Polynomial Chaos Based Uncertainty Propagation

Lecture 1: Uncertainty and Spectral Expansions

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Goals of this tutorial

- An overview of the key aspects of uncertainty quantification
- 2 Lectures
  - Lecture 1: Context and Fundamentals
    - Introduction to uncertainty
    - The various aspects of UQ
    - Spectral representation of random variables
  - Lecture 2: Forward Propagation and Inverse Problems
- Please do not hesitate to ask questions!!

Outline

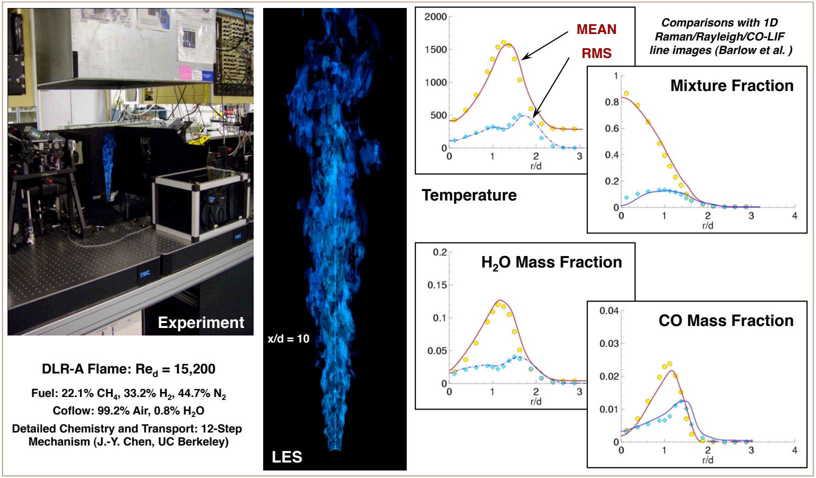
Aspects of Uncertainty Quantification

- Enabling predictive simulation
- Types of uncertainty
- UQ methodologies

Predictive simulations enable science-based design

- Empirical design can be inefficient and costly
  - Trial and error does not work well for complex systems
- Experiments not always feasible or permissible
  - Reliability of nuclear weapons
  - Climate change mitigation approaches
- Predictive simulations provide insight into the physics that drive complex systems
  - Identification of key mechanisms
  - Allows for rigorous optimization strategies

Model validation requires targeted experiments



Large Eddy Simulation (LES) validation on turbulent flame (courtesy J. Oefelein, SNL)

Predictive simulation requires careful assessment of all sources of error and uncertainty

- Numerical errors
    - Grid resolution
    - Time step
    - Time integration order
    - Spatial derivative order
    - Tolerance on iterative solvers
    - Condition number of matrices
- Uncertainties
    - Initial and boundary conditions
    - Model parameters
    - Model equations
    - Coupling between models
    - Sampling noise in particle models
    - Stochastic forcing terms

Governing equations for LES simulation of multiphase reacting flow

- Mass:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}) + \nabla\cdot(\theta\overline{\rho}\tilde{\mathbf{u}}) = \overline{\dot{\rho}}_s$$

- Momentum:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{\mathbf{u}}) + \nabla\cdot\left[\theta\left(\overline{\rho}\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}} + \frac{\mathcal{P}}{M^2}\mathbf{I}\right)\right] = \nabla\cdot(\theta\vec{\vec{\mathcal{T}}}) + \overline{\dot{\mathbf{F}}}_s$$

- Total Energy:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{e}_t) + \nabla\cdot[\theta(\overline{\rho}\tilde{e}_t + \mathcal{P})\tilde{\mathbf{u}}] = \nabla\cdot\left[\theta\left(\vec{\mathcal{Q}}_e + M^2(\vec{\vec{\mathcal{T}}}\cdot\tilde{\mathbf{u}})\right)\right] + \theta\overline{\dot{Q}}_e + \overline{\dot{Q}}_s$$

- Species:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\overline{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{\mathcal{S}}_i) + \theta\overline{\dot{\omega}}_i + \overline{\dot{\omega}}_{s_i}$$

- Spray Source Terms
- Composite Stresses/Fluxes
- Chemical Source Terms

Constitutive models provide closure for governing equations

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\mathbf{I} + \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)\right] - \overline{\rho}\left(\widetilde{\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}} - \tilde{\tilde{\mathbf{u}}} \otimes \tilde{\tilde{\mathbf{u}}}\right)$$

Smagorinsky sub-grid scale model

Dynamic modeling and reacting flows involve additional complexity

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla\cdot\tilde{\mathbf{u}})\mathbf{I} + \left(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\mathbf{u}}^T\right)\right] \; - \; \overline{\rho}\left(\tilde{\mathbf{u}} \,\widetilde{\otimes}\, \tilde{\mathbf{u}} - \tilde{\tilde{\mathbf{u}}} \otimes \tilde{\tilde{\mathbf{u}}}\right)$$

- Energy Flux:

$$\vec{\mathcal{Q}}_e = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr}\right)\frac{C_p}{Re}\nabla\tilde{T} + \sum_{i=1}^{N} \tilde{h}_i \vec{\mathcal{S}}_i \; - \; \overline{\rho} C_p \left(\widetilde{\tilde{T}\tilde{\mathbf{u}}} - \tilde{\tilde{T}}\tilde{\tilde{\mathbf{u}}}\right)$$

- Mass Flux:

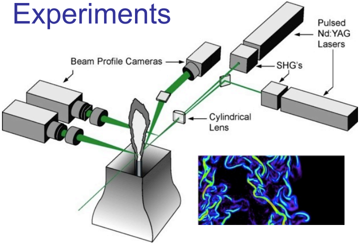
$$\vec{\mathcal{S}}_i = \left(\frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i}\right)\frac{1}{Re}\nabla\tilde{Y}_i \; - \; \overline{\rho}\left(\widetilde{\tilde{Y}_i\tilde{\mathbf{u}}} - \tilde{\tilde{Y}}_i\tilde{\tilde{\mathbf{u}}}\right)$$

Coefficients C_R, Pr_t, and Sc_{t_i} Evaluated Dynamically as Functions of Space and Time

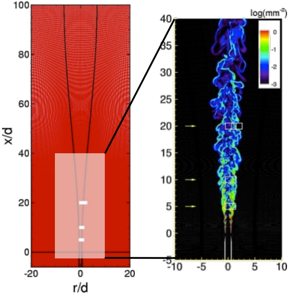
Does additional complexity provide more accuracy and less uncertainty?

