Uncertainty Modeling using Polynomial Chaos Expansion

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Outline

Introduction

- Uncertainty is a doubt. A doubt asking how accurately a model is describing the process it is trying to explain and how does it's uncertainty affect the output.
- Polynomial chaos expansion is a technique used to quantify said uncertainties by re-writing the models as SPDEs and solving them.

Polynomial Chaos Expansion

A Polynomial Chaos Expansion (PCE) is a way of writing one random variable as a function of another random variable with a known distribution.

- If $u(X, \omega)$ is the process we are interested in, we may represent as the series $\sum_{i=0}^{\infty} u_i(X)\psi_i(\xi)$.
- ξ is a vector of orthonormal random variables, $\psi(\xi)$ are known orthogonal polynomials. These orthogonal polynomials have a weight function that is precisely the pdf of ξ.
- The choice of ξ and ψ is free and can be chosen by the type of system.
- We truncate the expansion to P+1 terms with $P + 1 = \frac{(N+K)!}{(N!)(K!)}$, N is the number of random variables in the vector and K is the highest degree of the polynomial.

PCE Contd

- We denote $\psi_n(x)$ as a polynomial of degree n. A set of polynomials $\{\psi_i(x)\}_{i=0}^n$ is orthogonal if : $\int_D \psi_n(x)\psi_m(x)W(x)dx = h_n\delta_{nm}, n, m \in \mathbb{N}$, where D is the support of the polynomial, W is a specified weight function and $h_i s$ are non-zero constants.
- The set $\{\psi_i(x)\}_{i=0}^n$ is the polynomial basis used for the PCE, $E[\psi_0] = 1, E[\psi_i] = 0, \forall i \geq 1$.
- $E[u(X, \omega)] = E[\sum_{i=0}^P u_i(X)\psi_i] = u_0(X)$
- $Var(u(X, \omega)) = Var(\sum_{i=0}^P u_i(X)\psi_i) = E[(u(X, \omega) - u_0(X))^2] = E[(\sum_{i=1}^P u_i(X)\psi_i)^2]$
- We can approximate the pdf of $u(X, \omega)$ by sampling from the distribution of ψ and using the samples in the PCE.

Example: Poisson Problem

We try to understand the process of UQ using PCE with this example.

- Domain : $D = (x, y) : x \in [-1, 1], y \in [-1, 1]$ and Ω be the sample space with $\omega \in \Omega$
- $\alpha(\omega)\left[\nabla^2 u(x, y, \omega)\right] = 1$ on $D \times \Omega$, the solution is 0 on the boundary.
- $\alpha(\omega)$ is a constant random variable uniformly distributed over $[1, 3]$.
- We choose Legendre Polynomial and shift ξ to $\xi + 2$, so as to follow $U[1, 3]$.
- We discretise the space using the centered difference scheme, and solve a system thus obtained.
- We obtain the expectation and standard deviation of the solution.

Example: Poisson Problem Contd

We substitute the PCE in the place of $u(x, y, \omega)$. Then multiply with $\psi_k, \forall k = 0, 1, ..., P$ and take inner product.

- $(\xi + 2) \sum_{i=0}^{P} (\nabla^2 u_i(x, y))\psi_i(\xi) = 1$.
- The system becomes:

$$\sum_{i=0}^{P} (\nabla^2 u_i) \langle \psi_i(\xi)(\xi + 2)\psi_k(\xi) \rangle = \langle \psi_k(\xi) \rangle, D \times \Omega$$

$$u_k(x, y, \omega) = 0, \partial D \times \Omega$$

- In matrix form:

$$(CL)u_i(x, y, \omega) = f$$

$$u_k(x, y, \omega) = 0, \partial D \times \Omega$$

$$C = \begin{pmatrix} <\psi_0(\xi+2)\psi_0> & <\psi_0(\xi+2)\psi_1> & \cdots & <\psi_0(\xi+2)\psi_P> \\ <\psi_1(\xi+2)\psi_0> & <\psi_1(\xi+2)\psi_1> & \cdots & <\psi_1(\xi+2)\psi_P> \\ \vdots & \vdots & \ddots & \vdots \\ <\psi_P(\xi+2)\psi_0> & <\psi_P(\xi+2)\psi_1> & \cdots & <\psi_P(\xi+2)\psi_P> \end{pmatrix}$$

L is the 5 point stencil.

