


An introduction to surrogate modelling for uncertainty quantification in computational sciences

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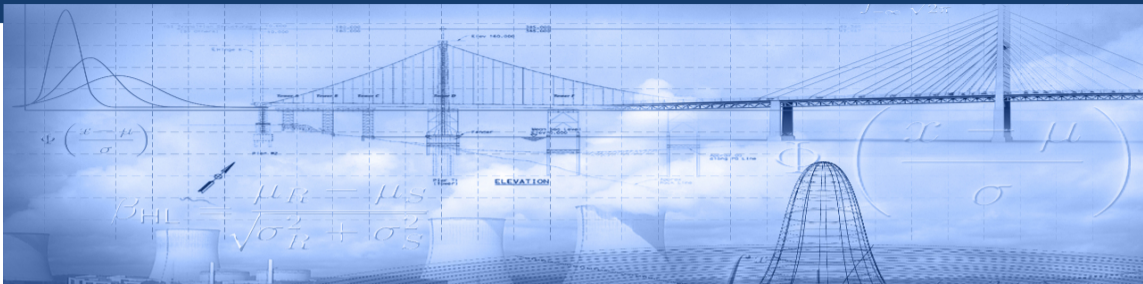
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An introduction to surrogate modelling for uncertainty quantification in computational sciences

Bruno Sudret

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Computational models in engineering

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

A computational model combines:

- A **mathematical description** of the physical phenomena (governing equations), *e.g.* mechanics, electromagnetism, fluid dynamics, etc.
- **Discretization techniques** which transform continuous equations into linear algebra problems
- Algorithms to **solve** the discretized equations

$$\operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f} = \mathbf{0}$$

$$\boldsymbol{\sigma} = \mathbf{D} \cdot \boldsymbol{\varepsilon}$$

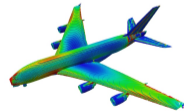
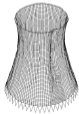
$$\boldsymbol{\varepsilon} = \frac{1}{2} \left(\nabla \boldsymbol{u} + {}^T \nabla \boldsymbol{u} \right)$$



Computational models in engineering

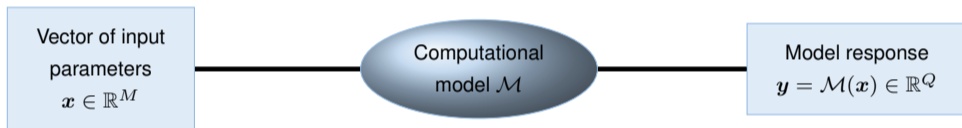
Computational models are used:

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

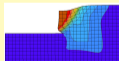


Computational models: the abstract viewpoint

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



- Geometry
- Material properties
- Loading

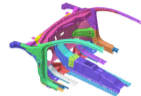


- Analytical formula
- Finite element model
- Comput. workflow

- Displacements
- Strains, stresses
- Temperature, etc.

Real world is uncertain

- Differences between the **designed** and the **real** system:
 - Dimensions (tolerances in manufacturing)
 - Material properties (e.g. variability of the stiffness or resistance)
- **Unforecast exposures**: exceptional service loads, natural hazards (earthquakes, floods, landslides), climate loads (hurricanes, snow storms, etc.), accidental human actions (explosions, fire, etc.)



Outline

Introduction

Uncertainty quantification: why surrogate models?

