Approximating processes of stochastic diffusion models under spatial uncertainty

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Abstract. This paper deals with the construction of approximate numerical processes of mixed diffusion models under spatial uncertainty in the diffusion coefficient and the source term. After discretization, the stochastic discrete problem is solved using a stochastic separation of the variables method.
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1 Introduction

Mathematical models are useful to describe reality up to certain point. Individual behaviour may be erractic, but aggregate behaviour is often quite predictable. Spatial uncertainty is frequent in Geostatistics descriptions of natural variables. Examples of such variables are, pressure, temperature and wind velocity in the atmosphere, concentrations of pollutants in a contamined site, see [Chilés and Delfiner, 1999]. Wave propagation problems in random media have been studied in [Keller, 1963]. A different approach to numerical stochastic methods for diffusion models where the spatial uncertainty is a Brownian motion is developed in [Kloeden and Platen, 1992] using Ito stochastic calculus. In this paper we study stochastic diffusion problems of the form

$$u_t = [p(x)u_x]_x + F(x,t) \quad , \quad 0 < x < 1 \quad , \quad t > 0 \tag{1}$$

$$a_1 u(0,t) + a_2 u_x(0,t) = 0 \quad , \quad t > 0, \quad |a_1| + |a_2| > 0, \tag{2}$$

$$b_1 u(1,t) + b_2 u_x(1,t) = 0 \quad , \quad t > 0, \quad |b_1| + |b_2| > 0, \tag{3}$$

$$u(x,0) = f(x) \quad , \quad 0 \le x \le 1, \tag{4}$$

where the diffusion coefficient $p(x)$ is assumed to be a stochastic process and for each t fixed, $F(x,t)$ is also a stochastic process. Here $f(x)$ is a deterministic function and h_1 and h_2 are constants. Chance of randomness can affect in any of the following ways:

- uncertainty as to the diffusion properties of the medium which the diffusion takes place,
- random variations of the internal influences of the system undergoing diffusion,

- random external sources to the medium in which the diffusion takes place.

For the particular case where $F(x,t) = 0$ and $p(x)$ is a constant random variable, problem has been recently treated in [Cortés *et al.*, 2005a].

This paper is organized as follows. Section 2 studies random discrete Sturm-Liouville problem and random discrete Fourier series. In section 3 the way for obtaining an exact series solution process is summarized and problem (1)-(4) is discretized and an explicit solution process of the stochastic discretized model is given by means of a random eigenfunctions method. Section 4 includes an illustrative example.

2 Random discrete Sturm-Liouville problems

For the sake of clarity in the presentation we recall some concepts, notations and results related to the mean square stochastic calculus, that may be found in [Soong, 1973]. Let $(\Omega, \mathcal{F}, P)$ be a probability space. A real random variable (r.v.) $Y : \Omega \to R$ is said to be continuous if its distribution function F_Y is continuous and almost everywhere differentiable. In this case, its density function is defined by

$$g_Y(y) = \frac{dF_Y(y)}{dy}.$$

If Y satisfies the additional property

$$E\left[Y^2\right] = \int_{-\infty}^{+\infty} y^2 g_Y(y) dy < +\infty, \tag{5}$$

then Y is said to be a second order random variable (2-r.v.) and the integral in (5) is the expectation of Y^2. If $\{p(x)\}_{x\in I}$ is a real stochastic process on the probability space $(\Omega, \mathcal{F}, P)$, we say that it is a second order process (2-s.p.), if $E\left[p^2(x)\right] < +\infty$, for all $x \in I$.

