ETH zürich

ETH Library

Computational methods for uncertainty quantification and sensitivity analysis of complex systems

Labex MS2T - Seminar February 14th, 2013 Université Technologique de Compiègne

Presentation

Author(s):
Sudret, Bruno

Publication date:
2013

Permanent link:
https://doi.org/10.3929/ethz-a-010060753

Rights / license:
In Copyright - Non-Commercial Use Permitted

This page was generated automatically upon download from the ETH Zurich Research Collection.
For more information, please consult the Terms of use.

DEPARTMENT OF CIVIL, ENVIRONMENTAL AND GEOMATIC ENGINEERING
CHAIR OF RISK, SAFETY & UNCERTAINTY QUANTIFICATION

Computational methods for uncertainty quantification and sensitivity analysis of complex systems

B. Sudret

Labex MS2T - Université Technologique de Compiègne

Outline

1. Introduction to uncertainty quantification
2. Polynomial chaos expansions
   - Polynomial chaos basis
   - Computing the coefficients
   - Post-processing
3. Sensitivity analysis in multiscale problems
   - Single model / independent variables
   - Imbricated models: the issue of correlation
   - Distribution-based sensitivity indices
   - Covariance-based sensitivity indices
4. Application example
   - Mechanical example: composite beam
   - Tolerance analysis

Some common engineering structures

Cattenom nuclear power plant (France)

Cormet de Roselend dam (France)

Military satellite

Airbus A380

Bladed disk

Computational models

- Modern engineering has to address problems of increasing complexity in various fields including infrastructures (civil engineering), energy (civil/mechanical engineering), aeronautics, defense, etc.

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

  - a mathematical description of the physics (*e.g.* mechanics, acoustics, heat transfer, electromagnetism, etc.)

  - numerical algorithms that solve the resulting set of (*e.g.* partial differential) equations: finite element-, finite difference-, finite volume- methods, boundary element methods)

Computational models

Simulation models are calibrated and validated through comparison with lab experiments and *in situ* / full scale measurements. Once they are validated, these models may be run with different sets of input parameters in order to:

- explore the design space at low cost
- optimize the system w.r.t to cost criteria
- assess the robustness of the system w.r.t. uncertainties

Sources of uncertainty

- Differences between the designed and the real system in terms of material/physical properties and dimensions (tolerancing)
- Unforecast exposures: exceptional service loads, natural hazards (earthquakes, floods), climate loads (hurricanes, snow storms, etc.)

Global framework for managing uncertainties

Step B

Quantification of sources of uncertainty

Step A

Model(s) of the system

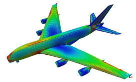
Assessment criteria

Step C

Uncertainty propagation

Random variables

Computational model



Moments

Probability of failure

Response PDF

Step C'

Sensitivity analysis

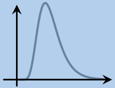
Global framework for managing uncertainties

Step B
Quantification of sources of uncertainty

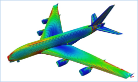
Step A
Model(s) of the system
Assessment criteria

Step C
Uncertainty propagation

Random variables



Computational model



Moments
Probability of failure
Response PDF

Step C'
Sensitivity analysis

Global framework for managing uncertainties

Step B

Quantification of sources of uncertainty

Step A

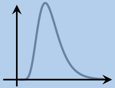
Model(s) of the system

Assessment criteria

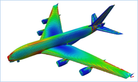
Step C

Uncertainty propagation

Random variables



Computational model



Moments

Probability of failure

Response PDF

Step C'

Sensitivity analysis

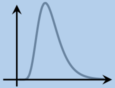
Global framework for managing uncertainties

Step B
Quantification of sources of uncertainty

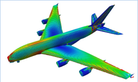
Step A
Model(s) of the system
Assessment criteria

Step C
Uncertainty propagation

Random variables



Computational model



Moments
Probability of failure
Response PDF

Step C'
Sensitivity analysis

Step A: computational models (civil & mechanical engineering)

Vector of input parameters $\boldsymbol{x} \in \mathbb{R}^M$	Computational model $\mathcal{M}$	Model response $\boldsymbol{y} = \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}^N$

- geometry
- material properties
- loading

- analytical formula
- finite element model
- etc.

- displacements
- strains, stresses
- temperature, etc.

Step A: computational models (civil & mechanical engineering)

Vector of input parameters $\boldsymbol{x} \in \mathbb{R}^M$	Computational model $\mathcal{M}$	Model response $\boldsymbol{y} = \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}^N$
• geometry • material properties • loading	• analytical formula • finite element model • etc.	• displacements • strains, stresses • temperature, etc.

Step B: probabilistic models of input parameters

No data exist

- expert judgment for selecting the input PDF's of $\boldsymbol{X}$
- literature, data bases (*e.g.* on material properties)
- maximum entropy principle

Input data exist

- classical statistical inference
- Bayesian statistics when data is scarce but there is some prior information

Data on output quantities

- inverse probabilistic methods and Bayesian updating techniques

Step B: probabilistic models of input parameters

No data exist

- expert judgment for selecting the input PDF's of $\boldsymbol{X}$
- literature, data bases (*e.g.* on material properties)
- maximum entropy principle

Input data exist

- classical statistical inference
- Bayesian statistics when data is scarce but there is some prior information

Data on output quantities

- inverse probabilistic methods and Bayesian updating techniques

Step B: probabilistic models of input parameters

No data exist

- expert judgment for selecting the input PDF's of $\boldsymbol{X}$
- literature, data bases (*e.g.* on material properties)
- maximum entropy principle

Input data exist

- classical statistical inference
- Bayesian statistics when data is scarce but there is some prior information

Data on output quantities

- inverse probabilistic methods and Bayesian updating techniques

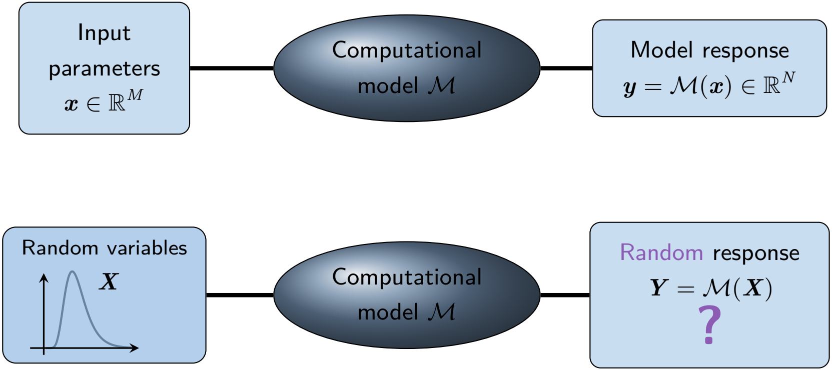
Step C: principles of uncertainty propagation

Input parameters $\boldsymbol{x} \in \mathbb{R}^M$ — Computational model $\mathcal{M}$ — Model response $\boldsymbol{y} = \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}^N$

Random variables $\boldsymbol{X}$

— Computational model $\mathcal{M}$ — Random response $\boldsymbol{Y} = \mathcal{M}(\boldsymbol{X})$?

