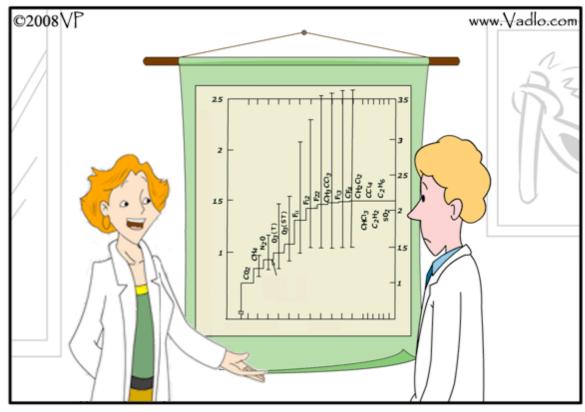


Uncertainty Quantification in Computational Science

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Did you really have to show the error bars?

The global picture



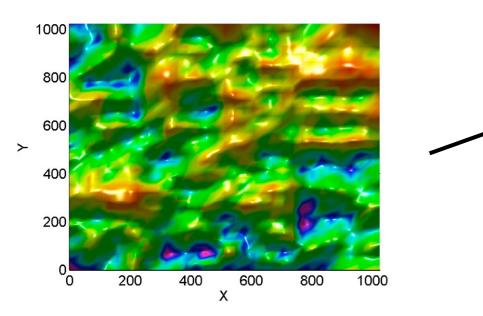
- Lecture I Introduction to UQ
 - Motivation, terminology, background, Wiener chaos expansions.
- Lecture II Stochastic Galerkin methods
 Formulation, extensions, polynomial chaos, and examples.
- Lecture III Stochastic Collocation methods Motivation, formulation, high-d integration, and examples.
- Lecture IV Extensions, challenges, and open questions Geometric uncertainty, ANOVA expansions, and discussion of open questions.

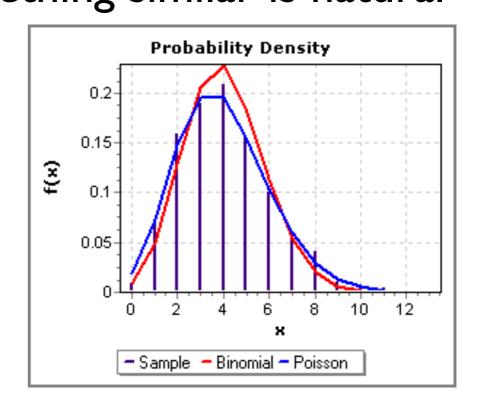
On smoothness



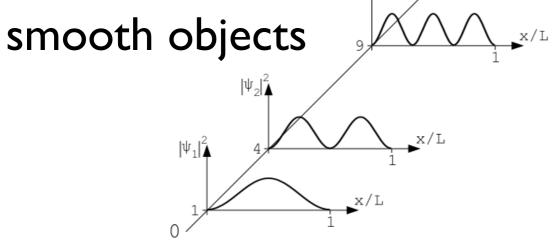
The assumption of smoothness is on the random variable - not on the solution - in MC something similar is natural

Imagine an experiment

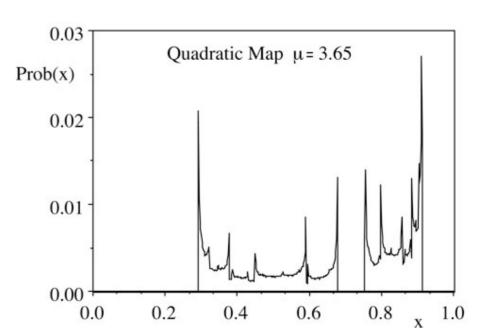




After the fit, evolution often also leads to



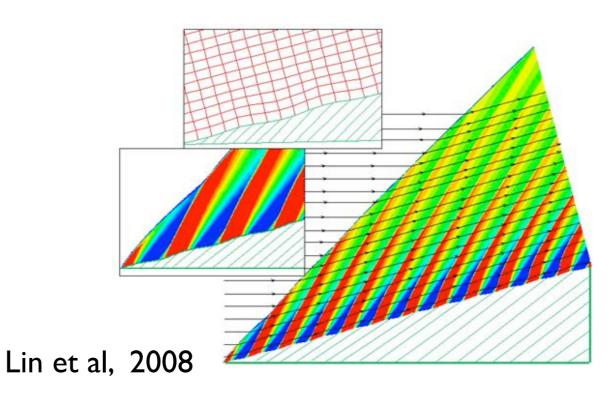
In this case, we are all out of luck



The local picture



- A brief reminder
- Stochastic Galerkin methods for ODEs
- Stochastic Galerkin methods for PDEs
- Extensions to non-Gaussian variables
- Summary



A brief reminder



Through a series of arguments we realized

- We need to be able to quantify with the impact of uncertainty in modeling of complex systems.
- While MC is tested and tried, its cost is problematic for complex systems and/or high accuracy requirements
- For many systems the random variables have smooth densities and this we should explore
- We introduced the Wiener Chaos expansion for this purpose

A brief reminder



We introduced the homogeneous Chaos expansion

$$f_N(\mathbf{X}) = \sum_{|i|=0}^{N} \hat{f}_i \Phi_i(\mathbf{X}) \in \mathsf{P}_N^d \quad \dim \mathsf{P}_N^d = \binom{N+d}{N} = \frac{(N+d)!}{N!d!}$$

to represent functions of d-dimensional random vectors

$$\mathbf{X} = (X_1, \dots, X_d)$$

$$F_{X_i}(x_i) = P(X_i \le x_i)$$

$$F_X = F_{X_1} \times \dots \times F_{X_d}$$

Here we defined the Chaos polynomial

$$\Phi_i(\mathbf{X}) = \Phi_{i_1}(X_1) \times \ldots \times \Phi_{i_d}(X_d)$$
$$\mathsf{E}[\Phi_i(\mathbf{X})\Phi_j(\mathbf{X})] = \int \Phi_i(\mathbf{x})\Phi_j(\mathbf{x}) \, dF_X(x) = \gamma_i \delta_{ij} \qquad \gamma_i = \mathsf{E}[\Phi_i^2]$$

For Gaussian variables, these are known as Hermite Poly.



Let us now see how we can use these development

We consider again the simple ODE

$$\frac{du}{dt}(t,Z) = -\alpha(Z)u, \qquad u(t=0,Z) = \beta,$$

Let us assume that $\alpha \sim N(\mu, \sigma^2)$ and express it as

$$\alpha_N(Z) = \sum_{i=0}^N a_i H_i(Z), \qquad a_0 = \mu, \qquad a_1 = \sigma, \qquad a_i = 0, \quad i > 1.$$

Similarly for the deterministic initial condition

$$\beta_N = \sum_{i=0}^N b_i H_i(Z), \qquad b_0 = \beta, \qquad b_i = 0, \quad i > 0,$$

Note: This is very simple for illustration only!



