Sparse polynomial chaos expansions for solving high-dimensional UQ problems

Author(s):
Sudret, Bruno

Publication Date:
2015

Permanent Link:
https://doi.org/10.3929/ethz-a-010583137

Rights / License:
In Copyright - Non-Commercial Use Permitted
Sparse polynomial chaos expansions for solving high-dimensional UQ problems

Bruno Sudret

1st International Conference on Uncertainty Quantification in Computational Sciences and Engineering
Chair of Risk, Safety and Uncertainty quantification

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

- Structural reliability analysis
- **Polynomial chaos expansions** and stochastic finite element methods
- Gaussian process modelling (Kriging)
- Bayesian model calibration and stochastic inverse problems
- Global sensitivity analysis
- Reliability-based design optimization

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

Complex engineering systems are designed using computational models that are based on:

- A mathematical description of the physics
- Numerical algorithms that solve the resulting set of (e.g. partial differential) equations, e.g. finite element models

Computational models are used:

- Together with experimental data for calibration purposes
- To explore the design space ("virtual prototypes")
- To optimize the system w.r.t cost constraints
- To assess its robustness w.r.t uncertainty and its reliability
Sources of uncertainty

- 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), climate loads (hurricanes, snow storms, etc.)
Uncertainty quantification in engineering and applied sciences

- Uncertainty quantification arrives on top of well defined simulation procedures (legacy codes)
- State-of-the-art computational models are complex: coupled problems (thermo-mechanics), plasticity, large strains, contact, buckling, etc.
- A single simulation is already costly (e.g. several hours)
- The input variables modelling aleatory uncertainty are often non Gaussian. The size of the input random vector is typically $10-100$

Need for non intrusive and parsimonious methods for uncertainty quantification
Outline

1 Introduction

2 Polynomial chaos expansions: small dimension
   - PCE basis
   - Computing the coefficients
   - Post-processing

3 Sparse polynomial chaos expansions
   - Why sparse PCE?
   - How sparse PCE?
   - Application: global sensitivity analysis in hydrogeology

4 Time-variant problems
   - Introduction
   - Non linear Duffing oscillator
Polynomial chaos expansions in a nutshell

Ghanem & Spanos (1991); Xiu & Karniadakis (2002); Soize & Ghanem (2004)

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

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

where:

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

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

- **Univariate** orthogonal polynomials \( \{ P_k^{(i)}, k \in \mathbb{N} \} \) are built for each input variable \( X_i \):

\[
\left\langle P_j^{(i)}(x_i), P_k^{(i)}(x_i) \right\rangle = \int P_j^{(i)}(x_i) P_k^{(i)}(x_i) f_{X_i}(x_i) \, dx_i = \gamma_j^{(i)} \delta_{jk}
\]

- **Normalization**:

\[
\Psi_j^{(i)} = P_j^{(i)} / \sqrt{\gamma_j^{(i)}} \quad i = 1, \ldots, M, \quad j \in \mathbb{N}
\]

- **Tensor product construction**

\[
\Psi_\alpha(x) \overset{\text{def}}{=} \prod_{i=1}^{M} \Psi_{\alpha_i}^{(i)}(x_i) \quad \mathbb{E} [\Psi_\alpha(X) \Psi_\beta(X)] = \delta_{\alpha \beta}
\]
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
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
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

- The joint CDF is defined through its marginals and copula

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

- Rosenblatt or Nataf isoprobabilistic transform is used
Truncation scheme

- For practical computation, a truncated series is defined:

\[ Y = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(X) \]

- The classical truncation scheme contains all multi-indices of total degree \(|\alpha| \overset{\text{def}}{=} \sum_{i=1}^{M} \alpha_i\) smaller than \(p\)

\[ \mathcal{A}^{M,p} = \{ \alpha \in \mathbb{N}^M : |\alpha| \leq p \} \quad \text{card} \ \mathcal{A}^{M,p} \equiv P = \binom{M + p}{p} \]

