{-3}	0.26	2937	1.43×10^{-3}	0.101
3.45	6.64×10^{-4}	0.49	3581	6.46×10^{-4}	0.31	3711	6.34×10^{-4}	0.11
3.50	2.50×10^{-4}	0.66	3691	2.44×10^{-4}	0.35	3767	2.50×10^{-4}	0.18
3.55	9.95×10^{-5}	1.09	4349	8.85×10^{-5}	0.39	4390	8.87×10^{-5}	0.24
3.60	3.28×10^{-5}	1.48	4600	2.89×10^{-5}	0.50	4686	3.03×10^{-5}	0.33
3.65	7.56×10^{-6}	1.87	5354	7.06×10^{-6}	0.58	5354	6.86×10^{-6}	0.79

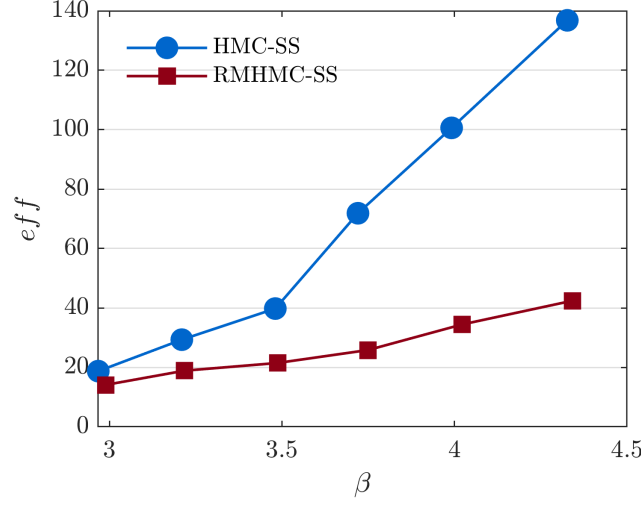


Figure 9: The eff - β curves for various methods

5.2.3. Posterior failure probability for static structural analysis

Consider a shear-frame structure shown in Figure 10. The first and second story masses are 1.65×10^4 and 1.61×10^4 [kg], respectively. The inter-story stiffnesses are parameterized as $k_1 = \bar{k}_1 x_1$ and $k_2 = \bar{k}_2 x_2$, where $\bar{k}_1 = \bar{k}_2 = 2.97 \times 10^7$ [N/m] and $\mathbf{x} = [x_1, x_2]^\top$ are independent random variables following a lognormal distribution with mean [1.3, 0.8] and unit standard deviations. After introducing observations on natural frequencies, the posterior distribution of $\mathbf{x}$ can be expressed as [33]

$$\pi_{\mathcal{D}}(\mathbf{x}) \propto \exp \left[-\frac{J(\mathbf{x})}{2\epsilon^2} \right] \pi(\mathbf{x}),$$

$$J(\mathbf{x}) = \sum_{j=1}^2 \lambda_j^2 \left[\frac{f_j^2(\mathbf{x})}{\tilde{f}_j^2} - 1 \right]^2, \quad (30)$$

where $\pi(\mathbf{x})$ is prior distribution of $\mathbf{x}$, and $\tilde{f}_j$ is the observed natural frequencies of the structure. In this example, we set the observed natural frequencies $\tilde{f}_1$ and $\tilde{f}_2$ to 3.13 and 9.83 [Hz], respectively, $\epsilon = 1/\sqrt{8}$ and $\lambda_1 = \lambda_2 = 1$. The lateral forces F_1 and F_2 are set to 1.50×10^5 and 2.50×10^5 [N], respectively.

The limit-state function is defined as

$$G(\mathbf{x}) = r - \max(\mathbf{d}(\mathbf{x})), \quad (31)$$

where $\mathbf{d} = [d_1, d_2]$ represents the first and second interstory drift. The threshold r is set to 5% of the story height h , corresponding to the serviceability limit state, and we set $h = 3$ [m]. Note that the interstory drift is defined as the relative displacement between two consecutive stories divided by the height.

