Polynomial chaos expansions for sensitivity analysis

B. Sudret

Chair of Risk, Safety & Uncertainty Quantification

Ecole ASPEN – May 9th, 2014 – Les Houches
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

- Random variables
- Computational model
- Distribution
  - Mean, std. deviation
  - Probability of failure

**Step C’**
Sensitivity analysis

---

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

- **Random variables**
- **Computational model**
- **Distribution**
  - Mean, std. deviation
  - Probability of failure

**Step C’**
Sensitivity analysis

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

Random variables
Computational model
Distribution
Mean, std. deviation
Probability of failure

Step C'
Sensitivity analysis

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

Random variables

Computational model

Distribution
Mean, std. deviation
Probability of failure

**Step C’**
Sensitivity analysis

Outline

1. Polynomial chaos expansions
   - Polynomial chaos basis
   - Computation of the expansion coefficients
   - Error estimation and validation

2. Application to sensitivity analysis
   - Sobol’ indices
   - PC-based Sobol’ indices

3. Application examples
   - Ishigami function
   - Morris function
   - Marelli function
The input parameters are modelled by a random vector $X$ over a probabilistic space $(\Omega, \mathcal{F}, P)$ such that $P(dx) = f_X(x) \, dx$

The response random vector $Y = M(X)$ is considered as an element of $L^2(\Omega, \mathcal{F}, P)$

A basis of multivariate orthogonal polynomials is built up with respect to the input PDF (assuming independent components)

The response random vector $Y$ is completely determined by its coordinates in this basis
Spectral approach

- The input parameters are modelled by a random vector $X$ over a probabilistic space $(\Omega, \mathcal{F}, \mathbb{P})$ such that $\mathbb{P}(dx) = f_X(x) \, dx$

- The response random vector $Y = \mathcal{M}(X)$ is considered as an element of $L^2(\Omega, \mathcal{F}, \mathbb{P})$

- A basis of multivariate orthogonal polynomials is built up with respect to the input PDF (assuming independent components)

- The response random vector $Y$ is completely determined by its coordinates in this basis
Spectral approach

- The input parameters are modelled by a random vector $X$ over a probabilistic space $(\Omega, \mathcal{F}, \mathbb{P})$ such that $\mathbb{P}(d\mathbf{x}) = f_X(x) \, dx$

- The response random vector $Y = \mathcal{M}(X)$ is considered as an element of $L^2(\Omega, \mathcal{F}, \mathbb{P})$

- A basis of multivariate orthogonal polynomials is built up with respect to the input PDF (assuming independent components)

- The response random vector $Y$ is completely determined by its coordinates in this basis

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

where:

- $y_{\alpha}$: coefficients to be computed (coordinates)
- $\Psi_{\alpha}(X)$: basis
Univariate orthogonal polynomials

For each marginal distribution \( f_{X_i}(x_i) \) one can define a functional inner product:

\[
\langle \phi_1, \phi_2 \rangle_i = \int_{D_i} \phi_1(x) \phi_2(x) f_{X_i}(x_i) \, dx_i
\]

and a family of orthogonal polynomials \( \{P_k^{(i)} \}, \ k \in \mathbb{N} \} \) such that:

\[
\langle P_j^{(i)}, P_k^{(i)} \rangle = \int P_j^{(i)}(x) P_k^{(i)}(x) f_{X_i}(x) \, dx = a_i^j \delta_{jk}
\]

Classical families

<table>
<thead>
<tr>
<th>Type of variable</th>
<th>Weight function</th>
<th>Orthogonal polynomials</th>
<th>Hilbertian basis ( \psi_k(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>([-1,1]) ( f(x)/2 )</td>
<td>Legendre ( P_k(x) )</td>
<td>( P_k(x)/\sqrt{2k+1} )</td>
</tr>
<tr>
<td>Gaussian</td>
<td>( \frac{1}{\sqrt{2\pi}} e^{-x^2/2} )</td>
<td>Hermite ( H_{c_k}(x) )</td>
<td>( H_{c_k}(x)/\sqrt{k!} )</td>
</tr>
<tr>
<td>Gamma</td>
<td>( x^a e^{-x} 1_{\mathbb{R}^+}(x) )</td>
<td>Laguerre ( L_k^a(x) )</td>
<td>( L_k^a(x)/\sqrt{\Gamma(k+a+1)/k!} )</td>
</tr>
<tr>
<td>Beta</td>
<td>([-1,1]) ( (1-x)^a (1+x)^b )</td>
<td>Jacobi ( J_k^{a,b}(x) )</td>
<td>( J_k^{a,b}(x)/\Gamma(a,b,1) )</td>
</tr>
</tbody>
</table>

