

# Geometric insight into the challenges of solving high-dimensional reliability problems

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**ABSTRACT:** In this paper we adopt a geometric perspective to highlight the challenges associated with solving high-dimensional reliability problems. Adopting a geometric point of view we highlight and explain a range of results concerning the performance of several well-known reliability methods.

We start by investigating geometric properties of the  $N$ -dimensional Gaussian normal space and the distribution of samples in such a space or in a subspace corresponding to a failure domain. Next, we discuss Importance Sampling (IS) in high dimensions. We provide a geometric understanding to why IS does generally not work in high dimensions (Au and Beck 2003). We furthermore challenge the significance of "design point" when dealing with strongly nonlinear problems. We conclude by showing that for the general high-dimensional nonlinear reliability problems the selection of an appropriate IS density is practically impossible.

Next, we discuss the simulation of samples using Markov Chain Monte Carlo (MCMC) methods. Firstly, we provide a geometric explanation as to why the standard Metropolis-Hastings (MH) algorithm does "not work" in high-dimensions. We then explain why the modified Metropolis-Hastings (MMH) algorithm introduced by Au and Beck (2001) overcomes this problem. A study of the correlation of samples obtained using MMH as a function of different parameters follows. Such study leads to recommendations for fine-tuning the MMH algorithm. Finally, the MMH algorithm is compared with the MCMC algorithm proposed by Katafygiotis and Cheung (2006) in terms of the correlation of samples they generate.

**Keywords:** Reliability; Importance sampling; Subset simulation; Markov Chains; Dynamic analysis.

## 1 GEOMETRIC PROPERTIES OF HIGH-DIMENSIONAL GAUSSIAN SPACE

In practical applications random parameters of a system can usually be generated by appropriate transformation of independent standard Gaussian variables. So let us start with the investigation of the geometric properties of the  $N$ -dimensional standard Gaussian space and the distribution of samples in such a space.

Let  $\theta = (\theta_1, \dots, \theta_N)$  be a random vector in  $\mathbb{R}^N$  where each of its components follows the standard Gaussian distribution:

$$\theta_i \sim \mathcal{N}(0, 1), \quad i = 1, \dots, N. \quad (1)$$

By definition the square of the Euclidean norm of  $\theta$  is distributed according to the chi-square distribution with  $N$  degrees of freedom:

$$R^2 = \sum_{i=1}^N \theta_i^2 \sim \chi_N^2 \quad (2)$$

As  $N$  tends to infinity, the distribution of  $R^2$  tends to normality (by Central Limit Theorem). In particular, it becomes more and more symmetric. However, the tendency is slow: the skewness is  $\sqrt{8/N}$ . The probability density function (PDF) and cumulative distribution function (CDF) for  $N = 10^3$  are plotted in Fig. 1.

It can be shown that  $\sqrt{2R^2}$  is approximately normally distributed with mean  $\sqrt{2N - 1}$  and unit variance. Hence the norm of the random vector  $\|\theta\| = R$  is also approximately a Gaussian random variable:

$$R \stackrel{\text{app}}{\approx} \mathcal{N}\left(\sqrt{N - 1/2}, 1/2\right) \approx \mathcal{N}\left(\sqrt{N}, 1/2\right), \quad (3)$$

when  $N \rightarrow \infty$ . This means that the huge part of probability mass in the  $N$ -dimensional standard Gaussian space belongs in the ring, so called Important Ring,

$$\sqrt{N} - r < R < \sqrt{N} + r, \quad (4)$$

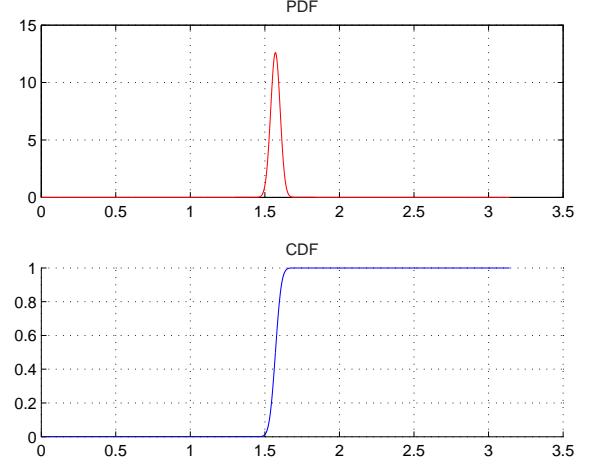
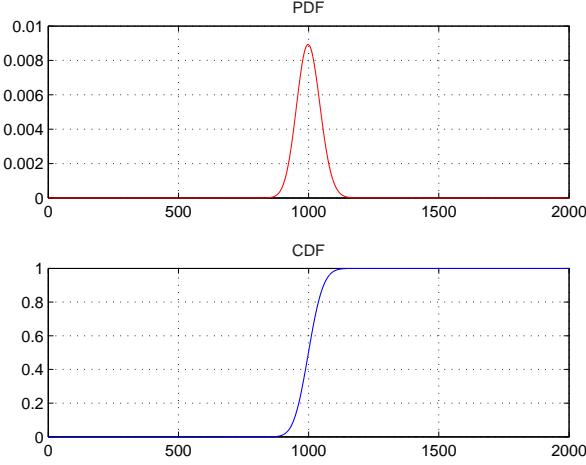


Figure 1: Probability Density Function and Cumulative Distribution Function of chi-square distribution with  $N = 10^3$  degrees of freedom

where  $r$  depends on the amount of probability mass that we want to contain inside the Important Ring. For example, if  $N = 10^3$  and  $r = 3.46$  the probability of the corresponding Important Ring is more than  $1 - 10^{-6}$ . Thus, any sample  $\theta \in \mathbb{R}^N$  distributed according to the high-dimensional standard Gaussian distribution will lie with extremely large probability in the Important Ring.

