

Generation of Random Process Realizations Via Markov Chain Monte Carlo

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It is often necessary to generate realizations of nonstationary random processes for the simulation of random environments. A framework useful for modeling nonstationary random processes is the Karhunen-Loeve (KL) expansion; a strength and shortcoming is that its description involves a stochastic vector of zero-mean, unit variance, uncorrelated random variables that are not necessarily jointly Gaussian, and not necessarily independent. These facts can make it difficult to simulate the random process accurately. However, the Markov chain Monte Carlo technique, when coupled to a multi-variate kernel density estimator, presents a tractable approach to the simulation problem. This paper discusses the tools, mentioned here, required to generate realizations of nonstationary random process realizations, and presents a numerical example.

INTRODUCTION

Practically all the environments to which structural dynamic systems are subjected are realizations of random processes. That is, the environments that excite systems, whether described in the time domain or in a transform space, cannot be predicted precisely in advance of their measurement. For example, random vibration environments are the prototypical stochastic environments that excite structures. But, beyond those environments, others, like mechanical shock environments, are also random processes. That is, most shock environments are signals that come from a source that has a formal, probabilistic description. Of course, measures of mechanical environments, like the shock response spectrum, are themselves random processes because they are simply well-defined transformations of random processes. Some valuable capabilities in the representation and analysis of randomly excited structural dynamic systems are the facilities to model a random source, then generate realizations of the source.

A compact framework for describing general random processes is the Karhunen-Loeve (KL) expansion (Traina, et al. [7], Ghanem and Spanos [1], Masri, et al. [2], Paez and Hunter [3], [4]). The KL expansion models a random process as a mean function plus a random deviation from the mean. The random deviation from the mean is the product of normalized shape functions, amplitude constants, and randomizing variates. (The specifics of the expansion will be covered later.) The random variates come from a multi-variate random source, i.e., a vector random variable. The random variates in the KL expansion are guaranteed uncorrelated, but not statistically independent. So if the random process is Gaussian distributed, then the vector random variable has a joint Gaussian distribution. If the random process is not Gaussian distributed, then the vector random variable has some distribution other than a joint Gaussian distribution. In this latter case, it is usually difficult to characterize the joint distribution of the vector random variable, and therefore, it is difficult to generate realizations of the random process.

However, an empirical/numerical construct is available for the description of joint probability density functions (PDF) known only through data they produce. This is the kernel density estimator (KDE), and it is useful for

characterizing joint probability density functions in up to a few dimensions. The KDE is described, for example, in Silverman [6]. It is particularly useful for describing the joint PDFs of vector random variables, where the random variables are dependent and non-Gaussian. But even though the expression of the KDE in terms of measured data is simple and direct, it presents a form that is not convenient for generating multi-variate realizations of the represented random vector.

The Markov chain Monte Carlo (MCMC) method is an efficient numerical technique for the generation of multi-variate realizations from a vector random source, when the joint PDF of the source is known. It is described, for example, in Press [5]. It uses a Markov chain random sampling scheme to develop multi-variate random vector realizations, and then determines whether or not the realizations are acceptable samples of the target source.

This investigation develops (1) the KL expansion as an efficient means for modeling general random processes, (2) the KDE as a framework for modeling the joint PDF of the jointly distributed random variables in the KL expansion, and (3) the MCMC construct to generate realizations of the underlying random vector in the KL expansion representation of the random process of interest. Once these things are done, a practical problem and its data are described, and the simulation technique developed here is applied to it.