<table>
<thead>
<tr>
<th>(M \backslash p)</th>
<th>2</th>
<th>3</th>
<th>5</th>
<th>7</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>6</td>
<td>10</td>
<td>21</td>
<td>36</td>
<td>66</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td>20</td>
<td>56</td>
<td>120</td>
<td>286</td>
</tr>
<tr>
<td>5</td>
<td>21</td>
<td>56</td>
<td>252</td>
<td>792</td>
<td>3,003</td>
</tr>
<tr>
<td>10</td>
<td>66</td>
<td></td>
<td></td>
<td></td>
<td>184,756</td>
</tr>
<tr>
<td>50</td>
<td>1,326</td>
<td></td>
<td></td>
<td></td>
<td>75,394,027,566</td>
</tr>
<tr>
<td>100</td>
<td>5,151</td>
<td>176,851</td>
<td>96,560,646</td>
<td>26,075,972,546</td>
<td>46,897,636,623,981</td>
</tr>
</tbody>
</table>

Curse of dimensionality
Outline

1. Introduction

2. Polynomial chaos expansions: small dimension
   - PCE basis
   - Computing the coefficients
   - Post-processing

3. Sparse polynomial chaos expansions

4. Time-variant problems
Various methods for computing the coefficients

Intrusive approaches

- Historical approaches: projection of the equations residuals in the Galerkin sense
  Ghanem et al.; Le Maître et al., Babuska, Tempone et al.; Karniadakis et al., etc.
- Proper generalized decompositions
  Nouy et al., 2007-10

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
  $\mathcal{X} = \{x^{(i)} \in \mathcal{D}_X, i = 1, \ldots, n\}$ of the input parameters
- Different classes of methods are available:
  - projection: by simulation or quadrature
    Matthies & Keese, 2005; Le Maître et al.
  - stochastic collocation
    Xiu, 2007-09; Nobile, Tempone et al., 2008; Ma & Zabaras, 2009
  - least-square minimization
    Berveiller et al., 2006; Blatman & S., 2008-11
Statistical approach: least-square minimization

Principle

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

\[ Y = \mathcal{M}(X) = \sum_{\alpha \in A} y_\alpha \Psi_\alpha(X) + \varepsilon_P \equiv Y^T \Psi(X) + \varepsilon_P(X) \]

where:

\[ Y = \{ y_\alpha, \alpha \in A \} \equiv \{ y_0, \ldots, y_{P-1} \} \quad (P \text{ unknown coef.}) \]

\[ \Psi(x) = \{ \Psi_0(x), \ldots, \Psi_{P-1}(x) \} \]

Least-square minimization

The unknown coefficients are estimated by minimizing the mean square residual error:

\[ \hat{Y} = \arg \min E \left[ (Y^T \Psi(X) - \mathcal{M}(X))^2 \right] \]
Least-Square Minimization: discretized solution

Ordinary least-square (OLS)

- An estimate of the mean square error (sample average) is minimized:

\[
\hat{Y} = \arg \min_{Y \in \mathbb{R}^P} \frac{1}{n} \sum_{i=1}^{n} (Y^T \Psi(x^{(i)}) - M(x^{(i)}))^2
\]

Procedure

- Select an experimental design and evaluate the model response

\[
M = \{ M(x^{(1)}), \ldots, M(x^{(n)}) \}^T
\]

- Compute the experimental matrix

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

- Solve the resulting linear system

\[
\hat{Y} = (A^T A)^{-1} A^T M
\]

Simple is beautiful!
Error estimators

- In least-squares analysis, the generalization error is defined as:

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

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

- The empirical error based on data set \( \mathcal{X} \):

\[ E_{emp} = \frac{1}{n} \sum_{i=1}^{n} \left( \mathcal{M}(x^{(i)}) - \mathcal{M}^{PC}(x^{(i)}) \right)^2 \]

is a poor estimator (overfitting):

- Model validation shall be carried out with independent data

Leave-one-out cross validation
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)

\[
E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \left( M(\mathbf{x}^{(i)}) - M_{PC \setminus i}(\mathbf{x}^{(i)}) \right)^2
\]

- Computing directly 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 \( \mathbf{A}(\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \)
**Algorithm 1: OLS**

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

- Due to the orthogonality of the basis functions \( \mathbb{E} [\Psi_\alpha(X)\Psi_\beta(X)] = \delta_{\alpha\beta} \)
  and using \( \mathbb{E} [\Psi_\alpha \neq 0] = 0 \) the statistical moments read:

  \[
  \text{Mean:} \quad \hat{\mu}_Y = y_0 \\
  \text{Variance:} \quad \hat{\sigma}_Y^2 = \sum_{\alpha \in \mathcal{A} \setminus 0} y_\alpha^2
  \]

