Polynomial Chaos

Workshop on Uncertainty Analysis & Estimation (ACC 2015)

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What is polynomial chaos theory?

It provides a non-sampling based method to determine evolution of uncertainty in dynamical system, when there is probabilistic uncertainty in the system parameters.

Consider a dynamical system

- $\dot{x} = -ax$, $x(t_0) = x_0$ is given (known)
- \blacksquare a is an unknown parameter in the range [0,1] (equally likely values)

Polynomial chaos theory helps us answer these questions

- How does x(t) evolve for various values of a?
- \blacksquare What is the ensemble behavior of x (mean, variance, PDF)?

Monte-Carlo Approach

Summary of Steps

- $\dot{x} = -ax$, $x(t_0) = 1$
- lacksquare a is an unknown parameter in the range [0,1] (equally likely values)
- Sample $a \in [0,1]$
- Plot x(t) for every value of a
- Estimate statistics from data

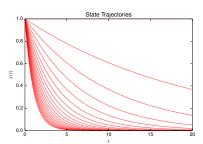
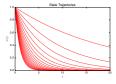


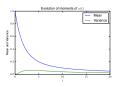
Figure: Sample paths

Monte-Carlo Approach

Solution Interpretation



(a) Sample paths



(b) Moments



Polynomial Chaos

Basic Idea

■ Approximate x(t,a), solution of $\dot{x} = -ax$ as

$$\hat{x}(t,a) \approx \sum_{i} x_i(t)\phi_i(a)$$

- \bullet $\phi_i(a)$ are known polynomials of parameter a
- \blacksquare $x_i(t)$ are unknown time varying coefficients
- Determine $x_i(t)$ that minimises equation error $e(t,a) = \dot{\hat{x}} a\hat{x}$
 - ▶ Galerkin Projection: minimize $||e(t,a)||_2$
 - ▶ Stochastic Collocation: set e(t, a) = 0 at certain locations
- Resulting system
 - ▶ is in higher dimensional state space
 - doesn't involve parameter a

Galerkin Projection

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Stochastic Finite Element

Generalized Formulation

■ Let system be

$$\dot{x} = f(x, \Delta),$$

where state $oldsymbol{x} \in \mathbb{R}^n$ and parameter $oldsymbol{\Delta} \in \mathcal{D}_{oldsymbol{\Delta}} \subseteq \mathbb{R}^d$

- More precisely, $\Delta:=\Delta(\omega)$ is a \mathbb{R}^d -valued continuous random variable
- ω is an event in the probability space (Ω, \mathcal{F}, P)
- \blacksquare A second order process ${\pmb x}(t,{\pmb \Delta}(\omega))$ can be expressed by polynomial chaos as

$$x(t, \Delta(\omega)) = \sum_{i=0}^{\infty} x_i(t)\phi_i(\Delta(\omega))$$

■ In practice, approximate with finite terms

$$m{x}(t,m{\Delta}) pprox \hat{m{x}}(t,m{\Delta}) = \sum_{i=0}^{N} m{x}_i(t) \phi_i(m{\Delta})$$

Reduced Order System

1. Dynamics

$$\dot{x}=f(x,\Delta),$$
 (n differential equations)

2. Proposed solution

$$\hat{\boldsymbol{x}}(t, \boldsymbol{\Delta}) = \sum_{i=0}^{N} \boldsymbol{x}_i(t) \phi_i(\boldsymbol{\Delta})$$

Residue

$$e(t, \boldsymbol{\Delta}) := \dot{\hat{x}} - f(\hat{x}, \boldsymbol{\Delta})$$

4. Set projection on basis function to zero (best \mathcal{L}_2 solution)

$$\langle e(t, \Delta), \phi_i(\Delta) \rangle = 0$$
, for $i = 0, 1, \dots, N$

5. This gives n(N+1) ordinary differential equations to determine n(N+1) unknowns $\boldsymbol{x}_i(t) \in \mathbb{R}^n$

Inner product

Define

$$\langle \boldsymbol{e}(t,\boldsymbol{\Delta}),\phi_i(\boldsymbol{\Delta})\rangle := \int_{\mathcal{D}_{\boldsymbol{\Delta}}} \boldsymbol{e}(t,\boldsymbol{\Delta})\phi_i(\boldsymbol{\Delta}) p(\boldsymbol{\Delta}) d\boldsymbol{\Delta},$$

where $p(\Delta)$ is the probability density function of Δ .

Also

$$\mathsf{E}\left[e(t, \Delta)\phi_i(\Delta)\right] := \int_{\mathcal{D}_{\Delta}} e(t, \Delta)\phi_i(\Delta)p(\Delta)d\Delta$$

Therefore.

$$\langle \boldsymbol{e}(t, \boldsymbol{\Delta}), \phi_i(\boldsymbol{\Delta}) \rangle \equiv \mathbf{E} \left[\boldsymbol{e}(t, \boldsymbol{\Delta}) \phi_i(\boldsymbol{\Delta}) \right]$$

Basis Functions

Basis functions are such that

$$\mathbf{E}\left[\phi_i(\mathbf{\Delta})\phi_j(\mathbf{\Delta})\right] = 0$$
, when $i \neq j$

i.e. orthogonal w.r.t $p(\Delta)$

$$\int_{\mathcal{D}_{\Delta}}\phi_i(\mathbf{\Delta})\phi_j(\mathbf{\Delta})p(\mathbf{\Delta})d\mathbf{\Delta}=0, \text{ when } i\neq j$$

Distribution	Polynomial Basis Function	Support
Uniform: $\frac{1}{2}$	Legendre	$x \in [-1,1]$
Standard Normal: $\frac{1}{\sqrt{2\pi}}e^{-\frac{1}{2}x^2}$	Hermite	$x \in (-\infty, \infty)$
Beta: $\frac{1}{B(\alpha,\beta)}x^{\alpha-1}(1-x)^{\beta-1}$	Jacobi	$x \in [0, 1]$
Gamma: $\frac{x^{k-1}e^{-\frac{x}{\theta}}}{\theta^k\Gamma(k)}$	Laguerre	$x \in (0, \infty)$

Basis Functions (contd.)

