Sensitivity analysis and polynomial chaos for differential equations

Dongbin Xiu

Department of Mathematics, Purdue University

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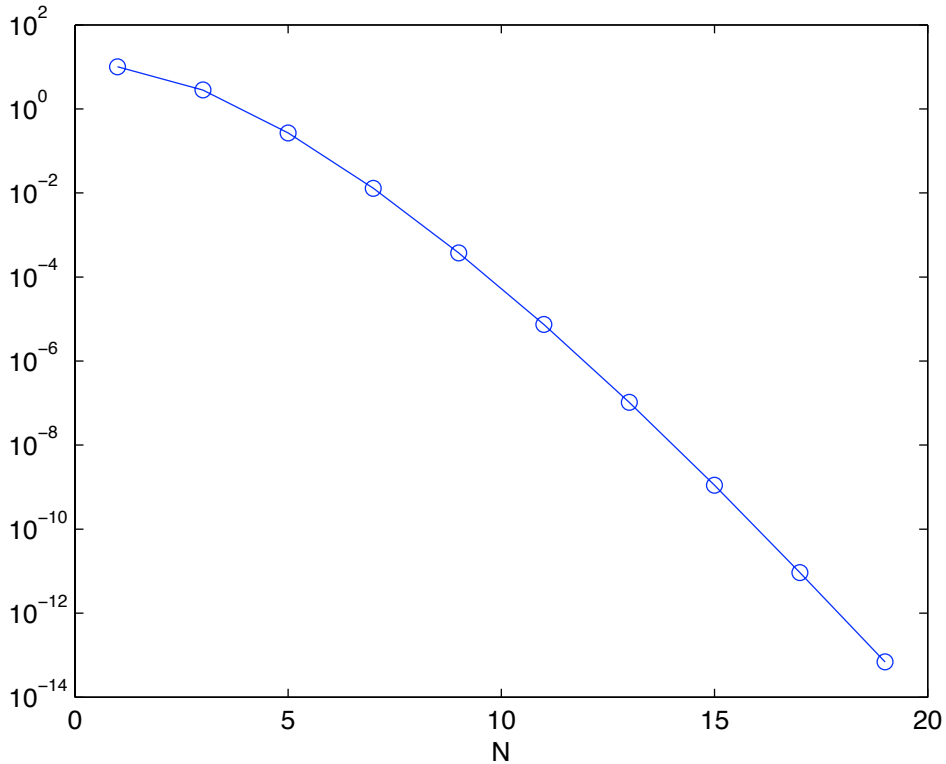
Outline

- Basic approximation theory
- Formulation of SPDE
  - "Basic-er" probability facts
  - Sensitivity analysis
- Generalized polynomial chaos
- Numerical methods
  - Stochastic Galerkin
  - Stochastic collocation

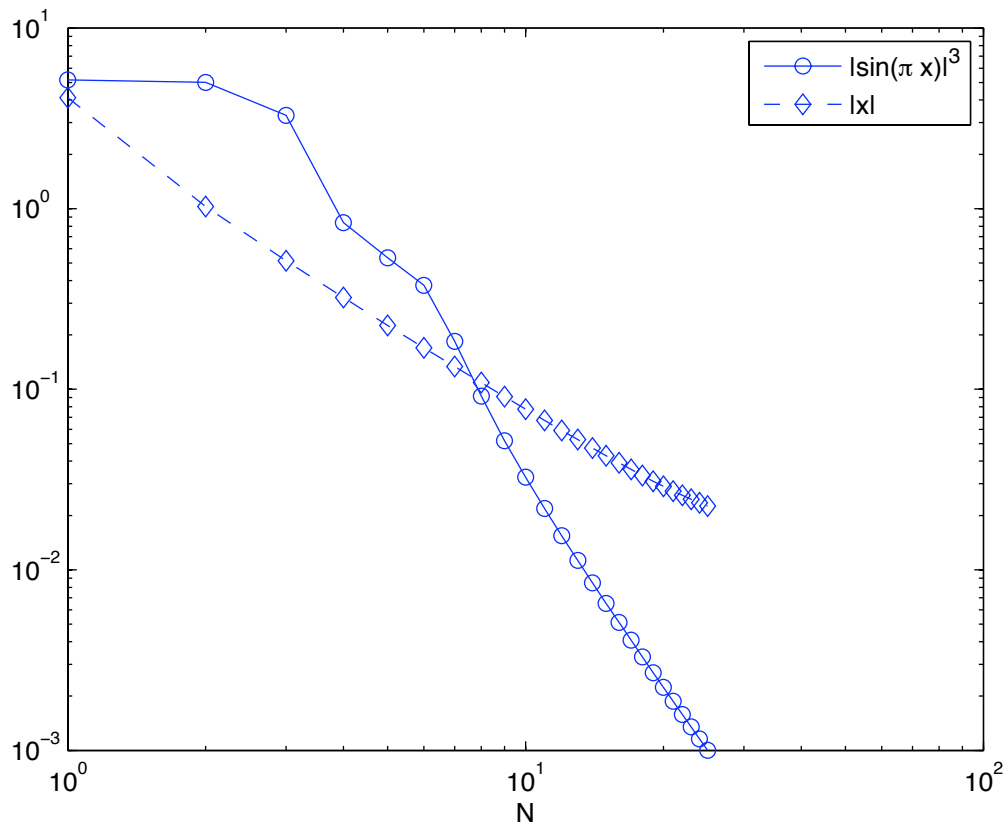
• *Xiu, Numerical methods for stochastic computations, Princeton Univ. Press, 2010*