Distribution of the QoI

- The PCE can be used as a response surface for sampling:

  \[
  \eta_j = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(x_j) \quad j = 1, \ldots, n_{\text{big}}
  \]

- The PDF of the response is estimated by histograms or kernel smoothing
Sensitivity analysis

Goal

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

Hoeffding-Sobol’ decomposition

\[
X \sim \mathcal{U}([0,1]^M)
\]

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

\[
= M_0 + \sum_{u \subset \{1, \ldots, M\}} M_u(x_u) \quad (x_u \overset{\text{def}}{=} \{x_{i_1}, \ldots, x_{i_s}\})
\]

- 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’ (1993); Saltelli et al. (2000)

B. Sudret (Chair of Risk, Safety & UQ)
Sobol’ indices

Total variance:

\[ D \equiv \text{Var} [\mathcal{M}(X)] = \sum_{\mathcal{U} \subseteq \{1, \ldots, M\}} \text{Var} [\mathcal{M}_\mathcal{U}(X_\mathcal{U})] \]

- Sobol’ indices:

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

- First-order Sobol’ indices:

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

Quantify the additive effect of each input parameter separately

- Total Sobol’ indices:

\[ S_i^T \overset{\text{def}}{=} \sum_{\mathcal{U} \supseteq i} S_u \]

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

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

Interaction sets

\[ \forall \ u \overset{\text{def}}{=} \{i_1, \ldots, i_s\} : \ A_u = \{\alpha \in A : k \in u \iff \alpha_k \neq 0\} \]

\[ \mathcal{M}_{\text{PC}}(x) = \mathcal{M}_0 + \sum_{u \subset \{1, \ldots, M\}} \mathcal{M}_u(x_u) \quad \text{where} \quad \mathcal{M}_u(x_u) \overset{\text{def}}{=} \sum_{\alpha \in A_u} y_{\alpha} \Psi_{\alpha}(x) \]

PC-based Sobol’ indices

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

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

1. Introduction

2. Polynomial chaos expansions: small dimension

3. Sparse polynomial chaos expansions
   - Why sparse PCE?
   - How sparse PCE?
   - Application: global sensitivity analysis in hydrogeology

4. Time-variant problems
Why are sparse representations relevant?

- Elastic truss structure
- \( M = 10 \) independent input variables
  (loads / Young’s moduli / cross sections)
- PCE of degree \( p = 5 \) (3,003 coefficients)
Low-rank truncation schemes

Ockham’s razor

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

Sparsity-of-effects principle

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 $\alpha$:

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

Definition

- The $q$-norm of a multi-index $\alpha$ is defined by:

$$||\alpha||_q \equiv \left( \sum_{i=1}^{M} \alpha_i^q \right)^{1/q}, \quad 0 < q \leq 1$$

- The hyperbolic truncation sets read:

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

Limit cases

- $q = 1$: standard truncation scheme (all polynomials of maximal total degree $p$)
- $q \to 0$: additive model (no interaction)
Hyberbolic truncation sets

$q = 1$

$q = 0.75$

$q = 0.5$
For a given value of $0 < q \leq 1$, the **index of sparsity** tends to zero when $M$ and $p$ increase.
How to get sparse expansions?

- 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, (Bayesian) compressive sensing

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

Least Angle Regression

- Least Angle Regression (LAR) solves the LASSO problem for different values of the penalty constant in a single run

- The various PC expansions obtained have $1, 2, \ldots, \min(n, |A|)$ terms

Efron et al. (2004)
Least angle regression
Implementation

Consider a 3-dimensional vector

\[ \Psi_{\alpha_3} \]

\[ a_3 \rightarrow \Psi_{\alpha_2} \rightarrow a_2 \rightarrow a_1 \rightarrow \Psi_{\alpha_1} \]

\[ Y = \mathcal{M}(X) \]
The algorithm is initialized with $Y^{(0)} = 0$. The residual is $R = Y = \mathcal{M}(X)$.