Throughout this paper a random variable will mean a 2-r.v. and a stochastic process will denote a 2-s.p. If $\{p(x)\}_{x\in I}$ is a 2-s.p., its covariance function is the deterministic function $\Gamma_{pp}(r,s) = E[p(r)p(s)] - E[p(r)]\, E[p(s)]$, for $(r,s) \in I \times I$. If Y is a 2-r.v., then $\|Y\| = \sqrt{E[Y^2]}$ is a norm and the set of all 2-r.v.'s endowed with this norm is a Banach space denoted by L_2, [Soong, 1973, chap.4]. From the Cauchy-Schwarz property in L_2, we recall that if X and Y are two 2-r.v.'s in L_2, then

$$\|XY\| \le \|X\|\, \|Y\|\,. \tag{6}$$

A sequence of 2-r.v.'s $\{Y_n\}$ converges in mean square (m.s.) to a 2-r.v. Y as $n \to \infty$ if

$$\lim_{n\to\infty} \|Y_n - Y\|^2 = \lim_{n\to\infty} E\left[|Y_n - Y|^2\right] = 0. \tag{7}$$

This type of convergence is called mean square convergence. A 2-s.p. $\{p(x)\}_{x\in I}$ is m.s. continuous if, for $x, x+\tau \in I$, one satisfies

$$\lim_{\tau\to 0} \|p(x+\tau) - p(x)\| = 0. \tag{8}$$

Let N be the set of all natural numbers including zero. If $a < b$ are two natural numbers in N, we denote $N(a,b) = \{a, a+1, \ldots, b\}$.

Let $p(i)$, $r(i)$ be 2-r.v., $p(i) : \Omega \to R$, $r(i) : \Omega \to R$ such that

$$\left.\begin{array}{l} p(i)(\omega) > 0 \ , \ \omega \in \Omega \ , \ i \in N(0,K) \\ r(i)(\omega) > 0 \ , \ \omega \in \Omega \ , \ i \in N(1,K) \end{array}\right\} \tag{9}$$

and let α, β be real numbers. If Δ denotes the forward difference operator defined by $\Delta u(i) = u(i+1) - u(i)$, then a boundary value problem of the form

$$\left.\begin{array}{l} \Delta\left(p(i-1)\Delta u(i-1)\right) + \lambda r(i)u(i) = 0 \ , \ i \in N(1,K) \\ u(0) = \alpha u(1) \quad , \quad u(K+1) = \beta u(K) \ , \end{array}\right\} \tag{10}$$

is called a random discrete Sturm-Liouville problem. Note that for each event $\omega \in \Omega$, the problem

$$\left.\begin{array}{l} \Delta\left(p(i-1)(\omega)\Delta u(i-1)\right) + \lambda r(i)(\omega)u(i) = 0 \ , \ i \in N(1,K) \\ u(0) = \alpha u(1) \quad , \quad u(K+1) = \beta u(K) \ , \end{array}\right\} \tag{11}$$

is a deterministic discrete Sturm-Liouville problem, see [Agarwal, 1991, p.663]. A problem (11) has exactly K real eigenvalues $\lambda_m(\omega)$, $1 \le m \le K$, which are distinct, and corresponding to each eigenvalue $\lambda_m(\omega)$ there exist an eigenfunction $\phi_m(i)(\omega)$, $i \in N(1,K)$. These eigenfunctions $\phi_m(i)(\omega)$, $1 \le m \le K$ are mutually orthogonal with respect to weight function $r(i)(\omega)$, i.e.,

$$\sum_{l=1}^{K} r(l)(\omega)\phi_\mu(l)(\omega)\phi_\nu(l)(\omega) = 0 \quad , \quad \text{if} \quad \mu \neq \nu. \tag{12}$$

In particular, these eigenfunctions $\phi_m(i)(\omega)$ are linearly independent on the set $N(1,K)$. Eigenpairs $(\lambda_m(\omega), \phi_m(i)(\omega))$ of the Sturm-Liouville problem (11) for each $\omega \in \Omega$, are easily computed as eigenpairs of the matrix eigenvalue problem

$$R^{-1}(\omega)A(\omega)u = \lambda u \quad , \tag{13}$$

where

$$R(\omega) = \operatorname{diag}\left(r(1)(\omega), r(2)(\omega), \ldots, r(K)(\omega)\right) \quad , \tag{14}$$

and if we denote

$$\left.\begin{array}{l} s(i)(\omega) = p(i)(\omega) + p(i-1)(\omega) \ , \ i \in N(1,K) \\ \overline{s}(1)(\omega) = \quad s(1)(\omega) - \alpha p(0)(\omega) \quad , \overline{s}(K)(\omega) = s(K)(\omega) - \beta p(K)(\omega) \end{array}\right\} , \tag{15}$$

