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Procedia Engineering 199 (2017) 1122–1127

Procedia Engineering

www.elsevier.com/locate/procedia

X International Conference on Structural Dynamics, EURODYN 2017

Markov Chain Monte Carlo Simulation Methods for Structural Reliability Analysis

Carsten Proppe[a]

[a]*Chair of Engineering Mechanics, Karlsruhe Institute of Technology, Kaiserstr. 10, Bdg. 10.23, 76131 Karlsruhe, Germany*

Abstract

Two Markov chain Monte Carlo simulation methods for reliability estimation, subset simulation and the moving particles algorithm, are compared. To this end, both low-dimensional and high-dimensional test cases are considered. The investigation sheds light on the avoidance of correlated samples in both algorithms, notably on the necessity of a burn-in period and the influence of a metamodel.

Peer-review under responsibility of the organizing committee of EURODYN 2017.

Keywords: Reliability Estimation; Markov Chain Monte Carlo Simulation; Subset Simulation; Moving Particles Algorithm

1. Introduction

Markov Chain Monte Carlo (MCMC) algorithms provide an important class of reliability estimation methods. The samples that are generated by these algorithms are not independent, but still identically distributed, if the Markov chain is in stationary state. The ergodic theorem and the central limit theorem for reversible Markov chains yield the convergence and the asymptotic unbiasedness of the estimator. An MCMC based algorithm that is widely used for reliability estimation is subset simulation [3], which is based on the estimation of conditional probabilities for nested sets. In contrast to many other MCMC algorithms, subset simulation does not require a burn-in of the Markov chain, because the seeds of the Markov chains are already distributed according to the target distribution [4]. On the other hand, MCMC with the classical Metropolis-Hastings (MH) algorithm suffers from a high rejection rate in conjunction with subset simulation, especially for high-dimensional reliability estimation, cf. [2]. Therefore, a componentwise MH algorithm has been introduced in [3].

In subset simulation, the size of the nested sets is usually chosen such that the conditional probabilities are equal to 0.1, i.e. 90% of the samples are discarded and need to be recomputed from the remaining 10% that serve as seeds. This leads in general to less than ten nested sets. Having too few nested sets would lead to a similar inefficiency as for direct MCS. In [3], it is argued that having much more nested sets would lead to an increase in the total number

* Corresponding author. Tel.: +49-721-608-46822 ; fax: +49-721-608-46070.
E-mail address: author@institute.xxx

1877-7058
Peer-review under responsibility of the organizing committee of EURODYN 2017.
10.1016/j.proeng.2017.09.226

of samples, which again decreases the efficiency of subset simulation. However, it is worthwhile to consider the limit case, where only a single sample is discarded and recomputed. This leads to a maximum number of nested sets. Such an MCMC based algorithm, called moving particles algorithm, has been introduced in [6] and [7] for reliability estimation. Markov chains were generated either by means of the classical MH algorithm or by directly sampling from a transition kernel.

Here subset simulation and the moving particles algorithm for reliability estimation are compared. Therefore, the componentwise MH algorithm of [3] has been implemented for both MCMC algorithms. Examples comprise low- as well as high-dimensional test cases with emphasis on accuracy, efficiency and acceptance rate. The objective is to shed some light on specific features of these two MCMC based algorithms. The paper is organized as follows: in the next section, subset simulation and the moving particles algorithm are introduced. Following this, the test cases and the test methodology are briefly presented. The test results are discussed and explanations for the observed phenomena are given. Finally, a summary of the observed phenomena and recommendations for off-the-shelf application of the simulation algorithms are given.

2. Markov Chain Monte Carlo Simulation

2.1. Subset Simulation

Subset Simulation is based on nested sets, $F_1 \supset F_2 \supset \dots F_M$, where $F_M = \{\boldsymbol{\theta} \in \mathbb{R}^n | g(\boldsymbol{\theta}) < 0\}$ denotes the failure region and $g(\boldsymbol{\theta})$ is the performance function. If $\boldsymbol{\theta}$ is a vector of random variables, the failure probability is given by

$$P_f = P_{F_1} \prod_{i=1}^{M-1} P(F_{i+1}|F_i). \tag{1}$$

The rather small failure probability is written as the product of larger probabilities that can be estimated with less effort. However, the estimation of the conditional probabilities requires the application of MCMC simulations, because the corresponding conditional probability density function is not known explicitly. In subset simulation, N_s parallel Markov chains are started from seeds that for step $i-1$ lie in F_i and propagated by a componentwise MH algorithm [3]. A weak correlation of the samples produced by the Markov chain is necessary for a reduction of the coefficient of variation for the conditional probability $P_{i+1} = P(F_{i+1}|F_i)$.