Experimental data is used to calibrate models

Experiments



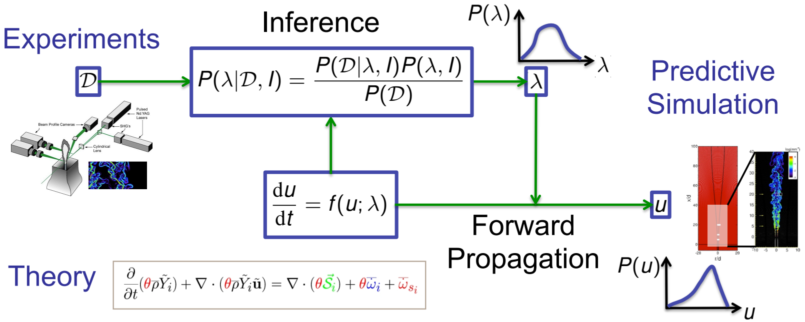
Predictive Simulation



$$\frac{\partial}{\partial t}(\theta\bar{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\bar{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{S}_i) + \theta\bar{\dot{\omega}}_i + \bar{\dot{\omega}}_{s_i}$$

Theory

UQ methods extract information from all sources to enable predictive simulation



- UQ not just about propagating uncertainties
- The term UQ covers a wide range of methods

UQ assesses confidence in model predictions and allows resource allocation for fidelity improvements

- Parameter inference
  - Determine parameters from data
  - Characterize uncertainties in inferred parameters
- Propagate input uncertainties through computational models
  - Account for uncertainty from all sources
  - Resolve coupling between sources
- Analysis
  - Sensitivity analysis
  - Attributions
- Model calibration, validation, selection, averaging

Types of uncertainty

- Epistemic uncertainty
  - Variable has one particular value, but it is not known
  - Reducible: by taking more measurements, we can get to know the value of the variable better
  - Examples
    - The mass of the planet Neptune
    - Ocean temperature at a particular point and time
- Aleatory uncertainty
  - Intrinsic or inherent uncertainty: variable is random; different value each time it is observed
  - Irreducible: taking more measurements will not reduce uncertainty in the value of the variable
  - Examples:
    - Collisions interactions in molecular systems
    - Sampling noise

Point of view matters

- Epistemic versus aleatory sometimes depends on scale level
  - In fully resolved turbulent simulations, velocity field near a wall is deterministic
  - In mesoscale channel flow, near wall velocity field is turbulent forcing term (aleatory)
  - In macroscale channel flow, near wall velocity field provides friction term (epistemic)
- These lectures follow the Bayesian view: probability represents the degree of belief in the value of a variable

Many UQ approaches are available, filling specific needs

Estimation of model/parametric uncertainty

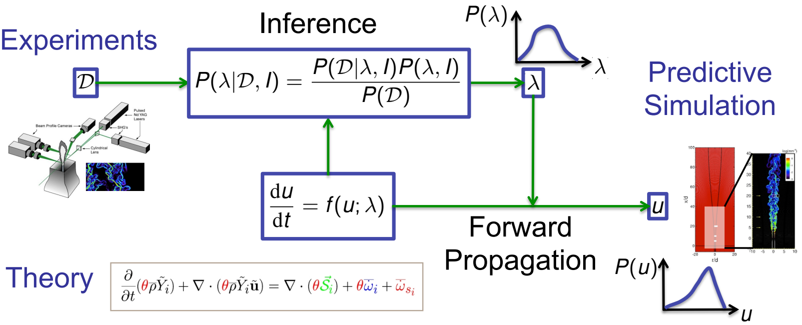
- Expert opinion, data collection
- Regression analysis, fitting, parameter estimation
- Bayesian inference of uncertain models/parameters

Forward propagation of uncertainty in models

- Local sensitivity analysis (SA) and error propagation
- Fuzzy logic; Evidence theory — interval math
- Probabilistic framework — Global SA / stochastic UQ
  - Random sampling, statistical methods (*e.g.* Monte-Carlo)
  - Spectral Polynomial Chaos (PC) Galerkin methods
    - Intrusive or non-intrusive
  - Collocation, interpolants, regression, ... PC/other

Outline

This section focuses on representation of random variables with Polynomial Chaos Expansions (PCEs)



- PCEs are a way to compactly represent random variables
- Often used as a way to characterize parametric uncertainties

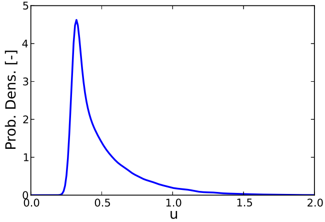
Polynomial Chaos Expansions (PCEs)

- Representation of random variables with PCEs
- Projection of random variables onto PCEs
- PC basis types
- Convergence of PCEs
- Analysis of PCEs

Polynomial Chaos Expansions Represent Random Variables

$$u = \sum_{k=0}^{P} u_k \psi_k(\xi)$$

- u: Random Variable (RV) represented with 1D PCE
- u_k: PC coefficients (deterministic)
- ψ_k: 1D Hermite polynomial of order k
- ξ: Gaussian RV