Figure 1: EXPECTED VALUES OF PCE COEFFICIENTS

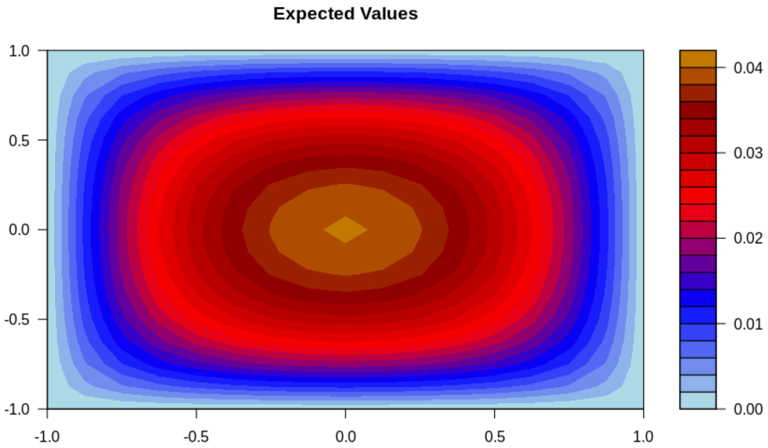
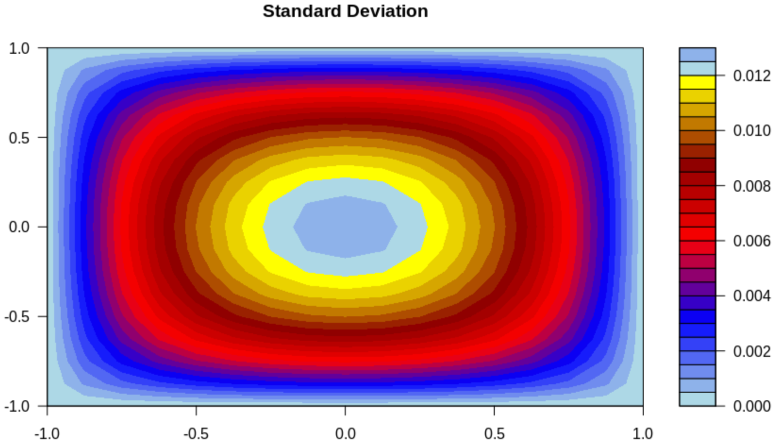


Figure 2: STANDARD DEVIATIONS OF PCE COEFFICIENTS



Logistic Growth-Diffusion Equation

We extend our understanding of PCE through the Poisson problem to the logistic growth-diffusion equation

$$\frac{\partial u(x,y,t)}{\partial t} = u(x,y,t)r\left(1-\left(\frac{u(x,y,t)}{K}\right)^{\theta}\right) + d\left(\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2}\right) \tag{1}$$

- A system has been developed for $\theta = 1$ using the ADI method.
- Employed appropriate linearisation techniques.
- There are two systems for each half time step.

LGDE Contd1

- $\frac{\partial}{\partial t}\sum_{i=0}^{P} u_i(x,y,t,\omega)\psi_i(\xi(\omega)) =$
$r\sum_{i=0}^{P} u_i(x,y,t,\omega)\psi_i(\xi(\omega))\left(1-\left(\frac{\sum_{i=0}^{P} u_i(x,y,t,\omega)\psi_i(\xi(\omega))}{K}\right)\right)+$
$d\nabla^2\sum_{i=0}^{P} u_i(x,y,t,\omega)\psi_i(\xi(\omega))$
- On multiplying with ψ_k and taking expectation and rearranging the terms, we get :

$$
\begin{aligned}
< \psi_k^2 > (u_k)_t = \sum_{l=0}^{P}(u_l) < \psi_l(\xi+1)\psi_k > -\frac{1}{K}\sum_{l=0}^{P}(u_l)^2 < \psi_l^2(\xi+1)\psi_k > - \\
\frac{2}{K}\sum_{m=1}^{P}\sum_{l=0}^{m-1}(u_l u_m) < \psi_l\psi_m(\xi+1)\psi_k > +d\left((u_k)_{xx}+(u_k)_{yy}\right) < \psi_k^2 >, k=0,1,\cdots,P
\end{aligned}
$$

where $(u_k)_t = \frac{\partial}{\partial t}u(x,y,t,\omega), (u_k)_{xx} = \frac{\partial^2}{\partial x^2}u(x,y,t,\omega), (u_k)_{yy} = \frac{\partial^2}{\partial y^2}u(x,y,t,\omega)$

