Polynomial Chaos SAND2017-8196C Uncertainty Quantification

Topic 1: UQ Methods / PDF assignment

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Acknowledgements

Cosmin Safta Khachik Sargsyan Kenny Chowdhary Habib Najm Prashant Rai	Sandia National Laboratories Livermore, CA
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As well as Katy Jarvis, Sarah de Bord, Sarah Castorena, Majid Latif, Katherine Johnston, and many others ...

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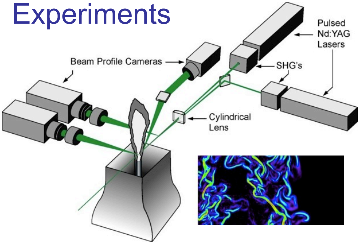
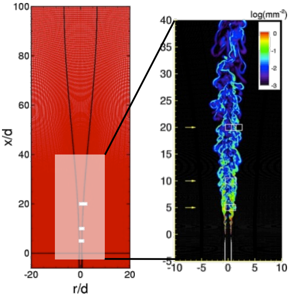
Aspects of Uncertainty Quantification

Experimental data is used to calibrate models

Experiments



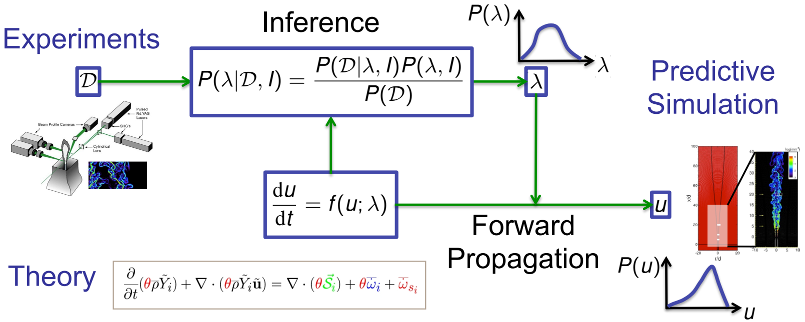
Predictive Simulation



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

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:
    - Collision interactions in molecular systems
    - Sampling noise

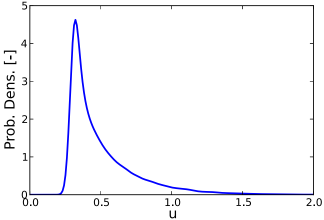
Epistemic or aleatory can depend on point of view

- 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

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

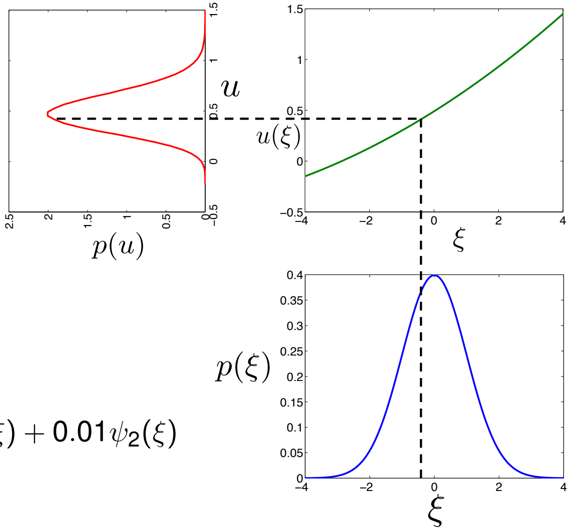


$$u = 0.5 + 0.2\psi_1(\xi) + 0.1\psi_2(\xi)$$

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

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

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

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 $\boldsymbol{\alpha}^{\boldsymbol{i}} = (\alpha_1^i, \alpha_2^i, \ldots, \alpha_n^i)$,

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

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

Obtaining PC coefficients for arbitrary random variables is not trivial

- 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

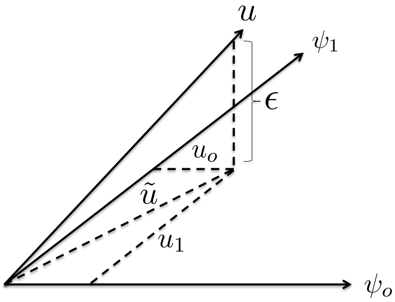
The PC basis functions are orthogonal with respect to the probability measure of the associated RVs

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

where,

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

Orthogonality enables a Galerkin projection to determine the PC coefficients



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

$$\Rightarrow \qquad u_i = \frac{\langle u \Psi_i \rangle}{\left\langle \Psi_i^2 \right\rangle}$$

