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Bayesian Subset Simulation: a kriging-based subset simulation algorithm for the estimation of small probabilities of failure

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Abstract: The estimation of small probabilities of failure from computer simulations is a classical problem in engineering, and the Subset Simulation algorithm proposed by Au & Beck (Prob. Eng. Mech., 2001) has become one of the most popular method to solve it. Subset simulation has been shown to provide significant savings in the number of simulations to achieve a given accuracy of estimation, with respect to many other Monte Carlo approaches. The number of simulations remains still quite high however, and this method can be impractical for applications where an expensive-to-evaluate computer model is involved.

We propose a new algorithm, called Bayesian Subset Simulation, that takes the best from the Subset Simulation algorithm and from sequential Bayesian methods based on kriging (also known as Gaussian process modeling). The performance of this new algorithm is illustrated using a test case from the literature. We are able to report promising results. In addition, we provide a numerical study of the statistical properties of the estimator.

Keywords: Computer experiments, Sequential design, Subset Simulation, Probability of failure

1. INTRODUCTION

In this paper, we propose an algorithm called *Bayesian Subset Simulation* (BSS), that combines the Bayesian decision-theoretic framework from our previous studies [1, 2] with the Subset Simulation algorithm [3].

Let $\Gamma = \{x \in \mathbb{X} : f(x) > u\}$ denote the excursion set of a function $f : \mathbb{X} \rightarrow \mathbb{R}$ above a threshold $u \in \mathbb{R}$. We are interested in estimating the probability $\alpha(u) := P_{\mathbb{X}}(\Gamma)$, which corresponds to the probability of failure of a system for which f is a function of performance (see, e.g., [2]). If the probability $\alpha(u)$ is small, estimating it using the Monte Carlo estimator $\hat{\alpha}_m^{\text{MC}} = 1/m \sum_{i=1}^m \mathbb{1}_{f(X_i) > u}$, $X_i \stackrel{\text{i.i.d.}}{\sim} P_{\mathbb{X}}$, requires a large number of evaluations of f . If the performance function f is expensive to evaluate, this leads to use a large amount of computational resources, and in some cases, it may be even impossible to proceed in reasonable time. Estimating small probabilities of failure with moderate computational resources is a challenging topic.

When $\alpha(u)$ is small, the main problem with the estimator $\hat{\alpha}_m^{\text{MC}}$ is that the sample size m must be large in order to get a reasonably high probability of observing at least a few samples in Γ . In the literature, importance sampling methods have been considered to generate more samples in the failure region Γ . However, the success of this kind of methods relies greatly on prior knowledge about the failure region Γ and on a relevant choice for the proposal sampling distribution.

The idea of Subset Simulation is to decompose the difficult problem of generating samples in the failure region into a series of easier problems, by introducing intermediate failure events. Let $u_0 = -\infty < u_1 < u_2 < \dots < u_T = u$ be a sequence of increasing thresholds and define a corresponding sequence of decreasing excursion sets $\Gamma_0 := \mathbb{X} \supseteq \Gamma_1 \supseteq \dots \supseteq \Gamma_T := \Gamma$, where $\Gamma_t := \{x \in \mathbb{X} : f(x) > u_t\}$, $t = 1, \dots, T$. Notice that

$\Gamma_t = \bigcap_{i=1}^t \Gamma_i$. Then, using the properties

$$\begin{cases} \alpha(u_0) = 1, \\ \alpha(u_{t+1}) = \alpha(u_t) P_{\mathbb{X}}(\Gamma_{t+1}|\Gamma_t), \quad t \geq 0, \end{cases} \quad (1)$$

$\alpha(u)$ can be rewritten as a product of conditional probabilities:

$$\alpha(u) = P_{\mathbb{X}}(\Gamma_T) = \prod_{t=0}^{T-1} P_{\mathbb{X}}(\Gamma_{t+1}|\Gamma_t). \quad (2)$$

Thus, the idea of Subset Simulation is to replace the problem of estimating the small probability $\alpha(u)$ by that of estimating the *higher* conditional probabilities $P_{\mathbb{X}}(\Gamma_{t+1}|\Gamma_t)$, $0 \leq t < T$.

