

Polynomial Chaos

Uncertainty Quantification

SAND2015-0639PE

Lecture 3: Characterization of Random Variables and Processes

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and many others ...

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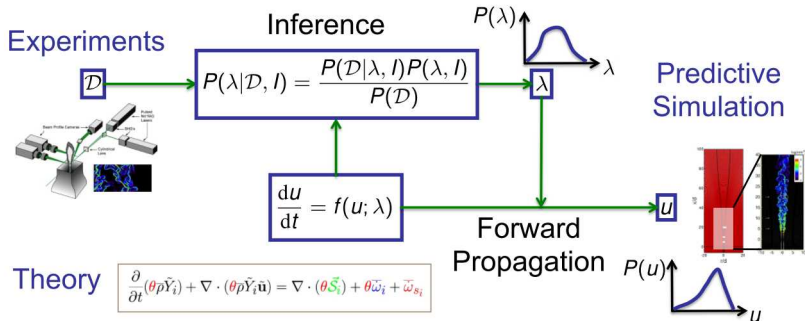
Goals of This Tutorial

- 4 Lectures
 - Lecture 1: Context and Fundamentals
 - Lecture 2: Forward Propagation
 - Lecture 3: Characterization
 - Sensitivity Analysis
 - Representing Arbitrary Random Variables
 - Representing Random Fields
 - Lecture 4: Bayesian Inference – UQ Software

Outline

- ➊ Introduction
- ➋ Sensitivity Analysis
- ➌ Representing Arbitrary RVs
- ➍ Representing Random Fields
- ➎ References

Sensitivity analysis gives insight into key sources of uncertainty



- Obtaining global sensitivity analysis from PCEs
 - Identify dominant sources of uncertainty
 - Attribution

PC Postprocessing: global sensitivity information is readily obtained from PCE

$$g(\xi_1, \dots, \xi_d) = \sum_{k=0}^P c_k \psi_k(\xi)$$

- Global sensitivity analysis $\equiv$ Variance decomposition
- Total variance

$$\text{Var}[g(\xi)] = \sum_{k>0} c_k^2 \|\psi_k\|^2$$

PC Postprocessing: Main Effect and Joint Sensitivity Indices

- Main effect sensitivity indices

$$S_i = \frac{\text{Var}[\mathbb{E}(g(\xi|\xi_i))]}{\text{Var}[g(\xi)]} = \frac{\sum_{k \in \mathbb{I}_i} c_k^2 \|\psi_k\|^2}{\sum_{k > 0} c_k^2 \|\psi_k\|^2}$$

- $\mathbb{I}_i$ is the set of bases with only ξ_i involved
- S_i is the uncertainty contribution that is due to i -th parameter only
- Joint sensitivity indices

$$S_{ij} = \frac{\text{Var}[\mathbb{E}(g(\xi|\xi_i, \xi_j))]}{\text{Var}[g(\xi)]} - S_i - S_j = \frac{\sum_{k \in \mathbb{I}_{ij}} c_k^2 \|\psi_k\|^2}{\sum_{k > 0} c_k^2 \|\psi_k\|^2}$$

- $\mathbb{I}_{ij}$ is the set of bases with only ξ_i and ξ_j involved
- S_{ij} is the uncertainty contribution that is due to (i, j) parameter pair

PC Postprocessing: Total Effect Sensitivity Indices

- Total effect sensitivity indices

$$T_i = 1 - \frac{\text{Var}[\mathbb{E}(g(\xi|\xi_{-i}))]}{\text{Var}[g(\xi)]} = \frac{\sum_{k \in \mathbb{I}_i^T} c_k^2 \|\psi_k\|^2}{\sum_{k > 0} c_k^2 \|\psi_k\|^2}$$

- The notation ξ_{-i} indicates terms that do not have ξ_i in them
- $\mathbb{I}_i^T$ is the set of bases with ξ_i involved, including all its interactions
- The sum of all T_i is usually > 1

Sensitivity indices are directly computable from PC

$$g(\xi) = \sum_{k=0}^P c_k \Psi_k(\xi)$$

Consider dimensionality $d = 3$, total order $p = 2$,
number of PC terms $P + 1 = (d + p)! / (d! p!) = 10$.

$$g(\xi_1, \xi_2, \xi_3) = c_0 + c_1 \psi_1(\xi_1) + c_2 \psi_1(\xi_2) + c_3 \psi_1(\xi_3) + \\ + c_4 \psi_2(\xi_1) + c_5 \psi_1(\xi_1) \psi_1(\xi_2) + c_6 \psi_1(\xi_1) \psi_1(\xi_3) + c_7 \psi_2(\xi_2) + c_8 \psi_1(\xi_2) \psi_1(\xi_3) + c_9 \psi_2(\xi_3)$$

Variance contributions

$$\text{Var}(g) = 0 + c_1^2 \langle \psi_1^2 \rangle + c_2^2 \langle \psi_1^2 \rangle + c_3^2 \langle \psi_1^2 \rangle + \\ + c_4^2 \langle \psi_2^2 \rangle + c_5^2 \langle \psi_1^2 \rangle \langle \psi_1^2 \rangle + c_6^2 \langle \psi_1^2 \rangle \langle \psi_1^2 \rangle + c_7^2 \langle \psi_2^2 \rangle + c_8^2 \langle \psi_1^2 \rangle \langle \psi_1^2 \rangle + c_9^2 \langle \psi_2^2 \rangle$$

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Main effect sensitivities ξ_1 ξ_2 ξ_3

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Total sensitivities $\xi_1 \quad \xi_2 \quad \xi_3$

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Joint sensitivities (ξ_1, ξ_2) (ξ_1, ξ_3) (ξ_2, ξ_3)

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Joint sensitivities (ξ_1, ξ_2) (ξ_1, ξ_3) (ξ_2, ξ_3)

PC Postprocessing: Sampling-Based Approaches

$$g(\xi_1, \dots, \xi_d) = \sum_{k=0}^P c_k \psi_k(\xi)$$

- In some cases, need to resort to Monte-Carlo estimation, e.g.
 - Piecewise-PC with irregular subdomains
 - Output transformations, e.g. build PC for $\log g(\xi)$, but inquire sensitivity with respect to $g(\xi)$
- A brute-force sampling of $\text{Var}[\mathbb{E}(g(\xi|\xi_i))]$ is extremely inefficient.

PC Postprocessing: Sampling-Based Approaches

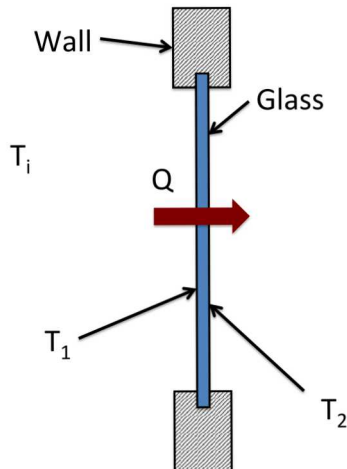
- Tricks are available, given a single set of sampled input [\[Saltelli, 2002\]](#). E.g., use

$$\mathbb{E}[g(\boldsymbol{\xi}|\xi_i)^2] = \mathbb{E}[g(\boldsymbol{\xi}|\xi_i)g(\boldsymbol{\xi}'|\xi_i)] = \frac{1}{N-1} \sum_{r=1}^N g(\boldsymbol{\xi}^{(r)})g(\tilde{\boldsymbol{\xi}}^{(r)}),$$

where $\tilde{\boldsymbol{\xi}}$ is $\boldsymbol{\xi}'$ with i -th element replaced by ξ_i .

- Similar formulae available for joint sensitivity indices.
- Con: as all Monte-Carlo algorithms, converges slowly.
- Pro: sampling is cheap.