- The most correlated regressor is $\Psi_{\alpha_1}$.
Least angle regression
Implementation

- A move in the direction $\Psi_{\alpha_1}$ is carried out so that the residual $Y - a_1^{(1)} \Psi_{\alpha_1}$ becomes equicorrelated with $\Psi_{\alpha_1}$ and $\Psi_{\alpha_2}$
- The 1-term sparse approximation of $Y$ is $a_1^{(1)} \Psi_{\alpha_1}$

$Y = \mathcal{M}(X)$
Least angle regression

Implementation

A move is jointly made in the direction $\Psi_{\alpha_1} + \Psi_{\alpha_2}$ until the residual becomes equicorrelated with a third regressor.
Least angle regression
Implementation

A move is jointly made in the direction $\Psi_{\alpha_1} + \Psi_{\alpha_2}$ until the residual becomes equicorrelated with a third regressor.
Least angle regression

Implementation

This gives the 2-term sparse approximation
Least angle regression

Implementation

- In finite dimension, LAR eventually yields the same results as projection in $P$ steps.

Efron et al., 2004
Least angle regression
Path of solutions

- A path of solutions is obtained containing $1, 2, \ldots, \min(n, |A|)$ terms.
- Leave-one-out error $E_{LOO}$ is computed for each solution and the best model (smallest error) is selected.

\[
E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{M(x^{(i)}) - M_{PC}(x^{(i)})}{1 - h_i} \right)^2
\]

$h_i$: $i$-th diagonal term of matrix $A(A^T A)^{-1} A^T$ and $A_{ij} = \Psi_j(x^{(i)})$
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 $q \in \mathbb{Q}$ 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. $(p^{*}, q^{*}) = \text{arg min } e_{\text{LOO}}(p, q)$
15. **Return** Optimal sparse basis $A^{*}(p, q)$, PCE coefficients, $e_{\text{LOO}}(p^{*}, q^{*})$
Tolerance-driven sparse PCE: wrap up

Algorithm 3: Tolerance-driven Sparse PCE

1: Input
2: Initial and max. computational budget $n_{ini}$, $n_{max}$ batch size $B$
3: Target error TOL
4: Initialization
5: Apply LARbasedPCE($n_{ini}$), return $e_{LOO}(n_{ini})$
6: Enrich ED
7: $n \leftarrow n_{ini}$
8: while ($e_{LOO}(n) > TOL$) & ($n + B \leq n_{max}$) do
9:   Enrich ED: $\mathcal{X} \leftarrow \mathcal{X} \cup \{x^{(1)}, \ldots, x^{(B)}\}$
10:  $n \leftarrow n + B$
11:  Apply LARbasedPCE($n$)
12: end
13: Return Final ED size $n$, optimal sparse basis and PCE coefficients, $e_{LOO}(n)$
Outline

1. Introduction
2. Polynomial chaos expansions: small dimension
3. Sparse polynomial chaos expansions
   - Why sparse PCE?
   - How sparse PCE?
   - Application: global sensitivity analysis in hydrogeology
4. Time-variant problems
The UQLab framework

**UQLab ...**

... The Uncertainty Quantification Laboratory

"Make uncertainty quantification available for anybody, in any field of applied science and engineering"

- Matlab-based core managing system (MODEL / INPUT / ANALYSIS objects)
  - Modules: surrogate models (Gaussian processes / polynomial chaos expansions), sensitivity analysis, reliability analysis
  - Dispatcher to HPC infrastructure
Geological model

- Idealized model of the Paris Basin
- Two-dimensional cross section
  
  \( (25 \text{ km long} / 1,040 \text{ m depth}) \text{ with } 5 \times 5 \text{ m mesh} (10^6 \text{ elements}) \)
- 15 homogeneous layers

- Steady-state flow with Dirichlet boundary conditions:

\[
\nabla \cdot (K \cdot \nabla H) = 0
\]
Mean lifetime expectancy

Definition

The Mean Lifetime Expectancy $MLE(x)$ is the time required for a molecule of water at point $x$ to get out of the boundaries of the model.

