# Conditional sampling using affine invariant ensemble MCMC: application to subset simulation

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## ABSTRACT

Subset simulation (SS) is an attractive method that is simple to implement and results in unbiased estimates for reliability analysis in high dimensional applications. Often the high coefficient of variation of the SS estimator is attributed to sampling fluctuation and correlation among the Markov Chain Monte Carlo (MCMC) samples. In this work, we use an ensemble MCMC sampler, which is known to produce independent samples with lower correlation lag for certain types of distributions, to generate samples for estimating the intermediate probabilities. The algorithm is particularly effective for estimating failure probabilities when random variables are highly correlated and non-Gaussian and therefore cannot be mapped to standard normal variables.

## 1 Introduction

The safety of a structure is quantified in terms of its probability of satisfactory performance, often termed as reliability. This safety can be defined in terms of system level reliability or component level reliability. The basic premise is the definition of performance criterion and quantification of uncertainties associated with the structural and loading patterns. Defining a function $G(\boldsymbol{U})$ such that $G(\boldsymbol{U}) < 0$ denotes the unsatisfactory performance of the system, the probability of failure, $P_F = 1 - R$, where $R$ is the reliability, is defined as $P_F = P[G(\boldsymbol{U}) < 0]$. Here $\boldsymbol{U}$ is a $n \times 1$ vector of uncorrelated standard normal random variables representing the uncertainties in the structure under considerations, say material properties, loading and boundary conditions, etc. It is typically assumed that correlated non-Gaussian random variables can be transformed into $\boldsymbol{U}$ through a suitable reversible transformation (Der Kiureghian and Liu, 1986). When the uncertainties are quantified in terms of random processes, it is assumed that an equivalent discretized random variable representation is possible (Sudret and Der Kiureghian, 2000; Ghanem and Spanos, 2003). Mostly, the $P_F$ is very small, rendering a brute force Monte Carlo simulation ineffective. Sampling strategies with the ability to control the variance have been developed to tackle this issue (Schuëller and Stix, 1987; Engelund and Rackwitz, 1993; Au and Beck, 2001; Schuëller and Pradlwarter, 2007; Sundar, 2013; Sundar and Manohar, 2014b; Au and Patelli, 2016).

Subset simulation (SS) Au and Beck (2001) has emerged as the widely used tool for reliability estimation in the recent years. The versatility of this method has led to the development of several variants in diverse fields (Au and Beck, 2003; Katafygiotis and Cheung, 2005, 2007; Song et al., 2009; Hsu and Ching, 2010; Bourinet et al., 2011; Papadopoulos et al., 2012; Sundar and Manohar, 2014a). Recent advances in the subset simulation methodology have been directed

towards development of efficient conditional sampling strategies (Santoso et al., 2011; Miao and Ghosn, 2011; Zuev et al., 2012; Papaioannou et al., 2015; Wang et al., 2017; Sundar, 2017). However, the general consensus is that for high dimensional problems, the component-wise Modified Metropolis Hastings (MMH) algorithm proposed in the original subset simulation method is the most robust and efficient.

As in many other reliability methods, algorithms for subset simulation have typically assumed that the input parameters can be expressed as uncorrelated normal random variables. In many cases, however, they cannot. While the subset simulation method itself poses no theoretical restrictions and does not require this treatment, to date there has been no investigation (to the author's knowledge) of the most appropriate conditional sampling method to employ for subset simulation when input distributions are non-Gaussian, anisotropic, and/or degenerate and cannot be easily transformed to standard normals. In fact, many times these distributions cannot even be sampled directly and Markov Chain Monte Carlo (MCMC) methods must be employed to draw samples from them.

One of the most important features of any MCMC algorithm for conditional sampling in subset simulation is the correlation between subsequent states of the chain (samples), which should be minimized to the extent possible. In fact, Au and Beck Au and Beck (2001), derive analytical relations approximating the coefficient of variation of probability of failure estimates from subset simulation in terms of the MCMC correlations. Minimizing correlation in the chains is extremely difficult to achieve for highly anisotropic/degenerate distributions such that even samples generated using the MMH may have very long correlation length. One set of methods that are especially effective in such cases are the class of affine invariant ensemble MCMC samplers (Goodman and Weare, 2010), which have been shown to reduce the correlation length by an order of magnitude or more over MMH for highly anisotropic/degenerate distributions. In this work, a versions of the affine invariant ensemble sampler utilizing so-called "stretch moves" is employed for conditional sampling in subset simulation.