LGDE Contd2

- We proceed to solve this using ADI method.
- We choose grid spacing $\Delta x, \Delta y$ in x and y directions and Δt time spacing. We discretise time derivative using forward differencing and the Laplacian using central differencing scheme. We let there be B grid cells in each spatial domain.
- In the first direction, we move in x direction keeping y same in first half time step $(n, n+\frac{1}{2})$.
- In the next direction along y keeping x constant in time interval $(n+\frac{1}{2}, n+1)$.
- The linearisation has been done in the following way :
  $(u_l) = ((u_l)^{(n+1/2)} + (u_l)^{(n)})/2$
  $(u_l)^2 = ((u_l)^{(n+1/2)}(u_l)^{(n)})$

LGDE Contd3

- On substituting the PCE in both directions and rearranging terms, we get the following two systems.
- We have $A1_k U_k(n+0.5) = B1_k$ for the first direction and $A2_k U_k(n+1) = B2_k$ for each $k = 0, 1, 2, ..., P$, which is a system of N-1 equations each. There are two more equations say (0,0.5) and (N,0.5) and (0,1) and (N,1), at i,j=0 and N that contain fictitious points which we can find using suitable boundary conditions or let them be zero.
- Equation (0,0.5) is $a_0(u_{k(-1,j)}^{n+1/2}) = rhs1_{k_{0,j}} - b_{0_{(0,j)}}(u_0)_{(0,j)}^{(n+1/2)} - b_0(u_0)_{(0,j)}^{(n+1/2)}$

LGDE Contd4

- $$A1_k = \begin{pmatrix} b_{k(1,j)} & a_0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ a_0 & b_{k(2,j)} & a_0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & a_0 & b_{k(2,j)} & a_0 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & a_0 & b_{k(N-3,j)} & a_0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_0 & b_{k(N-2,j)} & a_0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & a_0 & b_{k(N-1,j)} \end{pmatrix}$$

$$A2_k = \begin{pmatrix} -f_{k(i,1)} & c_0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ c_0 & -f_{k(i,2)} & c_0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & c_0 & -f_{k(i,3)} & c_0 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & c_0 & -f_{k(i,N-3)} & c_0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & c_0 & -f_{k(i,N-2)} & c_0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & c_0 & -f_{k(i,N-1)} \end{pmatrix}$$

LGDE Contd5

- $U_k(n+0.5) = \begin{pmatrix} u_{k(1,j)}^{(n+1/2)} \\ u_{k(2,j)}^{(n+1/2)} \\ u_{k(3,j)}^{(n+1/2)} \\ \\ \vdots \\ u_{k(N-3,j)}^{(n+1/2)} \\ u_{k(N-2,j)}^{(n+1/2)} \\ u_{k(N-1,j)}^{(n+1/2)} \end{pmatrix}, U_k(n+1) = \begin{pmatrix} u_{k(i,1)}^{(n+1)} \\ u_{k(i,2)}^{(n+1)} \\ u_{k(i,3)}^{(n+1)} \\ \\ \vdots \\ u_{k(i,N-3)}^{(n+1)} \\ u_{k(i,N-2)}^{(n+1)} \\ u_{k(i,N-1)}^{(n+1)} \end{pmatrix}$
- $B1_k = \begin{pmatrix} rhs1_{1_{(i,j)}} - a_0 u_{k(0,j)}^{(n+1/2)} \\ rhs1_{2_{(i,j)}} \\ rhs1_{3_{(i,j)}} \\ \\ \vdots \\ rhs1_{N-3_{(i,j)}} \\ rhs1_{N-2_{(i,j)}} \\ rhs1_{N-1_{(i,j)}} - a_0 u_{k(N,j)}^{(n+1/2)} \end{pmatrix}, U_k(n+1) = \begin{pmatrix} rhs2_{1_{(i,j)}} - c_0 u_{k(i,0)}^{(n+1)} \\ rhs2_{2_{(i,j)}} \\ rhs2_{3_{(i,j)}} \\ \\ \vdots \\ rhs2_{N-3_{(i,j)}} \\ rhs2_{N-2_{(i,j)}} \\ rhs2_{N-1_{(i,j)}} - c_0 u_{k(i,N)}^{(n+1)} \end{pmatrix}$

