ETH zürich

Risk, Safety & Uncertainty Quantification

# Surrogate models for global sensitivity analysis - Old and New

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Chair of Risk, Safety and Uncertainty Quantification

ETH Zurich

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# Chair of Risk, Safety and Uncertainty quantification

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

## Research topics

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

`http://www.rsuq.ethz.ch`

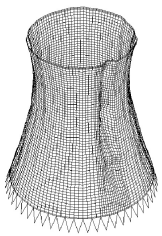
# Computational models in engineering

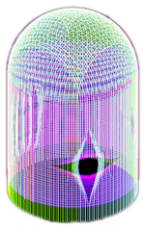
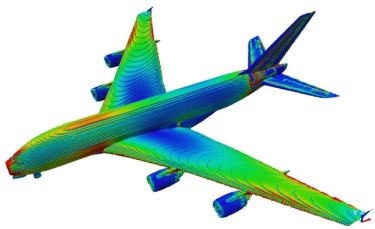
Complex engineering systems are designed and assessed using computational models, a.k.a simulators that comprise:

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

Computational models are used:

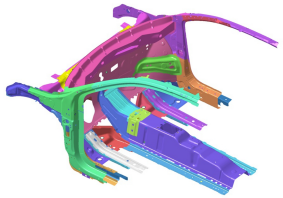
- Together with experimental data for calibration purposes
- To explore the design space ("virtual prototypes")
- To optimize the system (*e.g.* minimize the mass) under performance constraints
- To assess its robustness w.r.t uncertainty and its reliability



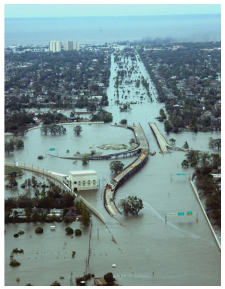



# Real world is uncertain

- 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/malevolent human actions (explosions, fire, etc.)



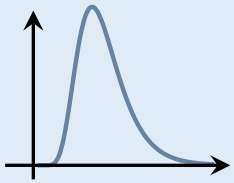
# Global framework for uncertainty quantification

**Step B**
Quantification of sources of uncertainty

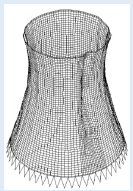
**Step A**
Model(s) of the system
Assessment criteria

**Step C**
Uncertainty propagation

Random variables



Computational model



Moments
Probability of failure
Response PDF

**Step C'**
Sensitivity analysis

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

# Surrogate models for uncertainty quantification

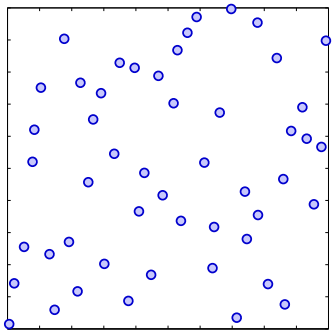
A surrogate model $\tilde{\mathcal{M}}$ is an approximation of the original computational model $\mathcal{M}$ with the following features:

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

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

# Ingredients for building a surrogate model

- Select an experimental design $\mathcal{X}$ that covers at best the domain of input parameters: Latin hypercube sampling (LHS), low-discrepancy sequences



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

# Advantages of surrogate models

## Usage

$$\underset{\text{hours per run}}{\mathcal{M}(\boldsymbol{x})} \quad \approx \quad \underset{\text{seconds for } 10^6 \text{ runs}}{\tilde{\mathcal{M}}(\boldsymbol{x})}$$

## Advantages

- Non-intrusive methods: based on runs of the computational model, exactly as in Monte Carlo simulation
- Construction suited to high performance computing: "embarrassingly parallel"

## Challenges

- Need for rigorous validation
- Communication: advanced mathematical background

Efficiency: 2-3 orders of magnitude less runs compared to Monte Carlo

# Outline

# Polynomial chaos expansions in a nutshell

Ghanem & Spanos (1991); Sudret & Der Kiureghian (2000); Xiu & Karniadakis (2002); Soize & Ghanem (2004)

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

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

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

  where :

