On MCMC algorithm for Subset Simulation

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Abstract

A new Markov Chain Monte Carlo (MCMC) algorithm for Subset Simulation was recently proposed by imposing a joint Gaussian distribution between the current sample and the candidate. It coincides with the limiting case of the original independent-component algorithm where each random variable is represented by an infinite number of hidden variables. The algorithm is remarkably simple as it no longer involves the explicit choice of proposal distribution. It opens up a new perspective for generating conditional failure samples and potentially allows more direct and flexible control of algorithm through the cross correlation matrix between the current sample and the candidate. While by definition the cross correlation matrix need not be symmetric, this article shows that it must be so in order to satisfy detailed balance and hence to produce an unbiased algorithm. The effect of violating symmetry on the distribution of samples is discussed and insights on acceptance probability are provided.

Keywords: Detailed balance, Rare Event, Markov Chain Monte Carlo, Monte Carlo, Subset Simulation

1. Introduction

In a risk assessment problem let $\mathbf{X}=[X_1,\ldots,X_n]^T$ be the set of uncertain parameters modeled by random variables. Without loss of generality $\{X_i\}_{i=1}^n$ are assumed to be standard Gaussian (zero mean and unit variance) and i.i.d. (independent and identically distributed). Dependent non-Gaussian random variables can be constructed from Gaussian ones by proper transformation [1]. One important problem in risk assessment is the determination of failure probability $P(F)$ for a specified failure event F, which can be formulated as an n-dimensional integral or an expectation:

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$$P(F) = \int I(\mathbf{x} \in F)\phi(\mathbf{x})d\mathbf{x} = E[I(\mathbf{X} \in F)] \quad (1)$$

where $I(\cdot)$ is the indicator function, equal to 1 if its argument is true and zero otherwise; $\mathbf{x} = [x_1,..., x_n]^T$ denotes the parameter value of $\mathbf{X}$; and

$$\phi(\mathbf{x}) = (2\pi)^{-n/2} \exp(-\frac{1}{2}\sum_{i=1}^{n} x_i^2) \quad (2)$$

is the n-dimensional standard Gaussian probability density function (PDF).

Direct Monte Carlo method [2][3] is the most robust method for estimating the failure probability regardless of problem complexity but it is not efficient for small probabilities. Advanced Monte Carlo methods aim at reducing the variance of estimators beyond direct Monte Carlo but in doing so they lose application robustness [4]. Subset Simulation is a method that is found to play a balance between efficiency and robustness [5][6]. It is based on the idea that a small failure probability can be expressed as the product of larger conditional probabilities of intermediate failure events, thereby potentially converting a rare event simulation problem into a sequence of more frequent ones.

The efficient generation of conditional failure samples, i.e., samples that are conditional on intermediate failure events, is pivotal to Subset Simulation. This is conventionally performed using an independent-component Markov Chain Monte Carlo (MCMC) algorithm [5][7][8], which is applicable for high dimensional problems and makes the algorithm robust to applications. In Step I, given the current sample $\mathbf{X} = [X_1,..., X_n]^T$, each component X_i' $(i = 1,..., n)$ of the candidate is generated independently by MCMC. In Step II, the candidate $\mathbf{X}' = [X_1',..., X_n']^T$ is accepted as the next sample if it lies in F; otherwise the current sample is taken as the next sample.

By imposing a joint Gaussian distribution between the current sample and the candidate, a new algorithm for Step I was recently proposed (Section 3.3 in [9]). Each component X_i' $(i = 1,..., n)$ of the candidate is generated independently as a Gaussian variable with mean $\rho_i X_i$ and variance $1 - \rho_i^2$, where $\rho_i \in (0,1)$ is a parameter chosen by user and can be seen as the correlation between X_i' and X_i. This algorithm is remarkably simple and the candidate $\mathbf{X}'$ is always different from the current sample $\mathbf{X}$. It is directly controlled through the correlations $\{\rho_i\}_{i=1}^n$ and the explicit choice of proposal PDF is no longer required. It coincides with the limiting case of the original independent-component algorithm where each random variable is represented by an infinite number of hidden variables [10].

