Uncertainty propagation using polynomial chaos expansions

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The Chair carries out research projects in the field of uncertainty quantification for engineering problems with applications in structural reliability, sensitivity analysis, model calibration and reliability-based design optimization.

Research topics

- Uncertainty modelling for engineering systems
- Structural reliability analysis
- Surrogate models (polynomial chaos expansions, Kriging, support vector machines)
- Bayesian model calibration and stochastic inverse problems
- Global sensitivity analysis
- Reliability-based design optimization

http://www.rsuq.ethz.ch
Computational models in engineering

Complex engineering systems are designed and assessed using computational models, a.k.a simulators.

A computational model combines:

- A mathematical description of the physical phenomena (governing equations), e.g. mechanics, electromagnetism, fluid dynamics, etc.

- Discretization techniques which transform continuous equations into linear algebra problems

- Algorithms to solve the discretized equations

\[
\begin{align*}
\nabla \cdot D &= \rho \\
\nabla \cdot B &= 0 \\
\n\nabla \times E &= -\frac{\partial B}{\partial t} \\
\n\nabla \times H &= J + \frac{\partial D}{\partial t}
\end{align*}
\]
Computational models in engineering

Computational models are used:

- Together with experimental data for *calibration* purposes
- To explore the design space ("*virtual prototypes"")
- To *optimize* the system (e.g. minimize the mass) under performance constraints
- To assess its *robustness w.r.t* uncertainty and its *reliability*
Computational models: the abstract viewpoint

A computational model may be seen as a black box program that computes quantities of interest (QoI) (a.k.a. model responses) as a function of input parameters.

- **Vector of input parameters** \( \mathbf{x} \in \mathbb{R}^M \)
- **Computational model** \( M \)
- **Model response** \( y = M(\mathbf{x}) \in \mathbb{R}^Q \)

- **Geometry**
- **Material properties**
- **Loading**
- **Analytical formula**
- **Finite element model**
- **Comput. workflow**
- **Displacements**
- **Strains, stresses**
- **Temperature, etc.**
Real world is uncertain

- Differences between the **designed** and the **real** system:
  - Dimensions (tolerances in manufacturing)
  - Material properties (e.g. variability of the stiffness or resistance)

- Unforecast exposures: exceptional service loads, natural hazards (earthquakes, floods, landslides), climate loads (hurricanes, snow storms, etc.), accidental human actions (explosions, fire, etc.)
Outline

1 Introduction

2 Global framework for uncertainty quantification

3 Polynomial chaos basis
   Orthogonal polynomials
   Multivariate basis

4 Computing the coefficients and post-processing
   Projection
   Ordinary Least-squares (OLS)
   Sparse PCE
   Post-processing the coefficients

5 Application examples
   Truss structure
   Hydrogeology
   Structural dynamics
Global framework for uncertainty quantification

**Step A**
Model(s) of the system  
Assessment criteria

**Step B**
Quantification of sources of uncertainty

**Step C**
Uncertainty propagation

**Step C’**
Sensitivity analysis

**Step C: uncertainty propagation**

**Goal:** estimate the uncertainty / variability of the quantities of interest (QoI) $Y = M(X)$ due to the input uncertainty $f_X$

- Output statistics, *i.e.* mean, standard deviation, etc.

$$
\mu_Y = \mathbb{E}_X [M(X)]
$$

$$
\sigma^2_Y = \mathbb{E}_X [(M(X) - \mu_Y)^2]
$$

- Distribution of the QoI

- Probability of exceeding an admissible threshold $y_{adm}$

$$
P_f = \mathbb{P} (Y \geq y_{adm})
$$
Uncertainty propagation using Monte Carlo simulation

**Principle:** Generate *virtual prototypes* of the system using random numbers

- A sample set \( \mathcal{X} = \{x_1, \ldots, x_n\} \) is drawn according to the input distribution \( f_X \)
- For each sample the quantity of interest (resp. performance criterion) is evaluated, say \( \mathcal{Y} = \{M(x_1), \ldots, M(x_n)\} \)

- The set of quantities of interest is used for moments-, distribution- or reliability analysis
Advantages/Drawbacks of Monte Carlo simulation

**Advantages**

- Universal method: only rely upon sampling random numbers and running repeatedly the computational model

- Sound statistical foundations: convergence when $N_{MCS} \to \infty$

- Suited to High Performance Computing: “embarrassingly parallel”

**Drawbacks**

- **Statistical uncertainty**: results are not exactly reproducible when a new analysis is carried out (handled by computing confidence intervals)

- **Low efficiency**: convergence rate $\propto 1/\sqrt{N_{MCS}}$

The “scattering” of Y is investigated point-by-point: if two samples $x_i, x_j$ are almost equal, two independent runs of the model are carried out
Spectral approach

Heuristic

Instead of considering the random output $Y = \mathcal{M}(X)$ through samples, i.e. $Y = \{\mathcal{M}(x_i), i = 1, \ldots, n\}$, $Y$ is represented by a series expansion

$$Y = \sum_{j=0}^{+\infty} y_j Z_j$$

where:

- $\{Z_j\}_{j=0}^{+\infty}$ is a numerable set of random variables that forms a basis of a suitable space $\mathcal{H} \supset Y$

- $\{y_j\}_{j=0}^{+\infty}$ is the set of coordinates of $Y$ in this basis
Spectral approach

Questions to solve

- What is the relevant mathematical framework (i.e. abstract space \( H \)) to represent random variables \( Y = M(X) \)?

- How to construct a basis of this space of \( \{Z_j\}_{j=0}^{+\infty} \)?

- How to compute the coefficients? (truncation scheme)

- How to interpret the results in terms of meaningful engineering quantities?
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Polynomial chaos expansions in a nutshell

- Consider the input random vector $\mathbf{X}$ (dim $\mathbf{X} = M$) with given probability density function (PDF) $f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^{M} f_{X_i}(x_i)$

- Assuming that the random output $Y = \mathcal{M}(\mathbf{X})$ has finite variance, it can be cast as the following polynomial chaos expansion:

$$Y = \sum_{\alpha \in \mathbb{N}^M} y_\alpha \Psi_\alpha(\mathbf{X})$$

where :

- $\Psi_\alpha(\mathbf{X}) :$ basis functions
- $y_\alpha :$ coefficients to be computed (coordinates)

- The PCE basis $\{\Psi_\alpha(\mathbf{X}), \alpha \in \mathbb{N}^M\}$ is made of multivariate orthonormal polynomials
Orthogonal polynomials

Definition

- A **monic** polynomial of degree \( n \) reads:
  \[
  p_n(x) = x^n + a_{n-1} x^{n-1} + \cdots + a_0
  \]

- A sequence of monic polynomials \( \{\pi_k, k \geq 0\} \) is **orthogonal** with respect to a weight function \( w : x \in D_X \mapsto \mathbb{R}^+ \) if:
  \[
  \langle \pi_k, \pi_l \rangle_w \overset{\text{def}}{=} \int_{D_X} \pi_k(x) \pi_l(x) w(x) \, dx = \gamma_k^2 \delta_{kl}
  \]
  where \( \delta_{kl} : \text{Kronecker symbol} \)

that is:

- \( \langle \pi_k, \pi_l \rangle_w = 0 \) if \( k \neq l \)
- \( \langle \pi_k, \pi_k \rangle_w = \|\pi_k\|^2_w = \gamma_k^2 \)
Orthogonal polynomials

Canonical representation

- The sequence of powers \( \{1, x, x^2, \ldots \} \) forms a basis of the space of polynomials.
- This basis is however not orthogonal with respect to classical weight functions.

