HYPERCUBE POINT CONCENTRATION SAMPLING TECHNIQUE

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Abstract

A new sampling technique referred to as the hypercube point concentration sampling technique is proposed. This sampling technique is based on the concepts of the Latin hypercube sampling technique and the point concentration method. In the proposed technique, first, the probability density function of the random variables is replaced by a sufficiently large number of probability concentrations with magnitudes and locations determined from the moments of the random variables. In other words, the probability density function is replaced by the probability mass function determined based on the point estimate method. The probability mass function is then used with the Latin hypercube sampling technique to obtain samples. For evaluating statistics of a complicated performance function of an engineering system, the proposed technique could be more efficient than the Latin hypercube sampling technique since for a given simulation cycle the required number of evaluations of the performance function in the former is less than that in the latter. The proposed sampling technique is illustrated through numerical examples.

Introduction

Many random variables are involved in an engineering system. Direct or simple Monte Carlo method and efficient reliability methods such as the first-order and second-order reliability methods (Madsen et al. 1986) can be employed to carry out probabilistic assessment of the system. The reliability methods are almost exclusively used to estimate the probability of failure while the Monte Carlo method are employed to calculate the statistics of the responses or the probability of failure of the system. Although the direct Monte Carlo method is simple to use, however it can be computationally intensive. To reduce the number of simulation cycles, more efficient simulation methods can be used (Iman and Conover 1980, Rubinstein 1981).

In this study, a new sampling technique is proposed. This new sampling technique is based on the Latin hypercube sampling (LHS) technique and the point estimate method (Rosenblueth 1975, 1981). In the LHS technique (Iman and Conover 1980), the domain of the random variables is partitioned into many mutually exclusive and collectively exhaustive hypercubes. The hypercubes that do not have common domain in subspaces are selected randomly; and a point within each of the selected hypercubes is chosen randomly for the analysis. For the proposed technique, the marginal probability density functions of the random variables are replaced by probability mass functions with a sufficiently large number of concentrations. The locations and their associated probability concentrations are obtained based on Rosenblueth's point estimate method (Rosenlueth 1975, 1981). The probability mass functions are then used with the Latin hypercube sampling technique to generate values of the random variables for the simulation analysis. The advantage of the new technique is that it requires less number of evaluations of the performance function of the system than the LHS technique. This is because several generated samples are likely to fall into a same concentration point. The proposed technique is described in detail in the following, and is illustrated by numerical examples.

Background and discussions

Latin Hypercube sampling

Consider that the performance of an engineering system, Z, is a function of a set of s random variables X, $X = [X_1, \dots, X_s]$,

$$Z = h(X) , (1)$$

where $h(\bullet)$ is a deterministic function. The mathematical expectation of Z^k or the k-th moments of Z, $E(Z^k)$, is defined as,

$$E(Z^{k}) = \int_{\Omega} (h(\mathbf{x}))^{k} f_{\mathbf{X}}(\mathbf{x}) d\mathbf{x} , \qquad (2)$$

where Ω represents the domain of X, and $f_X(x)$ is the joint probability density function of X. The mean of Z, m_Z , equals E(Z), and the variance of Z, σ_Z^2 , equals $E(Z^2) - m_Z^2$. The probability that Z is less than or equal to a given value z_p , P_f , can be expressed as,

$$P_f = \int_{g \le 0} f_X(\mathbf{x}) d\mathbf{x} , \qquad (3)$$

where $g \le 0$ represents the domain of Z- $z_p \le 0$.

Integrals in Eqs. (2) and (3) can be estimated using the simple simulation technique. Alternatively, the more efficient LHS technique can be employed (Iman and Conover 1980). According to this technique, for practical applications with independent random variables, the generation of Latin hypercube samples of size n could be carried out as follows. The domain of each random variable is divided into n mutually exclusive and collectively exhaustive intervals, and one value is selected randomly in each interval according to the probability distribution of the random variable. A value is randomly selected from the n values for each of the random variables to form the first Latin hypercube sample. The remaining n-1 values for each of the random variables are used to form the second Latin hypercube sample. That is, a value is randomly selected from the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables are used to form the second Latin hypercube sample. That is, a value is randomly selected from the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the n-1 remaining values for each of the random variables to form the second Latin hypercube sample.

