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Hamiltonian Monte Carlo methods for Subset Simulation in reliability analysis

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ABSTRACT

This paper studies a non-random-walk Markov Chain Monte Carlo method, namely the Hamiltonian Monte Carlo (HMC) method in the context of Subset Simulation used for reliability analysis. The HMC method relies on a deterministic mechanism inspired by Hamiltonian dynamics to propose samples following a target probability distribution. The method alleviates the random walk behavior to achieve a more effective and consistent exploration of the probability space compared to standard Gibbs or Metropolis-Hastings techniques. After a brief review of the basic concepts of HMC method and its computational details, two algorithms are proposed to facilitate the application of HMC method to Subset Simulation in reliability analysis. Next, the behavior of the two HMC algorithms is illustrated using simple probability distribution models. Finally, the accuracy and efficiency of Subset Simulation employing the two HMC algorithms are tested using various reliability examples in both Gaussian and non-Gaussian spaces.

1. Introduction

Since analytical solutions of general reliability problems either at component or system level are usually unavailable, approximate reliability methods such as first- and second-order reliability methods [1,2], response surface methods [3,4], and Monte Carlo simulation (MCS) techniques [5–8] have gained wide popularity. Compared with other reliability methods, MCS has the benefits of being accurate, insensitive to the complexity of limit-state functions and straightforward to implement. On the other hand, the efficiency of MCS depends on magnitude of the estimated probability. Since most practical reliability problems are characterized by small failure probabilities, the MCS scheme using the original probability density function can be computationally inefficient and often infeasible. To enhance the efficiency of MCS, variance-reduction Monte Carlo methods have been developed. One powerful variance-reduction Monte Carlo method which has been widely used in reliability analysis is Subset Simulation [7]. The method expresses the failure domain of interest as the intersection of a sequence of nested intermediate failure domains, and the failure probability of interest is expressed as a product of conditional probabilities associated with the intermediate failure domains. Since the conditional probabilities are significantly larger than the target failure probability the computational cost of Subset Simulation is significantly lower than the crude MCS method. The challenge of the scheme, which consists of evaluating the intermediate conditional probabilities, is overcome by using efficient Markov Chain Monte Carlo (MCMC) methods. It is noted that approaches essentially similar to Subset Simulation have been independently developed for other statistical computing applications under the names, Sequential Monte Carlo method (or Particle Filters) [9] and Annealed Importance Sampling [10].

The crucial step in Subset Simulation is to obtain random samples according to a sequence of probability distributions that are conditional on nested intermediate failure domains. The efficiency and accuracy of Subset Simulation is directly affected by those of the MCMC algorithm used to produce random samples representing the conditional distributions in the sequence. In the current practice of Subset Simulation, various random-walk-based MCMC methods [11,12] are employed to generate samples based on each conditional distribution model in the sequence. In this paper, a non-random-walk MCMC method, namely the Hamiltonian Monte Carlo (HMC) method [13,14], is studied in the context of Subset Simulation for reliability analysis. The HMC method employs a deterministic mechanism inspired by Hamiltonian dynamics to propose samples for a target probability distribution. The method alleviates the random-walk behavior to achieve a more effective and consistent exploration of the probability space compared to standard Gibbs or Metropolis-Hastings techniques.

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Originally developed in 1987 by Duane et al. [13] under the name "Hybrid Monte Carlo" method for lattice field theory simulations in Lattice Quantum Chromodynamics, the HMC method has been introduced to mainstream statistical computing starting from the work of Neal [15] in 1993. The popularity of the HMC method has grown rapidly in recent years, and has proven a remarkable success in various statistical applications [16–18]. The HMC method has been applied to Bayesian analysis of structural engineering problems [19,20]. However, to our knowledge, the application of the HMC to reliability analysis has never been studied. Motivated by this perspective, the paper studies the application of HMC to Subset Simulation for reliability analysis. In this context, the accuracy and efficiency of the HMC are investigated and compared with the conventional random-walk Metropolis-Hastings algorithm.