Heat Transfer through a Window



$$h_i(T_i - T_1) = k_w \frac{(T_1 - T_2)}{d_w}$$

$$k_w \frac{(T_1 - T_2)}{d_w} = h_o(T_2 - T_o)$$

T_o 6 Uncertain, Gaussian parameters

$$T_i = 293\text{K}, \sigma = 0.5\%$$

$$T_o = 273\text{K}, \sigma = 0.5\%$$

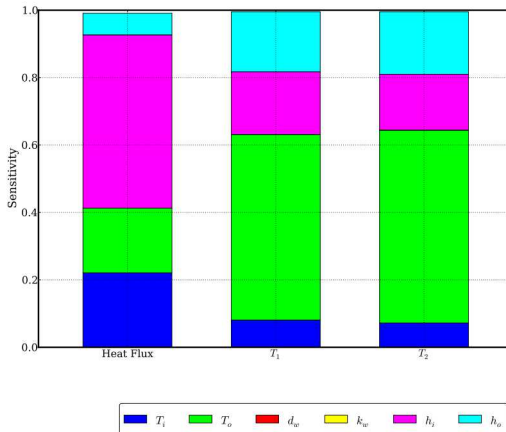
$$d_w = 0.01\text{m}, \sigma = 1\%$$

$$k_w = 1\text{W/mK}, \sigma = 5\%$$

$$h_i = 2\text{W/m}^2\text{K}, \sigma = 15\%$$

$$h_o = 6\text{W/m}^2\text{K}, \sigma = 15\%$$

Outputs are most sensitive to ambient temperatures and convective heat transfer coefficients

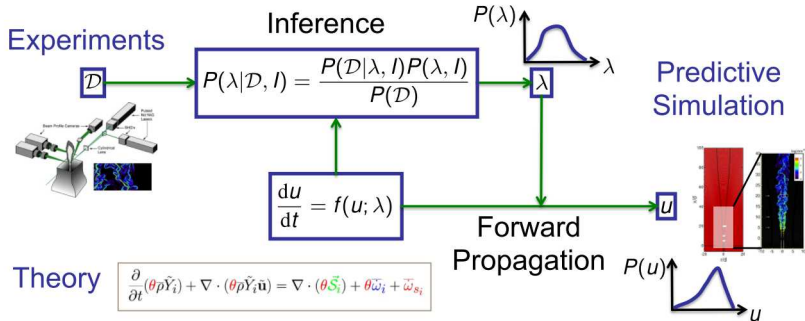


- Main effect sensitivities
 - Sum to 1 only if coupling terms do not matter
- k_w has minimal contribution due to its low uncertainty

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Obtaining PCEs for Uncertain Inputs

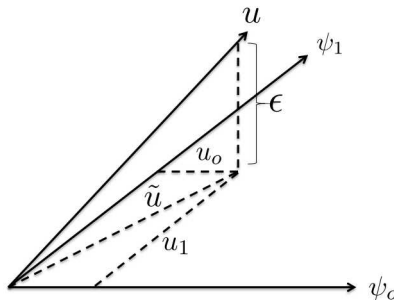


- Representation of uncertain inputs λ with PCEs

Obtaining PC coefficients for arbitrary random variables is not trivial

- Characterizing PCEs for uncertain inputs is a really difficult problem
- Inputs specified in a variety of ways, and often incomplete
 - Probability density function
 - Samples, *e.g.* from inverse problem solution
 - Expert opinion (*e.g.* “about 3.5”)
- Particular case of a random variable specified by a PDF is generally tractable

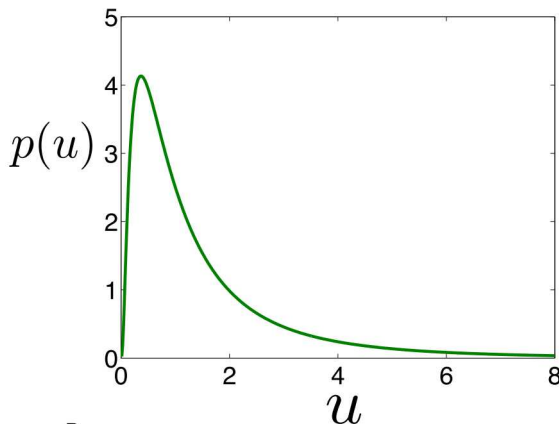
Orthogonality enables a Galerkin projection to determine the PC coefficients



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

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

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



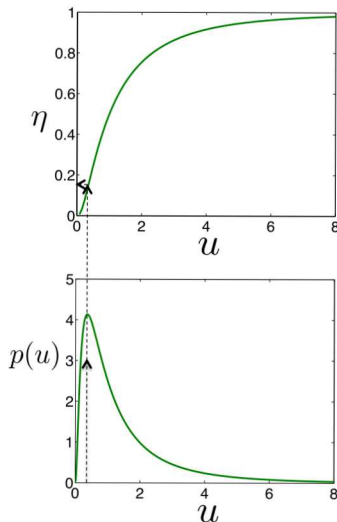
$$u = \sum_{k=0}^P u_k \Psi_k(\xi) \quad \Rightarrow \quad u_i = \frac{\langle u \Psi_i(\xi) \rangle}{\langle \Psi_i^2 \rangle}$$

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

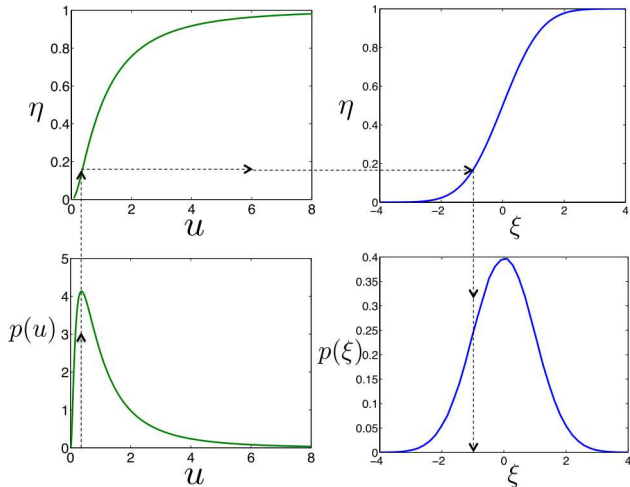
$$F(u) = \int_{-\infty}^u p(s) ds$$

- $F(u)$ 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
- $u = F^{-1}(\Phi(\xi))$

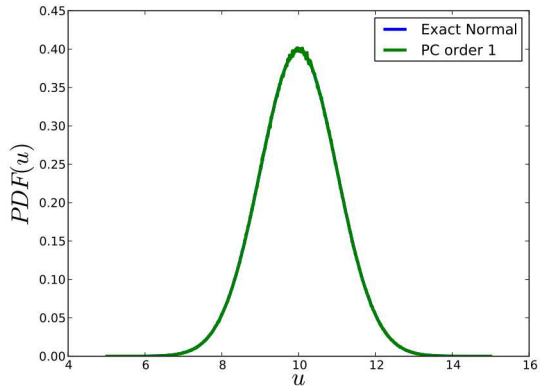


$$\langle u \Psi_i(\xi) \rangle = \int \underbrace{F^{-1}(\Phi(\xi))}_u \Psi_i(\xi) w(\xi) d\xi$$

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

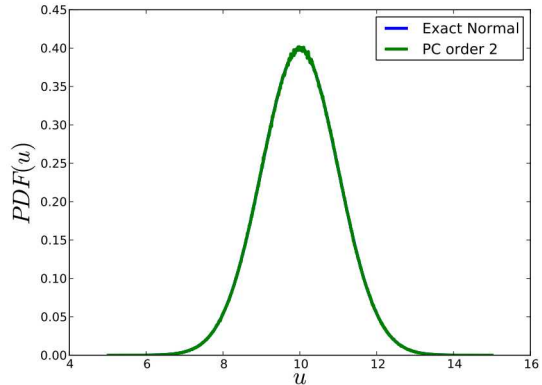
$$\begin{aligned}u &= \sum_{k=0}^P u_k \psi_k(\xi) \\ &= u_0 + u_1 \xi\end{aligned}$$



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

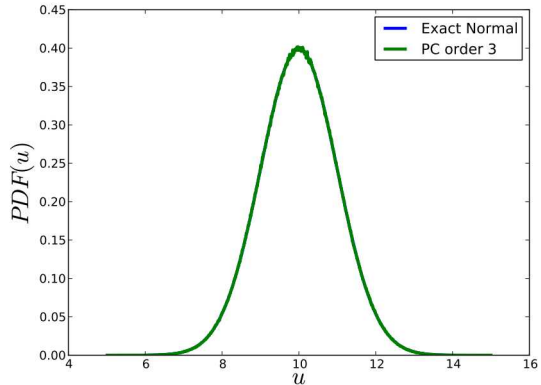
$$\begin{aligned}u &= \sum_{k=0}^P u_k \psi_k(\xi) \\ &= u_0 + u_1 \xi + u_2 (\xi^2 - 1)\end{aligned}$$