Besides the transition kernel of the MCMC algorithm, the most influential parameter of subset simulation are the sets F_i, for which sets of equal conditional probability $p_0 = P(F_{i+1}|F_i)$ are preferred. Given p_0, the sets are obtained from a percentile estimation for the performance function. The failure probability is then given by

$$p_0^{M-1} \hat{P}_M, \tag{2}$$

where $\hat{P}_M$ is the estimate for $P(F_M|F_{M-1})$.

2.2. Moving Particles

The moving particles algorithm can be considered as subset simulation with a maximum number of steps. Thus, in each step, only one sample is discarded and resampled by a Markov chain that takes as seed one of the retained samples. As for subset simulation, the algorithm starts with a direct MCS. For each step, the values $g(\boldsymbol{\theta}_i)$, $i = 1, ..., N_s$, of the N_s samples are ranked. The sample with the maximum value of the performance function is moved: MCMC is carried out starting from one of the remaining samples and the final state of the Markov chain is accepted, if the value of the performance function could be reduced. Otherwise, the sample is simply replaced by the seed of the Markov chain. Here, the same algorithm as for subset simulation is applied for the generation of the Markov chains.

Instead of computing the probability of failure from eq. (2), each initial sample is moved until it reaches the failure region and the number of moves is count. As has been shown in [6], the number of moves to get an initial sample into the failure region follows a Poisson distribution with parameter $\lambda = \log \frac{1}{p_F}$. The estimator for the parameter of the Poisson distribution is

$$\hat{\lambda} = \frac{\sum_{i=1}^{N_s} M_i}{N_s}, \tag{3}$$

where M_i denotes the number of moves until seed i reaches the failure state.

In order to obtain an unbiased estimate, it is mandatory that the trajectories of the Poisson process generated from the initial samples remain independent until the samples finally reach the failure domain. In [7], two means are proposed to maintain the independence:

- Burn-in: The Markov chain simulation is carried out with a burn-in period. The burn-in should ensure the independence of the candidate and the seed of the Markov chain.
- Seed avoidance: Repeated use of the same seed for the Markov chain should be avoided. Once a sample has been used as seed, the sample and its offspring should not be used as seed again.

While the moving particles algorithm can be considered as a special case of subset simulation, there are several differences with respect to the original subset simulation algorithm:

- In subset simulation, the number of steps is rather small; however, the number of steps in the moving particles algorithm is maximal.
- In subset simulation, only p_0 (usually 10%) of the samples are retained in each step and serve as seed for the Markov chains. In contrast, only one sample is resampled in each step of the moving particles algorithm, and the seed can be selected among the other samples.
- The moving particles algorithm has a clear interpretation from Poisson process theory, but requires that all initial samples finally reach the failure region.

3. Test Cases

Test cases have been considered with standardized parameters for the algorithms in order to investigate the robustness, accuracy and efficiency of both simulation methods. The aim was to find out whether the simulation methods can be applied off-the-shelf without fine tuning to a specific problem. The low dimensional test cases were those summarized in [9], Table 1. They allowed to carry out parameter studies for the number of initial samples and the Markov chain transition kernel. Moreover, for the moving particles algorithm, the influence of a burn-in period, a seed selection strategy and a low-rank metamodel have been investigated. Following this, both algorithms were applied to high-dimensional examples, a paraboloid with discretely varying principal curvatures, [10], example 4, and a single-degree-of-freedom oscillator with 1500 random variables, [3], example 1, with a threshold value $b = 1.5$.

For each test case and each set of parameters, 100 simulation runs were carried out from which the mean probability of failure, the mean number of performance function evaluations and the mean acceptance rate have been observed. The coefficient of variation of the results was so small that only mean results will be shown.

For the MCMC with MH algorithm, two acceptance rates can be defined:

- Level 1: Acceptance of the pre-candidate by the MH algorithm.
- Level 2: Acceptance of the candidate sample. For subset simulation, the candidate sample at step i must lie in F_i, while for the moving particles algorithm, the value of the performance function must decrease.