Basics of polynomial chaos expansions

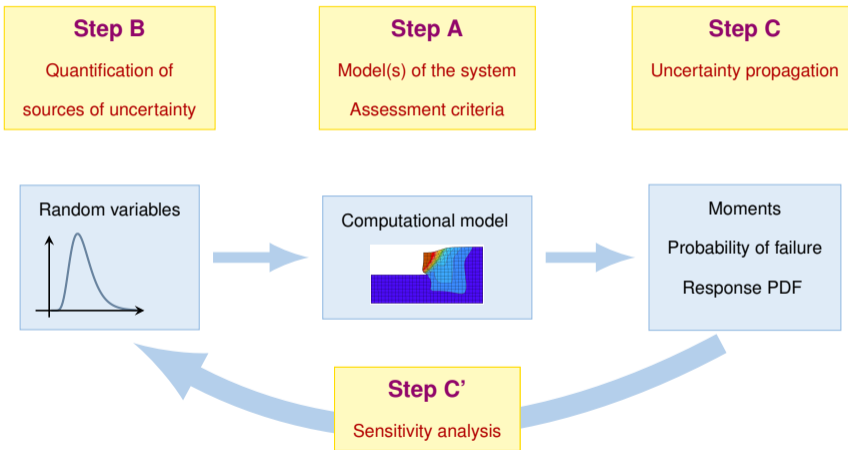
- PCE basis and coefficients

- Sparse PCE

- Post-processing

Conclusions

Global framework for uncertainty quantification



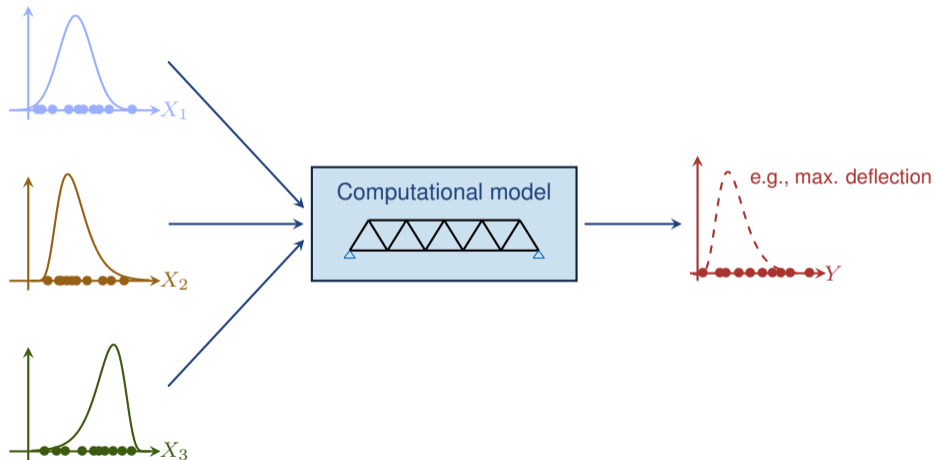
B. Sudret, Uncertainty propagation and sensitivity analysis in mechanical models – contributions to structural reliability and stochastic spectral methods (2007)

Uncertainty propagation using Monte Carlo simulation

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

- A sample set $\mathcal{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is drawn according to the input distribution $f_{\mathbf{X}}$
- For each sample the quantity of interest (resp. performance criterion) is evaluated, say $\mathcal{Y} = \{\mathcal{M}(\mathbf{x}_1), \dots, \mathcal{M}(\mathbf{x}_n)\}$
- The set of model outputs is used for moments-, distribution- or reliability analysis

Uncertainty propagation using Monte Carlo simulation



Advantages/Drawbacks of Monte Carlo simulation

Advantages

- Universal method: only rely upon **sampling** random numbers and running repeatedly the computational model
- Sound statistical foundations: convergence when $n \rightarrow \infty$
- Suited to **High Performance Computing**: “embarrassingly parallel”

Drawbacks

- **Statistical uncertainty**: results are not exactly reproducible when a new analysis is carried out (handled by computing **confidence intervals**)
- **Low efficiency**: convergence rate $\propto n^{-1/2}$

Surrogate models for uncertainty quantification

A **surrogate model** $\tilde{\mathcal{M}}$ is an **approximation** of the original computational model \mathcal{M} with the following features:

- It assumes some regularity of the model \mathcal{M} and some general functional shape
- It is built from a **limited** set of runs of the original model \mathcal{M} called the **experimental design**
 $\mathcal{X} = \{\mathbf{x}^{(i)}, i = 1, \dots, n\}$



Simulated data

- It is **fast to evaluate!**

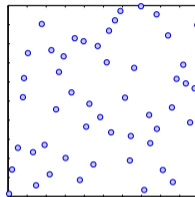
Surrogate models for uncertainty quantification

| Name | Shape | Parameters |
|------------------------------------|--|---|
| Polynomial chaos expansions | $\tilde{\mathcal{M}}(\mathbf{x}) = \sum_{\alpha \in \mathcal{A}} a_{\alpha} \Psi_{\alpha}(\mathbf{x})$ | a_{α} |
| Low-rank tensor approximations | $\tilde{\mathcal{M}}(\mathbf{x}) = \sum_{l=1}^R b_l \left(\prod_{i=1}^M v_l^{(i)}(x_i) \right)$ | $b_l, z_{k,l}^{(i)}$ |
| Kriging (a.k.a Gaussian processes) | $\tilde{\mathcal{M}}(\mathbf{x}) = \boldsymbol{\beta}^T \cdot \mathbf{f}(\mathbf{x}) + Z(\mathbf{x}, \boldsymbol{\omega})$ | $\boldsymbol{\beta}, \sigma_Z^2, \boldsymbol{\theta}$ |
| Support vector machines | $\tilde{\mathcal{M}}(\mathbf{x}) = \sum_{i=1}^m a_i K(\mathbf{x}_i, \mathbf{x}) + b$ | \mathbf{a}, b |
| (Deep) Neural networks | $\tilde{\mathcal{M}}(\mathbf{x}) = f_n(\dots f_2(b_2 + f_1(b_1 + \mathbf{w}_1 \cdot \mathbf{x}) \cdot \mathbf{w}_2))$ | \mathbf{w}, b |