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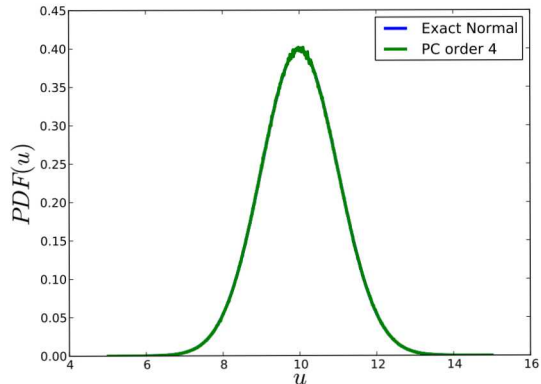
- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 3

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



PC Illustration: PC Expansion for a Normal RV

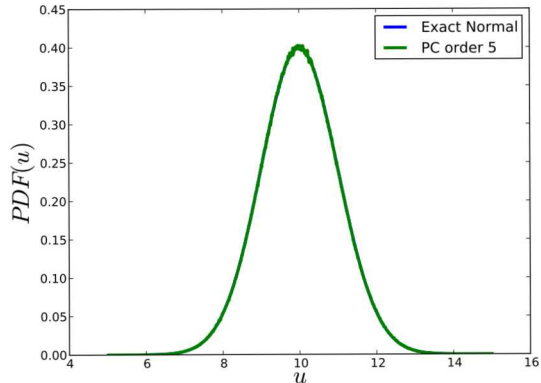
- Wiener-Hermite PCE constructed for a Normal RV
- PCE-sampled PDF superposed on true PDF
- Order = 4



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

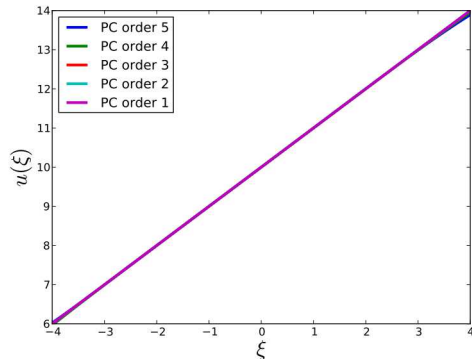
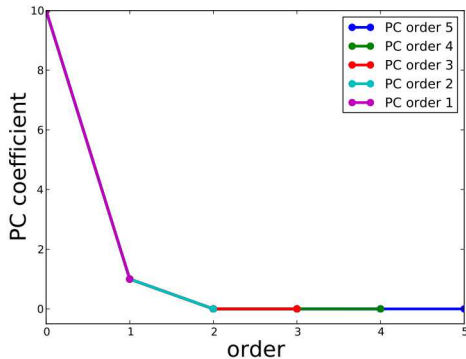
PC Illustration: PC Expansion for a Normal RV

- 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

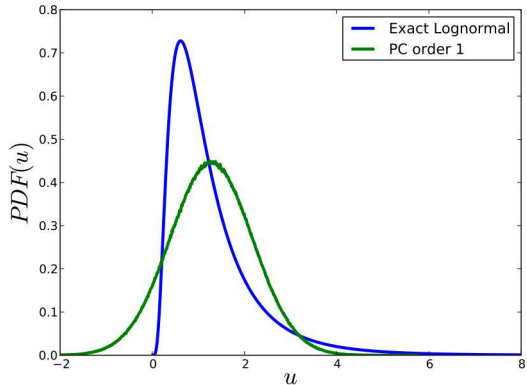


- First order Wiener-Hermite PCE exact for a normal RV
- Linear function of ξ
- Higher order terms are negligible

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

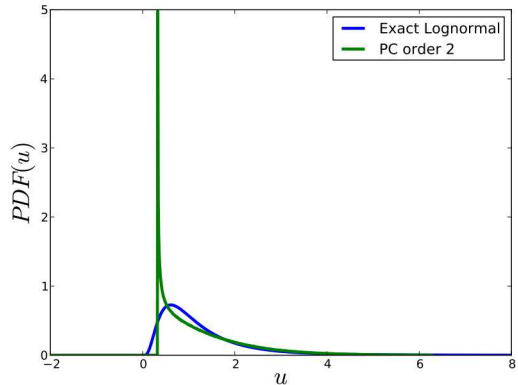
$$\begin{aligned}u &= \sum_{k=0}^P u_k \psi_k(\xi) \\ &= u_0 + u_1 \xi\end{aligned}$$



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

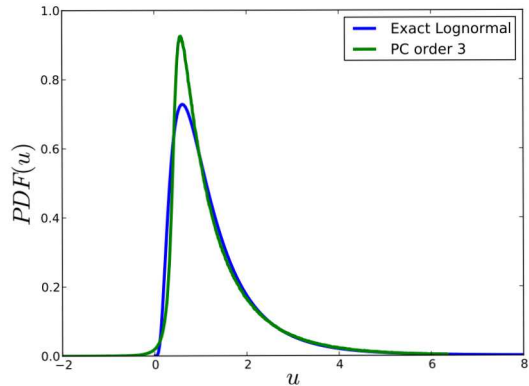
$$\begin{aligned} u &= \sum_{k=0}^P u_k \Psi_k(\xi) \\ &= u_0 + u_1 \xi + u_2 (\xi^2 - 1) \end{aligned}$$



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

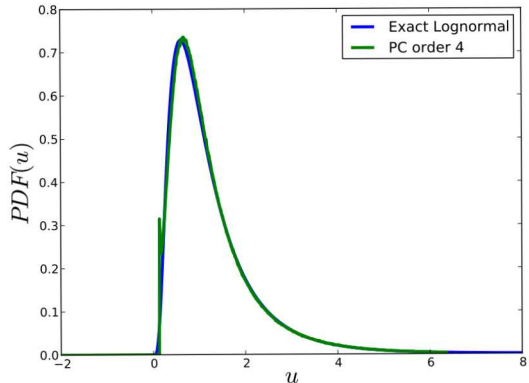
$$\begin{aligned}u &= \sum_{k=0}^P u_k \Psi_k(\xi) \\&= u_0 + u_1 \xi + u_2 (\xi^2 - 1) + u_3 (\xi^3 - 3\xi)\end{aligned}$$



PC Illustration: WH PCE for a Lognormal RV

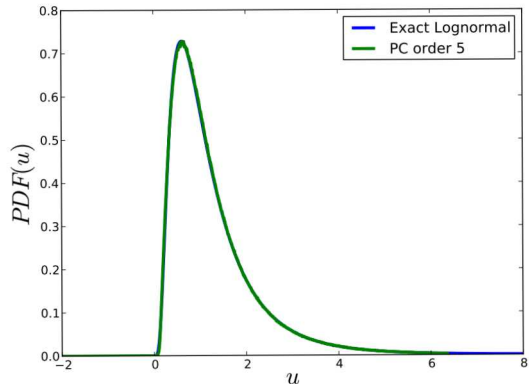
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 4

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



PC Illustration: WH PCE for a Lognormal RV

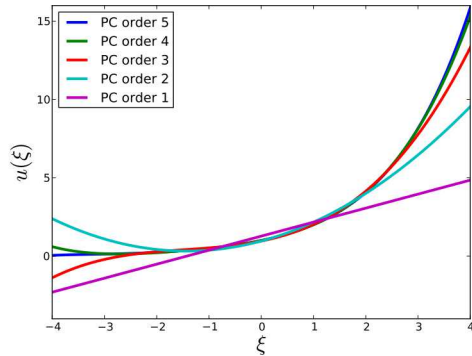
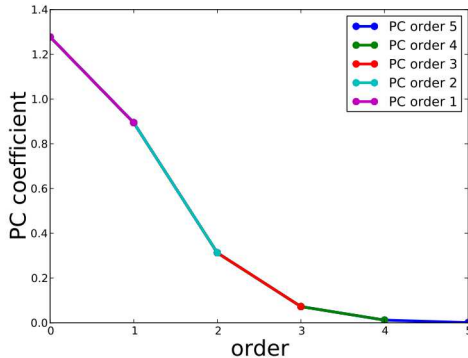
- Wiener-Hermite PCE constructed for a Lognormal RV
- PCE-sampled PDF superposed on true PDF
- Order = 5