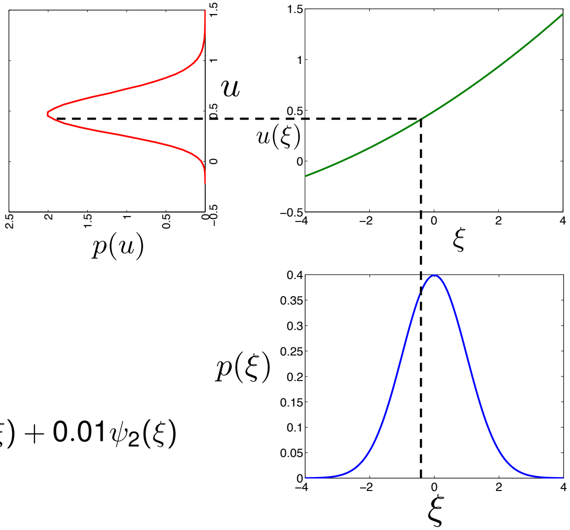


$$u = 0.5 + 0.2\psi_1(\xi) + 0.1\psi_2(\xi)$$

Expansion in terms of functions of random variables multiplied with deterministic coefficients

- Set of deterministic PC coefficients fully describes RV
- Separates randomness from deterministic dimensions

PCEs are a functional map from standard RVs to the represented RV



$$u = 0.5 + 0.2\psi_1(\xi) + 0.01\psi_2(\xi)$$

One-Dimensional Hermite Polynomials

$$\begin{aligned}\psi_0(\xi) &= 1 \\ \psi_k(\xi) &= (-1)^k e^{\xi^2/2} \frac{\mathrm{d}^k}{\mathrm{d}\xi^k} e^{-\xi^2/2}, \qquad k = 1, 2, \dots\end{aligned}$$

$$\psi_1(\xi) = x, \quad \psi_2(\xi) = \xi^2 - 1, \quad \psi_3(\xi) = \xi^3 - 3\xi, \ \dots$$

The Hermite polynomials form an orthogonal basis over $[-\infty, \infty]$ with respect to the inner product

$$\langle \psi_i \psi_j \rangle \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi_i(\xi)\psi_j(\xi) w(\xi) d\xi = \delta_{ij} \left\langle \psi_i^2 \right\rangle$$

where $w(\xi) = e^{-\xi^2/2}$ is the weight function.
Note that $\frac{e^{-\xi^2/2}}{\sqrt{2\pi}}$ is the density of a standard normal random variable

Multidimensional Hermite Polynomials

The multidimensional Hermite polynomial $\Psi_i(\xi_1, \ldots, \xi_n)$ is a tensor product of the 1D Hermite polynomials, with a suitable multi-index $\boldsymbol{\alpha^i} = (\alpha_1^i, \alpha_2^i, \ldots, \alpha_n^i)$,

$$\Psi_i(\xi_1, \ldots, \xi_n) \;=\; \prod_{k=1}^{n} \psi_{\alpha_k^i}(\xi_k)$$

For example, 2D Hermite polynomials:

i	p	Ψ_i	α^i
0	0	1	(0,0)
1	1	ξ_1	(1,0)
2	1	ξ_2	(0,1)
3	2	$\xi_1^2 - 1$	(2,0)
4	2	$\xi_1\xi_2$	(1,1)
5	2	$\xi_2^2 - 1$	(0,2)
...	...	...	...

Multidimensional Polynomial Chaos Expansion

$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi_1, \ldots, \xi_n)$$

- u: Random Variable (RV) represented with multi-D PCE
- u_k: PC coefficients (deterministic)
- Ψ_k: Multi-D Hermite polynomials up to order p
- ξ_i: Gaussian RV
- n: Dimensionality of stochastic space
- $P+1$: Number of PC terms: $P+1 = \frac{(n+p)!}{n!p!}$

The number of dimensions represents the number of independent inputs, degrees of freedom for u

- E.g. one stochastic dimension per uncertain model parameter
- Contributions from each uncertain input can be identified

Polynomial Chaos Expansions (PCEs)

- Representation of random variables with PCEs
- Projection of random variables onto PCEs
- PC basis types
- Convergence of PCEs
- Analysis of PCEs

Obtaining PC coefficients for arbitrary random variables

- This is a hard problem in general
- Random Variable can be specified in a variety of ways, but often incomplete
  - Probability Density Function (PDF)
  - Samples
  - Expert opinion (*e.g.* “somewhere between 2 and 4”)
- Particular case of a random variable specified by a PDF is generally tractable

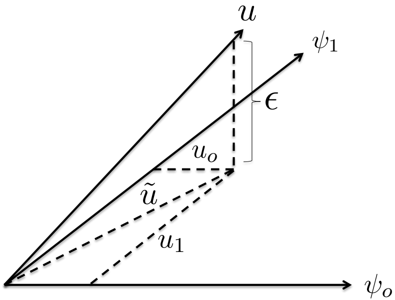
The PC basis functions are orthogonal with respect to the probability measure of the associated RVs.

$$
\begin{aligned}
\langle \Psi_i \Psi_j \rangle &\equiv \int \ldots \int \Psi_i(\boldsymbol{\xi}) \Psi_j(\boldsymbol{\xi}) g(\xi_1) g(\xi_2) \cdots g(\xi_n) \mathrm{d}\xi_1 \mathrm{d}\xi_2 \cdots \mathrm{d}\xi_n \\
&= \prod_{k=1}^{n} \left\langle \psi_{\alpha_k^i}(\xi_k) \psi_{\alpha_k^j}(\xi_k) \right\rangle = \delta_{ij} \left\langle \Psi_i^2 \right\rangle
\end{aligned}
$$

where,

$$
g(\xi) = \frac{e^{-\xi^2/2}}{\sqrt{2\pi}}
$$

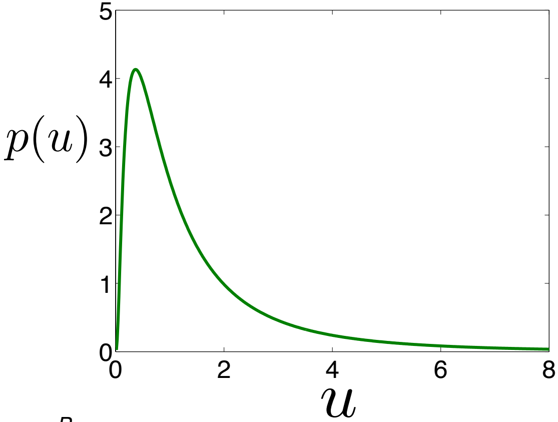
Orthogonality enables a Galerkin projection to determine the PC coefficients.



$$u \approx \sum_{k=0}^{P} u_k \Psi_k \quad \Rightarrow \quad \langle \Psi_i u \rangle = \sum_{k=0}^{P} u_k \langle \Psi_i \Psi_k \rangle = u_i \langle \Psi_i^2 \rangle$$

$$\Rightarrow \quad u_i = \frac{\langle u \Psi_i \rangle}{\langle \Psi_i^2 \rangle}$$

Galerkin projection requires functional relationship between random variable and germ of PCE.