LGDE Contd6

- $a_k = \frac{-d}{(\Delta x)^2}$
- $b_{k_{(i,j)}} = \frac{2<\psi_k^2>}{\Delta t} - \frac{<\psi_k(\xi+1)\psi_k>}{2} + \frac{(u_k)^n_{(i,j)}}{K} < \psi_k^2(\xi+1)\psi_k > + \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)^n_{(i,j)} < \psi_l\psi_k(\xi+1)\psi_k > + \frac{2d}{(\Delta x)^2} < \psi_k^2 >$
- $c_k = \frac{d}{(\Delta y)^2} < \psi_k^2 >$
- $d_{k_{(i,j)}} = \frac{2<\psi_k^2>}{\Delta t} + \frac{<\psi_k(\xi+1)\psi_k>}{2} - \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)^n_{(i,j)} < \psi_l\psi_k(\xi+1)\psi_k > - \frac{2d<\psi_k^2>}{(\Delta y)^2}$
- $e_{k_{(i,j)}} = \sum_{l=0,l\neq k}^{P}(u_l)^n_{(i,j)} < \psi_l(\xi+1)\psi_k > - \sum_{l=0,l\neq k}^{P}(u_l^2)^n_{(i,j)} < \psi_l^2(\xi+1)\psi_k > - \frac{2}{K}\sum_{m=1,m\neq k}^{P}\sum_{l=0,l\neq k}^{m-1}(u_l u_m)^n_{(i,j)} < \psi_l\psi_m(\xi+1)\psi_k >$
- $f_{k_{(i,j)}} = \frac{2<\psi_k^2>}{\Delta t} - \frac{<\psi_k(\xi+1)\psi_k>}{2} + \frac{(u_k)^{(n+1/2)}_{(i,j)}}{K} < \psi_k^2(\xi+1)\psi_k > + \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)^{(n+1/2)}_{(i,j)} < \psi_l\psi_k(\xi+1)\psi_k > + \frac{2d}{(\Delta y)^2} < \psi_k^2 >$
- $g_{k_{(i,j)}} = \frac{2<\psi_k^2>}{\Delta t} + \frac{<\psi_k(\xi+1)\psi_k>}{2} - \frac{1}{K}\sum_{l=0,l\neq k}^{P}(u_l)^{(n+1/2)}_{(i,j)} < \psi_l\psi_k(\xi+1)\psi_k > - \frac{2d<\psi_k^2>}{(\Delta x)^2}$
- $h_{k_{(i,j)}} = \sum_{l=0,l\neq k}^{P}(u_l)^{(n)+1/2}_{(i,j)} < \psi_l(\xi+1)\psi_k > - \sum_{l=0,l\neq k}^{P}(u_l^2)^n_{(i,j)} < \psi_l^2(\xi+1)\psi_k > - \frac{2}{K}\sum_{m=1,m\neq k}^{P}\sum_{l=0,l\neq k}^{m-1}(u_l u_m)^n_{(i,j)} < \psi_l\psi_m(\xi+1)\psi_k >$
- $rhs1_{k_{(i,j)}} = c_k(u_k)^{(n)}_{(i,j-1)} + d_{k_{(i,j)}}(u_k)^{(n)}_{(i,j)} + c_k(u_k)^{(n+1/2)}_{(i,j+1)} + e_{k_{(i,j)}}.$
- $rhs2_{k_{(i,j)}} = a_k(u_k)^{(n+1/2)}_{(i-1,j)} - g_{k_{(i,j)}}(u_k)^{(n+1/2)}_{(i,j)} + a_k(u_k)^{(n+1/2)}_{(i+1,j)} - h_{k_{(i,j)}}.$

Future Work

- Further study concepts to be able to develop system incorporating variable random variable.
- Finish solving developed system.
- Develop systems for various values of θ.
- Try out various random variables.

References

1. Probability and Measure theory, R. Ash, Catherine D.
2. Linear Algebra, K. Hoffman, R. Kunze.
3. The Wiener-Askey polynomial chaos for stochastic differential equations, D. Xiu
4. Stochastic Processes and Orthogonal Polynomials, W. Schoutens.
5. A Primer on Stochastic Galerkin methods, Paul Constantine.
6. Numerical methods for Stochastic computations, D. Xiu.
7. Individual based modeling of population growth and diffusion in discrete time, N. Tkachenko et al.