Uncertainty Quantification Methods with Applications

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Outline

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1. Polynomial Chaos
2. Stochastic Collocation

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1. **Polynomial Chaos**
2. **Stochastic Collocation**
3. **Karhunen-Loève**
4. **Applications**
   - Electromagnetics
   - Hydropower

Motivating Applications

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- Electromagnetic interrogation

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To solve problems and make informed decisions we need to both quantify these input uncertainties, and quantify the effect on the outputs of the models, usually expected values and variances.

Popular UQ Methods

- Polynomial Chaos [Wiener, 1938; Xiu, PhD Dissertation, 2004]

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- Karhunen-Loève expansion [Kosambi, 1943; Karhunen, 1947]

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- Stochastic Collocation [Tatang, PhD Dissertation, 1994]
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- Karhunen-Loève expansion [Kosambi, 1943; Karhunen, 1947]
  - Principal component analysis for functions

Outline

Polynomial Chaos: Simple example

Consider the first order, constant coefficient, linear ODE

$$\dot{y} = -ky, \quad k = k(\xi) = \xi, \quad \xi \sim \mathcal{N}(0,1).$$

We apply a Polynomial Chaos expansion in terms of orthogonal Hermite polynomials H_j to the solution y:

$$y(t,\xi) = \sum_{j=0}^{\infty} \alpha_j(t)\phi_j(\xi), \quad \phi_j(\xi) = H_j(\xi).$$

The Hermite polynomials H_j's are orthogonal with respect to the weighting function given by the probability density function of the Gaussian random variable. I.e., define the weighted inner product

$$\langle f, g \rangle_W = \int_\Gamma f(\xi)g(\xi)W(\xi)d\xi.$$

then

$$\langle \phi_j, \phi_i \rangle_W = \langle \phi_i, \phi_i \rangle_W \delta_{ij}.$$

- Why orthogonal?
  To allow the coefficients of the expansion to be easily computed using a projection.
- Why wrt Gaussian density?
  So that

$$\mathbb{E}[y] := \int_{\Gamma} y(t,\xi)W(\xi)d\xi = \langle y, 1\rangle_W = \alpha_0(t).$$

and variance is $\alpha_1^2 + \alpha_2^2 + \ldots + \alpha_p^2$.

Triple recursion formula

Then the ODE $\dot{y} = -\xi y$ becomes

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\phi_j(\xi) = -\sum_{j=0}^{\infty} \alpha_j(t)\xi\phi_j(\xi).$$

We can eliminate the explicit dependence on ξ by using the triple recursion relation for Hermite polynomials

$$\xi H_j = jH_{j-1} + H_{j+1}.$$

Thus

$$\sum_{j=0}^{\infty} \dot{\alpha}_j\ \phi_j + \alpha_j\ (j\phi_{j-1} + \phi_{j+1}) = 0.$$

Galerkin Projection onto span($\{\phi_i\}_{i=0}^{p}$)

To get a finite dimensional approximation,

$$y(t,\xi) \approx \sum_{j=0}^{p} \alpha_j(t)\phi_j(\xi) =: y^p(t,\xi),$$

we take the weighted inner product of the ODE with each basis function corresponding to $i = 0, \ldots, p$

$$\sum_{j=0}^{\infty} \dot{\alpha}_j(t)\langle \phi_j, \phi_i \rangle_W + \alpha_j(t)(j\langle \phi_{j-1}, \phi_i \rangle_W + \langle \phi_{j+1}, \phi_i \rangle_W) = 0.$$

Using orthogonality, $\langle \phi_j, \phi_i \rangle_W = \langle \phi_i, \phi_i \rangle_W \delta_{ij}$, we have simply

$$\dot{\alpha}_i \langle \phi_i, \phi_i \rangle_W + (i+1)\alpha_{i+1}\langle \phi_i, \phi_i \rangle_W + \alpha_{i-1}\langle \phi_i, \phi_i \rangle_W = 0, \quad i = 0, \ldots, p,$$

(let $\alpha_{-1}(t)$ and $\alpha_{p+1}(t)$ be identically zero).

Deterministic ODE system

Letting $\vec{\alpha}$ represent the vector containing $\alpha_0(t), \ldots, \alpha_p(t)$ the (modal) system of ODEs can be written

$$\dot{\vec{\alpha}} + M\vec{\alpha} = \vec{0},$$

with

$$M = \begin{bmatrix} 0 & 1 & & & \\ 1 & 0 & 2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & p \\ & & & 1 & 0 \end{bmatrix}$$

Generalizations

For any choice of family of orthogonal polynomials, there exists a triple recursion formula. Given the arbitrary relation

$$\xi\phi_j = a_j\phi_{j-1} + b_j\phi_j + c_j\phi_{j+1}$$

(with $\phi_{-1} = 0$) then the matrix above becomes

$$M = \begin{bmatrix} b_0 & a_1 & & & \\ c_0 & b_1 & a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & a_p \\ & & & c_{p-1} & b_p \end{bmatrix}$$

Generalized Polynomial Chaos

Table: Popular distributions and corresponding orthogonal polynomials.