Map of mean lifetime expectancy (nominal case)
Probabilistic model of porosity / conductivity

Nominal conductivity ($K_x$) vs. porosity

<table>
<thead>
<tr>
<th>Layer</th>
<th>$K_x$ [m/s]</th>
<th>$\phi$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>K3</td>
<td>9.01E-09</td>
<td>0.0100</td>
</tr>
<tr>
<td>K1-K2</td>
<td>4.53E-09</td>
<td>0.1150</td>
</tr>
<tr>
<td>L2c</td>
<td>1.10E-06</td>
<td>0.1389</td>
</tr>
<tr>
<td>L2b</td>
<td>3.46E-07</td>
<td>0.1110</td>
</tr>
<tr>
<td>L2a</td>
<td>1.62E-07</td>
<td>0.1139</td>
</tr>
<tr>
<td>L1b</td>
<td>1.49E-05</td>
<td>0.1604</td>
</tr>
<tr>
<td>L1a</td>
<td>1.17E-06</td>
<td>0.1549</td>
</tr>
<tr>
<td>C3ab</td>
<td>4.59E-08</td>
<td>0.0984</td>
</tr>
<tr>
<td>C2</td>
<td>1.99E-13</td>
<td>0.1580</td>
</tr>
<tr>
<td>C1</td>
<td>1.89E-06</td>
<td>0.0470</td>
</tr>
<tr>
<td>D4</td>
<td>1.65E-05</td>
<td>0.0905</td>
</tr>
<tr>
<td>D3</td>
<td>1.76E-06</td>
<td>0.1016</td>
</tr>
<tr>
<td>D2</td>
<td>2.62E-07</td>
<td>0.0623</td>
</tr>
<tr>
<td>D1</td>
<td>3.23E-06</td>
<td>0.0688</td>
</tr>
<tr>
<td>T</td>
<td>1.95E-12</td>
<td>0.0810</td>
</tr>
</tbody>
</table>

In each layer, bounds on porosity: $\phi_i \sim U[\phi_{i\text{min}}, \phi_{i\text{max}}]$

Deterministic mapping to the conductivity

$log_{10}(K_i x) = f_i(\phi_i)$ (layer-dependent)
Other parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Notation</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>(\phi^i), (i = 1, \ldots, 15)</td>
<td>([\phi_{min}^i, \phi_{max}^i])</td>
</tr>
<tr>
<td>Anisotropy of hydraulic conductivity tensor</td>
<td>(A_K^i), (i = 1, \ldots, 15)</td>
<td>([0.01, 1])</td>
</tr>
<tr>
<td>Euler angle of hydraulic conductivity tensor</td>
<td>(\theta^i), (i = 1, \ldots, 15)</td>
<td>([-30, 30] (°))</td>
</tr>
<tr>
<td>Longitudinal component of dispersivity tensor</td>
<td>(\alpha_L^i), (i = 1, \ldots, 15)</td>
<td>([5, 25])</td>
</tr>
<tr>
<td>Anisotropy of dispersivity tensor</td>
<td>(A_\alpha^i), (i = 1, \ldots, 15)</td>
<td>([5, 25])</td>
</tr>
</tbody>
</table>

Hydraulic gradient \((10^{-3} m/m)\)

<table>
<thead>
<tr>
<th>Sequence</th>
<th>(\nabla H)</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dogger sequence</td>
<td>(\nabla H_D)</td>
<td>([0.64, 0.96])</td>
</tr>
<tr>
<td>Oxfordian sequence</td>
<td>(\nabla H_O)</td>
<td>([2.40, 3.60])</td>
</tr>
<tr>
<td>Top of the model</td>
<td>(\nabla H_{top})</td>
<td>([2.72, 4.08])</td>
</tr>
</tbody>
</table>

78 independent variables with uniform distributions
Polynomial chaos expansions

- **Experimental design** of size 2,000 (Maximin Latin Hypercube Sampling).
  Independent validation set of size 2,000
- **Truncation scheme:** \( p = 8, \ q = 0.5 \)
- **Sparse basis size:** 185 / Full-basis size \( 5.3 \times 10^{10} \). Only 68 out of 78 parameters are included

\[
\text{err}_{\text{LOO}} = 0.056488 \quad \text{err}_G = 0.07591
\]

Training set

Validation set
• Uncertainties on the porosities (and associated conductivities) drive the MLE uncertainty
• Second-order effects have been identified