The Gaussian candidate concept was generalized to introduce correlation between the components of the candidate. It was proposed that the candidate $\mathbf{X}'$ be generated as a Gaussian vector with mean $\mathbf{RX}$ and covariance matrix $\mathbf{C} = \mathbf{I} - \mathbf{RR}^T$, where $\mathbf{I} \in R^{n \times n}$ denotes the identity matrix; and $\mathbf{R} \in R^{n \times n}$ is the cross covariance matrix between $\mathbf{X}'$ and $\mathbf{X}$, in the sense that $E[\mathbf{X}'\mathbf{X}^T] = \mathbf{R}E[\mathbf{XX}^T]$. By definition $\mathbf{R}$ need not be symmetric. In [9], symmetry was not explicitly imposed in deriving the properties of the algorithm, although the numerical examples assumed diagonal (hence symmetric) $\mathbf{R}$. The objective of this article is to clarify whether $\mathbf{R}$ needs to be symmetric. It will be shown that for detailed balance to hold, and hence the algorithm be unbiased, $\mathbf{R}$ must be symmetric. The effect of violating symmetry will be discussed and insights are provided for acceptance probabilities. Clarifications are also given on the derivation in [9] regarding the issue of symmetry.

2. Detailed balance and symmetry requirement

Consider using the generalized algorithm mentioned in the last section to generate samples distributed as the conditional PDF $\phi(\mathbf{x} | F) = \phi(\mathbf{x}) I(\mathbf{x} \in F) / P(F)$. Here F can denote any intermediate failure event in Subset Simulation. Let the current sample be $\mathbf{X}$ and the next sample be $\mathbf{Y}$. MCMC produces the conditional failure samples by ensuring the transition PDF from $\mathbf{X}$ to $\mathbf{Y}$ to satisfy the ‘detailed balance condition’, also known as ‘reversibility condition’:

$$p_{\mathbf{Y}|\mathbf{X}}(\mathbf{y} | \mathbf{x}) \phi(\mathbf{x} | F) = p_{\mathbf{Y}|\mathbf{X}}(\mathbf{x} | \mathbf{y}) \phi(\mathbf{y} | F) \qquad \mathbf{x}, \mathbf{y} \in R^n \qquad (3)$$

That is, the arguments $\mathbf{x}$ and $\mathbf{y}$ can be swapped. The following standard arguments [5] allow one to reduce detailed balance to the consideration of the transition PDF from the current sample to the candidate $\mathbf{X}'$, i.e., $p_{\mathbf{X}'|\mathbf{X}}(\cdot | \cdot)$. First, the equality holds trivially when $\mathbf{x} = \mathbf{y}$ and so it suffices to consider $\mathbf{x} \neq \mathbf{y}$. Since Step II ensures that all samples lie in F, it suffices to check detailed balance for only those states in F, i.e.,

$$p_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}\,|\,\mathbf{x})\phi(\mathbf{x}) = p_{\mathbf{Y}|\mathbf{X}}(\mathbf{x}\,|\,\mathbf{y})\phi(\mathbf{y}) \qquad \mathbf{x} \neq \mathbf{y},\ \mathbf{x},\mathbf{y} \in F \tag{4}$$

where $\phi(\cdot\,|\,F)$ has been replaced by $\phi(\cdot)$. This reduces to considering the case where the candidate in Step I is accepted in Step II, for which $\mathbf{Y} = \mathbf{X}'$. Detailed balance then reduces to requiring

$$p_{\mathbf{X}'|\mathbf{X}}(\mathbf{y}\,|\,\mathbf{x})\phi(\mathbf{x}) = p_{\mathbf{X}'|\mathbf{X}}(\mathbf{x}\,|\,\mathbf{y})\phi(\mathbf{y}) \qquad \mathbf{x} \neq \mathbf{y},\ \mathbf{x},\mathbf{y} \in F \tag{5}$$