KARHUNEN-LOEVE EXPANSION

We assume that the random source under consideration will be sampled at discrete values of a parameter (like time or frequency), and that every sample will have finite duration and the same number of points. Denote the random process of interest $X_{rp} = \{X_j, j = 0, \dots, n-1\}$; the random process may be nonstationary, or a finite segment of a stationary random process. Assume, further, that we have M measured realizations of the random process, and that they are denoted $\mathbf{x}_m, m = 1, \dots, M$. Each signal, \mathbf{x}_m , is an $n \times 1$ vector of real values and a realization of the random process X_{rp} . The entire collection of realizations may be collected in the matrix of column vectors $\mathbf{X}_0 = [\mathbf{x}_1 \ \mathbf{x}_1 \ \dots \ \mathbf{x}_M]$. As stated previously, our objective is to generate n_r additional random process realizations using the KL expansion, a KDE, and MCMC sampling.

The KL expansion requires, first, an estimate of the random process mean. It is

$$\bar{\mathbf{x}} = \frac{1}{M} \sum_{m=1}^M \mathbf{x}_m \quad (1)$$

where the sample mean is an $n \times 1$ vector. Next, define a matrix of mean-normalized realizations

$$\mathbf{X} = [(\mathbf{x}_1 - \bar{\mathbf{x}}) \ (\mathbf{x}_1 - \bar{\mathbf{x}}) \ \dots \ (\mathbf{x}_M - \bar{\mathbf{x}})] \quad (2)$$

The matrix \mathbf{X} has dimension $n \times M$. Use the matrix of normalized realizations to estimate the stochastic process auto- and cross-covariances.

$$\hat{\mathbf{C}}_{\mathbf{X}\mathbf{X}} = \frac{1}{M-1} \mathbf{X}\mathbf{X}^T \quad (3)$$

The dimension of $\hat{\mathbf{C}}_{\mathbf{X}\mathbf{X}}$ is $n \times n$, and the i^{th} row- j^{th} column element denotes the estimated covariance between the random variables X_i and X_j , the i^{th} and j^{th} elements of the random process X_{rp} .

Compute the eigenvalue decomposition of the estimated covariance matrix.

$$\hat{\mathbf{C}}_{\mathbf{X}\mathbf{X}} = \mathbf{V}\mathbf{W}\mathbf{V}^T \quad (4)$$

where the matrix V has dimension $n \times n$, and the columns of V are the eigenvectors of the estimated covariance matrix, and the diagonal matrix W has dimension $n \times n$, and contains the eigenvalues of the estimated covariance matrix. The eigenvectors are normalized so as to be orthonormal, i.e., $V^T V = I$, where I is the $n \times n$ identity matrix. The eigenvalues contained in W are nonnegative. The autocovariance estimate matrix can usually be accurately approximated using only a fraction of the columns of V and terms in W . We retain only the largest diagonal terms of W in w , and the corresponding columns of V in v . Then the approximation

$$\hat{C}_{XX} = v w v^T \quad (5)$$

can be written. When n_0 terms are retained in the approximation, the dimension of v is $n \times n_0$, and the dimension of w is $n_0 \times n_0$.

We can now use the sample mean \bar{x} , and the factors of the approximate eigenvalue expansion v and w , to write the approximate KL expansion of the stochastic process.

$$X_{rp} \cong v w^{1/2} U + \bar{x} \quad (6)$$

where U is an $n_0 \times 1$ vector of mean-zero, unit-variance uncorrelated random variables. In this context, the shapes contained in the columns of the matrix v are sometimes called the principal shapes of the KL expansion. The diagonal elements of the matrix $w^{1/2}$ are called the amplitudes of the KL expansion.

The realizations of U that correspond to the stochastic process realizations $X_0 = [x_1 \ x_1 \ \dots \ x_M]$ can be evaluated through inversion of Eq. (6).

$$u^{(real)} = w^{-1/2} v^T X = \begin{bmatrix} u_1^{(real)} & u_2^{(real)} & \dots & u_M^{(real)} \end{bmatrix} \quad (7)$$

where X is the matrix of mean-normalized realizations of the random process. The sample mean of the $u_m^{(real)}, m = 1, \dots, M$, is a zero vector, and the sample covariance (or correlation) is the $n_0 \times n_0$ identity matrix. Because the parameters of the KL expansion expression of Eq. (6) are based on estimates of the random process mean and covariance, the KL expansion is an estimate of the underlying random process. Because only a portion of the components of W and V are included in w and v , the KL expansion is only an approximation of the estimate of the random process.