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

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

# Multivariate polynomial basis

## Univariate polynomials

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

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

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

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

## Tensor product construction

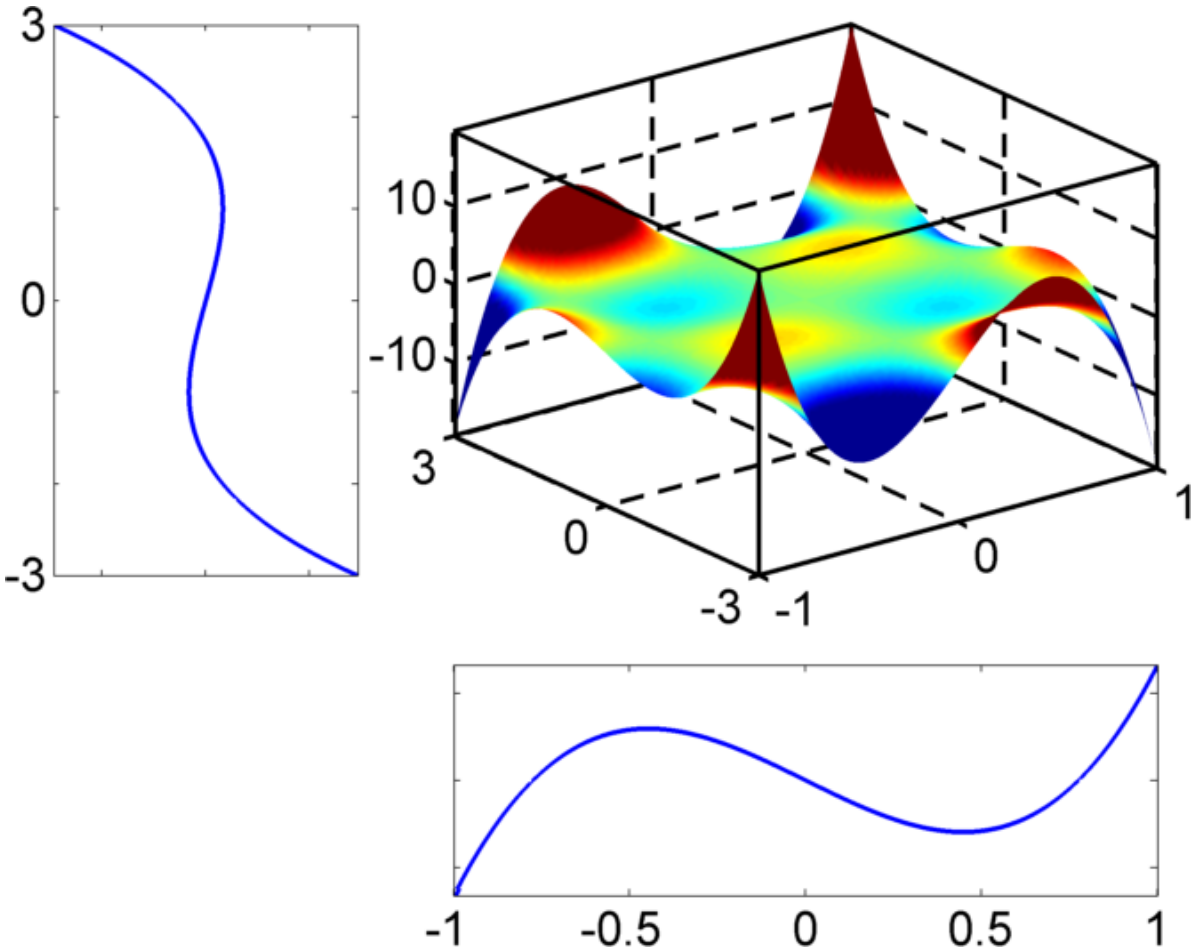
$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \overset{\text{def}}{=} \prod_{i=1}^{M} \Psi_{\alpha_i}^{(i)}(x_i) \qquad \mathbb{E}\left[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})\Psi_{\boldsymbol{\beta}}(\boldsymbol{X})\right] = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$$

where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_M)$ are multi-indices (partial degree in each dimension)

# Example: $M = 2$

Xiu & Karniadakis (2002)

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




- $X_1 \sim \mathcal{U}(-1, 1)$: Legendre polynomials
- $X_2 \sim \mathcal{N}(0, 1)$: Hermite polynomials

# Outline

# 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:

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

where : $\mathbf{Y} = \{y_{\boldsymbol{\alpha}}, \boldsymbol{\alpha} \in \mathcal{A}\} \equiv \{y_0, \ldots, y_{P-1}\}$ ($P$ unknown coef.)

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

## Least-square minimization

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

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

# Discrete (ordinary) least-square minimization

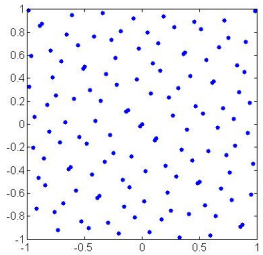
An estimate of the mean square error (sample average) is minimized:

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

## Procedure

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

$$\mathbf{M} = \left\{\mathcal{M}(\boldsymbol{x}^{(1)}), \ldots, \mathcal{M}(\boldsymbol{x}^{(n)})\right\}^\mathsf{T}$$



- Compute the experimental matrix

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

- Solve the resulting linear system

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

Simple is beautiful !

# Error estimators

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

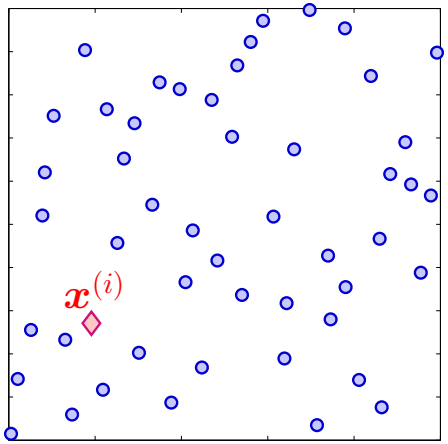
$$E_{gen} = \mathbb{E}\left[\left(\mathcal{M}(\boldsymbol{X}) - \mathcal{M}^{\mathsf{PC}}(\boldsymbol{X})\right)^2\right] \qquad \mathcal{M}^{\mathsf{PC}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} y_{\boldsymbol{\alpha}}\, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$$

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

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

Cross-validation techniques

# Leave-one-out cross validation




- An experimental design $\mathcal{X} = \{\boldsymbol{x}^{(j)},\ j = 1, \ldots, n\}$ is selected
- Polynomial chaos expansions are built using all points but one, *i.e.* based on $\mathcal{X} \backslash \boldsymbol{x}^{(i)} = \{\boldsymbol{x}^{(j)},\ j = 1, \ldots, n,\ j \neq i\}$

- Leave-one-out error (PRESS)

$$E_{LOO} \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} \left( \mathcal{M}(\boldsymbol{x}^{(i)}) - \mathcal{M}^{PC \backslash i}(\boldsymbol{x}^{(i)}) \right)^2$$

- Analytical derivation from a single PC analysis

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

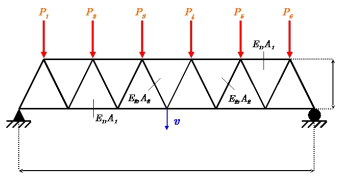
where $h_i$ is the $i$-th diagonal term of matrix $\mathbf{A}(\mathbf{A}^\mathsf{T}\mathbf{A})^{-1}\mathbf{A}^\mathsf{T}$