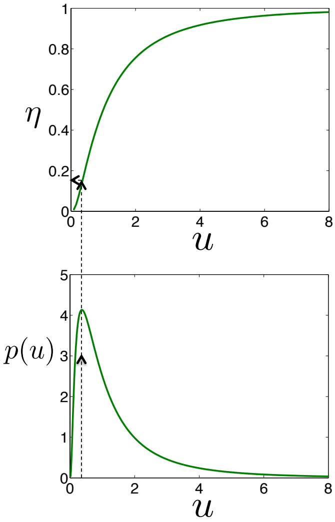
$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi) \qquad \Rightarrow \qquad u_i = \frac{\langle u \, \Psi_i(\xi) \rangle}{\langle \Psi_i^2 \rangle}$$

Cumulative Distribution Function (CDF) maps arbitrary random variable to a uniform random variable

- Consider u with PDF $p(u)$
- CDF of u is given by

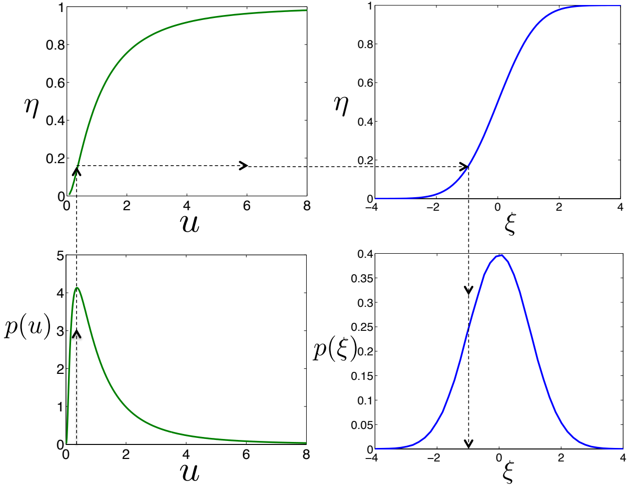
$$F(u) = \int_{-\infty}^{u} p(s)ds$$

- $F(u)$ maps u to η, uniform on $[0, 1]$



Inverse CDF mapping enables Galerkin Projection

- $\eta = F(u)$
- $\eta = \Phi(\xi)$ maps uniform η to normal RV ξ
- $u = F^{-1}(\Phi(\xi))$

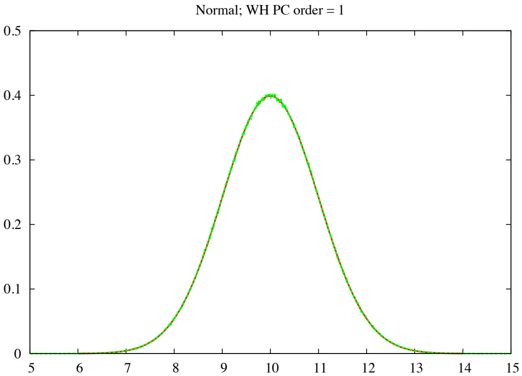


$$\langle u\, \Psi_i(\xi) \rangle = \int \underbrace{F^{-1}(\Phi(\xi))}_{u} \Psi_i(\xi) w(\xi) d\xi$$

PC Illustration: PC Expansion for a Normal RV

- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 1

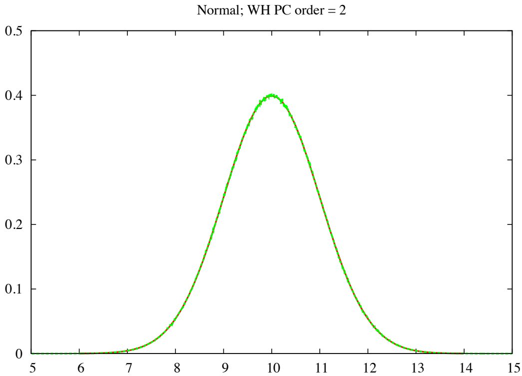
$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1 \xi
\end{aligned}
$$



PC Illustration: PC Expansion for a Normal RV

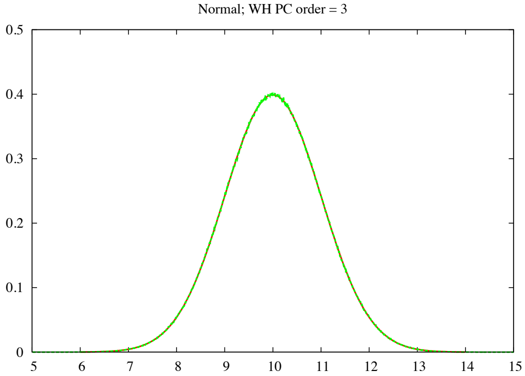
- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 2

$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1 \xi + u_2(\xi^2 - 1)
\end{aligned}
$$



PC Illustration: PC Expansion for a Normal RV

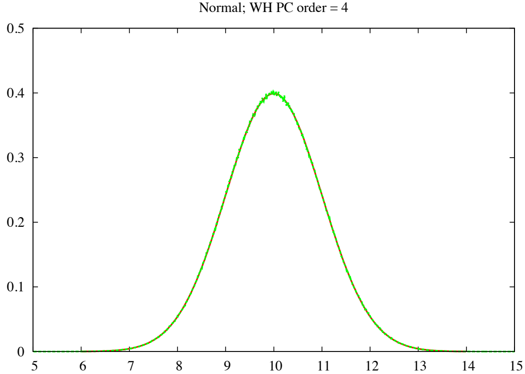
- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 3