Distribution	Polynomial	Support
Gaussian	Hermite	$(-\infty, \infty)$
gamma	Laguerre	$[0, \infty)$
beta	Jacobi	$[a, b]$
uniform	Legendre	$[a, b]$

Note: other random variables may be approximated by a non-linear function (e.g., Taylor expansion) of one of these random variables.

Spectral convergence

- Any set of orthogonal polynomials can be used in the truncated expansion, but there may be an optimal choice.
- If the polynomials are orthogonal with respect to weighting function $W(\xi)$, and k has PDF $W(k)$, then it can be shown that the PC solution converges exponentially in terms of p.
- In practice, approximately 4 are generally sufficient.

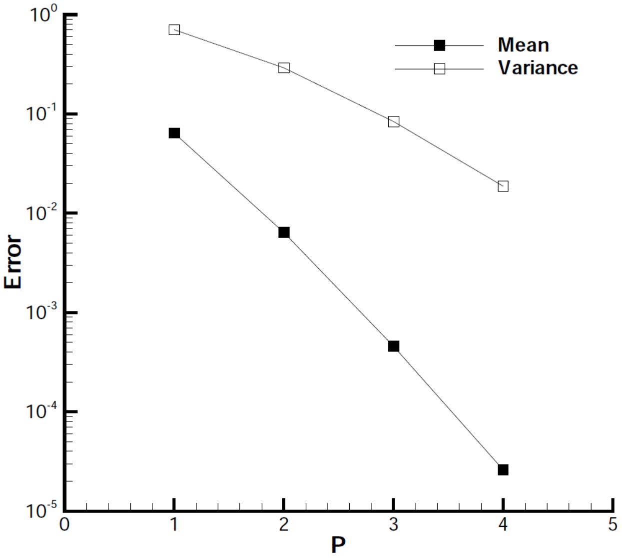

Figure: Error with Gaussian random variable by Hermitian Chaos [Xiu].

More Generalizations [McKenzie]

Consider the non-homogeneous ODE

$$\dot{y} + ky = g(t), \quad k = k(\xi) = \sigma\xi + \mu,$$

then

$$\dot{\alpha}_i + \sigma\left[(i+1)\alpha_{i+1} + \alpha_{i-1}\right] + \mu\alpha_i = g(t)\delta_{0i}, \quad i = 0, \ldots, p,$$

or the deterministic ODE system

$$\dot{\vec{\alpha}} + (\sigma M + \mu I)\vec{\alpha} = g(t)\vec{e_1}.$$

Note: eigenvalues of the $(p+1) \times (p+1)$ Jacobi matrix M are roots of the $p+1$ degree orthogonal polynomial.

Example

Consider the ODE

$$\dot{y} + ky = 0, \quad y(0) = 1, \quad k \sim \mathcal{U}[0,2].$$

We apply Legendre Chaos expansions with $p = 2$ to arrive at the modal system

$$\dot{\vec{\alpha}} + A\vec{\alpha} = \vec{0}, \qquad \vec{\alpha}(0) = [1,0,0]^T$$

where

$$A = (\sigma M + \mu I) = \begin{bmatrix} 1 & \frac{1}{3} & 0 \\ 1 & 1 & \frac{2}{5} \\ 0 & \frac{2}{3} & 1 \end{bmatrix}$$

which has eigenvalues 1.7746, 1, and 0.2254.
Diagonalizing A we can find the modal solutions, for instance,
$\alpha_0 = 0.2778 \exp(-1.7746\ t) + 0.4444 \exp(-t) + 0.2778 \exp(-0.2254\ t)$.

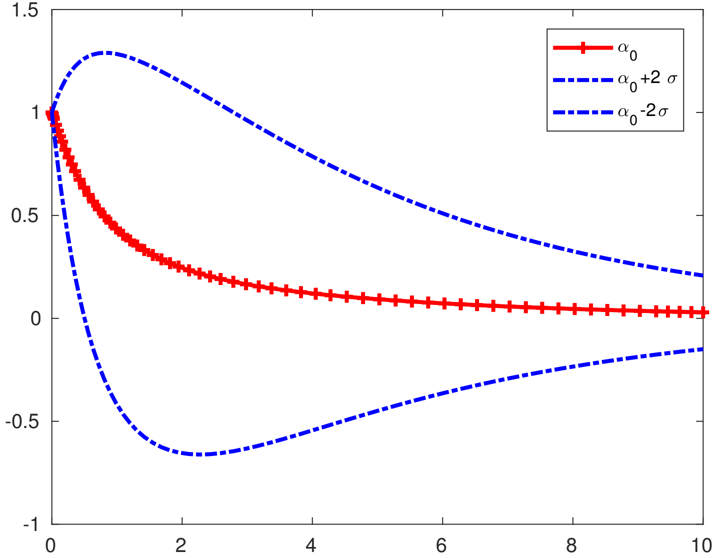

Figure: Mean and confidence intervals using $p = 2$.