In [3], a standard Monte Carlo simulation method is used to estimate $P_{\mathbb{X}}(\Gamma_1) = P_{\mathbb{X}}(\Gamma_1|\Gamma_0)$. For the other conditional probabilities, a Markov Chain Monte Carlo method is used to simulate samples in Γ_t , and then $P_{\mathbb{X}}(\Gamma_{t+1}|\Gamma_t)$ is estimated using a Monte Carlo method. Due to the direct use of Monte Carlo method, the number of evaluations needed remains still quite high. For many practical applications where the performance function corresponds to an expensive-to-evaluate computer model, it is not applicable. Note that the Subset Simulation algorithm has recently caught the attention of the Sequential Monte Carlo (SMC) community: using standard tools from the SMC literature, [4] derives several theoretical results about some very close versions of the Subset Sampling algorithm.

In this work, we propose an algorithm that takes advantage of a Gaussian process prior about f in order to decrease the number of evaluations needed to estimate the conditional probabilities $P_{\mathbb{X}}(\Gamma_{t+1}|\Gamma_t)$. The Gaussian process model makes it possible to assess the uncertainty about the position of the intermediate excursion sets Γ_t , given a set of past evaluation results. The idea has its roots in the field of design and analysis of computer experiments (see, e.g., [5, 6, 7, 8, 9, 10, 11]). More specifically, kriging-based sequential strategies for the estimation of a probability of failure are closely related to the field of Bayesian global optimization [12, 13, 14, 15, 16, 17].

The paper is organized as follows. In Section 2, we give a detailed presentation of our new Bayesian Subset Simulation algorithm. In Section 3, we apply the algorithm on an example from the literature, and we perform numerical simulations to investigate the performance of the proposed algorithm. A comparison with Subset Simulation and classical Monte Carlo methods is provided. Finally, we conclude in Section 4.

Remark. An algorithm involving kriging-based adaptive sampling and Subset Simulation has been recently proposed by V. Dubourg and co-authors [18, 19] to address the problem of Reliability-Based Design Optimization (RBDO). Their approach is different from the one proposed in this paper, which addresses the problem of reliability analysis.

2. BAYESIAN SUBSET SIMULATION ALGORITHM

2.1. Algorithm

Our objective is to build an estimator of $\alpha(u_T)$ from the evaluations results of f at a number of points $X_1, X_2, \dots, X_N \in \mathbb{X}$. Let ξ be a random process modeling our prior knowledge about f , and for each $n \geq 0$, denote by \mathcal{F}_n the σ -algebra generated by $X_1, \xi(X_1), \dots, X_n, \xi(X_n)$. A natural Bayesian estimator of $\alpha(u_t)$ using n_t evaluations is the posterior mean

$$\hat{\alpha}_t = E_{n_t}(\alpha(u_t)) = E_{n_t} \left(\int_{\mathbb{X}} \mathbb{1}_{\xi > u_t} dP_{\mathbb{X}} \right) = \int_{\mathbb{X}} g_t dP_{\mathbb{X}}, \quad (3)$$

where $g_t : x \in \mathbb{X} \mapsto \mathbb{P}_{n_t}(\xi(x) > u_t)$ and \mathbb{E}_n (resp. \mathbb{P}_n) denotes the conditional expectation (resp. conditional probability) with respect to \mathcal{F}_n (see [2]). Note that, $g_t(x)$ can be readily computed for any x using kriging (see, e.g., [2]).