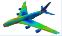
Step C: principles of uncertainty propagation



Step C: uncertainty propagation methods

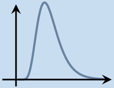
Computational model

Step A



Probabilistic model

Step B



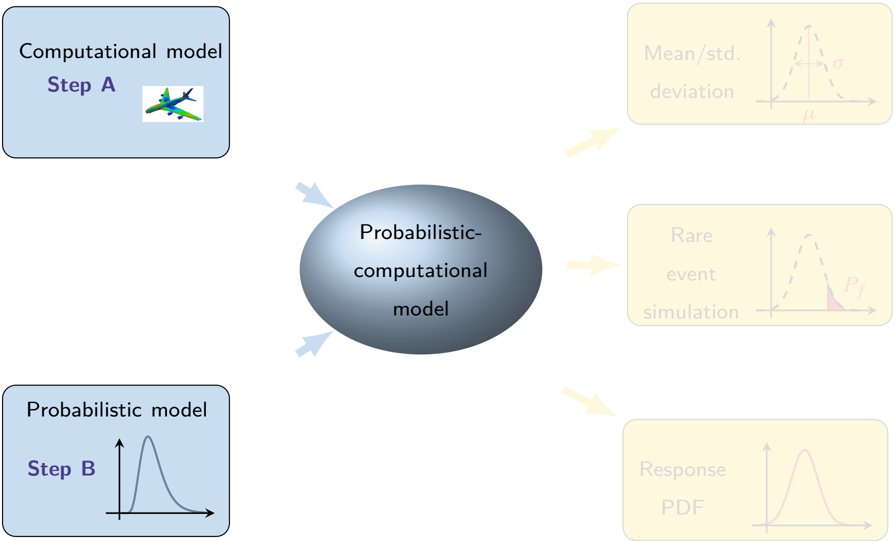
Probabilistic-computational model

Mean/std. deviation

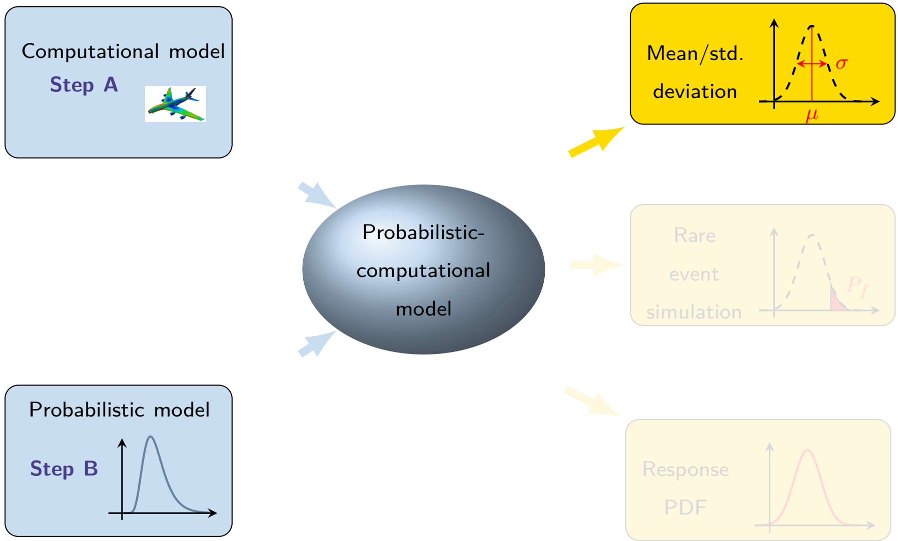
Rare event simulation

Response PDF

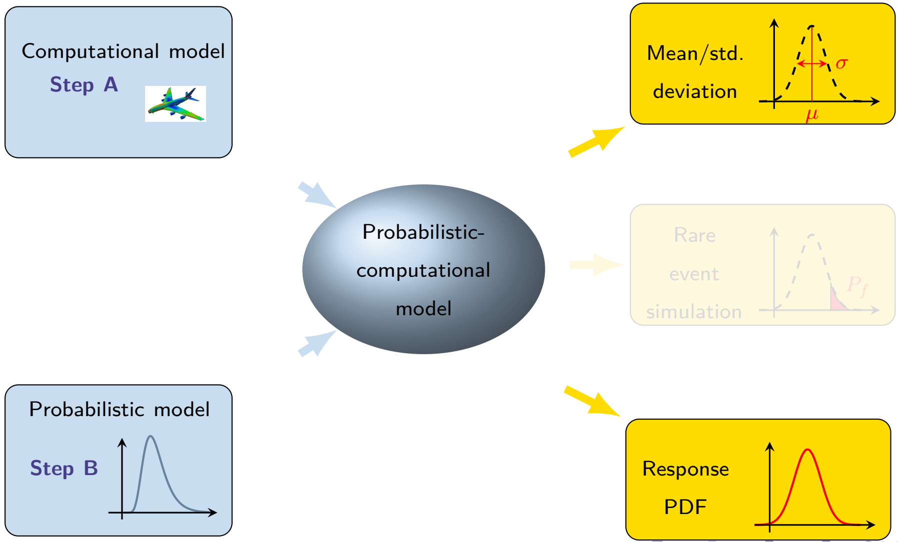
Step C: uncertainty propagation methods



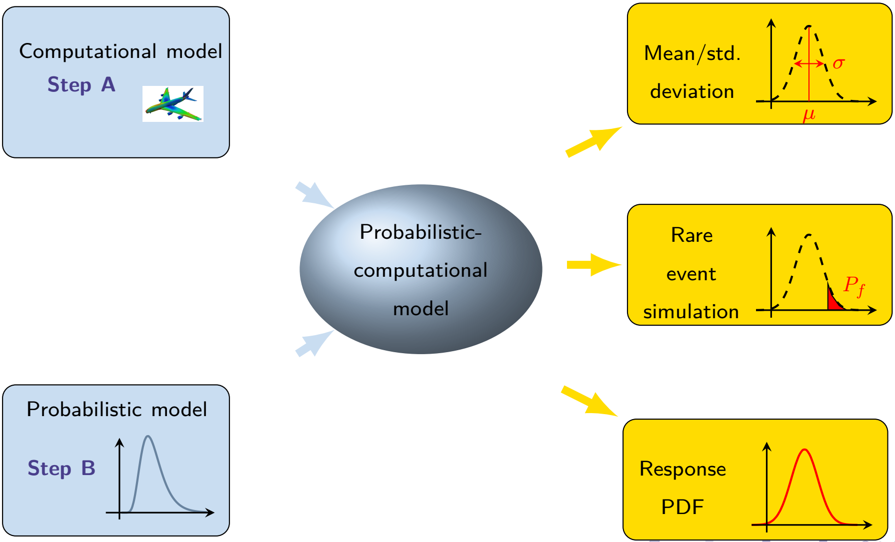
Step C: uncertainty propagation methods



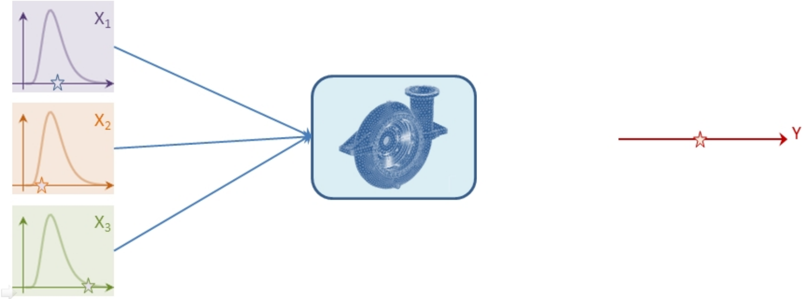
Step C: uncertainty propagation methods



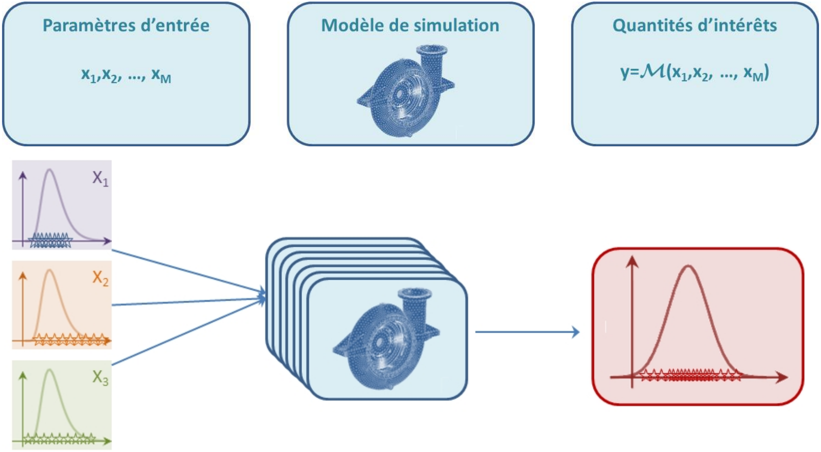
Step C: uncertainty propagation methods



Monte Carlo simulation



Monte Carlo simulation



Monte Carlo simulation

Principles

- The input random variables are sampled according to their joint PDF $f_{\boldsymbol{X}}(\boldsymbol{x})$.
- For each sample $\boldsymbol{x}^{(i)}$, the response $\mathcal{M}(\boldsymbol{x}^{(i)})$ is computed (possibly time-consuming).
- The response sample set $\mathfrak{M} = \{\mathcal{M}(\boldsymbol{x}^{(1)}), \ldots, \mathcal{M}(\boldsymbol{x}^{(n)})\}^{\mathsf{T}}$ is used to compute statistical moments, probabilities of failure or estimate the response distribution (histogram, kernel density estimation).

Monte Carlo simulation

Advantages

- This is a universal method, *i.e.* which does not depend on the type of model $\mathcal{M}$.
- It is statistically well defined: convergence, confidence intervals, etc.
- It is non intrusive, *i.e.* it is based on repeated runs of the computational model as a black box.
- It is suited to distributed computing (clusters of PCs).

Drawbacks

- The "scattering" of Y is investigated point-by-point: if two samples $\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}$ are almost equal, two independent runs of the model are carried out.
- The convergence rate is low ($\propto N^{-1/2}$).

