Spectral Methods for Uncertainty Quantification

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UTOPIÆ Uncertainty Treatment and Optimisation in Aerospace Engineering
Handling the unknown at the edge of tomorrow

PhD course on UQ - DTU

Overview

Objectives of the lecture

- Introduce Parametric Uncertainty Quantification & Propagation
- Discuss a first spectral expansion: the Karhunen-Loève decomposition
- Formalism and essential ingredients of Wiener's PC expansions
- Generalize finite dimensional PC expansions to arbitrary measures
- Shortly discuss alternative construction approaches.

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Simulation framework.

Basic ingredients

- Understanding of the physics involved (optional?):
  selection of the **mathematical model**.
- **Numerical method**(s) to solve the model.
- Specify a set of **data**:
  select a system among the class spanned by the model.

Simulation framework.

Basic ingredients

- Understanding of the physics involved (optional?):
  selection of the **mathematical model**.
- **Numerical method**(s) to solve the model.
- Specify a set of **data**:
  select a system among the class spanned by the model.

Simulation errors

- **Model errors**: physical approximations and simplifications.
- **Numerical errors**: discretization, approximate solvers, finite arithmetics.
- **Data error: boundary/initial conditions, model constants and parameters, external forcings, . . .**

Sources of data uncertainty

- Inherent **variability** (*e.g.* industrial processes).
- **Epistemic** uncertainty (*e.g.* model constants).
- **May not be fully reducible, even theoretically**.

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Probabilistic framework

- Define an abstract probability space $(\Theta, \mathcal{A}, d\mu)$.
- Consider **data** D as **random** quantity: $D(\theta), \ \theta \in \Theta$.
- **Simulation output** S is **random** and on $(\Theta, \mathcal{A}, d\mu)$.

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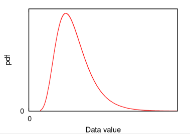
- **Simulation output** S is **random** and on $(\Theta, \mathcal{A}, d\mu)$.
- **Data D and simulation output S are dependent random quantities (through the mathematical model $\mathcal{M}$):**

$$\mathcal{M}(S(\theta), D(\theta)) = 0, \quad \forall \theta \in \Theta.$$

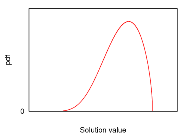
Propagation of data uncertainty

Data density



$$\mathcal{M}(S, D) = 0$$

Solution density



- **Variability** in model output: numerical error bars.
- Assessment of **predictability**.
- Support **decision making process**.
- What type of information (abstract quantities, confidence intervals, density estimations, structure of dependencies, ...) one needs?

Deterministic methods

- **Sensitivity analysis** (adjoint based, AD, . . .): local.
- **Perturbation techniques**: limited to low order and simple data uncertainty.
- **Neumann expansions**: limited to low expansion order.
- **Moments** method: closure problem (non-Gaussian / non-linear problems).

Simulation techniques — Monte-Carlo

Spectral Methods

Deterministic methods

Simulation techniques — Monte-Carlo

- Generate a **sample set of data** realizations and compute the corresponding **sample set of model ouput**.
- Use sample set based **random estimates** of abstract characterizations (moments, correlations, . . .).
- Plus: **Very robust** and re-use **deterministic codes**: (parallelization, complex data uncertainty).
- Minus: **slow convergence of the random estimates** with the sample set dimension.

Spectral Methods

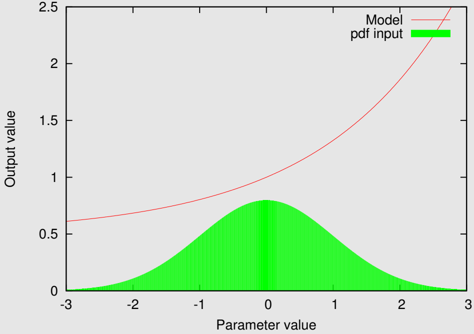
Deterministic methods

Simulation techniques — Monte-Carlo

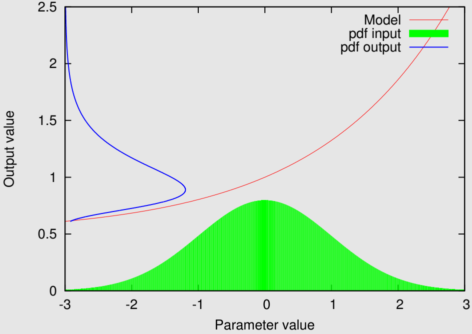
Spectral Methods

- Parameterization of the data with random variables (RVs).
- $\perp$ projection of solution on the (L_2) space spanned by the RVs.
- Plus: **arbitrary level of uncertainty, deterministic approach, convergence rate, information contained**.
- Minus: **parameterizations** (limited # of RVs), **adaptation of simulation tools** (legacy codes), **robustness** (non-linear problems, non-smooth output, . . .).
- **Not suited for model uncertainty**