# Curse of dimensionality

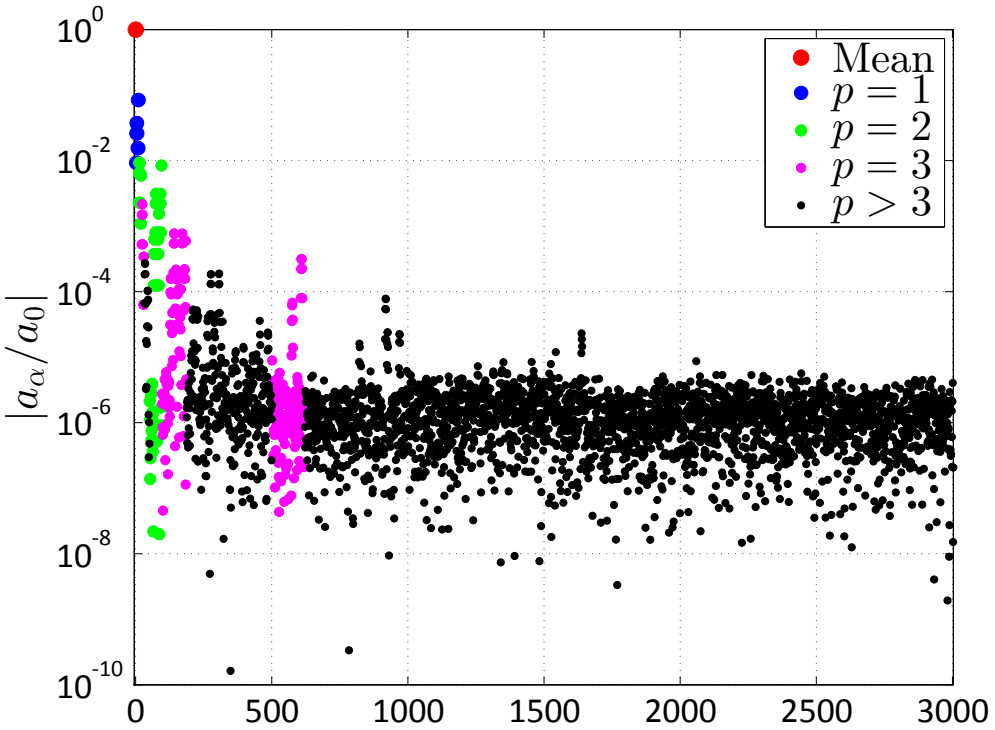
- The cardinality of the truncation scheme $\mathcal{A}^{M,p}$ is $P = \dfrac{(M+p)!}{M!\,p!}$
- Typical computational requirements: $n = OSR \cdot P$ where the oversampling rate is $OSR = 2 - 3$

However ... most coefficients are close to zero !

## Example



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



# Compressive sensing approaches

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

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

$$\boldsymbol{y}_{\boldsymbol{\alpha}} = \arg\min \frac{1}{n} \sum_{i=1}^{n} \left( \mathrm{Y}^{\mathsf{T}} \boldsymbol{\Psi}(\boldsymbol{x}^{(i)}) - \mathcal{M}(\boldsymbol{x}^{(i)}) \right)^2 + \lambda \parallel \boldsymbol{y}_{\boldsymbol{\alpha}} \parallel_1$$

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

## Least Angle Regression

Efron *et al.* (2004)
Blatman & Sudret (2011)

- Least Angle Regression (LAR) solves the LASSO problem for different values of the penalty constant in a single run without matrix inversions
- Leave-one-out cross validation error allows one to select the best model

# Outline

# Low-rank tensor representations

## Rank-1 function

A rank-1 function of $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}}$ is a product of univariate functions of each component:

$$w(\boldsymbol{x}) = \prod_{i=1}^{M} v^{(i)}(x_i)$$

## Canonical low-rank approximation (LRA)

A canonical decomposition of $\mathcal{M}(\boldsymbol{x})$ is of the form Nouy (2010)

$$\mathcal{M}^{\mathrm{LRA}}(\boldsymbol{x}) = \sum_{l=1}^{R} b_l \left( \prod_{i=1}^{M} v_l^{(i)}(x_i) \right)$$

where:

- $R$ is the rank (# terms in the sum)
- $v_l^{(i)}(x_i)$ are univariate function of $x_i$
- $b_l$ are normalizing coefficients

# Low-rank tensor representations

## Polynomial expansions

Doostan et al., 2013

By expanding $v_l^{(i)}(X_i)$ onto a polynomial basis orthonormal w.r.t. $f_{X_i}$ one gets:

$$\widehat{Y} = \sum_{l=1}^{R} b_l \left( \prod_{i=1}^{M} \left( \sum_{k=0}^{p_i} z_{k,l}^{(i)} P_k^{(i)}(X_i) \right) \right)$$

where:

- $P_k^{(i)}(X_i)$ is $k$-th degree univariate polynomial of $X_i$
- $p_i$ is the maximum degree of $P_k^{(i)}$
- $z_{k,l}^{(i)}$ are coefficients of $P_k^{(i)}$ in the $l$-th rank-1 term

## Complexity

Assuming an isotropic representation ($p_i = p$), the number of unknown coefficients is $R(p\,M + 1)$

Linear increase with dimensionality $M$

# Greedy construction of the LRA

Chevreuil et al. (2015); Konakli & Sudret (2016)

- A greedy construction is carried out by iteratively adding rank-1 terms. The $r$-th approximation reads $\widehat{Y}_r = \mathcal{M}_r(\boldsymbol{X}) = \sum_{l=1}^{r} b_l w_l(\boldsymbol{X})$
- In each iteration, alternate least-squares are used (correction and updating steps)