In particular, if the *n* mutually exclusive and collectively exhaustive intervals have equal probability, the *k*-th moments of *Z* is estimated as the average of the sum of the function $(h(x))^k$ evaluated at each of the sample points; and the probability of failure P_f defined in Eq. (3) is approximated by the ratio of the number of sample points where $h(x)-z_p \le 0$ to *n*.

Rosenblueth's point estimate method

The point estimate method is developed to evaluate approximately the moments of Z based on the first few statistical moments of X (Rosenblueth 1975, 1981). The method does not require the knowledge of the probability distribution of X except their statistical moments such as the means, standard deviations, correlation coefficients and skewness coefficients. The method basically replaces the original probability density functions of random variables by probability concentrations with magnitudes of the concentrations and locations determined from the moments of the random variables. In particular, if Z is a function of only one random variable X, and two point concentration (i.e., two-point estimate method) is considered for the random variable X, the locations x_j and magnitudes p_j of the concentrations are given by (Rosenblueth 1975, 1981),

$$x_j = m_X + \xi_j \sigma_X, j = 1,2 \tag{4}$$

and,

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$$p_{j} = (-1)^{j} \xi_{3-j} / \left(2\sqrt{1 + (\lambda_{X}/2)^{2}} \right), \ j = 1, 2,$$
(5)

where $\xi_j = \lambda_X / 2 + (-1)^{3-i} \sqrt{1 + (\lambda_X / 2)^2}$ and j = 1, 2, and μ_X , σ_X and λ_X are, respectively, the mean, standard deviation, and coefficient of skewness of *X*. Using these concentrations the mean of *Z*, for example, can be approximated by,

$$E(Z) \approx \sum_{i=1}^{n} p_i h(x_i) , \qquad (6)$$

where n = 2. If Z is a polynomial of degree less than 4, Eq. (6) will provide an exact mean of Z.

In general, if *n* concentrations are considered, x_j and p_j , $j = 1, 2, \dots, n$, of the concentrations can be obtained by solving the following 2n equations,

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ \vdots & \vdots & \ddots & \vdots \\ (x_1)^{2n-1} & (x_2)^{2n-1} & \cdots & (x_n)^{2n-1} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{bmatrix} = \begin{bmatrix} m_0 \\ m_1 \\ \vdots \\ m_{2n-1} \end{bmatrix},$$
(7)

where m_j is the *j*-th moment of X with respect to the origin. In such a case, the use of *n* concentrations matches the first 2n-1 moments of the random variable X. Therefore, if Z is a polynomial of degree $\leq 2n-1$, the estimated mean of Z by using Eq. (6) with *n* concentrations is exact.

Discussions

Consider the case that Z, Z = h(X), is a function of a random variable X. We discretize the domain of X into two mutually exclusive and collectively exhaustive intervals I_i , i = 1,2. The probability of the *i*-th interval p_{Ii} is given by $p_{Ii} = P(X \in I_i)$. According to the LHS technique we randomly select a sample $x_{si}, i = 1,2$, from I_i and calculate the expected value of Z using,

$$E(Z) \approx \sum_{i=1}^{n} p_{li} h(x_{si}), \qquad (8)$$

where n = 2. This approximation, which uses only two samples, is unlikely to be accurate or satisfactory even for when h(X) is a linear function of *X*. Clearly, we can overcome this by using Rosenblueth's two-point estimate method but with the following "sampling" interpretation so that we can extend it later. We replace the original probability distribution function of *X* according to Rosenblueth's two-point estimate method leading to x_j and p_j , j = 1,2, given by Eqs. (4) and (5). We divide the space into two intervals such that the cumulative probability distribution function

for the *i*-th interval
$$I_i$$
 varies from $\sum_{j=0}^{l-1} p_j$ to $\sum_{j=0}^{l} p_j$ where $p_0 = 0$, *i*=1 and 2. Therefore, the

probability of the *i*-th interval I_i , p_{1i} , equals p_i We randomly select a sample x_{si} from the interval I_i which is equal to the location of the *i*-th concentration x_i obtained according to Rosenblueth's two-point estimate method. Based on this sampling scheme the approximation to E(Z) calculated by using Eq. (8) is identical to Eq. (6) since $p_{1i} = p_i$, and $x_{si} = x_i$. As already mentioned such an approximation is exact if h(X) is a polynomial of degree less than 4. Therefore, one has judiciously selected the "sample" points for a sampling technique to become much more efficient. It is noteworthy that a similar observation can be made when *n* samples are employed.