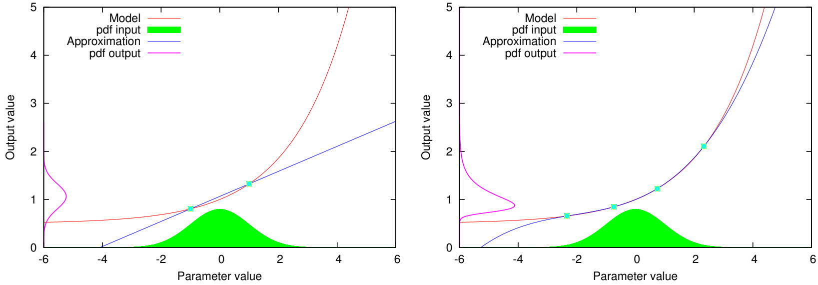
Propagation of data uncertainty



Propagation of data uncertainty

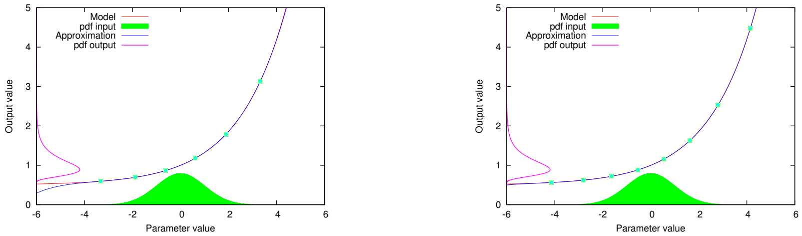


- Large number of parameters
- Costly model evaluation (PDE)
- Estimation of $p(S)$ is not the end of the story!



Approximate the model output $S(D)$ through a functional representation of the form

$$S(D) \approx \sum_{k=0}^{\mathrm{P}} S_k \Psi_k(D) \doteq S^{\mathrm{P}}(D)$$



$$S(D) \approx \sum_{k=0}^{\mathrm{P}} S_k \Psi_k(D) \doteq S^{\mathrm{P}}(D)$$

- Exploit (whenever possible) the smoothness of $S(D)$ to have a fast convergence of $S^{\mathrm{P}}(D)$ toward $S(D)$
- Determine S^{P} at a low computational cost
- Base UQ analysis on the surrogate $S^{\mathrm{P}}(D)$ (cheap evaluations).

Example (Elliptic equations)

Let $\Omega \in \mathbb{R}^2$ be a closed domain, and the Dirichlet problem

$$\begin{aligned} \nabla \cdot (\nu(\boldsymbol{x})\nabla u(\boldsymbol{x})) &= -f(\boldsymbol{x}) && \forall \boldsymbol{x} \in \Omega, \\ u(\boldsymbol{x}) &= 0 && \boldsymbol{x} \in \partial\Omega. \end{aligned}$$

with $0 < \epsilon < \nu(\boldsymbol{x}) < +\infty$ and f given.
Introducing a suitable functional space $V := H_0^1$, the solution $u \in V$ is such that

$$\begin{aligned} a(u, v; \nu) &= b(v) && \forall v \in V, \\ a(u, v; \nu) &= \int_\Omega \nu \nabla u \cdot \nabla v d\boldsymbol{x} && b(v) = \int_\Omega f v d\boldsymbol{x}. \end{aligned}$$

The solution is unique.

Example (Uncertainty)

The unique solution to

$$a(u, v; \nu) = b(v) \qquad \forall v \in V,$$

depends (continuously) on ν: $u := u(\boldsymbol{x}, \nu)$

Now, if ν is uncertain and model as a random process defined on a probability space $(\Theta, \Sigma, d\mu)$

$$(\Omega \times \Theta) \ni (\boldsymbol{x} \times \theta) \mapsto \nu(\boldsymbol{x}, \theta) \in \mathbb{R}.$$

$\nu(\cdot, \theta)$ is a function with domain Ω, $\nu(\boldsymbol{x}, \cdot)$ is a random variable.

$\implies u(\boldsymbol{x}, \nu)$ **is now random, we write** $U(\boldsymbol{x}, \theta)$.

The stochastic solution $U(\boldsymbol{x}, \theta)$ solves almost surely

$$a(U(\cdot, \theta), v; \nu(\theta)) = b(v) \qquad \forall v \in V.$$

We need to compute $U(\boldsymbol{x}, \theta)$.

Example (Spectral expansion)

Often $U(\boldsymbol{x}, \theta)$ is smooth in $\boldsymbol{x}$ and with respect to $\nu(\theta)$. We seek for a spectral approximation using a **rapidly converging** series

$$U(\boldsymbol{x}, \theta) = \sum_{n \geq 0} u_n(\boldsymbol{x}) \eta_n(\theta),$$

where $u_n(\boldsymbol{x}) \in V$ and $\eta_n(\theta)$ is defined on $(\Theta, \Sigma, d\mu)$.

Table of content

Consider a stochastic process $U(\boldsymbol{x}, \theta)$ (say the solution of the stochastic elliptic problem). We seek for the spectral expansion of U as

$$U(\boldsymbol{x}, \theta) = \sum_{n \geq 0} u_n(\boldsymbol{x}) \eta_n(\theta),$$

Denote

- (u, v) the inner product in $L^2(\Omega)$ equipped with the norm $\| \cdot \|_2$
- $\mathbb{E}[\cdot]$ the expectation operator

and assume $\mathbb{E}[U(\boldsymbol{x}, \cdot)] = 0$ and $U \in L^2(\Omega, \Theta)$: $\mathbb{E}\left[U(\boldsymbol{x}, \cdot)^2\right] < +\infty$, $\|U(\cdot, \theta)\|_2 < +\infty$
How to define the best m-terms truncated expansion

$$U(\boldsymbol{x}, \theta) \approx \sum_{n=1}^{m} u_n(\boldsymbol{x}) \eta_n(\theta)?$$

Hint: the m-terms expansion minimizes the approximation error

$$\epsilon(m)^2 = \mathbb{E}\left[\left\| U - \sum_{n=1}^{m} u_n \eta_n \right\|_2^2\right],$$

- The solution is not unique: $\|u_n\|_2 = 1$
- The spatial modes u_n are the **eigenfunctions** of the auto-correlation kernel

$$(\Omega \times \Omega) \ni (\boldsymbol{x}, \boldsymbol{y}) \mapsto K(\boldsymbol{x}, \boldsymbol{y}) = \mathbb{E}\left[U(\boldsymbol{x}, \cdot)U(\boldsymbol{y}, \cdot)\right] \in \mathbb{R}.$$