The prior and posterior distributions of $\mathbf{x}$ and the limit-state function are illustrated in Figure 11. Now the HMC-SS and RMHMC-SS are used to estimate the failure probability corresponding to the posterior distribution of $\mathbf{x}$. Similar to the previous example, the reference solution is obtained from 50 runs of MCMC with 10^6 samples for each run. The results are reported in Table 5.

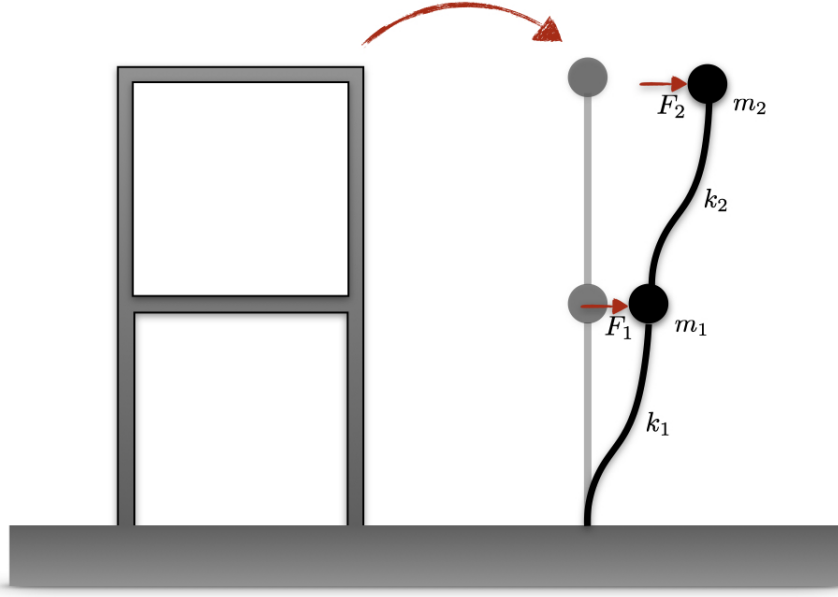


Figure 10: Structural archetype.

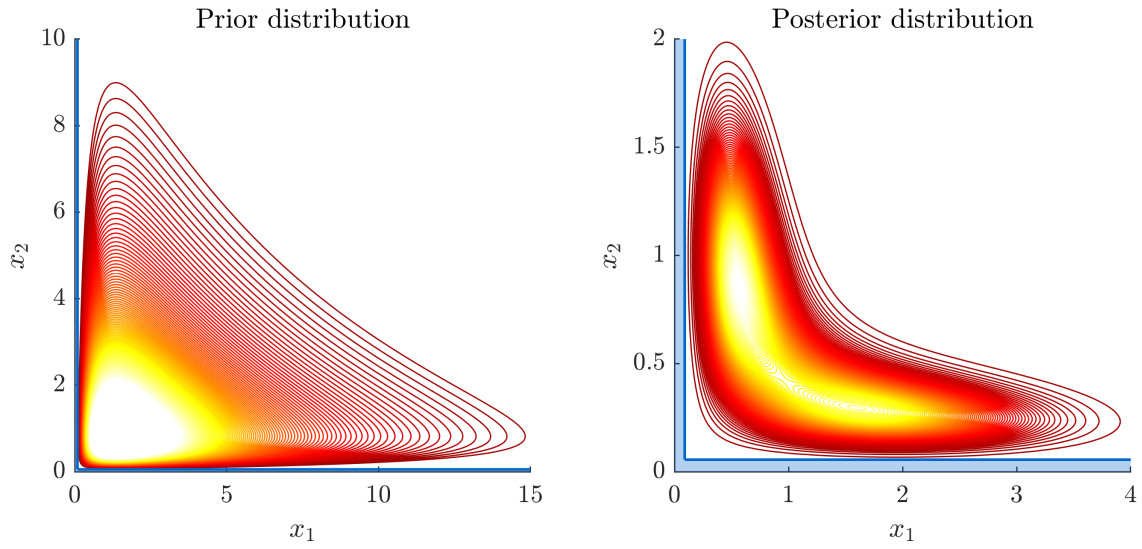


Figure 11: **The prior distribution $\pi(\mathbf{x})$ and the posterior distribution $\pi(\mathbf{x}|\tilde{f})$.** The blue line represents the limit-state surface, and the shaded area represents the failure domain.