In this investigation, the level 2 acceptance rate has been monitored exclusively.

The simulation platform was Matlab with FERUM [11]. To this end, the moving particles simulation algorithm has been added to FERUM and extensions to the subset simulation algorithm were made.

4. Results

Figures 1 and 2 display the influence of the number of initial samples on the accuracy and the efficiency of the simulation algorithms for the low-dimensional test cases. While increasing the number of initial samples increases the accuracy, the efficiency is decreased. The number of initial samples needed for subset simulation is larger than for the moving particles algorithms, which is due to the fact that 90% of the samples are discarded in each simulation step. A good balance between accuracy and efficiency is obtained for the moving particles algorithm with 200 initial

samples and for subset simulation with 2000 initial samples. The number of initial samples does not influence the mean level 2 acceptance rate very much.

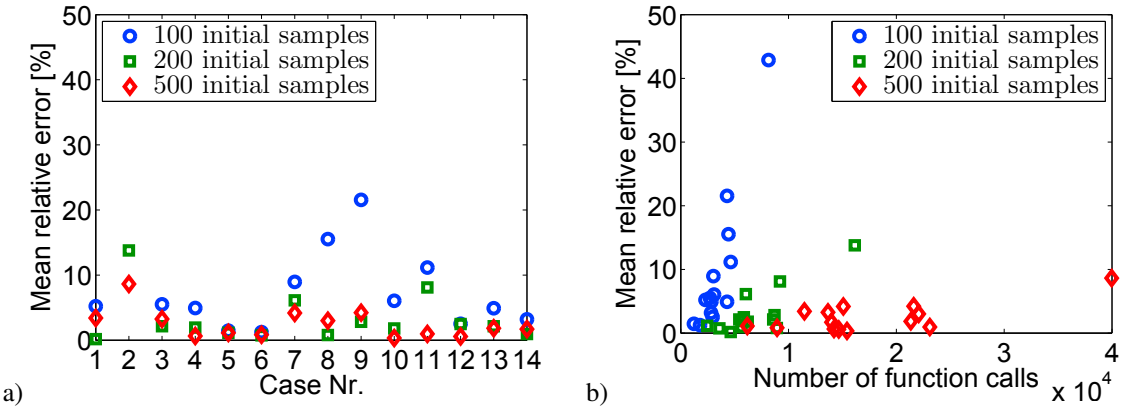

Fig. 1. Moving particles algorithm. Influence of the number of initial samples.

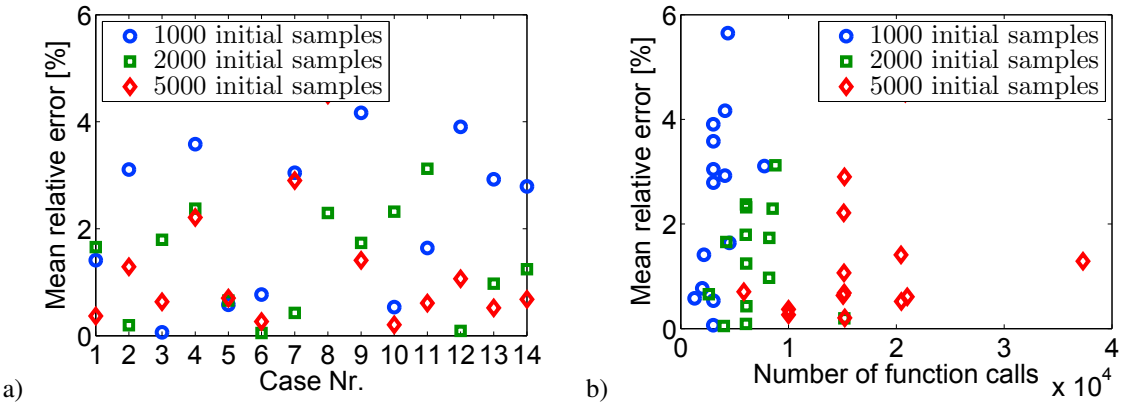

Fig. 2. Subset simulation. Influence of the number of initial samples.