Now let us fix one particular direction (here direction means a ray passing through zero), say  $e = (1, 0, \dots, 0)$ , and explore the distribution of the angle  $\alpha = \hat{\theta}e$  between this direction and a random vector  $\theta$ . By definition

$$\begin{aligned} f_\alpha(\alpha_0)d\alpha &= P(\alpha_0 \leq \alpha \leq \alpha_0 + d\alpha) \\ &= P(\alpha_0 \leq \hat{\theta}e \leq \alpha_0 + d\alpha), \end{aligned} \quad (5)$$

where  $f_\alpha$  is the PDF of  $\alpha$ . Since the Gaussian space is isotropic (there are no preferable directions) and any point that lies along a particular ray forms the same angle with  $e$ , we can simplify the problem by considering the  $(N - 1)$ -dimensional sphere of unit radius. On this sphere all points are uniformly distributed. Therefore,  $f_\alpha(\alpha_0)$  is proportional to the geometric volume of part of this sphere:

$$f_\alpha(\alpha_0) \sim Vol(\Omega_{\alpha_0}), \quad (6)$$

$$\Omega_{\alpha_0} = \{\theta \in \mathbb{S}_1^{N-1} : \hat{\theta}e = \alpha_0\} \quad (7)$$

If  $\langle \cdot, \cdot \rangle$  denotes the standard scalar product in  $\mathbb{R}^N$  then  $\langle \theta, e \rangle = \theta_1$ . On the other hand  $\langle \theta, e \rangle = \|\theta\| \|e\| \cos \hat{\theta}e$ . Therefore

$$\Omega_{\alpha_0} = \{\theta \in \mathbb{S}_1^{N-1} : \theta_1 = \cos \alpha_0\} \quad (8)$$

Figure 2: Probability Density Function and Cumulative Distribution Function of angle  $\alpha$

One can rewrite (8) as the intersection of the hypersphere  $\mathbb{S}_1^{N-1}$  with the hyperplane  $\{\theta_1 = \cos \alpha_0\}$ :

$$\Omega_{\alpha_0} = \mathbb{S}_1^{N-1} \cap \pi_{\alpha_0}^{N-1}, \quad (9)$$

$$\pi_{\alpha_0}^{N-1} = \{\theta \in \mathbb{R}^N : \theta_1 = \cos \alpha_0\}. \quad (10)$$

This intersection can be easily evaluated.

$$\left\{ \begin{array}{l} \theta_1^2 + \dots + \theta_N^2 = 1 \\ \theta_1 = \cos \alpha_0. \end{array} \right. \Leftrightarrow \quad (11)$$

$$\theta_2^2 + \dots + \theta_N^2 = \sin^2 \alpha_0. \quad (12)$$

Thus, the region in which we are interested is a  $(N - 2)$ -dimensional sphere of radius  $\sin \alpha_0$ :

$$\Omega_{\alpha_0} = \mathbb{S}_{\sin \alpha_0}^{N-2}. \quad (13)$$

It is well known that the volume of a  $k$ -dimensional sphere is proportional to the radius in the power  $k$ . So we have:

$$f_\alpha(\alpha_0) \sim Vol(\Omega_{\alpha_0}) \sim \sin^{N-2} \alpha_0. \quad (14)$$

Finally, we can obtain that the PDF and CDF of  $\alpha$  (Fig. 2) are correspondingly equal to

$$f_\alpha(\alpha) = \frac{\sin^{N-2} \alpha}{\int_0^\pi \sin^{N-2} \alpha d\alpha} \quad (15)$$

$$F_\alpha(\alpha) = \frac{\int_0^\alpha \sin^{N-2} \alpha d\alpha}{\int_0^\pi \sin^{N-2} \alpha d\alpha} \quad (16)$$

From this result and by plotting these distributions for large  $N$  it follows that if we fix the particular direction  $e$  then a sample  $\theta \in \mathbb{R}^N$  that is distributed according to the high-dimensional standard Gaussian distribution will be with high probability almost perpendicular to this direction.

Although we proved this result for the specific direction  $e = (1, 0, \dots, 0)$  this also holds for arbitrary  $e$  since the Gaussian space is isotropic.

This also can be argued in a more intuitive way. If  $\theta$  is such a sample then

$$\cot^2 \alpha = \frac{\theta_1^2}{\theta_2^2 + \dots + \theta_N^2} \quad (17)$$

Since  $\theta_i$  are independent and identically distributed random variables we have that expectation:

$$E[\cot^2 \alpha] = \frac{1}{N-1} \rightarrow 0 \text{ as } N \rightarrow \infty. \quad (18)$$

Therefore

$$\alpha \rightarrow \pi/2 \text{ as } N \rightarrow \infty. \quad (19)$$

## 2 IMPORTANCE SAMPLING

Consider the problem of computing failure probability. The probability of failure can be simply expressed as:

$$p_F = \int_{\mathbb{R}^N} I_F(\theta) q(\theta) d\theta \quad (20)$$

where  $F \subseteq \mathbb{R}^N$  is the failure domain,  $I_F$  is the indicator function ( $= 1$  if  $\theta \in F$ ,  $= 0$  otherwise) and  $\theta$  represents the random parameters of the system with joint PDF  $q$ <sup>1</sup>.

Among all procedures developed for estimation of  $p_F$ , a prominent position is held by simulation methods. In standard Monte Carlo simulations the integral (20) is interpreted as mathematical expectation:

$$p_F = E_q[I_F] \quad (21)$$

and, keeping in mind the Law of Large Numbers, the following estimator is used:

$$p_F^{mc} = \frac{1}{n} \sum_{k=1}^n I_F(\theta^{(k)}), \quad \theta^{(k)} \sim q(\cdot) \quad (22)$$

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<sup>1</sup>Without limiting the generality the random vector  $\theta = (\theta_1, \dots, \theta_N)$  will be considered to be standard Gaussian with independent components (any vector can be appropriately transformed to a vector that is indeed distributed like this). So

$$q(\theta) = \prod_{i=1}^N q_i(\theta_i) = \prod_{i=1}^N \mathcal{N}_{(0,1)}(\theta_i) = \frac{1}{(\sqrt{2\pi})^N} \exp\left(-\frac{\|\theta\|^2}{2}\right)$$

The statistical error of unbiased estimators is most appropriately measured by the coefficient of variation. In the case of standard Monte Carlo:

$$\delta_{mc} = \sqrt{\frac{(1-p_F)}{np_F}} \quad (23)$$

The main advantage of standard Monte Carlo is independence of the dimensionality  $N$  of the random vector  $\theta$ . Its main disadvantage is its inefficiency in estimating small failure probabilities because of the large number of samples ( $\sim 1/p_F$ ) needed to achieve an acceptable level of accuracy.

So standard Monte Carlo is not applicable in the case of small failure probabilities (even in a one-dimensional case). Importance Sampling is a variance reduction method aiming to improve the standard Monte Carlo method.