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

$$= u_0 + u_1 \xi + u_2 (\xi^2 - 1) + u_3 (\xi^3 - 3\xi) + u_4 (\xi^4 - 6\xi^2 + 3) + u_5 (\xi^5 - 10\xi^3 + 15\xi)$$

PC Illustration: WH PCE for a Lognormal RV



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

Constructing an n D PCE for a RV with a Given PDF

- Given RV $z \in \mathbb{R}$ with PDF: $g(z)$, define:

$$z = \sum_{i=0}^P z_i \Psi_i(\xi_1, \xi_2, \dots, \xi_n), \quad P + 1 = \frac{(n + p)!}{n!p!}$$

- No general procedure
- Construct PCE as model choice to represent what is known about RV
- Can choose $\{n, p\}$ and the mode strengths by ensuring accurate capture of
 - the PDF $g(z)$
 - select moments of z
 - some observable of interest $\phi(z)$

Multivariate Normal Approximation (MVN)

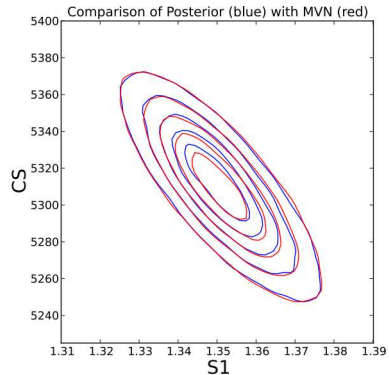
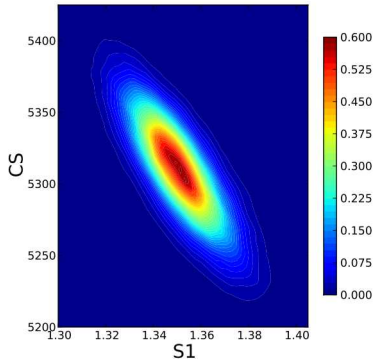
- Many distributions are unimodal and somewhat shaped like Gaussians
- MultiVariate Normal approximations capture mean and correlation structure of the random variables
- Easy to extract from a set of samples
 - In 1D: just compute mean and standard deviation:
 $u = u_0 + u_1 \xi$
 - Multi-D: Cholesky factorization of covariance

$$C = LL^T$$

$$u = L\xi$$

```
# Compute mean parameter values
par_mean = numpy.mean(samples,axis=0)
# Compute the covariance
par_cov = numpy.cov(samples,rowvar=0)
# Compute the Cholesky Decomposition
chol_lower = numpy.linalg.cholesky(par_cov)
```

MVN Approximation of Distribution from Samples



$$\begin{aligned} S_1 &= 1.351 + 0.01367\xi_1 \\ CS &= 5310 - 26.25\xi_1 + 20.26\xi_2 \end{aligned}$$

Rosenblatt Transformation for Multi-D RVs

- Assume samples of multi-D RVs are (*e.g.* from MCMC sampling of posterior parameter distribution)
- Rosenblatt transformation maps any (not necessarily independent) set of random variables $(\lambda_1, \dots, \lambda_d)$ to uniform i.i.d.'s $\{\eta_i\}_{i=1}^d$ (Rosenblatt, 1952).

$$\eta_1 = F_1(\lambda_1)$$

$$\eta_2 = F_{2|1}(\lambda_2|\lambda_1)$$

$$\vdots$$

$$\eta_d = F_{d|d-1,\dots,1}(\lambda_d|\lambda_{d-1}, \dots, \lambda_1)$$

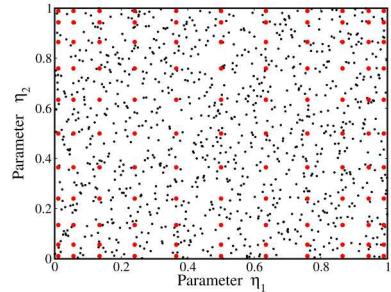
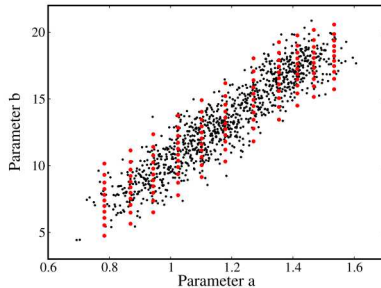
- Rosenblatt transformation is a multi-D generalization of 1D CDF mapping.
- Conditional CDFs are harder to evaluate in high dimensions

Rosenblatt transformation of a given sample set requires KDE

- Given samples $\{\lambda^{(n)}\}_{n=1}^N$ of the random variable $\lambda = (\lambda_1, \dots, \lambda_d)$
- Kernel Density Estimation (KDE) is needed to compute conditional CDFs

$$\begin{aligned}
 \eta_k &= F_{k|k-1, \dots, 1}(\lambda_k | \lambda_{k-1}, \dots, \lambda_1) = \\
 &= \int_{-\infty}^{\lambda_k} p_{k|k-1, \dots, 1}(\lambda'_k | \lambda_{k-1}, \dots, \lambda_1) d\lambda'_k = \int_{-\infty}^{\lambda_k} \frac{p_{k, \dots, 1}(\lambda'_k, \lambda_{k-1}, \dots, \lambda_1)}{p_{k-1, \dots, 1}(\lambda_{k-1}, \dots, \lambda_1)} d\lambda'_k \\
 &\approx \frac{1}{h\sqrt{2\pi}} \int_{-\infty}^{\lambda_k} \frac{\sum_{n=1}^N \exp\left(-\frac{(\lambda_1 - \lambda_1^{(n)})^2 + \dots + (\lambda'_k - \lambda_k^{(n)})^2}{2h^2}\right)}{\sum_{n=1}^N \exp\left(-\frac{(\lambda_1 - \lambda_1^{(n)})^2 + \dots + (\lambda_{k-1} - \lambda_{k-1}^{(n)})^2}{2h^2}\right)} d\lambda'_k \\
 &= \int_{-\infty}^{\lambda_k} \frac{\sum_{n=1}^N \exp\left(-\frac{(\lambda_1 - \lambda_1^{(n)})^2 + \dots + (\lambda_{k-1} - \lambda_{k-1}^{(n)})^2}{2h^2}\right) \times \frac{1}{h\sqrt{2\pi}} \exp\left(-\frac{(\lambda'_k - \lambda_k^{(n)})^2}{2h^2}\right)}{\sum_{n=1}^N \exp\left(-\frac{(\lambda_1 - \lambda_1^{(n)})^2 + \dots + (\lambda_{k-1} - \lambda_{k-1}^{(n)})^2}{2h^2}\right)} d\lambda'_k \\
 &= \frac{\sum_{n=1}^N \exp\left(-\frac{(\lambda_1 - \lambda_1^{(n)})^2 + \dots + (\lambda_{k-1} - \lambda_{k-1}^{(n)})^2}{2h^2}\right) \times \Phi\left(\frac{\lambda_k - \lambda_k^{(n)}}{h}\right)}{\sum_{n=1}^N \exp\left(-\frac{(\lambda_1 - \lambda_1^{(n)})^2 + \dots + (\lambda_{k-1} - \lambda_{k-1}^{(n)})^2}{2h^2}\right)},
 \end{aligned}$$

Rosenblatt transformation enables Galerkin projection



$(a, b) = R^{-1}(\xi_1, \xi_2)$ ensures a well-defined quadrature integration

$$a = \sum_{k=0}^P a_k \Psi_k(\xi)$$

$$a_k \propto \int \underbrace{R_a^{-1}(\xi)}_a \Psi_k(\xi) w(\xi) d\xi$$

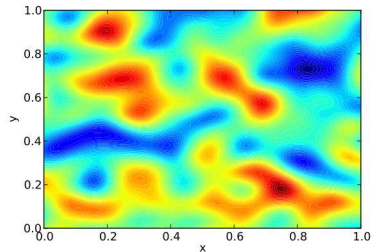
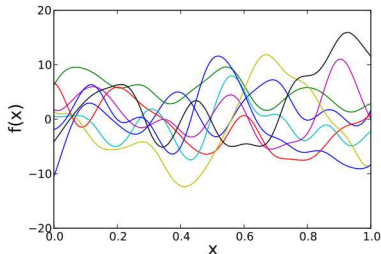
$$b = \sum_{k=0}^P b_k \Psi_k(\xi)$$

$$b_k \propto \int \underbrace{R_b^{-1}(\xi)}_b \Psi_k(\xi) w(\xi) d\xi$$

Outline

- ➊ Introduction
- ➋ Sensitivity Analysis
- ➌ Representing Arbitrary RVs
- ➍ Representing Random Fields
- ➎ References