We now seek solutions of the form

$$v_N(t,Z) = \sum_{i=0}^{N} \hat{v}_i H_i(Z)$$

To find the N+1 unknown we apply the Galerkin procedure

$$\mathsf{E}\left[\frac{dv_N}{dt}H_k\right] = -\mathsf{E}[\alpha_N v_N H_k], \ \forall k = 0, \dots, N$$

Yielding

$$\frac{d\hat{v}_k}{dt} = -\frac{1}{\gamma_k} \sum_{i=0}^N \sum_{j=0}^N a_i \hat{v}_j e_{ijk} \qquad \forall k = 0, \dots, N, \qquad e_{ijk} = \mathsf{E}[H_i H_j H_k]$$
$$\hat{v}_k(0) = b_k, \qquad 0 \le k \le N.$$

Can now be solved using a standard method

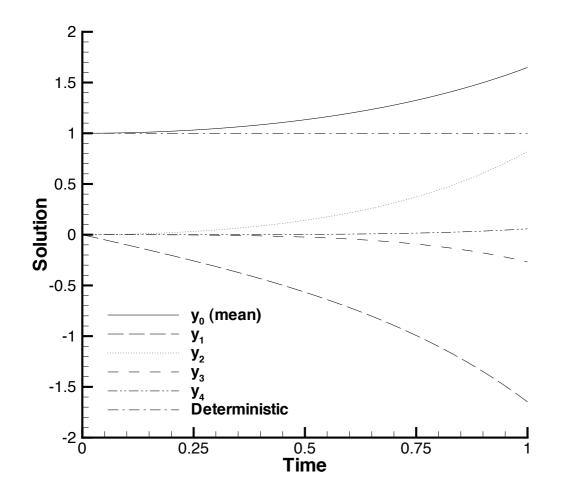


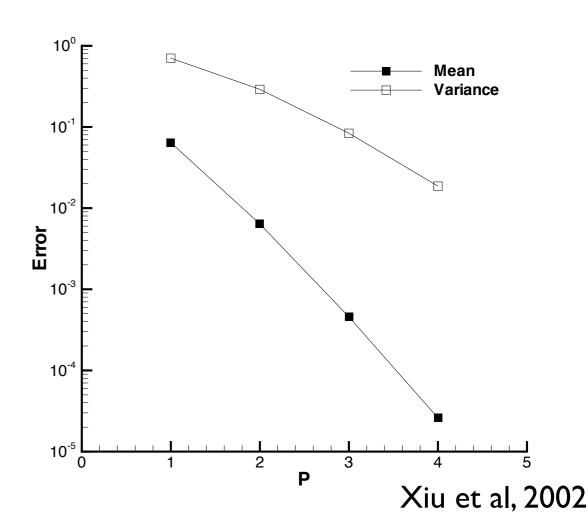
Define (N+I)x(N+I) matrix

$$A_{jk} = -\frac{1}{\gamma_k} \sum_{i=0}^{N} a_i e_{ijk},$$

to recover the system

$$\frac{d\mathbf{v}}{dt}(t) = \mathbf{A}^T \mathbf{v}, \qquad \mathbf{v}(0) = \mathbf{b},$$







A few observations are worth making

- Solving with the mean coefficients is not sufficient
- A stochastic scalar problem becomes a deterministic system
- Some work is needed to derive system and matrix entries $e_{ijk} = \mathsf{E}[H_i H_j H_k]$
- System is only coupled with multiplicative randomness
- Spectral convergence is clear, i.e., we have recovered the benefits of global expansions from PDE solvers



Let us briefly discuss the generalization to general SDEs

$$\frac{du(\mathbf{X},t)}{dt} = f(\alpha(\mathbf{X}), u, t) + g(\beta(\mathbf{X}), t), \quad u(\mathbf{X}, 0) = h(\gamma(\mathbf{X}))$$

Parameters depends on d-dimensional random space

$$\alpha(\mathbf{X}) = (\alpha_1(\mathbf{X}), \dots, \alpha_k(\mathbf{X}))$$

$$\beta(\mathbf{X}) = (\beta_1(\mathbf{X}), \dots, \beta_l(\mathbf{X}))$$

$$\mathbf{X} = (X_1, \dots, X_d)$$

$$\gamma(\mathbf{X}) = (\gamma_1(\mathbf{X}), \dots, \gamma_l(\mathbf{X}))$$

As in the simple case they are expanded in Chaos expansion

$$\alpha_{N}(\mathbf{X}) = \sum_{|i|=0}^{N} \hat{\alpha}_{i} \Phi_{i}(\mathbf{X}) \quad \beta_{N}(\mathbf{X}) = \sum_{|i|=0}^{N} \hat{\beta}_{i} \Phi_{i}(\mathbf{X}) \quad \gamma_{N}(\mathbf{X}) = \sum_{|i|=0}^{N} \hat{\gamma}_{i} \Phi_{i}(\mathbf{X})$$

$$\hat{\alpha}_{i} = \frac{1}{\gamma_{i}} \mathsf{E}[\alpha(\mathbf{X}) \Phi_{i}(\mathbf{X})] \quad \hat{\beta}_{i} = \frac{1}{\gamma_{i}} \mathsf{E}[\beta(\mathbf{X}) \Phi_{i}(\mathbf{X})] \quad \hat{\gamma}_{i} = \frac{1}{\gamma_{i}} \mathsf{E}[\gamma(\mathbf{X}) \Phi_{i}(\mathbf{X})]$$



Now proceed and express the solution as

$$u_N(\mathbf{X}, t) = \sum_{|i|=0}^{N} \hat{u}_i(t) \Phi_i(\mathbf{X})$$

Applying a Galerkin approach yields the system to solve

$$\frac{d}{dt}\mathsf{E}[u\,\Phi_k] = \frac{d\hat{u}_k}{dt} = \mathsf{E}[f(\alpha_N,u_N)\,\Phi_k] + \mathsf{E}[g(\beta_N)\,\Phi_k], \quad \forall |k| = 0,\dots, N$$

$$\hat{u}_k(0) = \frac{1}{\gamma_k}\mathsf{E}[h(\gamma_N)\,\Phi_k], \quad |k| = 0,\dots, N$$

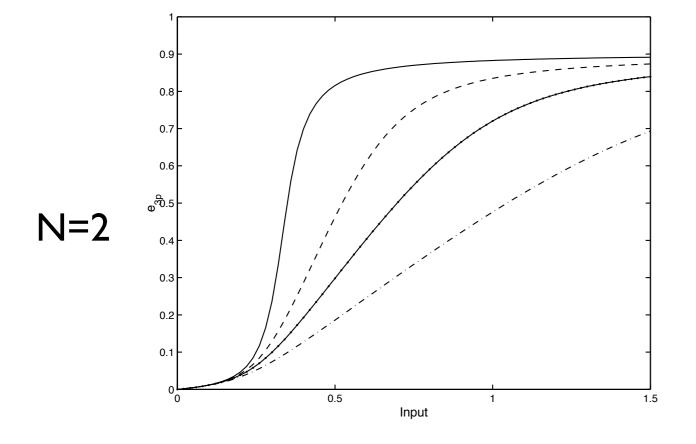
- Total number of variables $\frac{(N+d)!}{N!d!} \sim \frac{N^a}{d!}$
- Generally terms $\mathsf{E}[f(\alpha_N,u_N)\,\Phi_k]$ and $\mathsf{E}[g(\beta_N)\,\Phi_k]$ must be evaluated through quadrature