Sobol’ sensitivity indices

**Sobol’ sensitivity indices**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$S^{(1)}_i$</th>
<th>$S_{Tot}^i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nabla H$</td>
<td>0.0057</td>
<td></td>
</tr>
<tr>
<td>$A_\alpha$</td>
<td>0.0000</td>
<td></td>
</tr>
<tr>
<td>$\alpha_l$</td>
<td>0.0076</td>
<td></td>
</tr>
<tr>
<td>$\theta$</td>
<td>0.0029</td>
<td></td>
</tr>
<tr>
<td>$A_K$</td>
<td>0.0088</td>
<td></td>
</tr>
<tr>
<td>$\phi$</td>
<td>0.8664</td>
<td></td>
</tr>
</tbody>
</table>

**Total Sobol’ Indices**

**Sobol’ Indices Order 1**

- Uncertainties on the porosities (and associated conductivities) drive the MLE uncertainty
- Second-order effects have been identified

**Why sparse PCE?**

- **Sparse polynomial chaos expansions**
- **Time-variant problems**

**Application: global sensitivity analysis in hydrogeology**

**Why sparse PCE?**

- Sparse PCE for high-dimensional problems
- **Polynomial chaos expansions: small dimension**

**UNCECOMP - May 26th, 2015**

B. Sudret (Chair of Risk, Safety & UQ)
Sobol’ sensitivity indices: using 200 model runs

Only 200 model runs allow one to detect the important parameters out of 78
Outline

1. Introduction
2. Polynomial chaos expansions: small dimension
3. Sparse polynomial chaos expansions
4. Time-variant problems
   - Introduction
   - Non linear Duffing oscillator
Problem statement

**Premise:** In case of time-dependent governing equations, the response of the system is a time-dependent function:

\[ Y(t) = M(X; t) \]

- ordinary differential equations with random coefficients (chemical reactions)
- fluid dynamics
- structural dynamics (e.g. earthquake engineering)

**Time-frozen PCE**

- Consider the discretized deterministic solutions \( n_{TS} \) time steps:

\[ y_i(t_j) = M(x^{(i)}; t_j) \quad i = 1, \ldots, n, \quad j = 1, \ldots, n_{TS} \]

- Build up PCE independently at each time-instant (considered frozen)

\[ Y(t_j) = \sum_{\alpha \in A_{t_j}} y_{\alpha}(t_j) \Psi_{\alpha}(X) \]

Fails due to increasing complexity of the input/output map when \( t \to +\infty \)
Example: rigid body dynamics

Rotation of a rigid body described by Euler’s equations

\[
\begin{align*}
M_x &= I_{xx} \dot{\omega}_x - (I_{yy} - I_{zz}) \omega_y \omega_z \\
M_y &= I_{yy} \dot{\omega}_y - (I_{zz} - I_{xx}) \omega_z \omega_x \\
M_z &= I_{zz} \dot{\omega}_z - (I_{xx} - I_{yy}) \omega_x \omega_y
\end{align*}
\]

Reduced system

\[
\begin{align*}
\dot{x} &= yz \\
\dot{y} &= c \times xz \\
\dot{z} &= -xy
\end{align*}
\]

where \( c \sim U(-0.8, 0.6) \)

Mai & S., MascotNum Workshop, 2015

http://www.esa.int/spaceinimages/Missions/Rosetta
Different trajectories for various values of $c$
Stochastic dependence $y(c, t)$ for different time instants $t$
Time-frozen PCE: LOO error
Stochastic time warping

Heuristics

Introduce a virtual time scale $\tau$ such that the current trajectory $y(x(i), \tau)$ is “similar” to a reference trajectory

Measure of dissimilarity

$$\text{diss}[y(t), y_{ref}(t)] \overset{\text{def}}{=} \frac{\left| \int_0^T y(t) y_{ref}(t) \, dt \right|}{\sqrt{\int_0^T y^2(t) \, dt \cdot \int_0^T y_{ref}^2(t) \, dt}}$$

- It is the cross-correlation of the two signals
- Bounded between 0 and 1
Stochastic time warping: procedure

- Choose a reference trajectory $y_{ref}(t) = M(x_{ref}, t)$ where e.g. $x_{ref} = \mu x$