The efficiency of using *n* point concentrations depends on the efficiency in solving the system of nonlinear equations (Eq. (7)) to find x_j and p_j , $j = 1, 2, \dots, n$. The well known approach to solve Eq. (7) (Erdelyi et al. 1953) is to first find the zeros (i.e., x_i , $j = 1, 2, \dots, n$) of

the polynomial
$$\sum_{i=1}^{n} c_i x^i = 0$$
, where $c_n = 1$, and $c_j, j = 0, 1, \dots, n-1$, are obtained from,
 $M_{2n-2} \begin{bmatrix} c_0 & c_1 & \cdots & c_{n-1} \end{bmatrix}^T = -\begin{bmatrix} m_n & m_{n+1} & \cdots & m_{2n-1} \end{bmatrix}^T$, (9)
where $M_{2n-2} = \begin{bmatrix} m_0 & m_1 & \cdots & m_{n-1} \\ m_1 & m_2 & \cdots & m_n \\ \vdots & \vdots & \ddots & \vdots \\ m_{n-1} & m_n & \cdots & m_{2n-2} \end{bmatrix}$. The solution is then used to find p_i in Eq. (7).

The solution for x_j and p_j , does exist and p_j are larger than zero. This comes directly from a theorem in the orthogonal polynomials and quadrature formulas which state that (Erdelyi et al. 1953, Stroud and Secrest 1966):

For a non-negative weight function f(x) (in our case it represents probability density function), if m_i exist and $|M_{2n}| \neq 0$, a unique sequence of orthogonal polynomial $\{q_i(x)\}, i = 1, \dots, n$, (except normalization constants) can be constructed. $q_n(x)$ has *n* distinct roots (abscissas) which lie in the orthogonality interval. Using these *n* roots we can find the weights p_i such that,

$$\int_{\Omega} f(x)h(x)dx = \sum_{i=1}^{n} p_i h(x_i), \qquad (10)$$

is exact if h(x) is a polynomial of degree $\leq 2n-1$. Further, p_i are positive.

In other words, the above says that we can find the abscissas x_i and the positive weights p_i such that,

$$m_k = \int_{\Omega} x^k f(x) h(x) dx = \sum_{i=1}^n p_i x_i^k , \text{ or } m_k = \sum_{i=1}^n p_i x_i^k \text{ for } k = 1, 2, \dots, 2n-1,$$
(11)

which is equivalent to Eq. (7). Therefore, if some commonly used weighting functions can be transformed into the probability density functions by appropriate normalization constants, the obtained abscissas and weights for the Guassian quadrature formulas can be directly transformed into locations and probability concentrations in the point estimate method. There are three well known classical weighting functions associated with the Jacobi integration, the (generalized) Laguerre integration and the Hermite integration. With appropriate normalization constants, these weighting functions can be transformed into the beta distribution, the gamma distribution and the normal distribution. The correspondences between the abscissas and locations and between the weights and the probability concentrations for these cases are listed in Table 1. Note that the Legender integration is a particular case of the Jacobi integration. Values of the abscissas and weights for these quadrature formulas are tabulated in Stroud and Secrest (1966). They can also be calculated using the algorithms given in Press et al. (1992).