$A(\omega)$ is the symmetric tridiagonal matrix

$$A(\omega)=\begin{bmatrix} \overline{s}(1)(\omega) & -p(1)(\omega) & 0 & \cdots & 0 \\ -p(1)(\omega) & s(2)(\omega) & -p(2)(\omega) & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -p(K-2)(\omega) & s(K-1)(\omega) & -p(K-1)(\omega) \\ 0 & \cdots & 0 & -p(K-1)(\omega) & \overline{s}(K)(\omega) \end{bmatrix} \tag{16}$$

Thus, the eigenvalues and eigenfunctions of the random discrete Sturm-Liouville problem (10) are random variables whose statistical properties are determined by those of the random coefficients. See [Boyce, 1960] for the treatment of analogous of continuous Sturm-Liouville stochastic problems.

Under previous hypotheses and notation, if $\{u(i); 1 \leq i \leq K\}$ is a finite sequence of r.v.'s, or a discrete stochastic processes defined on a common sample space Ω, then for each $\omega \in \Omega$ the function $\{u(i)(\omega); i \in N(1, K)\}$ admits a series representation

$$u(i)(\omega) = \sum_{m=1}^{K} c_m(\omega)\phi_m(\omega)(i) \quad , \qquad i \in N(1, K) \tag{17}$$

where

$$c_m(\omega) = \frac{\sum_{i=1}^{K} r(i)(\omega)\phi_m(i)(\omega)u(i)(\omega)}{\sum_{i=1}^{K} r(i)(\omega)\left(\phi_m(i)(\omega)\right)^2} \quad , \tag{18}$$

is called the m-th discrete Fourier coefficient of $u(i)(\omega)$ with respect to $\{\phi_m(i)(\omega);\ 1 \leq m \leq K\}$ and (17) is the discrete Fourier series of the deterministic function $\{u(i)(\omega);\ i \in N(1, K)\}$, see [Agarwal, 1991, p.675].

Summarizing, under hypotheses (9) the random discrete Sturm-Liouville problem (10) admits exactly K real random eigenvalue variables λ_m, $1 \leq m \leq K$ and K real random eigenfunction variables $\phi_m(i)$, $1 \leq m \leq K$, so that each realization of problem (10), for $\omega \in \Omega$ fixed, described by (11), represents a deterministic discrete Sturm-Liouville problem. In a analogous way, given a discrete stochastic process $\{u(i);\ i \in N(1, K)\}$ defined on Ω, the m-th Fourier coefficient c_m defined by (18) is a random variable and

$$u(i) = \sum_{m=1}^{K} c_m\phi_m(i) \quad , \tag{19}$$

is the random Fourier series representation of the process $\{u(i);\ i \in N(1, K)\}$ with respect to the random eigenpairs $(\lambda_m, \phi_m(i))$ of the random Sturm-Liouville problem (10).

3 Approximating stochastic diffusion processes

An exact theoretical series solution process $u(x,t)$ of problem (1)-(4) of form

$$u(x,t) = \sum_{n\geq 1} \varphi_n(x) b_n(t), \tag{20}$$

can be obtained using a random continuous eigenfunction method, where $(\lambda_n, \varphi_n(x))$ is the random normalized eigenpair sequence associated to the Sturm-Liouiville problem

$$[p(x)X']' + \lambda X = 0, \quad 0 < x < 1 \tag{21}$$

$$a_1 X(0) + a_2 X'(0) = 0, \tag{22}$$

$$b_1 X(1) + b_2 X'(1) = 0, \tag{23}$$

and $b_n(t)$ is the random variable defined by

$$b_n(t) = \alpha_n e^{-\lambda_n t} + \int_0^t e^{-\lambda_n (t-s)} \gamma_n(s) ds, \tag{24}$$

