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STATISTICAL PRECONDITIONING IN SIMULATION OF STOCHASTIC VECTORS

Fumio Yamazaki* and Masanobu Shinozuka**

* Institute of Industrial Science, University of Tokyo, 7-22-1 Roppongi, Minato-ku, Tokyo 106, Japan.
** Dept. of Civil Engineering and Operations Research, Princeton University, Princeton, NJ 08544, USA.

ABSTRACT

A new stochastic vector simulation technique which realizes prescribed zero-mean vector and covariance matrix with a substantially smaller sample size than that of other existing methods has developed. The method utilizes the modal decomposition of the covariance matrix and the spectral representation of random processes. The ensemble-averaged means and covariance matrix and sample distribution by the proposed method are most favorably compared with those by the standard method.

KEYWORDS

Stochastic vector; modal decomposition; spectral representation; statistical preconditioning; eigenvalues; Monte Carlo simulation.

1. INTRODUCTION

Monte Carlo simulation techniques are of considerable usefulness for solving stochastic problems in the general area of engineering mechanics because of their versatility and algorithmic straightforwardness. However, the degree of accuracy of the resulting ensemble statistics such as mean values and standard deviations is, in general, satisfactorily high only when the sample size is sufficiently large. Hence, Monte Carlo simulation techniques usually require a substantial amount of computational effort. Referring specifically to stochastic field problems, the simulation and generation of sample functions can be performed by means of (1) spectral representation, (2) AR/ARMA modeling, and (3) covariance matrix decomposition procedures.

The spectral representation method [1,2] enables one to simulate stochastic fields and generate their sample functions resulting in highly accurate spatial statistics because of the periodicity and orthogonality of the trigonometric functions utilized. However, a large number of samples may be required in order to obtain stable ensemble statistics within a finite domain of space. The stability of the ensemble statistics of such sample functions is of great importance, particularly when they are used as an input to the finite element analysis. This is because the underlying ergodicity of the input stochastic field cannot be taken advantage of when the Monte Carlo solution calls for ensemble averaging on usually non-ergodic outputs of the finite element analysis.

The AR/ARMA model representation [3,4] of stochastic fields has recently received considerable attention. The advantage of this representation lies in the fact that substantially smaller memory space and CPU time are required for the generation of sample functions because of the recursive form of the equations. However, the method usually requires a larger sample size than the spectral representation does in order to achieve the same level of statistical accuracy.

The covariance matrix decomposition methods, such as by Cholesky decomposition and by modal decomposition, enable one to simulate discretized version of stochastic fields (stochastic vectors) if their correlation functions are given. Once the covariance matrix is constructed, these methods permit one to generate sample functions of nonhomogeneous multi-variate and multi-dimensional stochastic fields as easily as for those of homogeneous univariate one-dimensional stochastic fields. However, the methods may also require a large sample size until stable ensemble statistics can be obtained.

Considering these features of simulation techniques, a method of generating the samples of a stochastic vector with mean zero, which precisely reproduces the prescribed spatial correlation functions, is developed and numerical examples are provided.

2. Modal Decomposition of Covariance Matrix

The modal decomposition method is employed for the purpose of stochastic vector simulation. When dealing with a stochastic field which represents spatial variation of physical quantities (e.g., material properties), the field must be first discretized into a number of subdomains (e.g., finite elements). Then the stochastic vector is constructed using the representative value at each subdomain. There are two ways [5] in which to determine this representative value; (a) taking the value at the centroid of the element, and (b) taking the local average over the element. In this paper, we will use the method (a) assuming the discretization is fine enough.

If there are n finite elements in total and m material property parameters which exhibit random variability, there are $N=n\times m$ material property values. Thus, the stochastic field is reduced to a vector X of N-dimension as below:

$$\mathbf{X}=[\{\mathbf{X}^{(1)}\}^T\{\mathbf{X}^{(2)}\}^T\cdots\{\mathbf{X}^{(m)}\}^T]^T \text{ with } \mathbf{X}^{(i)}=[X_1^{(i)}\,X_2^{(i)}\cdots X_n^{(i)}]^T\quad (i=1,2,..,m) \qquad \cdots\cdots (1)$$