If Z, Z = h(X), is a function of *s* random variables, we can generate *n* samples according to the LHS technique and evaluate h(x) at these *n* sampling points in order to estimate the mean of E(Z). The number of random variables *s* does not change the fact that we need to evaluate *n* times the function h(x). However, if one uses the point estimate method with *n* concentrations for each random variable, one need to evaluate n^s times the function h(x). This can be extremely large and make the point estimate method unattractive. For example, n^s equals 9765625 for n = 5 and s = 10. In such a case, one is better off by using the LHS technique or any other simulation techniques. It is noted that the point estimate schemes with less number of concentrations that have reported in the literature (see Hong (1998) and the references listed thereafter) may also be employed. However, none of these schemes can appropriately take into account the cross terms of order higher than 3.

In short, the above indicates that the point estimate method is very efficient if we are

interested in a function of only one random variable, while the use of the LHS sampling technique is desirable if the number of random variables is large. In the following we propose a method that takes advantage of both of these methods.

Hypercube point concentration sampling

If Z is a function of s independent random variables, we replace each of the original probability distributions of the random variables by k probability concentrations whose locations and magnitudes are determined by the probability concentration method discussed in the previous section. Therefore, for the *i*-th random variable X_i , $i = 1, 2, \dots, s$, we have a "discrete" probability distribution function with locations and probability concentrations represented by $x_{i,j}$ and $p_{i,j}$, $j = 1, 2, \dots, k$. For k equal to 5, a schematic representation of the cumulative distribution function for the *i*-th random variable based on the above discretization is shown in Figure 1.



a) Representation according to point estimate method for k = 5



Now, for the *i*-th random variable we partition the range of the cumulative probability values (i.e., from 0 to 1) into mutually exclusive and collectively exhaustive *n* intervals each having a value $P_{i,m}$, $m = 1, 2, \dots, n$. This partition is based on the discrete representation of the probability

distribution function defined by $(x_{i,j}, p_{i,j})$, $i = 1, 2, \dots, s$, and $j = 1, 2, \dots, k$. For example, for *n* equal to 8 and k = 5, this partition is illustrated in Figure 1 again for the *i*-th random variable. Since there are *s* random variables, the sample space is partitioned into n^s cells (hypercubes) each with probability $P_{1,m1} \times P_{2,m2} \times P_{3,m3} \times \dots \times P_{s,ms}$ where *m*1 to *ms* can take values from 1 to *n*.

Given a random variable, for each of the partition, we randomly generate a sample. Let $s_{i,m}$ denote the randomly generated sample from the partition defined by $P_{i,m}$, $m = 1, 2, \dots, n$, for the *i*th random variable. The selected values $x_{i,m}$, $m = 1, 2, \dots, n$, must coincide with one of the $x_{i,j}$, $j = 1, 2, \dots, k$. Again, this is graphically illustrated in Figure 1 (in this particular case $x_{i,1} = x_{i,1}$, ${}_{s}x_{i,2} = {}_{s}x_{i,3} = x_{i,1}, {}_{s}x_{i,4} = {}_{s}x_{i,5} = x_{i,3}, {}_{s}x_{i,6} = {}_{s}x_{i,7} = x_{i,4}, {}_{s}x_{i,8} = x_{i,5}$). As in the LHS technique, we use these samples $s_{x_{i,m}}$, where $i = 1, 2, \dots, s$ and $m = 1, 2, \dots, n$, to form *n* samples x_i , $j = 1, 2, \dots, n$, in the s-dimension sample space. That is, the first sample x_1 is formed by randomly selecting a value from the *n* values for each of the random variables. This results in $\mathbf{x}_1 = (x_{1,k_1}, x_{2,k_2}, \dots, x_{s,k_s})$ and the probability associated with the cell from which the sample \mathbf{x}_1 was obtained, p_1 , equals $P_{1,k1} \times P_{2,k2} \times P_{3,k3} \times \cdots \times P_{s,ks}$ where each of $k1, k2, \dots, ks$, takes a values from 1 to *n*. The second sample x_2 and the probability associated with the cell from which the sample x_2 was obtained, p_2 , are formed in the same way but based only on the remaining n-1 values for each of the random variables. This process is continued until x_n and p_n is formed. Since the samples obtained in this way represent corners of the Hypercubes formed by the Point Concentrations we will refer this sampling technique as the HPCS technique.