In general

- \bullet $\{\phi_i(\Delta)\}\$ are orthogonal polynomials with weight $p(\Delta)$
- \blacksquare \mathcal{L}_2 exponential convergence in corresponding Hilbert functional space
- Askey scheme of hypergeometric polynomials for common $p(\Delta)$
 - Normal, uniform, beta, gamma, etc
- Numerically generate for arbitrary $p(\Delta)$:
 - Gram-Schmidt
 - Chebvshev
 - Gauss-Wigert
 - Discretized Stielties

Basis Functions (contd.)

Mixed Basis Functions

- Let $\Delta := [\Delta_1 \ \Delta_2]^T$, $\Delta_1 \ \Delta_2$ are independent - Δ_1 is uniform over [-1,1] $-\Delta_2$ is standard normal over $(-\infty, \infty)$
- What is the basis function for Δ ?
- \bullet $\{\phi_i(\Delta)\}$ is multivariate polynomial
 - $\{\psi_i(\Delta_1)\}$: Legendre polynomials
 - $\{\theta_k(\Delta_2)\}$: Hermite polynomials
 - $\{\phi_i(\Delta)\}$: tensor product of $\{\psi_i(\Delta_1)\}$ and $\{\theta_k(\Delta_2)\}$

Example: First Order Linear System

Consider system $\dot{x} = -ax$, where $a \in \mathcal{U}_{[0,1]}$ (uniform distribution)

- 1. Define $a(\Delta) := \frac{1}{2}(1+\Delta), \ \Delta \in \mathcal{U}_{[-1,1]}$ Now dynamics is $\dot{x} = -a(\Delta)x$.
- 2. Approximate solution as $\hat{x} = \sum_{i=0}^{N} x_i(t)\phi_i(\Delta)$
- Residue:

$$e(t, \Delta) := \dot{\hat{x}} - a(\Delta)\hat{x}$$
$$= \sum_{i=0}^{N} \dot{x}_i(t)\phi_i(\Delta) - a(\Delta)\sum_{i=0}^{N} x_i(t)\phi_i(\Delta)$$

Example: First Order Linear System (contd.)

4. Project residue on i^{th} basis function:

$$\begin{split} \langle e(t,\Delta), \phi_j(\Delta) \rangle &= \left\langle \sum_{i=0}^N \dot{x}_i(t) \phi_i(\Delta), \phi_j(\Delta) \right\rangle - \left\langle a(\Delta) \sum_{i=0}^N x_i(t) \phi_i(\Delta), \phi_j(\Delta) \right\rangle \\ &= \sum_{i=0}^N \dot{x}_i(t) \langle \phi_i(\Delta), \phi_j(\Delta) \rangle - \sum_{i=0}^N x_i(t) \langle a(\Delta) \phi_i(\Delta), \phi_j(\Delta) \rangle \end{split}$$

5. If $\langle \phi_i(\Delta), \phi_i(\Delta) \rangle = 0$ for $i \neq i$ (orthogonal)

$$\langle e(t,\Delta), \phi_j(\Delta) \rangle = \dot{x}_j \langle \phi_j(\Delta), \phi_j(\Delta) \rangle - \sum_{i=0}^N x_i(t) \langle a(\Delta)\phi_i(\Delta), \phi_j(\Delta) \rangle$$

6. $\langle e(t, \Delta), \phi_i(\Delta) \rangle = 0$ implies

$$\dot{x}_j = \frac{1}{\langle \phi_j(\Delta), \phi_j(\Delta) \rangle} \sum_{i=0}^{N} x_i(t) \langle a(\Delta) \phi_i(\Delta), \phi_j(\Delta) \rangle$$

7. This gives use N+1 ordinary differential equations

Example: First Order Linear System (contd.)

The equation

$$\dot{x}_j = \frac{1}{\langle \phi_j(\Delta), \phi_j(\Delta) \rangle} \sum_{i=0}^N x_i(t) \langle a(\Delta)\phi_i, \phi_j \rangle$$

in more compact form

$$\dot{x}_{j} = \frac{1}{\langle \phi_{j}(\Delta), \phi_{j}(\Delta) \rangle} \left[\langle a(\Delta)\phi_{0}(\Delta), \phi_{j}(\Delta) \rangle \quad \cdots \quad \langle a(\Delta)\phi_{N}(\Delta), \phi_{j}(\Delta) \rangle \right] \begin{pmatrix} x_{0} \\ \vdots \\ x_{N} \end{pmatrix}$$

Define $x_{pc} := (x_0 \ x_1 \ \cdots \ x_N)^T$, then

$$\dot{\boldsymbol{x}}_{pc} = \boldsymbol{A}_{pc} \boldsymbol{x}_{pc}$$

where

$$\boldsymbol{A}_{pc} := \boldsymbol{W}^{-1} \begin{bmatrix} \langle a(\Delta)\phi_0, \phi_0 \rangle & \cdots & \langle a(\Delta)\phi_N, \phi_0 \rangle \\ \vdots & & \vdots \\ \langle a(\Delta)\phi_0, \phi_N \rangle & \cdots & \langle a(\Delta)\phi_N, \phi_N \rangle \end{bmatrix}, \ \boldsymbol{W} := \operatorname{diag} \left(\langle \phi_0, \phi_0 \rangle & \cdots & \langle \phi_N, \phi_N \rangle \right)$$