Spectral Accuracy: exponential convergence



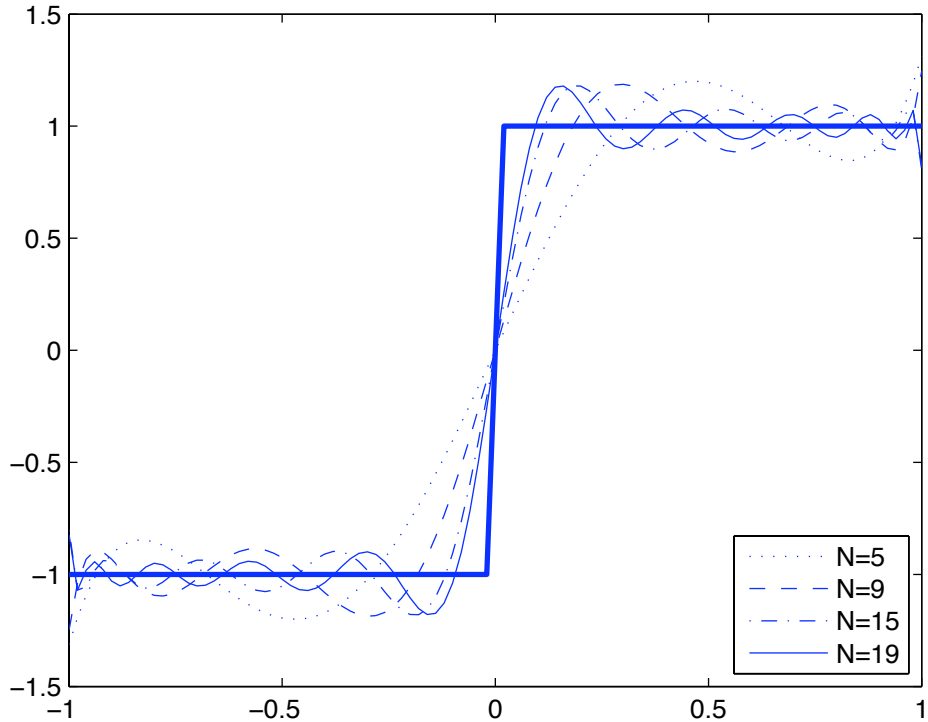
Projection error of $\cos(\pi x)$ by Legendre polynomials