Correction step: sequential updating of $\boldsymbol{z}_r^{(j)}$, $j = 1, \ldots, M$, to build $w_r$:

$$\boldsymbol{z}_r^{(j)} = \arg\min_{\boldsymbol{\zeta} \in \mathbb{R}^{p_j}} \left\| \mathcal{M} - \widehat{\mathcal{M}}_{r-1} - \left( \prod_{i \neq j} \sum_{k=0}^{p_i} z_{k,r}^{(i)} P_k^{(i)} \right) \left( \sum_{k=0}^{p_j} \zeta_k P_k^{(j)} \right) \right\|_{\mathcal{E}}^2$$

Updating step: evaluation of normalizing coefficients $\{b_1, \ldots, b_r\}$:

$$\boldsymbol{b} = \arg\min_{\boldsymbol{\beta} \in \mathbb{R}^{r}} \left\| \mathcal{M} - \sum_{l=1}^{r} \beta_l w_l \right\|_{\mathcal{E}}^2$$

# Outline

# Hoeffding-Sobol' decomposition

Consider a square integrable function $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}} \subset \mathbb{R}^M \mapsto \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}$, where the independent input parameters are modelled by a random vector $\boldsymbol{X} \sim f_{\boldsymbol{X}}$.

## Hoeffding-Sobol' decomposition

$$\begin{aligned}\mathcal{M}(\boldsymbol{X}) &= \mathcal{M}_0 + \sum_{i=1}^{M} \mathcal{M}_i(X_i) + \sum_{1 \leq i < j \leq M} \mathcal{M}_{i,j}(X_i, X_j) + \ldots + \mathcal{M}_{1,2,\ldots,M}(\boldsymbol{X}) \\ &= \mathcal{M}_0 + \sum_{\substack{\mathbf{u} \subset \{1,\ldots,M\} \\ \mathbf{u} \neq \emptyset}} \mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}),\end{aligned}$$

where $\mathbf{u} = \{i_1, \ldots, i_s\}$, $1 \leq s \leq M$, denotes a subset of $\{1, \ldots, M\}$ and $\boldsymbol{X}_{\mathbf{u}} = \{X_{i_1}, \ldots, X_{i_s}\}$

# Hoeffding-Sobol' decomposition

## Orthogonality of the summands

$$\mathbb{E}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\ \mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}})\right] = 0 \qquad \forall\ \mathbf{u}, \mathbf{v} \subset \{1, \ldots, M\},\ \mathbf{u} \neq \mathbf{v}$$

## Construction

Introducing the conditional effects:

$$\widetilde{\mathcal{M}}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}) = \mathbb{E}\left[\mathcal{M}(\boldsymbol{X})|\boldsymbol{X}_{\mathbf{u}}\right]$$

One gets:

$$\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}) = \widetilde{\mathcal{M}}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}) - \sum_{\substack{\mathbf{v} \subset \mathbf{u} \\ \mathbf{v} \neq \mathbf{u}}} \mathcal{M}_{\mathbf{v}}(\boldsymbol{X}_{\mathbf{v}}).$$

In particular, the univariate effects read:

$$\widetilde{\mathcal{M}}_i(X_i) = \mathcal{M}_i(X_i) = \mathbb{E}\left[\mathcal{M}(\boldsymbol{X})|X_i\right]$$

# Sobol' indices

## Variance decomposition

$$\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right] = \sum_{i=1}^{M} D_i + \sum_{1 \leq i < j \leq M} D_{i,j} + \ldots + D_{1,2,\ldots,M} = \sum_{\substack{\mathbf{u} \subset \{1,\ldots,M\} \\ \mathbf{u} \neq \emptyset}} D_{\mathbf{u}}$$

where $D_{\mathbf{u}}$ is the partial variance

## Sobol'indices

$$S_{\mathbf{u}} = \frac{D_{\mathbf{u}}}{D} = \frac{\mathrm{Var}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right]}$$

## Group indices and total' indices

$$\widetilde{S}_{\mathbf{u}} = \frac{\mathrm{Var}\left[\widetilde{\mathcal{M}}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right]} = \sum_{\substack{\mathbf{v} \subset \mathbf{u} \\ \mathbf{v} \neq \emptyset}} S_{\mathbf{v}}$$

$$\widetilde{S}^T_{\mathbf{u}} = 1 - \frac{\mathrm{Var}\left[\widetilde{\mathcal{M}}_{\sim\mathbf{u}}(\boldsymbol{X}_{\sim\mathbf{u}})\right]}{\mathrm{Var}\left[\mathcal{M}(\boldsymbol{X})\right]} = \sum_{\substack{\mathbf{v} \subset \{1,\ldots,M\} \\ \mathbf{v} \cap \mathbf{u} \neq \emptyset}} S_{\mathbf{v}}$$

# Sobol decomposition of a polynomial chaos expansions

Sudret CSM (2006), Reliab. Eng. Sys. Safety (2008)

Consider a polynomial chaos expansion $\mathcal{M}^{\mathrm{PCE}}(\boldsymbol{X}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$.

The mean and variance read:

$$\mathbb{E}\left[\mathcal{M}^{\mathrm{PCE}}(\boldsymbol{X})\right] = y_{\mathbf{0}} \qquad \mathrm{Var}\left[\mathcal{M}^{\mathrm{PCE}}(\boldsymbol{X})\right] = \sum_{\boldsymbol{\alpha} \in \mathcal{A} \setminus \{\mathbf{0}\}} {y_{\boldsymbol{\alpha}}}^2$$

## Summands of a PCE

$$\mathcal{M}^{\mathrm{PCE}}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}) = \sum_{\boldsymbol{\alpha} \in \mathcal{A}_{\mathbf{u}}} y_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}), \qquad \mathcal{A}_{\mathbf{u}} = \{\boldsymbol{\alpha} \in \mathcal{A} \mid \alpha_k \neq 0 \Leftrightarrow k \in \mathbf{u}\}$$