That is:

$$(Ku_n, v) = \lambda_n(u_n, v) \qquad v \in V.$$

Observe : K is a symmetric positive operator so the eigenfunctions are orthonormal: $(u_n, u_{n'}) = \delta_{nn'}$

The optimal decomposition is

$$U(\boldsymbol{x}\theta) \approx \sum_{n=1}^{m} \sqrt{\lambda_n} u_n(\boldsymbol{x}) \eta_n(\theta),$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$ and

$$\eta_n(\theta) = (U(\cdot, \theta), u_n), \quad \mathbb{E}[\eta_n] = 0, \quad \mathbb{E}\left[\eta_n^2\right] = 1.$$

- optimality and convergence in the mean-squared sense
- can be applied only if U is known
- how to represent the stochastic coefficient?

Example (Parametrization)

The KL expansion is often used to construct **parametrizations** of the uncertain model input which are known.
For instance, ν is frequently model as a log-normal random field:

$$\nu(\boldsymbol{x}, \theta) = C \exp G(\boldsymbol{x}, \theta),$$

where G is a zero-mean Gaussian random field with prescribed auto-correlation kernel $K_G(\boldsymbol{x}, \boldsymbol{y})$:

$$G(\boldsymbol{x}, \theta) \approx \sum_{n=1}^{m} g_n(\boldsymbol{x}) \xi_n(\theta),$$

where the ξ_n's are independent normalized Gaussian random variables. Setting $\boldsymbol{\xi} = (\xi_1 \cdots \xi_m)$, we finally seek for the **approximate** $U^m(\boldsymbol{x}, \boldsymbol{\xi})$ such that a.s.

$$a\left(U^m(\boldsymbol{x}, \boldsymbol{\xi}), v; \nu(\boldsymbol{x}, \boldsymbol{\xi})\right) = b(v) \quad \forall v \in V.$$

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Consider a $\mathbb{R}$-valued random variable defined on a probability space (Θ, Σ, dP):

$$U : \Theta \mapsto \mathbb{R}.$$

We denote $L^2(\Theta, dP)$ the space of second order random variables:

$$U \in L^2(\Theta, dP) \Leftrightarrow \mathbb{E}\left[U^2\right] := \int_\Theta U(\theta)^2 dP(\theta) < +\infty.$$

Let $\{\xi_i\}_{i=1}^{\infty}$ be a sequence of centered, normalized, mutually orthogonal (uncorrelated) Gaussian random variables:

$$\mathbb{E}[\xi_i] = 0, \quad \mathbb{E}\left[\xi_i \xi_j\right] = \delta_{i,j} \quad \forall\, i, j = 1, 2, \ldots$$

We denote for $p = 0, 1, 2, \ldots$:

- $\hat{\Gamma}_p$ the space of orthogonal polynomials in $\{\xi_i\}_{i=1}^{\infty}$ with degree $\leq p$.
- Γ_p the set of polynomials belonging to $\hat{\Gamma}_p$ and $\perp$ to $\hat{\Gamma}_{p-1}$.
- $\tilde{\Gamma}_p$ the (sub) space spanned by Γ_p.

We have

$$\hat{\Gamma}_p = \hat{\Gamma}_{p-1} \oplus \tilde{\Gamma}_p, \quad L^2(\Theta, dP) = \bigoplus_{p=0}^{p=\infty} \tilde{\Gamma}_p.$$

- $\tilde{\Gamma}_p$ is called the p-th Homogeneous Chaos.
- Γ_p is called the Polynomial Chaos of order p.
- Γ_p consists of orthogonal polynomials with degree p, involving all combinations of the r.v. $\{\xi_i\}$.

Note: functions of r.v. are r.v. themselves and are regarded as functionals.

Fundamental Result: [Wiener, 1938]

Any well-behaved random variable, *e.g.* second order ones, has a PC representation of the form

$$
\begin{aligned}
U(\theta) = & u_0\Gamma_0 + \sum_{i_1=1}^{\infty} u_{i_1}\Gamma_1(\xi_{i_1}(\theta)) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} u_{i_1,i_2}\Gamma_2(\xi_{i_1}(\theta),\xi_{i_2}(\theta)) \\
& + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} u_{i_1,i_2,i_3}\Gamma_3(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta)) \\
& + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2}\sum_{i_4=1}^{i_3} u_{i_1,i_2,i_3,i_4}\Gamma_4(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta),\xi_{i_4}(\theta)) + \dots
\end{aligned}
$$

The series converges in the mean-square sense:

$$
\lim_{p\to\infty} \mathbb{E}\left[\left(u_0\Gamma_0 + \cdots + \sum_{i_1=1}^{\infty}\cdots\sum_{i_p=1}^{i_{p-1}}\Gamma_p(\xi_{i_1},\cdots,\xi_{i_p}) - U\right)^2\right] = 0.
$$

PC expansion of U:

$$
\begin{aligned}
U(\theta) = & u_0\Gamma_0 + \sum_{i_1=1}^{\infty} u_{i_1}\Gamma_1(\xi_{i_1}(\theta)) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} u_{i_1,i_2}\Gamma_2(\xi_{i_1}(\theta),\xi_{i_2}(\theta)) \\
& + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} u_{i_1,i_2,i_3}\Gamma_3(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta)) \\
& + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2}\sum_{i_4=1}^{i_3} u_{i_1,i_2,i_3,i_4}\Gamma_4(\xi_{i_1}(\theta),\xi_{i_2}(\theta),\xi_{i_3}(\theta),\xi_{i_4}(\theta)) + \dots
\end{aligned}
$$

- We denote $\boldsymbol{\xi} := \{\xi_i\}_{i=1}^{\infty}$.
- We shall write $U(\boldsymbol{\xi})$ for the PC expansion of U.