Example

Consider a uniform random variable \( \mathcal{U}(-1, 1) \) with PDF \( w(x) = 1/2, \ x \in [-1, 1] \) and 0 otherwise:

\[
<x^p, x^q>_w = \int_{-1}^{1} x^{p+q} \frac{dx}{2} = \frac{1}{p+q+1} \quad \text{if } p + q \text{ even}
\]

The set of powers does NOT form an orthogonal basis:

\[
<x^p, x^q>_w \neq 0
\]
Basis of orthogonal polynomials

- Given the weight function $w$, there is a unique infinite sequence of monic orthogonal polynomials $\{\pi_k, k \geq 0\}$ where $\pi_0(x) \overset{\text{def}}{=} 1$

- This sequence may be built by the Gram-Schmidt orthogonalization procedure

- It satisfies a 3-term recurrence relation:

$$\pi_{k+1}(x) = (x - \alpha_k) \pi_k(x) - \beta_k \pi_{k-1}(x)$$

where:

$$\alpha_k = \frac{\langle x \pi_k, \pi_k \rangle_w}{\langle \pi_k, \pi_k \rangle_w}$$

$$\beta_k = \frac{\langle \pi_k, \pi_k \rangle_w}{\langle \pi_{k-1}, \pi_{k-1} \rangle_w}$$
Classical orthogonal polynomials

- Classical families of orthogonal polynomials have been discovered historically when solving various problems of physics, quantum mechanics, etc.
- The name of the researcher who first investigated their properties is attached to them.

<table>
<thead>
<tr>
<th>$\mathcal{D}_X$</th>
<th>Distribution</th>
<th>PDF $f_X \equiv w$</th>
<th>Family</th>
</tr>
</thead>
<tbody>
<tr>
<td>$[-1, 1]$</td>
<td>Uniform</td>
<td>$1/2$</td>
<td>Legendre</td>
</tr>
<tr>
<td>$\mathbb{R}$</td>
<td>Gaussian</td>
<td>$e^{-x^2/2}/\sqrt{2\pi}$</td>
<td>Hermite</td>
</tr>
<tr>
<td>$\mathbb{R}^+$</td>
<td>Exponential</td>
<td>$e^{-x}$</td>
<td>Laguerre</td>
</tr>
<tr>
<td>$[-1, 1]$</td>
<td>Beta</td>
<td>$(1-x)^\alpha(1+x)^\beta/B(\alpha+1, \beta+1)$</td>
<td>Jacobi</td>
</tr>
</tbody>
</table>

A.-M. Legendre (1752-1833)  C. Hermite (1822-1901)  E. Laguerre (1834-1886)  C. Jacobi (1804-1851)
Legendre polynomials are defined over $[-1, 1]$ so as to be orthogonal with respect to the uniform distribution:

$$w(x) = \frac{1}{2} \quad x \in [-1, 1]$$

- **Notation:** $P_n(x), n \in \mathbb{N}$
- **3-term recurrence**

$$P_0(x) = 1 \quad \text{;} \quad P_1(x) = x$$

$$(n + 1)P_{n+1}(x) = (2n + 1)xP_n(x) - nP_{n-1}(x)$$

- $P_n$ is solution of the ordinary differential equation

$$\left[(1 - x^2) P_n'(x)\right]' + n(n + 1) P_n(x) = 0$$
First Legendre polynomials

- The norm of the $n$-th Legendre polynomial reads:

$$\| P_n \|^2 = \langle P_n, P_n \rangle = \int_{-1}^{1} P_n^2(x) \cdot \frac{1}{2} \, dx = \frac{1}{2n+1}$$

- The orthonormal Legendre polynomials read:

$$\tilde{P}_n(x) = \sqrt{2n+1} P_n(x)$$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$P_n(x)$</th>
<th>$| P_n |^2$</th>
<th>$\tilde{P}_n(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>$x$</td>
<td>1/3</td>
<td>$\sqrt{3} P_1$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{2} (3x^2 - 1)$</td>
<td>1/5</td>
<td>$\sqrt{5} P_2$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{2} (5x^3 - 3x)$</td>
<td>1/7</td>
<td>$\sqrt{7} P_3$</td>
</tr>
<tr>
<td>4</td>
<td>$\frac{1}{8} (35x^4 - 30x^2 + 3)$</td>
<td>1/9</td>
<td>$\sqrt{9} P_4$</td>
</tr>
<tr>
<td>5</td>
<td>$\frac{1}{8} (63x^5 - 70x^3 + 15x)$</td>
<td>1/11</td>
<td>$\sqrt{11} P_5$</td>
</tr>
</tbody>
</table>
Hermite polynomials are defined over $\mathbb{R}$ so as to be orthogonal with respect to the Gaussian distribution:

$$w(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad x \in \mathbb{R}$$

- **Notation**: $He_n(x), \quad n \in \mathbb{N}$
- **3-term recurrence**:
  $$He_0(x) = 1 \quad ; \quad He_1(x) = x$$
  $$He_{n+1}(x) = x He_n(x) - n He_{n-1}(x)$$
- **Normalization**

$$\| He_n \|^2 = \int_{-\infty}^{+\infty} He_n^2(x) \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx = n! \quad n! = 1 \cdot 2 \cdot 3 \ldots n$$

- **The orthonormal Hermite polynomials read**:

$$\tilde{He}_n(x) = He_n(x)/\sqrt{n!}$$
Hermite polynomials

- $He_n$ is solution of the ordinary differential equation:

$$He''_n(x) - x He'_n(x) + n He_n(x) = 0$$

and satisfies:

$$He_n(x) = (-1)^n e^{x^2/2} \frac{d^n}{dx^n} \left(e^{-x^2/2}\right)$$

$$He'_n(x) = n He_{n-1}(x)$$

Important remark

In the literature, two families of Hermite polynomials (HP) are known:

- The “physicists’” HP are orthogonal w.r.t $e^{-x^2}$
- The “probabilists’” HP are orthogonal w.r.t the standard normal PDF $e^{-x^2/2}/\sqrt{2\pi}$
First Hermite polynomials

<table>
<thead>
<tr>
<th>n</th>
<th>$He_n(x)$</th>
<th>$|He_n|^2$</th>
<th>$\tilde{He}_n(x)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>$He_0$</td>
</tr>
<tr>
<td>1</td>
<td>$x$</td>
<td>1</td>
<td>$He_1$</td>
</tr>
<tr>
<td>2</td>
<td>$x^2 - 1$</td>
<td>2</td>
<td>$He_2/\sqrt{2}$</td>
</tr>
<tr>
<td>3</td>
<td>$x^3 - 3x$</td>
<td>6</td>
<td>$He_3/\sqrt{6}$</td>
</tr>
<tr>
<td>4</td>
<td>$x^4 - 6x^2 + 3$</td>
<td>24</td>
<td>$He_4/\sqrt{24}$</td>
</tr>
<tr>
<td>5</td>
<td>$x^5 - 10x^3 + 15x$</td>
<td>120</td>
<td>$He_5/\sqrt{120}$</td>
</tr>
</tbody>
</table>

\[
\tilde{H}_{e_n}(x) = \frac{H_{e_n}(x)}{\sqrt{n!}}
\]
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Multivariate polynomials

Tensor product of 1D polynomials

- One defines the multi-indices $\alpha = \{ \alpha_1, \ldots, \alpha_M \}$, of degree $|\alpha| = \sum_{i=1}^{M} \alpha_i$

- The associated multivariate polynomial reads:

$$\Psi_{\alpha}(x) \overset{\text{def}}{=} \prod_{i=1}^{M} P_{\alpha_i}^{(i)}(x_i)$$

where $P_{\alpha_i}^{(i)}$ is the univariate polynomial of degree $\alpha_i$ from the orthonormal family associated to variable $X_i$