$$\gamma_n(t) = \int_0^1 F(x,t) \varphi_n(x) dx, \tag{25}$$

$$\alpha_n = \int_0^1 f(x) \varphi_n(x) dx. \tag{26}$$

Under appropriate hypotheses it can be proved that $u(x,t)$ given by (20)-(26) is a well defined mean square convergent series, termwise mean square partially differentiable satisfying (1)-(4). In order to prove this fact it is necessary to find bounds of the eigenpairs $(\lambda_n(\omega), \varphi_n(x,\omega))$ of each deterministic realization

$$\left.\begin{array}{r} [p(x)(\omega)X']' + \lambda X = 0, \quad 0 < x < 1, \\ a_1 X(0) + a_2 X'(0) = 0, \\ b_1 X(1) + b_2 X'(1) = 0, \end{array}\right\}$$

using results of section 10.12 and 10.13 of [Birkhoff and Rota, 1965], the ideas developed in [Weinberger, 1965, p.135-137] and [Cortés *et al.*, 2005b] for deterministic eigenfunction method. For the sake of limitation in the extension of this paper we omit technical details of the proof, under the hypotheses

$$F(x,t) \quad \text{m.c. continuous} \tag{27}$$

$$F(x,t) \quad \text{twice m.c. differentiable with respect to} \quad x \tag{28}$$

$$\int_0^1 \frac{\partial^2 F}{\partial x^2}(x,t) dx \quad \text{uniformly bounded in } L_2 \text{ with respect to } t \in [0, \infty[\tag{29}$$

$$a_1 F(0,t) + a_2 F_x(0,t) = 0, \tag{30}$$

$$b_1F(1,t)+b_2F_x(1,t)=0. \tag{31}$$

We considering a stochastic discretization of the problem (1)-(4). Let us subdivide the domain $[0,1]\times[0,+\infty[$ into equal rectangles of sides $\Delta x=h$, $\Delta t=k$, and introduce coordinates of a typical mesh point $P(ih,jk)$; let us also put $u(ih,jk)=U(i,j)$, $F(ih,jk)=F(i,j)$ and $f(ih)=f(i)$. Let us approximate the partial derivatives

$$u_t(ih,jk)\approx\frac{U(i,j+1)-U(i,j)}{k}\quad;\quad u_x(ih,jk)\approx\frac{U(i+1,j)-U(i,j)}{h}$$

$$\begin{aligned}[p(x)u_x]_x(ih,jk)\approx{}&\frac{1}{h^2}\\ &\{p(i)U(i+1,j)-(p(i)+p(i-1))U(i,j)\\ &+p(i-1)U(i-1,j)\},\end{aligned}$$

and consider the discrete stochastic partial difference mixed problem

$$\begin{aligned}&-a\left\{p(i)U(i+1,j)-\left[p(i)+p(i-1)\right]U(i,j)+p(i-1)U(i-1,j)\right\}\\ &\qquad+\left[U(i,j+1)-U(i,j)\right]=kF(i,j)\quad,i\in N(1,K)\quad,\quad j\geq 0\end{aligned}\tag{32}$$

$$\alpha U(1,j)=U(0,j)\quad,\quad j\geq 0\quad,\tag{33}$$

$$U(K+1,j)=\beta U(K,j)\quad,\quad j\geq 0\quad,\tag{34}$$

$$U(i,0)=f(i)\quad,\quad 1\leq i\leq K\quad,\tag{35}$$

$$\left.\begin{array}{c} a=\frac{k}{h^2}=\frac{\Delta t}{(\Delta x)^2}\ ,\ h=\frac{1}{k}\ ,\ 1\leq i\leq K\quad j\geq 0\\ \alpha=\frac{a_2}{a_2-a_1h}\qquad,\qquad \beta=\frac{b_2-b_1h}{b_2}. \end{array}\right\}\tag{36}$$