## 2 Subset Simulation

In the subset simulation method the rare event probability $P_F$ is represented as a product of probability of more frequent events. That is, the failure event $F$ is expressed in terms of $M$ nested intermediate events $F_1, F_2, \cdots, F_M$ such that $F_1 \supset F_2 \supset \cdots \supset F_M$, and $F = \cap_{j=1}^{M} F_j$ resulting in $P_F = P(F_1)\prod_{j=2}^{M} P(F_j|F_{j-1})$. The probability $P(F_1)$ is computed through Monte Carlo simulations. The accuracy of the method heavily relies on the sampling strategy used to estimate the conditional probabilities $P(F_j|F_{j-1}), j = 2, 3, \cdots, M$, which in turn necessitates generation of samples from the conditional pdf $p_{\boldsymbol{U}}(\boldsymbol{u}|F_{j-1})$.

Several algorithms for the efficient construction of Markov chains have been proposed in the past, such as the Metropolis-Hastings (MH), the component-wise Modified Metropolis Hastings (MMH), the Metropolis-Hastings with delayed rejection, and the adaptive conditional sampling. These algorithms aim to achieve variance reduction through efficient sampling of the conditional space – lower rejection rate and sample correlation yielding estimates with low coefficient of variation. In the context of subset simulation, the Markov chains are constructed through a two-step acceptance/rejection criterion. Consider simulating from the conditional pdf $p(\boldsymbol{u}|F_j)$. Starting from a Markov chain state $\boldsymbol{x}$ and a proposal $q(\bullet|\boldsymbol{x})$, a prospective candidate state $\boldsymbol{y}$ is generated. In the first stage, the sample $\boldsymbol{y}$ is accepted/rejected with probability $\alpha = \min\{1, \frac{p(\boldsymbol{y})q(\boldsymbol{x}|\boldsymbol{y})}{p(\boldsymbol{x})q(\boldsymbol{y}|\boldsymbol{x})}\}$, and in the second stage is accepted/rejected based on whether the sample belongs to the failure region $F_j$.

Existing algorithms differ in their generation of the prospective state and the variations accompanying the first acceptance criterion. For example the MH algorithm uses a single $n-$dimensional

proposal pdf and a scalar $\alpha$ as an acceptance probability. The MMH or the component-wise MH algorithm proposed by Au and Beck however uses $n$ 1-dimensional proposal pdf's and a $n \times 1$ acceptance probability vector $\alpha$. Ideas based on repeated generations of the prospective state until the first acceptance criterion is satisfied have also been explored by a few researchers (Santoso et al., 2011; Miao and Ghosn, 2011; Au et al., 2012).

Papaioannou et al. (2015) proposed a conditional sampling strategy based on maintaining a specified correlation $\rho$ between the current state and prospective state. It was shown that the candidate states are always accepted without compromising the stationary distribution of the chain. This method can be interpreted as a special case of the M-H sampler with proposal distribution obtained by conditioning the joint normal distribution (Bernardo et al. (1998)) consisting of two independent standard normal random vectors with component-wise cross correlation coefficients. A value of $\rho$ close to one will increase the acceptance rate but will lead to a larger correlation of the new samples. By conducting numerical experiments, the authors conjecture that the optimal acceptance rate of 0.44 is optimal for subset simulation and further proposed to adjust the parameters of the conditional sampling method on the fly.

In spite of continued research in the development of conditional sampling schemes, it appears the MMH based original subset simulation method is still the first choice due to its simplicity and robustness to the dimension when input parameters are normal and uncorrelated. When input parameters are no so well-behaved, however, it is unclear what conditional sampling approach is most appropriate. The MMH method, for example, may have a very long correlation length (Goodman and Weare, 2010) which will induce a high coefficient of variation in the probability of failure estimate. In the subsequent sections, we discuss the

## 3 Affine invariant ensemble MCMC

Many of the most significant gains in probabilistic analysis including reliability analysis have come from numerical algorithms for approximate inference, particularly MCMC, which are designed to sample from a given probability distribution efficiently even in parameter spaces with large numbers of dimensions. The simplest and most commonly used MCMC algorithms are Metropolis-Hastings (MH) (Hastings, 1970; MacKay, 2003) and Gibbs sampling (Geman and Geman, 1984). In this work, we use a MH-based MCMC algorithm - Affine-invariant ensemble sampler proposed by Goodman and Weare (2010).