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	$[0, +\infty)$	$\frac{\xi^\alpha e^{-\xi}}{\Gamma(\alpha+1)}$	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: $\langle \psi_i \psi_j \rangle \equiv \int_a^b \psi_i(\xi)\psi_j(\xi) w(\xi) d\xi = \delta_{ij} \langle \psi_i^2 \rangle$

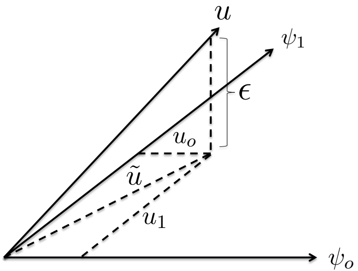
- Wiener-Askey scheme provides a hierarchy of possible continuous PC bases [Xiu and Karniadakis, 2002]
  - Legendre-Uniform is special case of Beta-Jacobi
- Input parameter domain often dictates the most convenient choice of PC
- Polynomials can also be tailored to be orthogonal w.r.t. chosen, arbitrary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

How do I know my PCE is converged?

- Approximation error in PCE is topic of a lot of research
- Rules of thumb:
  - Try to use a PC basis in terms of a random variable with a distribution similar to the uncertainties you expect to see
  - Higher order PC coefficients should decay
  - Increase order until results no longer change
  - Not always fail-proof ...

Propagation of Uncertain Inputs Represented with PCEs

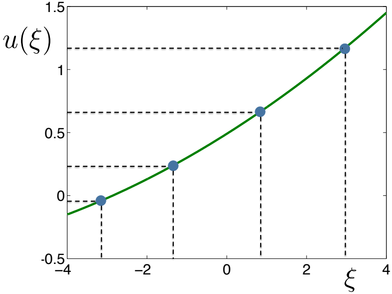
Galerkin Projection



$$u_k = \frac{\langle u\Psi_k\rangle}{\langle \Psi_k^2\rangle}, \quad k = 0, \dots, P$$

Residual orthogonal to space covered by basis functions

Collocation



Match PCE to random variable at chosen sample points: interpolation or regression

Galerkin projection methods are either intrusive or non-intrusive

- Use same projection but in different ways

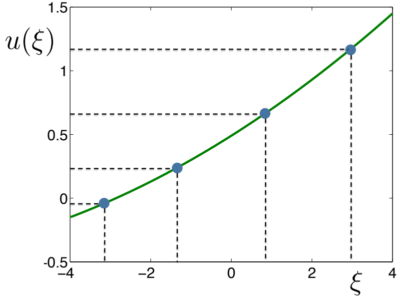
$$u_k = \frac{\langle u\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

- Intrusive methods apply Galerkin projection to governing equations
  - Results in set of equations for the PC coefficients
  - Requires redesign of computer code
  - PCEs for all uncertain variables in system
- Non-intrusive approaches apply Galerkin projection to outputs of interest
  - Sampling to evaluate projection operator
  - Can use existing code as black box
  - Only computes PCEs for quantities of interest

Collocation approaches are non-intrusive and minimize errors at sample points

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

$$i = 1, \ldots, N_c$$



- Use functional representation point of view
- Can use interpolation, e.g. Lagrange interpolants
- Or use regression approaches: $P + 1$ degrees of freedom to fit N_c points
- Can position points where most accuracy desired

Intrusive Galerkin projection reformulates original equations

- Assume $v = f(u; a, \lambda)$, with
  - a deterministic parameter(s)
  - λ uncertain parameter(s)
  - u, v variables of interest (deterministic or uncertain)
- Represent uncertain variables with PCEs

$$\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k(\xi), \qquad v = \sum_{k=0}^{P} v_k \Psi_k(\xi)$$

- Apply Galerkin projection to get PC coefficients of v

$$v_k = \frac{\langle v\Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle f(u; a, \lambda)\Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

- Results in larger, but deterministic set of equations

Projection of product: $v = \gamma\ \lambda$

- Assume $v = \gamma\ \lambda$, with $\gamma = \sum_{k=0}^{P} \gamma_k \Psi_k$, $\lambda = \sum_{k=0}^{P} \lambda_k \Psi_k$, and $v = \sum_{k=0}^{P} v_k \Psi_k$
- Galerkin projection

$$v_k = \frac{\langle v \Psi_k \rangle}{\langle \Psi_k^2 \rangle} = \frac{\langle (\gamma\ \lambda) \Psi_k \rangle}{\langle \Psi_k^2 \rangle}, \quad k = 0, \ldots, P$$

$$\begin{aligned}
\langle (\gamma\ \lambda) \Psi_k \rangle &= \left\langle \left(\sum_{i=0}^{P} \gamma_i \Psi_i \sum_{j=0}^{P} \lambda_j \Psi_j \right) \Psi_k \right\rangle \\
&= \left\langle \sum_{i=0}^{P} \sum_{j=0}^{P} \gamma_i \lambda_j \Psi_i \Psi_j \Psi_k \right\rangle \\
&= \sum_{i=0}^{P} \sum_{j=0}^{P} \gamma_i \lambda_j \langle \Psi_i \Psi_j \Psi_k \rangle
\end{aligned}$$