The set of multivariate polynomials $\{\Psi_{\alpha}(X), \alpha \in \mathbb{N}^M\}$ forms a basis of $L^2(\Omega, \mathcal{F}, \mathbb{P})$

$$Y = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_{\alpha}(X)$$
Example: \( M = 2 \)

\[ \alpha = [3, 3] \]

\[ \Psi_{(3, 3)}(x) = \tilde{P}_3(x_1) \cdot \tilde{H}e_3(x_2) \]

- \( X_1 \sim \mathcal{U}(-1, 1) \): Legendre polynomials
- \( X_2 \sim \mathcal{N}(0, 1) \): Hermite polynomials
Suppose that the input random vector has independent components:

\[ f_X(x) = \prod_{i=1}^{M} f_{X_i}(x_i) \]

and consider the tensor product polynomials \( \Psi_\alpha(x) = \prod_{i=1}^{M} P_{\alpha_i}^{(i)}(x_i) \) and \( \Psi_\beta(x) = \prod_{i=1}^{M} P_{\beta_i}^{(i)}(x_i) \). Then:

\[
E [\Psi_\alpha(X) \Psi_\beta(X)] = \int_{\mathcal{D}_X} \Psi_\alpha(x) \Psi_\beta(x) f_X(x) \, dx
\]

\[
= \int_{\mathcal{D}_X} \left( \prod_{i=1}^{M} P_{\alpha_i}^{(i)}(x_i) P_{\beta_i}^{(i)}(x_i) f_{X_i}(x_i) \right) \, dx
\]

\[
= \prod_{i=1}^{M} \left( \int_{\mathcal{D}_{X_i}} P_{\alpha_i}^{(i)}(x_i) P_{\beta_i}^{(i)}(x_i) f_{X_i}(x_i) \, dx_i \right) = \prod_{i=1}^{M} \delta_{\alpha_i \beta_i}
\]

\[
E [\Psi_\alpha(X) \Psi_\beta(X)] = \delta_{\alpha \beta}
\]
Isoprobabilistic transform

- Classical orthogonal polynomials are defined for reduced variables, e.g.:
  - standard normal variables $\mathcal{N}(0, 1)$
  - standard uniform variables $\mathcal{U}(-1, 1)$

- In practical UQ problems the physical parameters are modelled by random variables that are:
  - not necessarily reduced, e.g. $X_1 \sim \mathcal{N}(\mu, \sigma), X_2 \sim \mathcal{U}(a, b)$, etc.
  - not necessarily from a classical family, e.g. lognormal variable

Need for isoprobabilistic transforms
 Polynomial chaos basis  
 Multivariate basis

Isoprobabilistic transform

Independent variables

- Given the marginal CDFs $X_i \sim F_{X_i}$, $i = 1, \ldots, M$

- A one-to-one mapping to reduced variables is used:

  $$X_i = F_{X_i}^{-1} \left( \frac{\xi_i + 1}{2} \right) \quad \text{if } \xi_i \sim \mathcal{U}(-1, 1)$$

  $$X_i = F_{X_i}^{-1} (\Phi(\xi_i)) \quad \text{if } \xi_i \sim \mathcal{N}(0, 1)$$

- The best choice is dictated by the least non linear transform

General case: addressing dependence

- The joint CDF is defined through its marginals and copula

  $$F_X(x) = C (F_{X_1}(x_1), \ldots, F_{X_M}(x_M))$$

- Rosenblatt or Nataf isoprobabilistic transform is used
Standard truncation scheme

Premise

- The infinite series expansion cannot be handled in practical computations
- A truncated series must be defined

Standard truncation scheme

Consider all multivariate polynomials of total degree $|\alpha| = \sum_{i=1}^{M} \alpha_i$ less than or equal to $p$:

$$\mathcal{A}^{M,p} = \{ \alpha \in \mathbb{N}^M : |\alpha| \leq p \}$$

$$\text{card } \mathcal{A}^{M,p} \equiv P = \binom{M + p}{p}$$

$|\alpha| \leq 3$

$|\alpha| \leq 4$

$|\alpha| \leq 5$

$|\alpha| \leq 6$
Application example

**Computational model**

\[ Y = M(X_1, X_2) \]

**Probabilistic model**

\[ X_1 \sim \mathcal{N}(\mu, \sigma) \quad X_2 \sim \mathcal{U}(a, b) \]

**Isoprobabilistic transform**

\[ X_1 = \mu + \sigma \xi_1 \quad \xi_1 \sim \mathcal{N}(0, 1) \]
\[ X_2 = \frac{(a + b)}{2} + \frac{(b - a)}{2} \xi_2 \quad \xi_2 \sim \mathcal{U}(-1, 1) \]

**Univariate polynomials**

- Hermite polynomials in \( \xi_1 \), i.e. \( \tilde{H}_e_n(\xi_1) \)
- Legendre polynomials in \( \xi_2 \), i.e. \( \tilde{P}_n(\xi_2) \)

**Multivariate polynomials**

\[ \Psi_{\alpha_1, \alpha_2}(\xi_1, \xi_2) = \tilde{H}_e_{\alpha_1}(\xi_1) \cdot \tilde{P}_{\alpha_2}(\xi_2) \]
Truncation example

Third order truncation $p = 3$

All the polynomials of $\xi_1, \xi_2$ that are product of univariate polynomials and whose total degree is less than 3 are considered

<table>
<thead>
<tr>
<th>$j$</th>
<th>$\alpha$</th>
<th>$\Psi_\alpha \equiv \Psi_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>[0, 0]</td>
<td>$\Psi_0 = 1$</td>
</tr>
<tr>
<td>1</td>
<td>[1, 0]</td>
<td>$\Psi_1 = \xi_1$</td>
</tr>
<tr>
<td>2</td>
<td>[0, 1]</td>
<td>$\Psi_2 = \sqrt{3} \xi_2$</td>
</tr>
<tr>
<td>3</td>
<td>[2, 0]</td>
<td>$\Psi_3 = (\xi_1^2 - 1)/\sqrt{2}$</td>
</tr>
<tr>
<td>4</td>
<td>[1, 1]</td>
<td>$\Psi_4 = \sqrt{3} \xi_1 \xi_2$</td>
</tr>
<tr>
<td>5</td>
<td>[0, 2]</td>
<td>$\Psi_5 = \sqrt{5/4} (3\xi_2^2 - 1)$</td>
</tr>
<tr>
<td>6</td>
<td>[3, 0]</td>
<td>$\Psi_6 = (\xi_1^3 - 3\xi_1)/\sqrt{6}$</td>
</tr>
<tr>
<td>7</td>
<td>[2, 1]</td>
<td>$\Psi_7 = \sqrt{3/2} (\xi_1^2 - 1)\xi_2$</td>
</tr>
<tr>
<td>8</td>
<td>[1, 2]</td>
<td>$\Psi_8 = \sqrt{5/4} (3\xi_2^2 - 1)\xi_1$</td>
</tr>
<tr>
<td>9</td>
<td>[0, 3]</td>
<td>$\Psi_9 = \sqrt{7/4} (5\xi_2^3 - 3\xi_2)$</td>
</tr>
</tbody>
</table>

\[ \tilde{Y} \equiv \mathcal{M}^{PC}(\xi_1, \xi_2) = a_0 + a_1 \xi_1 + a_2 \sqrt{3} \xi_2 \\
+ a_3 (\xi_1^2 - 1)/\sqrt{2} + a_4 \sqrt{3} \xi_1 \xi_2 \\
+ a_5 \sqrt{5/4} (3\xi_2^2 - 1) + a_6 (\xi_1^3 - 3\xi_1)/\sqrt{6} \\
+ a_7 \sqrt{3/2} (\xi_1^2 - 1)\xi_2 + a_8 \sqrt{5/4} (3\xi_2^2 - 1)\xi_1 \\
+ a_9 \sqrt{7/4} (5\xi_2^3 - 3\xi_2) \]
Conclusions

- **Polynomial chaos expansions** allow for an intrinsic representation of the random response as a series expansion.