Spectral approach
Principle

- The random response $Y = \mathcal{M}(\boldsymbol{X})$ is considered as an element of a suitable vector space.
- A basis of this space is built up (with respect to the input joint PDF).
- The response random vector Y is completely determined by its coordinates in this basis:

$$Y = \sum_{j=0}^{\infty} y_j \, \Psi_j(\boldsymbol{X})$$

where:

  - y_j : coefficients to be computed (coordinates)
  - $\Psi_j(\boldsymbol{X})$: basis

Assumption: Y has a finite second moment, *i.e.* :

$$\mathbb{E}\left[Y^2\right] = \int Y^2(\omega) \, d\mathbb{P}(\omega) = \int \mathcal{M}^2(\boldsymbol{x}) \, f_{\boldsymbol{X}}(\boldsymbol{x}) \, d\boldsymbol{x} < \infty$$

Outline

Univariate orthogonal polynomials

Definition

- Suppose that the input random vector has independent components.

$$f_{\boldsymbol{X}}(\boldsymbol{x}) = \prod_{i}^{M} f_{X_i}(x_i)$$

- For each marginal distribution, define:

$$\langle \phi_1, \phi_2 \rangle_i = \int_{\mathcal{D}_i} \phi_1(x)\, \phi_2(x)\, f_{X_i}(x_i)\, dx_i$$

- By classical algebra one can build a family of orthogonal polynomials $\{P_k^i,\ k \in \mathbb{N}\}$ as follows:

$$\left\langle P_j^i, P_k^i \right\rangle = \int P_j^i(x)\ P_k^i(x)\ f_{X_i}(x)\, dx = a_j^i\ \delta_{jk}$$

Univariate orthogonal polynomials

Xiu & Karniadakis

Classical families

Type of variable	Weight function	Orthogonal polynomials	Hilbertian basis $\psi_k(x)$
Uniform	$\mathbf{1}_{]-1,1[}(x)/2$	Legendre $P_k(x)$	$P_k(x)/\sqrt{\frac{1}{2k+1}}$
Gaussian	$\frac{1}{\sqrt{2\pi}}\, e^{-x^2/2}$	Hermite $He_k(x)$	$He_k(x)/\sqrt{k!}$
Gamma	$x^a\, e^{-x}\, \mathbf{1}_{\mathbb{R}^+}(x)$	Laguerre $L_k^a(x)$	$L_k^a(x)/\sqrt{\frac{\Gamma(k+a+1)}{k!}}$
Beta	$\mathbf{1}_{]-1,1[}(x)\, \frac{(1-x)^a(1+x)^b}{B(a)\, B(b)}$	Jacobi $J_k^{a,b}(x)$	$J_k^{a,b}(x)/\mathfrak{J}_{a,b,k}$
		$\mathfrak{J}^2_{a,b,k} = \frac{2^{a+b+1}}{2k+a+b+1}$	$\frac{\Gamma(k+a+1)\Gamma(k+b+1)}{\Gamma(k+a+b+1)\Gamma(k+1)}$