The structure of this paper is as follows. Section 2 briefly reviews the Subset Simulation. Section 3 introduces general concepts of HMC. Section 4 develops the computational details of HMC algorithms for Subset Simulation method. Section 5 shows the behavior of HMC-based Subset Simulation using simple distribution models. Next, in both standard Gaussian space and non-Gaussian spaces, it is presented a series of numerical examples with analytical limit-state functions as well as structural reliability examples to test and demonstrate the validity of the method. Finally, Section 6 presents concluding remarks and future directions.

2. Subset simulation

In reliability analysis, the failure probability of a system with basic random variables $\mathbf{x} \in \mathbb{R}^n$ can be expressed by an integral,

$$P_f = \int_{\mathbb{R}^n} I_{\mathcal{F}}(\mathbf{x}) f(\mathbf{x}) d\mathbf{x} \tag{1}$$

where $I_{\mathcal{F}}(\cdot)$ is a binary indicator function which gives '1' if point $\mathbf{x}$ is within the failure domain $\mathcal{F}$, and '0' otherwise, and $f(\mathbf{x})$ is the joint probability density function (PDF) of $\mathbf{x}$. A common practice in reliability analysis is to apply a transformation to random variables $\mathbf{x}$, denoted by $\mathbf{x} = \mathrm{T}(\mathbf{u})$, so that $\mathbf{x}$ can be expressed in terms of independent standard Gaussian random variables $\mathbf{u}$. With the transformation, Eq. (1) can be rewritten as

$$P_f = \int_{\mathbb{R}^n} I_{\mathcal{F}}[\mathrm{T}(\mathbf{u})] \varphi(\mathbf{u}) d\mathbf{u} \tag{2}$$

where $\varphi(\mathbf{u})$ denotes the multivariate standard Gaussian PDF.

The Subset Simulation solution of Eq. (2) involves the construction of a sequence of nested intermediate failure domains, so that the failure domain of interest, $\mathcal{F}$, is expressed by

$$\mathcal{F} = \bigcap_{j=1}^{M} \mathcal{F}_j \tag{3}$$

where $\mathcal{F}_1 \supset \mathcal{F}_2 \supset ... \supset \mathcal{F}_M$, and $\mathcal{F} = \mathcal{F}_M$. The failure probability $P_f = \Pr(\mathbf{u} \in \mathcal{F})$ can be written as

$$\Pr(\mathbf{u} \in \mathcal{F}) = \prod_{j=1}^{M} \Pr(\mathbf{u} \in \mathcal{F}_j | \mathbf{u} \in \mathcal{F}_{j-1}) \tag{4}$$

where $\mathcal{F}_0 = \mathbb{R}^n$, thus $\Pr(\mathbf{u} \in \mathcal{F}_0) = 1$. Each $\Pr(\mathbf{u} \in \mathcal{F}_j | \mathbf{u} \in \mathcal{F}_{j-1})$ in Eq. (4) can be computed using

$$\Pr(\mathbf{u} \in \mathcal{F}_j | \mathbf{u} \in \mathcal{F}_{j-1}) = \int_{\mathbb{R}^n} I_{\mathcal{F}_j}(\mathbf{u}) \varphi(\mathbf{u}|\mathcal{F}_{j-1}) d\mathbf{u} \tag{5}$$

where $\varphi(\mathbf{u}|\mathcal{F}_{j-1})$ is the conditional/truncated multivariate standard Gaussian PDF. Using an MCMC technique to generate samples of $\varphi(\mathbf{u}|\mathcal{F}_{j-1})$, Eq. (5) can be evaluated by MCS, i.e.

$$\Pr(\mathbf{u} \in \mathcal{F}_j | \mathbf{u} \in \mathcal{F}_{j-1}) \cong \frac{1}{N} \sum_{i=1}^{N} I_{\mathcal{F}_j}(\mathbf{u}_i) \tag{6}$$

in which $\mathbf{u}_i$ are samples generated from conditional PDF $\varphi(\mathbf{u}|\mathcal{F}_{j-1})$. In implementations of Subset Simulation, the nested failure domains are chosen adaptively such that $\Pr(\mathbf{u} \in \mathcal{F}_j | \mathbf{u} \in \mathcal{F}_{j-1})$, $j = 1, 2, ..., M-1$, approximately equals to a specified percentile p_0. The failure probability is then estimated as follows

$$\widehat{P}_f = \frac{p_0^{M-1}}{N} \sum_{i=1}^{N} I_{\mathcal{F}_M}(\mathbf{u}_i) \tag{7}$$

where $\mathbf{u}_i$ are sampled from $\varphi(\mathbf{u}|\mathcal{F}_{M-1})$.