\( \delta_{jk} \) is the Kronecker delta, \( \psi_k(x) \) is the Hilbertian basis, and \( \Gamma \) is the gamma function.
Univariate orthogonal polynomials

For each marginal distribution \( f_{X_i}(x_i) \) one can define a functional inner product:

\[
\langle \phi_1, \phi_2 \rangle_i = \int_{D_i} \phi_1(x) \phi_2(x) f_{X_i}(x_i) \, dx_i
\]

and a family of orthogonal polynomials \( \{P^{(i)}_k, k \in \mathbb{N}\} \) such that:

\[
\langle P^{(i)}_j, P^{(i)}_k \rangle = \int P^{(i)}_j(x) P^{(i)}_k(x) f_{X_i}(x) \, dx = a^i_j \delta_{jk}
\]

### Classical families

<table>
<thead>
<tr>
<th>Type of variable</th>
<th>Weight function</th>
<th>Orthogonal polynomials</th>
<th>Hilbertian basis ( \psi_k(x) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniform</td>
<td>([-1, 1]), (e^{-x^2}/2)</td>
<td>Legendre (P_k(x))</td>
<td>(P_k(x)/\sqrt{2k+1})</td>
</tr>
<tr>
<td>Gaussian</td>
<td>(x^a e^{-x^2}/2)</td>
<td>Hermite (H_{ek}(x))</td>
<td>(H_{ek}(x)/\sqrt{k!})</td>
</tr>
<tr>
<td>Gamma</td>
<td>(x^a \cdot 1_{\mathbb{R}^+}(x))</td>
<td>Laguerre (L^a_k(x))</td>
<td>(L^a_k(x)/\sqrt{\Gamma(k+a+1)/k!})</td>
</tr>
<tr>
<td>Beta</td>
<td>([-1, 1]), ((1-x)^a (1+x)^b/B(a)/B(b))</td>
<td>Jacobi (J_{a,b}^k(x))</td>
<td>(J_{a,b}^k(x)/3^{a,b,k})</td>
</tr>
</tbody>
</table>

\(3^{a,b,k} = 2^{a+b+1}(k+a+1)(k+b+1)/(k+a+b+1)(k+1)\)
Multivariate polynomials

Let us define the multi-indices (tuples) $\alpha = \{\alpha_1, \ldots, \alpha_M\}$, of degree

$$|\alpha| = \sum_{i=1}^{M} \alpha_i.$$ 

The associated multivariate polynomial reads:

$$\Psi_\alpha(x) = \prod_{i=1}^{M} P^{(i)}_{\alpha_i}(x_i).$$

Orthonormality of the basis

$$\mathbb{E}[\Psi_\alpha(X)\Psi_\beta(X)] = \delta_{\alpha\beta} \quad (\text{Kronecker symbol: } \delta_{\alpha\beta} = 1 \text{ if } \alpha = \beta, \ 0 \text{ otherwise})$$

The set of multivariate polynomials $\{\Psi_\alpha, \alpha \in \mathbb{N}^M\}$ forms a basis of the space of second order variables:

$$Y = \sum_{\alpha \in \mathbb{N}^M} y_\alpha \Psi_\alpha(X)$$
The input random variables are first transformed into reduced variables (e.g. standard normal variables $\mathcal{N}(0, 1)$, uniform variables on $[-1,1]$, etc.):

$$X = \mathcal{T}(\xi) \quad \text{dim} \xi = M \quad \text{(isoprobabilistic transform)}$$

The model response is cast as a function of the reduced variables and expanded:

$$Y = \mathcal{M}(X) = \mathcal{M} \circ \mathcal{T}(\xi) = \sum_{\alpha \in \mathbb{N}^M} y_{\alpha} \Psi_\alpha(\xi)$$

A truncation scheme is selected and the associated finite set of multi-indices is generated, e.g.:

$$\mathcal{A}^{M,p} = \{ \alpha \in \mathbb{N}^M : |\alpha| \leq p \} \quad \text{card } \mathcal{A}^{M,p} \equiv P = \binom{M + p}{p}$$
Application example (1)