Normalization

- The classical orthogonal polynomials are not orthonormal: they may be normalized by dividing by $\sqrt{a_j^i}$:

$$\Psi_j^i = P_j^i/\sqrt{a_j^i} \quad i = 1, \ldots, M, \quad j \in \mathbb{N}$$

Multivariate polynomials

Tensor product of 1D polynomials

- One defines the multi-indices $\boldsymbol{\alpha} = \{\alpha_1, \ldots, \alpha_M\}$, of degree $|\boldsymbol{\alpha}| = \sum_{i=1}^{M} \alpha_i$
- The associated multivariate polynomial reads:

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

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

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

Practical implementation

- 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.):

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

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

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

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

$$\mathcal{A} = \{\boldsymbol{\alpha} \in \mathbb{N}^M \;:\; |\boldsymbol{\alpha}| \leq p\} \qquad \text{card } \mathcal{A} \equiv P = \binom{M+p}{p}$$

Outline

Regression approach

Principle

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

$$Y = \mathcal{M}(\boldsymbol{X}) = \sum_{j=0}^{P-1} y_j \, \Psi_j(\mathbf{X}) + \varepsilon_P \equiv \mathsf{Y}^{\mathsf{T}} \boldsymbol{\Psi}(\boldsymbol{X}) + \varepsilon_P$$

where: $\mathsf{Y} = \{y_0, \ldots, y_{P-1}\}$

$$\boldsymbol{\Psi}(\boldsymbol{x}) = \{\Psi_0(\boldsymbol{x}), \ldots, \Psi_{P-1}(\boldsymbol{x})\}$$

Mean-square minimization

The coefficients are gathered into a vector $\hat{\mathsf{Y}}$, and computed by minimizing the mean square error:

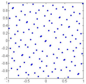
$$\boxed{\hat{\mathsf{Y}} = \arg\min \mathbb{E}\left[\left(\mathsf{Y}^{\mathsf{T}} \boldsymbol{\Psi}(\boldsymbol{X}) - \mathcal{M}(\boldsymbol{X})\right)^2\right]}$$

Regression: discretized solution

The discretized mean-square minimization reads:

$$\hat{\mathsf{Y}}^{reg} = \arg\min \frac{1}{n} \sum_{i=1}^{n} \left(\mathsf{Y}^{\mathsf{T}} \boldsymbol{\Psi}(\boldsymbol{x}^{(i)}) - \mathcal{M}(\boldsymbol{x}^{(i)}) \right)^2$$

- Select an experimental design $\mathcal{X} = \left\{ \boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(n)} \right\}^{\mathsf{T}}$ that covers at best the domain of variation of the parameters



- Evaluate the model response for each sample (exactly as in Monte carlo simulation)
$$\mathfrak{M} = \left\{ \mathcal{M}(\boldsymbol{x}^{(1)}), \dots, \mathcal{M}(\boldsymbol{x}^{(n)}) \right\}^{\mathsf{T}}$$
- Compute the experimental matrix
$$\mathbf{A}_{ij} = \Psi_j\left(\boldsymbol{x}^{(i)}\right) \quad i = 1, \dots, n\,;\ j = 0, \dots, P-1$$
- Solve the least-square minimization problem

$$\boxed{\hat{\mathbf{Y}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathsf{T}}\mathfrak{M}}$$

Validation of the surrogate model

Blatman (2009)
Blatman & Sudret (20010-11)

- 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, 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 regression approach
- This has lead to the development of sparse polynomial chaos expansions.

Error estimators
Coefficient of determination

The regression technique is based on the minimization of the mean square error. The generalization error is defined as:

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

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

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

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

$$R^2 = 1 - \frac{E_{emp}}{\hat{\mathbb{V}}[\mathcal{Y}]} \qquad \hat{\mathbb{V}}[\mathcal{Y}] = \frac{1}{n}(\mathcal{M}(\boldsymbol{x}^{(i)}) - \bar{\mathcal{Y}})^2$$

This error estimator may lead to overfitting

Error estimators

Leave-one-out cross validation

Principle

- In statistical learning theory, cross validation consists in splitting the experimental design $\mathcal{Y}$ in 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 $\boldsymbol{x}^{(i)}$, a polynomial chaos expansion is built using the following experimental design: $\mathcal{X} \backslash \boldsymbol{x}^{(i)} = \{\boldsymbol{x}^{(j)},\ j = 1, \ldots, n,\ j \neq i\}$, denoted by $\mathcal{M}^{PC\backslash i}(.)$.
- The predicted residual is computed in point $\boldsymbol{x}^{(i)}$:

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

- 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:

$$E_{LOO} = \frac{1}{n} \sum_{i=1}^{n} \Delta_i^2 \qquad Q^2 = 1 - \frac{E_{LOO}}{\hat{\mathbb{V}}[\mathcal{Y}]}$$

Post-processing of polynomial chaos expansions
Reminder

Polynomial chaos

$$Y = \mathcal{M}(\boldsymbol{X}) = \mathcal{M} \circ \mathcal{T}(\boldsymbol{\xi})$$

Truncated series

$$Y^{PC} = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$$

- The computed coefficients (“coordinates” of the random variable in the Hilbertian basis) are not the quantities of interest.
- Depending on the situation, the PDF, the statistical moments or quantiles of Y are of interest (*e.g.* low quantiles in structural reliability analysis) .

The PC expansion must be post-processed in order to get relevant information on the model response

Statistical moments

Mean value and variance

From the orthonormality of the polynomial chaos basis one gets:

$$\mathbb{E}\left[\Psi_{\boldsymbol{\alpha}}\right] = 0 \qquad \mathbb{E}\left[\Psi_{\boldsymbol{\alpha}}\Psi_{\boldsymbol{\beta}}\right] = 0$$

Mean value

$$\hat{\mu}_Y = y_0$$

The estimated mean value is the first term of the series.

Variance

$$\hat{\sigma}_Y^2 = \sum_{\boldsymbol{\alpha} \in \mathcal{A} \setminus \mathbf{0}} y_{\boldsymbol{\alpha}}^2$$

The estimated variance is computed as the sum of the squares of the remaining coefficients.

Probability density function

Principle

- The polynomial series expansion may be considered as a stochastic response surface, *i.e.* an analytical function of the input variables $\boldsymbol{\xi}$ (after some isoprobabilistic transform), that may be sampled easily using Monte Carlo simulation.
- A large sample set of reduced variables is drawn $\boldsymbol{\xi}$, say of size $n_{sim} = 10^5 - 10^6$:

$$\mathcal{X}_{sim} = \left\{ \boldsymbol{\xi}^{(j)}, \ j = 1, \ldots, n_{sim} \right\}$$

- The truncated series is evaluated onto this sample:

$$\mathcal{Y}_{sim} = \left\{ \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^{j}), \ j = 1, \ldots, n_{sim} \right\}$$

- The obtained sample set is plotted as an histogram or by kernel density smoothing.

Outline

Sensitivity analysis

Sobol' decomposition

Sobol', 1993
Saltelli *et al.* , 2000

- 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 $\mathcal{M} : \boldsymbol{x} \in [0,1]^M \to \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}$. The Sobol' decomposition reads:

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

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.