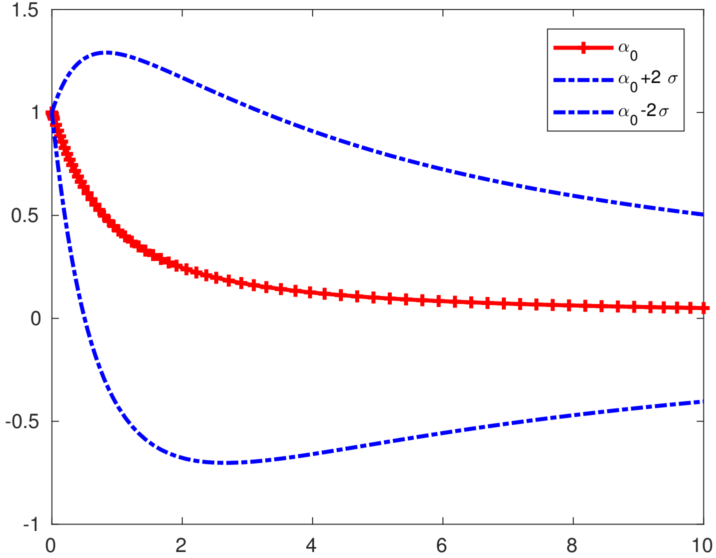

Figure: Mean and confidence intervals using $p = 20$.

Outline

Intrusive vs Non-intrusive

Each gPC expansion coefficient can be represented via a projection

$$\alpha_i(t) = \mathbb{E}[y(t,\vec{\xi})\phi_i(\vec{\xi})] = \int_\Gamma y(t,\vec{\xi})\phi_i(\vec{\xi})W(\vec{\xi})d\vec{\xi}.$$

- $\Gamma = \prod_{k=1}^N \Gamma_k$, $\Gamma_k = \xi_k(\Omega)$, where $(\Omega, \mathcal{F}, P)$ is a probability space
- $W(\vec{\xi})$ is a joint probability density of the random vector $\vec{\xi}$

The Polynomial Chaos method finds the coupled DE system for these coefficients, but this is *intrusive* as it changes the system we would like to solve (not good if we wish to reuse code from deterministic simulations).

Instead, the computation of the coefficients α_i, $i = 0, \ldots, p$ can be done *non-intrusively* with the use of the stochastic collocation method.

Stochastic Collocation and gPC

- Choose a set of collocation points $\mathbf{z}_j = (z_{j,1}, z_{j,2}, \ldots, z_{j,N}) \in \Gamma$ and weights w_j, $j = 1, \ldots, N_{cp}$.

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- Approximate the gPC expansion coefficients using Gaussian Quadrature

$$\alpha_i(t) = \mathbb{E}[y(t,\vec{\xi})\phi_i(\vec{\xi})] = \int_\Gamma y(t,\vec{\xi})\phi_i(\vec{\xi})W(\vec{\xi})d\vec{\xi} \approx \sum_{j=1}^{N_{cp}} w_j y(t,\mathbf{z}_j)\phi_i(\mathbf{z}_j).$$

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- Construct the N-variate, pth-order gPC approximation, if necessary

$$y^p(t,\vec{\xi}) = \sum_{i=0}^{M_p} \alpha_i(t)\phi_i(\vec{\xi}). \tag{1}$$

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$$y^p(t,\vec{\xi}) = \sum_{i=0}^{M_p} \alpha_i(t)\phi_i(\vec{\xi}). \tag{1}$$

- Or just use $\mathbb{E}[y(t,\vec{\xi})] \approx \alpha_0(t) \approx \sum_{j=1}^{N_{cp}} w_j y(t,\mathbf{z}_j)$, $\quad \mathrm{Var}[y(t,\vec{\xi})] \approx \sum_{i=1}^{M_p} \alpha_i(t)^2.$

Back to Example

Consider again the ODE

$$\dot{y} + ky = 0, \quad y(0) = 1, \quad k \sim \mathcal{U}[0,2].$$

Look up the Gauss-Legendre weights and nodes online for $N_{cp} = 3$ (they are actually just the roots of the 3rd degree Legendre polynomial):
$x_j \in \{0, \pm\sqrt{\frac{3}{5}}\}$ with weights $\frac{8}{9}$ and $\frac{5}{9}$.