Affine invariant samplers take advantage of the fact that a simple affine transformation is enough to make a poorly scaled distribution much easier to sample. Consider, for example, the distribution $\pi(x)$ that is poorly scaled. A general purpose MCMC algorithm will struggle to sample from $\pi(x)$ unless its parameters (i.e. the parameters of the proposal density) are well tuned, which may be challenging for example if $\pi(x)$ is implicitly defined, high dimensional, degenerate, or otherwise not well-behaved. However, the distribution of $Y = AX + b$, having undergone an affine transformation, having density

$$\pi_{A,b}(y) = \pi_{A,b}(Ax + b) \propto \pi(x)$$

may be well scaled and therefore much easier to sample. Goodman and Weare (2010) introduce the class of samplers referred to affine invariant, where the sequence of samples following the distribution $\pi_{A,b}(y)$, $Y(t)$, can be related through the affine transformation to a sequence following $\pi(x)$ by $Y(t) = AX(t) + b$.

Currently, there are no known general MCMC algorithms that produce sequences of affine invariant samples. Goodman and Weare (2010), however, propose a family of ensemble samplers with the affine invariant property. An ensemble sampler employs a set of $L$ independent chains that collectively (but not necessarily individually) sample from the target density. The basic

principle of ensemble samplers is that many walkers move through parameter space, and at each iteration each walker undergoes a trial move that is dependent on the positions of each of the other walkers, called the complementary ensemble, which provide information about the underlying distribution.

In this work, we employ the simplest of the affine invariant ensemble samplers which uses a so-called stretch move for each step of the Markov chain propagation. At step $t$, let $X(t)$ denote the $k^{th}$ walker. Using the stretch move, the proposed next sample in sequence $k$, denoted $Y$, is sample using one other sample from the ensemble $X_j, j \neq k$ as

$$Y = X_j + Z(X_k(t) - X_j)$$

where $Z$ is a random variable having density

$$g(z) \propto \frac{1}{\sqrt{z}}, \quad z \in \left[\frac{1}{a}, a\right] \tag{1}$$

where $a > 1$ is the only parameter necessary for implementation of the method. Here, we use $a = 2$. To satisfy detailed balance, the sample $Y$ is accepted with probability

$$\min\left\{1, Z^{n-1}\frac{\pi(Y)}{\pi(X_k(t))}\right\} \tag{2}$$

The algorithm is summarized in Algorithm 1 below (see also Foreman-Mackey et al. (2013) for more details)

**Algorithm 1** Affine-invariant ensemble MCMC - stretch move

1: Initialize the positions of the $L$ walkers, and suppose the positions of all the walkers are described by $\boldsymbol{x}(t)$ at iteration $t$
2: For each of the walkers $x_k(t), k = 1, 2, ..., L$ successively
3: Draw a random walker $x_j$ from the complementary ensemble $\boldsymbol{x}_{[k]}(t)$.
4: Generate a random variable $z$ from

$$g(z) \propto \frac{1}{\sqrt{z}}, z \in \left[\frac{1}{a}, a\right] \tag{3}$$

5: Propose a trial step $y$ that is called stretch move

$$y = x_j + z[x_k(t) - x_j] \tag{4}$$

6: Define the acceptance probability

$$\alpha = \min\left(1, z^{n-1}\frac{\pi(y)}{\pi(x_k(t))}\right) \tag{5}$$

where $n$ is the dimension of parameter space
7: Draw a random variable $r \sim U(0,1)$
8: Determine the next move

$$x_k(t+1) = \begin{cases} y & \text{if } r \leq \alpha \\ x_k(t) & \text{otherwise} \end{cases} \tag{6}$$

9: Iterate over $t$ from step 2 to obtain $\boldsymbol{x}(t+1)$

The affine invariant ensemble MCMC sampler has several advantages over conventional MCMC sampling algorithms. The major advantage of the algorithm is that it leverages an ensemble of Markov chains to adopt the proposal density through an invariant affine transformation. This greatly improves efficiency for anisotropic and degenerate densities – increasing the acceptance rate while at the same time significantly reducing correlation length and yielding independent samples more quickly. Another benefit is that this algorithm is largely "self-tuning," such that it only requires 1 tuning parameter, $a$, rather than $\sim n^2$ for most MH-based MCMC algorithms in an $n-$ dimensional parameter space. Both advantages are useful for improving the efficiency of subset simulation. The method is also easily parallelized such that $L$ steps can be taken concurrently.

## 4 Subset simulation with the affine invariant MCMC sampler

The affine invariant MCMC sampler can be integrated into the subset simulation algorithm with ease. In fact, because subset simulation samples from the conditional distribution by propagating one Markov chain for each sample originally lying in a conditional level, an ensemble already exists for each conditional density. The affine invariant ensemble sampler, however, has the effect of removing the condition that each chain individually follow the conditional density in favor of a looser condition that the ensemble must follow the conditional density. In so doing, it leverages the existing samples to propagate each chain. Upon acceptance of a given state, $X_k(t+1)$, the typical condition that the sample lies in the conditional domain $G(X_k(t+1)) < 0$, is checked and accepted or rejected.