## Conditional effects

$$\widetilde{\mathcal{M}}^{\mathrm{PCE}}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}}) = \sum_{\boldsymbol{\alpha} \in \widetilde{\mathcal{A}}_{\mathbf{u}}} y_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X}), \qquad \widetilde{\mathcal{A}}_{\mathbf{u}} = \{\boldsymbol{\alpha} \in \mathcal{A} \mid \alpha_i = 0 \; \forall \; i \notin \mathbf{u}\}$$

# Sobol indices from polynomial chaos expansions

Using:

$$D^{\mathrm{PCE}} = \mathrm{Var}\left[\mathcal{M}^{\mathrm{PCE}}(\boldsymbol{X})\right] = \sum_{\boldsymbol{\alpha}\in\mathcal{A}\setminus\{\mathbf{0}\}} {y_{\boldsymbol{\alpha}}}^2$$

one gets the:

- Sobol' indices

$$S_{\mathbf{u}} = \sum_{\boldsymbol{\alpha}\in\mathcal{A}_{\mathbf{u}}} {y_{\boldsymbol{\alpha}}}^2 / D^{\mathrm{PCE}}, \qquad \mathcal{A}_{\mathbf{u}} = \{\boldsymbol{\alpha}\in\mathcal{A} \mid \alpha_k \neq 0 \Leftrightarrow k \in \mathbf{u}\}$$

- Group Sobol' indices

$$\widetilde{S}_{\mathbf{u}}^{\mathrm{PCE}} = \sum_{\boldsymbol{\alpha}\in\widetilde{\mathcal{A}}_{\mathbf{u}}} {y_{\boldsymbol{\alpha}}}^2 / D^{\mathrm{PCE}}, \qquad \widetilde{\mathcal{A}}_{\mathbf{u}} = \{\boldsymbol{\alpha}\in\mathcal{A}\setminus\{\mathbf{0}\} \mid \alpha_i = 0 \ \forall\ i \notin \mathbf{u}\}$$

- Total Sobol' indices

$$\widetilde{S}_{\mathbf{u}}^{T,\mathrm{PCE}} = \sum_{\boldsymbol{\alpha}\in\widetilde{\mathcal{A}}_{\mathbf{u}}^{T}} {y_{\boldsymbol{\alpha}}}^2 / D^{\mathrm{PCE}}, \qquad \widetilde{\mathcal{A}}_{\mathbf{u}}^{T} = \{\boldsymbol{\alpha}\in\mathcal{A} \mid \exists\ i \in \mathbf{u} : \alpha_i > 0\}$$

# Outline

# Moments of LRA

Konakli & Sudret, Reliab. Eng. Sys. Safety (2016)

Consider the canonical decomposition:

$$\mathcal{M}^{\mathrm{LRA}}(\boldsymbol{X}) = \sum_{l=1}^{R} b_l \left( \prod_{i=1}^{M} \left( \sum_{k=0}^{p_i} z_{k,l}^{(i)} P_k^{(i)}(X_i) \right) \right)$$

## Mean value

$$\mathbb{E}\left[\mathcal{M}^{\mathrm{LRA}}(\boldsymbol{X})\right] = \sum_{l=1}^{R} \left[ b_l \cdot \prod_{i=1}^{M} z_{0,l}^{(i)} \right]$$

## Variance

$$D^{\mathrm{LRA}} \overset{\text{def}}{=} \mathrm{Var}\left[\mathcal{M}^{\mathrm{LRA}}(\boldsymbol{X})\right] = \sum_{l=1}^{R} \sum_{l'=1}^{R} b_l \, b_{l'} \left[ \prod_{i=1}^{M} \left( \sum_{k=0}^{p_i} z_{k,l}^{(i)} \, z_{k,l'}^{(i)} \right) - \prod_{i=1}^{M} z_{0,l}^{(i)} \, z_{0,l'}^{(i)} \right]$$

# Conditional effects

## Univariate effects

$$\widetilde{\mathcal{M}}_i^{\mathrm{LRA}}(X_i) = \sum_{l=1}^{R} b_l \left( \prod_{j \neq i}^{M} z_{0,l}^{(j)} \right) v_l^{(i)}(X_i)$$

## Conditional effects

$$\widetilde{\mathcal{M}}_{\mathbf{u}}^{\mathrm{LRA}}(\boldsymbol{X}_{\mathbf{u}}) = \sum_{l=1}^{R} b_l \left( \prod_{j \notin \mathbf{u}} z_{0,l}^{(j)} \right) \left( \prod_{i \in \mathbf{u}} v_l^{(i)}(X_i) \right)$$

## Group Sobol' indices

$$\widetilde{S}_{\mathbf{u}} = \left( \mathbb{E}\left[ \left( \widetilde{\mathcal{M}}_{\mathbf{u}}^{\mathrm{LRA}}(\boldsymbol{X}_{\mathbf{u}}) \right)^2 \right] - \mathcal{M}_{\mathbf{0}}^2 \right) / D^{\mathrm{LRA}}$$

with:

$$\mathbb{E}\left[ \left( \widetilde{\mathcal{M}}_{\mathbf{u}}^{\mathrm{LRA}}(\boldsymbol{X}_{\mathbf{u}}) \right)^2 \right] = \sum_{l=1}^{R} \sum_{l'=1}^{R} b_l \, b_{l'} \left( \prod_{j \notin \mathbf{u}} z_{0,l}^{(j)} \, z_{0,l'}^{(j)} \right) \left( \prod_{i \in \mathbf{u}} \left( \sum_{k=0}^{p_i} z_{k,l}^{(i)} \, z_{k,l'}^{(i)} \right) \right)$$

# Sobol and total Sobol indices

After some bookkeeping nightmare, one gets

- The first-order and group Sobol' indices at any order
- The total Sobol' indices