Computational model

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

Probabilistic model

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

Isoprobabilistic transform

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

Hermite polynomials

- Recurrence:

\[
\begin{align*}
H_{-1}(x) &= H_0(x) = 1 \\
H_{n+1}(x) &= x H_n(x) - n H_{n-1}(x)
\end{align*}
\]

where \( ||H_n||^2 = n! \)

- First (normalized) polynomials:

\[
\begin{align*}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= (x^2 - 1)/\sqrt{2} \\
P_3(x) &= (x^3 - 3x)/\sqrt{6}
\end{align*}
\]
Truncature scheme

Consider all multivariate polynomials of total degree \( |\alpha| = \sum_{i=1}^{M} \alpha_i \) less than or equal to \( p \).
Third order truncature $p = 3$

All the polynomials of $\xi_1, \xi_2$ that are product of univariate Hermite 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>$\Psi_2 = \xi_2$</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>$\Psi_4 = \xi_1 \xi_2$</td>
</tr>
<tr>
<td>5</td>
<td>[0, 2]</td>
<td>$\Psi_5 = (\xi_2^2 - 1)/\sqrt{2}$</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>$\Psi_7 = (\xi_1^2 - 1)\xi_2/\sqrt{2}$</td>
</tr>
<tr>
<td>8</td>
<td>[1, 2]</td>
<td>$\Psi_8 = (\xi_2^2 - 1)\xi_1/\sqrt{2}$</td>
</tr>
<tr>
<td>9</td>
<td>[0, 3]</td>
<td>$\Psi_9 = (\xi_2^3 - 3\xi_2)/\sqrt{6}$</td>
</tr>
</tbody>
</table>

$\tilde{Y} \equiv M_{PC}(\xi_1, \xi_2) = y_0 + y_1 \xi_1 + y_2 \xi_2 + y_3 (\xi_1^2 - 1)/\sqrt{2} + y_4 \xi_1 \xi_2 + y_5 (\xi_2^2 - 1)/\sqrt{2} + y_6 (\xi_1^3 - 3\xi_1)/\sqrt{6} + y_7 (\xi_1^2 - 1)\xi_2/\sqrt{2} + y_8 (\xi_2^2 - 1)\xi_1/\sqrt{2} + y_9 (\xi_2^3 - 3\xi_2)/\sqrt{6}$
Outline

1. Polynomial chaos expansions
   - Polynomial chaos basis
   - Computation of the expansion coefficients
   - Error estimation and validation

2. Application to sensitivity analysis

3. Application examples
Various methods for computing the coefficients

Intrusive approaches

- Historical approaches: projection of the equations residuals in the Galerkin sense


- Proper generalized decompositions

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
  - Stochastic collocation
  - Least-square minimization

Nouy, 2007-2010
**Statistical approach: least-square minimization**

**Principle**

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

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

where : \( Y = \{y_0, \ldots, y_{P-1}\} \)

\( \Psi(x) = \{\Psi_0(x), \ldots, \Psi_{P-1}(x)\} \)
Least-Square Minimization: continuous solution

Least-square minimization

The unknown coefficients are gathered into a vector \( \hat{Y} = \{ y_\alpha, \alpha \in A \} \), and computed by minimizing the mean square error:

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

Analytical solution (continuous case)

The least-square minimization problem may be solved analytically:

\[
\hat{y}_\alpha = E \left[ M(X) \Psi_\alpha(X) \right] \quad \forall \alpha \in A
\]

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

Resolution

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

\[
\hat{Y}_{L.S} = \arg \min \hat{E} \left[ (Y^{T} \Psi(X) - M(X))^2 \right]
\]

\[
= \arg \min \frac{1}{n} \sum_{i=1}^{n} (Y^{T} \Psi(x^{(i)}) - M(x^{(i)}))^2
\]
Least-Square Minimization: procedure

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

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

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

- Solve the least-square minimization problem
  \[ \hat{Y} = (A^T A)^{-1} A^T \mathcal{M} \]
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 ED

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

The thumb rule $n = k P$ where $k = 2 - 3$ is used
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 ED

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

The thumb rule \( n = kP \) where \( k = 2 \rightarrow 3 \) is used
1. Polynomial chaos expansions
   - Polynomial chaos basis
   - Computation of the expansion coefficients
   - Error estimation and validation

2. Application to sensitivity analysis

3. Application examples
The truncated series expansions are convergent in the mean square sense. However one does not know in advance where to truncate (problem-dependent).