Ingredients for building a surrogate model

- Select an **experimental design** \mathcal{X} that covers at best the domain of input parameters:
 - (Monte Carlo simulation)
 - **Latin hypercube sampling** (LHS)
 - Low-discrepancy sequences

- Run the computational model \mathcal{M} onto \mathcal{X} **exactly as in Monte Carlo simulation**



Ingredients for building a surrogate model

- Smartly post-process the data $\{\mathcal{X}, \mathcal{M}(\mathcal{X})\}$ through a **learning algorithm**

| Name | Learning method |
|--------------------------------|---|
| Polynomial chaos expansions | sparse grid integration, least-squares, compressive sensing |
| Low-rank tensor approximations | alternate least squares |
| Kriging | maximum likelihood, Bayesian inference |
| Support vector machines | quadratic programming |

- **Validate** the surrogate model, e.g. estimate a global error $\varepsilon = \mathbb{E} \left[(\mathcal{M}(\mathbf{X}) - \tilde{\mathcal{M}}(\mathbf{X}))^2 \right]$

Advantages of surrogate models

Usage

$$\mathcal{M}(\boldsymbol{x}) \approx \tilde{\mathcal{M}}(\boldsymbol{x})$$

hours per run seconds for 10^6 runs

Advantages

- **Non-intrusive methods**: based on runs of the computational model, exactly as in Monte Carlo simulation
- **Suited to high performance computing**: “embarrassingly parallel”

Challenges

- Need for rigorous **validation**
- **Communication**: advanced mathematical background

Efficiency

- 6-8 orders of magnitude (!) less CPU for a **single run**
- 2-3 orders of magnitude less runs compared to a full Monte Carlo simulation

Surrogate modelling vs. machine learning

| Features | Supervised learning | Surrogate modelling |
|--|--|--|
| Computational model \mathcal{M} | ✗ | ✓ |
| Probabilistic model of the input $\mathbf{X} \sim f_{\mathbf{X}}$ | ✗ | ✓ |
| Training data: $\mathcal{X} = \{(\mathbf{x}_i, y_i), i = 1, \dots, n\}$ | ✓ | ✓ |
| | Training data set (big data) | Experimental design (small data) |
| Prediction goal: for a new $\mathbf{x} \notin \mathcal{X}$, $y(\mathbf{x})$? | $\sum_{i=1}^m y_i K(\mathbf{x}_i, \mathbf{x}) + b$ | $\sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{x})$ |
| Validation (resp. cross-validation) | ✓ | ✓ |
| | Validation set | Leave-one-out CV |

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- PCE basis and coefficients

- Sparse PCE

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Polynomial chaos expansions in a nutshell

Ghanem & Spanos (1991; 2003); Xiu & Karniadakis (2002); Soize & Ghanem (2004)

- We assume here for simplicity that the input parameters are independent with $X_i \sim f_{X_i}$, $i = 1, \dots, M$
- PCE is also applicable in the general case using an isoprobabilistic transform $\mathbf{X} \mapsto \Xi$

The **polynomial chaos expansion** of the (random) model response reads:

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

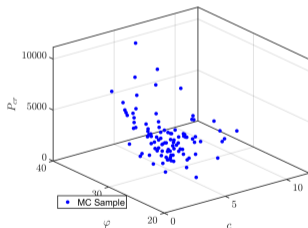
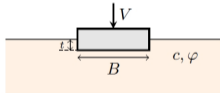
where:

- $\Psi_{\alpha}(\mathbf{X})$ are basis functions (**multivariate orthonormal polynomials**)
- y_{α} are **coefficients** to be computed (coordinates)

Sampling (MCS) vs. spectral expansion (PCE)

Whereas MCS explores the output space /distribution **point-by-point**, the polynomial chaos expansion assumes a generic structure (**polynomial function**), which better exploits the available information (**runs of the original model**)