# Outline

# Sobol' function

## Problem statement

$$\mathcal{M}(\boldsymbol{X}) = \prod_{i=1}^{20} \frac{|4X_i - 2| + c_i}{1 + c_i} \qquad X_i \sim \mathcal{U}(0, 1) \quad \text{independent uniform}$$

where:

$$\boldsymbol{c} = \{1, 2, 5, 10, 20, 50, 100, 500, 500, 500, \ldots, 500\}^{\mathsf{T}}$$

## Analytical solution for Sobol' indices

$$S_{i_1, \ldots, i_s} = \frac{1}{D} \prod_{i=i_1}^{i_s} D_i$$

where:

$$D_i = \frac{1}{3(1 + c_i)^2} \qquad D = \prod_{i=1}^{M} (D_i + 1) - 1$$

# Sobol' function – Results

## Quality of the surrogate models

**Generalization error – Experimental design: Sobol' sequences, validation set of size** $10^6$

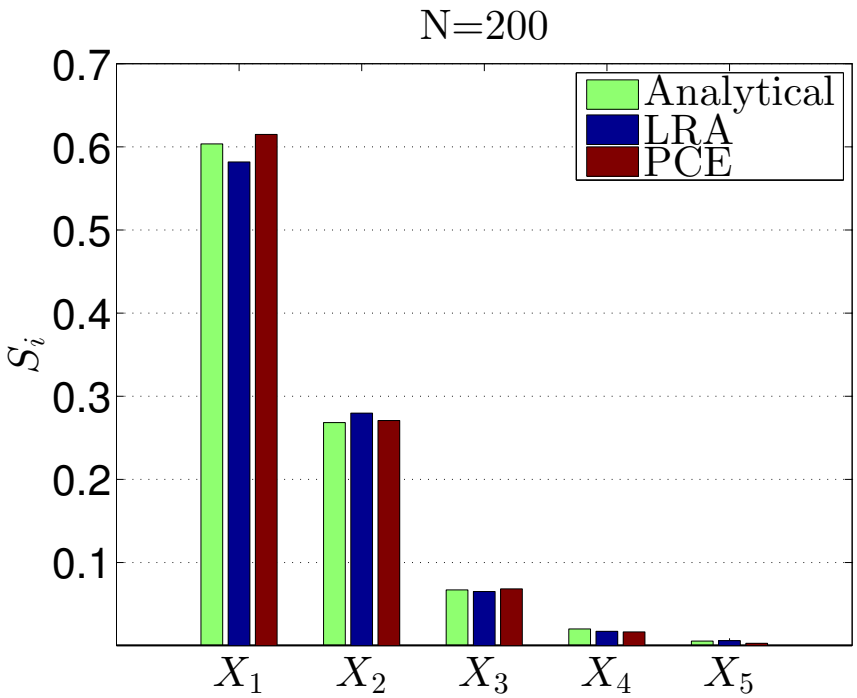
| N | $\widehat{err}_G^{\text{LRA}}$ | $\widehat{err}_G^{\text{PCE}}$ |
|---|---|---|
| 100 | $8.08 \cdot 10^{-2}$ | $5.46 \cdot 10^{-2}$ |
| 200 | $2.57 \cdot 10^{-2}$ | $3.64 \cdot 10^{-2}$ |
| 500 | $2.32 \cdot 10^{-3}$ | $1.45 \cdot 10^{-2}$ |
| 1,000 | $4.68 \cdot 10^{-4}$ | $6.34 \cdot 10^{-3}$ |
| 2,000 | $2.03 \cdot 10^{-4}$ | $2.48 \cdot 10^{-3}$ |

## Moments

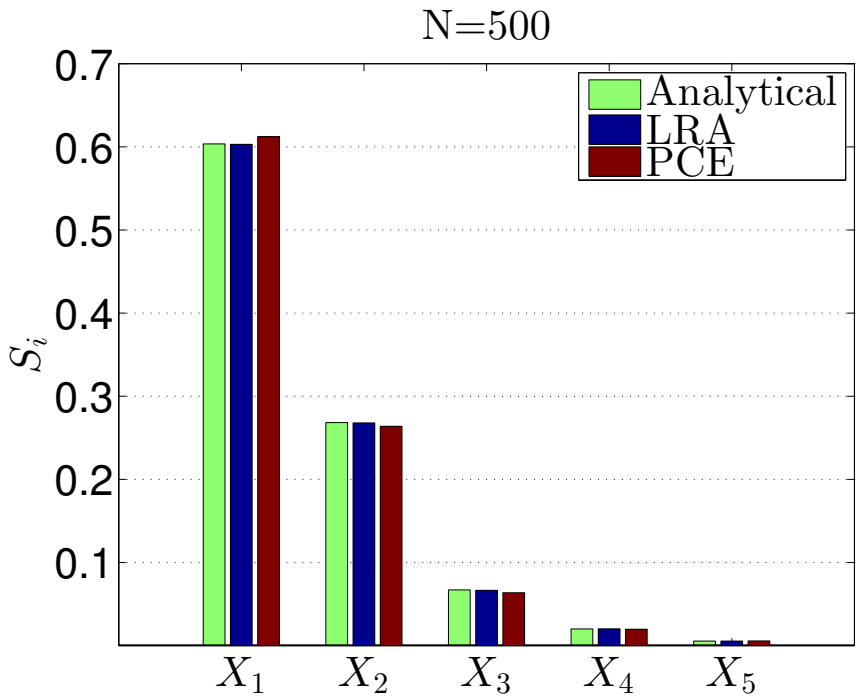
**Mean and standard deviation of response**

| | | $N = 200$ | | $N = 500$ | |
|---|---|---|---|---|---|
| | Analytical | LRA ($\varepsilon\%$) | PCE ($\varepsilon\%$) | LRA ($\varepsilon\%$) | PCE ($\varepsilon\%$) |
| $\mu_Y$ | 1.000 | 1.005 (0.5) | 0.998 ($-0.2$) | 1.000 (0.0) | 0.995 ($-0.5$) |
| $\sigma_Y$ | 0.3715 | 0.3820 (2.8) | 0.3424 ($-7.8$) | 0.3715 (0.0) | 0.3536 ($-4.8$) |