Most people truncate the series according to the total maximal degree of the polynomials, say \( p=2,3,4, \text{ etc.} \). Several values of \( p \) are tested until some kind of convergence is “empirically” observed.

The recent research deals with the development of error estimates:

- adaptive integration in the projection approach
- cross validation in the least-square minimization approach
The least-squares technique is based on the minimization of the mean square error. The generalization error is defined as:

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

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

It may be estimated by the empirical error using the already computed response quantities:

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

The coefficient of determination \( R^2 \) is often used as an error estimator:

\[ R^2 = 1 - \frac{E_{\text{emp}}}{\text{Var}[Y]} \]

\[ \text{Var}[Y] = \frac{1}{n} (\mathcal{M}(x^{(i)}) - \bar{Y})^2 \]

This error estimator leads to overfitting.
Error estimators
Leave-one-out cross validation

Principle

- In statistical learning theory, cross validation consists in splitting the experimental design $\mathcal{Y}$ into two parts, namely a *training set* (which is used to build the model) and a *validation set*.

- The leave-one-out technique consists in using each point of the experimental design as a single validation point for the meta-model built from the remaining $n - 1$ points.

- $n$ different meta-models are built and the error made on the remaining point is computed, then mean-square averaged.
Cross validation
Implementation

- For each $x^{(i)}$, a polynomial chaos expansion is built using the following experimental design: $\mathcal{X}\backslash x^{(i)} = \{x^{(j)} , j = 1, \ldots, n, j \neq i\}$, denoted by $\mathcal{M}^{PC\backslash i}(.)$.
- The predicted residual is computed in point $x^{(i)}$:

$$\Delta_i = \mathcal{M}(x^{(i)}) - \mathcal{M}^{PC\backslash i}(x^{(i)})$$

- The PRESS coefficient (predicted residual sum of squares) is evaluated:

$$PRESS = \sum_{i=1}^{n} \Delta_i^2$$

- The leave-one-out error and related $Q^2$ error estimator are computed:

$$E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \Delta_i^2 \quad Q^2 = 1 - \frac{E_{LOO}}{\text{Var}[Y]}$$
In practice one does not need to explicitly derive the $n$ different models $M^{PC\setminus i}(\cdot)$.

- In contrast, a single least-square analysis using the full ED is carried out. The predicted residual reads:

$$\Delta_i = M(x^{(i)}) - M^{PC\setminus i}(x^{(i)}) = \frac{M(x^{(i)}) - M^{PC}(x^{(i)})}{1 - h_i}$$

where $h_i$ is the $i$-th diagonal term of matrix $A(A^TA)^{-1}A^T$, where:

$$A_{ij} = \Psi_j(x^{(i)})$$

- Thus:

$$E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \left( \frac{M(x^{(i)}) - M^{PC}(x^{(i)})}{1 - h_i} \right)^2$$
Sparse PC expansions

- The LOO error allows one to assess a posteriori the accuracy of a given expansion
- Adaptive algorithms may be used based on a target accuracy
- Other truncation schemes (e.g. hyperbolic) may be used to decrease the computational cost
- The Least Angle regression algorithm allows one to compute sparse expansion within a candidate set of polynomials

Sparse expansions allows one to address problems of dimension $M = 20 - 500$
Outline

1. Polynomial chaos expansions

2. Application to sensitivity analysis
   - Sobol’ indices
   - PC-based Sobol’ indices

3. Application examples
Sensitivity analysis

Sobol’ decomposition

- Sensitivity analysis aims at quantifying what are the input parameters (or combinations thereof) that influence the most the response variability.
- Global sensitivity analysis relies on so-called variance decomposition techniques.