- Define a stochastic time transform:

$$\tau(X) = k(X) t + \phi(X)$$

- For each sample trajectory $\{y_i(t), i = 1, \ldots, n\}$, compute the appropriate rescaling:

$$(k_i, \phi_i) = \arg \min_{k, \phi} \text{diss}[y_i(kt + \phi), y_{ref}(t)]$$

- Compute a sparse PCE of the parameters of the time transform:

$$k(X) = \sum_{\alpha \in A} k_\alpha \Psi_\alpha(X) \quad \phi(X) = \sum_{\alpha \in A} \phi_\alpha \Psi_\alpha(X)$$

Mai & Sudret (2015)
Stochastic time warping: procedure

- In the virtual time scale, trajectories show much higher coherency. \( \tau \)-frozen PCE expansions apply:

\[
y(X, \tau) = \sum_{\alpha \in A} y_\alpha(\tau) \Psi_\alpha(X)
\]

Predictions for a new sample \( x^{(0)} \)

- Predict the trajectory in the virtual time scale

\[
y(x^{(0)}, \tau) = \sum_{\alpha \in A} y_\alpha(\tau) \Psi_\alpha(x^{(0)})
\]

- Predict the proper time warping:

\[
\tau(x^{(0)}) = k(x^{(0)}) t + \phi(x^{(0)})
\]

- Map back the predicted trajectory in the real time scale:

\[
y(x^{(0)}, t) = \sum_{\alpha \in A} y_\alpha \left( k(x^{(0)}) t + \phi(x^{(0)}) \right) \Psi_\alpha(x^{(0)})
\]
Application – non linear Duffing oscillator

Non-linear SDOF Duffing oscillator:

\[ \ddot{x}(t) + 2 \omega \zeta \dot{x}(t) + \omega^2 (x(t) + \epsilon x^3(t)) = 0 \]

Initial conditions: \( x(0) = 1, \quad \dot{x}(0) = 0 \)

Input: 3 uniform random variables

\[ \zeta = 0.05(1 + 0.05 \xi_1), \quad \xi_1 \sim U(-1, 1) \]
\[ \omega = 2\pi(1 + 0.2 \xi_2), \quad \xi_2 \sim U(-1, 1) \]
\[ \epsilon = -0.5(1 + 0.5 \xi_3), \quad \xi_3 \sim U(-1, 1) \]
Time-frozen PCE

LOO error vs. time

Predicted trajectory

- Actual model
- PCE prediction
Time-warped PCE

Rescaled trajectories

Predicted trajectory in real time $t$
Validation: mean and standard deviation (time-warping PCE)

Validation set: 10,000 Monte Carlo samples

Mean response

Standard deviation
Earthquake engineering applications

- Structural systems under earthquake excitation
- Parametrized input signal in high dimension:

\[ \hat{a}(t) = \alpha_1 t^{\alpha_2-1} \exp(-\alpha_3 t) \sum_{i=1}^{n} s_i(t, \lambda(t_i)) U_i \]

Goal

Predict the output trajectories through time-variant PCE, e.g. the interstorey drift
Conclusions

- Polynomial chaos expansions are a versatile tool for solving engineering uncertainty quantification problems

- Sparse expansions are extremely efficient for global sensitivity analysis (e.g. ~ x00 model runs for 50-100 input variables)

- An a posteriori built-in error estimator is available through leave-one-out cross validation, leading to adaptive methods (incl. adaptive experimental designs)

- Ingredients such as isoprobabilistic transforms, least-square analysis and low-rank truncation schemes are easy to understand

- ... and easy to implement in a general-purpose software
Outlook and ongoing projects

- More compact representations: **low-rank tensor approximations**
  Chevreuil et al. (2013), Konakli & Sudret, UNCECOMP’2015

- Optimal **small size** experimental designs and local error estimation:
  Polynomial-chaos based Kriging
  Kersaudy et al., JCP (2015); Schöbi & Sudret, IJUQ (2015)

- PCE expansions in case of imprecise probability description of the input parameters through **p-boxes**
  Schöbi & Sudret, ICASP (2015)

- Spectral likelihood expansions for solving Bayesian inverse problems
  Nagel & Sudret, PANACM (2015)
Questions ?

Acknowledgements:
K. Konakli, C.V. Mai, C. Lataniotis, S. Marelli, R. Schöbi

Thank you very much for your attention!

Chair of Risk, Safety & Uncertainty Quantification

http://www.rsuq.ethz.ch