Spectral Accuracy: algebraic convergence



Projection error of $|\sin(\pi x)|^3$ and $|x|$ by Legendre polynomials

Spectral Accuracy: Gibb's phenomenon

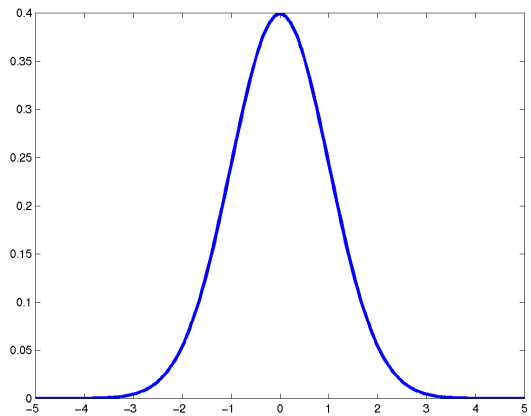


Legendre series expansion of sign function

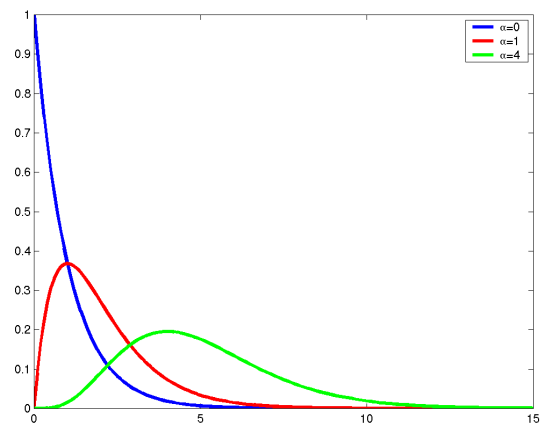
$$\mathrm{sgn}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (4n+3)(2n)!}{2^{2n+1}(n+1)!n!} P_{2n+1}(x).$$

Probability distribution: $F_X(x) = P(X < x) \in [0,1]$

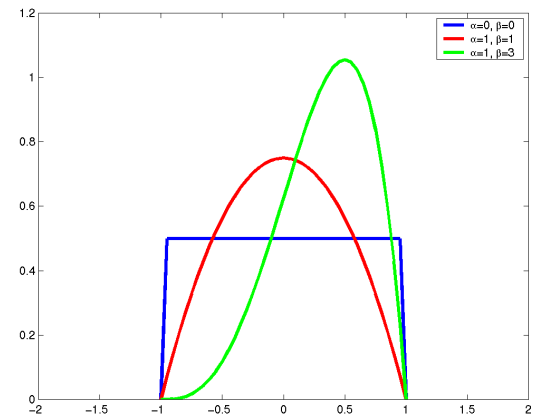
Probability density function (PDF): $\rho_X(x) = \dfrac{dF(x)}{dx}$



Gaussian distribution



Gamma distribution



Beta distribution

Expectation: $\mathbb{E}\big(g(X)\big) = \int g(x)\, dF_X(x) = \int g(x)\rho(x)\, dx$

Mean: $\mu_X = \mathbb{E}\big(X\big)$

Variance: $\sigma^2 = \mathbb{E}\Big(\big(X - \mu_X\big)^2\Big)$

Skewness: $\mathbb{E}\Big(\big(X - \mu_X\big)^3\Big)$

Kurtosis: $\mathbb{E}\Big(\big(X - \mu_X\big)^4\Big)$

(Re-)Formulation of PDE: Input Parameterization

$$\frac{\partial u}{\partial t}(t,x) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Goal:** To characterize the random inputs by a set of random variables
  - Finite number
  - Mutual independence
- **If inputs == parameters**
  - Identify the (smallest) independent set
  - Prescribe probability distribution
- **Else if inputs == fields/processes**
  - Approximate the field by a function of finite number of RVs
  - Well-studied for Gaussian processes
  - Under-developed for non-Gaussian processes
  - Examples: Karhunen-Loeve expansion, spectral decomposition, etc.

$$a(x,\omega) \approx \mu_a(x) + \sum_{i=1}^{d} \tilde{a}_i(x) Z_i(\omega)$$

The Reformulation

- **Stochastic PDE:**

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Solution:** $u(t,x,Z) : [0,T] \times \bar{D} \times \mathbb{R}^{n_Z} \to \mathbb{R}$

- Uncertain inputs are characterized by n_z random variables Z

- Probability distribution of Z is prescribed

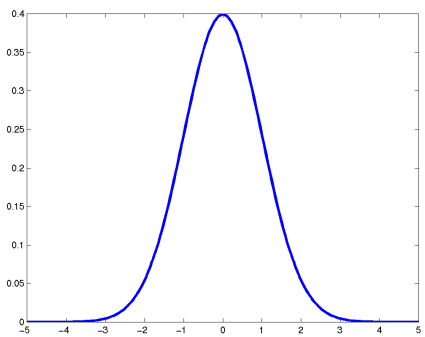
$$F_Z(s) = \Pr(Z \le s), \quad s \in \mathbb{R}^{n_Z}$$

Non-trivial task

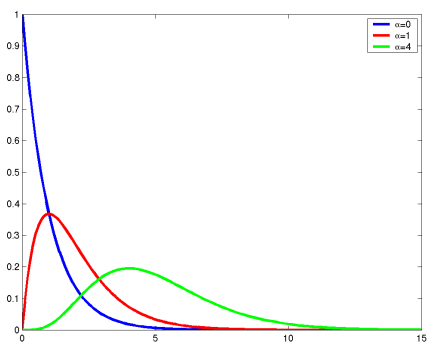
gPC Basis

- **Expectation:** $$\mathbb{E}\big(g(Z)\big) = \int_{\mathbb{R}} g(z)\rho(z)\,dz$$