Note that these are for $x \in [-1,1]$ and $W(x) = 1$. Need to shift and scale to get:
$z_j \in \{1.7746, 1, 0.2254\}$ with weights 0.2778, 0.4444 and 0.2778.

Thus, we have
$\alpha_0 = 0.2778 \exp(-1.7746\ t) + 0.4444 \exp(-t) + 0.2778 \exp(-0.2254\ t)$.

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In the case when the random coefficients, or more likely, the random forcing, are time varying, we seek a representation of these stochastic processes in terms of standard random variables so that we may apply gPC or SC methods.

Consider the case when all that is known about a random forcing process $Y_t(\omega)$ is its mean $\mu_Y(t)$ and its covariance function $C(t,s) = cov(Y_t, Y_s)$. Then the Karhunen-Loève expansion is given by

$$Y_t(\omega) = \mu_Y(t) + \sum_{i=1}^{\infty} \sqrt{\lambda_i}\, \psi_i(t)\, \xi_i$$

where the eigenpair (λ_i, ψ_i) solve the eigenvalue problem

$$\int_{\mathcal{T}} C(t,s)\, \psi_i(s) ds = \lambda_i\, \psi_i(t), \quad t \in \mathcal{T}$$

and $\{\xi_i\}$ are mutually uncorrelated zero-mean, unit-variance random variables.

Often the eigenvalues decay exponentially (faster for larger correlation length), thus justifying a truncated expansion as an approximation

$$Y_t(\omega) = \mu_Y(t) + \sum_{i=1}^{d} \sqrt{\lambda_i}\ \psi_i(t)\ \xi_i.$$

Since the computational complexity of gPC and SC grows exponentially with the dimension of the random space, we want as few random variables as possible.

One can show that of all the d dimensional expansions, KL is the best (minimizes means square error).

The total variance of the process is the sum of the eigenvalues, so we can estimate the error in the truncation at d by computing the percentage

$$\frac{\lambda_{d+1}}{\sum_{i=1}^{d+1} \lambda_i}.$$

Example

The covariance function for a Brownian Bridge process on $0 \leq t \leq 1$ (Brownian motion conditioned on $B(0) = B(1) = 0$) is

$$C_B(s,t) = \min(s,t) - st.$$

The eigenfunctions and eigenvalues are as follows

$$\lambda_n = (n\pi)^{-2},$$
$$\phi_n(t) = \sqrt{2}\sin\left(t/\sqrt{\lambda_n}\right).$$

Thus the KL expansion is

$$B_t(\omega) = \frac{\sqrt{2}}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\sin(n\pi\, t)\xi_n.$$

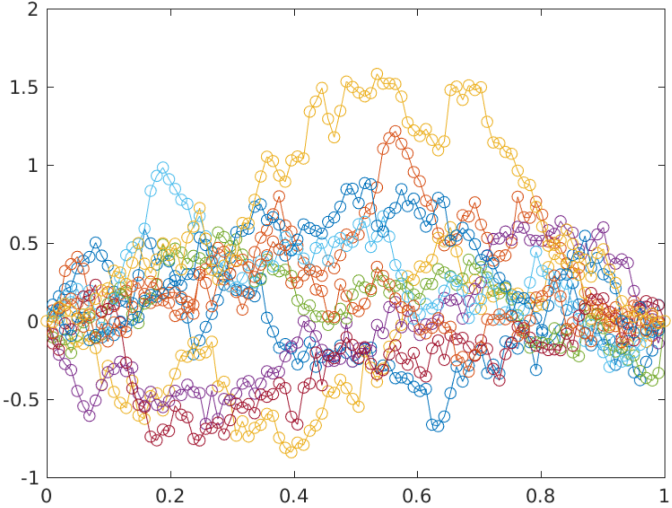

Figure: Realizations of the Brownian Bridge.

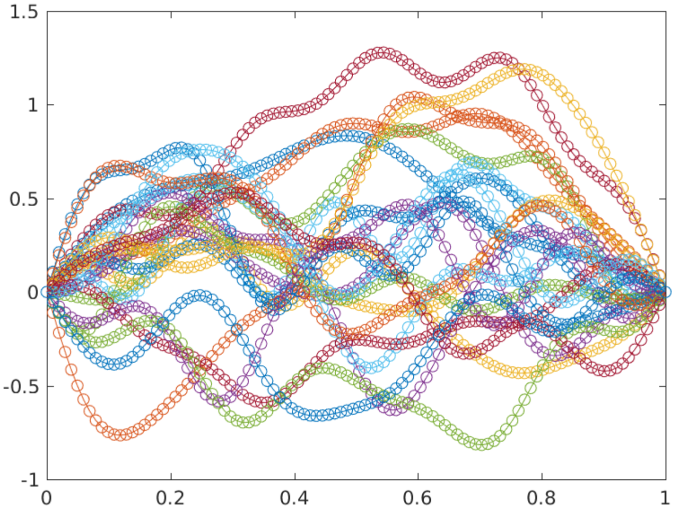

Figure: Realizations of the KL expansion of the Brownian Bridge with $d = 10$.