The basic idea of Importance Sampling is to generate samples that lie more frequently in the region of the failure domain with high PDF values. Roughly speaking standard Monte Carlo does not work because the vast majority of terms in the sum (22) are zero and only very few are equal to one. Using Importance Sampling we want instead of summing of 0's and 1's to consider a sum of many small numbers to approximate the failure probability.

Specifically, for any PDF  $q_{is}$  we can write:

$$\begin{aligned} p_F &= \int_{\mathbb{R}^N} I_F(\theta) q(\theta) d\theta \\ &= \int_{\mathbb{R}^N} \frac{I_F(\theta) q(\theta)}{q_{is}(\theta)} q_{is}(\theta) d\theta = E_{q_{is}} \left[ \frac{I_F q}{q_{is}} \right] \end{aligned} \quad (24)$$

and similarly to (22) we have:

$$p_F^{is} = \frac{1}{n} \sum_{k=1}^n \frac{I_F(\theta^{(k)}) q(\theta^{(k)})}{q_{is}(\theta^{(k)})}, \quad \theta^{(k)} \sim q_{is}(\cdot) \quad (25)$$

Note that standard Monte Carlo method is a special case of Importance Sampling when  $q_{is} = q$ .

The most important task in applying Importance Sampling is the construction of the importance sampling density (ISD)  $q_{is}$ . If it is "good" then we can get great improvement in efficiency.

What does it mean: "good" ISD? Let us consider an example. Suppose we know that a certain vector  $x$  belongs to the failure domain  $x \in F$ . It is natural to assume that in the neighbourhood of  $x$  there are more points from  $F$ . Thus, we can consider  $q_{is}$  to be a Gaussian PDF centered at  $x$ :

$$q_{is}(\theta) = \frac{1}{(\sqrt{2\pi})^N} \exp\left(-\frac{\|\theta - x\|^2}{2}\right). \quad (26)$$

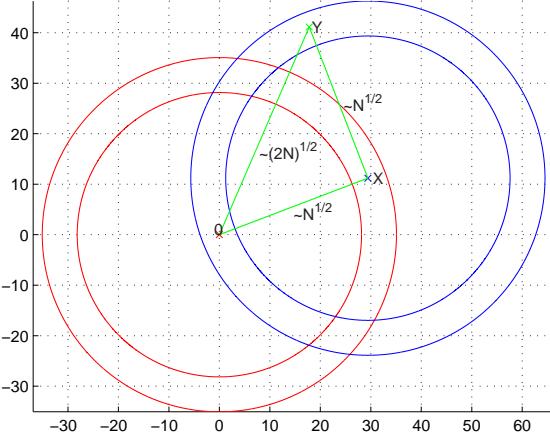


Figure 3: Vectors  $x, y \in \mathbb{R}^N$  are drawn from standard Gaussian and Gaussian centered at  $x$  distributions respectively,  $N = 1000$ .

As discussed in the previous section, the main part of probability mass is concentrated inside the Important Ring. This means that we can restrict the sample space and consider only the part of failure domain that belongs to the Important Ring, since the contribution of the remaining part of the failure domain to the probability  $p_F$  is comparatively very small. So we can consider that  $x$  belongs in the Important Ring. Again, from the previous section we know that the angle between the vectors  $x$  and  $(y - x)$ , where  $y$  is a random vector drawn from  $q_{is}$  is approximately equal to  $\pi/2$ . Moreover  $y$  will lie in the Important Ring corresponding to  $q_{is}$ . This is schematically shown in Fig. 3.

It follows that in high dimensions we will have:

$$\|x\| \approx \sqrt{N}, \quad \|y - x\| \approx \sqrt{N} \quad (27)$$

Therefore

$$\|y\| \approx \sqrt{2N} \quad (28)$$

Now the estimator (25) gives:

$$p_F^{is} = \frac{1}{n} \sum_{k=1}^n \frac{I_F(y^{(k)})q(y^{(k)})}{q_{is}(y^{(k)})}, \quad (29)$$

since each  $y^{(k)}$  is drawn from the Gaussian distribution centered at  $x$  and, therefore, satisfies (28), it follows from (27), (28) that the ratio

$$\frac{q(y^{(k)})}{q_{is}(y^{(k)})} \approx e^{-N/2}, \quad (30)$$

is extremely small in high dimensions. Thus, Importance Sampling leads to underestimation of  $p_F$ . A geometrical reason as to why this happens is that it is very unlikely to simulate points inside the Important Ring centered in zero.

### 3 DESIGN POINTS AND NONLINEAR PROBLEMS

The next question we discuss is the significance of design points when dealing with strongly nonlinear problems.

Basically, the calculation of the probability of failure  $p_F$  in (20) is the evaluation of the total probability volume corresponding to the failure domain  $F \in \mathbb{R}^N$  defined by  $g(\theta) < 0$ , where  $g(\cdot)$  denotes the limit-state function (LSF). The design point is defined as the point  $\theta^*$  on the limit-state surface  $\{\theta : g(\theta) = 0\}$  that is nearest to the origin when the random variables are assumed to have been transformed to the standard Gaussian space. Due to the rotational symmetry of standard Gaussian, the design point is the most likely realization of the random variables that gives rise to the failure event.

It is considered to be that design points play very important role in solving reliability problems. Without doubt this is true in the linear case. Consider a linear reliability problem with LSF expressed in terms of the standard Gaussian vector  $\theta$  as follows:

$$g(\theta) = a^t \theta + b, \quad (31)$$

where  $a \in \mathbb{R}^N$  and  $b$  are fixed coefficients. The design point  $\theta^*$  is then the point on the plane  $g(\theta) = 0$  that is located closest to the origin and can be easily calculated in terms of  $a$  and  $b$  as follows:

$$\theta^* = -\frac{b}{\|a\|^2} a \quad (32)$$

The norm of the design point is usually called reliability index:

$$\beta = \|\theta^*\| = \frac{b}{\|a\|} \quad (33)$$

It is well known that the failure probability corresponding to this linear failure domain is given in terms of  $\beta$  by the expression:

$$p_F = P(\theta : g(\theta) < 0) = 1 - \Phi(\beta), \quad (34)$$

where  $\Phi$  denotes the CDF of the standard Gaussian variable. So, the failure probability in the liner case is completely defined by the design point. In the case where the failure domain is almost linear the first order reliability method (FORM) based on (34) for the given design point provides a good approximation of  $p_F$ . In the case where the LSF

can be approximated by a second order polynomial function, the design point still plays a very important role and is the basis of the second order reliability method (SORM). However in nonlinear case the meaning of the design points is not so clear and is in need of research.