Table 5: Performance of RMHMC-SS for estimating reliability of uncertain structure

r	HMC-SS			RMHMC-SS			MCMC	
	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v	NG	$\hat{p}_f$	c.o.v
0.15	1.79×10^{-4}	1.48	4105	1.79×10^{-4}	0.63	4254	1.78×10^{-4}	0.17

Finally, it is of interest to note that instead of directly sampling from the Posterior distribution, another solution for the Bayesian reliability problems is to formulate the problem in the probability space of the prior distribution [34]. This approach essentially transforms the complexity of the posterior distribution into that of an equivalent limit-state function. A comparison of this approach with the direct RMHMC-SS approach can be an interesting topic for future studies.

6. Practical issues, limitations, and future directions

6.1. Multi-mode and topological shift in failure domains

In subset simulation, the Markov chains obtained from MCMC are relatively short and the newly generated samples may cluster in the vicinity of the seeds. Consequently, when the topology of $G(\mathbf{x}) = g$ changes dramatically with g (e.g., “mode-splitting” or “mode-merging” with varying g), the Markov chains may march into wrong directions. To illustrate this behavior, we consider a $\pi(\mathbf{x})$ as the two-dimensional Neal’s funnel distribution, and a limit-state function with the following form (a variant of [35])

$$G(\mathbf{x}) = \frac{0.6}{((x_1 + 5)^2/18 + (x_2 + 0.5)^2/60)^2 + 1} + \frac{0.6}{((x_1 - 5)^2/18 + (x_2 + 0.5)^2/60)^2 + 1} - 0.25. \quad (32)$$

The probability density and limit-state functions are shown in Figure 12. It can be seen from the figure that $G(\mathbf{x}) = g$ has a topological change (“mode-splitting”) as g increases. In the context of subset simulation, this implies that from $\mathcal{F}_1$ to $\mathcal{F}_M = \mathcal{F}$, the safe domain evolves from disconnected (with two modes) to connected.