Few important properties:

- Vanishing expectation: $\mathbb{E}[\Gamma_p] = 0$ for $p > 0$.
- One can express the expectation of U in the Gaussian space spanned by ξ_i with the measure

$$p_{\boldsymbol{\xi}}(\boldsymbol{y}) = \prod_{i=1}^{\infty} \frac{1}{\sqrt{2\pi}} \exp\left[-y_i^2/2\right].$$

- that is

$$\mathbb{E}[U] = \int_{\Theta} U(\theta) dP(\theta) = \int_{\Theta} U(\boldsymbol{\xi}(\theta)) dP(\theta)$$
$$= \int \cdots \int U(\boldsymbol{y}) p_{\boldsymbol{\xi}}(\boldsymbol{y}) d\boldsymbol{y} =: \langle U \rangle.$$

- The orthogonality of the polynomials is with regard to the Gaussian measure.

Truncated PC expansions: in practice a finite number of r.v. is used

$$\boldsymbol{\xi} = \{\xi_1, \cdots, \xi_N\}$$

N is called the stochastic dimension and $\boldsymbol{\xi}$ is often referred as the stochastic germ.

Example of two dimensional PC expansion:

$$\begin{aligned} U(\xi_1, \xi_2) = {} & u_0 \Gamma_0 + u_1 \Gamma_1(\xi_1) + u_2 \Gamma_2(\xi_2) \\ & + u_{11} \Gamma_2(\xi_1, \xi_1) + u_{21} \Gamma_2(\xi_2, \xi_1) + u_{22} \Gamma_2(\xi_2, \xi_2) \\ & + u_{111} \Gamma_3(\xi_1, \xi_1, \xi_1) + u_{211} \Gamma_3(\xi_2, \xi_1, \xi_1) + u_{221} \Gamma_3(\xi_2, \xi_2, \xi_1) \\ & + u_{222} \Gamma_3(\xi_2, \xi_2, \xi_2) + u_{1111} \Gamma_4(\xi_1, \xi_1, \xi_1, \xi_1) + \dots \end{aligned}$$

With the introduction of an indexation scheme, the expansion can be recast as

$$U(\boldsymbol{\xi}) = \sum_{k=0}^{\infty} u_k \Psi_k(\boldsymbol{\xi}), \quad u_k \in \mathbb{R}.$$

The u_k are the PC coefficients of U and Ψ_k are (orthogonal) polynomial. We here use the convention $\Psi_0 = \Gamma_0 = 1$.

1-D PC expansion:

Recall that the chaos polynomials are orthogonal wrt the probability density of ξ (centered, normalized, Gaussian):

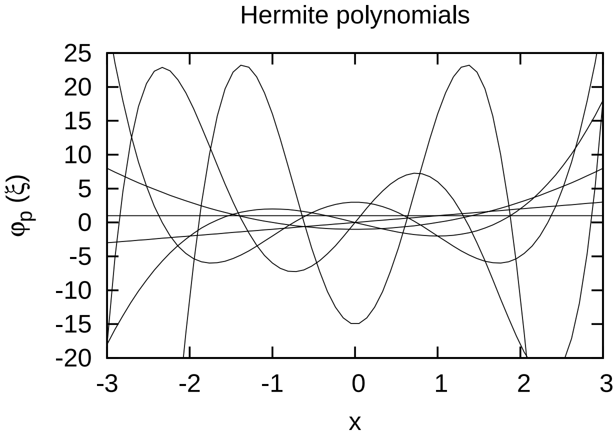
$$p_\xi(y) = \frac{1}{\sqrt{2\pi}} \exp\left[-y^2/2\right]. \quad (1)$$

By $\psi_p(\xi)$ we denote the 1D polynomial of order p.
Following the indexation convention, $\psi_0(\xi) = 1$.
The orthogonality condition is:

$$\mathbb{E}\left[\psi_i \psi_j\right] = \int_{\mathbb{R}} \psi_i(y)\psi_j(y)p_\xi(y)\mathrm{d}y = \delta_{ij}\left\langle \psi_i^2 \right\rangle.$$

- The ψ_i is the well known Hermite polynomial of degree i.
- the Hermite polynomials are normalized s.t. $\langle \psi_i^2 \rangle = i!$.

First Hermite polynomials (1-D):



One-dimensional Hermite polynomials, $\psi_p(\xi)$, for $p = 0, \ldots, 6$.

Multi-dimensional PC basis:
The N-variate polynomials Ψ_i are constructed as product of 1-D Hermite polynomials.
Let $\gamma := \{\gamma_1 \dots \gamma_{\mathrm{N}}\} \in \mathbb{N}^{\mathrm{N}}$ be a multi-index and $\lambda(p)$ the multi-index set

$$\lambda(p) = \left\{ \gamma \, : \, \sum_{i=1}^{\mathrm{N}} \gamma_i = p \right\}.$$

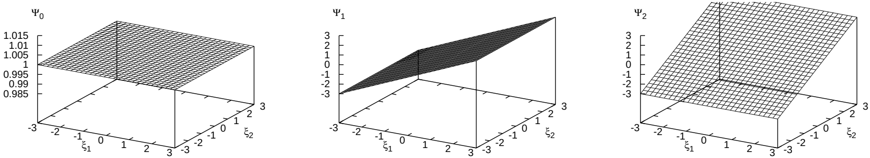
The p-th order polynomial chaos is constructed according to:

$$\Gamma_p = \left\{ \bigcup_{\gamma \in \lambda(p)} \prod_{\gamma_1}^{\gamma_{\mathrm{N}}} \psi_{\gamma_i}(\xi_i) \right\}.$$