Consider a model $\mathcal{M} : x \in [0, 1]^M \rightarrow \mathcal{M}(x) \in \mathbb{R}$. The Hoeffding-Sobol’ decomposition reads:

$$
\mathcal{M}(x) = \mathcal{M}_0 + \sum_{i=1}^{M} \mathcal{M}_i(x_i) + \sum_{1 \leq i < j \leq M} \mathcal{M}_{ij}(x_i, x_j) + \cdots + \mathcal{M}_{12...M}(x)
$$

where:
- $\mathcal{M}_0$ is the mean value of the function
- $\mathcal{M}_i(x_i)$ are univariate functions
- $\mathcal{M}_{ij}(x_i, x_j)$ are bivariate functions
- etc.
Sobol’ decomposition

Properties

- The functional decomposition is **unique** if the orthogonality of the terms (with respect to the uniform measure) is imposed \([0, 1]^M\), i.e. \(\{i_1, \ldots, i_s\} \neq \{j_1, \ldots, j_t\}\):

\[
\int_{[0,1]^M} M_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) M_{j_1 \ldots j_t}(x_{j_1}, \ldots, x_{j_t}) \, dx = 0
\]

- A construction definition of the terms is obtained by recurrence:

\[
M_i(x_i) = \int_{[0,1]^{M-1}} M(x) \, dx_{\sim i} - M_0
\]

\[
M_{ij}(x_i, x_j) = \int_{[0,1]^{M-2}} M(x) \, dx_{\sim \{ij\}} - M_i(x_i) - M_j(x_j) + M_0
\]

where \(\int_{[0,1]^{M-1}} (\cdot) \, dx_{\sim i}\) denoted the integration over all variables except for the \(i\)-th one.
Sobol’ indices

Variance decomposition

- Assume $X_i \sim \mathcal{U}(0, 1), \ i = 1, \ldots, M$ (possibly after some isoprobabilistic transform)

- Due to the orthogonality of the decomposition:

$$D \equiv \text{Var} [\mathcal{M}(\mathbf{X})] = \mathbb{E} \left[ (\mathcal{M}(\mathbf{X}) - \mathcal{M}_0)^2 \right]$$

$$= \mathbb{E} \left[ \left( \sum_{\{i_1, \ldots, i_s\} \subset \{1, \ldots, M\}} \mathcal{M}_{i_1 \ldots i_s}(X_{i_1}, \ldots, X_{i_s}) \right)^2 \right]$$

$$= \sum_{\{i_1, \ldots, i_s\} \subset \{1, \ldots, M\}} \mathbb{E} \left[ \mathcal{M}_{i_1 \ldots i_s}^2(X_{i_1}, \ldots, X_{i_s}) \right]$$
Partial variance

- Consider:

\[ D_{i_1 \ldots i_s} = \int_{[0,1]^s} M^2_{i_1 \ldots i_s}(x_{i_1}, \ldots, x_{i_s}) \, dx_{i_1} \ldots dx_{i_s} \]

- Then:

\[ D \equiv \text{Var} [Y] = \sum_{i=1}^{M} D_{i} + \sum_{1 \leq i < j \leq M} D_{ij} + \ldots + D_{12\ldots M} \]

- The *Sobol' indices* are obtained by normalization:

\[ S_{i_1 \ldots i_s} = \frac{D_{i_1 \ldots i_s}}{D} \]

They represent the fraction of the total variance \( \text{Var} [Y] \) that can be attributed to each input variable \( i \) (\( S_i \)) or combinations of variables \( \{i_1 \ldots i_s\} \).
First order and total Sobol’ indices

First order Sobol’ indices

\[ S_i = \frac{D_i}{D} \quad D_i = \text{Var}_{X_i} [M_i(X)] = \text{Var}_{X_i} [\mathbb{E} [M(X)|X_i = x_i]] \]

They quantify the (additive) effect of each input parameter separately, i.e. the reduction of variance to expect if \( X_i \) is set equal to \( x_i \)

Total Sobol’ indices

\[ S_i^T \overset{\text{def}}{=} \sum_{i \subseteq \{i_1 \ldots i_s\}} S_{i_1 \ldots i_s} \]

They quantify the total effect of \( X_i \) including the first order effect and the interactions with the other variables.
Outline

1. Polynomial chaos expansions

2. Application to sensitivity analysis
   - Sobol’ indices
   - PC-based Sobol’ indices

3. Application examples
Consider $Y = \mathcal{M}(X)$ where $X \sim f_X$ with independent components:

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

- Due to the orthogonality properties of the polynomial chaos basis, one gets:

$$\mathbb{E} [\Psi_{\alpha}(X)] = 0 \quad \mathbb{E} [\Psi_{\alpha}(X) \Psi_{\beta}(X)] = \delta_{\alpha\beta}$$