Firstly, we seek solutions of (32) with $F=0$, of the form

$$U(i,j)=H(i)G(j)\quad,\quad 1\leq i\leq K\quad j\geq 0\quad,\tag{37}$$

satisfying (33)-(34),

$$\begin{aligned}&-a\{p(i)H(i+1)-\left[p(i)+p(i-1)\right]H(i)\\ &\qquad+p(i-1)H(i-1)\}G(j)=-H(i)\left[G(j+1)-G(j)\right],\end{aligned}\tag{38}$$

$$H(0)=\alpha H(1)\quad,\quad H(K+1)=\beta H(K)\quad.\tag{39}$$

Adding the term $a\lambda G(j)H(i)$ to both members of (38), where λ is a real parameter, the resulting equation can be written in the form

$$\begin{aligned}&-a\left\{p(i)H(i+1)-\left[p(i)+p(i-1)-\lambda\right]H(i)+p(i-1)H(i-1)\right\}G(j)\\ &\qquad+H(i)\left\{G(j+1)-(1-a\lambda)G(j)\right\}=0.\end{aligned}\tag{40}$$

Note that equation (40) holds true if

$$p(i)H(i+1)-\left[p(i)+p(i-1)-\lambda\right]H(i)+p(i-1)H(i-1)=0,\ 1\leq i\leq K\ ,\tag{41}$$

and

$$G(j+1)-(1-a\lambda)G(j)=0 \quad , \quad j\geq 0 \quad . \tag{42}$$

Note that equation (41) together with (39) defines a random discrete Sturm-Liouville problem. Under hypothesis (9), such problem admits exactly K real distinct random eigenvalues functions λ_m, $1\leq m\leq K$, and corresponding to each eigenvalues r.v. λ_m there exists an eigenfunction r.v. $\phi_m(i)$, $1\leq i\leq K$. Now let us seek a solution process of the unhomogeneous problem (32)-(35) of the form

$$U(i,j)=\sum_{n=1}^{K}\phi_n(i)b_n(j) \quad , \tag{43}$$

where $b_n(j)$ are r.v. to be determined for $1\leq n\leq K$, $j\geq 0$ and $\{\phi_n(\cdot)\}_{n=1}^{K}$ are chosen so that they are orthonormal with respect to the weight function $r(i)=1$.

Let us take j fixed, and using the results of the section 2, let us consider the random discrete Fourier series expansion of the process $F(\cdot,j)$, see (17)-(19), given by

$$F(i,j)=\sum_{n=1}^{K}\gamma_n(j)\phi_n(i) \quad ; \quad \gamma_m(j)=\sum_{n=1}^{K}F(n,j)\phi_m(n) \quad , \tag{44}$$

with $1\leq i\leq K$, $j\geq 0$. Substituting (43) and (44) into (32) and taking account that $(\lambda_m,\phi_m(\cdot))$ is a random eigenpairs of problem (10), it follows that

$$\sum_{n=1}^{K}\left[b_n(j+1)-(1-a\lambda_n)b_n(j)-k\gamma_n(j)\right]\phi_n(i)=0 \quad . \tag{45}$$

Note that (45) holds if $b_n(j)$ satisfies the random difference equation

$$b_n(j+1)-(1-a\lambda_n)b_n(j)=k\gamma_n(j) \quad , \quad 1\leq n\leq K \quad , \quad j\geq 0 \quad . \tag{46}$$

The solution of the analogous deterministic problem, see [Agarwal, 1991, p.68], suggests the solution

$$b_n(j)=(1-a\lambda_n)^j b_n(0)+\sum_{l=0}^{j-1}k(1-a\lambda_n)^{j-1-l}\gamma_n(l) \quad , \quad j\geq 1 \quad . \tag{47}$$

¿From the initial condition $U(i,0)=f(i)$, one gets

$$b_n(0)=\sum_{i=1}^{K}f(i)\phi_n(i)=\alpha_n \quad , \quad 1\leq n\leq K \quad , \tag{48}$$

and by (43), (47), (48) one gets the approximating stochastic process

$$U(i,j)=\sum_{n=1}^{K}\alpha_n(1-a\lambda_n)^j\phi_n(i)+k\sum_{n=1}^{K}\sum_{l=0}^{j-1}(1-a\lambda_n)^{j-1-l}\gamma_n(l)\phi_n(i) \quad . \tag{49}$$

Once we have the approximating stochastic diffusion process (49) we may compute the expectation $E\left[U(i,j)\right]$ and the variance $V\left[U(i,j)\right]$ assuming the knowledge of the N-density function of both process $p(x)$ and $F(x,t)$, for a fixed value of t. In the following section an illustrative example is included. From the computational point of view the stability condition requires an appropriate size of the parameter $a = \frac{k}{h^2} = \frac{\Delta t}{(\Delta x)}$ so that

$$|1 - a\lambda_n| < 1, \quad 1 \le n \le K. \tag{50}$$

This condition guaranties that the values of any realization of the discrete process $U(i,j)$ remain bounded.