According to the generalized algorithm, given the current sample $\mathbf{X}$, the candidate $\mathbf{X}'$ is a Gaussian vector with mean $\mathbf{RX}$ and covariance matrix $\mathbf{C} = \mathbf{I} - \mathbf{RR}^T$. That is, for any $\mathbf{x},\mathbf{y} \in R^n$,

$$p_{\mathbf{X}'|\mathbf{X}}(\mathbf{y}\,|\,\mathbf{x}) = \phi(\mathbf{y};\mathbf{Rx},\mathbf{C}) = (2\pi)^{-n/2}\,|\,\mathbf{C}\,|^{-1/2} \exp\left[-\frac{1}{2}(\mathbf{y}-\mathbf{Rx})^T\mathbf{C}^{-1}(\mathbf{y}-\mathbf{Rx})\right] \tag{6}$$

where $\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})$ denotes the n-dimensional Gaussian PDF with mean $\mathbf{Rx}$ and covariance matrix $\mathbf{C}$ and evaluated at $\mathbf{y}$. Detailed balance in (5) therefore reads

$$\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})\phi(\mathbf{x}) = \phi(\mathbf{x};\mathbf{Ry},\mathbf{C})\phi(\mathbf{y}) \tag{7}$$

In an attempt to show (7), one tries to rewrite the LHS so that the roles of $\mathbf{x}$ and $\mathbf{y}$ can be swapped. This involves linear algebra dealing with the quadratic forms in the exponent of the Gaussian PDFs. As the key theoretical result in this article, it is shown in the appendix that the LHS of (7) can be rewritten as

$$\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})\phi(\mathbf{x}) = \phi(\mathbf{x};\mathbf{R}^T\mathbf{y},\mathbf{C}')\phi(\mathbf{y}) \tag{8}$$

where

$$\mathbf{C}' = \mathbf{I} - \mathbf{R}^T\mathbf{R} \tag{9}$$

Equation (8) says that $\mathbf{x}$ and $\mathbf{y}$ can be swapped but $\mathbf{R}$ should be replaced by $\mathbf{R}^T$ and $\mathbf{C}$ by $\mathbf{C}'$. Comparing the RHS of (7) and (8), it is now clear that detailed balance holds if and only if $\phi(\mathbf{x};\mathbf{Ry},\mathbf{C}) \equiv \phi(\mathbf{x};\mathbf{R}^T\mathbf{y},\mathbf{C}')$, i.e., one Gaussian PDF with mean $\mathbf{Ry}$ and covariance $\mathbf{C} = \mathbf{I} - \mathbf{RR}^T$ is identical to another Gaussian PDF with mean $\mathbf{R}^T\mathbf{y}$ and covariance $\mathbf{C}' = \mathbf{I} - \mathbf{R}^T\mathbf{R}$. This holds if and only if $\mathbf{R}$ is symmetric.

3. Distribution of the next sample

It is instructive to consider the effect of a general (asymmetric) $\mathbf{R}$ on the distribution of the next sample. According to the generalized algorithm, the transition PDF from the current sample $\mathbf{X}$ to the next sample $\mathbf{Y}$ is given by

$$p_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}\,|\,\mathbf{x}) = \phi(\mathbf{y};\mathbf{Rx},\mathbf{C})I(\mathbf{y}\in F) + \delta(\mathbf{y}-\mathbf{x})[1-P_A(\mathbf{x})] \tag{10}$$

where $\delta(\cdot)$ is the Dirac-Delta function; and

$$P_A(\mathbf{x}) = P(\mathbf{X}'\in F\,|\,\mathbf{X}=\mathbf{x}) = \int \phi(\mathbf{z};\mathbf{Rx},\mathbf{C})I(\mathbf{z}\in F)d\mathbf{z} \tag{11}$$

is the acceptance probability in Step I given that the current sample is at $\mathbf{x}$. Check that $p_{\mathbf{Y}|\mathbf{X}}(\cdot\,|\,\mathbf{x})$ integrates to 1:

$$\begin{aligned}\int p_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}\,|\,\mathbf{x})d\mathbf{y} &= \int \phi(\mathbf{y};\mathbf{Rx},\mathbf{C})I(\mathbf{y}\in F)d\mathbf{y} + \int \delta(\mathbf{y}-\mathbf{x})[1-P_A(\mathbf{x})]d\mathbf{y} \\ &= P(\mathbf{X}'\in F\,|\,\mathbf{X}=\mathbf{x}) + [1-P_A(\mathbf{x})] = 1\end{aligned} \tag{12}$$