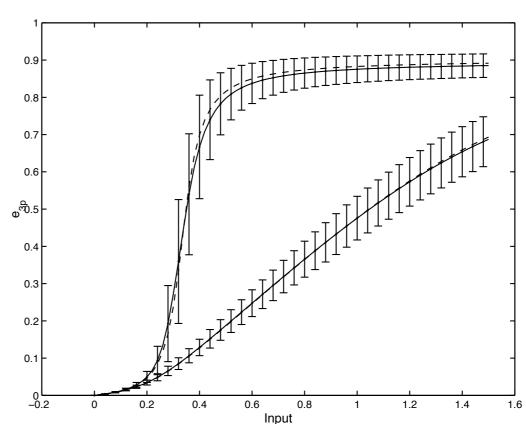


Consider a biological cell-signal problem

$$\begin{split} \frac{de_{1p}}{dt} &= \frac{I(t)}{1 + G_4 e_{3p}} \frac{V_{\max,1}(1 - e_{1p})}{K_{m,1} + (1 - e_{1p})} - \frac{V_{\max,2} e_{1p}}{K_{m,2} + e_{1p}}, \qquad K_{m,1-6} = 0.2 \\ \frac{de_{2p}}{dt} &= \frac{V_{\max,3} e_{1p}(1 - e_{2p})}{K_{m,3} + (1 - e_{2p})} - \frac{V_{\max,4} e_{2p}}{K_{m,4} + e_{2p}}, \qquad < V_{max} >= (0.5, 0.15, 0.15, 0.15, 0.25, 0.05) \\ \frac{de_{3p}}{dt} &= \frac{V_{\max,5} e_{2p}(1 - e_{3p})}{K_{m,5} + (1 - e_{3p})} - \frac{V_{\max,6} e_{3p}}{K_{m,6} + e_{3p}}. \end{split}$$
 I(t) is a control parameter

<u>Model</u> $V_{max,i} = \langle V_{max} \rangle (1 + \sigma X_i)$ $\sigma = 0.1$ $f_{X_i} = U(-1,1)$





Xiu, 2007



Consider as example a genetic toggle switch

$$\frac{du}{dt} = \frac{\alpha_1}{1 + v^{\beta}} - u,$$

$$\frac{dv}{dt} = \frac{\alpha_2}{1 + \omega^{\gamma}} - v,$$

$$\omega = \frac{u}{(1 + [IPTG]/\mathcal{K})^{\eta}}$$

Model

$$\alpha(\mathbf{X}) = <\alpha > (1 + \sigma \mathbf{X})$$

$$f_{X_i} = U(-1,1)$$

$$\langle \alpha \rangle = (156.25, 15.6, 2.5, 1, 2.0015, 2.9618 \times 10^{-5})$$

$$\sigma = 0.1$$

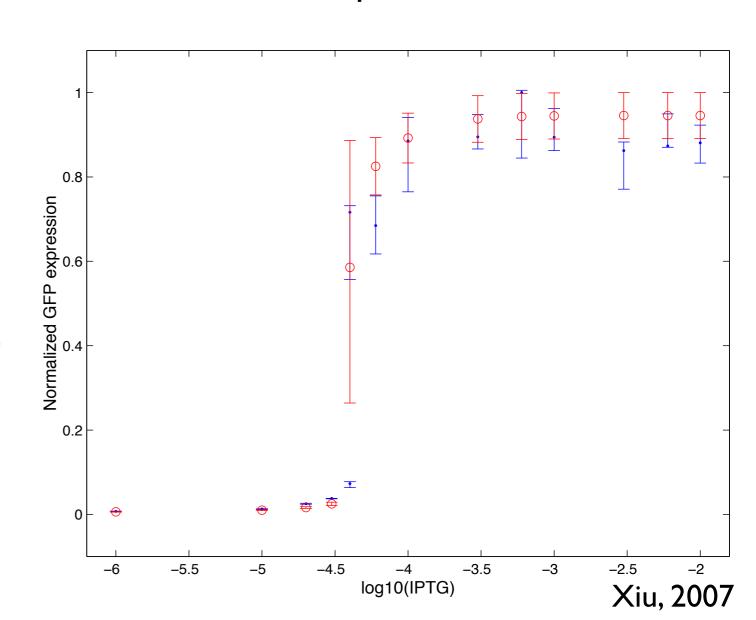
Experimental data

Computation results

$$N=2$$

$$\alpha = (\alpha_1, \cdots, \alpha_6) = (\alpha_1, \alpha_2, \beta, \gamma, \eta, \mathscr{K})$$

IPTG is a control parameter





Lets summarize our results for SDEs

- Approach is systematic
- SDE scalar problems leads to deterministic coupled systems of ODEs
- Results for both linear and non-linear are convincing and the potential for savings significant.

What changes for SPDEs?



Consider the general SPDE

$$\begin{cases} u_t(x, t, \omega) = \mathcal{L}(u), & D \times (0, T] \times \Omega, \\ \mathcal{B}(u) = 0, & \partial D \times [0, T] \times \Omega, \\ u = u_0, & D \times \{t = 0\} \times \Omega, \end{cases}$$

Assume that the uncertainty can be represented by

$$Z = (Z_1, \ldots, Z_d)$$

to recover the recognizable formulation

$$\begin{cases} u_t(x, t, Z) = \mathcal{L}(u), & D \times (0, T] \times \mathbb{R}^d, \\ \mathcal{B}(u) = 0, & \partial D \times [0, T] \times \mathbb{R}^d, \\ u = u_0, & D \times \{t = 0\} \times \mathbb{R}^d. \end{cases}$$



Let us first consider the elliptic problem

$$\begin{cases} \nabla \cdot [\kappa(x;\omega)\nabla u(x;\omega)] = f(x;\omega), & (x;\omega) \in D \times \Omega \\ u(x;\omega) = g(x;\omega), & (x;\omega) \in \partial D \times \Omega \end{cases}$$

We continue as before

$$\kappa_N(x, Z(\omega)) = \sum_{n=0}^N \hat{\kappa}_n(x) \Phi_n(Z)$$

$$f_N(x, Z(\omega)) = \sum_{n=0}^N \hat{f}_n(x) \Phi_n(Z) \qquad g_N(x, Z(\omega)) = \sum_{n=0}^N \hat{g}_n(x) \Phi_n(Z)$$

and seek solutions of the form

$$u_N(x, Z(\omega)) = \sum_{n=0}^{N} \hat{u}_n(x)\Phi_n(Z)$$



Inserting this into the PDE yields

$$\sum_{n=0}^{N} \sum_{m=0}^{N} \left[\nabla \cdot (\hat{\kappa}_n \nabla \hat{u}_m) \right] \Phi_n \Phi_m = \sum_{n=0}^{N} \hat{f}_n \Phi_n$$

Applying the Galerkin procedure yields

$$\sum_{n=0}^{N} \sum_{m=0}^{N} \left[\nabla \cdot (\hat{\kappa}_n \nabla \hat{u}_m) \right] e_{mnk} = \hat{f}_k \mathsf{E}[\Phi_k^2]$$

$$e_{mnk} = \mathsf{E}[\Phi_m \, \Phi_n \, \Phi_k]$$

with boundary conditions

$$\hat{u}_n = \mathsf{E}[g_N \, \Phi_n]$$

Essentially the same as for the SDE



Requires the solution of N+1 coupled of the form

$$\sum_{m=0}^{N} \nabla \cdot (\tilde{\kappa}_{mk} \nabla \hat{u}_m) = \hat{f}_k \gamma_k \qquad \qquad \tilde{\kappa}_{mk} = \sum_{n=0}^{N} \hat{\kappa}_n e_{mnk}$$

In space you can discretize as you prefer to recover

$$Au = f$$

where (u,f) are (N+1)xDOF long vectors.

Procedure requires solvers to be rewritten.