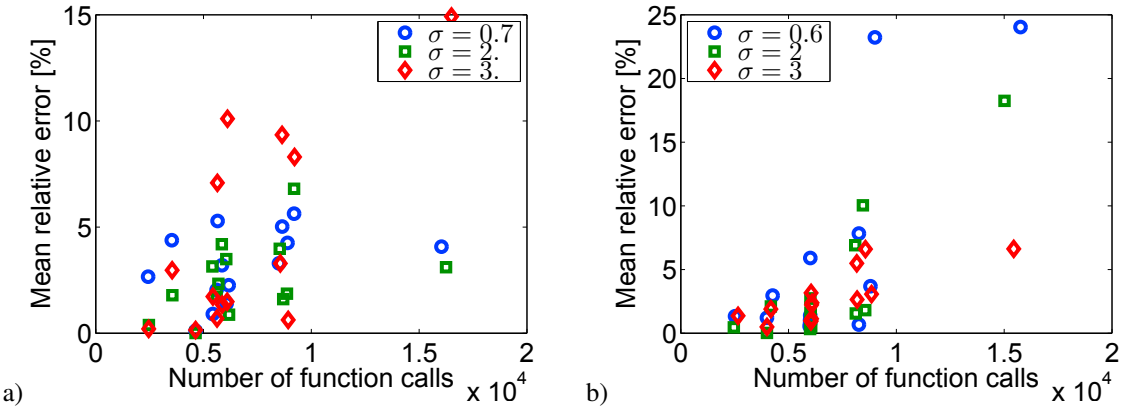

Fig. 3. Influence of σ. a) Moving particles algorithm. b) Subset simulation

Figure 3 displays the influence of the standard deviation on the moving particles algorithm and on subset simulation. It can be seen that higher values for the standard deviation are more appropriate for subset simulation. This can be explained by the fact that for subset simulation, there are only few different seeds for the Markov chains available.

For subset simulation and the moving particles algorithm, there is a clear dependence of the level 2 acceptance rate on the standard deviation σ of the normal densities. As has been reported previously (cf. [12] and [5]), a medium range of the level 2 acceptance rate leads to efficient estimations of the failure probability. For the moving particles algorithm, this medium level is attained for smaller values of the standard deviation. It is also noted that the level 2 acceptance rate is rather independent of the probability of failure.

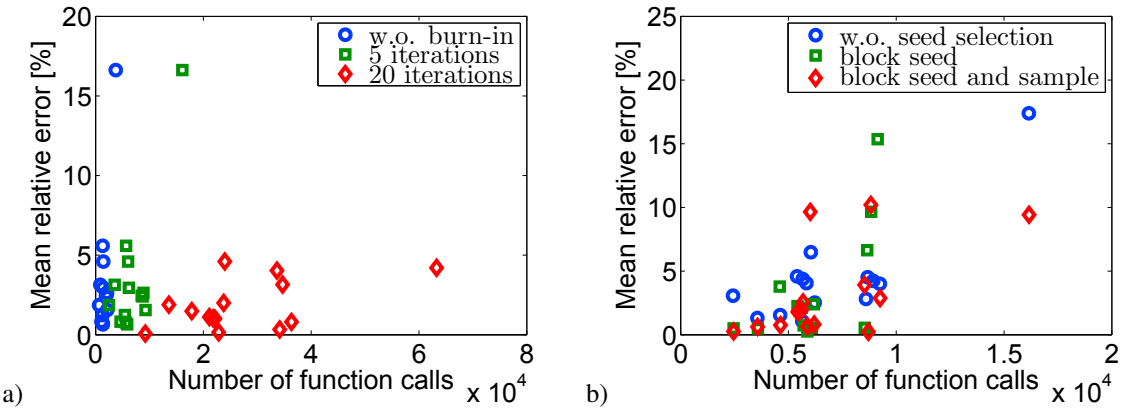

Fig. 4. Moving particles algorithm with MH kernel. a) Influence of the burn-in period b) Influence of seed selection strategies.

Figure 4 summarizes the influence of the burn-in period on the efficiency and various seed selection strategies on the accuracy of the moving particles algorithm. The results underline that a burn-in period is mandatory for the moving particles algorithm. However, a burn-in period of 20 samples as proposed in the literature leads to a high number of performance function calls. It was found that a shorter burn-in period (about 5 samples) is a good compromise between accuracy and effort.