Reduced Order System

Therefore

In general

$$\underbrace{\dot{x} = f(x, \Delta)}_{\text{stochastic in } \mathbb{R}^n} \xrightarrow{\mathsf{Polynomial Chaos}} \underbrace{\dot{x}_{pc} = F_{pc}(x_{pc})}_{\text{deterministic in } \mathbb{R}^{n(N+1)}}$$

where
$$m{x}_{pc} := egin{pmatrix} m{x}_0 \ dots \ m{x}_N \end{pmatrix}$$
 and $\hat{m{x}} = \sum_{i=0}^N m{x}_i(t) \phi_i(\Delta)$

Initial Condition Uncertainty

Transform uncertainty in dynamics as

$$\dot{m{x}} = m{f}(m{x}, m{\Delta}) \xrightarrow{\mathsf{Polynomial Chaos}} \dot{m{x}}_{pc} = m{F}_{pc}(m{x}_{pc})$$

$$m{x}_{pc} := egin{pmatrix} m{x}_0 \ dots \ m{x}_N \end{pmatrix}$$
 and $\hat{m{x}} = \sum_{i=0}^N m{x}_i(t) \phi_i(m{\Delta})$

Let I.C. uncertainty be: $x_0(\Delta)$

Initialize $oldsymbol{x}_{pc}$ as

$$\boldsymbol{x}_i(t_0) := \langle \boldsymbol{x}_0(\boldsymbol{\Delta}), \phi_i(\boldsymbol{\Delta}) \rangle$$

Random variable Δ is

Basis functions $\phi_i(\Delta)$ are defined w.r.t Δ

Linear Systems

Consider Linear System

$$\dot{m x} = m A(m \Delta)m x, ext{ with } m x(t_0) := m x_0(m \Delta), ext{ and } m \Delta := egin{pmatrix} m \Delta_0 \ m \Delta_p \end{pmatrix}$$

- System has random parameters in A matrix and I.C.
- $lacksquare x \in \mathbb{R}^n$ and $oldsymbol{\Delta} \in \mathbb{R}^d$
- lacksquare Define basis function vector $oldsymbol{\Phi}(oldsymbol{\Delta}) := \left(\phi_0(oldsymbol{\Delta}) \cdots \phi_N(oldsymbol{\Delta})
 ight)^T$
- Approximate solution is

$$\hat{oldsymbol{x}} := \sum_{i=0}^N oldsymbol{x}_i \phi_i(oldsymbol{\Delta}) = oldsymbol{X} oldsymbol{\Phi}(oldsymbol{\Delta}),$$

$$X = [x_0 \ x_1 \ \cdots \ x_N] \in \mathbb{R}^{n \times (N+1)}$$

Linear Systems (contd.)

Approximate solution

$$\hat{oldsymbol{x}} = oldsymbol{X} oldsymbol{\Phi}(oldsymbol{\Delta}), \, oldsymbol{X} = [oldsymbol{x}_0 \,\, oldsymbol{x}_1 \,\, \cdots \,\, oldsymbol{x}_N]$$

Define

$$oldsymbol{x}_{pc} := \mathsf{vec}\left(oldsymbol{X}
ight) \equiv egin{pmatrix} oldsymbol{x}_0 \ dots \ oldsymbol{x}_N \end{pmatrix}$$

Therefore,

$$\begin{array}{rcl} \operatorname{vec}\left(\hat{x}\right) & = & \operatorname{vec}\left(X\Phi\right) \\ & \hat{x} & = & \left(\Phi^T \otimes \boldsymbol{I}_n\right) \! \boldsymbol{x}_{pc} & \operatorname{vec}\left(ABC\right) \equiv (\boldsymbol{C}^T \otimes A) \operatorname{vec}\left(B\right) \end{array}$$

Linear Systems (contd.)

Residue

$$egin{array}{lll} e(t,\Delta) &:=& \dot{\hat{x}} - A(\Delta) \hat{x} = \dot{X} \Phi(\Delta) - A(\Delta) X \\ \mathrm{vec}\,(e) = e &=& \mathrm{vec}\left(\dot{X} \Phi(\Delta) - A(\Delta) X \Phi(\Delta)
ight) \\ &=& \left(\Phi^T \otimes I_n\right) \dot{x}_{pc} - \left(\Phi^T(\Delta) \otimes A(\Delta)\right) x_{pc} \end{array}$$

$$\langle \boldsymbol{e}, \phi_i(\boldsymbol{\Delta}) \rangle = 0$$
 implies

$$\dot{m{x}}_i = \left(\left\langle \phi_i(m{\Delta}), \phi_i(m{\Delta}) \right
angle \otimes m{I}_n
ight)^{-1} \left\langle m{\Phi}^T(m{\Delta}) \otimes m{A}(m{\Delta}), \phi_i(m{\Delta})
ight
angle m{x}_{pc}$$

Linear Systems (contd.)

Deterministic linear dynamics

$$\dot{oldsymbol{x}}_{pc} = oldsymbol{A}_{pc} \, oldsymbol{x}_{pc}$$

 $\boldsymbol{x}_{pc} \in \mathbb{R}^{n(N+1)}, \boldsymbol{A}_{pc} \in \mathbb{R}^{n(N+1) \times n(N+1)}$

A_{pc} is defined as

$$m{A}_{pc} := (m{W} \otimes m{I}_n)^{-1} egin{bmatrix} \left\langle m{\Phi}^T \otimes m{A}(m{\Delta}), \phi_0
ight
angle \\ & dots \\ \left\langle m{\Phi}^T \otimes m{A}(m{\Delta}), \phi_N
ight
angle \end{bmatrix}$$

Recall

$$W := \operatorname{diag}(\langle \phi_0, \phi_0 \rangle \cdots \langle \phi_N, \phi_N \rangle)$$