Projection of product: $v = \gamma\,\lambda$

$$\Rightarrow v_k = \sum_{i=0}^{P}\sum_{j=0}^{P}\gamma_i\lambda_j\frac{\langle\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle} = \sum_{i=0}^{P}\sum_{j=0}^{P}\gamma_i\lambda_j C_{ijk}$$

- $C_{ijk} = \dfrac{\langle\Psi_i\Psi_j\Psi_k\rangle}{\langle\Psi_k^2\rangle}$
- The C_{ijk} tensor can be computed up front for any given PC order and dimension and stored for use whenever two RVs are multiplied
- This tensor is sparse, *i.e.* many of its elements are zero

Non-intrusive Galerkin Projection

$$u_k = \frac{\langle u\Psi_k\rangle}{\langle \Psi_k^2\rangle} = \frac{1}{\langle \Psi_k^2\rangle}\int u\Psi_k(\xi)w(\xi)d\xi, \quad k = 0,\dots,P$$

Evaluate projection integrals numerically

- Pick samples of uncertain parameters, e.g. $b(\xi) = \sum b_k\psi_k(\xi)$ by sampling ξ
- Run deterministic forward model for each of the sampled input parameter values $b^i = b(\xi^i)$
- Integration using random sampling or quadrature methods

Reconstruct uncertain model output

$$u(x,t;\theta) = \sum_{k=0}^{P} u_k(x,t)\Psi_k(\xi(\theta))$$

Random Sampling Approaches for Galerkin Projection

- Evaluate integral through sampling

$$\int u\Psi_k(\xi)w(\xi)d\xi = \frac{1}{N_s}\sum_{i=1}^{N_s} u(\xi^i)\Psi_k(\xi^i)$$

- Samples are drawn according to the distribution of ξ
  - Monte-Carlo (MC)
  - Latin-Hypercube-Sampling (LHS)
- Pros:
  - Can be easily made fault tolerant
  - Sometimes random samples is all we have
- Cons: slow convergence, but less dependent on number of stochastic dimensions

Quadrature Approaches for Galerkin Projection

- Use numerical quadrature rules to evaluate integrals

$$\int u\Psi_k(\xi)w(\xi)d\xi = \sum_{i=1}^{N_q} q^i u(\xi^i)\Psi_k(\xi^i)$$

- The N_q ξ^i are quadrature points, with corresponding weights q^i
- Choice of quadrature points important for accuracy
  - Also referred to as *deterministic sampling* approach
- Pros:
  - Can use existing codes as black box to evaluate $u(\xi^i)$
  - Embarrassingly parallel
- Cons: Tensor product rule for d dimensions requires N_q^d samples

Gauss quadrature rules are very efficient

$$\int u\Psi_k(\xi)w(\xi)d\xi = \sum_{i=1}^{N_q} q^i u(\xi^i)\Psi_k(\xi^i)$$

- In one dimension, N_q quadrature points can integrate polynomial of order $2N_q - 1$ exactly
- Gauss-Hermite and Gauss-Legendre quadrature tailored to specific choices of the weight function $w(\xi)$

Further Reading

An (incomplete) list of references about the material covered

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Polynomial Chaos Based Uncertainty Quantification

Topic 2: Sensitivity Analysis

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Reservoirs UQ Workshop – Aug 1-3, 2017

QUANTIFICATION OF UNCERTAINTY IN EXTREME SCALE COMPUTATIONS
QUEST

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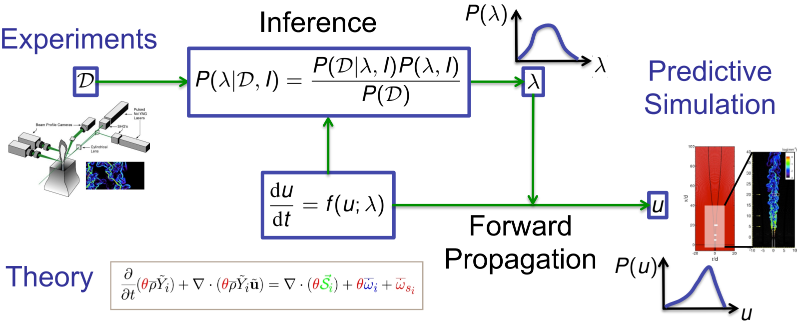
Sensitivity analysis gives insight into key sources of uncertainty



