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Numerical solution of the Karhunen–Loeve integral equation with examples based on various kernels derived from the Nataf procedure

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ABSTRACT

An efficient solution of the Karhunen–Loeve (KL) integral equation is developed based on an expansion in Legendre polynomials and also an expansion in the eigenfunctions of the Markov exponential kernel for which analytic results are available. We solve the integral equation with the kernels arising from the Nataf procedure for eight different stochastic processes, viz: Markov, uniform, step, triangular, Rayleigh, exponential, log-normal and log-uniform. It may be shown that use of the Markov eigenfunctions leads to a significant improvement in computing speed over that from the Legendre polynomials. We also discuss some curious behavior associated with the convergence of the Markov eigenfunctions.

1. Introduction

Recent contributions to the literature (Le Maitre and Knio, 2010; Ghanem and Spanos, 2003) have shown that the random aspects of a system may be analyzed by means of an expansion of the random parameter in terms of the eigenfunctions of a certain integral equation; the Karhunen–Loeve equation. While it is relatively simple to solve this equation analytically for the Markov exponential kernel, it is not so easy for other types of kernel which are directly related to the correlation function of the random process. This is especially so when non-Gaussian processes are involved (Park et al., 2015). There is therefore some merit in investigating efficient ways to solve this integral equation numerically and to compare the resulting eigenfunctions and eigenvalues for different correlation functions.

To illustrate the procedure, we remind the reader that in a spatially random medium one way to represent the randomness is to write the desired random parameter in the form:

$$f(\mathbf{x},\xi)=\bar{f}(\mathbf{x})+\sum_{n=1}^{N}\sqrt{\lambda_n}g_n(\mathbf{x})\xi_n \tag{1}$$

where N is chosen to give a desired accuracy. ξ_n are Gaussian random variables with zero mean and unit variance. The functions $g_n(\mathbf{x})$ are the eigenfunctions of the integral equation below and λ_n are the associated eigenvalues.

$$\int_D d\mathbf{x}'K(\mathbf{x},\mathbf{x}')g_n(\mathbf{x}')=\lambda_n g_n(\mathbf{x}) \tag{2}$$

The kernel $K(\mathbf{x},\mathbf{x}')$ is the covariance function of $f(\mathbf{x},\xi)$ defined by,

$$\begin{aligned}K(\mathbf{x},\mathbf{x}')&=\langle f(\mathbf{x},\xi)-\bar{f}(\mathbf{x})f(\mathbf{x}',\xi)-\bar{f}(\mathbf{x}')\rangle\\&=\sum_{n=1}^{N}\lambda_n g_n(\mathbf{x})g_n(\mathbf{x}')\end{aligned} \tag{3}$$

where in arriving at Eq. (3), we have used the fact that the eigenfunctions $g_n(\mathbf{x})$ obey the orthonormality condition

$$\int_D d\mathbf{x}g_n(\mathbf{x})g_m(\mathbf{x})=\delta_{nm} \tag{4}$$

A practical example of the above procedure would be in the description of a multiplying medium in which the fissile and/or absorbing material is randomly dispersed in a moderator such as in the pebble bed reactor. In such a case, the random variable $f(\mathbf{x},\xi)$ would be the number density $N(\mathbf{x},\xi)$ which arises in the macroscopic cross section.

In this note we wish to describe a method for solving Eq. (2). For illustrative purposes we assume one-dimension but the method can also be extended to higher dimensional problems. Thus we consider a uniform slab of thickness a for which Eq. (2) becomes,

$$\int_0^a dx'K(x,x')g_n(x')=\lambda_n g_n(x) \tag{5}$$

The choice of $K(x,x')$ will be made later. Neutrons will diffuse through this slab but their subsequent behavior is not the concern

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of the present work which is to show how the macroscopic cross sections are affected by spatial randomness and how they may be represented mathematically in the transport equation.

2. Theory of the method

We solve Eq. (5) by writing the solution in the form (Corngold, 1957):

$$g_n(x) = \sum_{k=0}^{N} g_{n,k} P_k\left(\frac{2x-a}{a}\right) \tag{6}$$

where $P_n(w)$ are the Legendre polynomials and we also note the orthogonality condition

$$\int_0^a dx P_n\left(\frac{2x-a}{a}\right) P_m\left(\frac{2x-a}{a}\right) = \frac{a}{2}\int_{-1}^{1} dt P_n(t)P_m(t) = \frac{a}{2n+1}\delta_{nm} \tag{7}$$

For practical reasons the sum in Eq. (6) is truncated at $k = N$. Inserting Eq. (6) into the integral Eq. (5), we find after multiplying by $P_\ell\left(\frac{2x-a}{a}\right)$ and integrating over $x(0, a)$, the following set of homogeneous algebraic equations for the expansion coefficients $g_{n,k}$,

$$\frac{a}{2\ell+1}\lambda_n g_{n,\ell} = \sum_{k=0}^{N} g_{n,k}\int_0^a dx P_\ell\left(\frac{2x-a}{a}\right)\int_0^a dx' P_k\left(\frac{2x'-a}{a}\right)K(x,x') \tag{8}$$

For simplicity, and because it is usually the case, we assume that the kernel is of the displacement type, i.e. $K(x,x') = K(|x-x'|) = \sigma_G^2\rho_G(|x-x'|)$, where σ_G^2 is the variance and $\rho_G(|x|)$ is the correlation function. That being so, we may symmetrise Eq. (8) to the form

$$\lambda_n\frac{g_{n,\ell}}{\sqrt{2\ell+1}} = \frac{a}{4}\sum_{k=0}^{N}\frac{g_{n,k}}{\sqrt{2k+1}}\sqrt{(2\ell+1)(2k+1)}\int_{-1}^{1} dt P_\ell(t) \times \int_{-1}^{1} dt' P_k(t')K\left(\frac{a}{2}|t-t'|\right) \tag{9}$$