Our first goal is to provide a feeling on how the nonlinear failure domain and the corresponding design point look like in the case of a nonlinear dynamic problem.

### 3.1 Duffing oscillator subjected to white noise

This nonlinear elastic system is taken from Koo et al (2005). Consider the Duffing oscillator defined by

$$m\ddot{x}(t) + c\dot{x}(t) + k[x(t) + \gamma x(t)^3] = f(t) \quad (35)$$

with  $m = 1000$  kg,  $c = 200\pi$  Ns/m,  $k = 1000(2\pi)^2$  N/m, and  $\gamma = 1$  m $^{-2}$ , and assume the input is white-noise with intensity  $S_0 = 10^6$  N $^2$ s/rad. Then in the discrete form  $f(t)$  is a vector of pulses  $f = (f_1, \dots, f_N) = \sigma\theta$ , where  $\sigma = \sqrt{2\pi S_0/\Delta t}$  and  $\theta$  is a standard Gaussian random vector. As described by Der Kiureghian and Li (1996) most events of interest in random vibration analysis can be represented in terms of the instantaneous failure event

$$E_\tau = \{x(\tau) > x_0\}, \quad (36)$$

i.e., the event that the response at a specified time  $\tau$  exceeds a specified threshold  $x_0$ . The corresponding failure domain is:

$$F_\tau = \{\theta : x(\tau) > x_0\}, \quad (37)$$

We consider the specific time instance  $\tau = 12$  s, three different thresholds  $x_0 = K\sigma_0$ , where  $K = 3, 4, 5$  and  $\sigma_0^2 = \pi S_0/ck$  is the stationary response variance for the linear case ( $\gamma = 0$ ). We use  $\Delta t = 0.01$  so that the dimension  $\dim \theta = N = \tau/\Delta t + 1 = 1201$ .

If the threshold is too large, then the probability  $p_F = P(F_\tau)$  is small and the intersection of  $F_\tau$  with a random 2-dimensional plane is zero. Let  $\theta^*$  and  $\theta_L^*$  denote the design points for the nonlinear and for the linear ( $\gamma = 0$ ) problems correspondingly. Then, the 2-dimensional plane  $\pi(\theta^*, \theta_L^*)$  formed by  $\theta^*$  and  $\theta_L^*$  contains failure points for sure. Note, that  $\theta^*$  can be found using a mirror-image excitation (Koo et al. 2005). In Fig. 4, 5, 6 the intersections  $F_\tau \cap \pi(\theta^*, \theta_L^*)$  for  $K = 3, 4, 5$  are shown. The concentric circles are the intersection of the Important Ring with this plane and the rays shown are the directions of  $\theta^*$  and  $\theta_L^*$ .

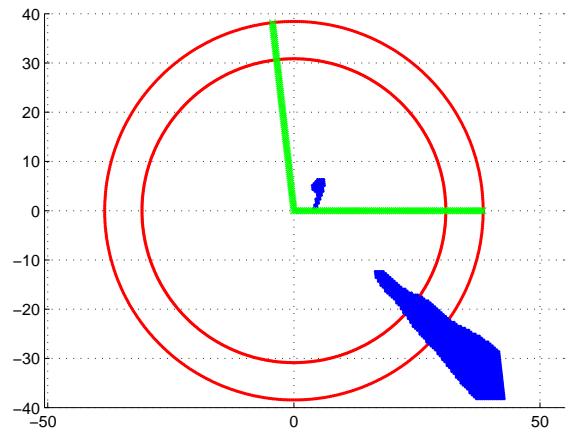


Figure 4: The intersection of failure domain  $F_\tau$  with the 2-dimensional plane  $\pi(\theta^*, \theta_L^*)$  for  $K = 3$ .

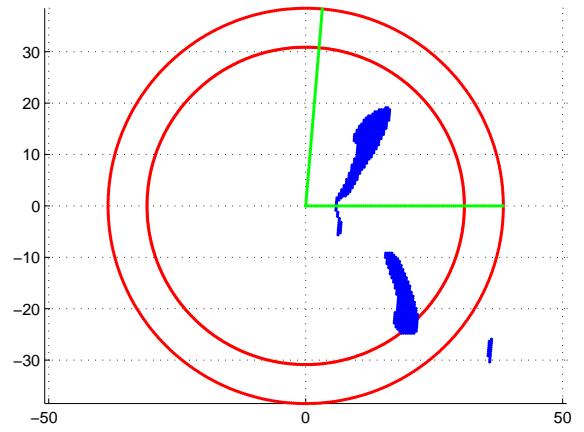


Figure 5: The intersection of failure domain  $F_\tau$  with the 2-dimensional plane  $\pi(\theta^*, \theta_L^*)$  for  $K = 4$ .

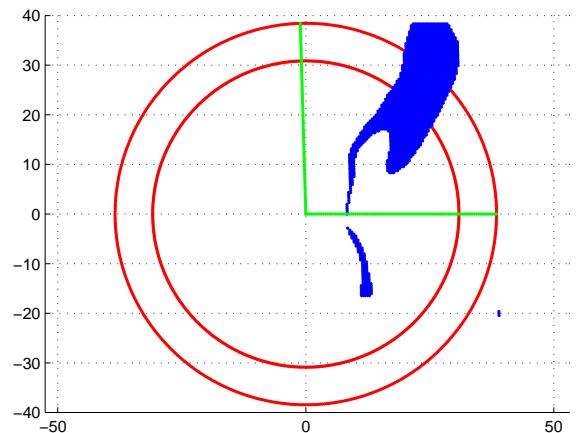


Figure 6: The intersection of failure domain  $F_\tau$  with the 2-dimensional plane  $\pi(\theta^*, \theta_L^*)$  for  $K = 5$ .