Assume now that $\mathbb{P}_{\mathbb{X}}$ has a probability density function $p_{\mathbb{X}}$ and consider the sequence of probability density functions q_t , $0 \leq t \leq T$, defined by

$$q_t(x) = \frac{1}{\widehat{\alpha}_t} p_{\mathbb{X}}(x) g_t(x). \quad (4)$$

We can write a recurrence relation similar to (1) for the sequence of Bayesian estimators $\widehat{\alpha}_t$:

$$\widehat{\alpha}_t = \int g_t(x) p_{\mathbb{X}}(x) dx = \widehat{\alpha}_{t-1} \int \frac{g_t(x)}{g_{t-1}(x)} q_{t-1}(x) dx. \quad (5)$$

The idea of our new algorithm, that we call Bayesian Subset Simulation, is to construct recursively a Monte Carlo approximation $\widehat{\alpha}_T$ of the Bayesian estimator $\widehat{\alpha}_t$, using (5) and sequential Monte Carlo simulation (SMC) (see, e.g., [20]) for the evaluation of the integral with respect to q_{t-1} on the right-hand side. More precisely, denoting by m the size of the Monte Carlo sample, we will use the recurrence relation

$$\widehat{\alpha}_t = \widehat{\alpha}_{t-1} \times \frac{1}{m} \sum_{i=1}^m \frac{g_t(Y_{t-1}^i)}{g_{t-1}(Y_{t-1}^i)}, \quad 1 \leq t \leq T, \quad (6)$$

where variables $Y_{t-1}^1, \dots, Y_{t-1}^m$ are distributed according to¹ the density q_{t-1} , which leads to

$$\widehat{\alpha}_T = \prod_{t=0}^{T-1} \frac{1}{m} \sum_{i=1}^m \frac{g_{t+1}(Y_t^i)}{g_t(Y_t^i)}. \quad (7)$$

The connection between the proposed algorithm and the original Subset Simulation algorithm is clear from the similarity between the recurrence relations (1) and (5), and the use of SMC simulation in both algorithms to construct recursively a “product-type” estimator of the probability of failure (see also in [20], Section 3.2.1, where this type of estimator is mentioned in a very general SMC framework).

Our choice for the sequence of densities q_1, \dots, q_T also relates to the original Subset Simulation algorithm. Indeed, note that $q_t(x) \propto \mathbb{E}_{n_t}(\mathbb{1}_{\xi > u_t} p_{\mathbb{X}})$, and recall that $\tilde{q}_t \propto \mathbb{1}_{\xi > u_t} p_{\mathbb{X}}$ is the distribution used in the Subset Simulation algorithm at stage t . (This choice of instrumental density is also used by [22, 23] in the context of a two-stage kriging-based adaptive importance sampling algorithm. This is indeed a quite natural choice, since $\tilde{q}_T \propto \mathbb{1}_{\xi > u} p_{\mathbb{X}}$ is the optimal instrumental density for the estimation of $\alpha(u)$ by importance sampling.)

2.2. Implementation

This section gives implementation details for our Bayesian Subset Simulation algorithm, the principle of which has been described in the Section 2.1. The pseudo-code for the algorithm is presented in Table 1.

The initial Monte Carlo sample $\mathbb{Y}_0 = \{Y_0^1, \dots, Y_0^m\}$ is a set of independent random variables drawn from the density $q_0 = p_{\mathbb{X}}$ —in other words, we start with a classical Monte Carlo simulation step. At each subsequent stage $t \geq 1$, a new sample \mathbb{Y}_t is produced from the previous one using the basic reweight/resample/move steps of SMC simulation (see [20] and the references therein). In this article, resampling is carried out using a multinomial sampling scheme, and the move step relies on a fixed-scan Metropolis-within-Gibbs algorithm as in [3] with a Gaussian-random-walk proposal distribution for each coordinate (for more information on these techniques, see, e.g., [24]).

¹By “distributed according to”, it is not meant that $Y_{t-1}^1, \dots, Y_{t-1}^m$ are independent and identically distributed. This is never the case in sequential Monte-Carlo techniques. What we mean is that the sample $Y_{t-1}^1, \dots, Y_{t-1}^m$ is *targetting* the density q_{t-1} in the sense of, e.g., [21].