Equation (6) indicates that in order to generate realizations of the random process, X_{rp} , it is necessary to generate realizations of the $n_0 \times 1$ random vector U . To generate realizations of the random vector U , we must first know the joint PDF of the random variables in the vector U .

KERNEL DENSITY ESTIMATOR

Every random vector U has a joint probability distribution. One description of the probability distribution is a joint PDF governing the behavior of the random variables in U , namely, $U_i, i = 1, \dots, n_0$. In some instances, the theoretical form for the distribution is known, however, in most practical situations, it is not. When sufficient realizations from the random vector are available, an empirical expression for the joint PDF can be written; it is the kernel density estimator (KDE). Let $u_m^{(real)}, m = 1, \dots, M$, be the ensemble of realizations of U expressed in Eq. (7). Each $u_m^{(real)}$ is an $n_0 \times 1$ vector of real numbers. In terms of these vectors the KDE is expressed

$$\hat{f}_U(\mathbf{u}) = \frac{1}{M} \sum_{m=1}^M \frac{1}{(2\pi\varepsilon^2)^{n_0/2}} \exp\left[-\frac{1}{2\varepsilon^2} \|\mathbf{u} - \mathbf{u}_m^{(real)}\|^2\right] \quad -\infty < \mathbf{u} < \infty \quad (8)$$

where ε is a smoothing parameter, and the symbol $\|\cdot\|$ refers to the operation of the norm – the square root of the sum of the squares of the elements of the vector that is the argument. Equation (8) is essentially a superposition of M , n_0 -variate, Gaussian PDFs with diagonal covariance matrix, and with each of the PDFs centered on a data vector, $\mathbf{u}_m^{(real)}$. Selection of the smoothing parameter is discussed in Silverman [6].

MARKOV CHAIN MONTE CARLO

As mentioned above, our objective is to generate realizations of the random process $\mathbf{X}_{rp} = \{\mathbf{X}_j, j = 0, \dots, n-1\}$, and Eq. (6) shows that this can be accomplished, approximately, by generating realizations of the random vector \mathbf{U} , whose empirical PDF is given by Eq. (8). We propose to generate samples from \mathbf{U} using the Markov chain Monte Carlo (MCMC) approach, and specifically, the Metropolis-Hastings (MH) implementation of MCMC (Press, [5]). Metropolis-Hastings sampling is a Bayesian technique for generating realizations of a multivariate random variable (a random vector) with prescribed PDF.

Metropolis-Hastings generates realizations of a random vector, \mathbf{U} , by specifying an initial realization $\mathbf{u}_0^{(MH)}$. When the vector $\mathbf{u}_0^{(MH)}$ is used in Eq. (8) as the argument, the quantity $\hat{f}_U(\mathbf{u}_0^{(MH)}) = L_U(\mathbf{u}_0^{(MH)})$ can be interpreted as the likelihood that the random vector \mathbf{U} would produce the realization $\mathbf{u}_0^{(MH)}$. Metropolis-Hastings next generates another realization of \mathbf{U} – a trial realization – by adding to $\mathbf{u}_0^{(MH)}$ an $n_0 \times 1$, vector random deviate $\boldsymbol{\delta}$. The characteristics of the random variable $\boldsymbol{\delta}$ are chosen so that the quantity

$$\mathbf{u}_{trial} = \mathbf{u}_0^{(MH)} + \boldsymbol{\delta} \quad (9)$$

yields realizations at least some of which lie in the vicinity of the vectors $\mathbf{u}_m^{(real)}, m = 1, \dots, M$. Next, the likelihood $L_U(\mathbf{u}_{trial})$ of \mathbf{u}_{trial} is computed, and used with $L_U(\mathbf{u}_0^{(MH)})$ to form the acceptance probability

$$p_{acc} = \min\left(\frac{L_U(\mathbf{u}_{trial})}{L_U(\mathbf{u}_0^{(MH)})}, 1\right) \quad (10)$$