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

PC Postprocessing: global sensitivity information is readily obtained from PCE

$$g(\xi_1, \ldots, \xi_d) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

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

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

PC Postprocessing: Main Effect and Joint Sensitivity Indices

- Main effect sensitivity indices

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

  - $\mathbb{I}_i$ 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

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

  - $\mathbb{I}_{ij}$ 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

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

  - 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

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

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

$$Var(g) = 0 + \; c_1^2\langle\psi_1^2\rangle \; + \; c_2^2\langle\psi_1^2\rangle \; + \; c_3^2\langle\psi_1^2\rangle \; +$$

$$+ \; c_4^2\langle\psi_2^2\rangle \; + \; c_5^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_6^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_7^2\langle\psi_2^2\rangle \; + \; c_8^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_9^2\langle\psi_2^2\rangle$$

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 $P + 1 = (d + p)!/(d!p!) = 10$.

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

Variance contributions

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

Main effect sensitivities $\boxed{\xi_1}$ ξ_2 ξ_3

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 $P + 1 = (d + p)!/(d!p!) = 10$.

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

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$$+ \; c_4\psi_2(\xi_1) \; + \; c_5\psi_1(\xi_1)\psi_1(\xi_2) \; + \; c_6\psi_1(\xi_1)\psi_1(\xi_3) \; + \; c_7\psi_2(\xi_2) \; + \; c_8\psi_1(\xi_2)\psi_1(\xi_3) \; + \; c_9\psi_2(\xi_3)$$

Variance contributions

$$Var(g) = 0 + \; c_1^2\langle\psi_1^2\rangle \; + \; c_2^2\langle\psi_1^2\rangle \; + \; c_3^2\langle\psi_1^2\rangle \; +$$

$$+ \; c_4^2\langle\psi_2^2\rangle \; + \; c_5^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_6^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_7^2\langle\psi_2^2\rangle \; + \; c_8^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; c_9^2\langle\psi_2^2\rangle$$

Main effect sensitivities $\xi_1 \quad \xi_2 \quad \xi_3$

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 $P + 1 = (d+p)!/(d!p!) = 10$.

$$g(\xi_1, \xi_2, \xi_3) = c_0 + c_1\psi_1(\xi_1) + c_2\psi_1(\xi_2) + c_3\psi_1(\xi_3) +$$
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Variance contributions

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

Total sensitivities ξ_1 ξ_2 ξ_3

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 $P + 1 = (d + p)!/(d!p!) = 10$.

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Variance contributions

$$Var(g) = 0 + c_1^2\langle\psi_1^2\rangle + \boxed{c_2^2\langle\psi_1^2\rangle} + c_3^2\langle\psi_1^2\rangle +$$
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Total sensitivities ξ_1 $\boxed{\xi_2}$ ξ_3

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$$g(\xi_1, \xi_2, \xi_3) = c_0 + \; c_1\psi_1(\xi_1) \; + \; c_2\psi_1(\xi_2) \; + \; \boxed{c_3\psi_1(\xi_3)} \; +$$

$$+ \; c_4\psi_2(\xi_1) \; + \; c_5\psi_1(\xi_1)\psi_1(\xi_2) \; + \; \boxed{c_6\psi_1(\xi_1)\psi_1(\xi_3)} + \; c_7\psi_2(\xi_2) \; + \; \boxed{c_8\psi_1(\xi_2)\psi_1(\xi_3)} + \boxed{c_9\psi_2(\xi_3)}$$

Variance contributions

$$Var(g) = 0 + \; c_1^2\langle\psi_1^2\rangle \; + \; c_2^2\langle\psi_1^2\rangle \; + \; \boxed{c_3^2\langle\psi_1^2\rangle} \; +$$

$$+ \; c_4^2\langle\psi_2^2\rangle \; + \; c_5^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle \; + \; \boxed{c_6^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle} + \; c_7^2\langle\psi_2^2\rangle \; + \; \boxed{c_8^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle} + \boxed{c_9^2\langle\psi_2^2\rangle}$$

Total sensitivities ξ_1 ξ_2 $\boxed{\xi_3}$

Sensitivity indices are directly computable from PC

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

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Variance contributions

$$Var(g) = 0 + c_1^2\langle\psi_1^2\rangle + c_2^2\langle\psi_1^2\rangle + c_3^2\langle\psi_1^2\rangle +$$

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Joint sensitivities $\boxed{(\xi_1, \xi_2)}$ (ξ_1, ξ_3) (ξ_2, ξ_3)

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 $P + 1 = (d + p)!/(d!p!) = 10$.