Suppose $\mathbf{X}$ is distributed as the conditional PDF $\phi(\mathbf{x}\,|\,F)$. Using the Theorem of Total Probability and (10), the PDF of $\mathbf{Y}$ is

$$\begin{aligned}p_{\mathbf{Y}}(\mathbf{y}) &= \int p_{\mathbf{Y}|\mathbf{X}}(\mathbf{y}\,|\,\mathbf{x})\phi(\mathbf{x}\,|\,F)d\mathbf{x} \\ &= \int I(\mathbf{y}\in F)\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})\phi(\mathbf{x}\,|\,F)d\mathbf{x} + \int \delta(\mathbf{y}-\mathbf{x})[1-P_A(\mathbf{x})]\phi(\mathbf{x}\,|\,F)d\mathbf{x}\end{aligned} \tag{13}$$

Using (8) and substituting $\phi(\mathbf{x}\,|\,F) = \phi(\mathbf{x})I(\mathbf{x}\in F)/P(F)$, the first integral is given by

$$\begin{aligned}&\int I(\mathbf{y}\in F)\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})\phi(\mathbf{x})I(\mathbf{x}\in F)P(F)^{-1}d\mathbf{x} \\ &= \int I(\mathbf{y}\in F)\phi(\mathbf{x};\mathbf{R}^T\mathbf{y},\mathbf{C}')\phi(\mathbf{y})I(\mathbf{x}\in F)P(F)^{-1}d\mathbf{x} \\ &= I(\mathbf{y}\in F)\phi(\mathbf{y})P(F)^{-1}\int \phi(\mathbf{x};\mathbf{R}^T\mathbf{y},\mathbf{C}')I(\mathbf{x}\in F)d\mathbf{x} \\ &= \phi(\mathbf{y}\,|\,F)P_{A'}(\mathbf{y})\end{aligned} \tag{14}$$

where

$$P_{A'}(\mathbf{y}) = \int \phi(\mathbf{x};\mathbf{R}^T\mathbf{y},\mathbf{C}')I(\mathbf{x}\in F)d\mathbf{x} \tag{15}$$

is the probability that a Gaussian vector with mean $\mathbf{R}^T\mathbf{y}$ and covariance $\mathbf{C}'$ lies in F.

The second integral in (13) is simply given by

$$\int \delta(\mathbf{y}-\mathbf{x})[1-P_A(\mathbf{x})]\phi(\mathbf{x}\,|\,F)d\mathbf{x} = [1-P_A(\mathbf{y})]\phi(\mathbf{y}\,|\,F) \tag{16}$$

Substituting (14) and (16) into (13) gives

$$p_{\mathbf{Y}}(\mathbf{y}) = \phi(\mathbf{y}\,|\,F) + [P_{A'}(\mathbf{y}) - P_A(\mathbf{y})]\phi(\mathbf{y}\,|\,F) \tag{17}$$

For general $\mathbf{R}$, $P_{A'}(\mathbf{y}) \neq P_A(\mathbf{y})$ and so $p_{\mathbf{Y}}(\mathbf{y})$ is different from the target PDF $\phi(\mathbf{y} \mid F)$. When $\mathbf{R}$ is symmetric, $\mathbf{C} = \mathbf{C}'$ and $P_{A'}(\mathbf{y}) = P_A(\mathbf{y})$ for all $\mathbf{y}$, and so $p_{\mathbf{Y}}(\mathbf{y}) \equiv \phi(\mathbf{y} \mid F)$.

To clarify, when $\mathbf{X}$ is a standard Gaussian vector, generating a Gaussian candidate $\mathbf{X}'$ with mean $\mathbf{RX}$ and covariance $\mathbf{C} = \mathbf{I} - \mathbf{RR}^T$ ensures it is also a standard Gaussian vector. The same also works when the mean is replace by $\mathbf{R}^T\mathbf{X}$ and the covariance by $\mathbf{C}' = \mathbf{I} - \mathbf{R}^T\mathbf{R}$. These are true no matter whether $\mathbf{R}$ is symmetric or not. For the next sample $\mathbf{Y}$ to have the target PDF $\phi(\mathbf{y} \mid F)$ (standard Gaussian conditional on failure), however, $\mathbf{R}$ must be symmetric.