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi)
\end{aligned}
$$

PC Illustration: PC Expansion for a Normal RV

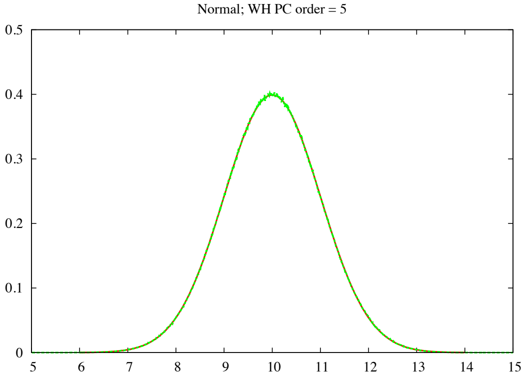
- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 4



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3)
\end{aligned}
$$

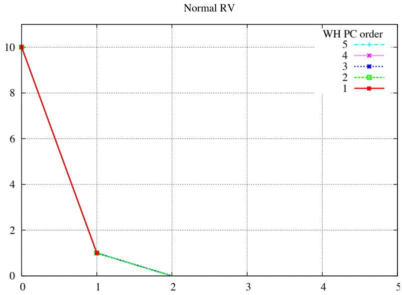
PC Illustration: PC Expansion for a Normal RV

- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 5



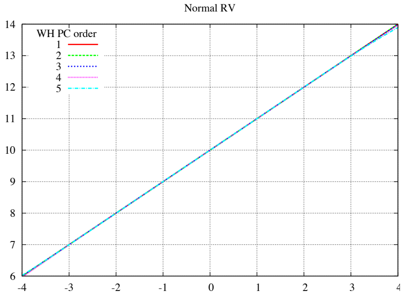
$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3) \\
&\quad + u_5(\xi^5 - 10\xi^3 + 15\xi)
\end{aligned}
$$

PC Illustration: WH PCE for a Normal RV



PC mode amplitudes

u_0–u_5



PC function $u(\xi)$

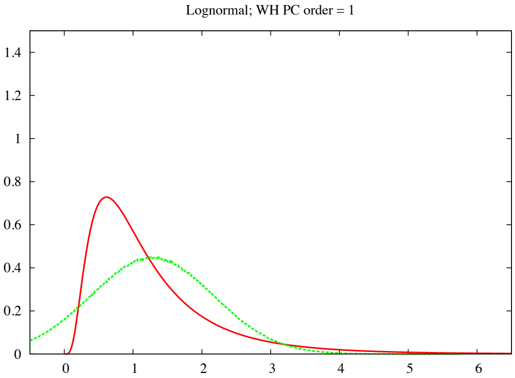
Order 1–5

- First order Wiener-Hermite PCE exact for a normal RV
- Linear function of ξ
- Higher order terms are negligible

PC Illustration: WH PCE for a Lognormal RV

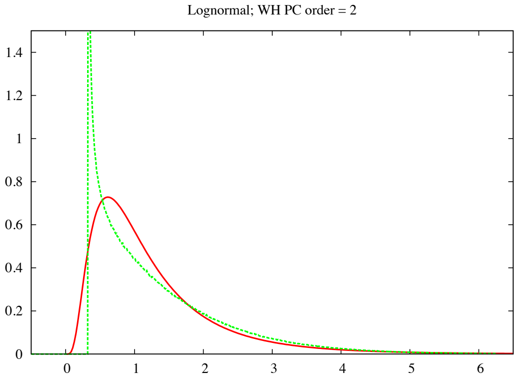
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 1

$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1 \xi
\end{aligned}
$$



PC Illustration: WH PCE for a Lognormal RV

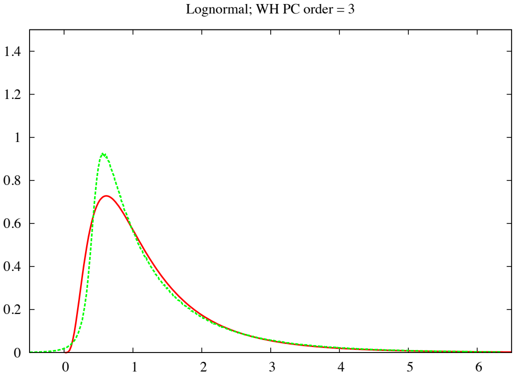
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 2



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1 \xi + u_2(\xi^2 - 1)
\end{aligned}
$$

PC Illustration: WH PCE for a Lognormal RV

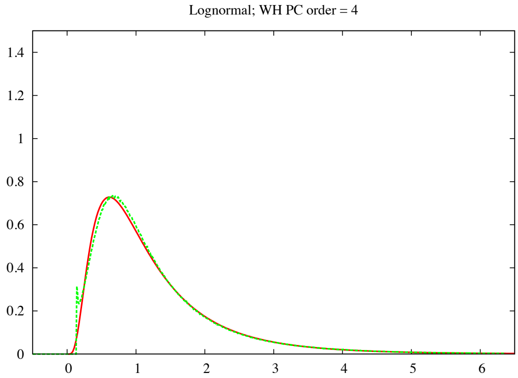
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 3



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1 \xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi)
\end{aligned}
$$

PC Illustration: WH PCE for a Lognormal RV

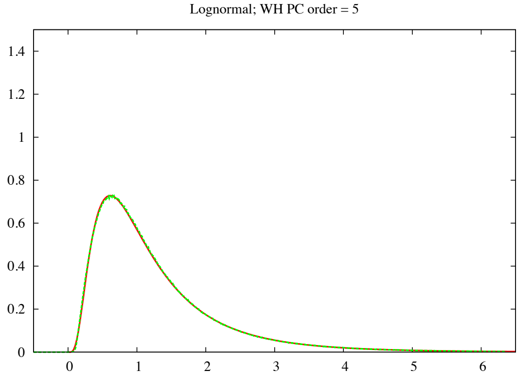
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 4