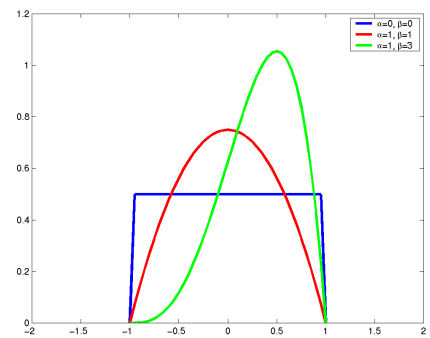
- **Orthogonality:** $$\int \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)\rho(z)\,dz = \mathbb{E}\big[\Phi_{\mathbf{i}}(Z)\Phi_{\mathbf{j}}(Z)\big] = \delta_{\mathbf{ij}}$$



Gaussian distribution



Gamma distribution



Beta distribution

$$\int_{-\infty}^{\infty} \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)e^{-z^2}\,dz = \delta_{\mathbf{ij}}$$

Hermite polynomial

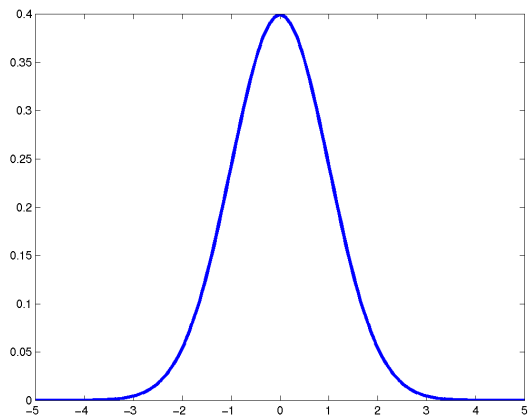
$$\int_{0}^{\infty} \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)e^{-z}\,dz = \delta_{\mathbf{ij}}$$

Laguerre polynomial

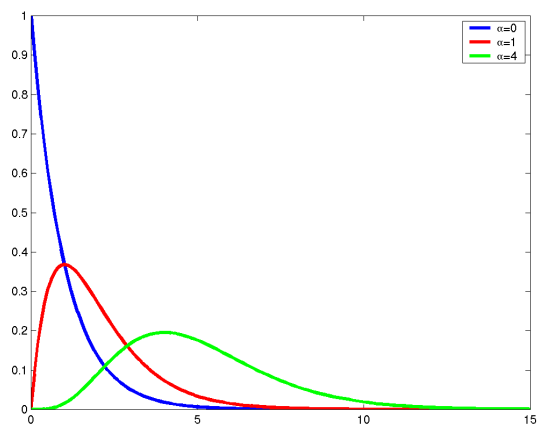
$$\int_{-1}^{1} \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)\,dz = \delta_{\mathbf{ij}}$$

Legendre polynomial

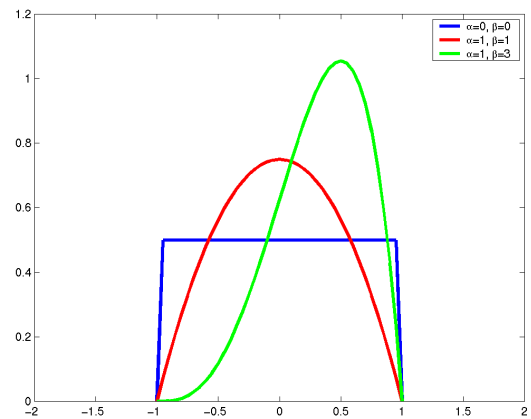
- **Continuous Cases**:
  - *Hermite* Polynomials ⟷ *Gaussian* Distribution
  - *Laguerre* Polynomials ⟷ *Gamma* Distribution
    (special case: *exponential* distribution)
  - *Jacobi* Polynomials ⟷ *Beta* Distribution
  - *Legendre* Polynomials ⟷ *Uniform* Distribution