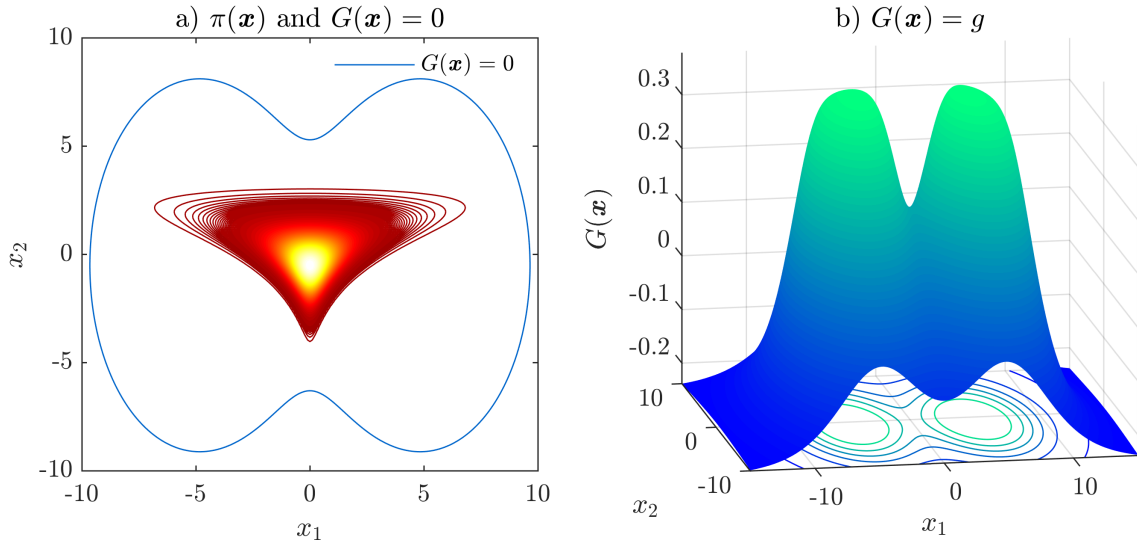


Figure 12: The probability density and limit-state functions.

Figure 13 and Figure 14 illustrate the samples drawn from the RMHMC-SS using $p_0 = 0.1$, $N = 1000$ and $p_0 = 0.6$, $N = 3000$, respectively. It is important to observe from the figures that increasing p_0 and

347 N would help the Markov chains get out of the local insignificant domains. Note that we cannot obtain a
348 result similar to Figure 14 using the HMC-SS approach.

349 A practical diagnosis for the possibility of being absorbed into the local insignificant minima/maxima is
350 to monitor the multi-mode behaviour of the probability estimate as the algorithm is run multiple times. For
351 this particular example, if the Markov chain proceeds to the correct domain, the probability estimate would
352 be at the scale of 10^{-4} ; while if the chain proceeds to the local insignificant domain, the probability estimate
353 would be at the scale of 10^{-10} . Therefore, if one observes two clusters of probability estimates, one may
354 expect the aforementioned issue has happened. Consequently, instead of averaging over all the probability
355 estimates, only considering the cluster around 10^{-4} would be more appropriate.

356 Finally, it is worth mentioning that RMHMC-SS is similar to a multi-start momentum driven stochastic
357 optimization algorithm. For a single run, the algorithm can march into a local minima where the probability
358 content is low. However, this is a common problem in the field of global optimization and a stochastic
359 algorithm has the advantage in that by repeated runs the risk of getting trapped decreases. A deterministic
360 algorithm can also employ a multiple run strategy with different starting points; however, it will also be more
361 difficult to escape from the local minima since the stochastic momentum is not present. In addition, the
362 aforementioned observation is more prominent for low dimensional problems, since in high dimensions the
363 model functions are typically more flat, and the saddle points become a new challenge. For the challenges
364 posed by saddle points, again, the stochastic momentum can be important and useful. A complete (and
365 mathematical) analysis of these problems is out of the scope of this paper while it is an active research
366 direction both in the reliability and optimization field.