Compact Representations of Random Fields



- Sometimes an uncertain input is a random field (also called stochastic process)
 - Friction coefficient along a wall
 - Thermal conductivity in heterogeneous material
 - Permeability in groundwater flow simulations
- Have infinitely many degrees of freedom
- To model effect of random fields on computations, need compact representation that captures key aspects of random field

Karhunen-Loève (KL) Expansions

- Assume stochastic process $F(x, \theta) : D \times \Theta \rightarrow \mathbb{R}$ an L^2 random field on D
- With covariance function $Cov(x, y)$
- F can be written as

$$F(x, \theta) = \langle F(x, \theta) \rangle_{\theta} + \sum_{k=1}^{\infty} \sqrt{\lambda_k} f_k(x) \xi_k$$

- $f_k(x)$: eigenfunctions of $Cov(x, y)$
- λ_k : corresponding eigenvalues, all positive
- ξ_k : uncorrelated random variables, unit variance
- Samples obtained by projecting realizations of F onto f_k
- Generally not independent
 - For Gaussian F , ξ_k are i.i.d. normal random variables
- The KLE is *optimal*: of all possible orthonormal bases for $L^2(\Theta \times D)$ the $\{f(x)\}$ minimize the mean-square error in a finite linear representation of $F(\cdot)$

KL Expansions - Numerical Approach - 1

- Covariance Matrix, $Cov(x, y) = \langle F(x, \theta)F(y, \theta) \rangle_{\theta}$:
 - specified analytically
 - estimated from samples
- Estimate eigenvalues and eigenvectors for the Fredholm equation of second kind:

$$\int Cov(x, y)f(y)dy = \lambda f(x)$$

KL Expansions - Numerical Approach - 2

- Nystrom algorithm for Fredholm equation

$$\sum_{i=1}^{N_p} w_i \text{Cov}(x, y_i) f(y_i) = \lambda f(x)$$

where w_i are the weights for the quadrature rule that uses N_p points y_i where realizations are provided.

- Further manipulation leads to the eigenvalue problem

$$Ag = \lambda g$$

where $A = WKW$ and $g = Wf$, with W being the diagonal matrix $W_{ii} = \sqrt{w_i}$ and $K_{ij} = \text{Cov}(x_i, y_j)$. Solutions consist of pairs of eigenvalues λ_k and eigenmodes $f_k = W^{-1}g_k$.

KL Expansions - Numerical Approach - 3

- Samples of random variables ξ_k are obtained by projecting realizations of the random process F on the eigenmodes f_k

$$\xi_k|_{\theta_l} = \langle F(x, \theta_l) - \langle F(x, \theta) \rangle_{\theta}, f_k(x) \rangle_x / \sqrt{\lambda_k}$$

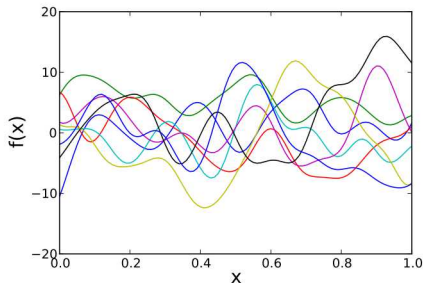
- ... or numerically

$$\xi_k|_{\theta_l} = \sum_{i=1}^{N_p} w_i (F(x_i, \theta_l) - \langle F(x_i, \theta) \rangle_{\theta}) f_k(x_i) / \sqrt{\lambda_k}$$

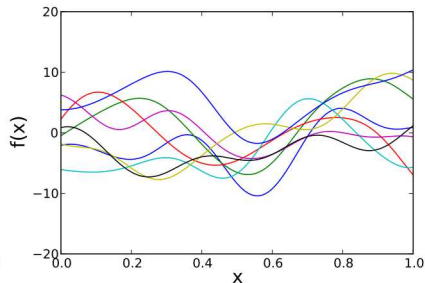
- If Gaussian process: automatically have first order WH PCE
- If not, same approaches as for converting RVs to PCEs applied to KL RVs

1D Gaussian Process: Realizations

$\delta = 0.1$



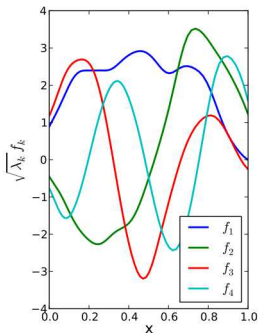
$\delta = 0.2$



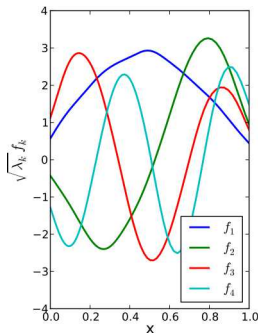
- Covariance $Cov(x_1, x_2) = \exp(-(x_1 - x_2)^2 / \delta^2)$
- Sample realizations are noisier as correlation length decreases

1D Gaussian Process: KL Modes for $\delta = 0.10$

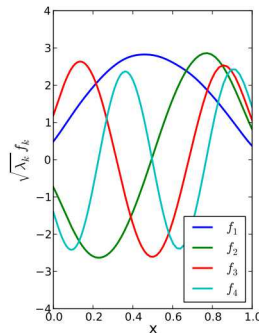
2^9 realizations



2^{13} realizations



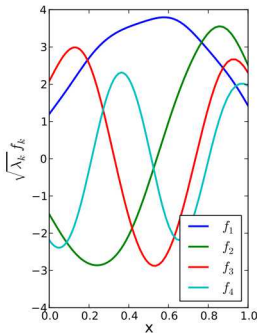
2^{17} realizations



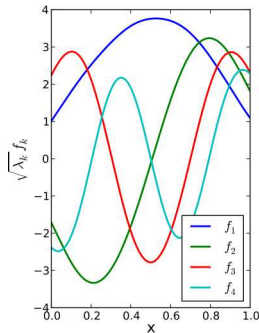
- Eigenmodes of the covariance matrix
 - Data covariance matrix constructed from $2^9 = 512$, $2^{13} = 8192$, and $2^{17} = 131072$ Gaussian process realizations
- Higher modes are more oscillatory

1D Gaussian Process: KL Modes for $\delta = 0.20$

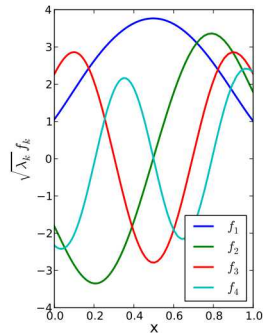
2^9 realizations



2^{13} realizations



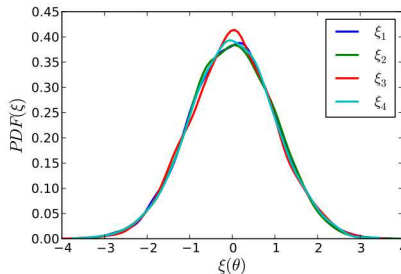
2^{17} realizations



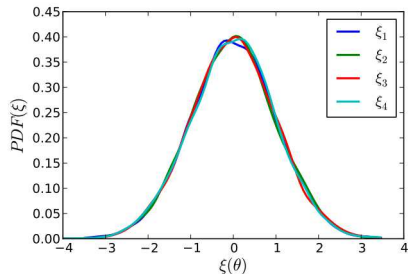
- Eigenmodes of the covariance matrix
 - Data covariance matrix constructed from $2^9 = 512$, $2^{13} = 8192$, and $2^{17} = 131072$ Gaussian process realizations
- Higher modes are more oscillatory