Gaussian distribution

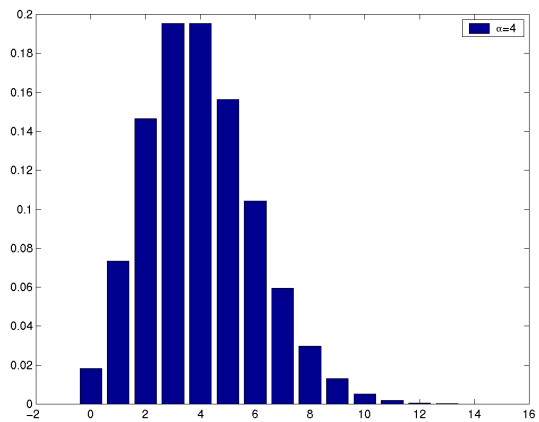


Gamma distribution

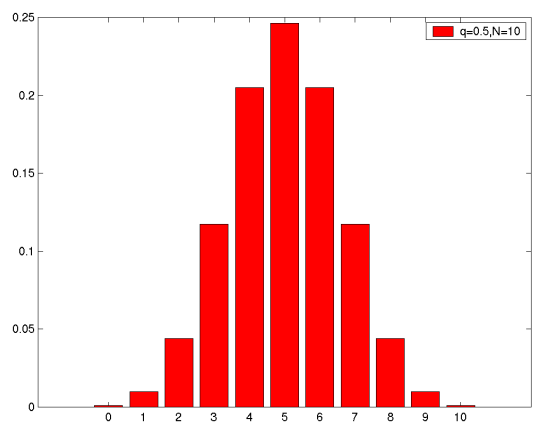


Beta distribution

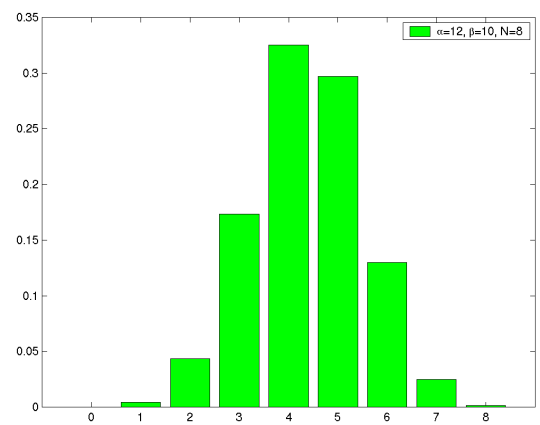
- **Discrete Cases :**
  - *Charlier* Polynomials ⟷ *Poisson* Distribution
  - *Krawtchouk* Polynomials ⟷ *Binomial* Distribution
  - *Hahn* Polynomials ⟷ *Hypergeometric* Distribution
  - *Meixner* Polynomials ⟷ *Pascal* Distribution