Lets consider a couple of examples

$$\frac{d}{dx} \left[\kappa(x; \omega) \frac{du}{dx}(x; \omega) \right] = 0, \qquad x \in [0, 1], \qquad u(0; \omega) = 0, \qquad u(1; \omega) = 1.$$

Diffusivity is assumed random

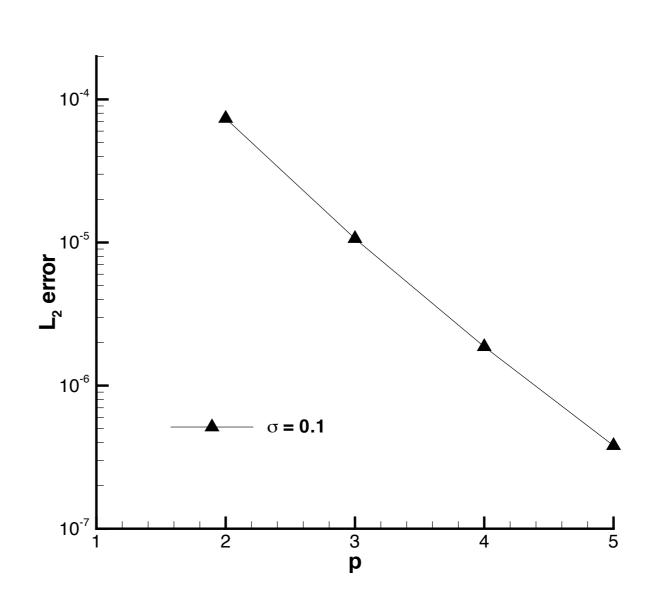
$$\kappa(x;\omega) = 1 + \epsilon(\omega)x,$$

<u>Model</u>

$$\epsilon(\omega) = \sigma X$$

$$f_X = \mathsf{N}(0,1)$$

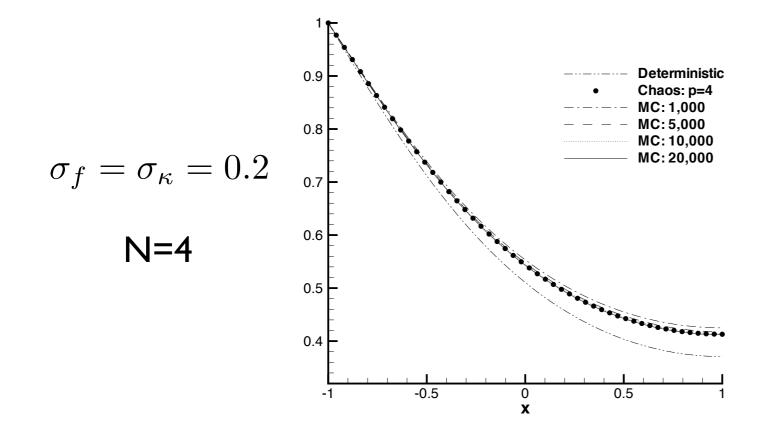
$$\sigma = 0.1$$

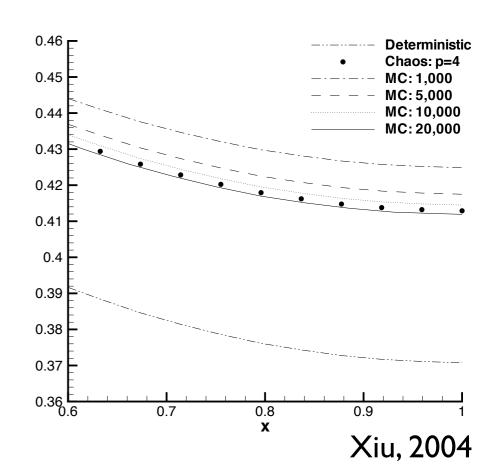




Consider a 2nd example

$$\nabla \cdot [\kappa(x, y; \omega) \nabla u(x, y; \omega)] = f(x, y; \omega), \qquad (x, y) \in [-1, 1] \times [-1, 1]$$
$$u(-1, y; \omega) = 1, \qquad \frac{\partial u}{\partial x}(1, y; \omega) = 0, \qquad u(x, -1; \omega) = 0, \qquad \frac{\partial u}{\partial y}(x, 1; \omega) = 0.$$







Let us also consider time dependent problems

$$\frac{\partial u(x, t, Z)}{\partial t} = c(Z) \frac{\partial u(x, t, Z)}{\partial x}, \quad x \in (-1, 1), \quad t > 0,$$

$$u(x, 0, Z) = u_0(x, Z).$$

$$u(1, t, Z) = u_R(t, Z), \quad c(Z) > 0,$$

$$u(-1, t, Z) = u_L(t, Z), \quad c(Z) < 0.$$

We proceed as before

$$v_N(x, t, Z) = \sum_{i=0}^{N} \hat{v}_i(x, t) \Phi_i(Z)$$

Applying the Galerkin procedure results in

$$\frac{\partial \hat{v}_k(x,t)}{\partial t} = \sum_{i=0}^{N} a_{ik} \frac{\partial \hat{v}_i(x,t)}{\partial x}, \qquad k = 0, \dots, N, \qquad a_{ik} = \mathsf{E}[c(Z) \, \Phi_i(Z) \, \Phi_k(Z)]$$

or the system

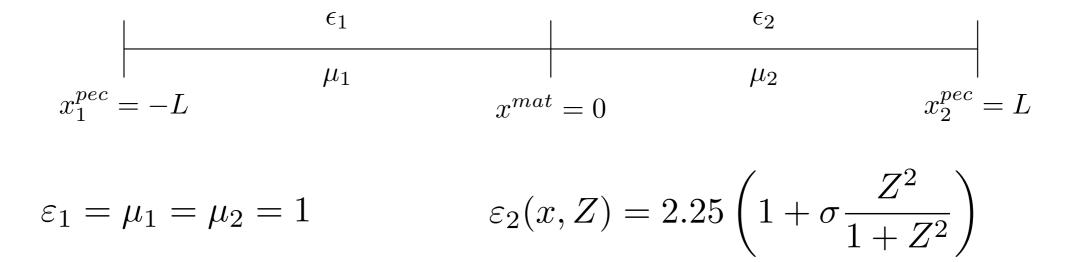
$$\frac{\partial \mathbf{v}(x,t)}{\partial t} = \mathbf{A} \frac{\partial \mathbf{v}(x,t)}{\partial x}.$$



Consider Maxwell's equations

$$\epsilon \frac{\partial \mathbf{E}^s}{\partial t} = \nabla \times \mathbf{H}^s + \sigma \mathbf{E}^s + \mathbf{S}^E,$$
$$\mu \frac{\partial \mathbf{H}^s}{\partial t} = -\nabla \times \mathbf{E}^s + \mathbf{S}^H,$$