Outline

Maxwell's Equations

$$
\begin{aligned}
\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} &= \nabla \times \mathbf{H} && \text{(Ampere)} \\
\frac{\partial \mathbf{B}}{\partial t} &= -\nabla \times \mathbf{E} && \text{(Faraday)} \\
\nabla \cdot \mathbf{D} &= \rho && \text{(Poisson)} \\
\nabla \cdot \mathbf{B} &= 0 && \text{(Gauss)}
\end{aligned}
$$

$\mathbf{E} =$	Electric field vector	$\mathbf{D} =$	Electric displacement
$\mathbf{H} =$	Magnetic field vector	$\mathbf{B} =$	Magnetic flux density
$\rho =$	Electric charge density	$\mathbf{J} =$	Current density

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$\boxed{\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} + \mathbf{P} \\ \mathbf{B} &= \mu \mathbf{H} + \mathbf{M} \\ \mathbf{J} &= \sigma \mathbf{E} + \mathbf{J}_s \end{aligned}}$$

$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Dispersive Dielectrics

The material response is modeled via the polarization with material parameters

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}.$$

- Debye model

$$\tau \dot{\mathbf{P}} + \mathbf{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)\mathbf{E}$$

  where $q = \{\epsilon_\infty, \epsilon_s, \tau\}$ and, in particular, τ is called the relaxation time.

- Lorentz model

$$\dot{\mathbf{P}} = \mathbf{J}$$

$$\dot{\mathbf{J}} + \frac{1}{\tau}\mathbf{J} + \omega_0^2 \mathbf{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)\omega_0^2 \mathbf{E}$$

  where $q = \{\epsilon_\infty, \epsilon_s, \tau, \omega_0\}$.

Frequency Domain

- Converting to frequency domain via Fourier transforms

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

  becomes

$$\hat{\mathbf{D}} = \epsilon(\omega)\hat{\mathbf{E}}$$

  where $\epsilon(\omega)$ is called the complex permittivity.

- Debye model gives

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + i\omega\tau}$$

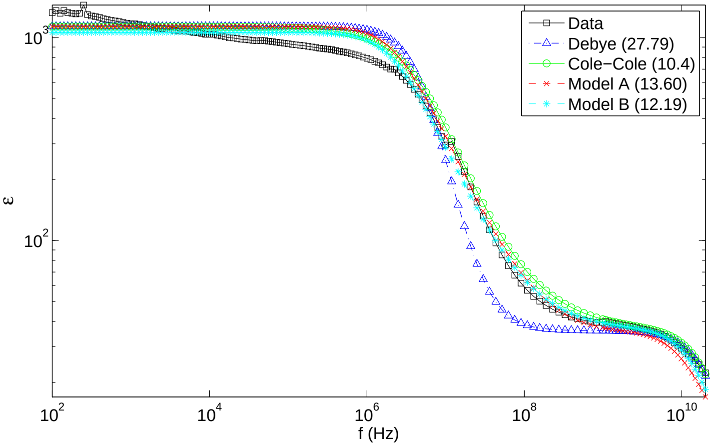

Figure: Real part of $\epsilon(\omega)$, called simply ϵ, or the permittivity. Model A refers to the Debye model with a uniform distribution on τ.

Random Polarization

We define the random polarization $\mathcal{P}(x, t; \tau)$ to be the solution to

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E$$

where τ is a random variable with PDF $f(\tau)$, for example,

$$f(\tau) = \frac{1}{\tau_b - \tau_a}$$

for a uniform distribution.

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for a uniform distribution.
The electric field depends on the macroscopic polarization, which we take to be the expected value of the random polarization at each point (x, t)

$$P(x, t; F) = \mathbb{E}[\mathcal{P}] := \int_{\tau_a}^{\tau_b} \mathcal{P}(x, t; \tau) f(\tau) d\tau.$$