Poisson distribution



Binomial distribution

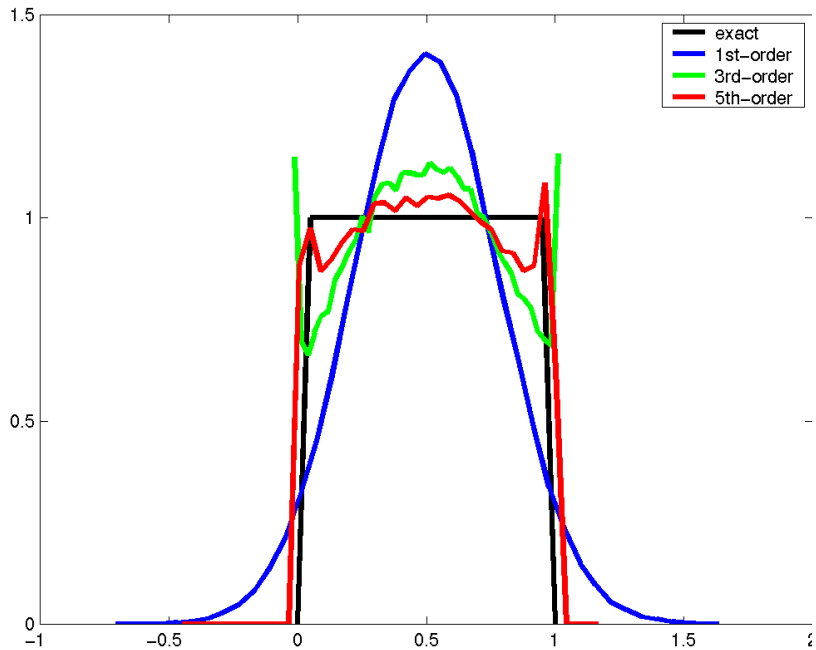


Hypergeometric distribution

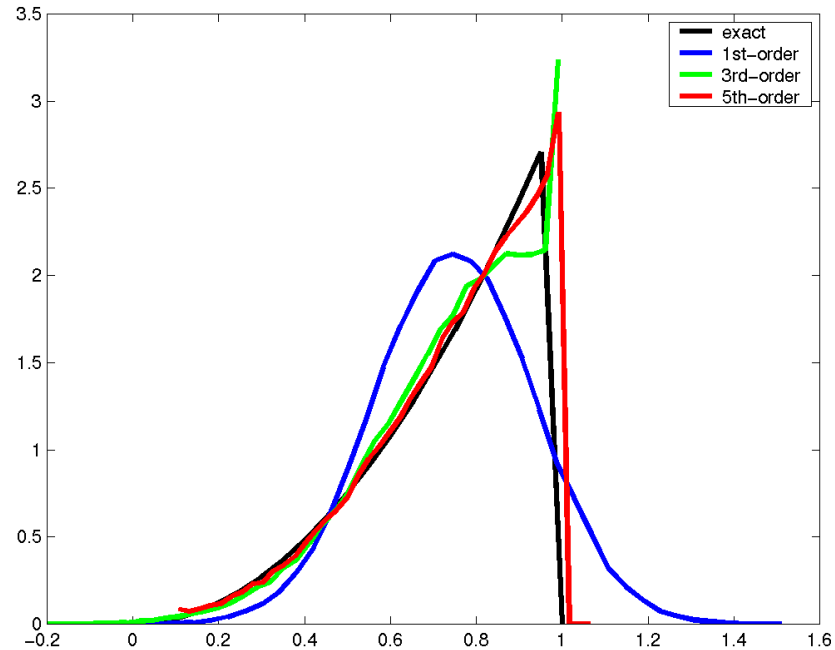
Hermite-Chaos Expansion of Beta Distribution

$$\text{PDF}: \quad f(x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha,\beta)}, \quad \alpha,\beta > 0, \quad 0 \le x \le 1$$

Uniform distribution : $\alpha = 1, \quad \beta = 1$



$\alpha = 3, \quad \beta = 1$



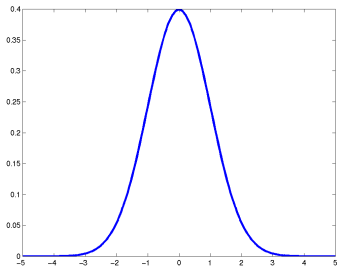
Exact PDF and PDF of 1st, 3rd, 5th-order Hermite-Chaos Expansions

gPC Basis: the Choices

- **Orthogonality:** $$\int \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)\rho(z)\,dz = \mathbb{E}\left[\Phi_{\mathbf{i}}(Z)\Phi_{\mathbf{j}}(Z)\right] = \delta_{\mathbf{ij}}$$

- **Example: Hermite polynomial**

$$\int_{-\infty}^{\infty} \Phi_{\mathbf{i}}(z)\Phi_{\mathbf{j}}(z)e^{-z^2}\,dz = \delta_{\mathbf{ij}}$$

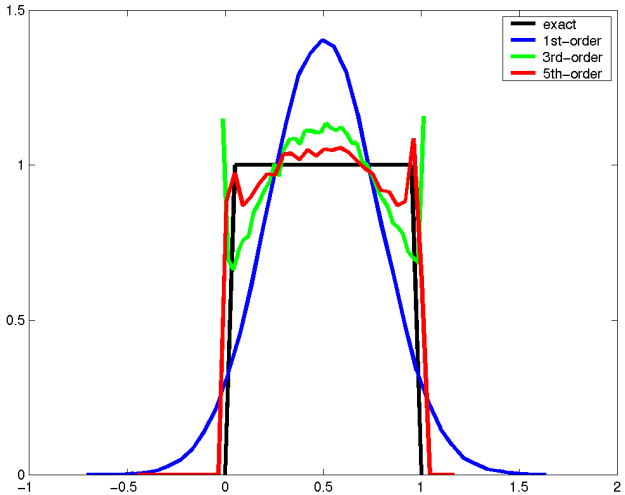


- **The polynomials:** *Z~N(0,1)*

$$\Phi_0 = 1, \quad \Phi_1 = Z, \quad \Phi_2 = Z^2 - 1, \quad \Phi_3 = Z^3 - 3Z, \quad \cdots$$

- **Approximation of arbitrary random variable:** Requires L^2 integrability

- **Example:** Uniform random variable
  - Convergence
  - Non-optimal
  - First-order Legendre is exact