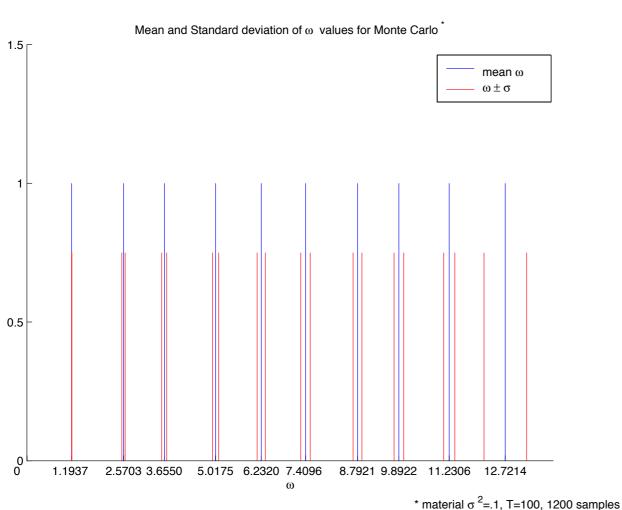
We first consider a ID cavity problem

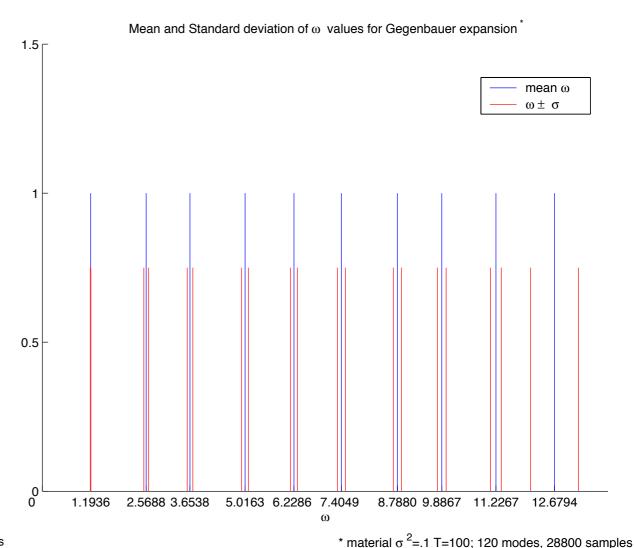


We wish to estimate sensitivity of eigenfrequencies



Direct comparison with MC





al 6 = 1, 1=100, 1200 samples

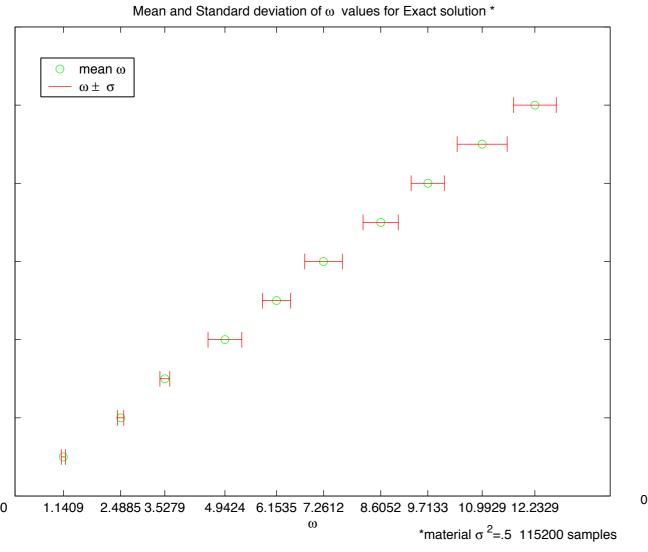
1200 samples

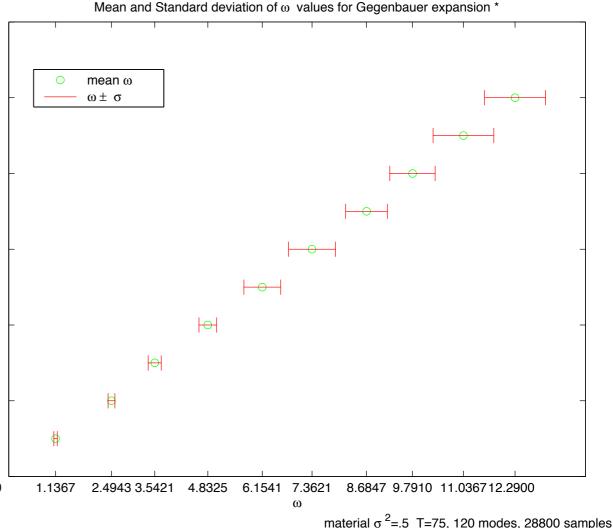
N = 120



Computation for large variation

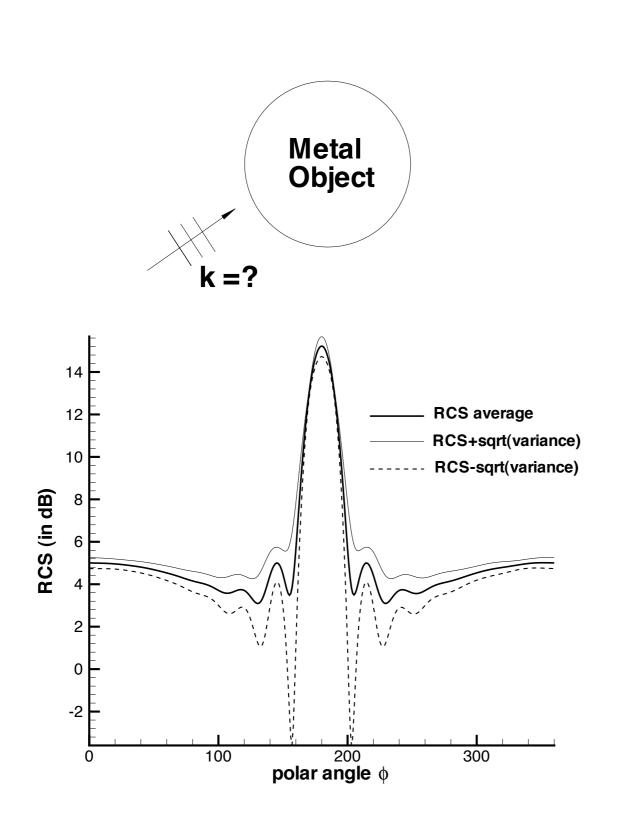
$$\sigma = 0.25$$

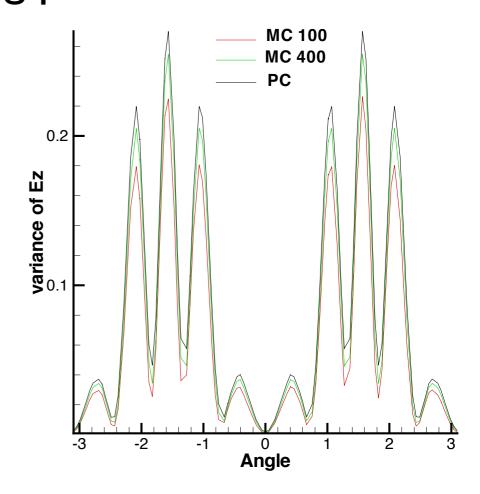






Let us also consider a 2D scattering problem



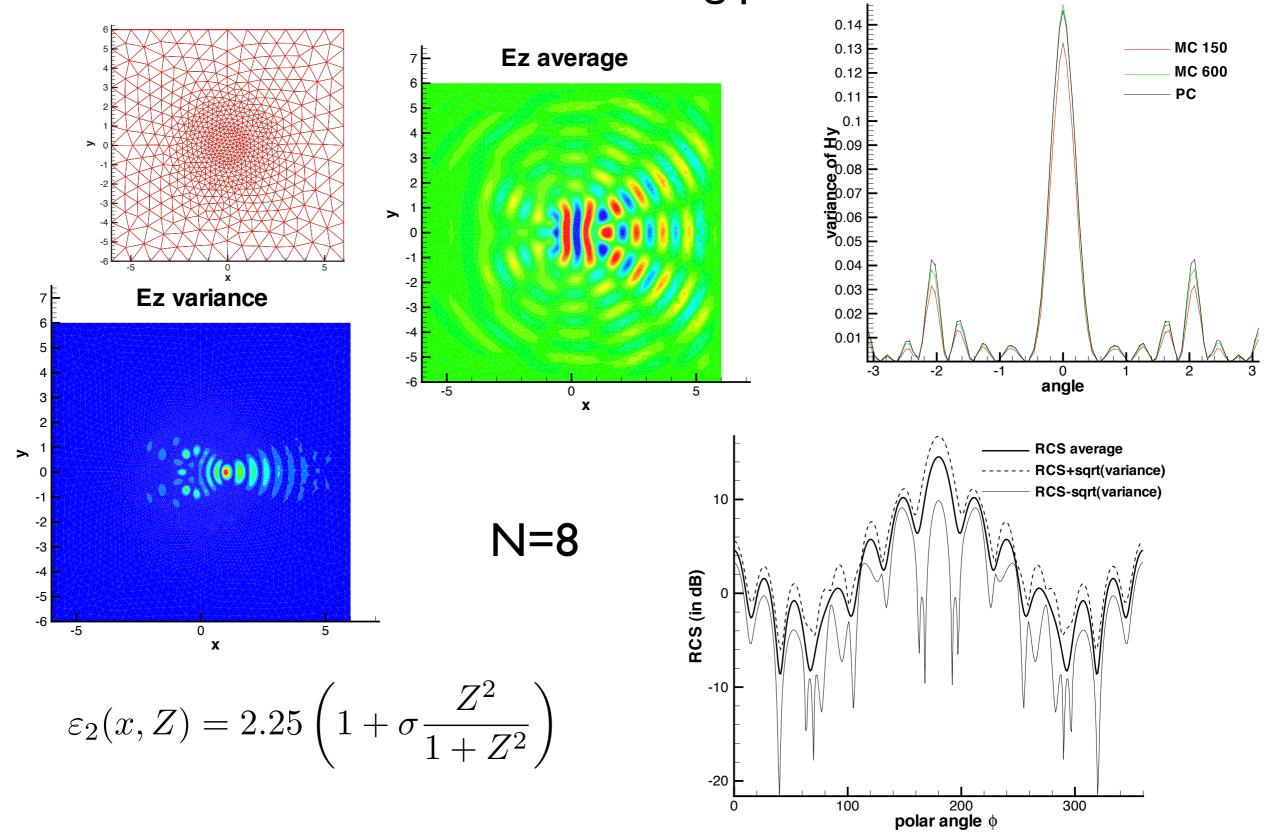


$$N=4$$

$$\mathbf{k}(Z) = [\cos(0.1Z), \sin(0.1Z)]$$



Consider a 2D material scattering problem

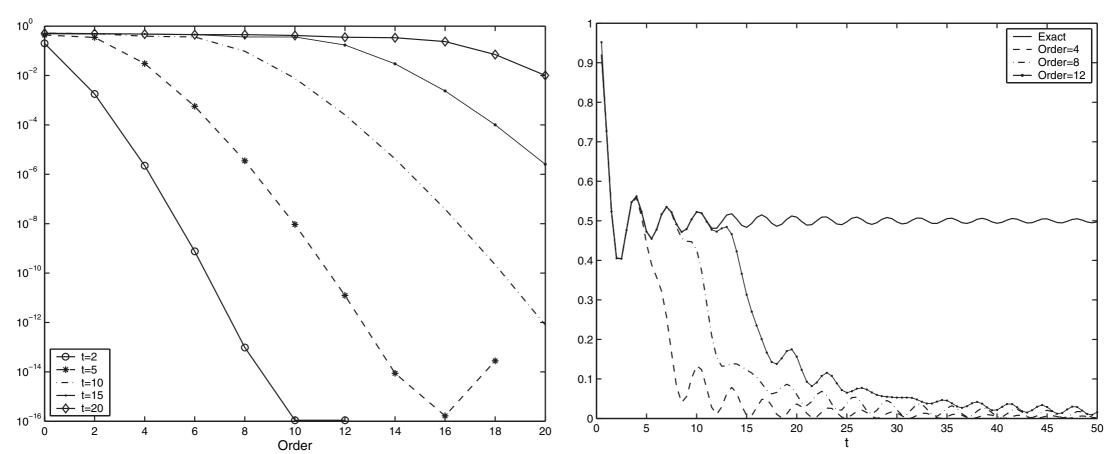




Let us again consider

$$\frac{\partial u(x,t,Z)}{\partial t} = c(Z)\frac{\partial u(x,t,Z)}{\partial x}, \quad x \in (-1,1), \quad t > 0,$$

Xiu, 2010



- Spectral convergence at fixed time as expected