Computation of Mean

Given
$$x(\Delta) := X\Phi(\Delta)$$

$$\mathbf{E}[x(\Delta)] = \mathbf{E}[X\Phi(\Delta)]$$

$$= X\mathbf{E}[\Phi(\Delta)]$$

$$= X(1 \ 0 \cdots 0)^{T}$$

$$= x_{0}$$

Also

$$\mathsf{E}\left[oldsymbol{x}(oldsymbol{\Delta})
ight] = \mathsf{E}\left[oldsymbol{\Phi}^T \otimes oldsymbol{I}_nig)oldsymbol{x}_{pc} = \left(oldsymbol{F}^T \otimes oldsymbol{I}_n
ight)oldsymbol{x}_{pc}
ight]$$

where $F^T = (1 \ 0 \ \cdots \ 0)$.

Computation of Variance

Given
$$\boldsymbol{x}(\boldsymbol{\Delta}) := \boldsymbol{X} \boldsymbol{\Phi}(\boldsymbol{\Delta})$$

$$\boldsymbol{x}(\boldsymbol{\Delta}) \boldsymbol{x}^T(\boldsymbol{\Delta}) = \boldsymbol{X} \boldsymbol{\Phi}(\boldsymbol{\Delta}) \boldsymbol{\Phi}^T(\boldsymbol{\Delta}) \boldsymbol{X}^T$$

$$\mathbf{E} \left[\boldsymbol{x}(\boldsymbol{\Delta}) \boldsymbol{x}^T(\boldsymbol{\Delta}) \right] = \mathbf{E} \left[\boldsymbol{X} \boldsymbol{\Phi}(\boldsymbol{\Delta}) \boldsymbol{\Phi}^T(\boldsymbol{\Delta}) \boldsymbol{X}^T \right]$$

$$= \boldsymbol{X} \mathbf{E} \left[\boldsymbol{\Phi}(\boldsymbol{\Delta}) \boldsymbol{\Phi}^T(\boldsymbol{\Delta}) \right] \boldsymbol{X}^T$$

$$= \boldsymbol{X} \begin{bmatrix} \langle \phi_0, \phi_0 \rangle & 0 & \dots & 0 \\ 0 & \langle \phi_1, \phi_1 \rangle & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \langle \phi_N, \phi_N \rangle \end{bmatrix} \boldsymbol{X}^T$$

$$= \boldsymbol{X} \boldsymbol{W} \boldsymbol{X}^T$$

Then

$$\mathbf{Var}\left[oldsymbol{x}
ight] := \mathsf{E}\left[\left(oldsymbol{x} - \mathsf{E}\left[oldsymbol{x}
ight]
ight)\left(oldsymbol{x} - \mathsf{E}\left[oldsymbol{x}
ight]
ight)^T
ight] = oldsymbol{X}(oldsymbol{W} - oldsymbol{F}oldsymbol{F}^T)oldsymbol{X}^T$$

Computation of Statistics – summary

Mean

$$\mathsf{E}\left[\boldsymbol{x}\right] = \boldsymbol{X}\boldsymbol{F} = \boldsymbol{x}_0$$

Variance

$$\operatorname{Var}[x] = X(W - FF^T)X^T$$

where

$$\boldsymbol{F} = \mathbf{E} \left[\boldsymbol{\Phi}(\boldsymbol{\Delta}) \right] = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \boldsymbol{W} = \mathbf{E} \left[\boldsymbol{\Phi} \boldsymbol{\Phi}^T \right] = \begin{bmatrix} \langle \phi_0, \phi_0 \rangle & 0 & \dots & 0 \\ 0 & \langle \phi_1, \phi_1 \rangle & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \langle \phi_N, \phi_N \rangle \end{bmatrix}$$

Polynomial Nonlinearity

Polynomials $x^n(\Delta)$, $x \in \mathbb{R}$ can be written as

$$x^{n}(\boldsymbol{\Delta}) = (\boldsymbol{X}\boldsymbol{\Phi}(\boldsymbol{\Delta}))^{n}$$
$$\langle x^{n}(\boldsymbol{\Delta}), \phi_{i}(\boldsymbol{\Delta}) \rangle = \langle (\boldsymbol{X}\boldsymbol{\Phi}(\boldsymbol{\Delta}))^{n}, \phi_{i} \rangle$$
$$= \sum_{i_{1}=0}^{N} \cdots \sum_{i_{n}=0}^{N} x_{i_{1}} \cdots x_{i_{n}} \langle \phi_{i_{1}} \cdots \phi_{i_{n}}, \phi_{i} \rangle$$

- Essentially integration of polynomials
 - analytical or numerical (exact).
- Inner product $\langle \phi_{i_1} \cdots \phi_{i_m}, \phi_i \rangle$
 - ► can be computed offline
 - stored in sparse, symmetric tensor

Rational polynomials

Functions such as $\frac{x^n(\Delta)}{y^m(\Delta)}$, $x,y\in\mathbb{R}$ can be approximated as

$$z(\mathbf{\Delta}) = \frac{x^{n}(\mathbf{\Delta})}{y^{m}(\mathbf{\Delta})}$$

$$Z\mathbf{\Phi}(\mathbf{\Delta}) = \frac{(X\mathbf{\Phi}(\mathbf{\Delta}))^{n}}{(Y\mathbf{\Phi}(\mathbf{\Delta}))^{m}}$$

$$(Y\mathbf{\Phi})^{m} Z\mathbf{\Phi} = (X\mathbf{\Phi})^{n}$$

$$\langle (Y\mathbf{\Phi})^{m} Z\mathbf{\Phi}, \phi_{i}) \rangle = \langle (X\mathbf{\Phi})^{n}, \phi_{i} \rangle, \quad i = \{0, 1, \dots, N\}$$