Without loss of generality, we can standardize each component of X to have zero-mean and unit variance. The correlational

characteristics of X can be specified by its covariance matrix:

$$\mathbf{C}_{XX}=\begin{bmatrix}\mathbf{C}_{XX}^{11} & \mathbf{C}_{XX}^{12} & \cdots & \mathbf{C}_{XX}^{1m}\\ \mathbf{C}_{XX}^{21} & \mathbf{C}_{XX}^{22} & \cdots & \mathbf{C}_{XX}^{2m}\\ \vdots & \vdots & \ddots & \vdots\\ \mathbf{C}_{XX}^{m1} & \mathbf{C}_{XX}^{m2} & \cdots & \mathbf{C}_{XX}^{mm}\end{bmatrix} \quad ; \quad \mathrm{Cov}[X_k^{(i)},X_l^{(j)}]=R_{X_iX_j}(\xi_{kl}) \qquad \cdots\cdots (2)$$

where the kl-component of the above submatrix $\mathbf{C}^{ij}_{XX}$ is determined from the auto- and cross-correlation functions between the stochastic vectors $\mathbf{X}^{(i)}$ and $\mathbf{X}^{(j)}$, and ξ_{kl} is the separation vector between the centroids of elements k and l. The covariance matrix $\mathbf{C}_{XX}$ is always symmetric regardless of the form of correlation functions. Hence the real eigenvalues and eigenvectors of $\mathbf{C}_{XX}$ are obtained by solving the following eigenequation:

$$\mathbf{C}_{XX}\Phi_X=\Phi_X\Lambda_X \quad \text{with} \quad \Phi_X=[\Phi_1\Phi_2\cdots\Phi_N]^T \qquad \cdots\cdots (3)$$

in which Φ_X is the modal matrix whose column vectors are orthogonal each other and have Euclidean lengths of 1 so that $\Phi_X^T\Phi_X=\mathbf{I}$, and Λ_X is the diagonal eigenvalue matrix whose diagonal members are numbered as follows: $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_N$.

It is not easy to directly generate a stochastic vector X whose components are correlated each other. Thus, a stochastic vector $\mathbf{Z}=[Z_1\,Z_2\cdots Z_N]^T$, whose components are Gaussian and independent each other and have zero-means and variances $\lambda_i\,(i=1,2,..,N)$, is generated first. Then, the correlated stochastic vector X is obtained by the transformation: $\mathbf{X}=\Phi_X\mathbf{Z}$. X is also Gaussian since it is represented by the linear combination of Gaussian random variables. If X exhibits non-Gaussian characteristics, the simulation technique for non-Gaussian fields [6] can be applied. The generated samples of X satisfy the target covariance matrix in ensemble sense. Considering the decaying feature of the eigenvalues, X may be approximated by its truncated form using only the first M ($M\leq N$) significant modes and corresponding independent random variables:

$$\mathbf{X}=\Phi_X\mathbf{Z}\approx[\Phi_1\Phi_2\cdots\Phi_M][Z_1\,Z_2\cdots Z_M]^T \qquad \cdots\cdots (4)$$

The error caused by the truncation can be evaluated by the normalized sum of eigenvalues up to the M-th mode as

$$P_\lambda(M)=\sum_{k=1}^{M}\lambda_k\Big/\sum_{k=1}^{N}\lambda_k=\sum_{k=1}^{M}\lambda_k/N \qquad \cdots\cdots (5)$$

The summation of all the eigenvalues represents the total power of variation of the stochastic vector. Thus, $P_\lambda(M)$ indicates the accuracy of generated samples after the truncation. M can usually be taken much smaller than N since the eigenvalues of higher-order modes are negligibly small except for white noise fields.

3. STATISTICAL PRECONDITIONING

Each component Z_i of the vector Z in Eq. 4 has zero-mean and variance λ_i. The standard method to generate Z's is to use a well-tested computer program that is supposed to generate independent standardized Gaussian random numbers. However, a common experience indicates that a fairly large sample size is necessary

for the simulated covariance matrix C^*_{ZZ} of Z to approach the target matrix C_{ZZ}. Especially, the off-diagonal terms of C^*_{ZZ} require a large sample size before they approach zero. Here, the sample covariance matrix and sample mean vector are obtained by

$$C^*_{ZZ} = \frac{1}{N_s}\sum_{j=1}^{N_s}[Z(j)\{Z(j)\}^T - \{\overline{Z}^*\}\{\overline{Z}^*\}^T] \quad ; \quad \overline{Z}^* = \frac{1}{N_s}\sum_{j=1}^{N_s} Z(j) \qquad \cdots\cdots (6)$$

where N_s is the sample size and $Z(j)$ is the j-th sample vector of Z.