1D Gaussian Process: KL Random Variables

$\delta = 0.1$

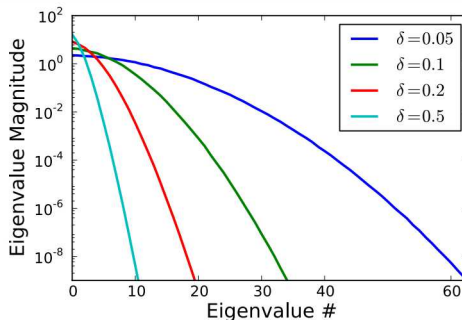


$\delta = 0.2$



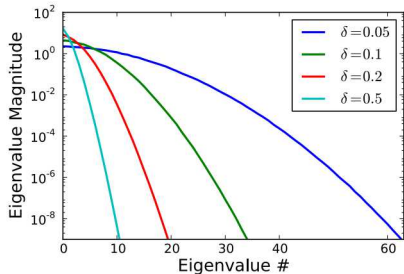
- Random variables obtained by projecting realizations onto KL modes
- Uncorrelated by construction
 - Also independent due to nature of Gaussian Process

1D Gaussian Process: Eigenvalue Spectrum



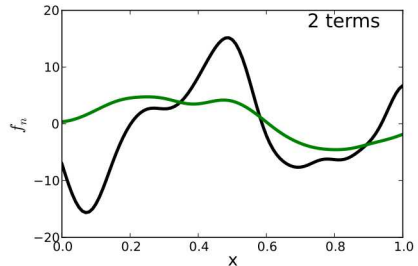
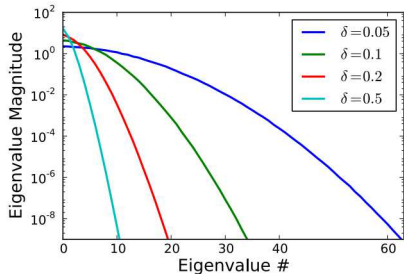
- Eigenvalue spectrum decays more slowly as correlation length decreases
 - More oscillatory modes needed to represent fluctuations in x
- KL expansion generally is truncated after enough modes are included to capture a specified fraction of the total variance

1D Gaussian Process: Reconstructed Realizations



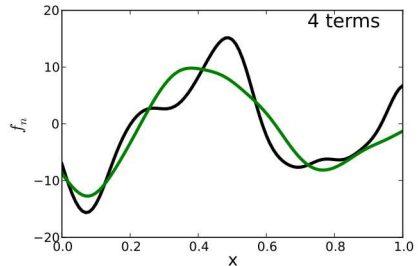
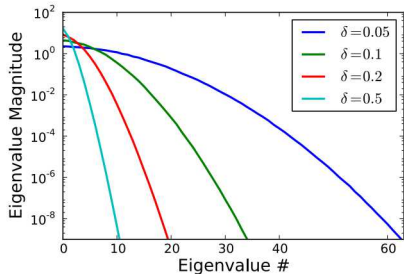
- Large scale features can be resolved with small number of modes
- Smaller scale features require higher modes

1D Gaussian Process: Reconstructed Realizations



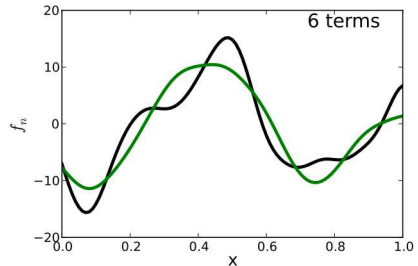
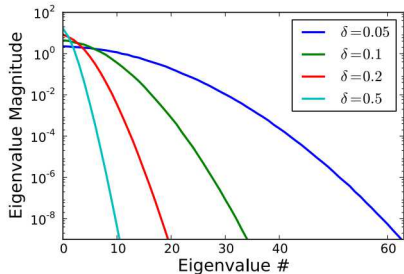
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1D Gaussian Process: Reconstructed Realizations



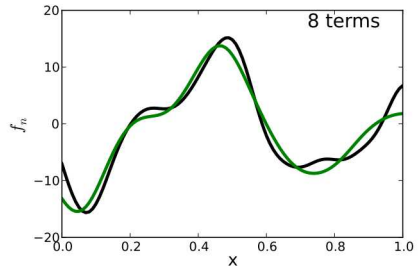
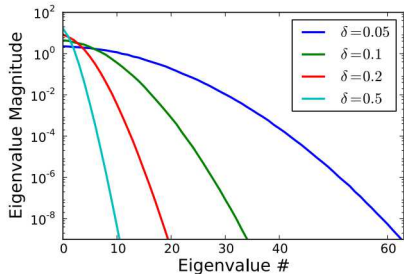
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1D Gaussian Process: Reconstructed Realizations



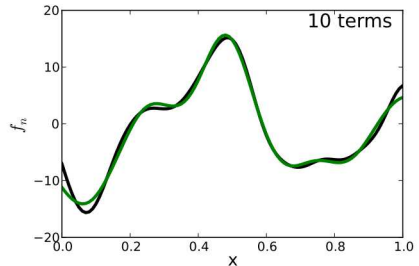
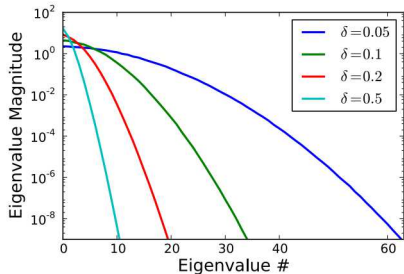
- Large scale features can be resolved with small number of modes
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1D Gaussian Process: Reconstructed Realizations



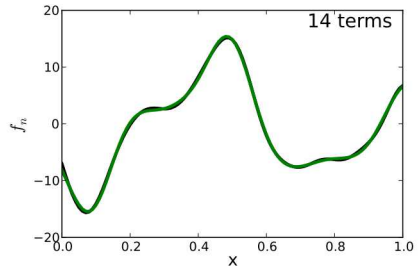
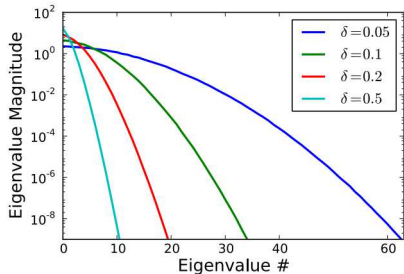
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1D Gaussian Process: Reconstructed Realizations



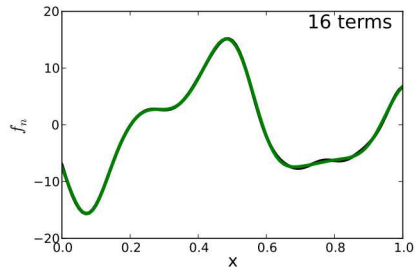
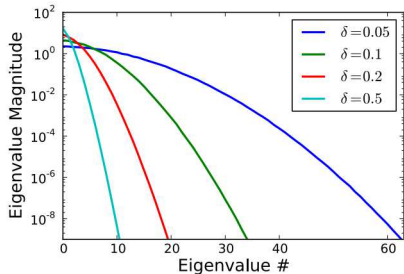
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1D Gaussian Process: Reconstructed Realizations



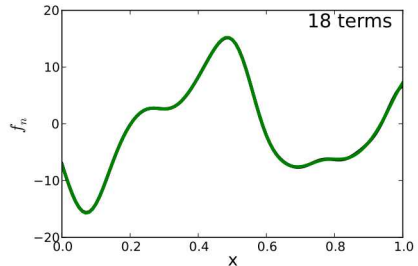
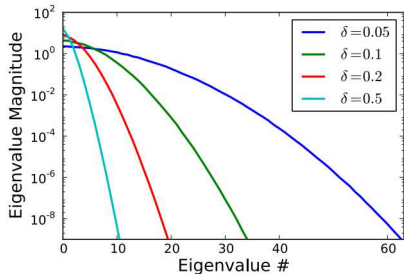
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1D Gaussian Process: Reconstructed Realizations



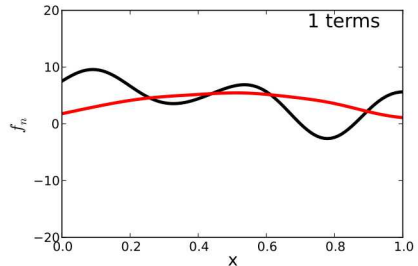
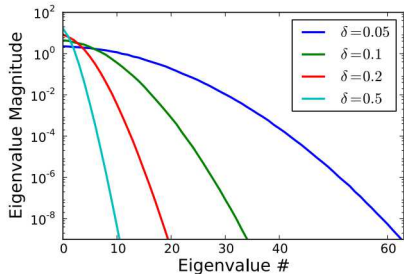
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1D Gaussian Process: Reconstructed Realizations