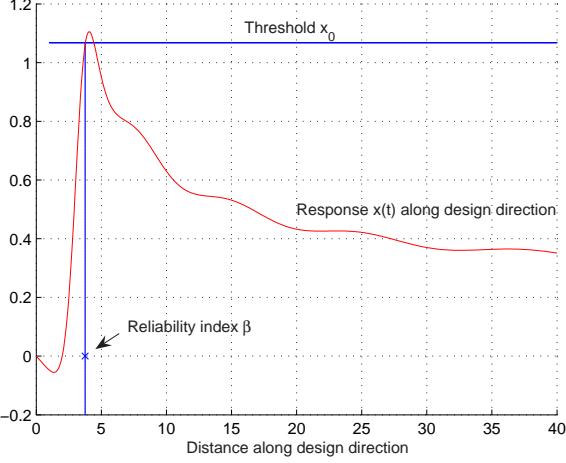


Figure 7: Response of Duffing oscillator along design point direction

The reliability index for this nonlinear problem is  $\beta = 3.76$ , with corresponding failure probability  $1 - \Phi(\beta) = 8.5 \cdot 10^{-5}$ . Note, that the true failure probability is equal to 0.0092 (Monte Carlo with  $10^4$  samples).

Let  $f_{\theta^*}$  be the excitation along the design point direction (design direction), i.e.

$$f_{\theta^*} = \sigma(s\theta^*), \quad (38)$$

where  $s$  is a scalar factor. The corresponding response  $x(\tau)$  at a specified time  $\tau$  is shown in Fig. (7). When  $s = 1$  we have an excitation that correspond to the design point itself and the response reaches the threshold  $x_0$ . Then there is a small period of exceedance of the threshold and after that the response begins to decrease so that around the Important Ring ( $s \sim \sqrt{N} = 34.64$ ) we have a safe region.

These pictures show that the design point itself as well as the direction of the design point can be of no consequence for searching the main parts of the failure domain (intersections of failure domain with the Important Ring).

### 3.2 Nonlinear failure domain of parabolic shape

The design points are usually used in conjunction with Importance Sampling for calculating the failure probability. For the first passage problem the failure domain  $F$  can be represent as a union of elementary failure regions  $F_i$ , defined similarly to (37) as exceedance at time  $t_i = i\Delta t$ :

$$F_i = \{\theta : x(t_i) > x_0\}, \quad i = 0, \dots, N = \frac{\tau}{\Delta t} \quad (39)$$

When the design points  $\theta_i^*$  are known, the ISD can be constructed as a weighted sum of Gaussian

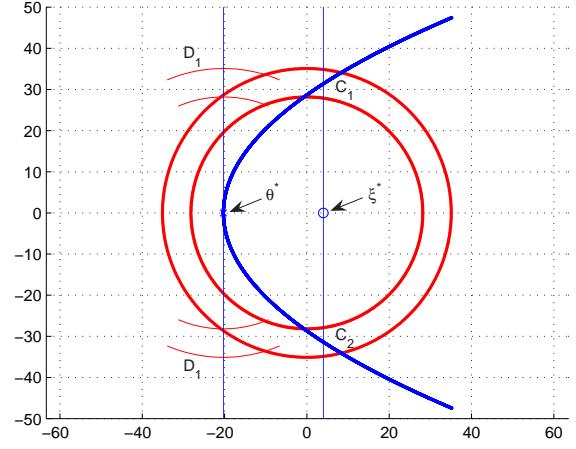


Figure 8: Failure domain of parabolic shape PDFs centered at the design points, i.e.:

$$q_{is}(\theta) = \sum_{i=1}^N w_i \mathcal{N}_{(0,1)}(\theta - \theta_i^*) \quad (40)$$

Our goal is to demonstrate that when the failure domain is strongly nonlinear Importance Sampling with ISD (40) can be feeble.

We consider a paraboloid in  $N$ -dimensional space defined as follows:

$$P : \quad x_1 = a \sum_{i=2}^N x_i^2 - b, \quad (41)$$

and define failure domain as the interior of this paraboloid:

$$F = \left\{ x \in \mathbb{R}^N : x_1 > a \sum_{i=2}^N x_i^2 - b \right\}. \quad (42)$$

The intersection of this high-dimensional failure domain with an arbitrary plane containing the  $x_1$  direction is shown in Fig. 8. We use  $a = 0.025$ ,  $b = 20.27$  and  $N = 1000$ . The probability of this parabolic failure domain calculated using standard MC simulation ( $10^4$  samples and 100 runs) is equal to  $p_F = 0.00142$  with c.o.v.  $\delta = 0.24$ .

However if we will use Importance Sampling method with Gaussian ISD centered at the design point  $\theta^* = (-b, 0, \dots, 0)$  we will get underestimation. For  $10^4$  samples and 20 runs we got  $p_F^{is} = 0$ . This happens because, as was explained in section 2, all samples generated from the Gaussian density centered at  $\theta^*$  will lie in the Important Ring centered at  $\theta^*$  and will be almost perpendicular to the fixed  $x_1$ -direction. In the 2-dimensional picture in Fig. 8 these regions are denoted as  $D_1$  and  $D_2$  which are not failure regions.

Suppose now that we know the shape of failure domain. Then from the previous discussion it is natural to use as ISD a Gaussian PDF  $\mathcal{N}(\xi^*, \sigma^2)$  centered at  $\xi^*$ , where  $\xi^*$  is a point along the  $x_1$ -direction, such that

$$P \cap \pi_{\xi^*}^\perp = P \cap \mathbb{S}_{\sqrt{N}}^{N-1}, \quad (43)$$

where  $\pi_{\xi^*}^\perp$  is a hyperplane passing through  $\xi^*$  and normal to the  $x_1$  direction,  $\mathbb{S}_{\sqrt{N}}^{N-1}$  is a hypersphere of radius  $\sqrt{N}$  (middle hypersphere in the Important Ring). In Fig. 8 points  $C_1$  and  $C_2$  belong to this intersection. Further, the variance  $\sigma^2$  of this Gaussian ISD has to be such that

$$E\|x - \xi^*\|^2 = \|\xi^* C_1\|^2, \quad x \sim \mathcal{N}(\xi^*, \sigma^2) \quad (44)$$

Since

$$E\|x - \xi^*\|^2 = N\sigma^2, \quad \|\xi^* C_1\|^2 = N - (\xi^*)^2 \quad (45)$$

we finally obtain:

$$\sigma^2 = \frac{N - (\xi^*)^2}{N}. \quad (46)$$

Now if we will use the described ISD then almost all samples will lie in the Important Ring, more precisely, in the neighbourhood of the  $(N - 2)$ -dimensional sphere defined by (43). In Fig. 8 this region corresponds to the neighbourhood of points  $C_1$  and  $C_2$ . Of course it is much better than the previous choice of ISD.

## 4 SUBSET SIMULATION

In the previous section we saw that getting information about the failure domain is quite difficult. Another approach for evaluating failure probability is Subset Simulation introduced by Au and Beck (2001).