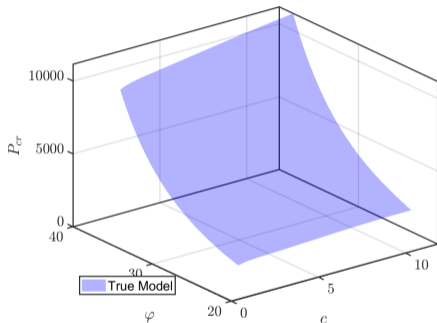
Example: load bearing capacity P_{cr} of a shallow foundation



Thousands (resp. millions) of points are needed to grasp the structure of the response (resp. capture the rare events)

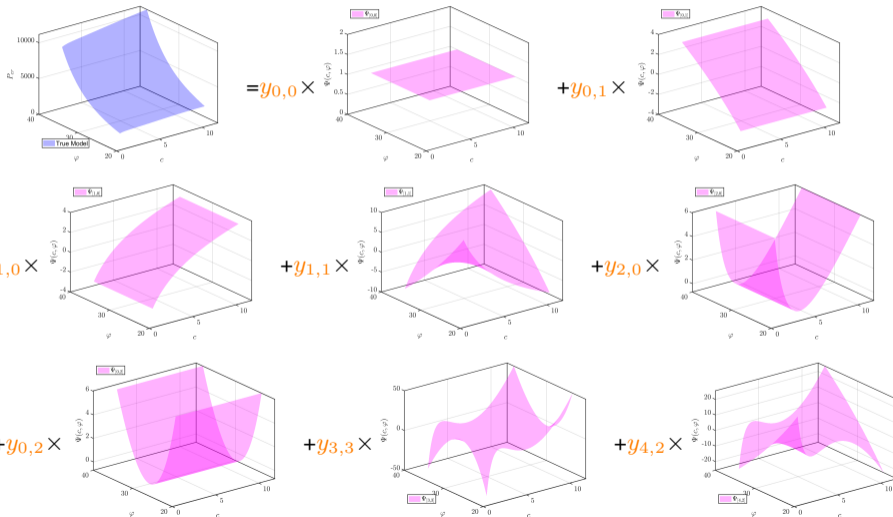
Defined as a function of the soil cohesion c and friction angle φ

Visualization of the PCE construction



= “Sum of **coefficients** \times **basic surfaces**”

Visualization of the PCE construction



Multivariate polynomial basis

Univariate polynomials

- For each input variable X_i , univariate orthogonal polynomials $\{P_k^{(i)}, k \in \mathbb{N}\}$ are built:

$$\langle P_j^{(i)}, P_k^{(i)} \rangle = \int P_j^{(i)}(u) P_k^{(i)}(u) f_{X_i}(u) du = \gamma_j^{(i)} \delta_{jk}$$

e.g., Legendre polynomials if $X_i \sim \mathcal{U}(-1, 1)$, Hermite polynomials if $X_i \sim \mathcal{N}(0, 1)$

- Normalization: $\Psi_j^{(i)} = P_j^{(i)} / \sqrt{\gamma_j^{(i)}} \quad i = 1, \dots, M, \quad j \in \mathbb{N}$

Tensor product construction

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

where $\alpha = (\alpha_1, \dots, \alpha_M)$ are multi-indices (partial degree in each dimension)

Computing the coefficients by least-square minimization

Isukapalli (1999); Berveiller, Sudret & Lemaire (2006)

Principle

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

$$Y = \mathcal{M}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X}) + \varepsilon_P \equiv \mathbf{Y}^{\top} \Psi(\mathbf{X}) + \varepsilon_P(\mathbf{X})$$

where : $\mathbf{Y} = \{y_{\alpha}, \alpha \in \mathcal{A}\} \equiv \{y_0, \dots, y_{P-1}\}$ (P unknown coefficients)

$$\Psi(\mathbf{x}) = \{\Psi_0(\mathbf{x}), \dots, \Psi_{P-1}(\mathbf{x})\}$$

Least-square minimization

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

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

Discrete (ordinary) least-square minimization

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

$$\hat{\mathbf{Y}} = \arg \min_{\mathbf{Y} \in \mathbb{R}^P} \frac{1}{n} \sum_{i=1}^n (\mathbf{Y}^\top \boldsymbol{\Psi}(\mathbf{x}^{(i)}) - \mathcal{M}(\mathbf{x}^{(i)}))^2$$