$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3)
\end{aligned}
$$

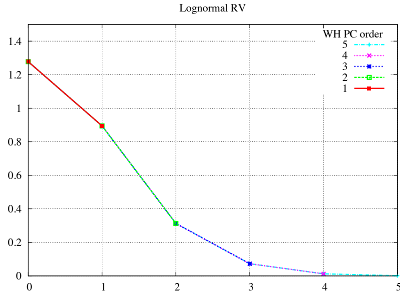
PC Illustration: WH PCE for a Lognormal RV

- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 5



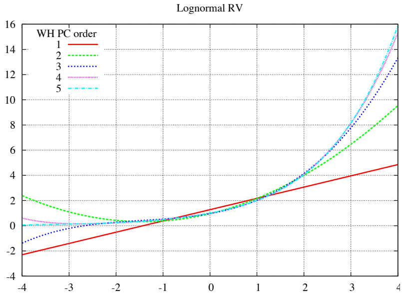
$$
\begin{aligned}
u &= \sum_{k=0}^{P} u_k \Psi_k(\xi) \\
&= u_0 + u_1\xi + u_2(\xi^2 - 1) + u_3(\xi^3 - 3\xi) + u_4(\xi^4 - 6\xi^2 + 3) \\
&\quad + u_5(\xi^5 - 10\xi^3 + 15\xi)
\end{aligned}
$$

PC Illustration: WH PCE for a Lognormal RV



PC mode amplitudes

u_0–u_5



PC function $u(\xi)$

Order 1–5

- Fifth-order Wiener-Hermite PCE represents the given Lognormal well
- Higher order terms are negligible

Polynomial Chaos Expansions (PCEs)

- Representation of random variables with PCEs
- Projection of random variables onto PCEs
- PC basis types
- Convergence of PCEs
- Analysis of PCEs

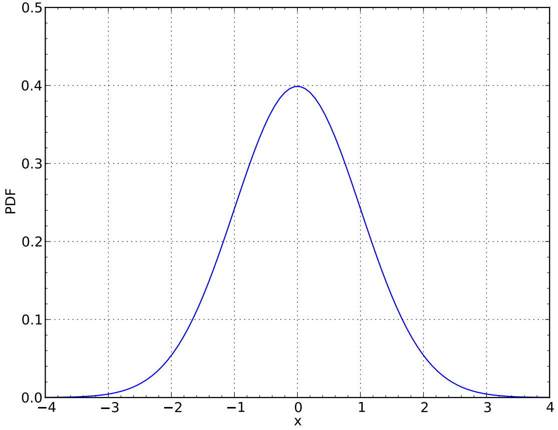
Generalized Polynomial Chaos

PC Type	Domain	Density $w(\xi)$	Polynomial	Free parameters
Gauss-Hermite	$(-\infty,+\infty)$	$\frac{1}{\sqrt{2\pi}}e^{-\frac{\xi^2}{2}}$	Hermite	none
Legendre-Uniform	$[-1,1]$	$\frac{1}{2}$	Legendre	none
Gamma-Laguerre	$[0,+\infty)$	$\frac{x^\alpha e^{-\xi}}{\Gamma(\alpha+1)}$	Laguerre	$\alpha > -1$
Beta-Jacobi	$[-1,1]$	$\frac{(1+\xi)^\alpha(1-\xi)^\beta}{2^{\alpha+\beta+1}B(\alpha+1,\beta+1)}$	Jacobi	$\alpha > -1, \beta > -1$

Inner product: $\langle\psi_i\psi_j\rangle \equiv \int_a^b \psi_i(\xi)\psi_j(\xi)w(\xi)d\xi = \delta_{ij}\left\langle\psi_i^2\right\rangle$

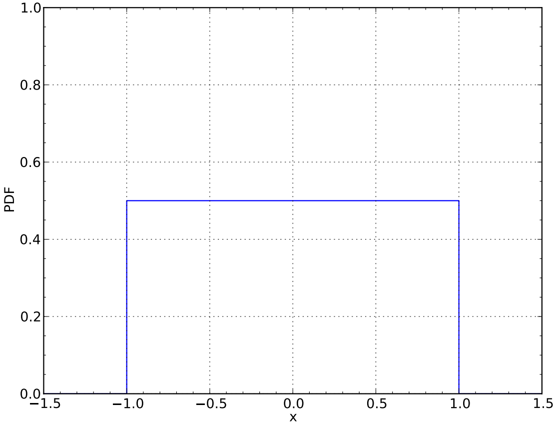
- Wiener-Askey scheme provides a hierarchy of possible continuous PC bases [Xiu and Karniadakis, 2002]
  - Legendre-Uniform is special case of Beta-Jacobi
- Input parameter domain often dictates the most convenient choice of PC
- Polynomials can also be tailored to be orthogonal w.r.t. chosen, arbitrary density

Normal Distribution



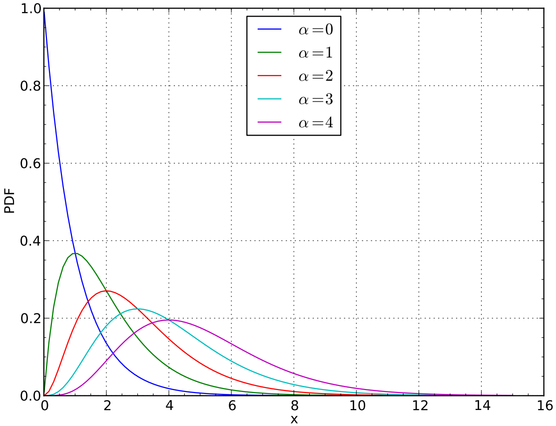
- Most commonly used density in PCEs
- Support on $(-\infty, +\infty)$