The main idea of this method is as follows. Given the original failure domain  $F$  let  $F_1 \supset \dots \supset F_n = F$  be a filtration, in other words a sequence of failure events so that  $F_k = \bigcap_{i=0}^k F_i$ . Using the definition of conditional probability it can be shown that,

$$p_F = P(F_1) \prod_{i=1}^{n-1} P(F_{i+1}|F_i) \quad (47)$$

The main observation is that, even if  $p_F$  is small, by choosing  $n$  and  $F_i, i = 1, \dots, n - 1$  appropriately, the conditional probabilities can be made large enough for efficient evaluation by simulation.

In engineering applications the failure event usually can be expressed in terms of exceedance of some demand-capacity ratio and, therefore, the probability of failure can be written in the form  $p_F = P(X > b)$ , where  $X$  is the response variable and  $b$  is a critical threshold. The sequence of intermediate failure events  $\{F_1, \dots, F_{n-1}\}$  can then be chosen as  $F_i = \{X > b_i\}$  for some intermediate thresholds  $b_1 < \dots < b_{n-1} = b$ . During Subset Simulation,  $b_1, \dots, b_{n-1}$  are adaptively chosen such that all probabilities  $P(F_1), P(F_2|F_1), \dots, P(F_n|F_{n-1})$  are equal to, say,  $p_0 = 0.1$ .

Let us briefly recall how Subset Simulation works. We start by simulating  $n$  samples  $\{\theta_0^k, k = 1, \dots, n\}$  by standard Monte Carlo simulation. Perform  $n$  system analyses to obtain the corresponding response values  $\{X(\theta_0^k), k = 1, \dots, n\}$ . Then the first intermediate threshold  $b_1$  is adaptively chosen as the  $((1 - p_0)n - 1)$ -th value in the ascending list of response values, so that the sample estimate for  $P(F_1) = P(X > b_1)$  is equal to  $p_0$ . There are  $n p_0$  samples among  $\{\theta_0^k, k = 1, \dots, n\}$  whose response  $X$  is greater than  $b_1$ , and hence lie in  $F_1$ . These samples are distributed as  $q(\cdot|F_1)$  and provide "seeds" for simulating additional samples. Starting from each of these samples Markov chain Monte Carlo simulation (MCMC) is used to obtain an additional  $(1 - p_0)n$  samples, making up a total of  $n$  conditional samples  $\{\theta_1^k, k = 1, \dots, n\}$  distributed according to  $q(\cdot|F_1)$ . The intermediate threshold  $b_2$  is then adaptively chosen as the  $((1 - p_0)n - 1)$ -th value in the ascending list of  $\{X(\theta_1^k), k = 1, \dots, n\}$ , and it defines the next intermediate failure event  $F_2 = \{X > b_2\}$ . The sample estimate for  $P(F_2|F_1)$  is automatically equal to  $p_0$ . Repeating this process, one can generate conditional samples for higher conditional levels until the target failure probability level has been reached.

### 4.1 Original Metropolis algorithm

Metropolis algorithm belongs to the class of very powerful techniques, called Markov chain Monte Carlo simulations, for simulating samples according to an arbitrary distribution. In these methods samples are simulated as the states of a Markov chain which has the target distribution as its stationary distribution.

The significance of Metropolis algorithm to the Subset simulation is that it allows to construct Markov chain with  $q(\cdot|F_i)$  as its stationary distribution. Therefore, we can use this algorithm for simulating new samples starting from "seeds" that

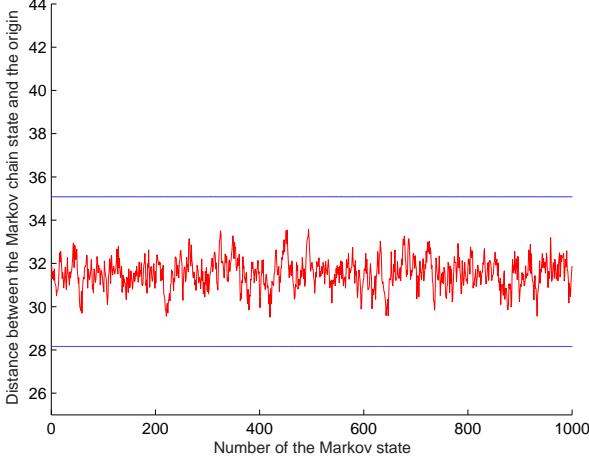


Figure 9: Markov chain starting from random Gaussian vector and governing by modified Metropolis algorithm,  $N = 10^3$ .

were obtained in the previous step of Subset Simulation. Even if the current sample is not distributed as  $q(\cdot|F_i)$ , the limiting distribution property of Markov chain guarantees that the distribution of simulated samples will tend to  $q(\cdot|F_i)$  as the number of Markov steps increases.

Given a current sample  $\theta^{(1)}$  (a "seeds" point) the original Metropolis algorithm works as follows.

Let  $p(\xi|\theta)$ , called proposal PDF, be a  $N$ -dimensional PDF for  $\xi$  centered at  $\theta$  with symmetry property  $p(\xi|\theta) = p(\theta|\xi)$ . Generate a sequence of samples  $\{\theta^{(1)}, \theta^{(2)}, \dots\}$  starting from a given sample  $\theta^{(1)}$  by computing  $\theta^{(k+1)}$  from  $\theta^{(k)}$  as follows:

1. *Generate candidate state  $\tilde{\theta}$ .* Simulate  $\xi$  according to  $p(\cdot|\theta)$ . Compute the ratio  $r = q(\xi)/q(\theta^{(k)})$ . Set  $\tilde{\theta} = \xi$  with probability  $\min\{1, r\}$  or set  $\tilde{\theta} = \theta^{(k)}$  with the remaining probability.
2. *Accept/Reject  $\tilde{\theta}$ .* If  $\tilde{\theta} \in F_i$  accept it as a next step, i.e.  $\theta^{(k+1)} = \tilde{\theta}$ ; otherwise reject it and take the current sample as a next step of Markov chain  $\theta^{(k+1)} = \theta^{(k)}$ .

Au and Beck (2001) realized that the original Metropolis algorithm does not work in high dimensions.