- Thus the mean and variance:

$$M_0 = \mathbb{E} [\mathcal{M}(X)] = y_0$$

$$D = \text{Var} [\mathcal{M}(X)] = \sum_{\substack{\alpha \in \mathbb{N}^M \\alpha \neq 0}} y_{\alpha}^2$$
**Interaction sets**

Let $\mathcal{A}_u$ be the set of multi-indices depending \textbf{exactly} on the subset of variables $u = \{i_1, \ldots, i_s\}$:

$$\mathcal{A}_u = \left\{ \alpha \in \mathbb{N}^M : k \in u \Leftrightarrow \alpha_k \neq 0 \right\} \bigcup_{u \subset \{1, \ldots, M\}} \mathcal{A}_u = \mathbb{N}^M$$

**Sobol’ decomposition**

By unicity of the Sobol’ decomposition one gets ($x_u \overset{\text{def}}{=} \{x_{i_1}, \ldots, x_{i_s}\}$):

$$\mathcal{M}(x) = \mathcal{M}_0 + \sum_{u \subset \{1, \ldots, M\}} \mathcal{M}_u(x_u)$$

where:

$$\mathcal{M}_u(x_u) \overset{\text{def}}{=} \sum_{\alpha \in \mathcal{A}_u} y_\alpha \Psi_\alpha(x)$$
Partial variances

The partial variances $D_u \overset{\text{def}}{=} D_{i_1...i_s} = \text{Var} \left[ M_u(X) \right]$ are obtained by summing up the square of selected PC coefficients.

First order contribution

$$D_i = \sum_{\alpha \in A_i} y_\alpha^2$$

$$A_i = \left\{ \alpha \in \mathbb{N}^M : \alpha_i > 0, \alpha_j \neq i = 0 \right\}$$

Higher order contribution

$$D_u = \sum_{\alpha \in A_u} y_\alpha^2$$

$$A_{i_1...i_s} = \left\{ \alpha \in \mathbb{N}^M : k \in u \Leftrightarrow \alpha_k > 0 \right\}$$

The Sobol’ indices come after normalization:

$$S_u = \frac{D_u}{D}$$
**Sobol’ decomposition from PC expansions**

Sudret (2006-08) ; Blatman & S. (2010)

First order indices

\[
S_i = \sum_{\alpha \in \mathcal{A}_i} y_{\alpha}^2 / D \\
\mathcal{A}_i = \{ \alpha \in \mathbb{N}^M : \alpha_i > 0, \alpha_j \neq i = 0 \}
\]

Higher order indices

\[
S_{i_1, \ldots, i_s} = \sum_{\alpha \in \mathcal{A}_{i_1, \ldots, i_s}} y_{\alpha}^2 / D \\
\mathcal{A}_{i_1, \ldots, i_s} = \{ \alpha \in \mathbb{N}^M : k \in \{i_1, \ldots, i_s\} \Leftrightarrow \alpha_j \neq 0 \}
\]

Total indices

\[
S_{i}^T = \sum_{\alpha \in \mathcal{A}_{i}^T} y_{\alpha}^2 / D \\
\mathcal{A}_{i}^T = \{ \alpha \in \mathbb{N}^M : \alpha_i > 0 \}
\]
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

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

<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 = \xi_2 )</td>
</tr>
<tr>
<td>3</td>
<td>[2, 0]</td>
<td>( \Psi_3 = (\xi_2^2 - 1)/\sqrt{2} )</td>
</tr>
<tr>
<td>4</td>
<td>[1, 1]</td>
<td>( \Psi_4 = \xi_1 \xi_2 )</td>
</tr>
<tr>
<td>5</td>
<td>[0, 2]</td>
<td>( \Psi_5 = (\xi_2^2 - 1)/\sqrt{2} )</td>
</tr>
<tr>
<td>6</td>
<td>[3, 0]</td>
<td>( \Psi_6 = (\xi_2^3 - 3\xi_1)/\sqrt{6} )</td>
</tr>
<tr>
<td>7</td>
<td>[2, 1]</td>
<td>( \Psi_7 = (\xi_2^2 - 1)\xi_2/\sqrt{2} )</td>
</tr>
<tr>
<td>8</td>
<td>[1, 2]</td>
<td>( \Psi_8 = (\xi_2^2 - 1)\xi_1/\sqrt{2} )</td>
</tr>
<tr>
<td>9</td>
<td>[0, 3]</td>
<td>( \Psi_9 = (\xi_2^3 - 3\xi_2)/\sqrt{6} )</td>
</tr>
</tbody>
</table>