- The basis functions are **multivariate orthonormal polynomials** (based on the input distribution).

- In practice, the input vector is first transformed into **independent reduced variables** for which classical orthogonal polynomials are well-known.

- A **truncation scheme** shall be introduced for practical computations, e.g. by selecting the maximal degree of the polynomials.

- Next step is the computation of the **expansion coefficients**.
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2. Global framework for uncertainty quantification
3. Polynomial chaos basis
4. Computing the coefficients and post-processing
   - Projection
   - Ordinary Least-squares (OLS)
   - Sparse PCE
   - Post-processing the coefficients
5. Application examples
Various methods for computing the coefficients

Intrusive approaches

- Historical approaches: projection of the equations residuals in the Galerkin sense
- Proper generalized decompositions
  Nouy, 2007-2012

Non intrusive approaches

- Non intrusive methods consider the computational model $\mathcal{M}$ as a black box
- They rely upon a design of numerical experiments, i.e. a $n$-sample $\mathcal{X} = \{\mathbf{x}^{(i)} \in \mathcal{Dx}, i = 1, \ldots, n\}$ of the input parameters
- Different classes of methods are available:
  - Projection: by simulation or quadrature
  - Stochastic collocation
  - Least-square minimization
Projection

Polynomial chaos expansion

\[ Y = \mathcal{M}(X) = \sum_{\beta \in \mathbb{N}^M} y_\beta \Psi_\beta(X) \]

By multiplying by \( \Psi_\alpha \) and taking the expectation one gets:

\[ \mathbb{E}[Y \Psi_\alpha(X)] = \sum_{\beta \in \mathbb{N}^M} y_\beta \mathbb{E}[\Psi_\alpha(X) \Psi_\beta(X)] = y_\alpha \]

Estimation techniques

\[ y_\alpha = \mathbb{E}[Y \Psi_\alpha(X)] = \int_{\mathcal{D}_X} \mathcal{M}(x) \Psi_\alpha(x) f_X(x) \, dx \]

Computation by full- or Smolyak quadrature
One-dimensional quadrature rules

Consider the following weighted integral, for some positive weight function $w : x \in \mathcal{D}_X \mapsto \mathbb{R}^+$

$$\mathcal{I}[g] = \int_{\mathcal{D}_X} g(x) w(x) \, dx$$

- A $n$-point quadrature rule is defined by

$$\mathcal{I}[g] \approx Q^n[g] \overset{\text{def}}{=} \sum_{k=1}^{n} \omega_k \, g(x_k)$$

where

- $\{\omega_k, k = 1, \ldots, n\}$ are the integration weights
- $\{x_k, k = 1, \ldots, n\}$ are the integration nodes
Gaussian quadrature rules

A Gaussian quadrature rule with \( n \) nodes reads:

\[
\int_{\mathbb{D}_X} g(x) w(x) \, dx \approx Q^G[g] \overset{\text{def}}{=} \sum_{j=1}^{n} \omega_j^G g(x_j^G)
\]

where:

- The nodes \( \{x_j^G, j = 1, \ldots, n\} \) are the zeros of the \( n \)-th orthogonal \( \pi_n \) w.r.t to \( w \)

- The weights are given by:

\[
\omega_j^G = \frac{<\pi_{n-1}, \pi_{n-1}>}{\pi'_n(x_j^G).\pi_{n-1}(x_j^G)}
\]

The degree of exactness is \( d = 2n - 1 \). It is the largest possible degree of exactness
Multidimensional quadrature

Higher dimensions

Consider the $M$-dimensional integral: $\mathcal{I}(h) \equiv \int_{D \subset \mathbb{R}^M} h(x) f_x(x) \, dx$

where $h(.)$ is a function to be integrated against the weight function $f_x(.)$:

$$f_x(x) = f_{X_1}(x_1) \cdots f_{X_M}(x_M)$$

The tensorized quadrature scheme consists in replacing each integral by a summation, thus the nested summations:

$$Q^n(h) \equiv Q^{(n_1, \ldots, n_M)}(h) \equiv \sum_{i_1=1}^{n_1} \cdots \sum_{i_M=1}^{n_M} \omega_{i_1} \cdots \omega_{i_M} h(x_{i_1}, \ldots, x_{i_M})$$

Computing the integral requires $n_1 \times \cdots \times n_M$ evaluations of the integrand.
Back to the computation of chaos coefficients ($M > 1$)

Each polynomial chaos coefficient $y_\alpha$ reads:

$$y_\alpha = \int_{D_X} M(x) \Psi_\alpha(x) f_X(x) \, dx$$

- **Integrand**: $h(x) := M(x) \Psi_\alpha(x)$
- **Order**: $n_i = p + 1, \quad i = 1, \cdots, M$

$$\hat{y}_\alpha \equiv Q^{(p+1, \cdots, p+1)}(h)$$

$$= \sum_{i_1=1}^{p+1} \cdots \sum_{i_M=1}^{p+1} \omega_{i_1} \cdots \omega_{i_M} M(x_{i_1}, \cdots, x_{i_M}) \Psi_\alpha(x_{i_1}, \cdots, x_{i_M})$$

**Computational cost**: $(p + 1)^M$ evaluations of the model
Computational cost

- The cost increases exponentially with $M$: $N = (p + 1)^M$
- Normal industrial (and research!) settings allow at most $O(100)$ model evaluations
- Industrial problems often use more than 10 variables!
- In some cases, they are very non-linear ($p > 5$)

<table>
<thead>
<tr>
<th>$M$</th>
<th>$p$</th>
<th>$N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>3</td>
<td>16</td>
</tr>
<tr>
<td></td>
<td>5</td>
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<td>3</td>
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</tr>
<tr>
<td></td>
<td>5</td>
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</tr>
<tr>
<td>10</td>
<td>3</td>
<td>1,048,576</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td>60,466,176</td>
</tr>
</tbody>
</table>

Need for a more efficient scheme in high dimensions
Smolyak quadrature: sparse grids

Smolyak sparse quadrature rule

\[ Q_{Smolyak}^{M,k} = \sum_{k+1 \leq |i| \leq k+M} (-1)^{M+k-|i|} \cdot \binom{M-1}{k + M - |i|} \cdot Q^i \]

where:

\[ i = i_1, i_2, \ldots, i_M, \quad |i| = i_1 + \ldots + i_M \in \mathbb{N} \]

and

\[ Q^i = Q^{i_1} \otimes \ldots \otimes Q^{i_M} \]

Smolyak integration scheme is exact for PC expansions of max. degree \( p \) using \( k = p \)
Outline

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4 Computing the coefficients and post-processing
   - Projection
   - Ordinary Least-squares (OLS)
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   - Post-processing the coefficients

5 Application examples
Statistical approach: least-square minimization

Berveiller et al. (2006)

Principle

The exact (infinite) series expansion is considered as the sum of a truncated series and a residual:

\[ Y = \mathcal{M}(X) = \sum_{j=0}^{P-1} y_j \Psi_j(X) + \varepsilon_P \equiv Y^T \Psi(X) + \varepsilon_P \]

where:

- \( Y = \{y_0, \ldots, y_{P-1}\} \)
- \( \Psi(x) = \{\Psi_0(x), \ldots, \Psi_{P-1}(x)\} \)
Computing the coefficients and post-processing