- Resolution requirement is time-dependent



One easily proves the following result

$$\mathsf{E}[\|u - u_N\|^2] \le \frac{C}{N^{2m-1}}t$$

m depends on smoothness in Z

Assume periodicity in x and write the solution as

$$\hat{u}_n(t,Z) = \hat{u}_n(0) \exp(inc(Z)t)$$

Shows that in Z the wavenumber to resolve is t-dependent

It is a property of the equation -- worst case scenario.

This remains a major practical challenge



Let us briefly consider nonlinear problems

$$\begin{cases} u_t + uu_x = vu_{xx}, & x \in [-1, 1], \\ u(-1) = 1 + \delta(Z), & u(1) = -1, \end{cases}$$

Assume again

$$v_N(x, t, Z) = \sum_{i=0}^{N} \hat{v}_i(x, t) \Phi_i(Z)$$

Following the same procedure yields

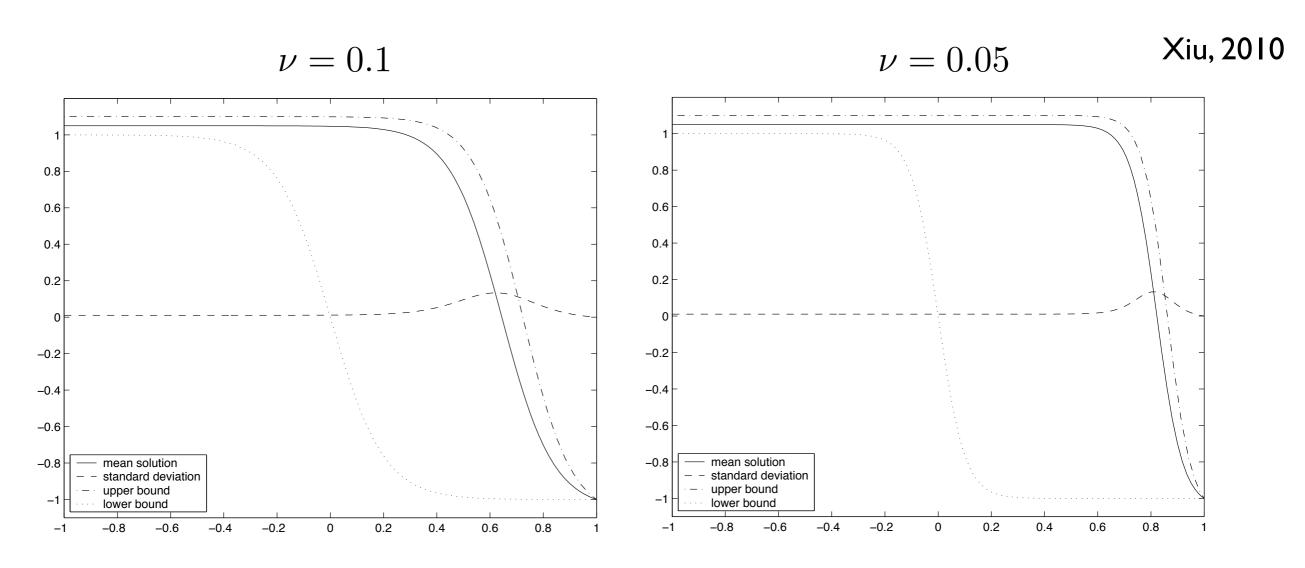
$$\frac{\partial \hat{v}_k}{\partial t} + \frac{1}{\gamma_k} \sum_{i=0}^{N} \sum_{j=0}^{N} \hat{v}_i \frac{\partial \hat{v}_j}{\partial x} e_{ijk} = \nu \frac{\partial^2 \hat{v}_k}{\partial x^2}, \qquad k = 0, \dots, N,$$