Variance

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

Sobol' indices

\[ S_1 = \frac{(y_1^2 + y_3^2 + y_6^2)}{D} \]
\[ S_2 = \frac{(y_2^2 + y_5^2 + y_9^2)}{D} \]
\[ S_{12} = \frac{(y_4^2 + y_7^2 + y_8^2)}{D} \]
Outline

1. Polynomial chaos expansions
2. Application to sensitivity analysis
3. Application examples
   - Ishigami function
   - Morris function
   - Marelli function
Ishigami function

Definition

\[ Y = \sin X_1 + a \sin^2 X_2 + b X_3^4 \sin X_1 \quad a = 7, \ b = 0.1 \]

where \( X_i \sim \mathcal{U}[-\pi, \pi] \) are independent uniform random variables

Analytical solution

\[ D = \frac{a^2}{8} + \frac{b \pi^4}{5} + \frac{b^2 \pi^8}{18} + \frac{1}{2} \]
\[ D_1 = \frac{b \pi^4}{5} + \frac{b^2 \pi^8}{50} + \frac{1}{2}, \quad D_2 = \frac{a^2}{8}, \quad D_3 = 0 \]
\[ D_{12} = D_{23} = 0, \quad D_{13} = \frac{8 b^2 \pi^8}{225}, \quad D_{123} = 0 \]
First order Sobol' indices

![Graph showing first order Sobol' indices](image)

<table>
<thead>
<tr>
<th>Index</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_1$</td>
<td>0.3138</td>
</tr>
<tr>
<td>$S_2$</td>
<td>0.4424</td>
</tr>
<tr>
<td>$S_3$</td>
<td>0</td>
</tr>
<tr>
<td>$S_{12}$</td>
<td>0</td>
</tr>
<tr>
<td>$S_{13}$</td>
<td>0.2436</td>
</tr>
<tr>
<td>$S_{23}$</td>
<td>0</td>
</tr>
</tbody>
</table>
First order Sobol’ indices

Sample size $N$

<table>
<thead>
<tr>
<th>$S_i - S_i^{(ref)}$</th>
</tr>
</thead>
</table>

$S_1$ (MCS)
$S_1$ (PC)
$S_2$ (MCS)
$S_2$ (PC)
$S_{13}$ (MCS)
$S_{13}$ (PC)
Total Sobol’ indices

![Graph showing total Sobol’ indices vs sample size.](image)

The graph illustrates the total Sobol’ indices ($S^T_i$) for different functions and sample sizes. The y-axis represents the Sobol’ indices, and the x-axis represents the sample size (N) ranging from 100 to 100,000. The different lines correspond to different functions and methods, such as MCS (Monte Carlo Simulation) and PC (Polynomial Chaos).
Total Sobol’ indices – small design and replication
Morris function

Definition

\[ Y = \beta_0 + \sum_{i=1}^{20} \beta_i w_i + \sum_{i<j}^{20} \beta_{ij} w_i w_j + \sum_{i<j<l}^{20} \beta_{ijl} w_i w_j w_l + \sum_{i<j<l<s}^{20} \beta_{ijls} w_i w_j w_l w_s \]

where:

\[ w_i = \begin{cases} 
2 \left(1.1 X_i / (X_i + 0.1) - 0.5\right) & \text{if } i = 3, 5, 7 \\
2 (X_i - 0.5) & \text{otherwise}
\end{cases} \]

and:

\[ X_i \sim \mathcal{U}(0, 1) \]

\[ \begin{align*}
\beta_i & = 20 & \text{for } i = 1, \ldots, 10 \\
\beta_{ij} & = -15 & \text{for } i = 1, \ldots, 6 \\
\beta_{ijl} & = -10 & \text{for } i = 1, \ldots, 5 \\
\beta_{ijls} & = 5 & \text{for } i = 1, \ldots, 4
\end{align*} \]

\[ \text{and } \beta_i = (-1)^i \text{ otherwise} \]

\[ \text{and } \beta_{ij} = (-1)^{i+j} \text{ otherwise} \]

\[ \text{and } \beta_{ijl} = 0 \text{ otherwise} \]

\[ \text{and } \beta_{ijls} = 0 \text{ otherwise} \]
Morris function

Sensitivity results

- Reference: \( N = 440,000 \) Monte Carlo simulations + bootstrap
- Adaptive sparse PC: \( Q^2_{tgt} = 0.9 \) (resp. 0.99)
## Morris function