Table 1: Algorithm of Bayesian Subset Simulation

a) Initialize (Stage 0):

1. Generate a MC sample $\mathbb{Y}_t = \{Y_0^1, \dots, Y_0^m\}$, drawn according to the distribution $P_{\mathbb{X}}$
2. Initial DoE $\mathcal{I}_n = \{(X_1, f(X_1)), \dots, (X_{n_0}, f(X_{n_0}))\}$ (maximin)
3. Choose kriging model, estimate parameters k_θ

b) At each stage $t(t = 1 \dots T)$:

1. Compute the kriging predictor \hat{f}_n^{t-1} , and choose threshold \tilde{u}^{t-1}
2. Select and evaluate N_t new points using a SUR sampling criterion for the threshold u_t .
3. Update \mathcal{I}_n , adjust intermediate threshold u_{t-1} according to \hat{f}_n^{t-1}
4. Regenerate a new sample \mathbb{Y}_t :
 - 4.1 **reweight**: calculate weights: $w_i^t \propto g_t(Y_{t-1}^i)/g_{t-1}(Y_{t-1}^i)$
 - 4.2 **resample**: generate a sample $\tilde{Y}_{t-1,i}$ according to weights
 - 4.3 **move**: for each $i \leq m$, $Y_t^i \sim K(\tilde{Y}_{t-1,i}, \cdot)$

c) The final probability of failure is calculated by

$$\hat{\alpha} = \prod_{t=0}^{T-1} \left(\frac{1}{m} \sum_{i=1}^m \frac{g_{t+1}(Y_t^i)}{g_t(Y_t^i)} \right)$$

A number N_t of evaluations of the performance function is done at each stage of the algorithm. This number is meant to be much smaller than the size m of the Monte Carlo sample—which would be the number of evaluations in the classical Subset Sampling algorithm. For the initialization stage ($t = 0$), we choose a space filling set of points \mathbb{Y}_0 as usual in the design of computer experiments [25]. At each subsequent stage, we use N_t iteration of a SUR sampling strategy [2] targeting the threshold u_t to select the evaluation points. Adaptive techniques to choose the sequence of thresholds and the number of points per stage are presented in the following sections.

Remark 1. *The resampling step could most certainly benefit from more elaborate schemes, such as the residual resampling scheme [26, 27, 28]. The comparison of resampling schemes is left for future work.*

2.3. Adaptive choice of the thresholds u_t

It can be proved that, for an idealized² Subset Simulation algorithm with fixed thresholds $u_0 < u_1 < \dots < u_T = u$, it is optimal to choose the thresholds to make all conditional probabilities $P_{\mathbb{X}}(\Gamma_{t+1} | \Gamma_t)$ equal to some constant value (see [4], Section 2.4). This leads to the idea of choosing the thresholds adaptively in such a way that, in the product estimate

$$\hat{\alpha}_T^{\text{SubSamp}} = \prod_{t=1}^T \frac{1}{m} \sum_{i=1}^m \mathbb{1}_{\Gamma_t}(Y_{t-1}^i),$$

²assuming that Y_t^1, \dots, Y_t^m are independent and identically distributed according to q_t .

each term but the last is equal to some predefined constant p_0 . In other words, u_t is chosen as the $(1 - p_0)$ -quantile of \mathbb{Y}_{t-1} . This idea was first suggested by [3] in Section 5.2, on the heuristic ground that the algorithm should perform well when the conditional probabilities are neither too small (otherwise they are hard to estimate) nor too large (otherwise a large number of stages is required). The asymptotic behavior of the resulting algorithm, when m is large, has been analyzed by [4].