In order to generate samples of a random vector Z that will exactly produce the target C_{ZZ} with a substantially small sample size, a trigonometric expansion is considered for the i-th component of the vector $Z(j)$:

$$Z_i(j) = \sqrt{2}C_i \sum_{m=1}^{N_f} \cos(\omega_k j\Delta t + \psi_k) \qquad (i=1,2,\cdots,N;\ j=1,2,\cdots,N_s) \qquad \cdots\cdots (7)$$

where $k=(m-1)N+i$, $C_i=\sqrt{\lambda_i/N_f}$, N_f is the number of cosines to be added, ψ_k a random phase angle uniformly distributed between 0 and 2π, and ω_k the k-th circular frequency.

Equation 7 has the form of well-known spectral representation for one-dimensional stationary stochastic processes although in this case, the j-axis indicates sample No., not the time step. If Δt, N_s and ω_k are determined properly, Eq. 7 exactly satisfies the target mean value and correlational characteristics for Z_i. It is possible to choose $N_f=1$ if the form of the distribution function of Z_i is not important. If, however, a large number of N_f is assumed, the sample distribution of Z_i will approach a Gaussian distribution by virtue of the central limit theorem. The fundamental period T of the sinusoids to be used for generation is $T=T_1=N_s\Delta t$ as shown in Fig. 1. Then the k-th frequency ω_k has a period T_k such that

$$\omega_k = 2\pi/T_k = 2\pi k/T \quad ; \quad T_k = T/k \qquad (k=1,2,\ldots,NN_f) \qquad \cdots\cdots (8)$$

Hence, there are k cycles of the sinusoids with frequency ω_k within duration T. In order to exactly satisfy the first two target moments by the corresponding ensemble statistics which represent the averaging with respect to j, the interval Δt is chosen to be 1/4 of the shortest period T_{NNf}:

$$\Delta t = T_{NN_f}/4 = \pi/(2\omega_{NN_f}) \qquad \cdots\cdots (9)$$

Under these assumptions, the sample mean value becomes zero:

$$Z^*_i = \frac{\sqrt{2}}{N_s} C_i \sum_{m=1}^{N_f}\sum_{j=1}^{N_s} \cos(\omega_k j\Delta t + \psi_k) = 0 \qquad \cdots\cdots (10)$$

Note that the existence of ψ_k in each cosine function does not influence this conclusion. The sample variance C^*_{ZZii} of Z_i can be shown to be λ_i by the following algebraic manipulation.

$$C^*_{ZZii} = \frac{1}{N_s}\sum_{j=1}^{N_s}[Z_i(j)]^2 = \frac{2}{N_s}C_i^2\sum_{j=1}^{N_s}\left\{\sum_{m=1}^{N_f}\cos(\omega_k j\Delta t + \psi_k)\right\}^2 = \lambda_i \qquad \cdots\cdots (11)$$

where the orthogonality of cosine functions are employed:

$$\sum_{j=1}^{N_s}\cos(\omega_\alpha j\Delta t + \psi_\alpha)\cos(\omega_\beta j\Delta t + \psi_\beta) = \begin{cases} 0 & (\text{if } \omega_\alpha \neq \omega_\beta) \\ N_s\cos(\psi_\alpha - \psi_\beta)/2 & (\text{if } \omega_\alpha = \omega_\beta) \end{cases} \qquad \cdots\cdots (12)$$

Using different sets of N_f frequencies for different Z's, the sample covariance of Z_i and Z_l can be shown to be zero:

$$C^*_{ZZil} = \frac{1}{N_s}\sum_{j=1}^{N_s} Z_i(j)\,Z_l(j) = 0 \qquad (\text{if } i \neq l) \qquad \cdots\cdots (13)$$

again due to the orthogonality of cosine functions.

Equations 10, 11 and 13 show that the target expected value and covariance matrix of Z are exactly reproduced by the sample size $N_s=T/\Delta t=4NN_f$. Note that the number N_f in Eq. 7 does not necessarily have to be identical for all values of i, although in this study N_f is assumed to be independent of i. This N_s will be a large number if N is large. However, by truncating the higher modes, N can be reduced to M as shown before.

The orthogonality of the cosine functions is also valid if $\omega_\alpha=\omega_\beta$ and $\psi_\beta=\psi_\alpha+\pi/2$ in Eq. 12. Hence one can conveniently use the same frequency twice from the following condition, still maintaining the orthogonality between Z_i and Z_l.

$$\omega_{k+M/2} = \omega_k \qquad \text{and} \qquad \psi_{k+M/2} = \psi_k + \pi/2 \qquad \cdots\cdots (14)$$

where k is such that $k=(m-1)M+i$ with $1\leqq i\leqq M/2$ and $1\leq m\leq N_f$. Then the sample size becomes

$$N_s = 4T_1/T_{N_fM/2} = 2MN_f \qquad (M: \text{even number}) \qquad \cdots\cdots (15)$$