Unicity under orthogonality conditions

Sensitivity analysis

Sobol' decomposition

Sobol', 1993
Saltelli *et al.* , 2000

- 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 $\mathcal{M} : \boldsymbol{x} \in [0,1]^M \to \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}$. The Sobol' decomposition reads:

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

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.

Unicity under orthogonality conditions

Sobol' indices
Independent input variables

Variance decomposition

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

- Due to the orthogonality of the decomposition:

$$
\begin{aligned}
D \equiv \mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right] &= \mathbb{E}\left[\left(\mathcal{M}(\boldsymbol{X}) - \mathcal{M}_0\right)^2\right] \\
&= \mathbb{E}\left[\left(\sum_{\{i_1, \ldots, i_s\} \subset \{1, \ldots, M\}} \mathcal{M}_{i_1 \ldots i_s}(X_{i_1}, \ldots, X_{i_s})\right)^2\right] \\
&= \sum_{\{i_1, \ldots, i_s\} \subset \{1, \ldots, M\}} \mathbb{E}\left[\mathcal{M}^2_{i_1 \ldots i_s}(X_{i_1}, \ldots, X_{i_s})\right]
\end{aligned}
$$

Sobol' indices

Partial variance

- Consider:

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

- Then:

$$\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right] = \sum_{i=1}^{M} D_i + \sum_{1 \leqslant i < j \leqslant M} D_{ij} + \dots + D_{12\dots M}$$

- The Sobol' indices are obtained by normalization:

$$S_{i_1\dots i_s} = \frac{D_{i_1\dots i_s}}{D}$$

They represent the fraction of the total variance $\mathrm{Var}\left[Y\right]$ that can be attributed to each input variable i (S_i) or combinations of variables $\{i_1 \dots i_s\}$

Link with PC expansions

Sudret, 2008

Sobol' decomposition *vs.* polynomial chaos expansions

- The truncated polynomial series may be sorted so as to emphasize the uni-, bi-, etc.- variate functions of the Sobol' decomposition, namely:

$$\begin{aligned}
\mathcal{M}_0 &= y_0 \\
\mathcal{M}_i(x_i) &= \sum_{\boldsymbol{\alpha} \in \mathcal{A}_i} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \qquad \mathcal{A}_i = \{\boldsymbol{\alpha} : \alpha_i > 0, \alpha_{j \neq i} = 0\} \\
&\dots \\
\mathcal{M}_{i_1 \dots i_s}(x_{i_1}, \, \dots \, , x_{i_s}) &= \sum_{\boldsymbol{\alpha} \in \mathcal{A}_{i_1, \, \dots \, , i_s}} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x})
\end{aligned}$$

$$\mathcal{A}_{i_1 \dots i_s} = \{\boldsymbol{\alpha} : \alpha_k > 0 \Leftrightarrow k \in (i_1, \, \dots \, , i_s)\}$$

The PC expansion readily provides a functional decomposition

Link with PC expansions

Computation of the Sobol' indices

- The partial variances $D_{i_1 \dots i_s}$ are obtained by summing up the square of selected PC coefficients.

$$D_i = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_i} y_{\boldsymbol{\alpha}}^2 \qquad \mathcal{A}_i = \{\boldsymbol{\alpha} : \alpha_i > 0, \alpha_{j \neq i} = 0\}$$

$$D_{i_1 \dots i_s} = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_{i_1, \dots, i_s}} y_{\boldsymbol{\alpha}}^2 \qquad \mathcal{A}_{i_1 \dots i_s} = \{\boldsymbol{\alpha} : \alpha_k > 0 \Leftrightarrow k \in (i_1, \dots, i_s)\}$$

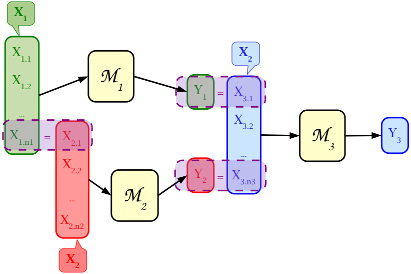
- The Sobol' indices come after normalization:

$$S_{i_1 \dots i_s} = \frac{D_{i_1 \dots i_s}}{D}$$

Once the PC expansion is available, the full set of Sobol' indices are obtained for free !

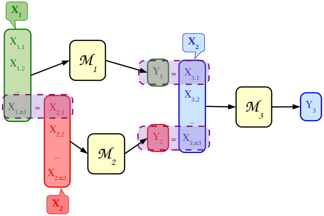
Outline

Characteristics of imbricated multiphysics models



- The computational workflow consists in an imbrication of models (multiscale/multiphysics analysis).
- Models of different levels have common parameters (*e.g.* geometrical dimensions for thermal, mechanical, acoustics problems).
- The output of micro-scale models is the input of the macro-scale models.

Impact on sensitivity analysis



Specificity of multi-level imbricated models

- The PDF of the parameters of the intermediate levels (margins + dependence structure (correlations)) is implicitely defined by uncertainty propagation.
- The appropriate statistical tools are non-parametric representation of the marginals and copula theory.

Wand & Jones (1995); Nelsen (1999)

- Sensitivity indices have to be defined in the case of dependent input variables.
- Two approaches have emerged recently: Caniou (2012)
  - Distribution-based sensitivity indices Borgonovo (2007, 2011)
  - Covariance decomposition Li & Rabitz (2010)

Distribution-based sensitivity indices

Borgonovo (2007)

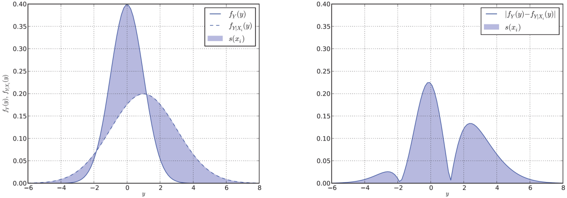
Heuristics

Schemes are taken from Caniou (2012)

If the PDF of the model response $Y = \mathcal{M}(\boldsymbol{X})$ is influenced by a given input parameter X_i then the conditional distribution $f_{Y|X_i}(y)$ shall significantly differ from $f_Y(y)$.