We can apply Polynomial Chaos method to our random polarization

$$\tau\dot{\mathcal{P}} + \mathcal{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)E, \quad \tau = \tau(\xi) = r\xi + r$$

resulting in

$$(rM + mI)\dot{\vec{\alpha}} + \vec{\alpha} = \epsilon_0(\epsilon_s - \epsilon_\infty)E\vec{e_1} =: \vec{g}$$

or

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

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The macroscopic polarization, the expected value of the random polarization at each point (t, x), is simply

$$P(t, x; F) = \alpha_0(t, x).$$

Applying the central difference approximation, based on the Yee scheme, Maxwell's equations with conductivity and polarization included

$$\epsilon \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \sigma E - \frac{\partial P}{\partial t}$$

and

$$\mu \frac{\partial H}{\partial t} = -\frac{\partial E}{\partial z}$$

become

$$\frac{E_k^{n+\frac{1}{2}} - E_k^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\epsilon}\frac{H_{k+\frac{1}{2}}^n - H_{k-\frac{1}{2}}^n}{\Delta z} - \frac{\sigma}{\epsilon}\frac{E_k^{n+\frac{1}{2}} + E_k^{n-\frac{1}{2}}}{2} - \frac{1}{\epsilon}\frac{P_k^{n+\frac{1}{2}} - P_k^{n-\frac{1}{2}}}{\Delta t}$$

and

$$\frac{H_{k+\frac{1}{2}}^{n+1} - H_{k+\frac{1}{2}}^n}{\Delta t} = -\frac{1}{\mu}\frac{E_{k+1}^{n+\frac{1}{2}} - E_k^{n+\frac{1}{2}}}{\Delta z}.$$

Note that while the electric field and magnetic field are staggered in time, the polarization updates simultaneously with the electric field.

Need a similar approach for discretizing the PC system

$$A\dot{\vec{\alpha}} + \vec{\alpha} = \vec{g}.$$

Applying second order central differences, as before, to $\vec{\alpha} = \vec{\alpha}(z_k)$:

$$A\frac{\vec{\alpha}^{n+\frac{1}{2}} - \vec{\alpha}^{n-\frac{1}{2}}}{\Delta t} + \frac{\vec{\alpha}^{n+\frac{1}{2}} + \vec{\alpha}^{n-\frac{1}{2}}}{2} = \frac{\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}}{2}.$$

Combining like terms gives

$$(2A + \Delta t I)\vec{\alpha}^{n+\frac{1}{2}} = (2A - \Delta t I)\vec{\alpha}^{n-\frac{1}{2}} + \Delta t\left(\vec{g}^{n+\frac{1}{2}} + \vec{g}^{n-\frac{1}{2}}\right)$$

Note that we first solve the discrete electric field equation for $E_k^{n+\frac{1}{2}}$ and plug in here (in $\vec{g}^{n+\frac{1}{2}}$) to update $\vec{\alpha}$.

Energy Decay and Stability

Theorem (Gibson2013)

For $n \geq 0$, let $\mathbf{U}^n = [H^n, E_x^n, E_y^n, \alpha_{0,x}^n, \ldots, \alpha_{0,y}^n, \ldots]^T$ be the solutions of the 2D TE mode Maxwell-PC Debye FDTD scheme with PEC boundary conditions. If the usual CFL condition for Yee scheme is satisfied $c\Delta t \leq \Delta z/\sqrt{2}$, then there exists the energy decay property

$$\mathcal{E}_h^{n+1} \leq \mathcal{E}_h^n$$

where

$$(\mathcal{E}_h^n)^2 = \left|\left|\sqrt{\mu_0}\overline{H}^n\right|\right|_H^2 + ||\sqrt{\epsilon_0\epsilon_\infty}\mathbf{E}^n||_E^2 + \left|\left|\frac{1}{\sqrt{\epsilon_0\epsilon_d}}\vec{\alpha}^n\right|\right|_\alpha^2.$$

Note: $\|\mathcal{P}\|_F^2 = \mathbb{E}[\|\mathcal{P}\|_2^2] = \|\mathbb{E}[\mathcal{P}]^2 + Var(\mathcal{P})\|_2^2 \approx \|\vec{\alpha}\|_\alpha^2.$

Energy decay implies that the method is stable and hence convergent.

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- Limitation: choice of polynomials depends on type of distribution.

Reservoir Operations

The broad context of the problem of interest is a PDE-constrained optimal control problem with uncertainty. In particular, one must

- meet electrical demand with hydro-power production
- mitigate flooding
- preserve ecological conditions
- possibly maximize revenue
- etc.

Reservoir Operations

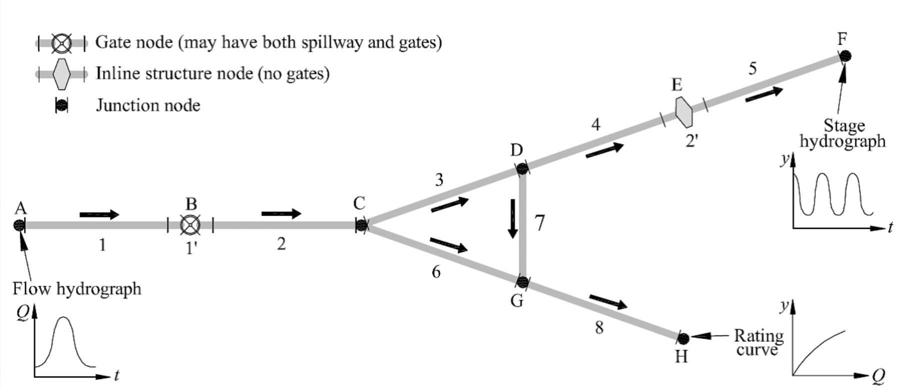
The broad context of the problem of interest is a PDE-constrained optimal control problem with uncertainty. In particular, one must

- meet electrical demand with hydro-power production
- mitigate flooding
- preserve ecological conditions
- possibly maximize revenue
- etc.

all without perfect knowledge of the system, the inflows, the demand, or prices.