Substituting Eq. 10 into Eq. 4,

$$X_s(j) = \sqrt{2}\sum_{i=1}^{M}\sum_{m=1}^{N_f}\phi_{si}\sqrt{\frac{\lambda_i}{N_f}}\cos(\omega_k j\Delta t + \psi_k) \qquad (s=1,2,\cdots,N) \qquad \cdots\cdots (16)$$

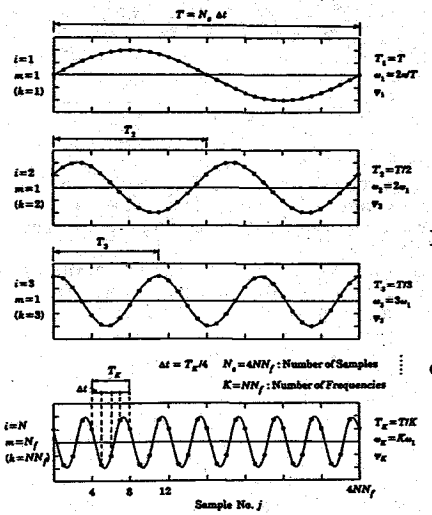

Fig. 1 Spectral Representation of $Z_i(j)$

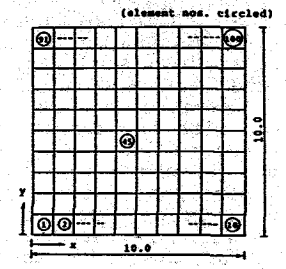

Fig. 2 Finite Element Discretization

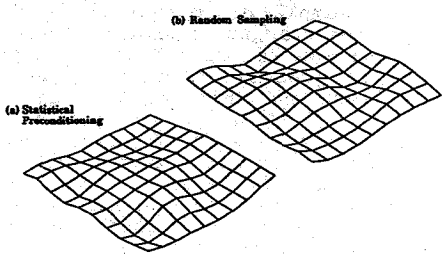

Fig. 3 Simulated Stochastic Fields

in which ϕ_{si} is the s-th component of vector ϕ_i. If $M \times N_f$ is large, $X_s(j)$ will have a Gaussian distribution asymptotically by virtue of the central limit theorem. Thus, even when $N_f=1$, $X_s(j)$ is asymptotically Gaussian if M is sufficiently large. It is noted that the sample mean value is still exactly equal to zero even after mode truncation, while the sample covariances are approximately equal to the target values. If the modes are not truncated, the sample covariances are identical to their targets.

4. NUMERICAL EXAMPLE

The efficacy of the statistical preconditioning technique is demonstrated using the finite element mesh shown in Fig. 2. The following auto-correlation function is assumed for a uni-variate two-dimensional stochastic field with a constant d=2.0.

$$R_{XX}(\xi) = \exp[-(|\xi|/d)^2] \qquad \cdots\cdots (17)$$

The sample size is taken as N_s=100 by choosing M=50 and N_f=1 in Eq. 15. This truncation represents more than 99% accuracy of the total power of the spatial variation. The ordinary simulation method based on the modal decomposition and the random sampling of the Z's is also carried out using the same sample size.

Two arbitrary sample stochastic fields generated by the two methods are shown in Fig. 3. There is no way in which the effect of preconditioning can be detected from this figure. However, a clear difference can be observed in Fig. 4 where the random variable $X_{45}(j)$ at element No. 45 is plotted as a function of the sample No. j. The random variables generated by the preconditioning method show periodic variation, while those by the random sampling method behave more like a white noise.

The target covariance matrix constructed from Eqs. 2 and 17 is graphically shown in Fig. 5. Similar figures for the sample covariance matrices are shown in Figs. 6 and 7. The covariance matrix generated by the preconditioning method is in perfect agreement with the target, while that by random sampling is quite erratic for the same sample size. A clearer demonstration of the same fact is shown in Fig. 8 where the sample covariance values along a straight line are plotted. In fact, a much larger sample size would be required for the random sampling method to produce target covariances acceptable in approximation. This indeed has been one of the major sources of discouragement for the use of Monte Carlo methods. The statistical preconditioning technique substantially alleviates this difficulty.

The sample distributions by the two methods are also compared with the target Gaussian distribution. 100 sample values at element No. 45 are plotted on a Gaussian probability paper in Fig. 9. The goodness of fit to the target Gaussian distribution with mean zero and unit standard deviation is about the same for both methods. If a larger sample size is selected, the simulated distributions will further approach a Gaussian distribution. Although only an example for a discretized uni-variate two-dimensional stochastic field is provided herein, the proposed method can deal with general Gaussian stochastic vectors.