4 Numerical example

Let us consider the stochastic problem

$$u_t = \left[p(x)u_x\right]_x + 4tv^3 \sin\left(\frac{3\pi}{2}x\right) \quad , \quad 0 < x < 1 \quad , \quad t > 0$$

$$u(0,t) = 0 \quad , \quad t > 0,$$
$$u_x(1,t) = 0 \quad , \quad t > 0,$$
$$u(x,0) = 1 \quad , \quad 0 \le x \le 1,$$

where $p(x) = v + \cos(vx)$, v is an uniform random variable defined on the interval $[0,1]$ and with the notation of section 3 we have $\alpha = 0$, $\beta = 1$. In the following tables we compare the expectation value $\widehat{E}\left[U(x,t)\right]$ and the variance $\widehat{V}\left[U(x,t)\right]$ of the discrete approximate process $U(i,j)$ given by (49) at the points $\left\{\left(\frac{i}{10}, 1\right); 1 \le i \le 9\right\}$ taking an appropriate time discretization $\Delta t = 1/400$ and several different space discretization $\Delta x = h$ so that the stability condition (50) is satisfied. This allows the comparison of the computed values in order to show the changes with respect to the uncertain variable x.

Note that the discrete approximate process $U(i,j)$ in our example is a function of the random variable v. Hence

$$E\left[U(i,j)\right] = \int_0^1 U(i,j)(v)dv \tag{51}$$

$$\begin{aligned} V\left[U(i,j)\right] &= E\left[U(i,j)^2\right] - \left(E\left[U(i,j)\right]\right)^2 \\ &= \int_0^1 U(i,j)^2(v)dv - \left(\int_0^1 U(i,j)(v)dv\right)^2 \end{aligned} \tag{52}$$

In the tables the numerical integration of previous expressions (51) and (52) are performed using composite Simpson's rule with 10 points.

(x,t)	$\widehat{E}\,[U(x,t)]$	$\widehat{u}(i,j)$	$\widehat{V}\,[U(x,t)]$
$(1/10,1)$	0.0068	0.0055	1.9×10^{-5}
$(2/10,1)$	0.0135	0.0108	7.5×10^{-5}
$(3/10,1)$	0.0198	0.0159	1.6×10^{-4}
$(4/10,1)$	0.0257	0.0206	2.7×10^{-4}
$(5/10,1)$	0.0310	0.0249	3.9×10^{-4}
$(6/10,1)$	0.0356	0.0286	5.1×10^{-4}
$(7/10,1)$	0.0393	0.0316	6.2×10^{-4}
$(8/10,1)$	0.0421	0.0339	7.1×10^{-4}
$(9/10,1)$	0.0439	0.0353	7.7×10^{-4}

Table 1. Numerical results for $K = 40$, $a = 1/4$.

(x,t)	$\widehat{E}\,[U(x,t)]$	$\widehat{u}(i,j)$	$\widehat{V}\,[U(x,t)]$
$(1/10,1)$	0.0066	0.0053	1.8×10^{-5}
$(2/10,1)$	0.0130	0.0104	7.2×10^{-5}
$(3/10,1)$	0.0192	0.0153	1.5×10^{-4}
$(4/10,1)$	0.0249	0.0198	2.6×10^{-4}
$(5/10,1)$	0.0300	0.0239	3.7×10^{-4}
$(6/10,1)$	0.0344	0.0275	4.9×10^{-4}
$(7/10,1)$	0.0380	0.0304	5.9×10^{-4}
$(8/10,1)$	0.0406	0.0325	6.8×10^{-4}
$(9/10,1)$	0.0423	0.0339	7.3×10^{-4}

Table 2. Numerical results for $K = 80$, $a = 1/4$.

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