Uniform Distribution



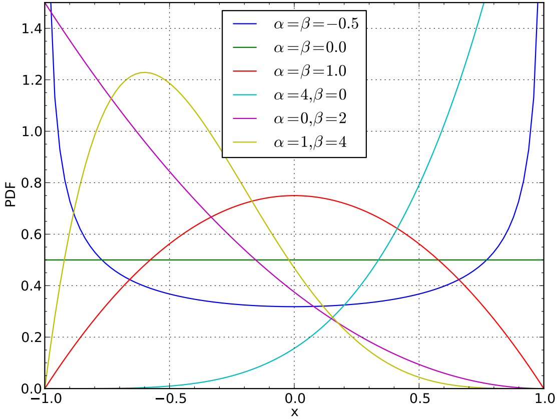
- Appropriate for variables with sharp bounds on their distribution
- Support on $[-1, 1]$

Gamma Distribution



- Useful to represent quantities that are strictly positive
- Support on $[0, +\infty)$

Beta Distribution



- Good for quantities that vary between set boundaries
- Can be tailored to preferentially weight some areas
- Support on $[-1, 1]$

Polynomial Chaos Expansions (PCEs)

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More Formally: Probability Spaces and Random Variables

- Let $(\Theta, \mathfrak{S}, \mathbb{P})$ be a probability space
  - Θ is an event space
  - $\mathfrak{S}$ is a σ-algebra on Θ
  - $\mathbb{P}$ is a probability measure on $(\Theta, \mathfrak{S})$
- Random variables are functions $\Xi : \Theta \to \mathbb{R}$ with a measure corresponding to their image:
  - if $\Xi^{-1}(A) \in \mathfrak{S}$, then define $\mu(A) = \mathbb{P}(\Xi^{-1}(A))$
  - $p(\xi) = d\mu/d\xi$: the density of the random variable Ξ (with respect to Lebesgue measure on $\mathbb{R}$)
  - Expectation: $\langle f \rangle = \int f\, d\mu = \int f\, p(\xi)\, d\xi$

Convergence of PC expansions

- General convergence theorems are subject of ongoing research
- Depends on the underlying random variables ξ
  - Wiener-Hermite Chaos has been well-studied
  - Generalized PC less so
- Ernst et al. 2011:
  - Let $\xi : \Theta \to \mathbb{R}^N$ such that for $i = 1, \ldots, N$ each $\xi_i : \Theta \to \mathbb{R}$, be a set of random variables
  - $\mathfrak{S}(\xi)$: σ-algebra generated by the set ξ
  - $L^2(\Theta, \mathfrak{S}(\xi), \mathbb{P})$: Hilbert space of real random variables defined on $(\Theta, \mathfrak{S}(\xi), \mathbb{P})$ with finite second moments
  - Any random variable in this σ-algebra can be represented with a Polynomial Chaos expansion with germ ξ

Convergence of PC expansions

- Proof does not state that any RV with finite variance can be represented with a PCE to arbitrary precision
  - In practice, one rarely knows how many degrees of freedom a RV has
  - Also, RV specification is rarely complete
  - In an engineering sense, the choice of the germ and the PCE order is seen as a model choice to represent what is known about a RV

How do I know my PCE is converged?

- Approximation error in PCE is topic of a lot of research
- Rules of thumb:
  - Higher order PC coefficients should decay
  - Increase order until results no longer change
  - Not always fail-proof ...

Polynomial Chaos Expansions (PCEs)

- Representation of random variables with PCEs
- Projection of random variables onto PCEs
- PC basis types
- Convergence of PCEs
- Analysis of PCEs
    - Moments
    - Probability Density Functions

Moments of RVs described with PCEs

$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi)$$

- Expectation: $\langle u \rangle = u_0$
- Variance σ^2

$$\begin{aligned}
\sigma^2 &= \left\langle (u - \langle u \rangle)^2 \right\rangle = \left\langle (\sum_{k=1}^{P} u_k \Psi_k(\xi))^2 \right\rangle \\
&= \left\langle \sum_{k=1}^{P} \sum_{j=1}^{P} u_j u_k \Psi_j(\xi) \Psi_k(\xi) \right\rangle \\
&= \sum_{k=1}^{P} \sum_{j=1}^{P} u_j u_k \left\langle \Psi_j(\xi) \Psi_k(\xi) \right\rangle = \sum_{k=1}^{P} u_k^2 \left\langle \Psi_k(\xi)^2 \right\rangle
\end{aligned}$$

Kernel Density Estimation to Get Probability Density Function of Random Variable Corresponding to PCEs

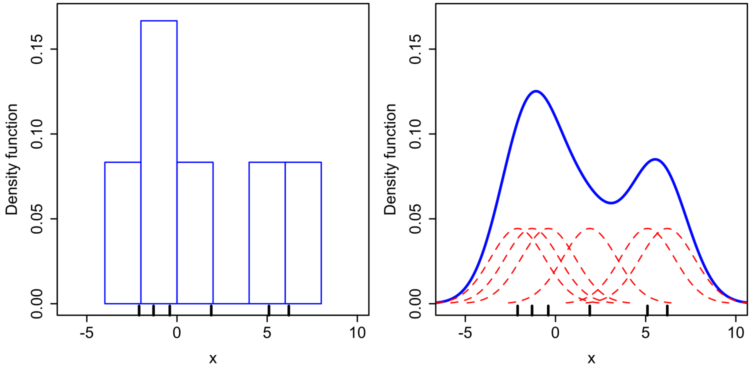
- PCE $u = \sum_{k=0}^{P} u_k \Psi_k(\xi)$ is cheap to sample
  - Brute-force sampling and bin samples into histogram
  - Use Kernel Density Estimation (KDE) to get smoother PDF with fewer samples u^i

$$\mathrm{PDF}(u) = \frac{1}{N_s h} \sum_{i=1}^{N_s} K\left(\frac{u - u^i}{h}\right)$$

    K is the kernel, h is the bandwidth.
  - Gaussian KDE is commonly used with $K(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$, leading to

$$\mathrm{PDF}(u) = \frac{1}{\sqrt{2\pi} N_s h} \sum_{i=1}^{N_s} \exp\left(-\frac{(u - u^i)^2}{2h^2}\right)$$