Least-Square Minimization: continuous solution

Least-square minimization

The unknown coefficients are gathered into a vector
\[ \mathbf{Y} = \{y_j, \ j = 0, \ldots, P - 1\} \], and computed by minimizing the mean square error:

\[ \hat{\mathbf{Y}} = \arg \min_{\mathbf{Y}} E \left[ (\mathbf{Y}^T \Psi(X) - M(X))^2 \right] \]

Analytical solution (continuous case)

The least-square minimization problem may be solved analytically:

\[ \hat{y}_j = E \left[ M(X) \Psi_j(X) \right] \quad \forall j = 0, \ldots, P - 1 \]

The solution is identical to the projection solution due to the orthogonality of the regressors
Least-Square Minimization: procedure

\[ \hat{Y} = \arg \min \hat{E} \left[ (Y^T \Psi(X) - M(X))^2 \right] = \arg \min_{y \in \mathbb{R}^P} \sum_{i=1}^{n} \left( M(x^{(i)}) - \sum_{j=0}^{P-1} y_j \Psi_j(x^{(i)}) \right)^2 \]

- Select an experimental design
  \[ X = \{ x^{(1)}, \ldots, x^{(n)} \}^T \]
  that covers at best the domain of variation of the parameters

- Evaluate the model response for each sample (exactly as in Monte carlo simulation)
  \[ M = \{ M(x^{(1)}), \ldots, M(x^{(n)}) \}^T \]

- Compute the experimental matrix
  \[ A_{ij} = \Psi_j(x^{(i)}) \quad i = 1, \ldots, n ; \quad j = 0, \ldots, P - 1 \]

- Solve the least-square minimization problem
  \[ \hat{Y} = (A^T A)^{-1} A^T M \]
Choice of the experimental design

Random designs

- Monte Carlo samples obtained by standard random generators
- Latin Hypercube designs that are both random and “space-filling”
- Quasi-random sequences (e.g. Sobol’ sequence)
Size of the experimental design

Size of the ED

The size $n$ of the experimental design shall be scaled with the number of unknown coefficients, e.g. $P = \binom{M+p}{p}$

- $n < P$ leads to an underdetermined system
- $n = P$ may lead to overfitting

The thumb rule $n = k \cdot P$ where $k = 2 - 3$ is used
In least-squares analysis, the **generalization error** is defined as:

\[
E_{\text{gen}} = \mathbb{E} \left[ (M(X) - M^{\text{PC}}(X))^2 \right]
\]

\[M^{\text{PC}}(X) = \sum_{\alpha \in A} y_{\alpha} \Psi_{\alpha}(X)\]

The **empirical error** based on the experimental design $\mathcal{X}$ is a poor estimator in case of overfitting:

\[
E_{\text{emp}} = \frac{1}{n} \sum_{i=1}^{n} \left( M(x^{(i)}) - M^{\text{PC}}(x^{(i)}) \right)^2
\]
Leave-one-out cross validation

- An experimental design
  \[ \mathcal{X} = \{ \mathbf{x}^{(j)}, \ j = 1, \ldots, n \} \] is selected

- Polynomial chaos expansions are built using all points but one, i.e. based on
  \[ \mathcal{X} \setminus \mathbf{x}^{(i)} = \{ \mathbf{x}^{(j)}, \ j = 1, \ldots, n, \ j \neq i \} \]

- Leave-one-out error (PRESS)
  \[
  E_{LOO} \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \left( M(\mathbf{x}^{(i)}) - M_{PC \setminus i}(\mathbf{x}^{(i)}) \right)^2
  \]

- Analytical derivation from a single PC analysis
  \[
  E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{M(\mathbf{x}^{(i)}) - M_{PC}(\mathbf{x}^{(i)})}{1 - h_i} \right)^2
  \]
  where \( h_i \) is the \( i \)-th diagonal term of matrix \( \mathbf{A}(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \)
Least-squares analysis: Wrap-up

**Algorithm 1:** Ordinary least-squares

1. **Input:** Computational budget \( n \)
2. **Initialization**
3. Experimental design \( \mathcal{X} = \{ x^{(1)}, \ldots, x^{(n)} \} \)
4. Run model \( \mathcal{Y} = \{ M(x^{(1)}), \ldots, M(x^{(n)}) \} \)
5. **PCE construction**
6. for \( p = p_{\text{min}} : p_{\text{max}} \) do
7. Select candidate basis \( \mathcal{A}^{M,p} \)
8. Solve OLS problem
9. Compute \( e_{\text{LOO}}(p) \)
10. end
11. \( p^* = \arg \min e_{\text{LOO}}(p) \)
12. **Return** Best PCE of degree \( p^* \)
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Curse of dimensionality

- The cardinality of the truncation scheme $A_{M,p}^M$ is $P = \frac{(M + p)!}{M!p!}$
- Typical computational requirements: $n = OSR \cdot P$ where the oversampling rate is $OSR = 2 - 3$

However ... most coefficients are close to zero!

Example

- Elastic truss structure with $M = 10$ independent input variables
- PCE of degree $p = 5$ ($P = 3,003$ coeff.)
Low-rank truncation schemes

Sparsity-of-effects principle – Ockham’s razor

"entia non sunt multiplicanda praeter necessitatem" (entities must not be multiplied beyond necessity)
W. Ockham (c. 1287-1347)

In most engineering problems, only low-order interactions between the input variables are relevant.

Use of low-rank monomials

Definition

The rank of a multi-index $\alpha$ is the number of active variables of $\Psi_\alpha$, i.e. the number of non-zero terms in $\alpha$

$$||\alpha||_0 = \sum_{i=1}^{M} 1\{\alpha_i > 0\}$$

Example: $M = 5, p = 5$, Legendre polynomial chaos

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$\Psi_\alpha$</th>
<th>Rank</th>
</tr>
</thead>
<tbody>
<tr>
<td>[0 0 0 3 0]</td>
<td>$\tilde{P}_3(x_4)$</td>
<td>1</td>
</tr>
<tr>
<td>[2 0 0 0 1]</td>
<td>$\tilde{P}_2(x_1) \cdot \tilde{P}_1(x_5)$</td>
<td>2</td>
</tr>
<tr>
<td>[1 1 2 0 1]</td>
<td>$\tilde{P}_1(x_1) \cdot \tilde{P}_1(x_2) \cdot \tilde{P}_2(x_3) \cdot \tilde{P}_1(x_5)$</td>
<td>4</td>
</tr>
</tbody>
</table>
Low-rank truncation set

Definition

\[ \mathcal{A}^{M,p,r} = \{ \alpha \in \mathbb{N}^M : |\alpha| \leq p, ||\alpha||_0 \leq r \} \quad r \leq p, \ r \leq M \]
Hyperbolic truncation sets

Sparsity-of-effects principle

In most engineering problems, only low-order interactions between the input variables are relevant

- \( q \)-norm of a multi-index \( \alpha \):
  \[
  ||\alpha||_q \equiv \left( \sum_{i=1}^{M} \alpha_i^q \right)^{1/q}, \quad 0 < q \leq 1
  \]

- Hyperbolic truncation sets:
  \[
  A_{q,p}^M = \{ \alpha \in \mathbb{N}^M : ||\alpha||_q \leq p \}
  \]

\[\text{Dim. input vector } M \begin{array}{c|c|c|c|c}
2 & 5 & 10 & 20 & 50 \\
|A_{q,p}^M| & 10^1 & 10^3 & 10^5 & 10^7 & 10^9 \\
\end{array}\]

- \( p = 3 \)
- \( p = 3, q = 0.5 \)
- \( p = 5 \)
- \( p = 5, q = 0.5 \)
- \( p = 7 \)
- \( p = 7, q = 0.5 \)
Compressive sensing approaches