$$g(\xi_1, \xi_2, \xi_3) = c_0 + c_1\psi_1(\xi_1) + c_2\psi_1(\xi_2) + c_3\psi_1(\xi_3) +$$

$$+ c_4\psi_2(\xi_1) + c_5\psi_1(\xi_1)\psi_1(\xi_2) + \boxed{c_6\psi_1(\xi_1)\psi_1(\xi_3)} + c_7\psi_2(\xi_2) + c_8\psi_1(\xi_2)\psi_1(\xi_3) + c_9\psi_2(\xi_3)$$

Variance contributions

$$Var(g) = 0 + c_1^2\langle\psi_1^2\rangle + c_2^2\langle\psi_1^2\rangle + c_3^2\langle\psi_1^2\rangle +$$

$$+ c_4^2\langle\psi_2^2\rangle + c_5^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle + \boxed{c_6^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle} + c_7^2\langle\psi_2^2\rangle + c_8^2\langle\psi_1^2\rangle\langle\psi_1^2\rangle + c_9^2\langle\psi_2^2\rangle$$

Joint sensitivities (ξ_1, ξ_2) $\boxed{(\xi_1, \xi_3)}$ (ξ_2, ξ_3)

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$$Var(g) = 0 + \; c_1^2\langle\psi_1^2\rangle \; + \; c_2^2\langle\psi_1^2\rangle \; + \; c_3^2\langle\psi_1^2\rangle \; +$$
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Joint sensitivities (ξ_1, ξ_2) (ξ_1, ξ_3) $\boxed{(\xi_2, \xi_3)}$

PC Postprocessing: Sampling-Based Approaches

$$g(\xi_1, \ldots, \xi_d) = \sum_{k=0}^{P} c_k \Psi_k(\boldsymbol{\xi})$$

- 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 $g(\boldsymbol{\xi})$, but inquire sensitivity with respect to $g(\boldsymbol{\xi})$
- A brute-force sampling of $Var[\mathbb{E}(g(\boldsymbol{\xi}|\xi_i)]$ is extremely inefficient.

PC Postprocessing: Sampling-Based Approaches

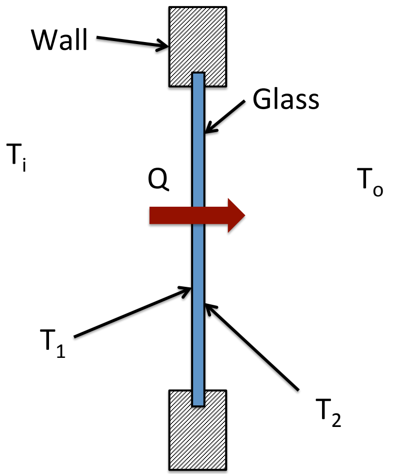
- Tricks are available, given a single set of sampled input [Saltelli, 2002]. E.g., use

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

  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

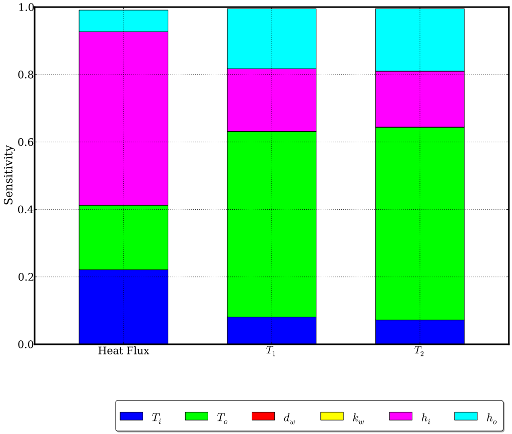


$$h_i(T_i - T_1) = k_w \frac{(T_1 - T_2)}{d_w}$$
$$k_w \frac{(T_1 - T_2)}{d_w} = h_o(T_2 - T_o)$$

6 Uncertain, Gaussian parameters

$$\begin{aligned}
T_i &= 293\mathrm{K}, \sigma = 0.5\% \\
T_o &= 273\mathrm{K}, \sigma = 0.5\% \\
d_w &= 0.01\mathrm{m}, \sigma = 1\% \\
k_w &= 1\mathrm{W/mK}, \sigma = 5\% \\
h_i &= 2\mathrm{W/m^2K}, \sigma = 15\% \\
h_o &= 6\mathrm{W/m^2K}, \sigma = 15\%
\end{aligned}$$

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

Further Reading

An (incomplete) list of references about the material covered

Polynomial Chaos Fundamentals

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Polynomial Chaos Based Uncertainty Quantification

Topic 3: Parameter Dependencies / Interactions

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Reservoirs UQ Workshop – Aug 1-3, 2017