More complex non-linearities become problematic

$$e^{u} \Rightarrow \mathbb{E}\left[e^{v_N}\Phi_k\right] = \int e^{\sum_i \hat{v}_i \Phi_i(z)} \Phi_k(z) dF_Z(z),$$



Consider the Burgers problem



$$\delta = (1 + 0.1Z)$$
$$f_Z = N[0, 1]$$

Referred to supersensitivity



- Galerkin approach reformulates SPDE to larger system of deterministic PDE
- The approach is systematic and applicable to general systems of SPDE's.
- Standard PDE solvers need to be rewritten but standard methods are applicable
- Main issue with nonlinear problems is cost.
- Advection dominated problems have special challenges

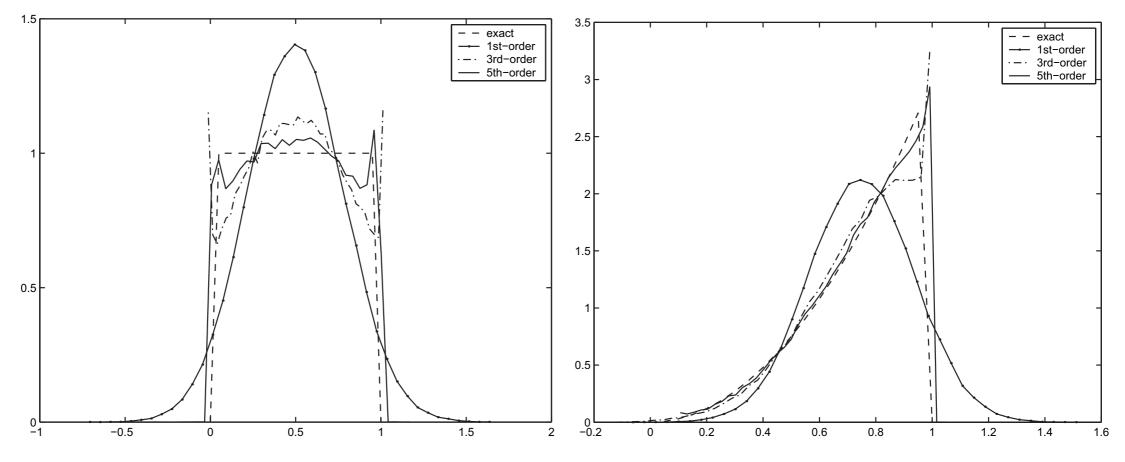


Focus has been on homogeneous Chaos expansions and Hermite polynomials as originally proposed by Wiener.

From the weak approximation results, we know this is ok

But is it a good idea?

Xiu, 2010



Approximation of uniform density

Approximation of Beta density



Recall that we introduced the polynomial chaos basis as

$$\mathsf{E}[\Phi_m(X)\Phi_n(X)] = \int \Phi_m(X(x))\Phi_n(X(x))\,dF_X(x) = \gamma_n \delta_{mn}$$

$$\gamma_n = \mathsf{E}[\Phi_n^2(X)]$$

and the Chaos expansion as

$$f(X) = \sum_{n=0}^{\infty} \hat{f}_n \Phi_n(X) \qquad \qquad \hat{f}_n = \frac{1}{\gamma_n} \mathsf{E}[f(X)\Phi_n(X)]$$

$$dF_X = \rho(x) dx$$

where the density is associated with the random variable

$$F_X = N[0,1]$$
 \Rightarrow $\rho(z) = \frac{1}{\sqrt{2\pi}} e^{-z^2/2}.$

This suggests that the suitable basis depends on the density

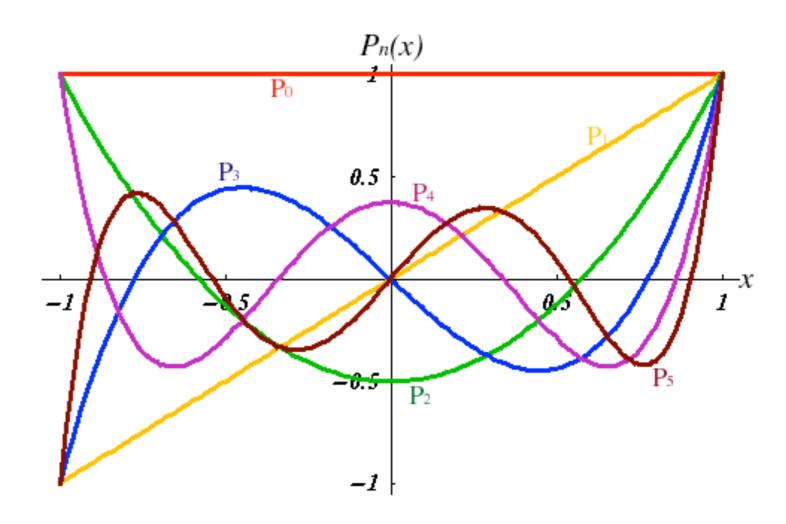


Uniformly distributed variables: U[-1,1]

Legendre polynomials

$$P_0(x) = 1$$
, $P_1(x) = x$, $P_2(x) = \frac{1}{2}(3x^2 - 1)$,...

$$\rho(x) = \frac{1}{2}$$





Beta-distributed variables: $B(\alpha, \beta)$

Jacobi polynomials:
$$P_0^{(\alpha,\beta)}(x)=1, \ P_1^{(\alpha,\beta)}(x)=\frac{1}{2}(\alpha-\beta+(\alpha+\beta+2)x),$$

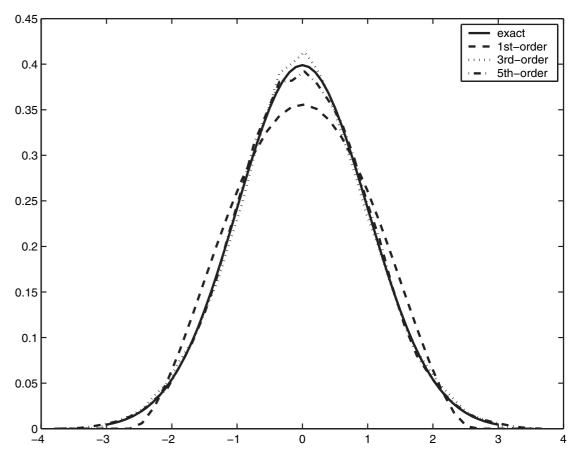
$$\rho(x) = C(\alpha, \beta)(1 - x)^{\alpha}(1 + x)^{\beta}, \ x \in [-1, 1], \ \alpha, \beta \ge 0$$

$$C(\alpha, \beta) = \frac{\Gamma(\alpha + \beta + 2)}{2^{\alpha + \beta + 1}\Gamma(\alpha + 1)\Gamma(\beta + 1)}$$

Well suited to model general densities.