Given X,Y solve system of linear equations to obtain Z

$$\begin{bmatrix} \left\langle \boldsymbol{\Phi}^T \otimes (\boldsymbol{Y}\boldsymbol{\Phi})^m, \phi_0 \right\rangle \\ \vdots \\ \left\langle \boldsymbol{\Phi}^T \otimes (\boldsymbol{Y}\boldsymbol{\Phi})^m, \phi_N \right\rangle \end{bmatrix} \boldsymbol{z}_{pc} = \begin{pmatrix} \langle (\boldsymbol{X}\boldsymbol{\Phi})^n, \phi_0 \rangle \\ \vdots \\ \langle (\boldsymbol{X}\boldsymbol{\Phi})^m, \phi_N \rangle \end{pmatrix} \text{Polynomial integrations}$$

Transcendental Functions

Let f(x) be a transcendental function:

 \blacksquare e.g. $x^a, e^x, x^{1/x}, \log(x), \sin(x), \text{ etc.}$

Use Taylor series expansion about mean

- Define $x := x_0 + d$, d is deviation from mean x_0
- Expand

$$f(x) = f(x_0 + d) = f(x_0) + f'(x_0)d + f''(x_0)\frac{d^2}{2!} + \cdots$$

■ Therefore

$$\langle f(x(\boldsymbol{\Delta})), \phi_i(\boldsymbol{\Delta}) \rangle \approx f(x_0) \langle 1, \phi_i \rangle + f'(x_0) \langle d, \phi_i \rangle + \frac{f''(x_0)}{2!} \langle d^2, \phi_i \rangle + \cdots$$

Transcendental Functions (contd.)

Taylor Series Approximation

$$\langle f(x(\boldsymbol{\Delta})), \phi_i(\boldsymbol{\Delta}) \rangle \approx f(x_0)\langle 1, \phi_i \rangle + f'(x_0)\langle d, \phi_i \rangle + \frac{f''(x_0)}{2!}\langle d^2, \phi_i \rangle + \cdots$$

- $\blacksquare \langle d^n, \phi_i \rangle$ is integration of polynomials
- Straightforward
- Computationally efficient
- Severe inaccuracies for higher order PC approximations

Remedies

- \blacksquare Approximate f(x) using polynomials, piecewise polynomials
- Non-intrusive: multi-dimensional integrals via sampling, tensor-product quadrature, Smolyak sparse grid, or cubature
- **Regression Approach**: \mathcal{L}_2 optimization

Example: First Order Linear System

Dvnamics:

$$\dot{x} = -a(\Delta)x,$$

$$a \in \mathcal{U}_{[0,1]}$$

Analytical Statistics:

$$\bar{x}(t) = \frac{1 - e^{-t}}{t}, \qquad \sigma(t) = \frac{1 - e^{-2t}}{2t} - \left(\frac{1 - e^{-t}}{t}\right)^2$$

Figure: Errors in estimates obtained from gPC for $\dot{x}=-a(\Delta)x$. Analytical: (red solid); gPC: 2^{nd} order(*), 3^{rd} order(o), $5^{th}(+)$.

Errors Due to Finite Terms

Dynamics:

$$\dot{x} = -a(\Delta)x, \qquad a \in \mathcal{U}_{[0,1]}$$

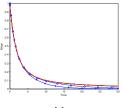
Analytical Solution:

$$x(t, \Delta) = x(t_0)e^{-a(\Delta)t}$$

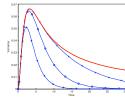
PC Solution:

$$\hat{x}(t,\Delta) = \sum_{i=0}^{P} x_i(t)\phi_i(\Delta)$$

Error: Finite term approximation of exponential.



(a) Mean



(b) Variance

Example: Eigen Analysis – Linear F-16 Aircraft

$$A(\boldsymbol{\Delta}) = \begin{bmatrix} 0.1658 & -13.1013 & -7.2748(1+0.2\Delta) & -32.1739 & 0.2780 \\ 0.0018 & -0.1301 & 0.9276(1+0.2\Delta) & 0 & -0.0012 \\ 0 & -0.6436 & -0.4763 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

- Linearized about flight condition $V = 160 \ ft/s$ and $\alpha = 35^o$
- Uncertainty due to damping term C_{xa}
- Difficult to model at high angle of attack
- 20% uncertainty about nominal

Example: Eigen Analysis – Linear F-16 Aircraft

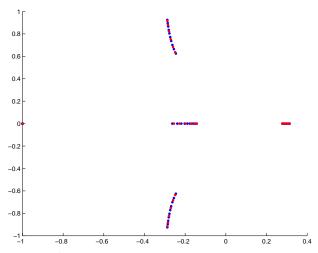


Figure: 5th Order PC ODE Eigen Values, Sampled ODE Eigen Values

Example: Eigen Analysis – Linear F-16 Aircraft

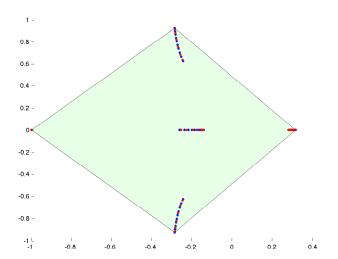
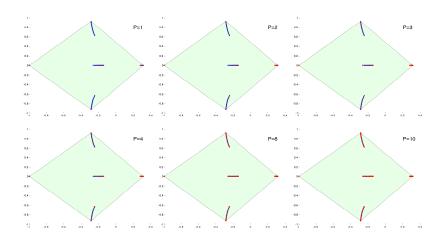


Figure: PC eigen values bounded by convex hull of sampled ODE eigen values (conservative!)*

Eigenvalues of the Jacobian of a Galerkin-Projected Uncertain ODE System, Sonday, et al.