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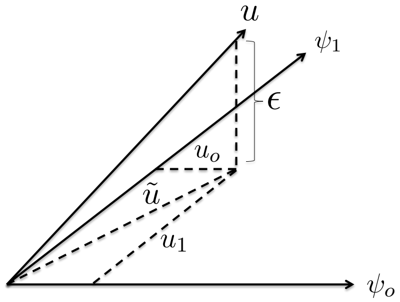
Obtaining PC coefficients for arbitrary random variables is not trivial

- 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

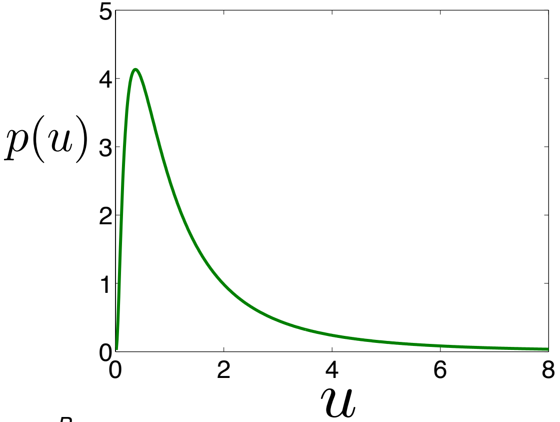
Orthogonality enables a Galerkin projection to determine the PC coefficients



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

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

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



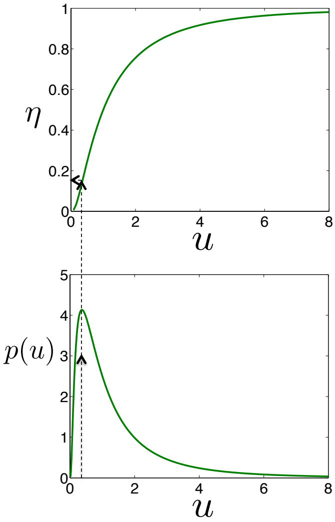
$$u = \sum_{k=0}^{P} u_k \Psi_k(\xi) \qquad \Rightarrow \qquad u_i = \frac{\langle u\, \Psi_i(\xi) \rangle}{\langle \Psi_i^2 \rangle}$$

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

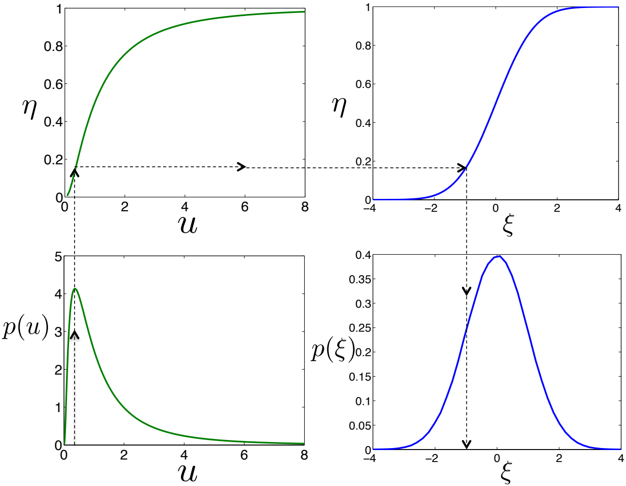
$$F(u) = \int_{-\infty}^{u} p(s)ds$$

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



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

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

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

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

- 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 $\phi(z)$

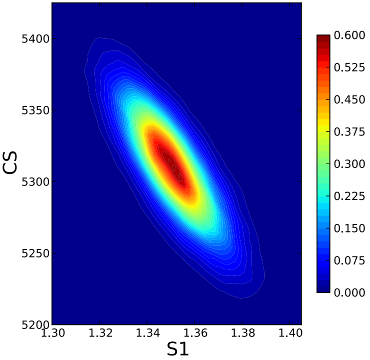
Multivariate Normal Approximation (MVN)

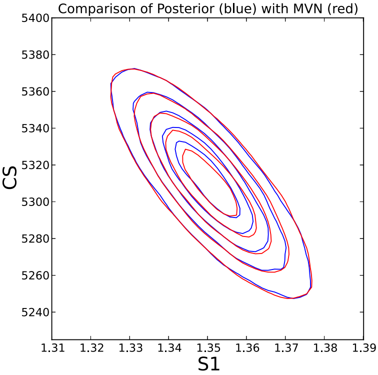
- Many distributions are unimodal and somewhat shaped like Gaussians
- MultiVariate Normal approximations capture mean and correlation structure of the random variables
- Easy to extract from a set of samples
  - In 1D: just compute mean and standard deviation: $u = u_0 + u_1\xi$
  - Multi-D: Cholesky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