In passing, it is noted that the so-called point estimate method [7] can generate a sample of a random variable so as to reproduce the first few moments exactly. The method, however, appears to be

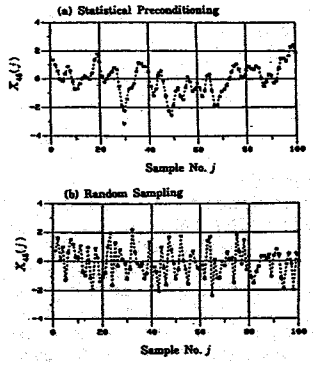

Fig. 4 Simulated Sample Variation

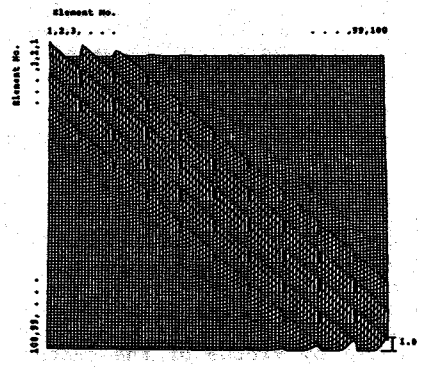

Fig. 5 Target Covariance Matrix

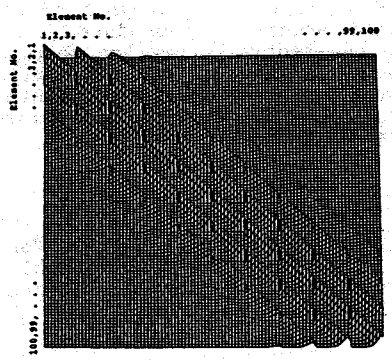

Fig. 6 Simulated Covariance Matrix by Statistical Preconditioning

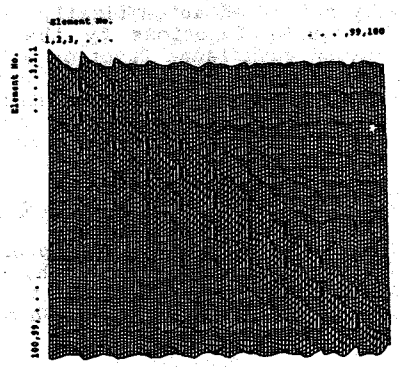

Fig. 7 Simulated Covariance Matrix by Random Sampling

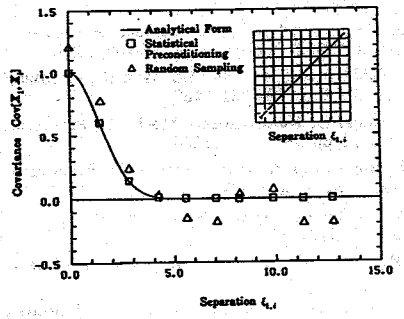

Fig. 8 Comparison of Analytical and Simulated Covariances

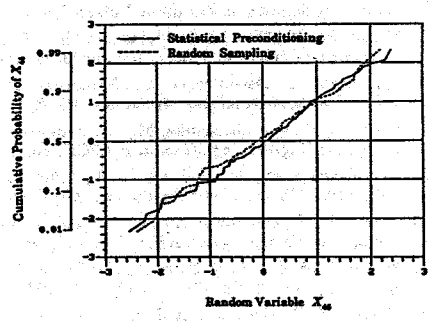

Fig. 9 Statistical Distributions of Simulated Random Variable X_{45}

of little value in generating sample functions of stochastic vectors. Similar difficulties exist for the Latin hypercube sampling technique [8] in which it is not easy to control the cross terms of the covariance matrix.

5. CONCLUSION

A method of generating sample functions of a mean zero stochastic vector which precisely reproduces the prescribed spatial correlation function is developed. The method is a hybrid approach of modal decomposition of the covariance matrix and spectral representation of random processes. The decaying feature of the eigenvalues of the covariance matrix and the orthogonality of the trigonometric functions are employed for generating independent random variables. The generated stochastic vector is Gaussian by virtue of the central limit theorem. For the central limit theorem to be valid, however, a reasonably large number of trigonometric functions must be summed up. This requirement is usually satisfied automatically in the process of modal synthesis.

The sample functions by the method precisely reproduces the prescribed covariance function with a substantially smaller sample size than that required by the standard random sampling technique. Thus the proposed technique will make the application of Monte Carlo methods to structural safety and reliability analysis involving stochastic vectors even more practical.

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