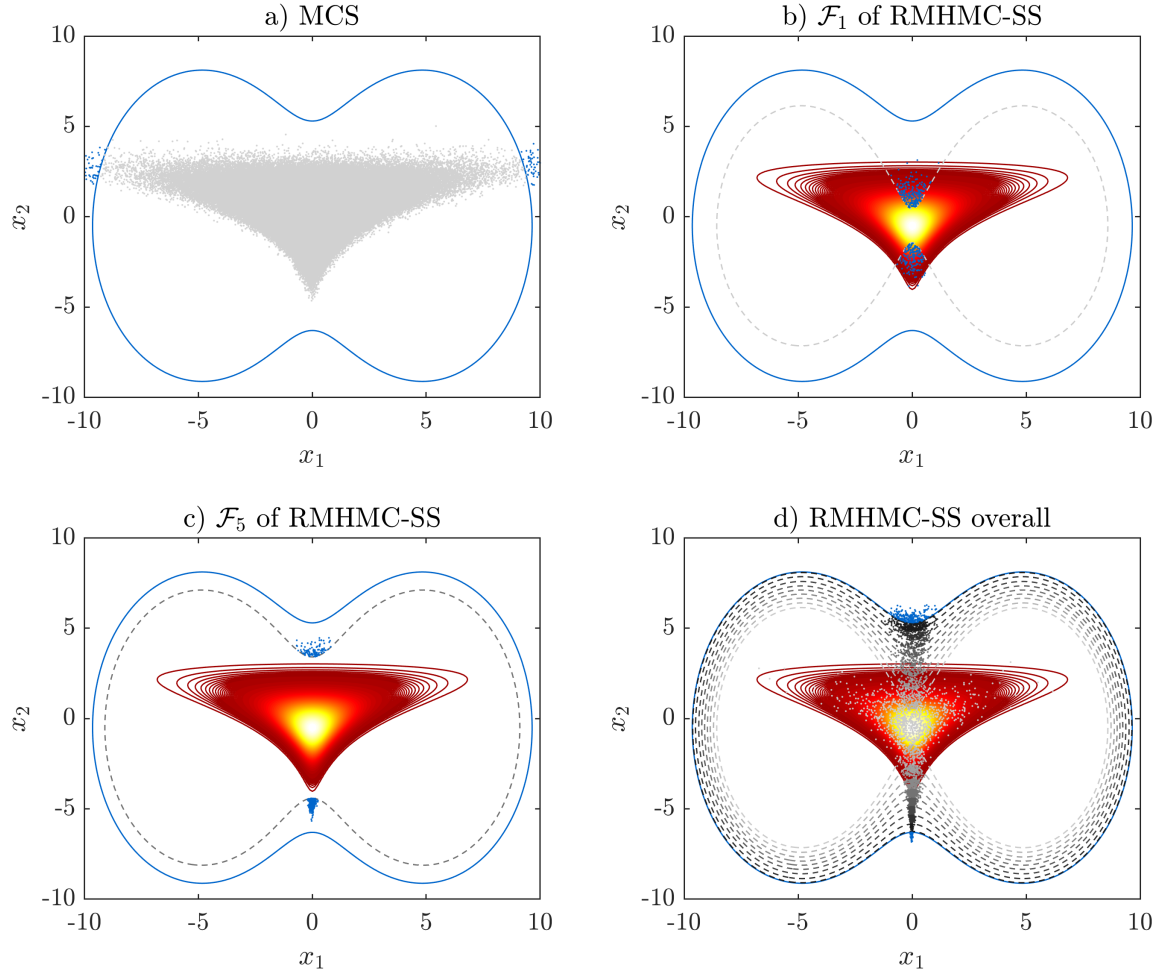


Figure 13: **The trajectories of RMHMC-SS using $p_0 = 0.1$ and $N = 1000$.** a) Samples obtained from MCS; those in the failure domain are marked with blue, those in the safe domain are marked with grey; b) Samples obtained from the first subset using RMHMC-SS; c) Samples obtained from the fifth subset using RMHMC-SS; d) The overall trajectories of RMHMC-SS.