The geometric reason of this inapplicability is that the same effect as shown in Fig. 3 arises. In each step of the original Metropolis algorithm the ratio  $r = q(\xi)/q(\theta^{(k)})$  will be extremely small for the reasons explained previously. Therefore, with extremely high probability one obtains repeated samples. Thus, a chain of practically meaningful length may consist of as few as a single sample. This yields Subset Simulation practically inapplicable.

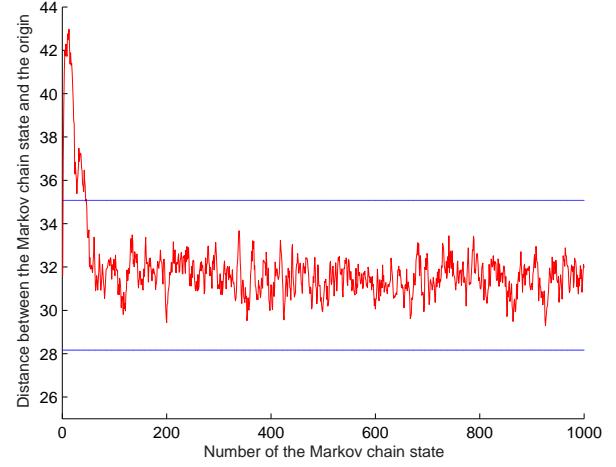


Figure 10: Markov chain starting from  $\hat{\theta} = (\sqrt{N}, 0, \dots, 0)$  and governing by modified Metropolis algorithm,  $N = 10^3$ .

#### 4.2 Modified Metropolis algorithm

The modified Metropolis algorithm differs from the original Metropolis algorithm in the way the candidate state  $\tilde{\theta}$  is generated. Instead of  $N$ -dimensional proposal PDF in the modified algorithm a 1-dimensional proposal PDF  $p(\xi_j|\theta_j)$ ,  $j = 1, \dots, N$  centered at  $\theta_j$  for each component is used. Being at state  $\theta$  the candidate for next state of Markov chain is generated as follows:

For each component  $j = 1, \dots, N$  simulate  $\xi_j$  from  $p(\cdot|\theta_j)$ . Compute the ratio  $r_j = q_j(\xi_j)/q_j(\theta_j)$ . Set  $\tilde{\theta}_j = \xi_j$  with probability  $\min\{1, r_j\}$  and set  $\tilde{\theta}_j = \theta_j$  with the remaining probability.

It can be shown analytically that in general modified Metropolis algorithm is applicable in high dimensions. This is intuitively clear, since when  $N$  is large, it is unlikely that the candidate state is equal to the current state, as this would mean that all  $N$  component candidate states  $\tilde{\theta}_j$  were rejected, which is highly unlikely.

Nevertheless there is a speculative chance that starting from a point inside the Important Ring, a Markov chain generated by modified Metropolis algorithm will leave it for a certain time.

Let us consider the following example. Let us forget for a moment the Acceptance/Rejection step, in other words we assume that the entire space  $\mathbb{R}^N$  is a failure domain, and consider a Markov chain starting from a random vector  $\hat{\theta}$  drawn from the  $N$ -dimensional standard Gaussian distribution and governed by modified Metropolis algorithm with proposal PDF  $p(\cdot|\theta_j) = \mathcal{N}(\theta_j, 1)$ . In Fig.9 the evolution of the length of Markov chain state is shown. The horizontal lines show the range of the Important Ring. Now let us consider the

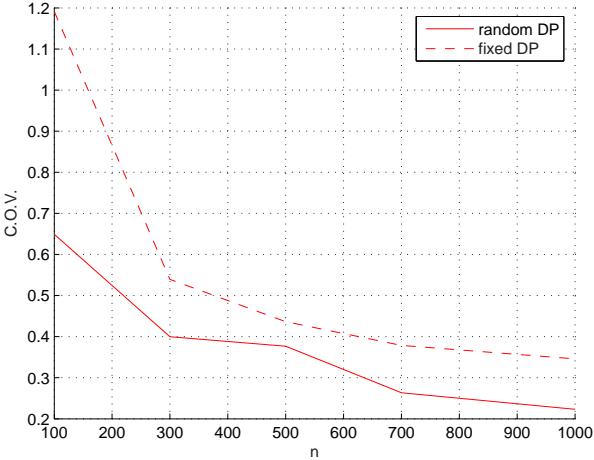


Figure 11: C.o.v. of estimators for liner failure domain probabilities with random and fixed design points.

same Markov chain but starting not from a random Gaussian vector. As initial state of the Markov chain we take vector  $\hat{\theta} = (\sqrt{N}, 0, \dots, 0)$ . This is a point within the Important Ring. The evolution of the length of the Markov chain state is shown in the Fig.10. As we can see from this picture at first the Markov chain jumps out of the Important Ring and only after approximately 50 steps returns to it.

This happens because the modified Metropolis algorithm assumes some structure while the standard Gaussian space has no structure. In the modified Metropolis algorithm there are special directions namely  $(0, \dots, 0, 1, 0, \dots, 0)$ , where 1 is on the  $j$ -th place ( $x_j$ -direction) and  $j = 1, \dots, N$ . However the standard Gaussian space is isotropic and has no special directions. The closer the initial state of a Markov chain to the  $x_j$ -direction the worse the modified Metropolis algorithm works. Of course the probability to obtain an initial state closely aligned to one of the coordinate is very small.

To prove this, consider a linear problem with LSF (31). As was mentioned before, for any design point lying on a hypersphere of the radius  $\beta$  the corresponding probability of linear failure domain will be given by (34).

Let us now apply Subset simulation with modified Metropolis Algorithm for evaluating the failure probabilities of two "equivalent" linear failure problems. The design point of the first problem is chosen as  $\theta_1^* = \beta \frac{x}{\|x\|}$ , where  $x$  is drawn from  $N$ -dimensional standard Gaussian distribution while that of the second problem is  $\theta_2^* = (\beta, 0, \dots, 0)$  for the first and second liner problems correspondingly. These failure domains have equal probabili-

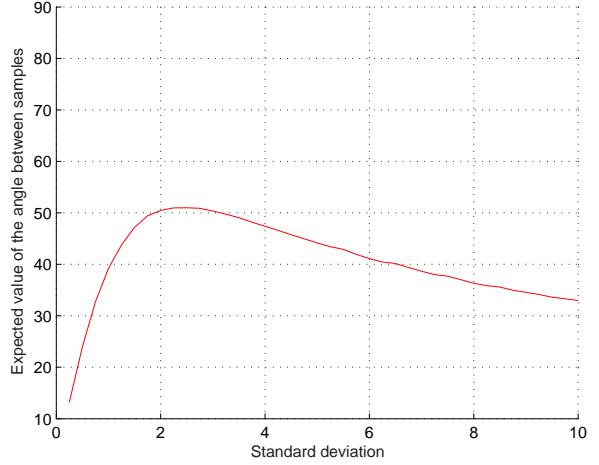


Figure 12: Dependence of expected value of angle between samples on standard deviation.

ties, since they have the same reliability index. In Fig. 11. the coefficients of variation (c.o.v.) for corresponding estimators for different values of  $n$  (number of samples in each intermediate Subset Simulation level) are shown. Here  $\beta = 3$ ,  $N = 10^3$  and 50 runs of the algorithm are used. Clearly in the second case the modified Metropolis algorithm works worse. This is due to the existence of preferable directions as explained earlier.