Ex:Approximation of Gaussian by $P^{(10,10)}(x)$

Effective truncated Gaussian

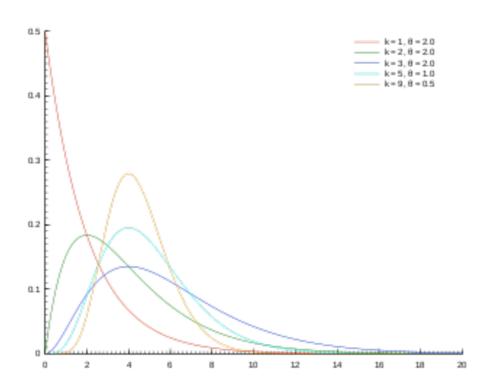




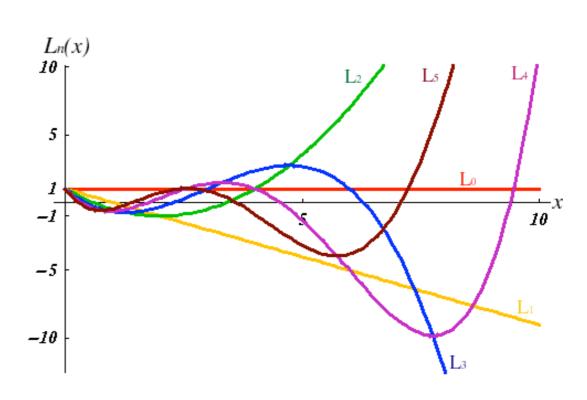
Gamma distributed variable: $\Gamma(r,c)$

Laguerre polynomials

$$L_0(x) = 1$$
, $L_1(x) = -x + 1$, $L_2(x) = \frac{1}{2}(x^2 - 4x + 2)$, ...



$$\rho(x) = x^{r-1} \frac{e^{-x/c}}{c^r \Gamma(r)}, \quad x \ge 0, \quad r, c > 0$$





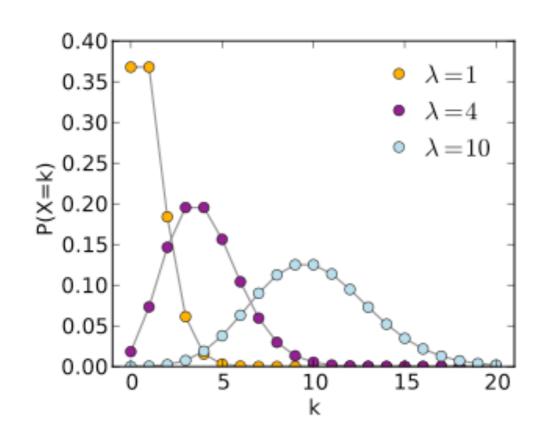
What about discrete random variables?

There is no essential difference

$$\mathsf{E}[\Phi_m(X)\Phi_n(X)] = \sum_i \Phi_m(x_i)\Phi_n(x_i)\rho_i = \gamma_n \delta_{nm}$$

This defines the appropriate Chaos basis

Ex: Poisson distribution



$$\rho(x) = \frac{\lambda^x e^{-\lambda}}{x!}, \quad x = 0, 1, 2, 3, \dots$$

Charlier polynomials is the appropriate basis



The much broader class of processes to consider is known as generalized Polynomial Chaos (gPC)

Continuous	Gaussian	Hermite	$(-\infty,\infty)$
	Gamma	Laguerre	$[0,\infty)$
	Beta	Jacobi	[a,b]
	Uniform	Legendre	[a,b]
Discrete	Poisson	Charlier	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk	$\{0, 1, \dots, N\}$
	Negative binomial	Meixner	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn	$\{0, 1, \dots, N\}$

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What about 'non-classic' cases?

Given a weight one can always constructed a corresponding orthogonal polynomial basis

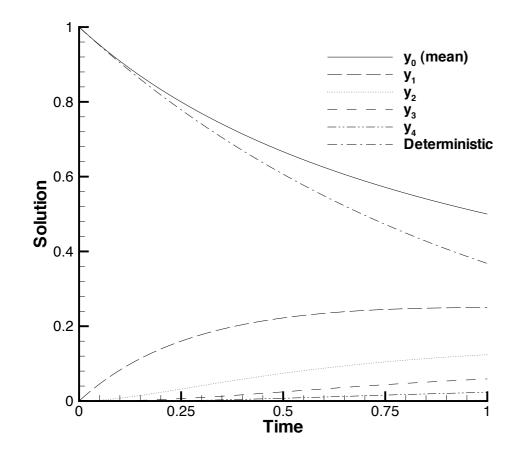


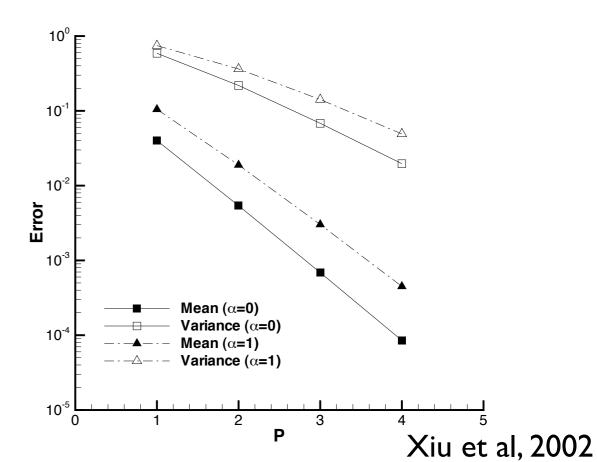
We consider again the simple ODE

$$\frac{du}{dt}(t,X) = -k(X)u, \quad u(0) = 1$$

Assume a Gamma distribution of the unknown -

$$k \sim \frac{e^{-x}x^{\alpha}}{\Gamma(\alpha+1)}$$
 $\mu = \bar{k} = \alpha+1, \ \sigma^2 = \alpha+1$





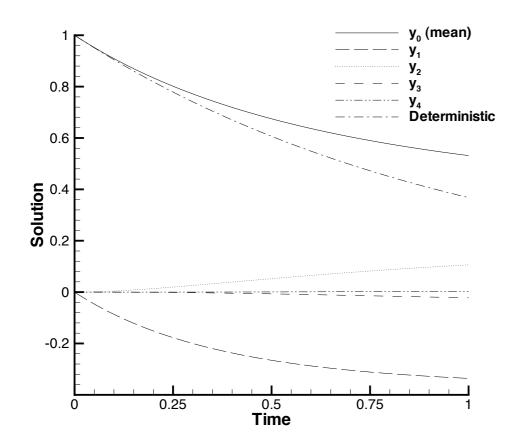


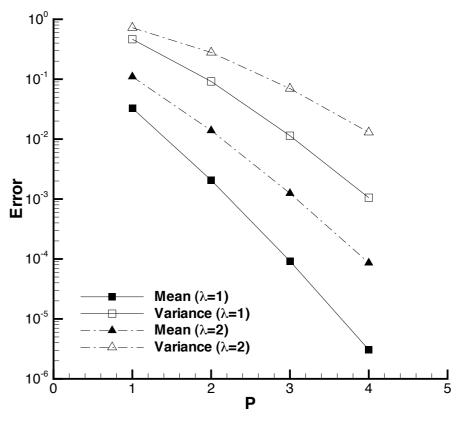
We consider again the simple ODE

$$\frac{du}{dt}(t,X) = -k(X)u, \quad u(0) = 1$$

Assume a Poisson distribution of the unknown -

$$k \sim \frac{e^{-\lambda}\lambda^x}{x!}$$
 $\mu = \bar{k} = \lambda, \quad \sigma^2 = \lambda$





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Summary



We have achieved quite a bit

- Developed and demonstrated the Stochastic Galerkin methods to quantify uncertainty in general problems
- Discussed both steady and time-dependent problems
- Introduced generalized Polynomial Chaos to most effectively deal with general random variables

Problems remain

- New solvers are required
- Computational cost