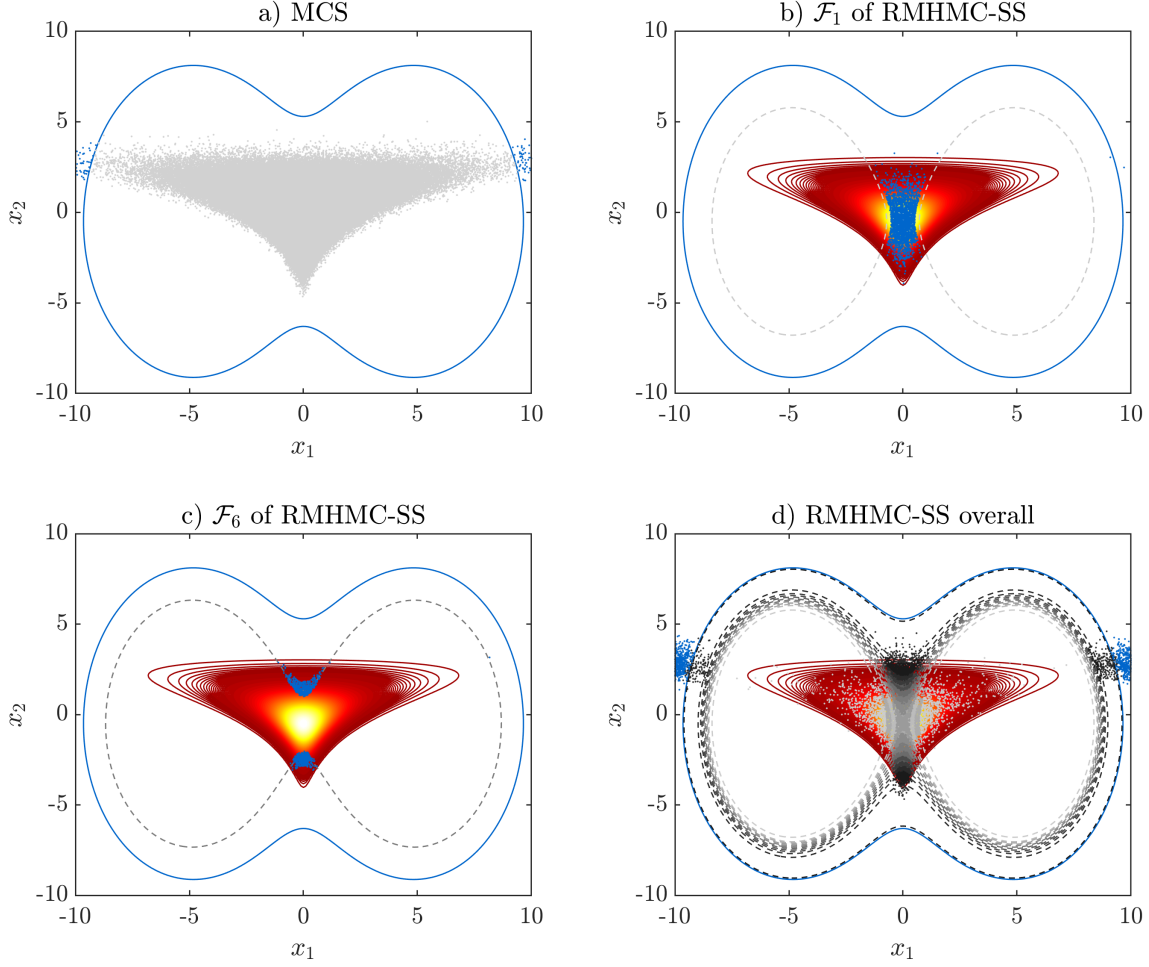


Figure 14: **The trajectories of RMHMC-SS using $p_0 = 0.6$ and $N = 3000$.** a) Samples obtained from MCS; those in the failure domain are marked with blue, those in the safe domain are marked with grey; b) Samples obtained from the first subset using RMHMC-SS; c) Samples obtained from the sixth subset using RMHMC-SS; d) The overall trajectories of RMHMC-SS.

6.2. Computational complexity of RMHMC-SS

Other than the limit-state function evaluations, the major computational effort of RMHMC lies in the Riemannian metric construction. If the original Hessian matrix cannot be directly used (i.e., not positive definite), the surrogate Hessian approach typically involves eigen-analysis on the original Hessian. The trade-off is that the more geometrical information we want to extract from the Hessian matrix, the more computational cost we may expect. Therefore, the study of effective sparsity constrained Riemannian metric is meaningful.

6.3. RMHMC-SS with bouncing

A possible extension of the current RMHMC-SS approach is to introduce the barrier bouncing mechanism to replace the rejection sampling. As studied in [10], the barrier bouncing based approach typically achieves fairly small c.o.v. at the cost of gradient computations of the limit-state function. For reliability problems with finite-element models, the requirement for gradient computations is not ideal. However, one possible solution is to consider the metamodeling technique. Another interesting direction is to construct a barrier bouncing based RMHMC-SS for Approximate Bayesian Computation.