Shift between f_Y and $f_{Y|X_i}$:

$$s(X_i) = \int_{\mathrm{D}_Y} \left| f_Y(y) - f_{Y|X_i}(y) \right| \, dy$$



Borgonovo's δ importance measure: expected shift

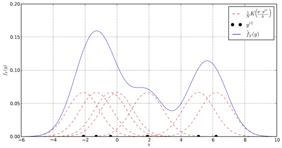
$$\delta_i \equiv \frac{1}{2}\mathbb{E}\left[s(X_i)\right] = \frac{1}{2} \int_{\mathrm{D}_{X_i}} \left[\int_{\mathrm{D}_Y} \left| f_Y(y) - f_{Y|X_i}(y) \right| \, dy \right] f_{X_i}(x_i) \, dx_i$$

Estimating the shift from PDFs

(Conditional) distributions are estimated by kernel smoothing techniques based on massive Monte Carlo simulation:

$$\hat{f}_Y(y) = \frac{1}{N_{MC}\, h} \sum_{l=1}^{N_{MC}} K\left(\frac{y - \mathcal{M}(\boldsymbol{y}^{(l)})}{h}\right)$$

$$e.g.\ \ K(t) = e^{-t^2/2}/\sqrt{2\pi}$$



h is the bandwidth parameter, *e.g.* $h \propto N_{MC}^{-1/5}$.

Shift estimation (inner integral)

$$s(x_i) = \int_{\mathcal{D}_Y} \left| f_Y(y) - f_{Y|X_i}(y) \right| \, dy$$

Computed by Gaussian quadrature

Expected shift (outer integral)

$$\mathbb{E}\left[s(X_i)\right] = \int_{\mathcal{D}_{X_i}} s(X_i)\, f_{X_i}(x_i)\, dx_i$$

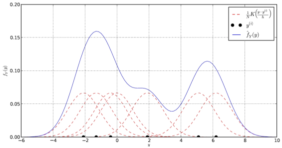
$$\approx \sum_{q=1}^{N_Q} \omega_q\, s(x_i^{(q)})$$

Estimating the shift from PDFs

(Conditional) distributions are estimated by kernel smoothing techniques based on massive Monte Carlo simulation:

$$\hat{f}_Y(y) = \frac{1}{N_{MC}\, h} \sum_{l=1}^{N_{MC}} K\left(\frac{y - \mathcal{M}(\boldsymbol{y}^{(l)})}{h}\right)$$

e.g. $K(t) = e^{-t^2/2} / \sqrt{2\pi}$



h is the bandwidth parameter, *e.g.* $h \propto N_{MC}^{-1/5}$.

Shift estimation (inner integral)

$$s(x_i) = \int_{\mathrm{D}_Y} \left| f_Y(y) - f_{Y|X_i}(y) \right| \, dy$$

Computed by Gaussian quadrature

Expected shift (outer integral)

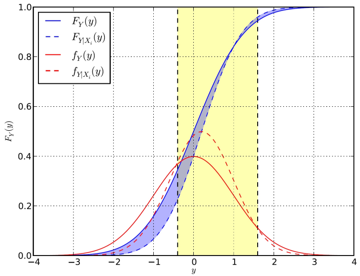
$$\mathbb{E}\left[s(X_i)\right] = \int_{\mathrm{D}_{X_i}} s(X_i)\, f_{X_i}(x_i)\, dx_i \approx \sum_{q=1}^{N_Q} \omega_q \, s(x_i^{(q)})$$

Estimating the shift from CDFs

Borgonovo *et al.* (2011)

Remarks

- The two nested integrals of functions derived from kernel PDF estimates are extremely expensive to compute and prone to numerical noise.
- The inner integral may be computed analytically though.



Schemes are taken from Caniou (2012)

Alternative scheme

$$s(X_i) = 2\,\mathbb{P}\left(f_Y(y) > f_{Y|X_i}(y)\right) - 2\,\mathbb{P}\left(f_Y(y) < f_{Y|X_i}(y)\right)$$

$$\delta_i = \mathbb{E}_{X_i}\left[F_Y(y_2) - F_Y(y_1) + F_{Y|X_i}(y_1) - F_{Y|X_i}(y_2)\right]$$

where (y_1, y_2) are the intersection points of the PDF and the conditional PDF, *i.e.* are the roots of:

$$f_Y(y) = f_{Y|X_i}(y)$$

Covariance-based sensitivity indices

Li, Rabitz *et al.* , 2010

Suppose a functional decomposition of the model exists, *e.g.* :

$$\mathcal{M}(\boldsymbol{x}) = \sum_{u \subset \{1, \dots, M\}} \mathcal{M}_u(\boldsymbol{x}_u)$$

NB : the summands $\mathcal{M}_u(\boldsymbol{x}_u)$ may not be orthogonal with respect to the probability measure associated with $f_{\boldsymbol{X}}$.

Covariance decomposition

$$\begin{aligned}\text{Var}\left[\mathcal{M}(\boldsymbol{X})\right] &= \text{Var}\left[\sum_{u \subset \{1, \dots, M\}} \mathcal{M}_u(\boldsymbol{X}_u)\right] \\ &= \sum_{u \subset \{1, \dots, M\}} \text{Var}\left[\mathcal{M}_u(\boldsymbol{X}_u)\right] + \sum_{u \subset \{1, \dots, M\}} \sum_{v \subsetneq u} \text{Cov}\left[\mathcal{M}_u(\boldsymbol{X}_u); \mathcal{M}_v(\boldsymbol{X}_v)\right]\end{aligned}$$

NB: in case of independence and Sobol' decomposition, the second term is zero.

Covariance-based sensitivity indices

Li, Rabitz *et al.* , 2010

Total sensitivity index

$$S_u^{(T)} = \mathrm{Cov}\left[\mathcal{M}_u(\boldsymbol{X}_u), \mathcal{M}(\boldsymbol{X})\right] / \mathrm{Var}\left[Y\right]$$

Structural sensitivity index

$$S_u^{(S)} = \mathrm{Var}\left[\mathcal{M}_u(\boldsymbol{X}_u)\right] / \mathrm{Var}\left[Y\right]$$

Correlative sensitivity index

$$S_u^{(C)} = S_u^{(T)} - S_u^{(S)}$$

- $S_u^{(C)} = 0$ on the case of independent input parameters and classical Sobol' functional decomposition.
- These indices are denoted respectively by S_{p_j}, $S_{p_j}^a$ and $S_{p_j}^b$ in Li, Rabitz *et al.* (2010).