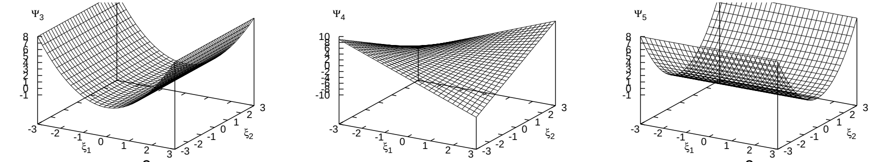
Example for $\mathrm{N} = 2$:

$$\begin{aligned} U(\xi_1, \xi_2) = {} & u_0\psi_0 + u_1\psi_1(\xi_1) + u_2\psi_1(\xi_2) + u_{11}\psi_2(\xi_1) + u_{21}\psi_1(\xi_2)\psi_1(\xi_1) \\ & + u_{22}\psi_2(\xi_2) + u_{111}\psi_3(\xi_1) + u_{211}\psi_1(\xi_2)\psi_2(\xi_1) \\ & + u_{221}\psi_2(\xi_2)\psi_1(\xi_1) + u_{222}\psi_3(\xi_2) + u_{1111}\psi_4(\xi_1) + \dots \end{aligned}$$

The Hermite polynomials for $p \leq 2$ $(\mathrm{N} = 2)$

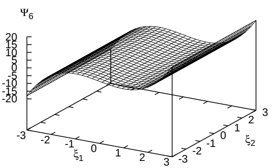


$\Psi_0 = 1$ $\Psi_1 = \xi_1$ $\Psi_2 = \xi_2$

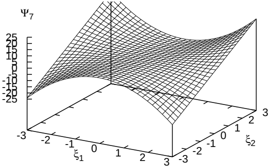


$\Psi_3 = \xi_1^2 - 1$ $\Psi_4 = \xi_1\xi_2$ $\Psi_5 = \xi_2^2 - 1$

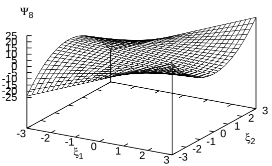
The Hermite polynomials for $p = 3$ ($\mathrm{N} = 2$)



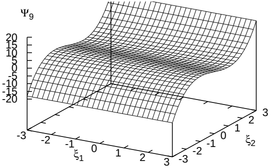
$\Psi_6 = \xi_1^3 - 3\xi_1$



$\Psi_7 = \xi_1^2\xi_2 - \xi_2$



$\Psi_8 = \xi_1\xi_2^2 - \xi_1$



$\Psi_9 = \xi_2^3 - 3\xi_2$

Truncated PC expansion

In addition to a finite number of random variables, N, we need to truncate the PC expansion to a finite order p

$$U(\xi) \approx U^{\mathrm{P}}(\xi) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi), \quad \mathrm{P}+1 = \frac{(\mathrm{N}+p)!}{\mathrm{N}!p!}$$

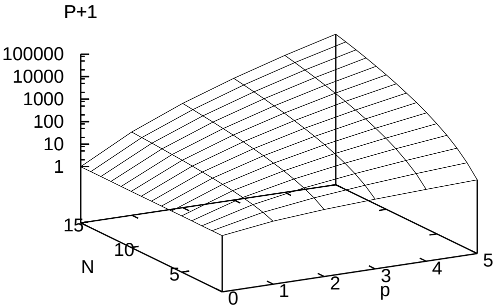
Dependence of $(\mathrm{P}+1)$ on N and p:

p/N	1	2	3	4	5	6
1	2	3	4	5	6	7
2	3	6	10	15	21	28
3	4	10	20	35	56	84

p/N	1	2	3	4	5	6
4	5	15	35	70	126	210
5	6	21	56	126	252	462
6	7	28	84	210	462	924

Fast increase with both N and p.

Other truncature strategies may be used.



Number of terms in the PC expansion plotted against the order, p, and the number of dimensions, N.

The truncated expansion of a random variable U is

$$U(\theta) \approx U^{\mathrm{P}}(\xi) + \epsilon(\mathrm{N}, p) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi) + \epsilon(\mathrm{N}, p).$$

The truncation error depends both on N and p.

The error is a random variable.

The expansion converges in the mean-square sense as N *and* p go to infinity [Cameron & Martin, 1947]:

$$\lim_{\mathrm{N}, p \to \infty} \left\langle \epsilon^2(\mathrm{N}, p) \right\rangle = 0.$$

In light of the dependence of P on the order and the number of random variables, the PC representation will be computationally efficient if the convergence is fast in both N and p.

Hilbert space (fixed finite N)

- The polynomials $\{\Psi_k\}_{k=0}^{\infty}$ forms an orthogonal basis of $L^2(\mathbb{R}^{\mathrm{N}}, p_{\boldsymbol{\xi}})$.
- $L^2(\mathbb{R}^{\mathrm{N}}, p_{\boldsymbol{\xi}})$ is equipped with the inner product

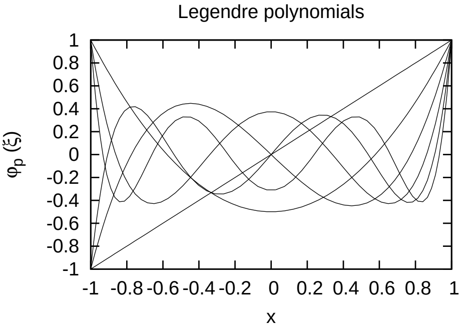
$$\langle U, V \rangle := \mathbb{E}\left[UV\right] = \int_{\mathbb{R}^{\mathrm{N}}} U(\boldsymbol{y})V(\boldsymbol{y})p_{\boldsymbol{\xi}}(\boldsymbol{y})d\boldsymbol{y}$$

  and norm $\|U\|_{L^2(\mathbb{R}^{\mathrm{N}}, p_{\boldsymbol{\xi}})} := \langle U, U \rangle^{1/2}$.
- The convergence of the truncated expansion $U^{\mathrm{P}} \to U$ depends on the probability law of U.
- For instance, if U is Gaussian, it has an exact first order expansion.
- Suggests the construction of polynomial spaces based on non-Gaussian distributions.