The estimator of the failure probability is biased because of the correlation of the samples [7] and the adaptive nature of the subsets [9]. The order of the bias is $O(N^{-1})$, which is negligible compare to the coefficient of variation (c.o.v.), $\delta_{\mathcal{F}}$, of the estimate. For a given run of the algorithm, an estimate of $\delta_{\mathcal{F}}$ is given as [7]

$$\delta_{\mathcal{F}}^2 \sim \sum_{j=1}^{M} \delta_j^2 \tag{8}$$

where δ_j is the c.o.v of the j-th subset which is given as follows

$$\delta_j = \sqrt{\frac{1-P_j}{NP_j}(1+\gamma_j)} \tag{9}$$

where $P_j = \Pr(\mathbf{u} \in \mathcal{F}_j | \mathbf{u} \in \mathcal{F}_{j-1})$ denotes the conditional probability, and γ_j is expressed as

$$\gamma_j = 2 \sum_{k=1}^{N/N_c - 1} \left(1 - \frac{kN_c}{N}\right) \rho_j(k) \tag{10}$$

where $N_c = p_0 N$ denotes the number of Markov chains at each subset level, and $\rho_j(k)$ is the average of the correlation coefficient at lag k of the stationary sequence $[I_{F_j}(\mathbf{u}_{j-1}^{(\frac{l-1}{p_0}+k)})$: $k = 1, ..., N/N_c]$, $l = 1, ..., N_c$, and $\rho_j(k)$ can be estimated directly from the sequence [7].

3. General concepts of Hamiltonian Monte Carlo method

This section provides a brief introduction of HMC method with the focus on its basic concepts. Detailed descriptions of the method can be found in [13,14]. Specifically, Section 3.1 introduces basic principles of Hamiltonian mechanics that are keys in formulating the HMC method. Then, Section 3.2 provides the ideas of HMC for sampling from a general distribution.

3.1. Hamiltonian mechanics

Hamiltonian mechanics was proposed to provide a reformulation of classical mechanics in a more abstract form, but later it made significant contributions to the development of statistical mechanics and quantum mechanics. The Hamiltonian Monte Carlo method uses a deterministic procedure inspired by Hamiltonian mechanics to generate samples based on the target probability distribution. In this section a brief introduction of Hamiltonian mechanics is first provided.

Hamiltonian mechanics describes the time evolution of a system in terms of position vector $\boldsymbol{q}$ and momentum vector $\boldsymbol{p}$. The dimension of $\boldsymbol{p}$ and $\boldsymbol{q}$ should be identical, and $(\boldsymbol{q}, \boldsymbol{p})$ defines a position-momentum phase space. The time evolution of the $(\boldsymbol{q}, \boldsymbol{p})$ system is governed by *Hamilton's equations* expressed by

$$\begin{aligned} \frac{d\boldsymbol{q}}{dt} &= \frac{\partial H}{\partial \boldsymbol{p}} \\ \frac{d\boldsymbol{p}}{dt} &= -\frac{\partial H}{\partial \boldsymbol{q}} \\ \frac{\partial H}{\partial t} &= -\frac{\partial L}{\partial t} \end{aligned} \tag{11}$$

where $L \equiv L(\boldsymbol{q}, \dot{\boldsymbol{q}}, t)$ is the *Lagrangian*, which (in the non-relativistic setting) corresponds to the discrepancy between kinetic energy and potential energy, or free energy; and $H = H(\boldsymbol{q}, \boldsymbol{p}, t)$ is the *Hamiltonian*,