Comparison of histograms and KDE



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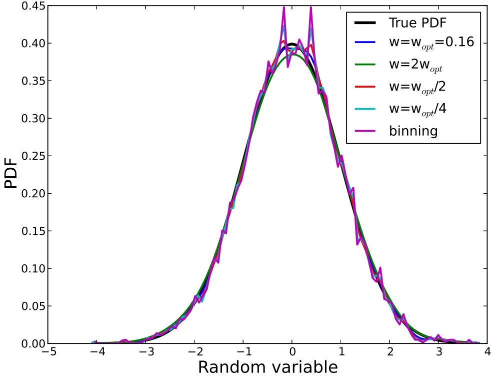
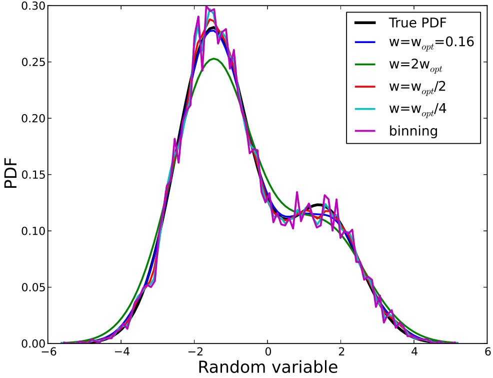
- Bandwidth *h* needs to be chosen carefully to avoid oversmoothing

KDE requires judicious choice of bandwidth h



- Scott's rule-of-thumb optimal for Gaussian RV: $h = N^{-\frac{1}{d+4}}$
- Smaller h makes KDE more accurate, but more noisy
- Binning is similar to smaller h case, for proper choice of N_{bins}

KDE requires judicious choice of bandwidth h



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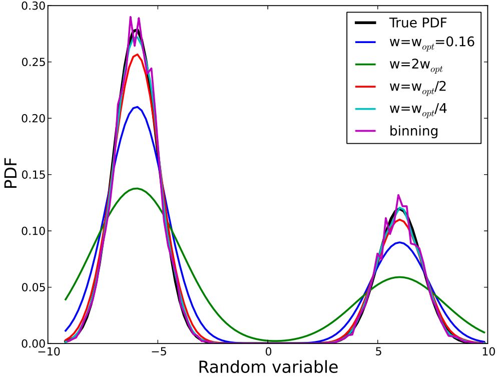

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Extra Material

- Analytical approach to obtain PDF of random variable

Probability Density Function of Random Variable Corresponding to PCEs – 1

- Assume one-dimensional PCE

$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi) = f(\xi)$$

- To evaluate PDF of u: $p_u(\cdot)$

$$p_u(u)du = \sum_{i}^{N} p_\xi(\xi^i)d\xi$$

where $\xi^1, \ldots, \xi^N$ are the N roots of $f(\xi) - u = 0$
Many possible ξ may give you this particular u and all of them contribute to the probability density at u.

Probability Density Function of Random Variable Corresponding to PCEs – 2

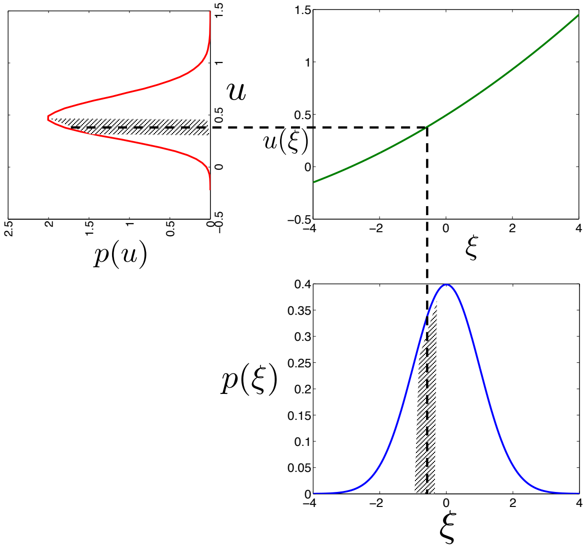
- More compactly

$$p_u(u) = \sum_{\xi \in R_u} \frac{p_\xi(\xi)}{|Df(\xi)|}$$

where $R_u = \xi : f(\xi) - u = 0$ and $|Df(\xi)| = |df/d\xi|$ evaluated at ξ

- Hard to generalize to multi-D PC expansions

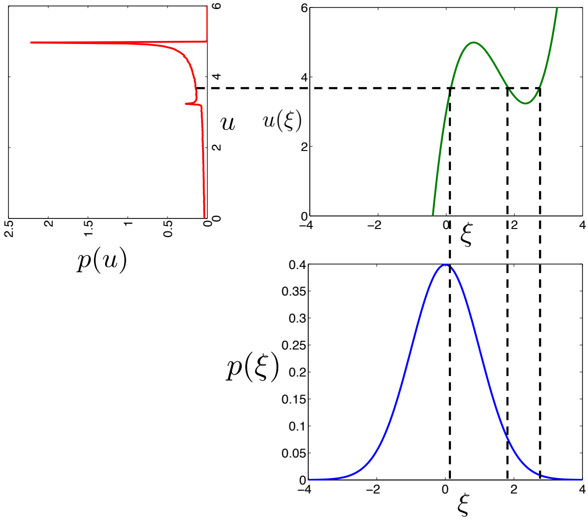
PCE to PDF for monotonic mapping between ξ and u



$$p_u(u) = \sum_{\xi \in R_u} \frac{p_\xi(\xi)}{|Df(\xi)|}$$

$$R_u = \xi : f(\xi) - u = 0$$
$$|Df(\xi)| = |df/d\xi|$$

PCE to PDF for non-monotonic mapping between ξ and u



$$p_u(u) = \sum_{\xi \in R_u} \frac{p_\xi(\xi)}{|Df(\xi)|}$$

$$R_u = \xi : f(\xi) - u = 0$$
$$|Df(\xi)| = |df/d\xi|$$

Further Reading

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