Blatman & Sudret (2011); Doostan & Owhadi (2011); Ian, Guo, Xiu (2012); Sargsyan et al. (2014); Jakeman et al. (2015); Sudret (2015)

- Sparsity in the solution can be induced by $\ell_1$-regularization:

$$y_\alpha = \arg \min \frac{1}{n} \sum_{i=1}^{n} \left( Y^T \Psi(x^{(i)}) - M(x^{(i)}) \right)^2 + \lambda \| y_\alpha \|_1$$

- Different algorithms: LASSO, orthogonal matching pursuit, Bayesian compressive sensing

Least Angle Regression

- Least Angle Regression (LAR) solves the LASSO problem for different values of the penalty constant in a single run without matrix inversion

- Leave-one-out cross validation error allows one to select the best model
Sparse PCE: wrap up

**Algorithm 2:** LAR-based Polynomial chaos expansion

1. **Input:** Computational budget \( n \)
2. **Initialization**
3. Sample experimental design \( \mathcal{X} = \{x^{(1)}, \ldots , x^{(n)}\} \)
4. Evaluate model response \( \mathcal{Y} = \{M(x^{(1)}), \ldots , M(x^{(n)})\} \)
5. **PCE construction**
6. for \( p = p_{\text{min}} : p_{\text{max}} \) do
7. for \( q \in Q \) do
8. Select candidate basis \( A_{q}^{M,p} \)
9. Run LAR for extracting the optimal sparse basis \( A^{*}(p, q) \)
10. Compute coefficients \( \{y_{\alpha}, \ \alpha \in A^{*}(p, q)\} \) by OLS
11. Compute \( e_{\text{LOO}}(p, q) \)
12. end
13. end
14. \( (p^{*}, q^{*}) = \arg \min e_{\text{LOO}}(p, q) \)
15. **Return** Optimal sparse basis \( A^{*}(p, q) \), PCE coefficients, \( e_{\text{LOO}}(p^{*}, q^{*}) \)
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Statistical moments

From the orthonormality of the polynomial chaos basis one gets:

\[ E[\Psi_\alpha(X)] = 0 \quad \text{for } \alpha \neq 0 \]
\[ E[\Psi_\alpha(X)\Psi_\beta(X)] = 0 \quad \text{for } \alpha \neq \beta \]

Mean value

\[ \hat{\mu}_Y = y_0 \]

The mean value is the first coefficient of the series

Variance

\[ \hat{\sigma}^2_Y \overset{\text{def}}{=} E\left[ (Y^{PC} - \hat{\mu}_Y)^2 \right] = E\left[ \left( \sum_{\alpha \in A \setminus 0} y_\alpha \Psi_\alpha(X) \right)^2 \right] \]

\[ \hat{\sigma}^2_Y = \sum_{\alpha \in A \setminus 0} y_\alpha^2 \]

The variance is computed as the sum of the squares of the remaining coefficients
Probability density function

**Principle**

The polynomial series expansion may be used as a **stochastic response surface**

- A large sample set $\xi$ of reduced variables is drawn, say of size $n_{sim} = 10^5 - 10^6$:
  \[ X_{sim} = \{ \xi_j, j = 1, \ldots, n_{sim} \} \]

- The truncated series is evaluated onto this sample:
  \[ Y_{sim} = \left\{ y_j = \sum_{\alpha \in A} y_\alpha \Psi_\alpha(\xi_j), j = 1, \ldots, n_{sim} \right\} \]

- The obtained sample set is plotted using **histograms or kernel density smoothing**
Computing the coefficients and post-processing

Post-processing the coefficients

**Probability density function**

**Kernel smoothing**

\[
\hat{f}_Y(y) = \frac{1}{n_{\text{sim}} h} \sum_{j=1}^{n_{\text{sim}}} K\left(\frac{y - \eta_j}{h}\right)
\]

- **Kernel function**: \( K(t) = \frac{1}{\sqrt{2\pi}} e^{-t^2/2} \)

- **Bandwidth**:

\[
h = 0.9 n_{\text{sim}}^{-1/5} \min(\hat{\sigma}_Y, (Q_{0.75} - Q_{0.25})/1.34)
\]

where \( Q_{0.75} - Q_{0.25} \) is the empirical inter-quartile computed from the sample
Step C’: sensitivity analysis

Goal

Global sensitivity analysis aims at quantifying which input parameter(s) (or combinations thereof) influence the most the response variability (variance decomposition)

- **Screening**: detect input parameters whose uncertainty has no impact on the output variability

- **Feature setting**: detect input parameters which allow one to best decrease the output variability when set to a deterministic value

- **Exploration**: detect interactions between parameters, i.e. joint effects not detected when varying parameters one-at-a-time

Sobol’ (1993); Saltelli et al. (2000)
Hoeffding-Sobol' decomposition

\[ M(x) = M_0 + \sum_{i=1}^{M} M_i(x_i) + \sum_{1 \leq i < j \leq M} M_{ij}(x_i, x_j) + \cdots + M_{12\ldots M}(x) \]

\[ = M_0 + \sum_{u \subseteq \{1, \ldots, M\}} M_u(x_u) \]

\( (x_u \overset{\text{def}}{=} \{x_{i_1}, \ldots, x_{i_s}\}) \)

- The summands satisfy the orthogonality condition:

\[ \int_{[0,1]^M} M_u(x_u) M_v(x_v) \, dx = 0 \quad \forall u \neq v \]
Sobol’ indices

Total variance:

\[ D \equiv \text{Var} [\mathcal{M}(X)] = \sum_{u \subset \{1, \ldots, M\}} \text{Var} [\mathcal{M}_u(X_u)] \]

- **Sobol’ indices:**

\[ S_u \overset{\text{def}}{=} \frac{\text{Var} [\mathcal{M}_u(X_u)]}{D} \]

- **First-order Sobol’ indices:**

\[ S_i = \frac{D_i}{D} = \frac{\text{Var} [\mathcal{M}_i(X_i)]}{D} \]

Quantify the additive effect of each input parameter separately

- **Total Sobol’ indices:**

\[ S_i^T \overset{\text{def}}{=} \sum_{u \supset i} S_u \]

Quantify the total effect of \( X_i \), including interactions with the other variables.
Link with PC expansions

Sobol decomposition of a PC expansion

Obtained by reordering the terms of the (truncated) PC expansion

\[ M_{PC}(X) \overset{\text{def}}{=} \sum_{\alpha \in A} y_\alpha \Psi_\alpha(X) \]

Interaction sets

For a given \( u \overset{\text{def}}{=} \{i_1, \ldots, i_s\} \):

\[ A_u = \{\alpha \in A : k \in u \Leftrightarrow \alpha_k \neq 0\} \]

\[ M_{PC}(x) = M_0 + \sum_{u \subset \{1, \ldots, M\}} M_u(x_u) \quad \text{where} \quad M_u(x_u) \overset{\text{def}}{=} \sum_{\alpha \in A_u} y_\alpha \Psi_\alpha(x) \]

PC-based Sobol’ indices

\[ S_u = D_u / D = \sum_{\alpha \in A_u} y_\alpha^2 / \sum_{\alpha \in A \setminus 0} y_\alpha^2 \]

The Sobol’ indices are obtained analytically, at any order from the coefficients of the PC expansion
Example

Computational model

\[ Y = \mathcal{M}(X_1, X_2) \]

Probabilistic model

\[ X_i \sim \mathcal{N}(\mu_i, \sigma_i) \]

Isoprobabilistic transform

\[ X_i = \mu_i + \sigma_i \xi_i \]

Chaos degree

\[ p = 3, \text{ i.e. } P = 10 \text{ terms} \]