$$
\begin{aligned}
C &= LL^T \\
u &= L\xi
\end{aligned}
$$

```
# 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 $(\lambda_1, \ldots, \lambda_d)$ to uniform i.i.d.'s $\{\eta_i\}_{i=1}^{d}$ (Rosenblatt, 1952).

$$
\begin{aligned}
\eta_1 &= F_1(\lambda_1) \\
\eta_2 &= F_{2|1}(\lambda_2|\lambda_1) \\
&\vdots \\
\eta_d &= F_{d|d-1,\ldots,1}(\lambda_d|\lambda_{d-1}, \ldots, \lambda_1)
\end{aligned}
$$

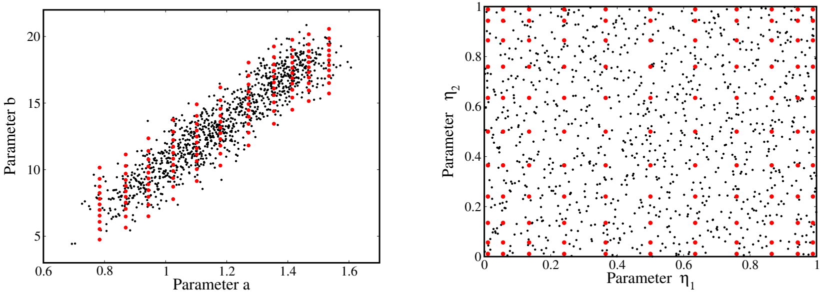
- Rosenblatt transformation is a multi-D generalization of 1D CDF mapping.
- Conditional CDFs are harder to evaluate in high dimensions

Rosenblatt transformation of a given sample set requires KDE

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

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

Rosenblatt transformation enables Galerkin projection



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

$$a = \sum_{k=0}^{P} a_k \Psi_k(\xi) \qquad a_k \propto \int \underbrace{R_a^{-1}(\xi)}_{a} \Psi_k(\xi) w(\xi) d\xi$$

$$b = \sum_{k=0}^{P} b_k \Psi_k(\xi) \qquad b_k \propto \int \underbrace{R_b^{-1}(\xi)}_{b} \Psi_k(\xi) w(\xi) d\xi$$

Further Reading

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Polynomial Chaos Based Uncertainty Quantification

Topic 4: Surrogate Models / Meta-models

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Reservoirs UQ Workshop – Aug 1-3, 2017

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Surrogate Models

- Approaches:
  - Polynomial Chaos Expansions
  - Gaussian Process Models
  - Low-rank Approximations
- Challenges:
  - High-dimensionality of input space
  - Computational cost of forward model

Mitigation Approaches

- High-Dimensionality:
  - Dimensionality reduction (sensitivity analysis)
  - Adaptive Sparse Quadrature approaches
  - Compressed Sensing
  - Low-rank approximations
- Computational Cost:
  - Multifidelity - Multilevel methods (see DAKOTA team)

Bayesian Compressed Sensing

- N training data points $(\boldsymbol{x}_n, u_n)$ and K basis terms $\Psi_k(\cdot)$
- Projection matrix $\boldsymbol{P}^{N\times K}$ with $\boldsymbol{P}_{nk} = \Psi_k(\boldsymbol{x}_n)$
- Find regression weights $\boldsymbol{c} = (c_0, \ldots, c_{K-1})$ so that

$$\boldsymbol{u} \approx \boldsymbol{P}\boldsymbol{c} \quad \text{or} \quad u_n \approx \sum_k c_k \Psi_k(\boldsymbol{x}_n)$$

- The number of polynomial basis terms grows fast; a p-th order, d-dimensional basis has a total of $K = (p+d)!/(p!d!)$ terms.