In Bayesian Subset Simulation, we propose to choose the thresholds adaptively using a similar approach. More precisely, considering the product form of the estimator (7), we suggest to choose u_t in such a way that

$$\frac{1}{m} \sum_{i=1}^m \frac{g_{t+1}(Y_t^i)}{g_t(Y_t^i)} = p_0.$$

The equation can be easily solved since the left-hand side is a strictly decreasing function of u_t .

Remark 2. Note that [4] proved that choosing adaptive levels in Subset Simulation introduces a positive bias of order $1/m$, which is negligible compared to its standard deviation.

2.4. Adaptive choice of the number N_t of evaluation at each stage

In this section, we propose a technique to choose adaptively the number N_t of evaluations of the performance function that must be done at each stage of the algorithm.

Let us assume that $t \geq 1$ is the current stage number; at the beginning of the stage, n_{t-1} evaluations of the performance function are available from previous stages. After several additional evaluations, the number of available observations of f is $n \geq n_{t-1}$. Then, for each $i \in \{1, \dots, m\}$, the probability of misclassification³ of $x \in \mathbb{X}$ with respect to the threshold u_t is

$$\tau_{t,n}(x) = \min\left(p_n(x, u_t), 1 - p_n(x, u_t)\right),$$

where $p_n(x, u) = \mathbb{E}_n(\mathbb{1}_{\xi(x) > u})$ (see [2]). We shall decide to stop adding new evaluations at stage t when

$$\frac{1}{m} \sum_{i=1}^m \tau_{t,n}(Y_{t-1}^i) \leq \eta,$$

for some prescribed $\eta > 0$.

3. NUMERICAL RESULTS

In this section, we apply the proposed algorithm on a simple 2D test case from the structural reliability literature. The problem under consideration is the deviation of a cantilever beam, with a rectangular cross-section, and subjected to a uniform load [29, 30]. The performance function is:

$$f(x_1, x_2) = 18.46154 - 7.476923 \times 10^{10} \frac{x_1}{x_2^3}. \quad (8)$$

The uncertain factors are x_1 and x_2 , which are supposed to be independent and normally distributed, as specified in Table 2. We use $u = 17.8$ as the threshold for the definition of the failure event. The probability of failure, which will be used as reference estimator, obtained using $\hat{\alpha}_m^{\text{MC}}$ with $m = 10^8$, is approximately 3.85×10^{-5} (with a coefficient variance of about $1/\sqrt{m\alpha} \approx 1.61\%$). Figure 1 shows the distribution of the input factors along with a contour plot of f . Notice that the failure region is quite far from the center region of the input distribution.

Table 2: Random input factors

Variable	Distribution	Mean m	Standard deviation σ
x_1	\mathcal{N}	0.001	0.0002
x_2	\mathcal{N}	250	37.5