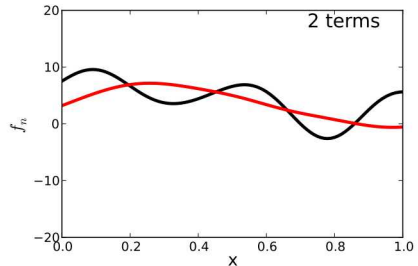
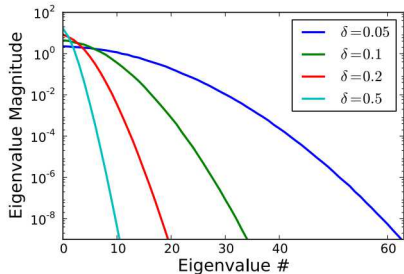
- Large scale features can be resolved with small number of modes
- Smaller scale features require higher modes

1D Gaussian Process: Reconstructed Realizations



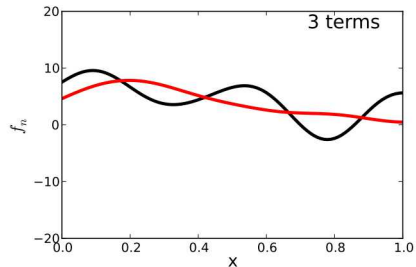
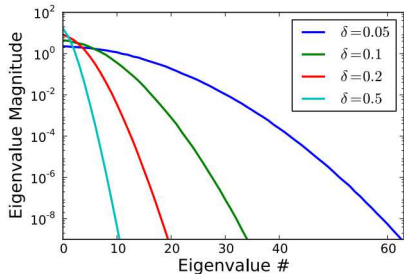
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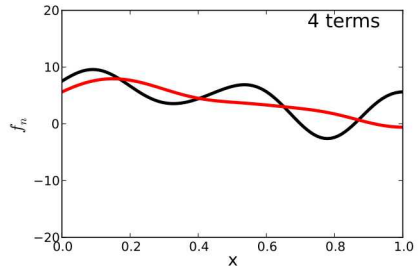
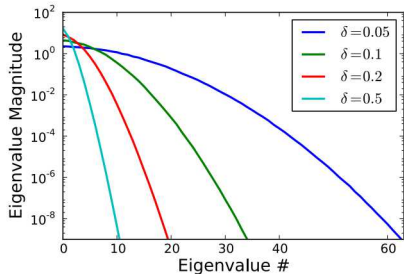
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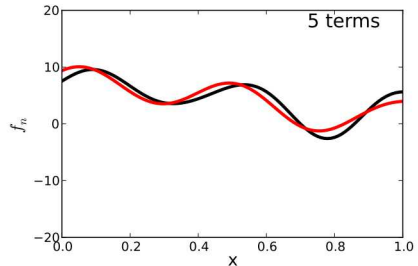
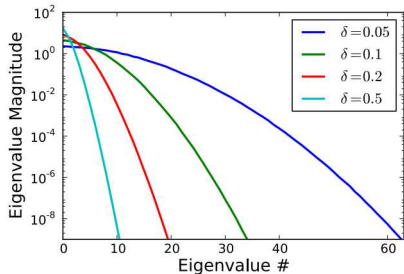
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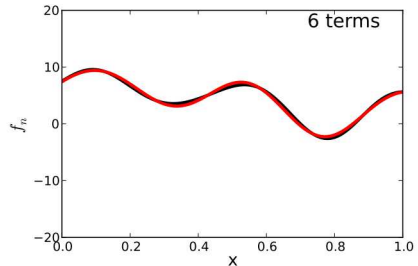
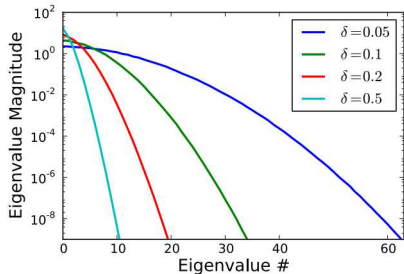
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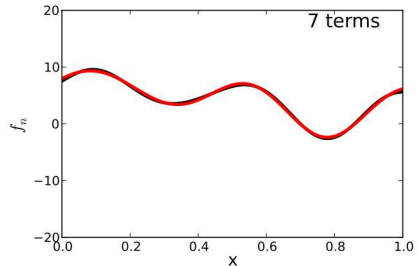
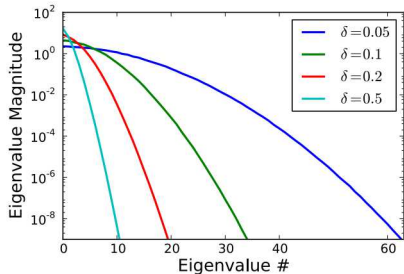
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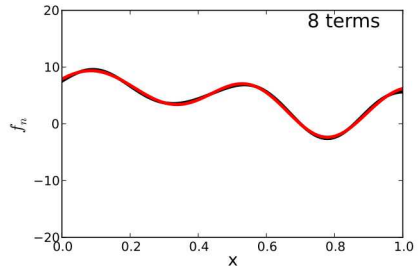
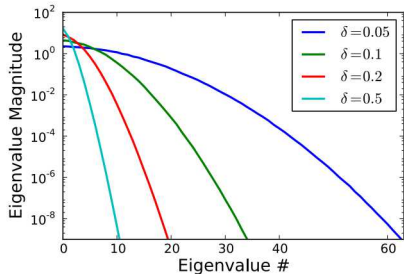
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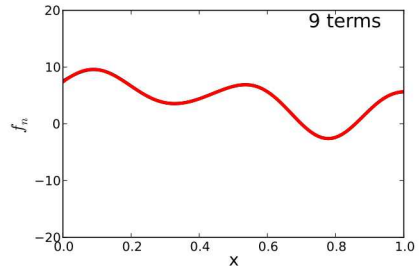
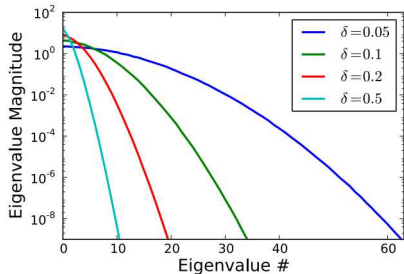
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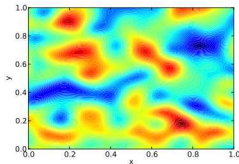
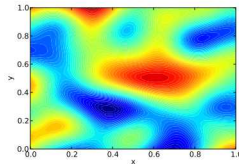
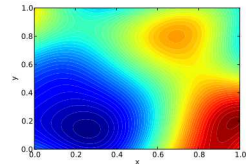
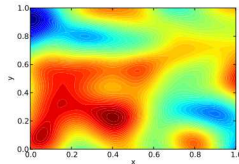
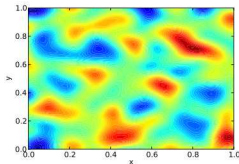
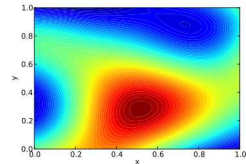
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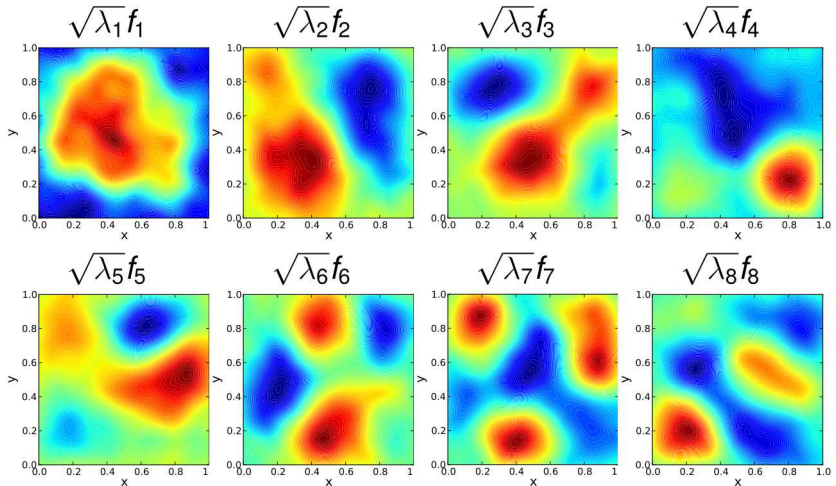
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KL of 2D Gaussian Process