Variance

\[ D = \sum_{j=1}^{9} a_j^2 \]

Sobol’ indices

\[ S_1 = \left( a_1^2 + a_3^2 + a_6^2 \right) / D \]
\[ S_2 = \left( a_2^2 + a_5^2 + a_9^2 \right) / D \]
\[ S_{12} = \left( a_4^2 + a_7^2 + a_8^2 \right) / D \]
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   - Truss structure
   - Hydrogeology
   - Structural dynamics
Elastic truss structures

10 independent input variables

- 4 describing the bars properties
- 6 describing the loads

Questions

PDF of the max. deflection, statistical moments, probability of failure

\[ V = \mathcal{M}^{FE} (E_1, E_2, A_1, A_2, P_1, \ldots, P_6) \]

Probabilistic model

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Name</th>
<th>Distribution</th>
<th>Mean</th>
<th>Std. Deviation</th>
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</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>( E_1, E_2 ) (Pa)</td>
<td>Lognormal</td>
<td>( 2.10 \times 10^{11} )</td>
<td>( 2.10 \times 10^{10} )</td>
</tr>
<tr>
<td>Hor. bars section</td>
<td>( A_1 ) (m²)</td>
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<td>( 2.0 \times 10^{-4} )</td>
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<tr>
<td>Vert. bars section</td>
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<td>Lognormal</td>
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<tr>
<td>Loads</td>
<td>( P_1-P_6 ) (N)</td>
<td>Gumbel</td>
<td>( 5.0 \times 10^4 )</td>
<td>( 7.5 \times 10^3 )</td>
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</tbody>
</table>
Isoprobabilistic transform

Lognormal and Gumbel distributions are transformed into reduced Gaussian variables

- **Lognormal variables** $E_1, E_2, A_1, A_2$

  
  \[
  X_i \sim \mathcal{L}\mathcal{N}(\lambda_i, \zeta_i) \\
  X_i = e^{\lambda_i + \zeta_i U_i} \quad U_i \sim \mathcal{N}(0, 1)
  \]

- **Gumbel variables** $P_1, \ldots, P_6$

  \[
  P_j \sim \mathcal{G}({\mu_j}, {\beta_j}) \quad F_{P_j}(x) = \exp \left[ -\exp \left[ -(x - {\mu_j})/{\beta_j} \right] \right]
  \]

  Thus:

  \[
  P_j = {\mu_j} - {\beta_j} \ln \left( -\ln \Phi(U_j) \right) \quad U_j \sim \mathcal{N}(0, 1)
  \]

  where the parameters $(\mu_j, \beta_j)$ are linked to the moments by:

  \[
  \mathbb{E}[P_j] = {\mu_j} + 0.577216 \beta_j \quad \sigma_{P_j} = \frac{\pi \beta_j}{\sqrt{6}}
  \]
# Full polynomial chaos expansions

## Comparison of methods

| Case | Degree | $P = |\mathcal{A}|$ | Method | Cost     |
|------|--------|----------------|--------|----------|
| A    | 2      | 66             | Quadrature | 59,049   |
| B    | 2      | 66             | Sparse quadrature | 231      |
| C$_1$| 2      | 66             | Least-squares ($n = 2P$) | 132      |
| C$_2$| 2      | 66             | Least-squares ($n = 3P$) | 198      |
| D    | 3      | 286            | Quadrature | 1,048,576|
| E    | 3      | 286            | Smolyak quadrature | 1,771    |
| F$_1$| 3      | 286            | Least-squares ($n = 2P$) | 572      |
| F$_2$| 3      | 286            | Least-squares ($n = 3P$) | 858      |
| G    | 4      | 1,001          | Smolyak quadrature | 10626    |
| H$_1$| 4      | 1,001          | Least-squares ($n = 2P$) | 2,002    |
| H$_2$| 4      | 1,001          | Least-squares ($n = 3P$) | 3,003    |
### Full polynomial chaos expansions

<table>
<thead>
<tr>
<th>Case</th>
<th>$\mu_V$</th>
<th>$\sigma_V$</th>
<th>$v_{95%}$</th>
<th>$v_{99%}$</th>
<th>Cost</th>
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<tr>
<td>B</td>
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<td>9.9030</td>
<td>10.9237</td>
<td>1,048,576</td>
</tr>
<tr>
<td>E</td>
<td>7.9400</td>
<td>1.1086</td>
<td>9.9037</td>
<td>10.9232</td>
<td>1,771</td>
</tr>
<tr>
<td>$F_1$</td>
<td>7.9392</td>
<td>1.1076</td>
<td>9.8987</td>
<td>10.9149</td>
<td>572</td>
</tr>
<tr>
<td>$F_2$</td>
<td>7.9394</td>
<td>1.1077</td>
<td>9.8991</td>
<td>10.9152</td>
<td>858</td>
</tr>
<tr>
<td>G</td>
<td>7.9401</td>
<td>1.1083</td>
<td>9.9006</td>
<td>10.9248</td>
<td>10,626</td>
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<td>$H_1$</td>
<td>7.9401</td>
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<td>9.9013</td>
<td>10.9236</td>
<td>2,002</td>
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<tr>
<td>$H_2$</td>
<td>7.9401</td>
<td>1.1083</td>
<td>9.9014</td>
<td>10.9239</td>
<td>3,003</td>
</tr>
</tbody>
</table>

**NB:** Reference values are obtained from $n = 10^6$ points (Sobol’ sequence)
Full PCE: Convergence curves

- Mean value
- Standard deviation

Models evaluated:
- Quadrature
- Sparse quadrature
- Regression (n=2*P)
- Regression (n=3*P)
Sparse polynomial chaos expansions

Set up

- The size of the experimental design is fixed to $n = 50, 100, 200, 500, 1000, 2000$. **Sobol points** are used.

- The standard truncation scheme is used ($q = 1$). Different candidate sets $A^{10,p}$ are used with $p = 2, 3, \ldots, 10$.

- The best **sparse expansion** is retained by cross-validation.

## Results

<table>
<thead>
<tr>
<th>$n$</th>
<th>$p_{opt}$</th>
<th>$A^{10,p_{opt}}$</th>
<th># Terms</th>
<th>Index of sparsity</th>
<th>$\epsilon_{LOO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>3</td>
<td>286</td>
<td>6</td>
<td>0.0210</td>
<td>2.9384e-01</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
<td>66</td>
<td>49</td>
<td>0.7424</td>
<td>3.4961e-03</td>
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<tr>
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<td>3</td>
<td>286</td>
<td>81</td>
<td>0.2832</td>
<td>1.6448e-03</td>
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<tr>
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<td>3</td>
<td>286</td>
<td>151</td>
<td>0.5280</td>
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<tr>
<td>1000</td>
<td>4</td>
<td>1001</td>
<td>381</td>
<td>0.3806</td>
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<tr>
<td>2000</td>
<td>5</td>
<td>3003</td>
<td>473</td>
<td>0.1575</td>
<td>1.9126e-06</td>
</tr>
</tbody>
</table>
Sparse polynomial chaos expansions

Set up
- The same calculations are carried out using a priori a hyperbolic truncation set with $q-$norm $q = 0.75$