Example: Spread of Spectrum – Linear F-16 Aircraft



Better characterization of spectrum spread is needed.

Example: Nonlinear System – Lorenz Attractor

Dvnamics:

$$\dot{x} = \sigma(y - x),$$
 $\dot{y} = x(\rho - z) - y,$ $\dot{z} = xy - \beta z.$

Initial Condition:

$$\left[x,y,z\right]^T = \left[1.50887, -1.531271, 25.46091\right]^T$$

Parameters:

$$\sigma = 10(1 + 0.1\Delta_1), \quad \rho = 28(1 + 0.1\Delta_2), \quad \beta = 8/3, \quad \Delta \in \mathcal{U}_{[-1,1]^2}.$$

$$\begin{split} x(t, \Delta) &\approx \sum_{i=0}^{P} x_i(t) \phi_i(\Delta) & \langle \phi_k^2 \rangle \dot{x}_k(t) = \sum_{i=0}^{P} \langle \sigma \phi_i \phi_k \rangle (y_i - x_i) \\ y(t, \Delta) &\approx \sum_{i=0}^{P} y_i(t) \phi_i(\Delta) & \langle \phi_k^2 \rangle \dot{y}_k(t) = \sum_{i=0}^{P} \langle \rho \phi_i \phi_k \rangle x_i - \sum_{i=0}^{P} \sum_{j=0}^{P} \langle \phi_i \phi_j \phi_k \rangle x_i z_j - \langle \phi_k^2 \rangle y_k \\ z(t, \Delta) &\approx \sum_{i=0}^{P} z_i(t) \phi_i(\Delta) & \langle \phi_k^2 \rangle \dot{z}_k(t) = \sum_{i=0}^{P} \sum_{j=0}^{P} \langle \phi_i \phi_j \phi_k \rangle x_i y_j - \beta \langle \phi_k^2 \rangle z_k \end{split}$$

Example: Nonlinear System – Lorenz Attractor

Integrals:

$$\langle \phi_k(\Delta)^2 \rangle$$

$$\langle \sigma(\Delta)\phi_i(\Delta)\phi_k(\Delta) \rangle$$

$$\langle \rho(\Delta)\phi_i(\Delta)\phi_k(\Delta) \rangle$$

$$\langle \phi_i(\Delta)\phi_j(\Delta)\phi_k(\Delta) \rangle$$

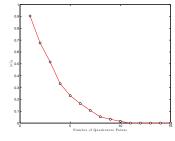


Figure: Error - Analytical vs Numerical Integration

- analytical
- numerical
 - non intrusive (blackbox)
 - quadratures defined by roots of $\phi_N(\cdot)$
 - tensor product of univariate quadratures
 - ► Here we use 7th order PC approximation
 - ► Highest order polynomial integrated is 21 in $\langle \phi_i(\boldsymbol{\Delta}) \phi_i(\boldsymbol{\Delta}) \phi_k(\boldsymbol{\Delta}) \rangle$
 - ightharpoonup N=11 will exactly integrate polynomials of order < 22.i.e.

$$\langle \phi_i(\Delta)\phi_j(\Delta)\phi_k(\Delta)\rangle = \sum_r w_r \phi_i(\Delta_r)\phi_j(\Delta_r)\phi_k(\Delta_r)$$

- Approximate for non polynomial integrands
- Multidimensional moments can be computed efficiently from products of one dimensional moments

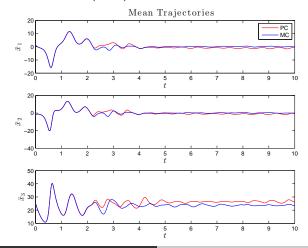
Example: Nonlinear System – Lorenz Attractor

MC: 1000 samples

PC: 7^{th} order approximation

■ using MATLAB rand(...)

36 basis functions



Stochastic Collocation

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Basic Idea

- Sample domain \mathcal{D}_{Δ} suitably
 - ▶ roots of basis functions $\phi(\Delta)$ same as Galerkin projection
 - ► multi-dimension samples ⇔ tensor product of roots or sparse grid
- Enforce stochastic dynamics at each sample point
 - ► Time varying coefficient at each sample point
- Interpolate (Lagrangian) for intermediate points

Algorithm

1. Given stochastic dynamics with uncertainty Δ

$$\dot{\boldsymbol{x}} = f(\boldsymbol{x}, \boldsymbol{\Delta})$$

- 2. For p^{th} order approximation:
 - ▶ sample domain \mathcal{D}_{Δ} with roots of p+1 order polynomial
 - ► tensor grid, sparse grid, etc.
 - ightharpoonup samples $\Delta := \{\Delta_i\}, i = 0, \cdots, p$.
- 3. Coefficient x_i evolves according to

$$\dot{oldsymbol{x}}_i = f(oldsymbol{x}_i, oldsymbol{\Delta}_i),$$
 deterministic solution

4. Approximate stochastic solution $\hat{x}(t, \Delta) := \sum_{i=1}^{n} \hat{x}_i(t, \Delta)$

$$\hat{\boldsymbol{x}}(t, \boldsymbol{\Delta}) := \sum_{i=0} \boldsymbol{x}_i(t) L_i(\boldsymbol{\Delta})$$

 L_i are Lagrangian interpolants $L_i(y) = \prod_{j=0, j \neq i}^p \frac{y-y_j}{y_i-y_j}$.