## 5 Numerical Illustration

We demonstrate the performance gain achieved using the affine invariant MCMC method through two numerical examples. The MMH and affine invariant methods are used for conditional sampling in the subset simulation method.

### 5.1 Degenerate Gaussian

For illustration purposes, we first consider a simple multidimensional linear performance function with standard Gaussian random variables as

$$G(\boldsymbol{U}) = \beta\sqrt{n} - \sum_{i=1}^{n} U_i \tag{7}$$

where $\boldsymbol{U}$ is an $n-$dimensional Gaussian random vector and $\beta$ is the Hasofer-Lind reliability index in the standard normal space having the property $P_f = \Phi(-\beta)$. This is a simple problem for most reliability methods in the standard normal space. Let us consider, however, that our true performance function $G(\boldsymbol{X})$ exists in a space of highly correlated Gaussian variables, $\boldsymbol{X}$, while maintaining the performance function in Eq. (7) in the standard normal space. That is, a linear transformation of $G(\boldsymbol{X})$ yields $G(\boldsymbol{U})$. Again, this problem is trivial if we know the transformation. For demonstration purposes let us, instead, image that we do not know the transformation and that we need to perform subset simulation in the space of $\boldsymbol{X}$ itself.

Consider $\mathbf{X}$ to have zero mean and covariance given by $C(X_i, X_i) = 1$ and $C(X_i, X_j) = \rho, \forall i \neq j$. Table 1 shows the mean probability of failure estimates for $\beta = 3$ for different values of the dimension $n$ and correlation coefficient $\rho$ using subset simulation (from 100 repeated trials) with 500 samples evaluated at each conditional level and each conditional level defined to have probability 0.1. The values in parentheses indicate the coefficient of variation and the log of the standard deviation of the $P_f$ estimates. Note that the second metric of error is used because

| $n\backslash\rho$ | | 0 | 0.9 | 0.99 | 0.9999 | 0.999999 | 0.99999999 |
|---|---|---|---|---|---|---|---|
| 2 | MMH | 1.36e-3 (39%, 0.4) | 1.83e-3 (46%, 0.5) | 1.43e-3 (68%, 0.8) | 1.08e-3 (128%, 3.2) | 1.12e-3 (132%, 9.6) | 1.10e-3 (130%, 7.7) |
| | AIE | 1.52e-3 (63%, 0.8) | 1.42e-3 (74%, 0.8) | 1.29e-3 (83%, 1.0) | 1.38e-3 (75%, 0.8) | 1.36e-3 (64%, 0.8) | 1.44e-3 (63%, 0.7) |
| 10 | MMH | 1.35e-3 (39%, 0.3) | 1.37e-3 (39%, 0.4) | 1.46e-3 (43%, 0.4) | 1.31e-3 (92%, 1.4) | 1.46e-3 (115%, 5.8) | 1.17e-3 (129%, 10.0) |
| | AIE | 1.42e-3 (87%, 2.2) | 1.42e-3 (92%, 1.3) | 1.34e-3 (91%, 2.0) | 1.37e-3 (79%, 1.9) | 1.31e-3 (92%, 1.5) | 1.50e-3 (80%, 1.9) |
| 50 | MMH | 1.43e-3 (35%, 0.3) | 1.36e-3 (33%, 0.3) | 1.39e-3 (32%, 0.3) | 1.40e-3 (82%, 0.8) | 1.39e-3 (96%, 2.2) | 1.46e-3 (126%, 8.0) |
| | AIE | 1.45e-3 (95%, 3.5) | 1.26e-3 (123%, 4.6) | 1.23e-3 (123%, 4.2) | 1.42e-3 (100%, 2.6) | 1.49e-3 (98%, 3.9) | 1.45e-3 (103%, 3.4) |

**Table 1:** Example 1: Probability of failure estimates and measures of error for subset simulation performed using the Modified Metropolis Hastings (MMH) algorithm and the Affine Invariant Ensemble (AIE) sampler for strongly correlated normal distributions. The numbers in parentheses are measures of error. First the coefficient of variation from 100 trials. Second, the log of the standard deviation of the estimates from 100 trials.

the coefficient of variation is insensitive to incorrect probability of failure estimates that greatly underestimate probability of failure but is very sensitive to its overestimation.