We can use these samples to estimate the expected value of Z, E(Z) from the statistic, S, defined by

$$S = \sum_{j=1}^{n} n^{s-1} p_j h(\mathbf{x}_j),$$
(12)

where p_i is the probability associated with the cell from which the sample x_i was obtained.

To show that the use of the above in estimating E(Z) is adequate, one can shown, following a similar proof given by Iman and Conover (1980), that S is an unbiased estimator of E(Z) when Z = h(x) is a polynomial of degree less than 2k-1 if k concentrations are employed to replace the probability distribution function.

Note that dependent random variables can be transformed into independent random variables by using the Rosenblatt transformation, and that if only the correlation coefficients between the dependent random variables are available (i.e., incomplete information), one could use the Nataf translation system to transform the correlated random variables into uncorrelated random variables (Madsen et al. 1986). For each of the independent random variables if its moments exist we can calculate $x_{i,j}$ and $p_{i,j}$ of the probability concentrations using Eq. (7). Alternatively, to avoid the evaluation of $x_{i,j}$ and $p_{i,j}$ we can transform the independent random variables into uniform, beta, exponential, gamma and/or normal variates since for these distributions $x_{i,j}$ and $p_{i,j}$ are readily available (see Table 1). In the transformed space, we can use the proposed HPCS technique to carry out the probabilistic analysis.

Illustrative numerical examples

Example 1. *Polynomial with two random variables*. Consider a simple example with Z defined by,

$$Z = \sum_{i=1}^{s} X_i^4 + \sum_{i=1}^{s} \sum_{j=i+1}^{s} X_i^2 X_j^2$$
(13)

where s = 2, X_1 and X_2 are independent normally distributed random variables with a mean of zero and standard deviation of one. It can be shown that the exact mean equals 7.

Guassian Integration formulas	Point estimate methods			
$\int_{\Omega_t} w(t)h(t)dt \approx \sum_{i=1}^n w_i h(t_i)$	$\int_{\Omega_X} f(x)h(x)dx \approx \sum_{i=1}^n p_i h(x_i)$			
Jacobi integration	Beta distribution			
$w(t) = (1-t)^{\alpha} (1+t)^{\beta}$	$f(x) = (b-x)^{\alpha} (a+x)^{\beta} / ((b-a)^{\alpha+\beta+1} B(\alpha,\beta)), \ \Omega_X \in (a,b)$			
$\Omega_t \in (-1,1)$	$p_{i} = w_{i} / ((b-a)^{\alpha+\beta+1} B(\alpha,\beta)), x_{i} = ((b-a)t_{i} + (b+a))/2$			
Legender integration	Uniform distribution			
$w(t) = 1, \ \Omega_t \in (-1,1)$	$f(x) = 1/(b-a), \ \Omega_X \in (a,b),$			
	$p_i = w_i / 2, x_i = ((b-a)t_i + (b+a))/2$			
Generalized Laguerre	Gamma distribution			
integration	$f(x) = \lambda^{\alpha+1} x^{\alpha} e^{-\lambda x} / \Gamma(\alpha+1), \ \Omega_X \in (0,\infty)$			
$w(t) = t^{\alpha} e^{-t}, \ \Omega_t \in (0, \infty)$	$p_i = w_i / \Gamma(\alpha + 1), x_i = t_i / \lambda$			
Laguerre integration	Exponential distribution			
$w(t) = e^{-t}, \ \Omega_t \in (0,\infty),$	$f(x) = \lambda e^{-\lambda x}, \ \Omega_X \in (0,\infty), \ p_i = w_i, x_i = t_i / \lambda$			
Hermite integration	Normal distribution			
$w(t) = e^{-t^2}, \ \Omega_t \in (-\infty, \infty)$	$f(x) = \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{1}{2}\left(\frac{x-m}{\sigma}\right)^2\right), \ \Omega_X \in (-\infty, \infty)$			
	$p_i = w_i / \sqrt{\pi}, x_i = m + t_i \sqrt{2}\sigma$			

Table 1. Relation between the locations, x_i , and probability concentrations, p_i , in the point estimate method and the abscissas, x_i' , and weights, w_i , of well known integration formulas.