Simple River System

Consider this simple network system



Unknowns: flow discharge upstream Q_u and downstream Q_d, water depth downstream y_d for each reach $i = 1, \ldots, 8$.

Simulation of Unsteady Flows

- Most free surface flows are unsteady and nonuniform.
- Unsteady flows in river systems are typically simulated using 1D models.

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- Unsteady flows in river systems are typically simulated using 1D models.

Saint-Venant equations: PDEs representing conservation of mass and momentum for a control volume:

$$B\frac{\partial y}{\partial t} + \frac{\partial Q}{\partial x} = 0, \tag{2}$$

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + gA\left(\frac{\partial y}{\partial x} + S_f - S_0\right) = 0, \tag{3}$$

where x is a distance along the channel in the longitudinal direction, t is time,
y is a water depth, Q is a flow discharge,
B is a width of the channel, g is an acceleration due to gravity,
A is a cross-sectional area of the flow, S_f is a friction slope, S_0 is a river bed slope.

Initial and boundary conditions are required to close the system.

Sources of Uncertainty

Hydrological conditions (particularly inflows) and power demand (and price) are the main sources of uncertainties.

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Chosen approach

- Parametrization of the uncertain inputs, such as stream inflows
- Stochastic representation of the solutions - discharge and water depth
- Robust optimization

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Assumptions on the uncertain inputs

- We have M predictions, $M > 1$, of the inflow function Q_{u_1}, forecast for the same points in time $\{t_j\}_{j=1}^{n}$.
- The logarithm of the inflow function Q_{u_1} can be represented as a Gaussian process.

Parametrization of the Stream Inflow

- $L_i(t_j) = \ln Q_{u_1,i}(t_j)$ is the value of the logarithm of the ith inflow at t_j.
- Expectation of the log stream inflow $\bar{L}$ and its covariance $C(t_j, t_k)$,

$$\begin{aligned}\bar{L}(t_j) &= \frac{1}{M}\sum_{i=1}^{M} L_i(t_j), \quad j = 1, \dots, n, \\ C(t_j, t_k) &= \frac{1}{M-1}\sum_{i=1}^{M}(L_i(t_j) - \bar{L}(t_j))(L_i(t_k) - \bar{L}(t_k)).\end{aligned}$$

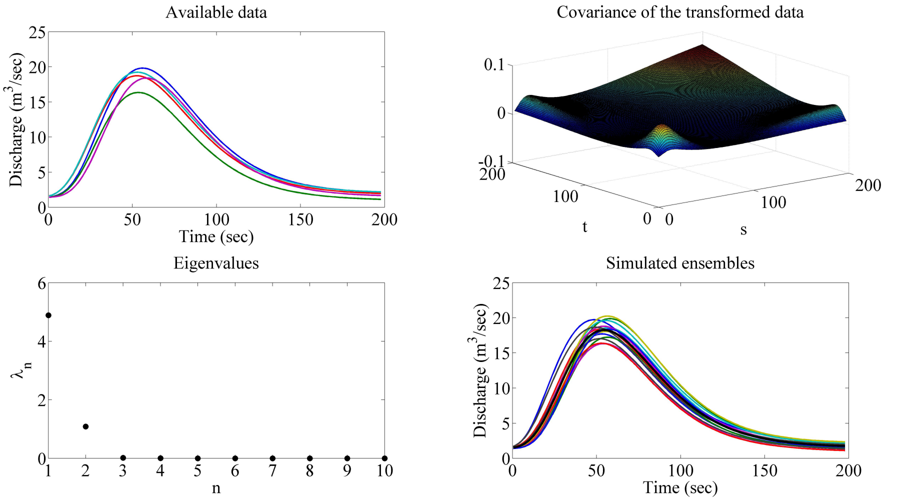
- $Q_{u_1}(t)$ can be represented as

$$Q_{u_1}(t) = exp\left(\bar{L}(t) + \sum_{k=1}^{\infty}\sqrt{\lambda_k}\psi_k(t)\xi_k\right).$$

- (λ_k, ψ_k): $\lambda\psi(t) = \int C(s,t)\psi(s)ds$.
- $\{\xi\}_{k=1}^{\infty}$ is a sequence of standard normal random variables.