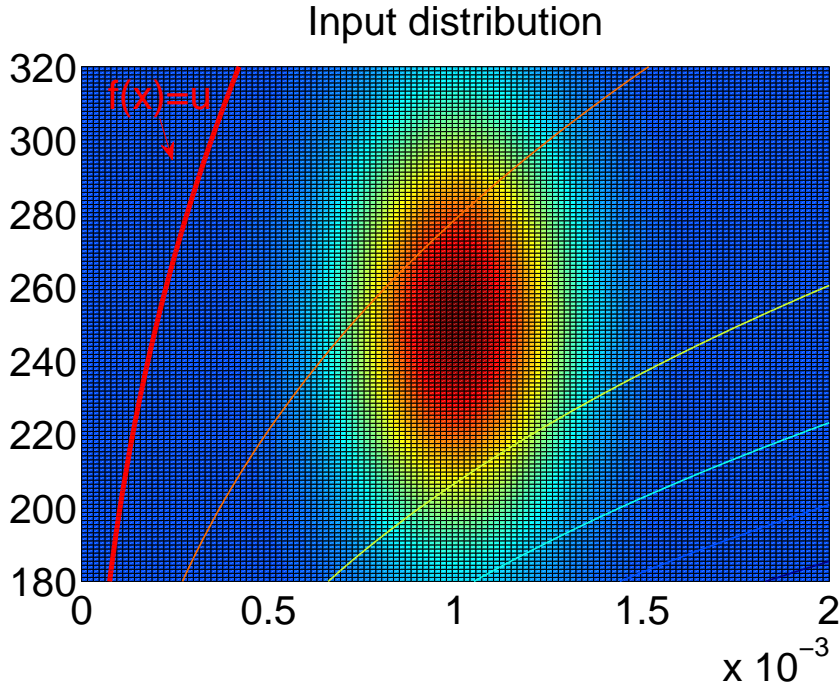


Figure 1: Input distribution and contour plot of the performance function

In the Bayesian Subset Simulation algorithm, we set an initial design of size $N_0 = 10$ which is equal to five times the dimension d of the input space (In the literature, very little is known about the problem of choosing N_0 , however some authors recommend to start with a sample size proportional to the dimension d , see [31]). Concerning the choice of N_0 , we decide to apply a greedy MAXMIN algorithm and sequentially choose the points which will maximize the minimal Euclidean distance between any two points in the initial Monte Carlo sample \mathbb{Y}_0 . At each stage, we choose a Monte Carlo sample of size $m = 1000$. A Gaussian process with constant unknown mean and a Matérn covariance function is used as our prior information about f . The parameters of the Matérn covariance functions are estimated on the initial design by REML (see, e.g., [32]). In this experiment, we follow the common practice of re-estimating the parameters of the covariance function during the sequential strategy, and update the covariance function after each evaluation. The target conditional probability between successive thresholds is set to $p_0 = 0.1$. The intermediate threshold u_t is chosen by the criterion (2.3). The proposal distribution q_t for a Gibbs sampling is a Gaussian distribution $\mathcal{N}(0, \sigma^2)$, where σ^2 is specified in Table 2. The stopping criterion for the adaptive SUR strategy is set to $\eta_t = 10^{-6}$ (for $t = 1, \dots, T - 1$) and $\eta_T = 10^{-7}$.

Figure 2 shows the Design of Experiment (DoE) selected by the algorithm at stage $t = 1, 2, 3$ and the last stage for one run. Table 3 lists the number of evaluations (rounded to integer) at each stage averaged over 50 runs. We can see that an average total of evaluations $N = \sum_{i=0}^T N_t = 104$ are needed for our proposed Bayesian Subset Simulation, while for Subset Simulation, the number is $1000 + 900 \times 4 = 4600$.

³See [2] Section 2.4 for more information

Table 3: Average number of evaluations at each stage.