Computation of Statistics

Mean

$$\mathbf{E}\left[oldsymbol{x}(t)
ight]pprox\mathbf{E}\left[\sum_{i=0}^{p}oldsymbol{x}_{i}(t)L_{i}(oldsymbol{\Delta})
ight]=\sum_{i=0}^{p}oldsymbol{x}_{i}(t)\mathbf{E}\left[L_{i}(oldsymbol{\Delta})
ight]$$

- Computation of $\mathbf{E}[L_i(\mathbf{\Delta})]$ involves high-dimensional polynomial integration
 - analytical
 - numerical: quadratures, sparse grids, etc
- Higher order statistics: similar to computation of mean.

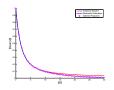
Example: Linear First Order System

Dynamics:

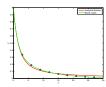
$$\dot{x} = -a(\Delta)x, \qquad a \in \mathcal{U}_{[0,1]}$$

Analytical Statistics:

$$\bar{x}(t) = \frac{1 - e^{-t}}{t},$$



(a) MC (3 samples)



Example: Nonlinear System – Lorenz Attractor

Dynamics:

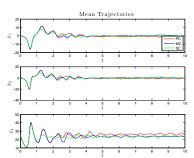
$$\dot{x} = \sigma(y - x),$$
 $\dot{y} = x(\rho - z) - y,$ $\dot{z} = xy - \beta z.$

Initial Condition:

$$[x, y, z]^T = [1.50887, -1.531271, 25.46091]^T$$

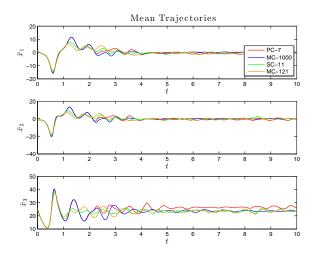
Parameters:

$$\sigma = 10(1 + 0.1\Delta_1), \quad \rho = 28(1 + 0.1\Delta_2), \quad \beta = 8/3, \quad \Delta \in \mathcal{U}_{[-1,1]^2}.$$



- MC: 1000 samples
 - ▶ using MATLAB rand(...)
- SC: 11 quadrature points
 - ► same as 7th order PC
 - ▶ 121 grid points in 2D
- SC performance is poor for nonlinear systems!

Example: Nonlinear System – Lorenz Attractor



SC performance is poor for nonlinear systems! But, better than MC with same sample budget.

Karhunen-Loève Expansion

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Basic Idea

Given a random process $X(t,\omega) := \{X_t(\omega)\}_{t \in [t_1,t_2]}$

- $X_t(\omega) \in \mathcal{L}_2(\Omega, \mathcal{F}, P)$ finite second moment $\mathcal{L}_2(\Omega, \mathcal{F}, P) := \{X : \Omega \mapsto \mathbb{R} : \int_{\Omega} |X(\omega)|^2 dP(\omega) < \infty\}$
- Auto Correlation

$$R_X(t_1, t_2) := \mathbf{E}[X_{t_1} X_{t_2}]$$

Auto Covariance

$$C_X(t_1,t_2) := R_X(t_1,t_2) - \mu_{t_1}\mu_{t_2} \ = R_X(t_1,t_2) - \mu^2$$
 stationary

lacksquare $C_X(t_1,t_2)$ is bounded, symmetric and positive definite, thus

$$C_X(t_1,t_2) = \sum_{i=0}^{\infty} \lambda_i f_i(t_1) f_i(t_2)$$
 spectral decomposition

where λ_i and $f_i(\cdot)$ are eigenvalues and eigenvectors of the covariance kernel.

Eigenvalues and Eigenfunctions

 \blacksquare λ_i and $f_i(\cdot)$ are solutions of

$$\int_{\mathcal{D}} C_X(t_1,t_2)\,f_i(t)\,dt_1 = \lambda_i\,f_i(t_2), \text{Fredholm integral equation of second kind}$$
 with
$$\int_{\mathcal{D}} f_i(t)f_j(t)dt = \delta_{ij}.$$

■ Write $X(t,\omega) := \bar{X}(t) + Y(t,\omega)$, where

$$Y(t,\omega) \stackrel{m.s.}{=} \sum_{i=0}^{\infty} \xi_i(\omega) \sqrt{\lambda_i} \, f_i(t), \text{ and } \xi_i(\omega) = \frac{1}{\lambda_i} \int_{\mathcal{D}} Y(t,\omega) f_i(t) dt.$$

- Reproducing Kernel Hilbert Space
 - Congruence between two Hilbert spaces!
 - $\{f_i(t)\} \mapsto X(t,\omega)$ or equivalently
 - \blacktriangleright $\{f_i(t)\} \mapsto \{\xi_i(\omega)\}\$

Solution of Integral Equation

■ Homogeneous Fredholm integral equation of the second kind,

$$\int_{\mathcal{D}} C_X(t_1,t_2) \, f_i(t) \, dt_1 = \lambda_i \, f_i(t_2)$$
 well studied problem

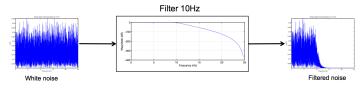
- $C_X(t_1,t_2)$ is bounded, symmetric, and positive definite, implies
 - 1. The set $f_i(t)$ of eigenfunctions is orthogonal and complete.
 - 2. For each eigenvalue λ_k , there correspond at most a finite number of linearly independent eigenfunctions.
 - 3. There are at most a countably infinite set of eigenvalues.
 - 4. The eigenvalues are all positive real numbers.
 - 5. The kernel $C_X(t_1,t_2)$ admits of the following uniformly convergent expansion

$$C_X(t_1, t_2) = \sum_{i=0}^{\infty} \lambda_i f_i(t_1) f_i(t_2)$$

Applicable to wide range of processes

Rational Spectra: Special Case

- 1D random process
- Stationary output of a linear filter, excited by white noise



■ Spectral density of the form $S(s^2) = H(j\omega)H(-j\omega) = \frac{N(s^2)}{D(s^2)}$

N and D are polynomials in s^2 such that

$$\int_{-\infty}^{\infty} S(-\omega^2) d\omega < \infty$$

 $s=j\omega$, here ω is frequency

- ▶ Degree of $D(s^2)$ must exceed degree of $N(s^2)$ by at least two.
- ▶ No roots of $D(s^2)$ on the imaginary axis
- $S(\omega) \ge 0$, \Rightarrow purely imaginary zeros of $N(s^2)$ of even multiplicity
- Finite dimensional Markovian process
 - ▶ effect of infinite past on the present is negligible

Important Kernel

Study specific kernel

$$C_X(t_1, t_2) = e^{-c|t_1 - t_2|}$$

1/c is the correlation time or length.