4. Acceptance probability

Further insights about the acceptance probabilities $P_A(\mathbf{y})$ and $P_{A'}(\mathbf{y})$ are presented for general $\mathbf{R}$. First, their integral with respect to $\phi(\mathbf{y})$ is equal to $P(F)$. Using (11),

$$\begin{aligned}
\int P_A(\mathbf{y})\phi(\mathbf{y})d\mathbf{y} &= \int\int I(\mathbf{z} \in F)\phi(\mathbf{z};\mathbf{Ry},\mathbf{C})\phi(\mathbf{y})d\mathbf{z}d\mathbf{y} \\
&= \int\int I(\mathbf{z} \in F)\phi(\mathbf{y};\mathbf{R}^T\mathbf{z},\mathbf{C}')\phi(\mathbf{z})d\mathbf{z}d\mathbf{y} \\
&= \int\left[\int \phi(\mathbf{y};\mathbf{R}^T\mathbf{z},\mathbf{C}')d\mathbf{y}\right]I(\mathbf{z} \in F)\phi(\mathbf{z})d\mathbf{z} \\
&= \int I(\mathbf{z} \in F)\phi(\mathbf{z})d\mathbf{z} \\
&= P(F)
\end{aligned} \tag{18}$$

where we have used (8) in the second equality and $\int \phi(\mathbf{y};\mathbf{Rz},\mathbf{C})d\mathbf{y} = 1$ in the fourth equality. The result in (18) is intuitive because generating a Gaussian vector with mean $\mathbf{RX}$ and covariance matrix $\mathbf{C} = \mathbf{I} - \mathbf{RR}^T$, and with $\mathbf{X}$ being standard Gaussian, will also give a standard Gaussian vector, whose probability of lying in F is clearly $P(F)$. Replacing $\mathbf{R}$ by $\mathbf{R}^T$ and $\mathbf{C}$ by $\mathbf{C}'$ in (18) shows that the same result holds for $P_{A'}(\mathbf{y})$, i.e.,

$$\int P_{A'}(\mathbf{y})\phi(\mathbf{y})d\mathbf{y} = P(F) \tag{19}$$

A more non-trivial result holds. Despite the fact that $P_{A'}(\mathbf{y}) \neq P_A(\mathbf{y})$, their integral with respect to $\phi(\mathbf{y} \mid F)$ are always the same:

$$\begin{aligned}
\int P_{A'}(\mathbf{y})\phi(\mathbf{y}\,|\,F)d\mathbf{y} &= \int\int I(\mathbf{x}\in F)\phi(\mathbf{x};\mathbf{R}^T\mathbf{y},\mathbf{C}')\times\phi(\mathbf{y})I(\mathbf{y}\in F)P(F)^{-1}d\mathbf{x}d\mathbf{y} \\
&= \int\int I(\mathbf{x}\in F)\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})\phi(\mathbf{x})I(\mathbf{y}\in F)P(F)^{-1}d\mathbf{x}d\mathbf{y} \\
&= \int\left[\int \phi(\mathbf{y};\mathbf{Rx},\mathbf{C})I(\mathbf{y}\in F)d\mathbf{y}\right]I(\mathbf{x}\in F)\phi(\mathbf{x})P(F)^{-1}d\mathbf{x} \\
&= \int P_A(\mathbf{x})\phi(\mathbf{x}\,|\,F)d\mathbf{x}
\end{aligned} \tag{20}$$

where we have used (8) in the second equality. This result in fact guarantees that the expression of $p_{\mathbf{Y}}(y)$ in (17) integrates to 1.