N_t	1	2	3	4	5
Sub-Sim	1000	900	900	900	900
Bayesian Sub-Sim	14	17	17	18	28

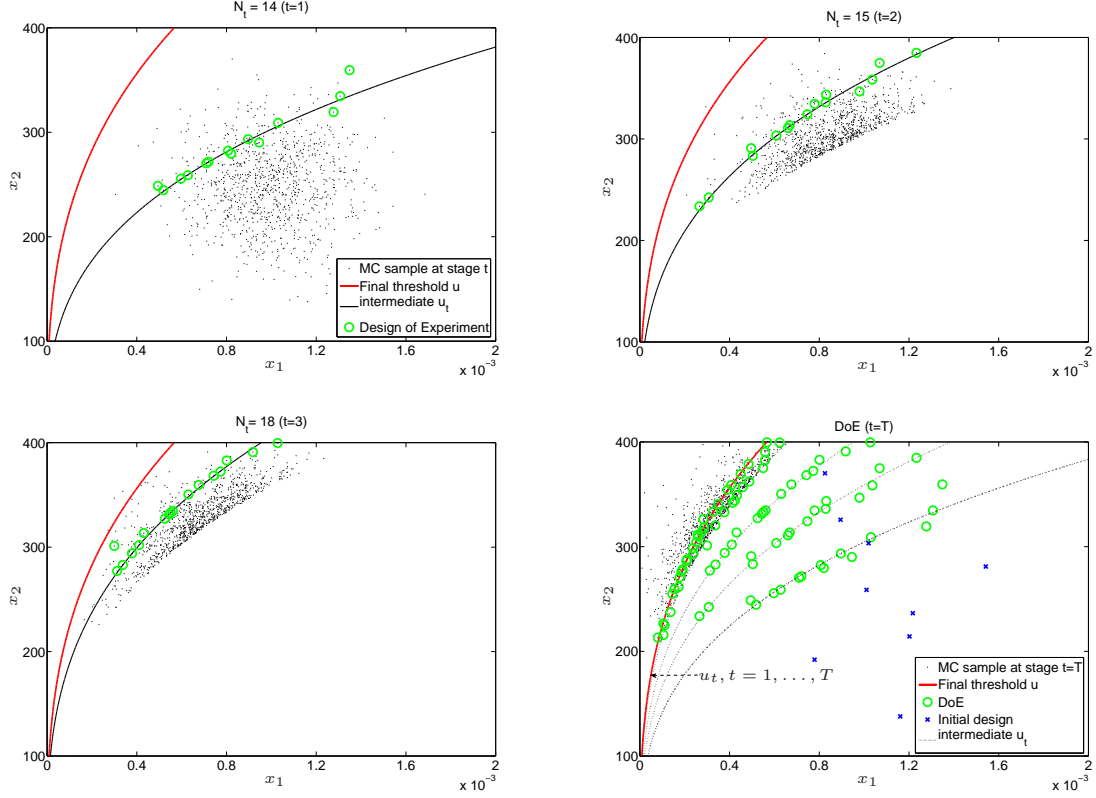


Figure 2: Evaluations selected by the Bayesian Subset Simulation strategy at stage $t = 1, 2, 3$ and the final Design of Experiment (DoE).

To evaluate the statistical properties of the estimator, we consider the absolute relative bias

$$\kappa = \left| \frac{E(\hat{\alpha}) - \alpha}{\alpha} \right| \quad (9)$$

and the coefficient of variation

$$\text{cov} = \frac{\delta(\hat{\alpha})}{\alpha}, \quad (10)$$

where $E(\hat{\alpha})$ is the average mean and $\delta(\hat{\alpha})$ is the standard deviation of the estimator $\hat{\alpha}$.

Table 4 shows the results of the comparison of our proposed Bayesian Subset Sampling algorithm with the Subset Simulation algorithm in [3]. Crude Monte Carlo sampling is used as the reference probability of failure. For the fairness of the comparison, we set the same intermediate probability $p_0 = 0.1$, and sample size $m = 1000$ in both methods. Fifty independent runs are performed to evaluate the average of both methods. For Bayesian Subset Simulation method, as N is different for each run, we show the minimal and maximal of N from 50 runs.

Table 4: Compare with Monte Carlo approach and Subset Simulation

Method	m	N	$\hat{\alpha}$ (10^{-5})	$\delta(\hat{\alpha})$ (10^{-5})	κ	cov
MCS	10^8	10^8	3.8500	0.062	0	1.6%
Sub-Sim	1000	4600	3.9078	2.470	1.5%	63.2%
Bayesian Sub-Sim	1000	[94, 109]	3.7020	0.618	4.4%	16.7%

4. CONCLUSION

In this paper, we propose a new algorithm called Bayesian Subset Simulation for estimating small probabilities of failure in a context of very expensive simulations. This algorithm combines the main ideas of the Subset Simulation algorithm and the SUR strategies developed in our recent work [2].

Our preliminary results show that the number of evaluations is dramatically decreased compared to the original Subset Simulation algorithm, while keeping a small bias and coefficient of variation.

Our future work will try to improve further the properties of our algorithm regarding the bias and the variance of the estimator. We shall also test and validate the approach on more challenging examples.

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