The quantity p_{acc} is the probability of acceptance of the trial realization, \mathbf{u}_{trial} , as a member of the ensemble of the random vector \mathbf{U} . Based on Eq. (10), when the likelihood, $L_U(\mathbf{u}_{trial})$, of the trial realization, \mathbf{u}_{trial} , is greater than or equal to the likelihood, $L_U(\mathbf{u}_0^{(MH)})$, of the current realization, $\mathbf{u}_0^{(MH)}$, the acceptance probability is one – the realization \mathbf{u}_{trial} is certain to be accepted as a realization of \mathbf{U} . When the likelihood of the trial realization, $L_U(\mathbf{u}_{trial})$, is less than the likelihood of the current realization, $L_U(\mathbf{u}_0^{(MH)})$, the acceptance probability is less than one, but typically nonzero – the realization \mathbf{u}_{trial} is accepted as a realization of \mathbf{U} with the probability $L_U(\mathbf{u}_{trial})/L_U(\mathbf{u}_0^{(MH)})$. Even relatively unlikely “outlier” realizations can, on occasion, be accepted as realizations of \mathbf{U} . To establish whether or not the trial realization, \mathbf{u}_{trial} , is accepted as a member of the ensemble of the random vector \mathbf{U} , we choose, at random, a number, r_0 , from a source that is uniformly distributed on the interval $[0,1]$. If r_0 is equal to or less than p_{acc} we accept the trial realization, \mathbf{u}_{trial} , as the next realization of \mathbf{U} in a sequence; if not we reject it. In equation form

$$\mathbf{u}_1^{(MH)} = \begin{cases} \mathbf{u}_{trial} & r_0 \leq P_{acc} \\ \mathbf{u}_0^{(MH)} & r_0 > P_{acc} \end{cases} \quad (11)$$

This procedure is repeated an arbitrary number of times to build up a collection of vectors each of which is a likely member of the ensemble of the random vector \mathbf{U} . The vector realizations of \mathbf{U} generated using the MH scheme are denoted $\mathbf{u}_j^{(MH)}, j = 1, \dots, n_{MH}$.

Numerous practical matters need to be treated before the MH procedure can be implemented in a specific case. Among others, the distribution of the vector innovation random source $\boldsymbol{\delta}$ needs to be developed. This is an art. The covariance of $\boldsymbol{\delta}$ needs to be small enough that most of the trial vectors are not rejected (because the innovations are too far from the collection $\mathbf{u}_m^{(real)}, m = 1, \dots, M$). This should not be too difficult, because the $\mathbf{u}_m^{(real)}, m = 1, \dots, M$, are known to have zero-mean and unit-variance, and to be uncorrelated. Further, when it is not certain that the starting realization $\mathbf{u}_0^{(MH)}$ is in the vicinity of the vectors $\mathbf{u}_m^{(real)}, m = 1, \dots, M$, then the first part of the generated sequence of vector random variates $\mathbf{u}_j^{(MH)}, j = 1, \dots, n_{MH}$, is discarded, and the latter part, only, of the sequence is retained. However, in the present case, for the reasons mentioned above, it is considered safe to use a starting vector, $\mathbf{u}_0^{(MH)}$, that is the $n_0 \times 1$, zero vector.