Results

<table>
<thead>
<tr>
<th>$n$</th>
<th>$p_{opt}$</th>
<th>$A^{10,p_{opt}}$</th>
<th># Terms</th>
<th>Index of sparsity</th>
<th>$\epsilon_{LOO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>2</td>
<td>66</td>
<td>19</td>
<td>0.2879</td>
<td>4.2476e-02</td>
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<tr>
<td>100</td>
<td>3</td>
<td>286</td>
<td>54</td>
<td>0.1888</td>
<td>3.8984e-03</td>
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<tr>
<td>200</td>
<td>4</td>
<td>1001</td>
<td>121</td>
<td>0.1209</td>
<td>3.9940e-04</td>
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<tr>
<td>500</td>
<td>5</td>
<td>3003</td>
<td>279</td>
<td>0.0929</td>
<td>4.0975e-05</td>
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<tr>
<td>1000</td>
<td>6</td>
<td>8008</td>
<td>579</td>
<td>0.0723</td>
<td>2.2236e-06</td>
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<tr>
<td>2000</td>
<td>7</td>
<td>19448</td>
<td>806</td>
<td>0.0414</td>
<td>1.5752e-07</td>
</tr>
</tbody>
</table>

- Higher degree terms are included (more sparsity)
- Better accuracy as measured by $\epsilon_{LOO}$
Sparse PCE: Convergence curves

Mean value

Standard deviation
Structural reliability analysis

Limit state function: \[ g(X) \equiv v_{\text{max}} - \mathcal{M}(E_1, E_2, A_1, A_2, P_1, \ldots, P_6) \]

Full PCE \[ p = 3, \text{ Smolyak quadrature (1,771 runs)} \]

<table>
<thead>
<tr>
<th>Threshold ( v_{\text{max}} ) (cm)</th>
<th>Reference</th>
<th>Smolyak quadrature</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( P_f )</td>
<td>( \beta )</td>
</tr>
<tr>
<td>10</td>
<td>4.31 \times 10^{-2}</td>
<td>1.71</td>
</tr>
<tr>
<td>11</td>
<td>8.70 \times 10^{-3}</td>
<td>2.37</td>
</tr>
<tr>
<td>12</td>
<td>1.50 \times 10^{-3}</td>
<td>2.96</td>
</tr>
<tr>
<td>14</td>
<td>3.49 \times 10^{-5}</td>
<td>3.97</td>
</tr>
<tr>
<td>16</td>
<td>6.03 \times 10^{-7}</td>
<td>4.85</td>
</tr>
</tbody>
</table>

† \( \beta = -\Phi^{-1}(P_f) \)

Sparse PC

<table>
<thead>
<tr>
<th>Reference (10^5 runs)</th>
<th>LAR (500 runs)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 cm</td>
<td>4.39e-02 ± 3.0%</td>
</tr>
<tr>
<td>11 cm</td>
<td>8.61e-03 ± 6.7%</td>
</tr>
<tr>
<td>12 cm</td>
<td>1.62e-03 ± 15.4%</td>
</tr>
<tr>
<td>13 cm</td>
<td>2.20e-04 ± 41.8%</td>
</tr>
</tbody>
</table>

B. Sudret (Chair of Risk, Safety & UQ)  UQ with polynomial chaos expansions   GRK1462 Summer School - Weimar 78 / 90
Outline

1 Introduction

2 Global framework for uncertainty quantification

3 Polynomial chaos basis

4 Computing the coefficients and post-processing

5 Application examples
   Truss structure
   Hydrogeology
   Structural dynamics
Example: sensitivity analysis in hydrogeology

- When assessing a nuclear waste repository, the Mean Lifetime Expectancy $\text{MLE}(x)$ is the time required for a molecule of water at point $x$ to get out of the boundaries of the system.

- Computational models have numerous input parameters (in each geological layer) that are difficult to measure, and that show scattering.
Geological model

Joint work with University of Neuchâtel


- **Two-dimensional idealized model** of the Paris Basin (25 km long / 1,040 m depth) with $5 \times 5$ m mesh ($10^6$ elements)

- **Steady-state flow** simulation with Dirichlet boundary conditions:

  $$\nabla \cdot (K \cdot \nabla H) = 0$$

- **15 homogeneous layers** with uncertainties in:
  - Porosity (resp. hydraulic conductivity)
  - Anisotropy of the layer properties (inc. dispersivity)
  - Boundary conditions (hydraulic gradients)

78 input parameters
Sensitivity analysis

Geometry of the layers

Conductivity of the layers

Question

What are the parameters (out of 78) whose uncertainty drives the uncertainty of the prediction of the mean life-time expectancy?
Sensitivity analysis: results

**Technique:** Sobol’indices computed from polynomial chaos expansions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\sum_j S_j$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\phi$ (resp. $K_x$)</td>
<td>0.8664</td>
</tr>
<tr>
<td>$A_K$</td>
<td>0.0088</td>
</tr>
<tr>
<td>$\theta$</td>
<td>0.0029</td>
</tr>
<tr>
<td>$\alpha_L$</td>
<td>0.0076</td>
</tr>
<tr>
<td>$A_\alpha$</td>
<td>0.0000</td>
</tr>
<tr>
<td>$\nabla H$</td>
<td>0.0057</td>
</tr>
</tbody>
</table>

**Conclusions**

- Only **200 model runs** allow one to detect the 10 important parameters out of 78
- Uncertainty in the porosity/conductivity of **5 layers** explain 86% of the variability
- Small interactions between parameters detected
The univariate effects of each variable are obtained as a straightforward post-processing of the PCE

\[
M_i(x_i) \overset{\text{def}}{=} \mathbb{E}[M(X)|X_i = x_i], \ i = 1, \ldots, M
\]
Polynomial chaos expansions in structural dynamics

Spiridonakos et al. (2015); Mai & Sudret, ICASP’2015; Mai et al., 2016

Premise

- For dynamical systems, the complexity of the map $x \mapsto M(x, t)$ increases with time.
- **Time-frozen PCE** does not work beyond first time instants

- Use of non linear autoregressive with exogenous input models (NARX) to capture the dynamics:

  $$y(t) = \mathcal{F}(x(t), \ldots, x(t - n_x), y(t - 1), \ldots, y(t - n_y)) + \epsilon_t$$

- Expand the NARX coefficients of different random trajectories onto a PCE basis

  $$y(t, \xi) = \sum_{i=1}^{n_g} \sum_{\alpha \in A_i} \vartheta_{i, \alpha} \psi_{\alpha}(\xi) g_i(z(t)) + \epsilon(t, \xi)$$
Application: earthquake engineering

- 2D steel frame with uncertain properties submitted to synthetic ground motions
- Experimental design of size 300

- Ground motions obtained from modulated, filtered white noise

\[ x(t) = q(t, \alpha) \sum_{i=1}^{n} s_i(t, \lambda(t_i)) \cdot \xi_i \quad \xi_i \sim \mathcal{N}(0, 1) \]

Rezaeian & Der Kiureghian (2010)
Application: earthquake engineering

Surrogate model of single trajectories

![Graph showing reference and PC-NARX models compared over time](image)

- Reference
- PC-NARX

$t (s)$ vs. $y(t) (m)$
Application examples  Structural dynamics

Application: earthquake engineering

First-storey drift

- PC-NARX calibrated based on 300 simulations
- Reference results obtained from 10,000 Monte Carlo simulations

PDF of max. drift

Fragility curves for two drift thresholds

\[ \delta_o = 0.021 \]

\[ \delta_o = 0.045 \]
Conclusions

- Uncertainty quantification for engineering applications require non-intrusive, parsimonious techniques to solve propagation, sensitivity and reliability problems.

- Polynomial chaos expansions represent the quantities of interest as a multivariate orthonormal polynomial series in the input variables.

- Coefficients can be computed by projection, ordinary least-square and compressive sensing.

- Post-processing of the series provides moments, quantiles, PDF, probabilities of failure, sensitivity indices, etc.

- Problems involving $O(10)$ input variables can be solved in $O(100)$ runs.
Questions?

Chair of Risk, Safety & Uncertainty Quantification
www.rsuq.ethz.ch

The Uncertainty Quantification Laboratory
www.uqlab.com

Thank you very much for your attention!