Various seed selection strategies have been tested. Figure 4 indicates that seed avoidance is beneficial to the accuracy of the simulation algorithm and that blocking the seed of the Markov chain and the generated sample (the offspring) for further use as seed of a Markov chain is a viable strategy to increase the efficiency.

Neither the length of the burn-in period nor the seed selection strategy had a significant influence on the level 2 acceptance rate.

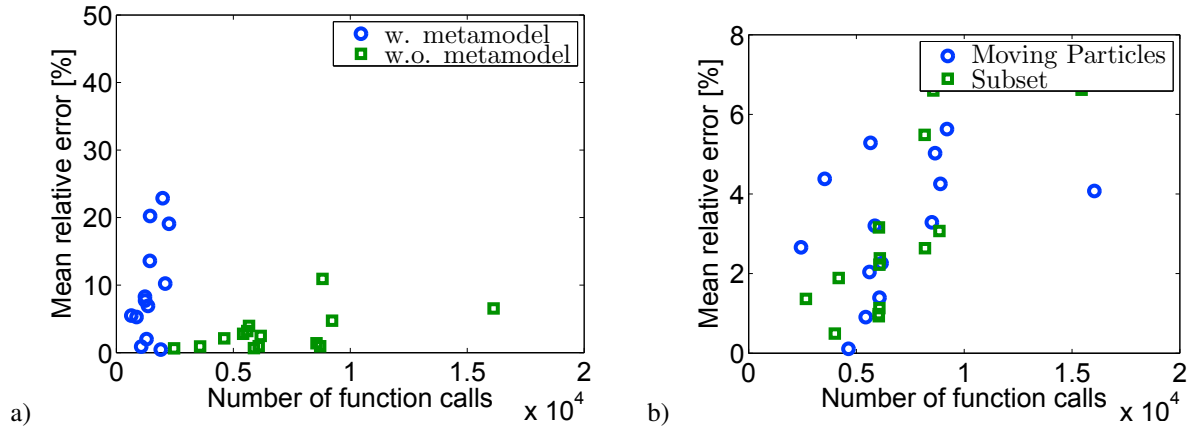

Fig. 5. a) Influence of a metamodel on the moving particles algorithm. b) Comparison of subset simulation and the moving particles algorithm.

As can be seen from Figure 5 a), the application of a metamodel during the burn-in period of the Markov chains for the moving particles algorithm will decrease the number of performance function calls, but increases at the same time the approximation error by about a factor of two, such that the quality of the obtained results is not acceptable anymore. Here, a low rank separated representation with 20 polynomial terms of order 10 that has been continuously updated (as described in [7]) has been applied.

The comparison of the moving particles algorithm and subset simulation, Figure 5 b), underlines that both algorithms lead to accurate predictions of the failure probability with similar efficiency. Finally, both algorithms have been applied to high-dimensional test cases, a single-degree-of-freedom oscillator with 1500 random variables and a paraboloid with varying curvatures. Both algorithms yielded results of same accuracy and efficiency. The level 2 acceptance rates were similar as for the low-dimensional test cases.

5. Conclusions

The aim of the simulation study was to investigate the suitability of two MCMC simulation algorithms, subset simulation and the moving particles algorithm, for off-the-shelf reliability computations.

The following conclusions conclusions can be drawn: A large initial sample size is beneficial for the accuracy of both algorithms, but decreases the efficiency in terms of performance function evaluations. Comparing the subset simulation algorithm to the moving particles algorithm, it was found that the subset simulation algorithm needs about a factor of ten more initial samples, as most of the initial samples are discarded during the move to the next subset simulation step. For the componentwise MH transition kernel, both algorithms tolerate a wide range of values for the standard deviation of the normal distribution. In order to obtain accurate results, the standard deviation for subset simulation must be higher than for the moving particles algorithm. A burn-in period is necessary in order to obtain a good accuracy of the moving particles algorithm. A seed selection strategy tends to increase the accuracy of the moving particles algorithm, but has nearly no influence on the level 2 acceptance rate.

For the efficiency, the differences between the moving particles and the subset simulation algorithm were rather small for the low- as well as the high-dimensional test cases. In conclusion, subset simulation and the moving particles algorithm seem to be well suited for off-the-shelf reliability estimations, but with a different setting for the most important parameters (σ and the initial sample size).

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