The results in Table 1 illustrate some important features of the application of the affine invariant sampler to conditional simulations for subset simulation. First, as the theory suggests, the accuracy of the estimates from the affine invariant are independent of the correlation. That is, as the joint distribution degenerates, the affine invariant maintains a consistent level of accuracy (i.e. same coefficient of variation). The MMH, on the other hand, begins to lose accuracy when the correlation becomes very strong such that the distribution is effectively one-dimensional. This happens because, as the component wise algorithm steps in each dimension, it has a very low acceptance rate because none of the step directions align with the one effective dimension of the problem.

We notice, however, that the accuracy of the affine invariant does not scale well with increasing dimension. While it maintains *consistent* accuracy across values of $\rho$, even for high dimension, the coefficient of variation is consistently higher than the MMH, which maintains its accuracy with increasing dimension but sees diminishing accuracy with increasing $\rho$.

### 5.2 Rosenbrock function

The second example considers a problem that is somewhat closer to the case where the affine invariant ensemble sampler is well-suited. In this case, the two-dimensional density follows a complex form that cannot necessarily be sampled directly (i.e. it requires MCMC methods to generate samples) and it has a strong dominant dimension that: (a) does not align with either dimension, and (b) changes throughout the parameter space.

Consider the random vector $\boldsymbol{X} = [X_1, X_2]$ having Rosenbrock probability density given by:

$$p(x_1, x_2) \propto \exp\left(-\frac{100(x_2 - x_1^2)^2 + (1 - x_1)^2}{20}\right) \tag{8}$$

Contours of the probability density are shown in Figure 1.

Goodman and Weare (2010) show that the affine invariant ensemble sampler (stretch moves) is especially efficient for sampling from this density – reducing the correlation length of the Markov chains by approximately one order of magnitude.

The performance function is taken as

$$g(\boldsymbol{X}) = 120 - X_2 - 3X_1 \tag{9}$$

The "true" probability of failure is estimated using $10^8$ Monte Carlo samples drawn using the affine invariant ensemble MCMC sampler to be 3.23e-3. Because the Rosenbrock cannot be sampled directly, we start the subset simulation by generating independent points using MCMC.

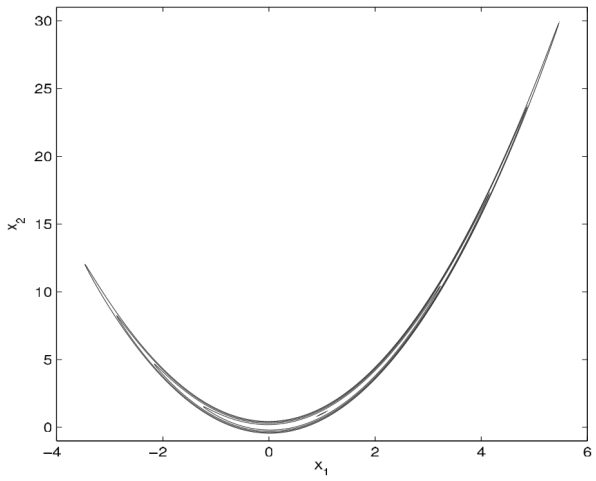


**Figure 1:** Rosenbrock probability density function

This is difficult to achieve because MCMC algorithms applied to this distribution have very long correlation length. To achieve independence using the MMH requires jumping of $\sim 163,000$ samples while the affine invariant requires jumping of $\sim 19,000$ samples (Goodman and Weare, 2010). This is critical because, if the initial samples are not independent, then the subset simulation algorithm cannot identify the conditional densities correctly and the probability of failure estimates will not be accurate. The conditional samples, by contrast, will not be independent and do not need to be – as is known from the subset simulation method (Au and Beck, 2001).

From an independent set of 500 MCMC samples, conditional samples are generated using the MMH and affine invariant ensemble sampler with stretch moves. We use 500 samples at each conditional level and a probability of 0.1 for each conditional level. The results are shown in Table 2. The results indicate a slight improvement in the estimator when using the affine invariant sampler, when compared to the MMH. The reported coefficient of variation is slightly lower for the affine invariant than for the MMH. But, these values are reported from only 20 independent trials. Moreover, the results have not been explored for varying MCMC parameters (MMH uses standard normal proposal and affine invariant uses $a = 2$). Further investigation of this problem is needed to establish a more careful comparison and identify the appropriate sampling method.

**Table 2:** Example 2: Mean $P_F$ and COV for 20 independent trials

| MCMC Algorithm | $P_F$ | COV |
|---|---|---|
| Component wise MH | $3.3150 \times 10^{-3}$ | 84% |
| Affine Invariant-stretch | $3.4431 \times 10^{-3}$ | 74% |

## Acknowledgments

This work has been supported by the US Office of Naval Research under award number N00014-16-1-2582 with Dr. Paul Hess as program officer.

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