To illustrate the above results, suppose failure is defined as $F=\{\mathbf{a}^T\mathbf{X}>b\}$ for some vector $\mathbf{a}\in R^n$ and scalar $b\in R$. Then the failure boundary is a hyperplane and it can be derived analytically (details omitted) that

$$P_A(\mathbf{y})=\Phi\left(-\frac{b-\mathbf{a}^T\mathbf{Ry}}{\sqrt{\mathbf{a}^T(\mathbf{I}-\mathbf{RR}^T)\mathbf{a}}}\right)\qquad P_{A'}(\mathbf{y})=\Phi\left(-\frac{b-\mathbf{a}^T\mathbf{R}^T\mathbf{y}}{\sqrt{\mathbf{a}^T(\mathbf{I}-\mathbf{R}^T\mathbf{R})\mathbf{a}}}\right) \tag{21}$$

Assume the following numerical values:

$$\mathbf{R}=\begin{bmatrix}0.5 & 0.3\\ 0.1 & 0.5\end{bmatrix}\qquad \mathbf{a}=\begin{bmatrix}1\\ 1.5\end{bmatrix}\qquad b=3$$

For $\mathbf{y}=[2\quad 1]^T$, (21) gives (3 significant digits) $P_A(\mathbf{y})=0.310$ and $P_{A'}(\mathbf{y})=0.422$, which are clearly different. The integrals in (19) and (20) are estimated by direct Monte Carlo. Averaging the values of $P_A(\mathbf{y})$ and $P_{A'}(\mathbf{y})$ with one million i.i.d. standard Gaussian samples of $\mathbf{y}$ confirms that $\int P_A(\mathbf{y})\phi(\mathbf{y})d\mathbf{y}$ and $\int P_{A'}(\mathbf{y})\phi(\mathbf{y})d\mathbf{y}$ are both equal to the theoretical value (3 significant digits) $P(F)=\Phi(-b/\sqrt{\mathbf{a}^T\mathbf{a}})=0.0480$. Averaging using the same set of samples but only over those with $\mathbf{a}^T\mathbf{y}>b$ (i.e., conditional on failure) gives estimates of $\int P_A(\mathbf{y})\phi(\mathbf{y}\,|\,F)d\mathbf{y}$ and $\int P_{A'}(\mathbf{y})\phi(\mathbf{y}\,|\,F)d\mathbf{y}$, which are both equal to 0.374 (3 significant digits). These findings are consistent with (19) and (20).

5. Remarks

Comments on the original derivation in [9] are in order. In Appendix A of the paper, detailed balance was shown by considering the Gaussian vector $\mathbf{U}=[\mathbf{U}_0;\mathbf{U}_1]\in R^{2n}$ with zero mean and covariance matrix

$$\mathbf{\Sigma}=\begin{bmatrix}\mathbf{I} & \mathbf{R}\\ \mathbf{R}^T & \mathbf{I}\end{bmatrix} \tag{22}$$

It was claimed that a) given $\mathbf{U}_1$, the vector $\mathbf{U}_0$ is marginally Gaussian with mean $\mathbf{RU}_1$ and covariance $\mathbf{I}-\mathbf{RR}^T$; and b) given $\mathbf{U}_0$, the vector $\mathbf{U}_1$ is marginally Gaussian with mean $\mathbf{RU}_0$ and covariance $\mathbf{I}-\mathbf{RR}^T$. By writing the joint PDF in two ways, i.e., $p_{\mathbf{U}_0\mathbf{U}_1}=p_{\mathbf{U}_1|\mathbf{U}_0}p_{\mathbf{U}_0}=p_{\mathbf{U}_0|\mathbf{U}_1}p_{\mathbf{U}_1}$, it was deduced that (see (43) of the paper), for any $\mathbf{u}_0,\mathbf{u}_1\in R^n$,

$$\phi(\mathbf{u}_1;\mathbf{Ru}_0,\mathbf{I}-\mathbf{RR}^T)\phi(\mathbf{u}_0)=\phi(\mathbf{u}_0;\mathbf{Ru}_1,\mathbf{I}-\mathbf{RR}^T)\phi(\mathbf{u}_1) \tag{23}$$

and hence detailed balance was concluded to hold.