Stochastic Galerkin

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Galerkin method:** Seek

$$u_N(t,x,Z) \triangleq \sum_{|\mathbf{k}|=0}^{N} \hat{u}_{\mathbf{k}}(t,x)\Phi_{\mathbf{k}}(Z)$$

Such that

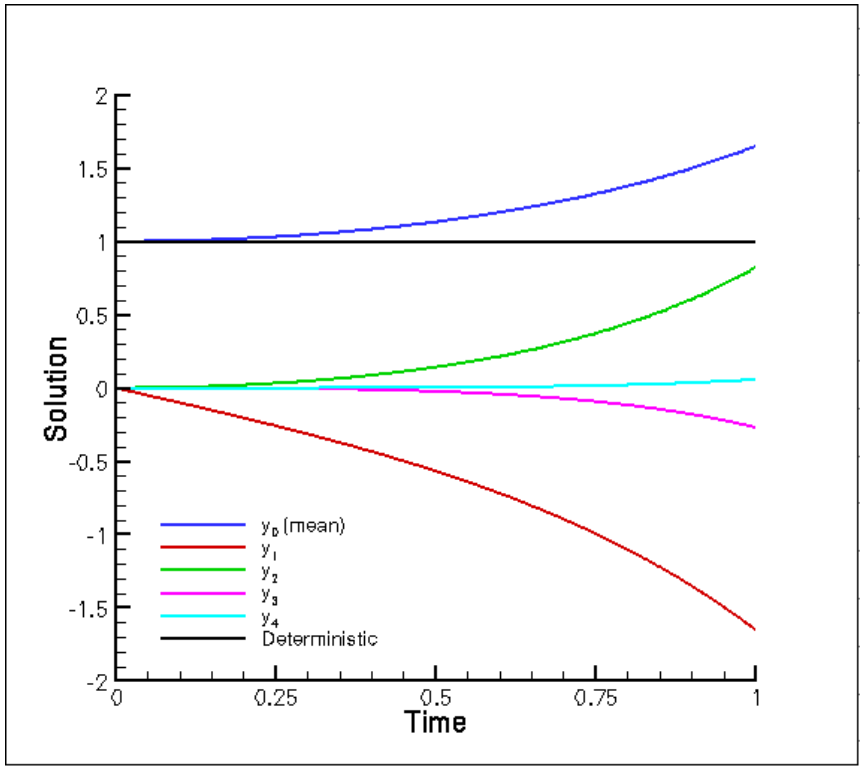
$$\mathbb{E}\left[\frac{\partial u_N}{\partial t}(t,x,Z)\Phi_{\mathbf{m}}(Z)\right] = \mathbb{E}\left[\mathcal{L}(u_N)\Phi_{\mathbf{m}}(Z)\right], \quad \forall |\mathbf{m}| \le N$$

- **The result:**
  - Residue is orthogonal to the gPC space
  - A set of deterministic equations for the coefficients
  - The equations are usually coupled – requires new solver

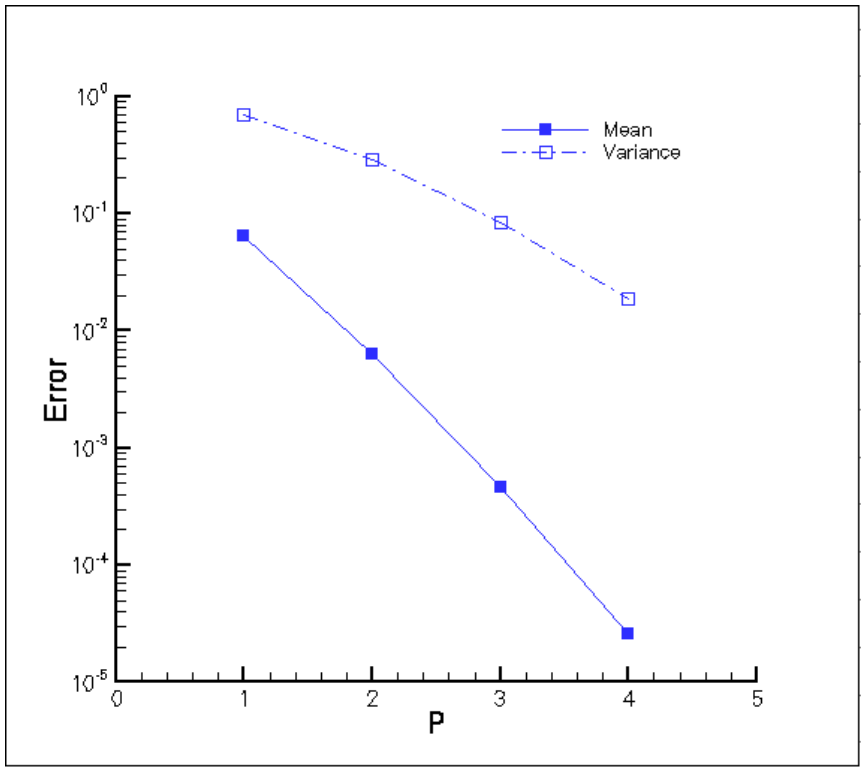
Continuous Distribution : Gaussian (Hermite-Chaos)