Generalized Polynomial Chaos (GPC) [Xiu & Karniadakis, 2002]

	Distribution ξ	Polynomials $\psi_k(\xi)$	Support
Continuous RV	Gaussian	Hermite	$(-\infty, \infty)$
	γ	Laguerre	$[0, \infty)$
	β	Jacobi	$[a, b]$
	Uniform	Legendre	$[a, b]$
Discrete RV	Poisson	Charlier	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk	$\{0, 1, 2, \dots, n\}$
	Negative binomial	Meixner	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn	$\{0, 1, 2, \dots, n\}$

Families of probability laws and corresponding families of orthogonal polynomials.



One-dimensional Legendre polynomials of order $p = 0, \dots, 6$.

- If the r.v. in $\boldsymbol{\xi}$ are independent,

$$p_{\boldsymbol{\xi}}(\boldsymbol{y}) = \prod_{i=1}^{\mathrm{N}} p_i(y_i),$$

the Ψ_k can be obtained by tensorization of one-dimensional polynomials constructed on the probability distribution of each ξ_i.

- We denote $\{\psi_l^{(i)}\}_{l=0}^{p}$ the family of 1-D polynomials with degree $\leq p$ orthogonal w.r.t. to the measure p_i associated to ξ_i, $i = 1, \cdots, \mathrm{N}$, that is

$$\int \psi_l(y)\psi_{l'}(y)p_i(y)dy = \delta_{l,l'} \int \psi_l(y)^2 p_i(y)dy.$$

- The m-th order GPC is constructed according to:

$$\Gamma_m^G = \left\{ \bigcup_{\gamma \in \lambda(m)} \prod_{\gamma_1}^{\gamma_{\mathrm{N}}} \psi_{\gamma_i}^{(i)}(\xi_i) \right\}, \quad \bigoplus_{m=0}^{m=p} \Gamma_m^G = \{\Psi_k\}_{k=0}^{k=\mathrm{P}}.$$

- For general distributions of the independent ξ_i, one can rely on numerical orthogonalization procedure (Gram-Schmidt) to construct the 1-D family of polynomials.
- Anticipating forthcoming lectures, one can think of using other types of functionals in the construction.
- These include piecewise polynomial functions, sine and cosine functions (uniform measure), wavelets, ...
- In fact any basis of the Hilbert space $L^2(\Xi, p_{\xi})$, where Ξ is the support of p_{ξ}.
- An important aspect to keep in mind is the dimension of the expansion.

(Really) Generalized PC: [Soize & Ghanem, 2004]
Case of a germ ξ **with dependent components** ξ_i

- The joint probability distribution p_{ξ} can not be factorized.
- Denote p_i the marginal distribution of ξ_i:

$$p_i(y) = \int \mathrm{d}y_1 \cdots \int \mathrm{d}y_{i-1} \int \mathrm{d}y_{i+1} \cdots \int \mathrm{d}y_{\mathrm{N}}\, p_{\xi}(y_1, \cdots, y_{\mathrm{N}}).$$

- Let $\{\phi_p^{(i)}(\xi)\}$ be the corresponding sets of 1-D polynomials satisfying

$$\left\langle \phi_p^{(i)}, \phi_{p'}^{(i)} \right\rangle_{p_i} \equiv \int \phi_p^{(i)}(y)\phi_{p'}^{(i)}(y) p_i(y)\mathrm{d}y = \delta_{pp'}.$$

(Really) Generalized PC: [Soize & Ghanem, 2004]
Case of a germ $\boldsymbol{\xi}$ **with dependent components** ξ_i

- The joint probability distribution $p_{\boldsymbol{\xi}}$ can not be factorized.
- Denote p_i the marginal distribution of ξ_i:

$$p_i(y) = \int dy_1 \cdots \int dy_{i-1} \int dy_{i+1} \cdots \int dy_N \, p_{\boldsymbol{\xi}}(y_1, \cdots, y_N).$$

- The Chaos function associated to the multi-index $\gamma \in \mathbb{N}^N$ writes

$$\Psi_\gamma(\boldsymbol{\xi}) = \left[\frac{p_1(\xi_1) \dots p_N(\xi_N)}{p_{\boldsymbol{\xi}}(\boldsymbol{\xi})} \right]^{1/2} \phi^{(1)}_{\gamma_1}(\xi_1) \dots \phi^{(N)}_{\gamma_N}(\xi_N).$$

- It can be checked that the Ψ's are orthogonal and form a basis of $L^2(\Xi, p_{\boldsymbol{\xi}})$.
- This is no more a polynomial expansion!

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- Let U^{P} be given by a truncated (G)PC expansion

$$U^{\mathrm{P}}(\boldsymbol{\xi}) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\boldsymbol{\xi}),$$

where the chaos polynomials $\{\Psi_0, \ldots, \Psi_{\mathrm{P}}\}$ are orthogonal (with the convention $\Psi_0 = 1$).