The identity in (8) shows that (23) is only true when $\mathbf{R}$ is symmetric. For general $\mathbf{R}$, the identity says that,

$$\phi(\mathbf{u}_1;\mathbf{Ru}_0,\mathbf{I}-\mathbf{RR}^T)\phi(\mathbf{u}_0)=\phi(\mathbf{u}_0;\mathbf{R}^T\mathbf{u}_1,\mathbf{I}-\mathbf{R}^T\mathbf{R})\phi(\mathbf{u}_1) \tag{24}$$

The issue in the argument leading to (23) stems from claim (b) above. The correct claim should be: given $\mathbf{U}_0$, the vector $\mathbf{U}_1$ is marginally Gaussian with mean $\mathbf{R}^T\mathbf{U}_0$ and covariance $\mathbf{I}-\mathbf{R}^T\mathbf{R}$. This follows from the standard result that for two jointly Gaussian vectors $X_1,X_2\in R^n$ with mean $\mu_1,\mu_2\in R^n$ and covariance matrices $\Sigma_{ij}=E[(X_i-\mu_i)(X_j-\mu_j)^T]\in R^{n\times n}$, given X_1, the vector X_2 is marginally Gaussian with mean $\mu_2+\Sigma_{21}\Sigma_{11}^{-1}(X_1-\mu_1)$ and covariance $\Sigma_{22}-\Sigma_{21}\Sigma_{11}^{-1}\Sigma_{12}$.

Appendix B in [9] assumed that $\mathbf{R}$ was symmetric so it was not affected by this issue. Neither was the adaptive algorithm in Section 3.4 or numerical examples in Section 4 affected because they assumed diagonal $\mathbf{R}$ (hence symmetric).

6. Conclusions

The identity in (8) provides the correct form of the joint PDF of the current sample and the candidate where the arguments are swapped. Based on this, detailed balance is shown to hold if and only if the cross correlation matrix is symmetric. A general expression for the PDF of the next sample has been derived in (17), which reveals the effect of violating symmetry. Insights on acceptance probabilities are also provided and illustrated with examples. The generalized algorithm opens up new possibilities for improving the efficiency of Subset Simulation and Monte Carlo algorithms in general. It is hoped that this article can contribute to clarifying basic theoretical issues for designing the cross correlation matrix or tuning the algorithm in future research.

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8. Appendix. Proof of identity (8)

To show (8), we express the LHS as

$$\phi(\mathbf{y};\mathbf{Rx},\mathbf{C})\phi(\mathbf{x}) = (2\pi)^{-n}|\mathbf{C}|^{-1}\exp\left[-\frac{1}{2}q(\mathbf{y},\mathbf{x})\right] \tag{25}$$

where

$$q(\mathbf{y},\mathbf{x}) = (\mathbf{y}-\mathbf{Rx})^T\mathbf{C}^{-1}(\mathbf{y}-\mathbf{Rx}) + \mathbf{x}^T\mathbf{x} \tag{26}$$

The proof is accomplished by showing $|\mathbf{C}|=|\mathbf{C}'|$ and

$$q(\mathbf{y},\mathbf{x}) = (\mathbf{x}-\mathbf{R}^T\mathbf{y})^T\mathbf{C}'^{-1}(\mathbf{x}-\mathbf{R}^T\mathbf{y}) + \mathbf{y}^T\mathbf{y} \tag{27}$$

where $\mathbf{C}' = \mathbf{I}-\mathbf{R}^T\mathbf{R}$ as defined in (9).

To show $|\mathbf{C}|=|\mathbf{C}'|$, we use the matrix determinant theorem [11], which says that for any matrices A,B,U,V of appropriate size,

$$|A+UBV| = |A||B||B^{-1}+VA^{-1}U| \tag{28}$$

Apply this with $A=\mathbf{I}$, $B=-\mathbf{I}$, $U=\mathbf{R}$ and $V=\mathbf{R}^T$ gives

$$|\mathbf{C}| = |\mathbf{I}-\mathbf{R}\mathbf{R}^T| = |\mathbf{I}||-\mathbf{I}||-\mathbf{I}^{-1}+\mathbf{R}^T\mathbf{I}^{-1}\mathbf{R}| = |\mathbf{I}-\mathbf{R}^T\mathbf{R}| = |\mathbf{C}'| \tag{29}$$