### Sparsity of the model

<table>
<thead>
<tr>
<th>Sensitivity indices</th>
<th>Sparse PCE</th>
<th>$Q_{\text{ISR}}^2 = 0.9$</th>
<th>$Q_{\text{ISR}}^2 = 0.99$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_4^7$</td>
<td>0.26</td>
<td>0.25</td>
<td></td>
</tr>
<tr>
<td>$S_5^3$</td>
<td>0.25</td>
<td>0.25</td>
<td></td>
</tr>
<tr>
<td>$S_6^2$</td>
<td>0.24</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>$S_7^0$</td>
<td>0.16</td>
<td>0.15</td>
<td></td>
</tr>
<tr>
<td>$S_8^1$</td>
<td>0.10</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>$S_9^2$</td>
<td>0.08</td>
<td>0.10</td>
<td></td>
</tr>
<tr>
<td>$S_{10}^1$</td>
<td>0.11</td>
<td>0.10</td>
<td></td>
</tr>
<tr>
<td>$S_{11}^0$</td>
<td>0.10</td>
<td>0.11</td>
<td></td>
</tr>
<tr>
<td>$S_{12}^0$</td>
<td>0.10</td>
<td>0.09</td>
<td></td>
</tr>
<tr>
<td>$S_{13}^0$</td>
<td>0.08</td>
<td>0.07</td>
<td></td>
</tr>
</tbody>
</table>

- **Full chaos:**
  \[ \text{card } \mathcal{A}_{20,11} = \binom{20+11}{11} = 84,672,315 \]

- **Hyperbolic truncature:**
  \[ \text{card } \mathcal{A}_{0.4}^{20,11} = 4,234 \]

LAR: 339 terms ($\text{IS}2 = 8\%$)
High dimensional example

Definition

\[
Y = 3 - \frac{5}{M} \sum_{k=1}^{M} kX_k + \frac{1}{M} \sum_{k=1}^{M} kX_k^3 + \ln \left( \frac{1}{3M} \sum_{k=1}^{M} k \left( X_k^2 + X_k^4 \right) \right) \\
+ X_1X_2^2 - X_5X_3 + X_2X_4 + X_{50} + X_{50}X_{54}^2
\]

- \( X \sim \mathcal{U}([1, 2])^M \), with \( X_{20} \in \mathcal{U}([1, 3]) \)
- Strongly non-linear
- Continuous and smooth function
- Well-located peaks in the sensitivity indices \( (X_2, X_{20}, X_{50}, X_{54}) \)
- Interactions: \( (X_1, X_2), (X_{50}, X_{54}) \)
Reference results

- Model response
- Total Sobol’ indices
- Second Order Sobol’ indices
Reference results

- Model response
- **Total Sobol’ indices**
- Second Order Sobol’ indices
Reference results

- Model response
- Total Sobol' indices
- **Second Order Sobol' indices**
Total Sobol' indices

PCE-based
(1200 model runs)

MCS-based
(1,760,000 model runs)
Conclusions

- Polynomial chaos expansions are a powerful technique for building surrogate models used in uncertainty quantification.
- They can be post-processed for moment- and sensitivity analysis straightforwardly. Sobol’ indices are obtained as a sum of squares of expansions coefficients.
- Sparse expansions can be obtained at an affordable cost for high-dimensional problems and used for screening purpose.
- Extensions for sensitivity problems with correlated inputs and to derivative-based sensitivity measures have been proposed.

Thank you very much for your attention!
Conclusions

- Polynomial chaos expansions are a powerful technique for building surrogate models used in uncertainty quantification.

- They can be post-processed for moment- and sensitivity analysis straightforwardly. Sobol’ indices are obtained as a sum of squares of expansions coefficients.

- Sparse expansions can be obtained at an affordable cost for high-dimensional problems and used for screening purpose.

- Extensions for sensitivity problems with correlated inputs and to derivative-based sensitivity measures have been proposed.

Thank you very much for your attention!

UQLab ...

... The Uncertainty Quantification Toolbox in Matlab