Procedure

- Select a truncation scheme, e.g. $\mathcal{A}^{M,p} = \{\boldsymbol{\alpha} \in \mathbb{N}^M : |\boldsymbol{\alpha}|_1 \leq p\}$
- Select an **experimental design** and evaluate the model response

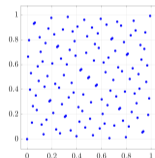
$$\mathbf{M} = \{\mathcal{M}(\mathbf{x}^{(1)}), \dots, \mathcal{M}(\mathbf{x}^{(n)})\}^\top$$

- Compute the experimental matrix

$$\mathbf{A}_{ij} = \Psi_j(\mathbf{x}^{(i)}) \quad i = 1, \dots, n; j = 0, \dots, P-1$$

- Solve the resulting **linear system**

$$\hat{\mathbf{Y}} = (\mathbf{A}^\top \mathbf{A})^{-1} \mathbf{A}^\top \mathbf{M}$$



Simple is beautiful !

Error estimators

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

$$E_{gen} = \mathbb{E} \left[(\mathcal{M}(\mathbf{X}) - \mathcal{M}^{PC}(\mathbf{X}))^2 \right] \quad \mathcal{M}^{PC}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X})$$

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

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

Leave-one-out cross validation

- From statistical learning theory, **model validation** shall be carried out using independent data

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

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

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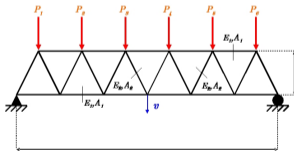
Conclusions

Curse of dimensionality

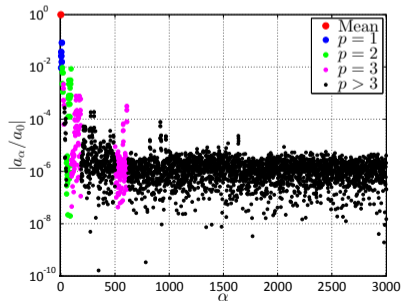
- The cardinality of the truncation scheme $\mathcal{A}^{M,p}$ is $P = \frac{(M+p)!}{M!p!}$
- Typical computational requirements: $n = OSR \cdot P$ where the **oversampling rate** is $OSR = 2 - 3$

However ... most coefficients are close to zero !

Example



- Elastic truss structure with $M = 10$ independent input variables
- PCE of degree $p = 5$ ($P = 3,003$ coefficients)



Compressive sensing approaches

Blatman & Sudret (2011); Doostan & Owhadi (2011); Sargsyan *et al.* (2014); Jakeman *et al.* (2015)

- Sparsity in the solution can be induced by ℓ_1 -regularization:

$$\mathbf{y}_\alpha = \arg \min \frac{1}{n} \sum_{i=1}^n \left(\mathbf{Y}^\top \boldsymbol{\Psi}(\mathbf{x}^{(i)}) - \mathcal{M}(\mathbf{x}^{(i)}) \right)^2 + \lambda \|\mathbf{y}_\alpha\|_1$$

- **Different algorithms:** LASSO, orthogonal matching pursuit, LARS, Bayesian compressive sensing, subspace pursuit, etc.

- State-of-the-art-review and comparisons available in:

Lüthen, N., Marelli, S. & Sudret, B. *Sparse polynomial chaos expansions: Literature survey and benchmark*, SIAM/ASA J. Unc. Quant., 2021, 9, 593-649 <https://doi.org/10.1137/20M1315774>

–, *Automatic selection of basis-adaptive sparse polynomial chaos expansions for engineering applications*, Int. J. Uncertainty Quantification, 2022, 12, 49-74

<https://doi.org/10.1615/Int.J.UncertaintyQuantification.2021036153>

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Post-processing sparse PC expansions

Statistical moments

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

$$\text{Mean: } \hat{\mu}_Y = y_0$$

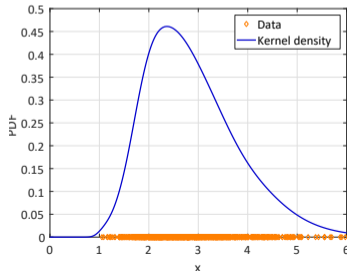
$$\text{Variance: } \hat{\sigma}_Y^2 = \sum_{\alpha \in \mathcal{A} \setminus \mathbf{0}} y_\alpha^2$$

Distribution of the QoI

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

$$\eta_j = \sum_{\alpha \in \mathcal{A}} y_\alpha \Psi_\alpha(\mathbf{x}_j) \quad j = 1, \dots, n_{big}$$