To show (27), expand the first term in (26):

$$q(\mathbf{y},\mathbf{x}) = \mathbf{y}^T\mathbf{C}^{-1}\mathbf{y} + \mathbf{x}^T(\mathbf{I}+\mathbf{R}^T\mathbf{C}^{-1}\mathbf{R})\mathbf{x} - \mathbf{y}^T\mathbf{C}^{-1}\mathbf{R}\mathbf{x} - (\mathbf{y}^T\mathbf{C}^{-1}\mathbf{R}\mathbf{x})^T \tag{30}$$

We use the matrix inverse lemma [11] to express $\mathbf{C}^{-1} = (\mathbf{I}-\mathbf{R}\mathbf{R}^T)^{-1}$ and $(\mathbf{I}+\mathbf{R}^T\mathbf{C}^{-1}\mathbf{R})$ in another form. For any matrices A,B,U,V of appropriate size, the lemma says that

$$(A+UBV)^{-1} = A^{-1} - A^{-1}U(B^{-1}+VA^{-1}U)^{-1}VA^{-1} \tag{31}$$

Applying the lemma with $A=\mathbf{I}$, $B=-\mathbf{I}$, $U=\mathbf{R}$ and $V=\mathbf{R}^T$ gives

$$\mathbf{C}^{-1} = (\mathbf{I}-\mathbf{R}\mathbf{R}^T)^{-1} = \mathbf{I} - \mathbf{R}(-\mathbf{I}+\mathbf{R}^T\mathbf{R})^{-1}\mathbf{R}^T = \mathbf{I} + \mathbf{R}(\mathbf{I}-\mathbf{R}^T\mathbf{R})^{-1}\mathbf{R}^T = \mathbf{I} + \mathbf{R}\mathbf{C}'^{-1}\mathbf{R}^T \tag{32}$$

Applying the lemma with $A=\mathbf{I}$, $B=\mathbf{C}^{-1}$, $U=\mathbf{R}^T$ and $V=\mathbf{R}$ gives

$$(\mathbf{I}+\mathbf{R}^T\mathbf{C}^{-1}\mathbf{R})^{-1} = \mathbf{I} - \mathbf{R}^T(\mathbf{C}+\mathbf{R}\mathbf{R}^T)\mathbf{R} = \mathbf{I} - \mathbf{R}^T\mathbf{R} = \mathbf{C}' \tag{33}$$

where we have used $\mathbf{C}+\mathbf{R}\mathbf{R}^T = \mathbf{I}$. Substituting $\mathbf{C}^{-1} = \mathbf{I}+\mathbf{R}\mathbf{C}'^{-1}\mathbf{R}^T$ from (32), the third term in (30) becomes

$$\mathbf{y}^T\mathbf{C}^{-1}\mathbf{R}\mathbf{x} = \mathbf{y}^T\mathbf{R}\mathbf{x} + \mathbf{y}^T\mathbf{R}\mathbf{C}'^{-1}\mathbf{R}^T\mathbf{R}\mathbf{x} = \mathbf{y}^T\mathbf{R}\mathbf{x} + \mathbf{y}^T\mathbf{R}\mathbf{C}'^{-1}(\mathbf{I}-\mathbf{C}')\mathbf{x} = \mathbf{y}^T\mathbf{R}\mathbf{C}'^{-1}\mathbf{x} \tag{34}$$

where in the second equality we have used $\mathbf{R}^T\mathbf{R} = \mathbf{I}-\mathbf{C}'$. Substituting (32) and (33) into the first and second term in (30), and using (34) for the last two terms,

$$q(\mathbf{y},\mathbf{x}) = \mathbf{y}^T\mathbf{y} + \mathbf{y}^T\mathbf{R}\mathbf{C}'^{-1}\mathbf{R}^T\mathbf{y} + \mathbf{x}^T\mathbf{C}'^{-1}\mathbf{x} - \mathbf{y}^T\mathbf{R}\mathbf{C}'^{-1}\mathbf{x} - (\mathbf{y}^T\mathbf{R}\mathbf{C}'^{-1}\mathbf{x})^T \tag{35}$$

This is identical to (27) after writing in complete square form in $\mathbf{x}$.

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