Numerical Experiments. Stochastic Parametrizations

Experiment: 5 predictions



Polynomial Chaos Representation of the Solutions

Goal: Given the parametrization of the uncertain inputs, provide the stochastic representation of the solutions.

Approach: Generalized Polynomial Chaos (gPC) Expansion.

Consider a flow discharge at the most downstream reach, Q_{d_8}. Its representation in terms of a degree p polynomial expansion

$$Q_{d_8}^p(t,\vec{\xi}) = \sum_{i=0}^{M_p} v_i(t)\phi_i(\vec{\xi}), \tag{4}$$

- $\vec{\xi} = (\xi_1, \xi_2, \ldots, \xi_N)$ are r.v. in the representation of Q_{u_1}
- $\{\phi_i\}_{i=0}^{M_p}$ are the N-variate orth. polynomial functions of degree up to p
- if $\{\xi_k\}$ are i.i.d. $N(0,1)$, $\{\phi_i\}_{i=0}^{M_p}$ are chosen as tensor products of univariate Hermite polynomials.
- $M_p < (N+p)!/(N!p!)$ (max number of polynomial basis functions)

Stochastic Collocation and gPC

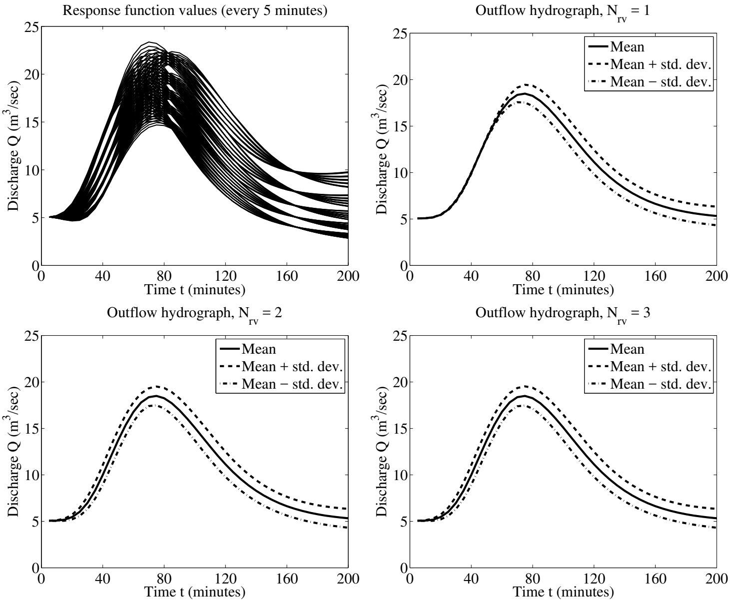
- Choose a set of collocation points $\mathbf{z}_j = (z_{j,1}, z_{j,2}, \ldots, z_{j,N}) \in \Gamma$ and weights w_j, $j = 1, \ldots, N_{cp}$.
- For each $j = 1, \ldots, N_{cp}$ evaluate the inflow function $Q_{u_1,j}(t) = Q_{u_1}(t, \mathbf{z}_j)$.
- Simulate deterministically the corresponding downstream flow $Q_{d_8,j}(t)$.
- Approximate the gPC expansion coefficients using Gaussian Quadrature

$$v_i(t) = \mathbb{E}[Q_{d_8}(t, \vec{\xi})\phi_i(\vec{\xi})] \approx \sum_{j=1}^{N_{cp}} w_j Q_{d_8}(t, \mathbf{z}_j)\phi_i(\mathbf{z}_j). \tag{5}$$

- Construct the N-variate, pth-order gPC approximation, if necessary

$$Q_{d_8}^{p}(t, \vec{\xi}) = \sum_{i=0}^{M_p} v_i(t)\phi_i(\vec{\xi}). \tag{6}$$

- Or just use $\mathbb{E}[Q_{d_8}(t, \vec{\xi})] \approx v_0(t), \quad \mathrm{Var}[Q_{d_8}(t, \vec{\xi})] \approx \sum_{i=1}^{M_p} v_i(t)^2.$


Response function values (every 5 minutes)
Discharge Q (m^3/sec)
Time t (minutes)
Outflow hydrograph, N_rv = 1
Outflow hydrograph, N_rv = 2
Outflow hydrograph, N_rv = 3
Mean
Mean + std. dev.
Mean − std. dev.
0
5
10
15
20
25
0
40
80
120
160
200

Summary

- We use KL expansions generated from sample means and sample covariances of reservoir inflow predictions
- If predictions not available, can use historical inflows to capture statistics
  - Not great for prediction, but easier to compute expected outflows with than ARMA models.
  - KL of ARMA models seem to work well!
- Have used KL on historical decisions to create a reduced order basis for decision space: works great!