- For limited data and large basis set ($N < K$) this is a sparse signal recovery problem $\Rightarrow$ need some regularization/constraints.

- Least-squares $\quad argmin_{\boldsymbol{c}} \{||\boldsymbol{u} - \boldsymbol{P}\boldsymbol{c}||_2\}$
- The 'sparsest' $\quad argmin_{\boldsymbol{c}} \{||\boldsymbol{u} - \boldsymbol{P}\boldsymbol{c}||_2 + \alpha||\boldsymbol{c}||_0\}$
- Compressive sensing $\quad argmin_{\boldsymbol{c}} \{||\boldsymbol{u} - \boldsymbol{P}\boldsymbol{c}||_2 + \alpha||\boldsymbol{c}||_1\}$

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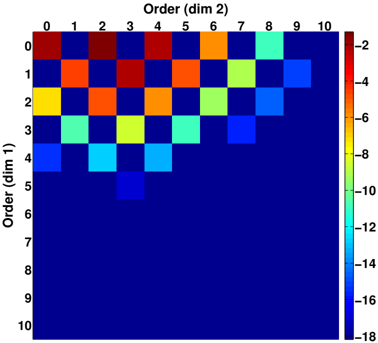
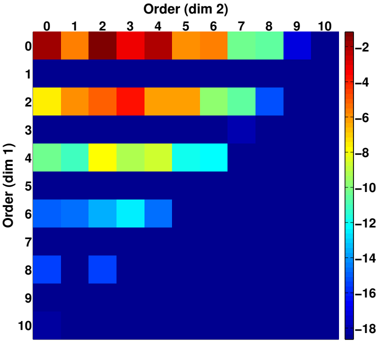
Bayesian Likelihood Prior

BCS removes unnecessary basis terms

$f(x,y) = \cos(x+4y)$ $\qquad$ $f(x,y) = \cos(x^2+4y)$

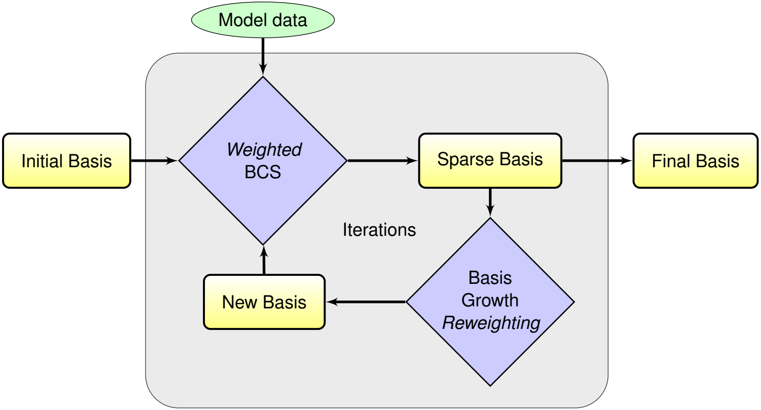




The square (i,j) represents the (log) spectral coefficient for the basis term $\psi_i(x)\psi_j(y)$.

Iterative Bayesian Compressive Sensing (iBCS)

- *Iterative BCS*: iteratively increase the order for the relevant basis terms while maintaining the dimensionality reduction [Sargsyan *et al.* 2014], [Jakeman *et al.* 2015].
- Combine basis growth and reweighting!



Low-Rank Approximations

- Univariate function representation: $p+1$ coefficients

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

- Multivariate function representation: $P+1 = \frac{(n+p)!}{n!p!}$

$$u(\xi_1, \ldots, \xi_n) = \sum_{k=0}^{P} u_k \prod_{i=1}^{n} \psi_{\alpha_i^k}(\xi_i)$$

- Low-rank approximation: $r * (p_1 + p_2 + \ldots + p_n)$

$$u(\xi_1, \ldots, \xi_n) = \sum_{k=1}^{r} w_k^{(1)}(\xi_1) \ldots w_k^{(n)}(\xi_n)$$

Minimization Problem for Coefficients

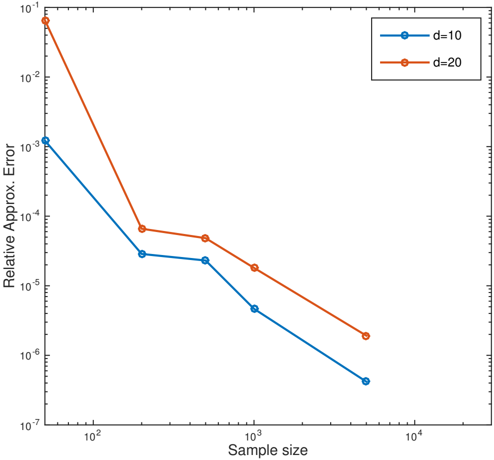
- Minimization problem:

$$\min_{\tilde{u}\in\mathcal{M}} \|u(\xi) - \tilde{u}(\xi)\|^2 + \lambda\mathcal{R}(\tilde{u}(\xi))$$

  where $\mathcal{M}$ is a suitable tensor subset (Canonical, Tensor Train) and $\mathcal{R}$ is a regularization function
- Selection of optimal rank r and regularization coefficient λ using cross validation
- Pros: Linear increase in parameters with dimension
- Cons: Non-linear optimization problem. Optimal approximation $\tilde{u}(\xi)$ is often not known

Low rank approximation of Genz Gaussian

- $u(\xi) = \exp\left(-\sum_{i=1}^{d} c^2(\xi_i - w)^2\right), \; c = 0.1, w = 0.5$
- $\mathcal{M}$: Canonical rank-r, $\mathcal{R}$: ℓ_1



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