Once the realizations of the random vector \mathbf{U} are obtained, they can be used with Eq. (6) to approximately define an ensemble of realizations of the random process \mathbf{X}_{rp} . The MH realizations are given by

$$\mathbf{X}^{(MH)} \cong \mathbf{v}\mathbf{w}^{1/2}\mathbf{U}^{(MH)} + \bar{\mathbf{x}} \quad (12)$$

where

$$\mathbf{U}^{(MH)} = \begin{bmatrix} \mathbf{u}_1^{(MH)} & \mathbf{u}_2^{(MH)} & \dots & \mathbf{u}_{n_{MH}}^{(MH)} \end{bmatrix} \quad (12a)$$

The matrix $\mathbf{X}^{(MH)}$ has dimension $n \times n_{MH}$, and each of its $n \times 1$ columns is an approximate realization of the random process.

NUMERICAL EXAMPLE

The data chosen for this study represent a normalized measure of the structural response at a single discrete location on a spacecraft exposed to a resonant motor burn event. The resonant burn event produces an oscillatory pressure fluctuation within the motor cavity that is very nearly sinusoidal in its character. However, at least with respect to the measured structural response, both the amplitude and frequency of the sinusoidal excitation are changing with time.

Due to the nature of this environment, the temporal data were analyzed using waterfall plots, which are simply a series of Fourier transforms computed for sequential segments of time. The result is a 3-dimensional spectral profile that shows how the amplitude and frequency content of the signal change with time.

For the purposes of this study it was decided that the change in amplitude as a function of frequency was the salient feature of the data so the maximum envelope of the projection of the time-specific waterfall plots onto the frequency-amplitude plane was used as the final measure of the environment. These will be called environment spectra in the following description. Figure 1 shows the environment spectra for an ensemble of 15 flights. The environment spectra are normalized so that the highest point on the most severe spectrum has a value of one.

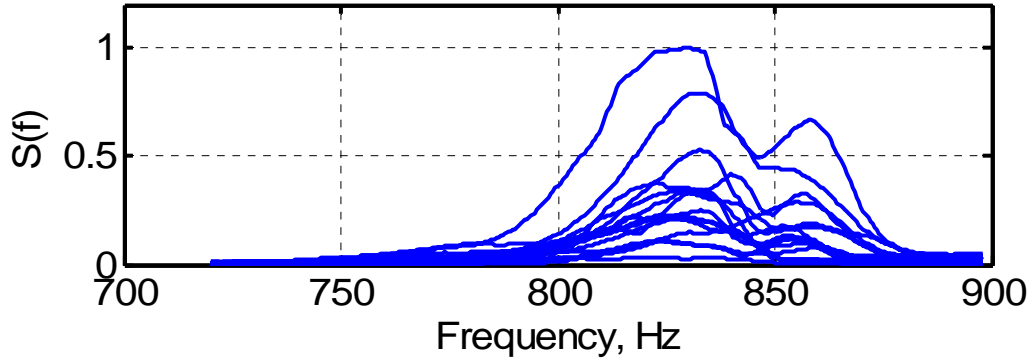


Figure 1. Realizations of environment spectra.

We judged, in this case, that it is more appropriate to model the random process that is the common logarithm of the environment spectra - the log-environment spectra. The common logarithms of the 15 curves in Figure 1 are shown in Figure 2. The mean of the logarithms is also shown in the graph.