If we use the LHS technique, samples for a typical run with 100 cycles are shown in Figure 2. These samples are obtained by partitioning the domain of each random variable into 100 intervals each with the same probability. Now if we replace the original probability distribution function of each of the random variables by 5 concentrations obtained using the point estimate method, the samples for a typical run with 100 cycles obtained by using the HPCS technique are also shown in Figure 2. Note that by using the HPCS, one need to carry out only 13 evaluations for this particular run because many samples fall into the same point.

By repeating the above analysis many times, the average value and the standard deviation of the mean of Z are shown in Figure 3. The results shown in the figure indicate that the accuracy of the proposed HPCS technique is comparable to that of LHS the technique.

Example 2. *Polynomial with many random variables*. Consider Eq. (13) but with *s* equal to 5. X_i , $i = 1, 2, \dots, s$, are independent normally distributed variates with a mean of zero and standard deviation of one.

We replace the original probability distribution function of each of the random variables by k concentrations based on the point estimate method. For k equal to 3, 4 and 5, the joint probability distribution of the random variables is represented, respectively, by 243, 1024 and 3125 probability concentrations. Using n partitions with equal probability of 1/n for each of the random variables and carrying out simulation analysis using the HPCS, the obtained results are shown in Table 2a. Also shown in the table is the number of evaluations of h(X), n_e , needed by the HPCS for the simulation runs carried out. Clearly, the results show that n_e is less than n

which represents the number of functional evaluations if the LHS technique is employed. The reduction in the computational effort is most significant if k is small and/or n large. Note that in all cases the obtained mean values are close to the exact value which is equal to 25.



Figure 2. Illustration of sample points for the LHS technique and the HPCS technique.



Figure 3. Mean and standard deviation of the mean of the performance function.

	<i>k</i> = 3		<i>k</i> = 4		<i>k</i> = 5				
		Estimated		Estimated		Estimated			
Ν	n _e	mean	n _e	mean	n _e	mean			
100	55	24.66	68	24.47	73	24.45			
500	115	24.98	168	24.76	205	24.76			
1000	162	25.20	235	25.01	304	25.25			
5000	224	24.96	408	24.98	594	24.97			
10000	236	25.04	517	24.94	757	25.05			

Table 2a. Results for Example 2 with s = 5.

Table 2b. Results for Example 2 with s = 10.

	<i>k</i> = 3		k = 4		<i>k</i> = 5	
		Estimated		Estimated		Estimated
n	n _e	mean	n _e	mean	n _e	mean
100	94	76.14	98	73.13	100	74.64
500	434	74.30	484	74.63	489	73.92
1000	795	75.15	929	75.32	974	74.90
5000	2915	74.78	3783	74.81	4444	74.75
10000	4713	74.86	6530	74.71	8095	74.83

Repeat this analysis but with s = 10. The obtained results are shown in Table 2b. Comparison of the results shown in Tables 2a and 2b suggests that n_e for s = 5 is smaller than that for s = 10. This is expected since in the latter for k equal to 3, 4 and 5, the joint probability distribution function of the random variables is represented, respectively, by 59049, 1048576, and 9765625 concentrations.

Summary and conclusions

A new sampling technique is proposed in this study. This sampling technique is based on salient features of the Latin hypercube sampling technique and the point concentration method. In this technique, the original probability density function of a random variable is replaced by k probability concentrations determined from the point estimate method. These probability concentrations are then used with the Latin hypercube sampling technique to obtain samples. It is shown that by using this technique an unbiased estimator of the expectation of a performance function that is a polynomial of degree less than 2k-1 can be obtained. For highly nonlinear functions, the proposed technique provides an approximate estimate and the error is due to terms of order higher than 2k-1.

Illustrative numerical examples indicate that the proposed technique could be more efficient than the Latin hypercube sampling technique since the former could significantly reduce the required number of evaluations of the performance function. This is particularly important when the numerical evaluation of the performance function is computationally intensive. Also the numerical results suggest that the proposed technique provides relatively stable and accurate results even for highly nonlinear performance functions.

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