Covariance-based indices using PC expansions
Principle

Functional decomposition

A truncated polynomial expansion is computed assuming that the parameters are independent:

$$\mathcal{M}(\boldsymbol{x}) \approx \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

- The terms are grouped according to their input parameters so as to build the functional decomposition:

$$\mathcal{M}_u(\boldsymbol{x}_u) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_u} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \qquad \mathcal{A}_u = \{\boldsymbol{\alpha} : k \in u \Leftrightarrow \alpha_k > 0\}$$

Covariance-based indices using PC expansions

Monte Carlo estimators

Caniou & Sudret (2012)

- A sample set $\mathcal{X} = \left\{ \boldsymbol{x}^{(i)}, i = 1, \ldots, N \right\}$ of size N is drawn according to the joint PDF $f_{\boldsymbol{X}}(\boldsymbol{x})$.
- Classical estimators are used:

$$\widehat{\mathrm{Var}\,[Y]} = \frac{1}{N-1} \sum_{i=1}^{N} \left(\mathcal{M}(\boldsymbol{x}^{(i)}) - \mu_{\mathcal{M}} \right)^2$$

$$\widehat{S_u^{(T)}} = \frac{1}{N-1} \sum_{i=1}^{N} \left(\mathcal{M}_u(\boldsymbol{x}^{(i)}) - \mu_{\mathcal{M}_u} \right) \left(\mathcal{M}(\boldsymbol{x}^{(i)}) - \mu_{\mathcal{M}} \right) / \widehat{\mathrm{Var}\,[Y]}$$

$$\widehat{S_u^{(S)}} = \frac{1}{N-1} \sum_{i=1}^{N} \left(\mathcal{M}_u(\boldsymbol{x}^{(i)}) - \mu_{\mathcal{M}_u} \right)^2 / \widehat{\mathrm{Var}\,[Y]}$$

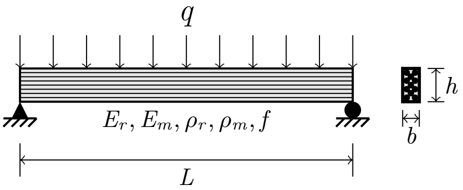
$$\widehat{S_u^{(C)}} = \widehat{S_u^{(T)}} - \widehat{S_u^{(S)}}$$

NB: all the functions are multivariate polynomials. $N = 10^5$ evaluations may be carried out in a matter of seconds.

Outline

Simply supported composite beam
Problem statement

A composite beam of length L and section $b \times h$ is made of a fraction f of carbon fibers (E_f, ρ_f) and a fraction $(1 - f)$ of epoxyde matrix (E_f, ρ_f).



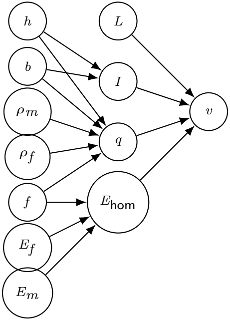
- The beam is loaded by its dead weight $q = \rho_{\text{hom}} g b h$:
- Of interest is the sensitivity of the maximum midspan deflection v to its input parameters:

$$v = \frac{5}{384} \frac{qL^4}{E_{\text{hom}} I}$$

Nested model and input variables

Models

$$E_{\text{hom}} = f\,E_f + (1-f)\,E_m$$
$$I = \frac{bh^3}{12}$$
$$q = [f\,\rho_r + (1-f)\,\rho_m]\,g\,h$$
$$v = \frac{5}{384}\,\frac{qL^4}{E_{\text{hom}}\,I}$$



Basic random variables

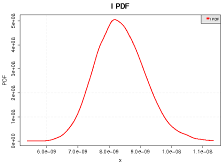
Parameter	Distribution	Mean	Coefficient of variation
L	Lognormal	2 m	1%
b	Lognormal	10 cm	3%
h	Lognormal	1 cm	3%
E_f	Lognormal	300 GPa	15%
E_m	Lognormal	10 GPa	15%
ρ_f	Lognormal	1800 kg·m^{-3}	3%
ρ_m	Lognormal	1200 kg·m^{-3}	3%
f	Lognormal	0.5	10%

Output of the intermediate variables

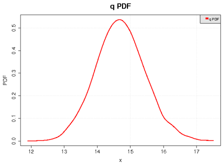
- PC expansions of the intermediate variables E_{hom}, q, I

$$
\begin{aligned}
E_{\text{hom}} &= \sum_{\boldsymbol{\alpha} \in \mathcal{A}_E} e_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \\
q &= \sum_{\boldsymbol{\alpha} \in \mathcal{A}_q} q_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}) \\
I &= \sum_{\boldsymbol{\alpha} \in \mathcal{A}_I} i_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})
\end{aligned}
$$

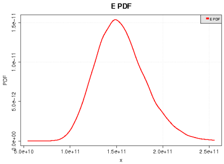
- Non parametric estimation of the margins (kernel smoothing with 10^4 points):



$\widehat{f_I}(i)$



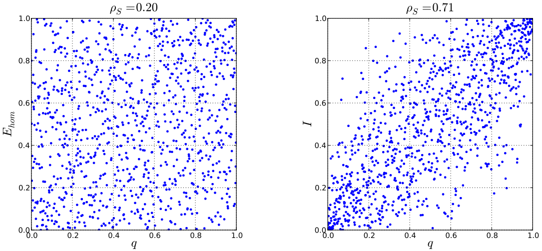
$\widehat{f_q}(q)$



$\widehat{f_{E_{\text{hom}}}}(e)$

Output of the intermediate variables
Correlation structure

- Estimation of the dependence structure : Gaussian copula based on the Spearman's rank correlation coefficients.



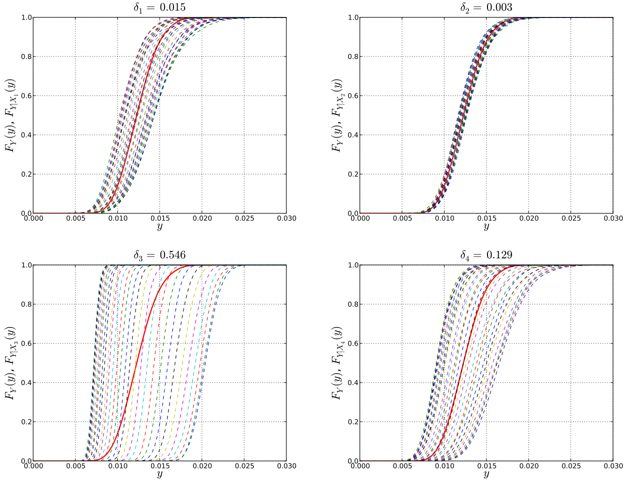
$\rho_S(q, E) = 0.20$ $\rho_S(q, I) = 0.71$

Last level uncertainty propagation

- Isoprobabilistic transform of L, I, q, E_{hom} into standard normal variates $\boldsymbol{U}$
- PC expansion of v and computation of distribution-based (resp. covariance-based) sensitivity indices

Results - Distribution-based indices

CDF and conditional CDF of the maximal deflection



Results

Parameter	δ^{CDF}	S	S^U	S^C
q	0.015	-0.08	0.09	-0.17
L	0.003	0.01	0.01	0.00
E_{hom}	0.546	0.89	0.94	-0.05
I	0.129	0.18	0.30	-0.12
Σ	0.693	1.00	1.34	-0.34

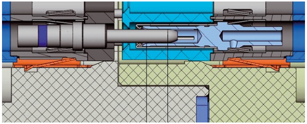
$$v = \frac{5}{384} \frac{qL^4}{E_{\text{hom}} I}$$

- The homogenized Young's modulus and the moment of inertia are the most important parameters.
- The distribution- and covariance-based indices give consistent results.
- The cov.-based index of q is negative due to the strong correlation between q and I which have opposite influences in the maximal displacement.