- Many applications.
- Other kernels also possible

Solve integral equation

$$\int_{\mathcal{D}} C_X(t_1, t_2) f_i(t) dt_1 = \lambda_i f_i(t_2).$$

Or equivalently solve

ODE:
$$\ddot{f}(t) + \omega^2 f(t) = 0$$
, $\omega^2 = \frac{2c - c^2 \lambda}{\lambda}$, $-a \le t \le a$

Boundary Condition: $cf(a) + \dot{f}(a) = 0$, $cf(-a) - \dot{f}(-a) = 0$.

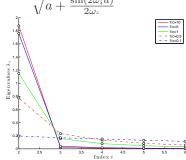
Basis Functions

Equivalently solve for ω , ω^*

Odd i

$$c - \omega \tan(\omega a) = 0, \quad \lambda_i = \frac{2c}{\omega_i^2 + c^2}$$

$$f_i(t) = \frac{\cos(\omega_i t)}{\sqrt{a + \frac{\sin(2\omega_i a)}{2\omega_i}}}$$

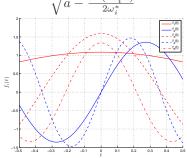


(a) Eigenvalues

Even i

$$c - \omega \tan(\omega a) = 0, \quad \lambda_i = \frac{2c}{\omega_i^2 + c^2} \quad \omega^* + c \tan(\omega^* a) = 0, \quad \lambda_i^* = \frac{2c}{\omega_i^{*2} + c^2}$$

$$f_i^*(t) = \frac{\sin(\omega_i^* t)}{\sqrt{a - \frac{\sin(2\omega_i^* a)}{2\omega_i^*}}}$$



(b) Eigenfunctions

Coefficients

Recall
$$X(t,\omega) := \bar{X}(t) + Y(t,\omega)$$
,

$$Y(t,\omega) \stackrel{m.s.}{=} \sum_{i=0}^{\infty} \xi_i(\omega) \sqrt{\lambda_i} f_i(t)$$
$$= \sum_{i=0}^{\infty} \left[\xi_i(\omega) \sqrt{\lambda_i} f_i(t) + \xi_i^*(\omega) \sqrt{\lambda_i^*} f_i^*(t) \right]$$

- \bullet $\xi_i(\omega), \xi_i^*(\omega)$ are uncorrelated random variables determined from $Y(t,\omega)$
- \bullet $\xi_i(\omega), \xi_i^*(\omega)$ model the distribution of amplitude of $Y(t,\omega)$
- \bullet $f_i(t), f_i^*(t)$ models the distribution of signal power over time or among frequencies

If $Y(t,\omega)$ is a Gaussian process

- \blacksquare $\xi_i(\omega), \xi_i^*(\omega)$ Gaussian independent random variables
- KL expansion is almost surely convergent

UQ Application

Dynamical system with process noise $n(t,\omega)$

$$\dot{x} = f(t, \Delta, x) + n(t, \omega)$$

Replace

$$n(t,\omega) \approx \sum_{i=0}^{N} \left[\xi_i(\omega) \sqrt{\lambda_i} f_i(t) + \xi_i^*(\omega) \sqrt{\lambda_i^*} f_i^*(t) \right]$$

Define new parameter vector

$$\mathbf{\Delta}' := \left(\mathbf{\Delta}^T, \xi_0, \xi_0^*, \cdots, \xi_N, \xi_N^*\right)^T$$

Rewrite dynamics as

$$\dot{x} = F(t, \Delta', x),$$

Process noise converted to parametric uncertainty.

- Use PC, SC, or simplified FPK equation to determine $x(t, \Delta')$
- Increases number of parameters ⇒ increases computational complexity

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- 2. A. Prabhakar and R. Bhattacharya, Analysis of Hypersonic Flight Dynamics with Probabilistic Uncertainty in System Parameters, AIAA GNC 2008.
- 3. A. Prabhakar, J. Fisher, R. Bhattacharva, Polynomial Chaos Based Analysis of Probabilistic Uncertainty in Hypersonic Flight Dynamics, AIAA Journal of Guidance, Control, and Dynamics, Vol.33 No.1 (222-234), 2010.
- 4. J. Fisher, R. Bhattacharya, Optimal Trajectory Generation with Probabilistic System Uncertainty Using Polynomial Chaos, Journal of Dynamic Systems, Measurement and Control, volume 133, Issue 1, January 2011.
- 5. J. Fisher, R. Bhattacharya, Linear Quadratic Regulation of Systems with Stochastic Parameter Uncertainties, Automatica, 2009.
- 6. Roger G. Ghanem. Pol D. Spanos, Stochastic Finite Elements: A Spectral Approach. Revised Edition (Dover Civil and Mechanical Engineering
- 7. Olivier Le Maitre, Omar M Knio, Spectral Methods for Uncertainty Quantification: With Applications to Computational Fluid Dynamics, Scientific Computation.
- 8. Dongbin Xiu, Numerical Methods for Stochastic Computations: A Spectral Method Approach, ISBN: 9780691142128, Princeton Press.