- The mathematical expectation of U is

$$\mathbb{E}\left[U^{\mathrm{P}}\right] = \left\langle U^{\mathrm{P}}(\boldsymbol{\xi})\right\rangle = \left\langle \Psi_0, U^{\mathrm{P}}(\boldsymbol{\xi})\right\rangle = \sum_{k=0}^{\mathrm{P}} u_k \left\langle \Psi_0, \Psi_k \right\rangle = u_0.$$

- Let U^{P} be given by a truncated (G)PC expansion

$$U^{\mathrm{P}}(\boldsymbol{\xi}) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\boldsymbol{\xi}),$$

where the chaos polynomials $\{\Psi_0, \dots, \Psi_{\mathrm{P}}\}$ are orthogonal (with the convention $\Psi_0 = 1$).

- Its variance $\sigma^2_{U^{\mathrm{P}}}$ is in turn

$$\sigma^2_{U^{\mathrm{P}}} = \mathbb{E}\left[\left(U^{\mathrm{P}} - \mathbb{E}\left[U^{\mathrm{P}}\right]\right)^2\right] = \mathbb{E}\left[\left(\sum_{k=1}^{\mathrm{P}} u_k \Psi_k\right)^2\right]$$
$$= \sum_{k,l=1}^{\mathrm{P}} u_k u_l \left\langle \Psi_k, \Psi_l \right\rangle = \sum_{k=1}^{\mathrm{P}} u_k^2 \left\langle \Psi_k^2 \right\rangle.$$

The variance of U^{P} is given as a weighted sum of its squared PC coefficients.

- Let U^{P} be given by a truncated (G)PC expansion

$$U^{\mathrm{P}}(\boldsymbol{\xi}) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\boldsymbol{\xi}),$$

  where the chaos polynomials $\{\Psi_0, \dots, \Psi_{\mathrm{P}}\}$ are orthogonal (with the convention $\Psi_0 = 1$).
- Similar expressions for the higher order moments of U^{P} in terms of its PC coefficients (but more complex).
- More complex statistical characterizations can be obtained by means of sampling strategies:
  1. sampling of Ξ with probability density $p_{\boldsymbol{\xi}}$,
  2. generation of realization of U^{P} by evaluating the PC expansion,
  3. analysis of the sample set (density estimation, probability of events, ...).
- Will be shown in subsequent lectures.

Consider a $\mathbb{R}^d$-random vectors: $\boldsymbol{U} : \Xi \mapsto \mathbb{R}^d$.
Denoting U_i the i-th component of the random vector, its truncated PC expansion writes

$$U_i(\boldsymbol{\xi}) \approx \sum_{k=0}^{\mathrm{P}} (u_i)_k \, \Psi_k(\boldsymbol{\xi}).$$

- The expansion of $\boldsymbol{U}$ can be recast in the vector form

$$\boldsymbol{U} = \sum_{k=0}^{\mathrm{P}} \boldsymbol{u}_k \Psi_k(\boldsymbol{\xi}),$$

  where $\boldsymbol{u}_k = ((u_1)_k \cdots (u_d)_k)^t \in \mathbb{R}^d$ is the vector containing the k-th PC coefficients of the random vector components.
- $\boldsymbol{u}_k$ is called the k-th stochastic mode of the random vector.

Consider a $\mathbb{R}^d$-random vectors: $\boldsymbol{U} : \Xi \mapsto \mathbb{R}^d$.
Denoting U_i the i-th component of the random vector, its truncated PC expansion writes

$$U_i(\boldsymbol{\xi}) \approx \sum_{k=0}^{\mathrm{P}} (u_i)_k \, \Psi_k(\boldsymbol{\xi}).$$

- Two components U_i and U_j are orthogonal iff

$$\sum_{k=0}^{\mathrm{P}} (u_i)_k (u_j)_k \left\langle \Psi_k^2 \right\rangle = 0.$$

- The correlation and covariance matrices of the vector $\boldsymbol{U}$ can be respectively expressed as:

$$\boldsymbol{r} = \sum_{k=0}^{\mathrm{P}} \boldsymbol{u}_k \boldsymbol{u}_k^T \left\langle \Psi_k^2 \right\rangle , \qquad \boldsymbol{c} = \sum_{k=1}^{\mathrm{P}} \boldsymbol{u}_k \boldsymbol{u}_k^T \left\langle \Psi_k^2 \right\rangle .$$

Consider a 2nd order stochastic process

$$\Omega \times \Theta \ni (\boldsymbol{x}, \theta) \mapsto U(\boldsymbol{x}, \theta) \in \mathbb{R}.$$

It PC approximation writes

$$U(\boldsymbol{x}, \theta) \approx U^{\mathrm{P}}(\boldsymbol{x}, \boldsymbol{\xi}(\theta)) = \sum_{k=0}^{\mathrm{P}} u_k(\boldsymbol{x}) \Psi_k(\boldsymbol{\xi}(\theta)).$$

- Functions $u_k : \boldsymbol{x} \in \Omega \mapsto \mathbb{R}$ are called the stochastic modes of U.
- Owing to the orthogonality of the chaos polynomials,

$$\mathbb{E}\left[U(\boldsymbol{x}, \cdot)\Psi_k\right] = \sum_l u_l(\boldsymbol{x}) \mathbb{E}\left[\Psi_l \Psi_k\right] = u_k(\boldsymbol{x}) \left\langle \Psi_l^2 \right\rangle .$$

- From the convention $\Psi_0 = 1$, $u_0(\boldsymbol{x})$ is the mean of the stochastic process

$$\mathbb{E}\left[U^{\mathrm{P}}(\boldsymbol{x}, \cdot)\right] = \sum_{k=0}^{\mathrm{P}} u_k(\boldsymbol{x}) \left\langle \Psi_k \right\rangle = u_0(\boldsymbol{x}).$$