 $\delta = 0.1$  $\delta = 0.2$  $\delta = 0.5$ 

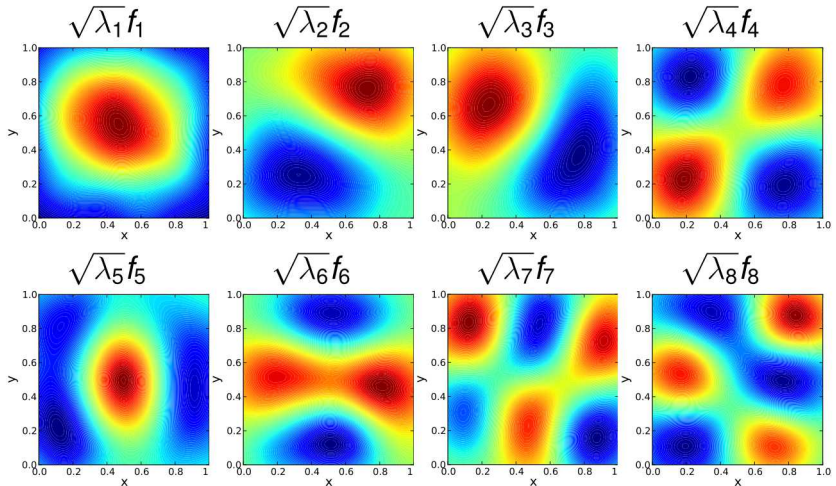
- 2D Gaussian Process with covariance:
 $Cov(x_1, x_2) = \exp(-||x_1 - x_2||^2/\delta^2)$
- Realizations are smoother as covariance length δ increases

2D KL - Modes for $\delta = 0.1$



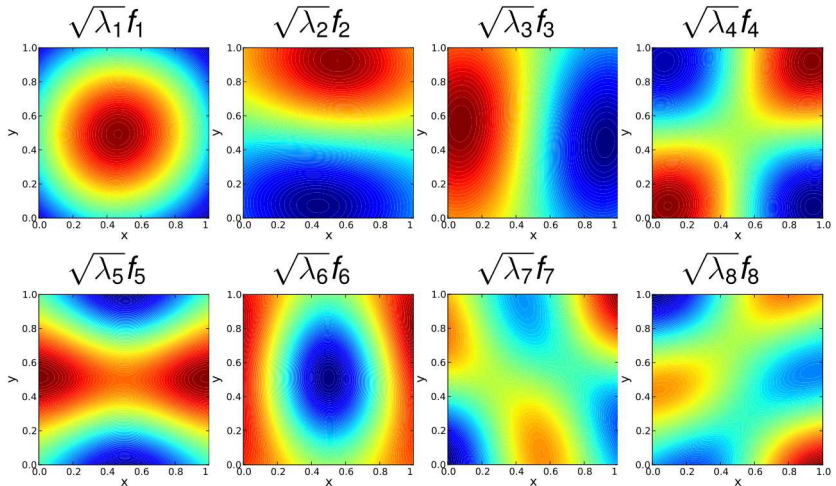
- Data covariance matrix constructed from $2^{12} = 4096$ Gaussian process realizations

2D KL - Modes for $\delta = 0.2$



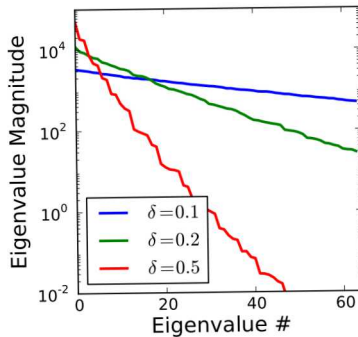
- Data covariance matrix constructed from $2^{12} = 4096$ Gaussian process realizations

2D KL - Modes for $\delta = 0.5$



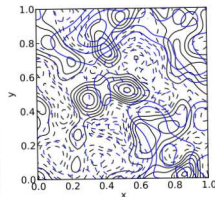
- Data covariance matrix constructed from $2^{12} = 4096$ Gaussian process realizations

2D KL - Eigenvalue Spectrum

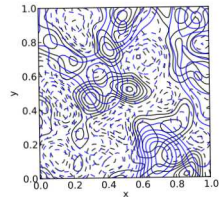


$\delta = 0.1$

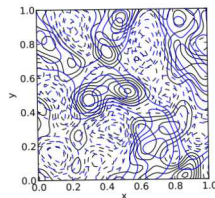
4 terms



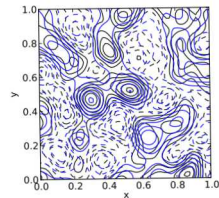
16 terms



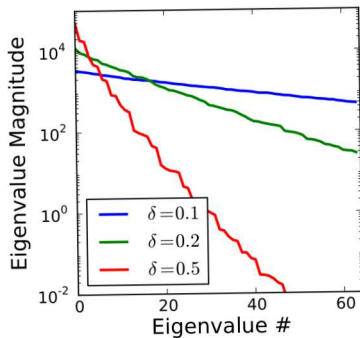
32 terms



64 terms

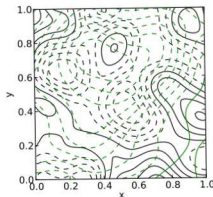


2D KL - Eigenvalue Spectrum

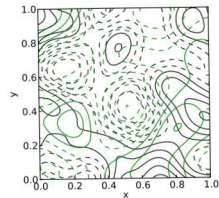


$\delta = 0.2$

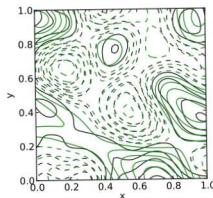
4 terms



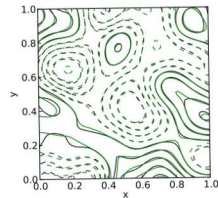
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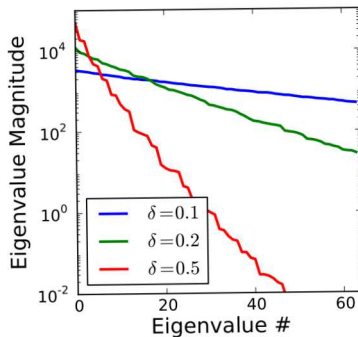
32 terms



64 terms

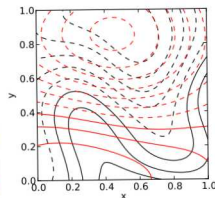


2D KL - Eigenvalue Spectrum

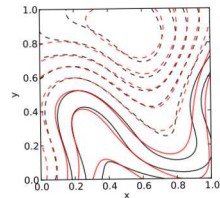


$\delta = 0.5$

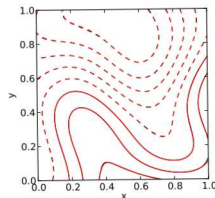
4 terms



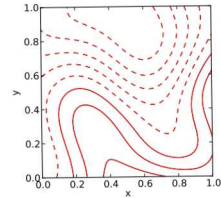
16 terms



32 terms



64 terms



KL: Summary

- The KL expansion allows a compact, finite dimensional representation of random fields
- Dimensionality reduction is strongest if eigenvalue spectrum decays rapidly
 - Long correlation length in random field realizations
 - Relatively narrow range of feature sizes
- A potential drawback is that many samples are needed to compute the covariance matrix accurately
 - 1000's of realizations were needed to get smooth eigenmodes in 2D examples shown earlier
- Often, a covariance function is assumed and the associated eigenmodes are used to parametrize an unknown random field

Further Reading

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- D. Xiu, "Numerical Methods for Stochastic Computations: A Spectral Method Approach", Princeton U. Press, 2010.
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- M. Rosenblatt, "Remarks on a Multivariate Transformation", *Ann. Math. Statist.*, 23:3, pp. 470-472, 1952.

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- R. E. Kass, B. P. Carlin, A. Gelman, and R. M. Neal, "Markov chain monte carlo in practice: A roundtable discussion," *The American Statistician*, vol. 52, no. 2, pp. 93–100, 1998.
- D.S. Sivia, "Data Analysis: A Bayesian Tutorial," Oxford Science, 1996.