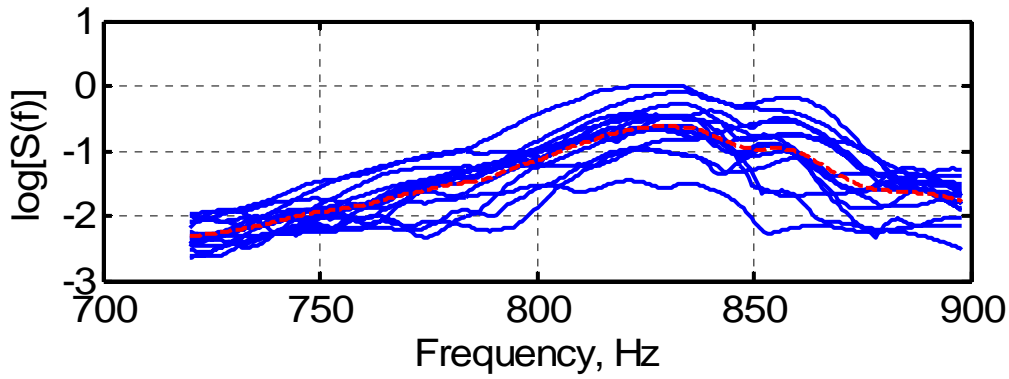


Figure 2. Common logarithms of the environment spectra of Figure 1. Sample mean curve is dashed line.

The KL expansion was computed and the parameters ν and \mathbf{w} were established. In this application, five components were retained in the KL expansion, i.e., $n_0 = 5$. The principal shapes of the KL expansion, ν , are plotted in Figure 3. The amplitudes of the KL expansion, $\text{diag}(\mathbf{w}^{1/2})$, are plotted in Figure 4.

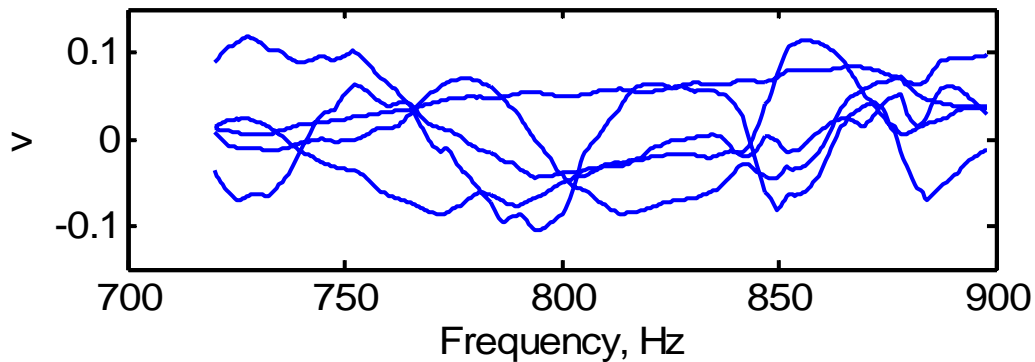


Figure 3. Principal shapes of the estimated KL expansion of the log-environment spectrum random process.

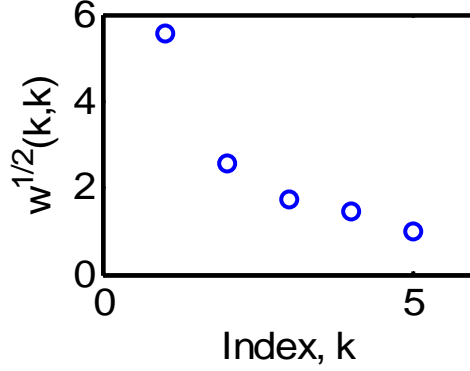
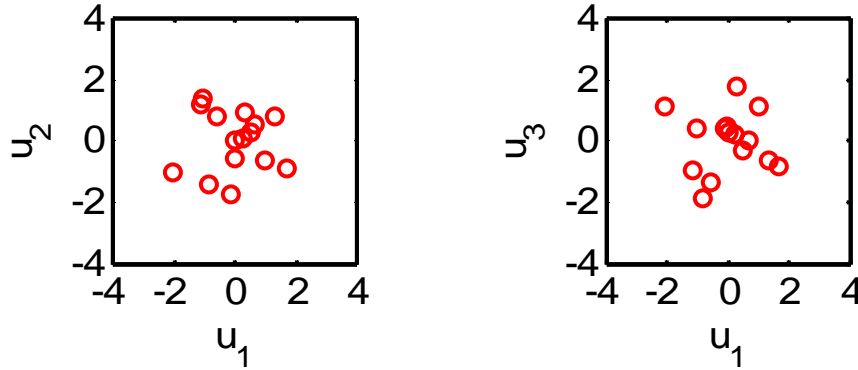


Figure 4. Amplitudes of the estimated KL expansion of the log-environment spectrum random process.