Consider a 2nd order stochastic process

$$\Omega \times \Theta \ni (\boldsymbol{x}, \theta) \mapsto U(\boldsymbol{x}, \theta) \in \mathbb{R}.$$

It PC approximation writes

$$U(\boldsymbol{x}, \theta) \approx U^{\mathrm{P}}(\boldsymbol{x}, \boldsymbol{\xi}(\theta)) = \sum_{k=0}^{\mathrm{P}} u_k(\boldsymbol{x}) \Psi_k(\boldsymbol{\xi}(\theta)).$$

- the correlation function of U^{P} expresses as

$$R_{U^{\mathrm{P}}}(\boldsymbol{x}, \boldsymbol{x}') = \left\langle U^{\mathrm{P}}(\boldsymbol{x}, \cdot) U^{\mathrm{P}}(\boldsymbol{x}', \cdot) \right\rangle = \left\langle \left(\sum_{k=0}^{\mathrm{P}} u_k(\boldsymbol{x}) \Psi_k \right) \left(\sum_{k=0}^{\mathrm{P}} u_k(\boldsymbol{x}') \Psi_k \right) \right\rangle$$

$$= \sum_{k=0}^{\mathrm{P}} \sum_{l=0}^{\mathrm{P}} u_k(\boldsymbol{x}) u_l(\boldsymbol{x}') \langle \Psi_k \Psi_l \rangle = \sum_{k=0}^{\mathrm{P}} u_k(\boldsymbol{x}) u_k(\boldsymbol{x}') \left\langle \Psi_k^2 \right\rangle.$$

- It shows that an infinite number of stochastic processes share the same correlation function.

Relation with the KL decomposition of $U(\boldsymbol{x},\theta)$ (zero mean S.P.)
Recall that U can be decomposed in

$$U(\boldsymbol{x},\theta)=\sum_l u_l^{(KL)}\sqrt{\lambda_l}\eta^l(\theta),\quad \left(u_k^{(KL)},u_l^{(KL)}\right)_\Omega=\delta_{kl},\quad \mathbb{E}\left[\eta^l\eta^{l'}\right]=\delta_{ll'}.$$

$u_l^{(KL)}$ are the eigenfunctions of the covariance function.

- $\eta^l\in L^2(\Theta,dP)$ has a PC expansion:
$$\eta^l(\theta)=\textstyle\sum_k \eta_k^l\Psi_k(\boldsymbol{\xi}(\theta)).$$
- Inserting the expansions of the η and rearranging the summations
$$U(\boldsymbol{x},\theta)=\sum_k\left[\sum_l u_l^{(KL)}(\boldsymbol{x})\sqrt{\lambda_l}\eta_k^l\right]\Psi_k(\boldsymbol{\xi}(\theta)).$$
- In addition, it comes
$$(u_k,u_{k'})_\Omega=\sum_l\sum_{l'}\sqrt{\lambda_l\lambda_{l'}}\left(u_l^{(KL)},u_{l'}^{(KL)}\right)_\Omega\eta_k^l\eta_{k'}^{l'}=\sum_l\lambda_l\eta_k^l\eta_{k'}^l$$
which in general is not zero.

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Truncated PC expansions can be used to approximate stochastic quantities U (random variables, vectors, fields, ...)
This calls for procedures / strategies to determine

- the number of **random variables** N in the germ (and eventually their distributions)
- the **polynomial order** p of the expansion
- the coefficients of the expansion (stochastic modes)

We distinguish two fundamentally different situations

1. the **particular situation** where, given the germ ξ, information on $U(\xi)$ can be assessed
2. the **general case** where only information on $U(\theta)$ is available can be assessed

$U(\xi)$ can be assessed:

This case corresponds to situation found in parametric uncertainty propagation, where for each realization $\xi(\theta)$ one can **compute / measure the particular realization** $U(\xi(\theta))$.

One can then exploit the mapping $\Xi \ni \xi \mapsto U(\xi)$

to compute the coefficients u_k in the expansion,

$$U(\xi) \approx U^P(\xi) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi)$$

For instance, exploiting the orthogonality of the Ψ

$$u_k = \frac{\langle U, \Psi_k \rangle}{\langle \Psi_k, \Psi_k \rangle} = \frac{1}{\langle \Psi_k, \Psi_k \rangle} \int_\Xi U(\boldsymbol{y}) \Psi_k(\boldsymbol{y}) p_{\boldsymbol{\xi}}(\boldsymbol{y}) d\boldsymbol{y}.$$

This is the L^2-projection of U onto $\mathrm{span}\{\Psi_k, k = 0, \dots, \mathrm{P}\}$.

Other type of projections and computational strategies will be extensively discussed in the following.

This is the most general situation where:

- a random quantity $U(\theta)$ has to be approximated by means of a PC expansion,
- $U(\theta)$ may be known partially or completely through, *e.g.*, **sample set of realizations, moments, estimated probability law, ...**
- from the **available information**, one need to define a germ, expansion order and to specify $U^{\mathrm{P}}(\xi(\theta))$ that approximate $U(\theta)$.

One cannot exploit the mapping $\Xi \ni \xi \mapsto U(\xi)$

to compute the coefficients u_k in the expansion,

$$U(\theta) \approx U^P(\xi(\theta)) = \sum_{k=0}^{\mathrm{P}} u_k \Psi_k(\xi(\theta))$$

as there is no *explicit* relation between $U(\theta)$ and $\xi(\theta)$.

This is the typical situation faced when constructing stochastic models of uncertainty in particular to model stochastic fields.

- It essentially amounts to the resolution of optimization problems to identify /estimate the germ and expansion order that best fit the available information.
- Optimization can be based on moments matching, likelihood, entropy maximization, . . .

Questions & Discussion