Outline

Tolerance analysis

- In industrial mass production, assembled products are made of individual parts that are prone to uncertainty in their dimensions due to the manufacturing processes.

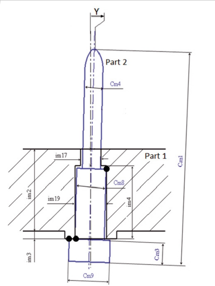


After Gayton *et al.* , Méca. Indus. (2011)

- Non-assembly problems may occur when some parts' real dimensions differ (even slightly) from their theoretical values.

- Predicting the probability of non-assembly prior to the mass production is of crucial importance. Probabilistic methods derived from structural reliability analysis have been recently proposed. Gayton *et al.* (2011)

Connector contact clearance



$$
\begin{aligned}
c &= \frac{cm_4 + cm_8 + cm_7}{2} \\
i &= \frac{ima_{17} + ima_{19} + ima_{20}}{2} \\
h &= ima_2 + ima_3 \\
\alpha &= \arccos\left(\frac{c}{\sqrt{i^2 + h^2}}\right) - \arccos\left(\frac{i}{\sqrt{i^2 + h^2}}\right) \\
r_2 &= \frac{\frac{ima_{19} + ima_{20}/2}{2} - \frac{cm_8 + cm_7/2}{2\cos(\alpha)}}{\tan(\alpha)} \\
z &= \frac{r_2}{\cos(\alpha)} + ((cm_9 + cm_{10}/2)/2 + cm_7/4)\tan(\alpha) \\
J_1 &= (cm_1 - cm_3 - z)\sin(\alpha) \\
J_2 &= \frac{cm_7}{4}\cos(\alpha) \\
J_3 &= \frac{cm_5 + cm_6}{2}\cos(\alpha) \\
Y &= J_1 + J_2 + J_3 \qquad (
\end{aligned}
$$

The axial deviation of an electrical connector pin is considered.

After Gayton *et al.* , Méca. Indus. (2011)

- The deviation is computed as a non linear function of 14 geometrical dimensions describing the geometry of the two parts and their respective position.
- Each dimension is characterized by a Gaussian variable.
- Since different surfaces are machined during the same operation, their dimensions are highly correlated, *e.g.* $\rho_S = 0.8$ between the three different diameters of the pin.

Results

Parameter	δ^{CDF}	S	S^U	S^C
cm_1	0.00	0.00	0.00	0.00
cm_3	0.00	0.00	0.00	0.00
cm_4	0.02	0.02	0.01	0.01
cm_5	0.11	0.15	0.15	0.00
cm_6	0.01	0.02	0.02	0.00
cm_7	0.30	0.52	0.51	0.01
cm_8	0.03	0.03	0.02	0.01
cm_9	0.00	0.00	0.00	0.00
cm_{10}	0.00	0.00	0.00	0.00
ima_2	0.01	0.00	0.00	0.00
ima_3	0.01	0.00	0.00	0.00
ima_{17}	0.07	0.11	0.05	0.06
ima_{19}	0.05	0.07	0.02	0.05
ima_{20}	0.07	0.09	0.03	0.06
Σ	0.68	1.00	0.81	0.19

After Caniou (2012)

- A set of 5 dimensions explain 94% of the variance of the pin deviation.
- Three of them are correlated input variables for which the correlated contribution of the cov.-based indices is larger than the uncorrelated part.
- The δ-indices are consistent.

- The results may be used for tolerance allocation, *i.e.* allocate smaller tolerance intervals to important dimensions.

Conclusions

- Complex systems are nowadays modelled by computational workflows that involve various submodels / physics / scales of description.
- The existing uncertainty propagation methods have to be adapted to the specific characteristics of these models:
  - large CPU demand: need for surrogate models, *e.g.* polynomial chaos expansions
  - statistical dependence between the meaningful intermediate parameters of the workflow
- Sensitivity indices have been developed for the case of models with dependent input parameters and can be used in the context of complex workflows:
  - distribution-based δ-indices
  - covariance-based indices

Conclusions

- Polynomial chaos expansions whose efficiency in moment-, reliability- and sensitivity analysis is well established show a new feature in this context, namely the functional decomposition of the computational model.

- Further work is required to make these methods available to the industry in a convenient format.

Thank you very much for your attention !

Conclusions

- Polynomial chaos expansions whose efficiency in moment-, reliability- and sensitivity analysis is well established show a new feature in this context, namely the functional decomposition of the computational model.
- Further work is required to make these methods available to the industry in a convenient format.

Thank you very much for your attention !

References

Blatman, G. (2009).
Adaptive sparse polynomial chaos expansions for uncertainty propagation and sensitivity analysis.
Ph. D. thesis, Université Blaise Pascal, Clermont-Ferrand.

Blatman, G. et B. Sudret (2010a).
An adaptive algorithm to build up sparse polynomial chaos expansions for stochastic finite element analysis.
Prob. Eng. Mech. 25(2), 183–197.

Blatman, G. et B. Sudret (2010b).
Efficient computation of global sensitivity indices using sparse polynomial chaos expansions.
Reliab. Eng. Sys. Safety 95, 1216–1229.

Blatman, G. et B. Sudret (2011).
Adaptive sparse polynomial chaos expansion based on Least Angle Regression.
J. Comput. Phys 230, 2345–2367.

Borgonovo, E. (2007).
A new uncertainty importance measure.
Reliab. Eng. Sys. Safety 92, 771–784.

Borgonovo, E., W. Castaings, et S. Tarantola (2011).
Moment-independent importance measures: new results and analytical test cases.
Risk Analysis 31(3), 404–428.

Caniou, Y. (2012).
Global sensitivity analysis for nested and multiscale models.
Ph. D. thesis, Université Blaise Pascal, Clermont-Ferrand.

Gayton, N., P. Beaucaire, J.-M. Bourinet, E. Duc, M. Lemaire, et L. Gauvrit (2011).
APTA: advanced probability-based tolerance analysis of products.
Mécanique & Industries 12(2), 71–85.

Li, G., H. Rabitz, P. Yelvington, O. Oluwole, F. Bacon, C. Kolb, et J. Schoendorf (2010).
Global sensitivity analysis for systems with independent and/or correlated inputs.
J. Phys.Chem. 114, 6022–6032.

Saltelli, A., K. Chan, et E. Scott (Eds.) (2000).
Sensitivity analysis.
J. Wiley & Sons.

Sobol', I. (1993).
Sensitivity estimates for nonlinear mathematical models.
Math. Modeling & Comp. Exp. 1, 407–414.

Sudret, B. (2008).
Global sensitivity analysis using polynomial chaos expansions.
Reliab. Eng. Sys. Safety 93, 964–979.

Xiu, D. et G. Karniadakis (2002).
The Wiener-Askey polynomial chaos for stochastic differential equations.
SIAM J. Sci. Comput. 24(2), 619–644.