- $du/dt = - Z\, y, \;\; u(t=0)=1$
- Z is a **Gaussian** random variable :

$$\text{PDF:} \;\; f_Z(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}$$



Solution of expansion coefficients



Convergence w.r.t. expansion terms

- 4th-order **Hermite-Chaos** expansion
- Exponential convergence rate

Stochastic Collocation

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

- **Collocation:** To satisfy governing equations at selected nodes
  - Allow one to use existing deterministic codes repetitively

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- **Sampling:** (solution statistics only)
  - Random (Monte Carlo)
  - Deterministic (lattice rule, tensor grid, cubature)

- **Stochastic collocation:** To construct **polynomial approximations**
  - Node selection is critical to efficiency and accuracy
  - More than sampling

Stochastic Collocation: Interpolation

$$\frac{\partial u}{\partial t}(t,x,Z) = \mathcal{L}(u) \quad + \text{ boundary/initial conditions}$$

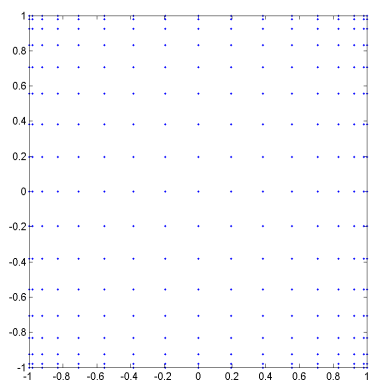
- **Definition:** Given a set of nodes and solution ensemble, find u_N in a proper polynomial space, such that $u_N \approx u$ in a proper sense.

- **Interpolation Approaches:**

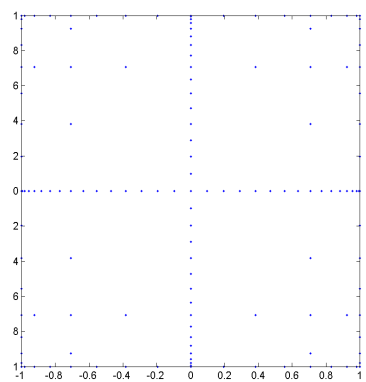
$$u_N(Z) = \sum_{j=1}^{Q} u(Z^j) L_j(Z)$$

$$L_i(Z^j) = \delta_{ij}, \quad 1 \le i, j \le Q$$

  - Dimension-by-dimension space filling



Tensor grids: inefficient



Sparse grids: more efficient

gPC-Collocation: Algorithm

Deterministic solver

1. Choose a nodal set $\left\{Z^j, \alpha^j\right\}_{j=1}^{Q}$ in $\mathbb{R}^{n_z}$

2. Solve for each $j = 1, \cdots, Q$,

$$\frac{\partial u}{\partial t}(t, x, Z^j) = \mathcal{L}(u), \quad \text{in } (0, T] \times D,$$

$$\mathcal{B}(u) = 0, \quad [0, T] \times \partial D,$$

$$u = u_0(x, Z^j), \quad \{t = 0\} \times D$$

Post-process

3. Evaluate the approximate gPC expansion coefficient

$$\hat{w}_{\mathbf{k}} = \sum_{j=1}^{Q} u(t, x, Z^j) \Phi_{\mathbf{k}}(Z^j) \alpha^j, \quad 0 \le |\mathbf{k}| \le N;$$

4. Construct the Nth-order gPC approximation

$$w_N(t, x, Z) = \sum_{|\mathbf{k}|=1}^{N} \hat{w}_{\mathbf{k}} \Phi_{\mathbf{k}}(Z).$$

- **Error bound:**

$$\varepsilon \triangleq \left\| u - w_N \right\|_{L^2(Z)} \le \left(\varepsilon_N^2 + \varepsilon_Q^2 + M \varepsilon_\Delta^2 C_Q^2 \right)^{1/2}$$

Error $\le$ Finite-term projection error + aliasing error + Numerical error