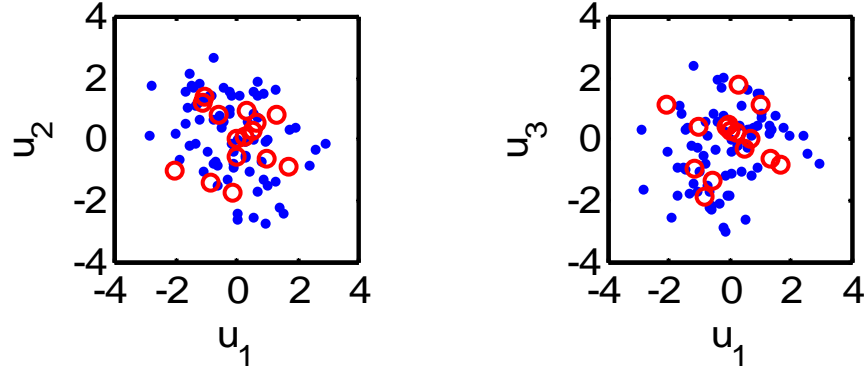
In view of the fact that the KL expansion includes five components, the random vector \mathbf{U} has dimension 5×1 , and because the approximation to the KL expansion of the log-environment spectrum random process is based on 15 measured realizations, $M = 15$, and we can evaluate the vectors $\mathbf{u}_m^{(real)}, m = 1, \dots, 15$. Of course, the vectors cannot be plotted in all their dimensions simultaneously because the plot would require five dimensions. We can, however, plot the realizations in two of their dimensions at a time using a scatter plot. Figure 5 shows the 15 realizations of the random variable U_2 (the second random variable in the random vector \mathbf{U}) plotted versus the 15 realizations of the random variable U_1 . Figure 6 is similar, plotting realizations of U_3 versus realizations of U_1 .



Figures 5 and 6. Realizations of U_2 versus realizations of U_1 , and realizations of U_3 versus realizations of U_1 .

The MCMC process was used to generate realizations $\mathbf{u}_j^{(MH)}, j = 1, \dots, n_{MH}$, of the of the random vector \mathbf{U} . Two-hundred realizations were generated, i.e., $n_{MH} = 200$, and partial results are shown in Figures 7 and 8, in the style of Figures 5 and 6. The realizations generated via the Metropolis-Hastings implementation of MCMC are shown by the blue dots, and the realizations from the identified KL model are shown as red circles. As before, Figure 7 plots realizations of U_2 versus realizations of U_1 , and Figure 8 plots realizations of U_3 versus realizations of U_1 . The two figures show that the MCMC-generated random variable realizations appear to satisfactorily represent the realizations that come directly from the KL model.

The realizations that correspond to the full vector realizations $\mathbf{u}_j^{(MH)}, j = 1, \dots, n_{MH}$, part of which are shown by the blue dots in Figures 7 and 8, were used in Eq. (12) to obtain realizations of the log-environment spectrum random process. The realizations are shown by the blue curves in Figure 9. The figure also includes the 15 realizations of the log-environment spectrum random process in red.



Figures 7 and 8. Realizations of U_2 versus realizations of U_1 , and realizations of U_3 versus realizations of U_1 . Realizations from the identified KL model are shown as red circles, and MCMC-generated realizations are shown as blue dots.