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



Sensitivity analysis

Goal

Sobol' (1993); Saltelli *et al.* (2008)

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

Hoeffding-Sobol' decomposition

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

$$\begin{aligned} \mathcal{M}(\mathbf{x}) &= \mathcal{M}_0 + \sum_{i=1}^M \mathcal{M}_i(x_i) + \sum_{1 \leq i < j \leq M} \mathcal{M}_{ij}(x_i, x_j) + \dots + \mathcal{M}_{12\dots M}(\mathbf{x}) \\ &= \mathcal{M}_0 + \sum_{\mathbf{u} \subset \{1, \dots, M\}} \mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \quad (\mathbf{x}_{\mathbf{u}} \stackrel{\text{def}}{=} \{x_{i_1}, \dots, x_{i_s}\}) \end{aligned}$$

- The summands satisfy the orthogonality condition:

$$\int_{[0,1]^M} \mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \mathcal{M}_{\mathbf{v}}(\mathbf{x}_{\mathbf{v}}) d\mathbf{x} = 0 \quad \forall \mathbf{u} \neq \mathbf{v}$$

Sobol' indices

Total variance:
$$D \equiv \text{Var} [\mathcal{M}(\mathbf{X})] = \sum_{\mathbf{u} \subset \{1, \dots, M\}} \text{Var} [\mathcal{M}_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})]$$

- Sobol' indices:

$$S_{\mathbf{u}} \stackrel{\text{def}}{=} \frac{\text{Var} [\mathcal{M}_{\mathbf{u}}(\mathbf{X}_{\mathbf{u}})]}{D}$$

- First-order Sobol' indices:

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

Quantify the **additive** effect of each input parameter **separately**

- Total Sobol' indices:

$$S_i^T \stackrel{\text{def}}{=} \sum_{\mathbf{u} \supset i} S_{\mathbf{u}}$$

Quantify the **total effect** of X_i , including interactions with the other variables.

Link with PC expansions

Sobol decomposition of a PC expansion

Sudret, CSM (2006); RESS (2008)

Obtained by reordering the terms of the (truncated) PC expansion $\mathcal{M}^{\text{PC}}(\mathbf{X}) \stackrel{\text{def}}{=} \sum_{\alpha \in \mathcal{A}} y_{\alpha} \Psi_{\alpha}(\mathbf{X})$

Interaction sets

For a given $\mathbf{u} \stackrel{\text{def}}{=} \{i_1, \dots, i_s\}$: $\mathcal{A}_{\mathbf{u}} = \{\alpha \in \mathcal{A} : k \in \mathbf{u} \Leftrightarrow \alpha_k \neq 0\}$

$$\mathcal{M}^{\text{PC}}(\mathbf{x}) = \mathcal{M}_0 + \sum_{\mathbf{u} \subset \{1, \dots, M\}} \mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \quad \text{where} \quad \mathcal{M}_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \stackrel{\text{def}}{=} \sum_{\alpha \in \mathcal{A}_{\mathbf{u}}} y_{\alpha} \Psi_{\alpha}(\mathbf{x})$$

PC-based Sobol' indices

$$S_{\mathbf{u}} = D_{\mathbf{u}}/D = \sum_{\alpha \in \mathcal{A}_{\mathbf{u}}} y_{\alpha}^2 / \sum_{\alpha \in \mathcal{A} \setminus \mathbf{0}} y_{\alpha}^2$$

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

Conclusions

- **Surrogate models** are unavoidable for solving uncertainty quantification problems involving costly computational models (e.g. finite element models)
- Depending on the analysis, specific surrogates are most suitable: **polynomial chaos expansions** for distribution- and sensitivity analysis, **Kriging** (and active learning) for reliability analysis
- **Sparse PCE and its extensions** (time warping, PC-NARX, PC-Kriging, DRSM, etc.) allow us to address a wide range of engineering problems, including **Bayesian inverse problems** (without the need for MCMC simulations)
- Techniques for constructing surrogates are **versatile, general-purpose** and **field-independent**
- All the presented algorithms are available in the general-purpose **uncertainty quantification software UQLab**

UQLab

The Framework for Uncertainty Quantification



OVERVIEW

FEATURES

DOCUMENTATION

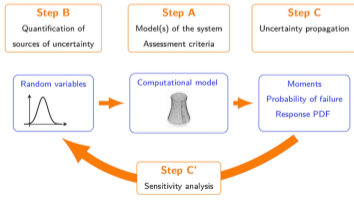
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| Italy | 221 |
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