Defining

$$\tilde{y}_\ell = \frac{g_{n,\ell-1}}{\sqrt{2\ell-1}} \tag{10}$$

and

$$\widetilde{\Delta}_{\ell,k} = \widetilde{\Delta}_{k,\ell} = \sqrt{(2\ell-1)(2k-1)}\int_{-1}^{1} dt P_{\ell-1}(t)\int_{-1}^{1} dt' P_{k-1}(t')K\left(\frac{a}{2}|t-t'|\right) \tag{11}$$

Eq. (9) is written:

$$\tilde{\lambda}\tilde{y}_\ell = \sum_{k=1}^{N}\tilde{y}_k\tilde{\Delta}_{\ell,k}, \quad (\ell = 1,2,\ldots,N) \tag{12}$$

with $\tilde{\lambda} = 4\lambda/a$. We have suppressed the subscript n but this will reappear when we reconstruct the eigenfunctions from Eq. (6). Eq. (12) constitute an eigenvalue problem which may be solved using a Fortran subroutine from the IMSL library. In order to normalise the eigenfunctions we return to Eq. (6) and write

$$A^2\int_0^a dx\left[\sum_{k=0}^{N} g_{n,k}P_k\left(\frac{2x-a}{a}\right)\right]^2 = 1$$

or

$$A^2\sum_{k=0}^{N}\sum_{k'=0}^{N} g_{n,k}g_{n,k'}\int_0^a dx P_k\left(\frac{2x-a}{a}\right)P_{k'}\left(\frac{2x-a}{a}\right) = 1 \tag{13}$$

Using the orthogonality of the Legendre polynomials, we find:

$$A^2 a\sum_{k=0}^{N}\frac{g_{n,k}^2}{2k+1} = A^2 a\sum_{k=1}^{N}\tilde{y}_k^2 = 1$$

from which we find the normalisation factor A. The normalised eigenfunction is therefore,

$$g_n(x) = \frac{1}{A_n}\sum_{k=0}^{N} g_{n,k}P_k\left(\frac{2x-a}{a}\right) \tag{14}$$

Clearly, both eigenvalues and eigenfunctions depend crucially on the value of N.

3. Numerical examples

To illustrate the above method we consider eight forms of kernel each of which appears in problems relating to reliability estimates and/or data uncertainty. It is not appropriate to go into the specific details of these kernels but a full account may be found in (Park et al., 2015).

- Type 1. Markov
$$K(|x|) = \sigma_G^2\rho_G(x) = \sigma_G^2 e^{-\mu|x|} \tag{15}$$
- Type 2. Nataf uniform
$$K(|x|) = \sigma_G^2\rho_G(x) = 2\sigma_G^2\sin\left(\frac{\pi}{6}e^{-\mu|x|}\right) \tag{16}$$
- Type 3. Nataf step (dichotomic)
$$K(|x|) = \sigma_G^2\rho_G(x) = \sigma_G^2\sin\left(\frac{\pi}{2}e^{-\mu|x|}\right) \tag{17}$$
- Type 4. Nataf triangular (see Appendix)
- Type 5. Nataf Rayleigh (see Appendix)
- Type 6. Nataf exponential (see Appendix)
- Type 7. Nataf log-normal $\rho_y(x)(e^{\hat{\sigma}^2}-1) = \left(e^{\hat{\sigma}^2\rho_G(x)}-1\right)$
- Type 8. Nataf log-uniform (see Appendix)

The covariance functions of types 2–8 are derived from the following Nataf equation (Nataf, 1962; Llango et al., 2013),

$$\sigma_y^2\rho_y(x) = \sum_{n=1}^{M} K_n^2(X)\rho_G^n(x) \tag{18}$$

where σ_y^2 and $\rho_y(x)$ are prescribed by the problem at hand, $K_n(X)$ is obtained by the Nataf procedure for stochastic process X (i.e. one of types 2–8) and $\rho_G(x)$ is the root of Eq. (18) which lies in the range $(-1, 1)$. In some cases, the summation in Eq. (18) may be performed analytically, e.g. in the above types 2, 3 and 7; in the other cases a root-finding procedure is necessary. The values of K_n^2 for types 4, 5, 6 and 8 are given in the Appendix.

While the use of types 2–8 in the integral equation does not admit of an analytical solution, for type 1 we may convert the integral equation to a second order differential equation from which the eigenvalues and eigenfunctions can be obtained analytically. This enables the accuracy of the approximate method described above to be assessed. The results obtained by solving the KL equation analytically with the Markov kernel are (Williams, 2006),

$$\tilde{g}_n(x) = \frac{\mu\sin(w_n x) + w_n\cos(w_n x)}{\sqrt{\mu + a(\mu^2 + w_n^2)/2}}, \quad \int_0^a dx\tilde{g}_n(x)\tilde{g}_m(x) = \delta_{nm} \tag{19}$$

where w_n are the roots of

$$\tan(wa) = \frac{2\mu w}{w^2-\mu^2} \tag{20}$$

and the eigenvalues are

$$\lambda_n = \frac{2\mu\sigma^2}{w_n^2+\mu^2} \tag{21}$$

σ^2 being the variance of the process described by $K(x, x')$.