In the implementation of Subset Simulation the choice of a proposal distribution is very important, since it governs the efficiency in generating the samples by MCMC. Let us again consider "free" Markov chain simulated by modified Metropolis algorithm when the entire space is a failure domain, i.e. there is no Acceptance/Rejection step. For each component we use a Gaussian proposal as before but instead of using unit variance we will consider it as a parameter:

$$p(\cdot | \theta_j) = \mathcal{N}(\theta_j, \sigma^2), \quad j = 1, \dots, N. \quad (48)$$

The question is how  $\sigma$  affects the correlation between samples. The expected value of the angle  $\alpha$  between two consecutive samples is a good parameter for measuring the correlation of the Markov chain states. The larger angle, the more independent samples and, therefore, more ergodic the chain. Furthermore, unlike distance between samples, the measured angle is independent on the dimension  $N$ . Clearly, standard Monte Carlo provides the best samples and for this method

$$E[\alpha] = \pi/2. \quad (49)$$

For the described one-parameter family of Markov chains the expected value of  $\alpha$  is shown in Fig. 12.

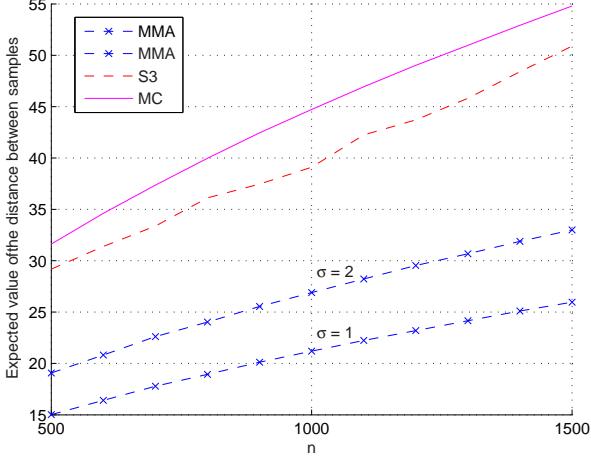


Figure 13: Dependence of expected value of distance between samples on dimension  $N$  for MMA, S3 and MC.

As we can see the "optimal" standard deviation is somewhere between 2 and 3.

Of course in real engineering applications the failure domain is a small part of parameter space and adopting too large standard deviation in the proposal PDF may lead to too many rejections in the second step of the modified Metropolis algorithm yielding a highly correlated chain.

#### 4.3 Spherical Subset Simulation Method ( $S^3$ )

A new MCMC algorithm was proposed by Katafygiotis and Cheung (2006). Given a sample  $\theta = Ru$ , where  $u = \theta/\|\theta\| \in \mathbb{S}^N$  is a vector of unit length and  $R = \|\theta\|$ , this algorithm works as follows. The algorithm consists of two steps. The first step involves sampling an intermediate failure point  $\theta' = Ru'$ , having the same length  $R$  as the current sample  $\theta$ . The second step involves radial sampling along the direction  $u'$  to obtain  $R'$ . The distinct sample  $\theta'' = R'u'$  is then the next state of the chain, i.e. it is accepted with probability one. For more details, refer to Katafygiotis and Cheung (2006). From a geometric point of view the advantage of this method is that it is consistent with the nature of the Gaussian space, namely there is no preferable directions as in the modified Metropolis algorithm.

First of all let us compare  $S^3$  with the modified Metropolis algorithm in terms of the correlation of samples they generate in  $\mathbb{R}^N$

From the description of the algorithm it is clear that the expectation of angle between samples generated by  $S^3$  method is equal to  $\pi/2$  as in standard Monte Carlo. Due to this fact we explore the expectation value of distance between samples that depends on the dimension  $N$ . The results for

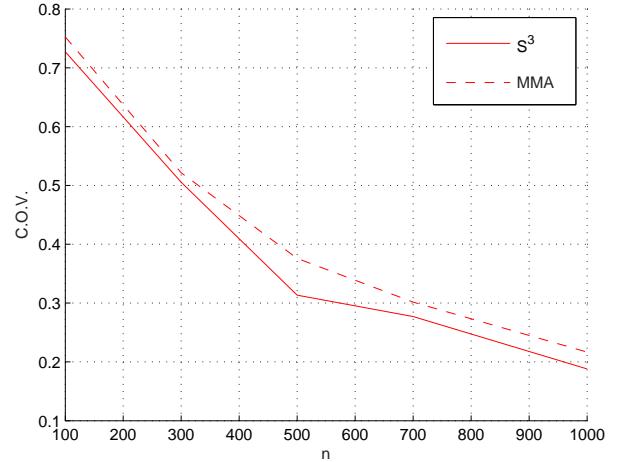


Figure 14: C.o.v. of estimators for liner failure domain probabilities.

modified Metropolis algorithm with  $\sigma = 1, 2, 3$ ,  $S^3$  method and standard Monte Carlo are presented in Fig. 13. We can see that in terms of distances between samples,  $S^3$  method is closer to Monte Carlo simulation.

Finaly let us consider a linear problem with the direction of the design point  $\theta^*$  being drawn from  $N$ -dimensional Gaussian distribution and evaluate the corresponding failure probability using Subset simulation with  $S^3$  method and MMA ( $\sigma = 1$ ). The c.o.v of these estimators are shown in Fig. 14. Here reliability index  $\beta = 3$  and 50 runs of each algorithms are used.

#### 5 ACKNOWLEDGMENTS

This research has been supported by the Hong Kong Research Grants Council under grants 614305 and CA04/05.EG01. This support is gratefully acknowledged.

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