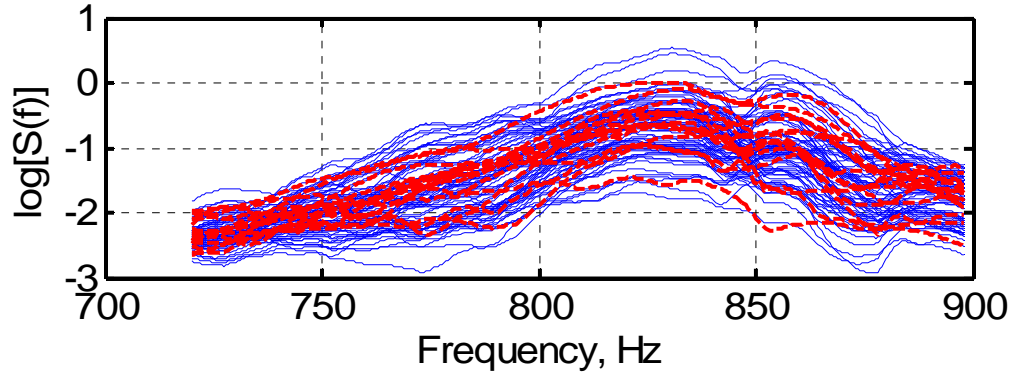


Figure 9. Realizations of the log-environment spectrum random process. MCMC-generated realizations (blue). Realizations from the KL model (red).

Of course, the random process realizations in Figure 9 could be transformed back into the original space by raising each point on each curve to the power 10. Further, though 200 MCMC realizations were generated for this example, an arbitrary number can be generated for user-defined purposes.

And given that realizations of the log-environment spectrum random process are available, the applications are only limited by the needs of the analyst. For example, if a test specification is required, a criterion that measures the severity of the specific log-environment spectrum realizations can be defined, and the generated realizations can be ranked according to the measure. The single log-environment spectrum that falls on the probability limit of the specification defines the test specification. For example, if a ninety percent conservative environment is sought and the severity criterion is the peak value of the realization, then the 200 peaks of the random process realizations shown by the blue curves in Figure 9 are evaluated, and the curve with the ninetieth percentile value defines the test specification.

CONCLUSIONS

A method for generating random process realizations via the Markov Chain Monte Carlo (MCMC) technique is described here. The method uses measured random process realizations to approximate a Karhunen-Loeve (KL) expansion for the random process. Next, it uses a kernel density estimator to characterize the joint probability density function of the underlying random vector in the KL expansion. Finally, the method uses the Metropolis-Hastings implementation of the MCMC technique to generate vector random variable realizations from the random source that is the underlying random vector in the KL expansion.

A specific example is given here, but the technique is useful for the generation of random process realizations from any random source where experimentally measured realizations are available.

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REFERENCES

1. Ghanem, R., Spanos, P., (1991), *Stochastic Finite elements: A Spectral Approach*, Springer-Verlag, New York.
2. Masri, S., Smyth, A., Traina, M., (1998) "Probabilistic Representation and Transmission of Nonstationary Processes in Multi-Degree-of-Freedom Systems," *Journal of Applied Mechanics*, ASME, Vol. 65, June, pp. 398-409.
3. Paez, T., Hunter, N., (2000), "Representation of Random Shock Via the Karhunen Loeve Expansion," *Proceedings of the 2000 Shock and Vibration Symposium*, SAVIAC, Shock and Vibration Information and Analysis Center.
4. Paez, T., Hunter, N., (2001), "Spectral Density Estimation – Welch's Method and the Karhunen-Loeve Expansion," *Proceedings of the 2001 Shock and Vibration Symposium*, SAVIAC, Shock and Vibration Information and Analysis Center.
5. Press, S. J., (2003), *Subjective and Objective Bayesian Statistics – Principles, Models, and Applications*, Wiley-Interscience, New York.
6. Silverman, B. W. (1986), *Density Estimation for Statistics and Data Analysis*, Chapman and Hall, New York.
7. Traina, M., Miller, R., Masri, S., (1984), "Orthogonal Decomposition and Transmission of Nonstationary Random Processes," in *Random Vibrations*, T. C. Huang, P. D. Spanos, eds., AMD-Vol. 65, ASME, New Orleans.