6.4. Credible interval of the probability estimator

In this study, the coefficient of variation (c.o.v.) is used to compare the variability of different methods. This together with an error measure provide a general evaluation on the efficiency and accuracy of the proposed RMHMC-SS approach. However, it is noted that the estimator of subset simulation is biased and skewed, and thus $\bar{p}_f \pm b \cdot c.o.v.$ may not be a good estimator on the credible interval. Typically, obtaining the credible intervals of failure probability estimates requires multiple analysis runs [34]. Therefore, further studies along this direction will be meaningful.

7. Conclusions

In this paper, the Riemannian Manifold Hamiltonian Monte Carlo (RMHMC) method is applied to subset simulation (SS) to solve reliability problems defined in non-Gaussian space. By constructing the Hamiltonian on the Riemannian manifold of the target probability space, the RMHMC makes use of the second-order geometrical information and provides effective route for Markov chain evaluations. The benefit of RMHMC becomes more prominent when the target probability space is with large curvature and high dimensionality. This property makes RMHMC-SS particularly attractive for reliability problems defined in highly curved non-Gaussian spaces, e.g. Bayesian reliability problems. A sequence of numerical examples is studied to test and verify the RMHMC-SS approach. It is shown in the examples that the RMHMC-SS shows superior performance for reliability problems defined in highly curved non-Gaussian spaces.

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Appendix A. Initialization of t_f

Algorithm 3: Initialization of t_f

Step 1 Select the $N \cdot p_0^2$ -th sample

- For the initial subset with N samples sorted according to ascending order of limit-state functions, select the $N \cdot p_0^2$ -th sample and denote it by $\mathbf{q}^{(N \cdot p_0^2)}$.

Step 2 Compute the time T required for $\mathbf{q}^{(N \cdot p_0^2)}$ to move to the boundary of $\mathcal{F}_1$

foreach $L = 1, 2, \dots$ do

$$\left(\mathbf{q}^{(N \cdot p_0^2)}, \mathbf{p}\right)^{(0)} \xrightarrow{L \text{ leapfrog steps (Eq.(11))}} \left(\mathbf{q}^{(N \cdot p_0^2)}, \mathbf{p}\right)^{(L)} ;$$

if $\left(\mathbf{q}^{(N \cdot p_0^2)}, \mathbf{p}\right)^{(L)}$ lies outside the subset $\mathcal{F}_1$ then

set $T = L \cdot \Delta t$;

break;

end

end

Step 3 Initialize t_f

- Repeatedly run Step 2 m times with the estimated T in each run denoted by T_i , initialize t_f as $\text{mean}[T_i]$.

Note that the Step 2 in Algorithm 3 introduces additional limit-state function evaluations. However, it is found the m in Algorithm 3 can be set to as low as 5 without significantly compromising the performance. Also note that even one uses a poor initial t_f , the adaptive nature of the method to select t_f would gradually correct t_f to a reasonable range.

Appendix B. Adaptive rule to select t_f in RMHMC-SS

Algorithm 4: Adaptive rule to select t_f in RMHMC-SS

- Compute the acceptance rate, denoted as α , for every chains N_α chains simulated.

- if $\alpha < \alpha_{low}$, in general it is suggested $\alpha_{low} = 0.3$ then

$$t_f \leftarrow (\bar{T}/2\pi) \sin^{-1} \left\{ \sin(2\pi t_f / \bar{T}) \exp[(\alpha - \alpha_{low})/2] \right\} ;$$

- else if $\alpha > \alpha_{up}$, in general it is suggested $\alpha_{up} = 0.5$ then

$$t_f \leftarrow (\bar{T}/2\pi) \sin^{-1} \left\{ \sin(2\pi t_f / \bar{T}) \exp[(\alpha - \alpha_{up})/2] \right\} ;$$

end

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