# Sobol' function – First order Sobol' indices

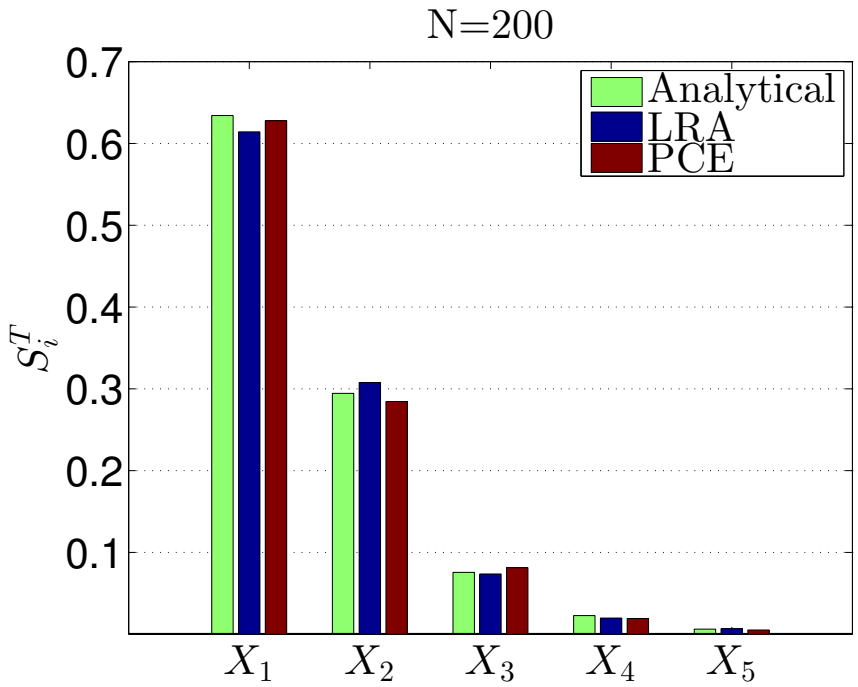



$N = 200$ **points**

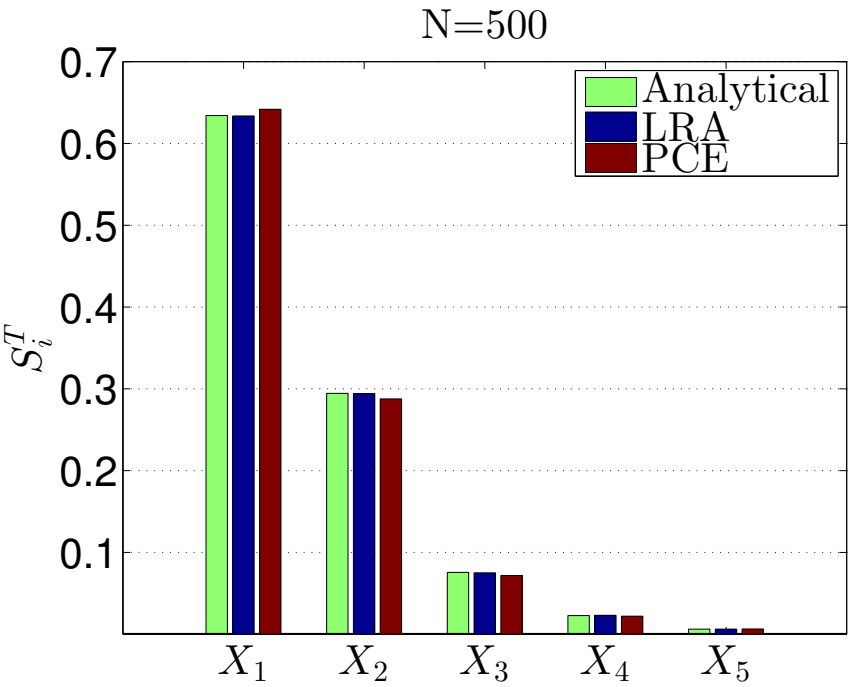



$N = 500$ **points**

# Sobol' function – Total Sobol' indices

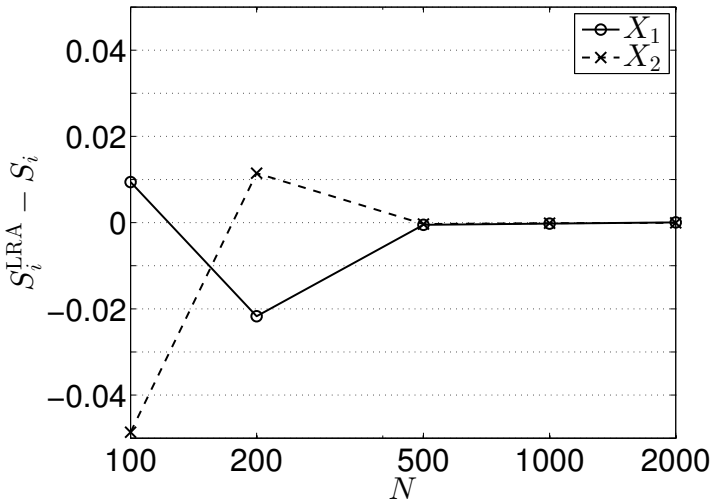



$N = 200$ **points**

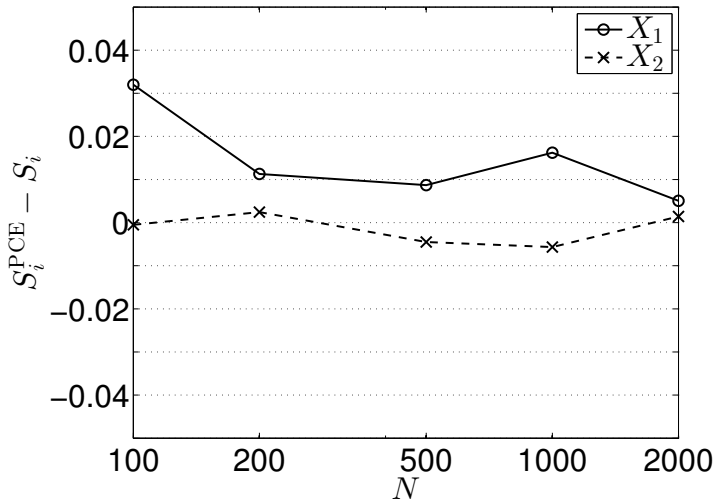



$N = 500$ **points**

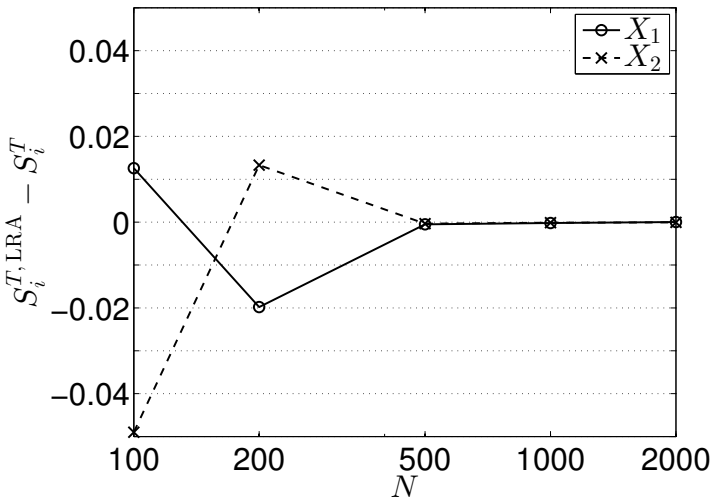
# Sobol' function – convergence



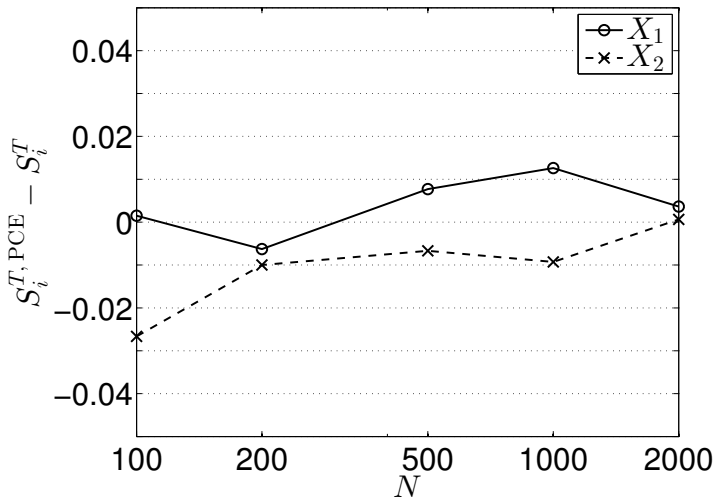

**LRA - First order indices**




**PCE - First order indices**

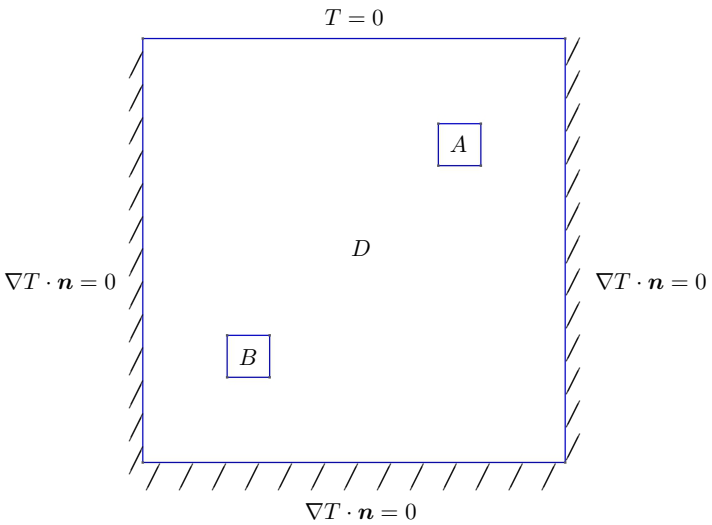



**LRA - Total indices**




**PCE - Total indices**

# Stationary heat conduction – problem statement




Heat conduction in $D = 1\mathrm{m} \times 1\mathrm{m}$

$$-\nabla(\kappa(\boldsymbol{z})\ \nabla T(\boldsymbol{z})) = 500\ I_A(\boldsymbol{z})$$

Thermal conductivity (lognormal random field)

$$\kappa(\boldsymbol{z}) = \exp[a_\kappa + b_\kappa\ g(\boldsymbol{z})] \qquad \left[\frac{\mathrm{W}}{^\circ\mathrm{C} \cdot \mathrm{m}}\right]$$

- $g(\boldsymbol{z})$: standard normal random field with:

$$\rho(\boldsymbol{z}, \boldsymbol{z}') = \exp\left(-\|\boldsymbol{z} - \boldsymbol{z}'\|^2/\ell^2\right)$$

$$\mu_\kappa = 1, \quad \sigma_\kappa = 0.3, \quad \ell = 0.2\ m$$

# Random field discretization

## Expansion Optimal Linear Estimation (EOLE)

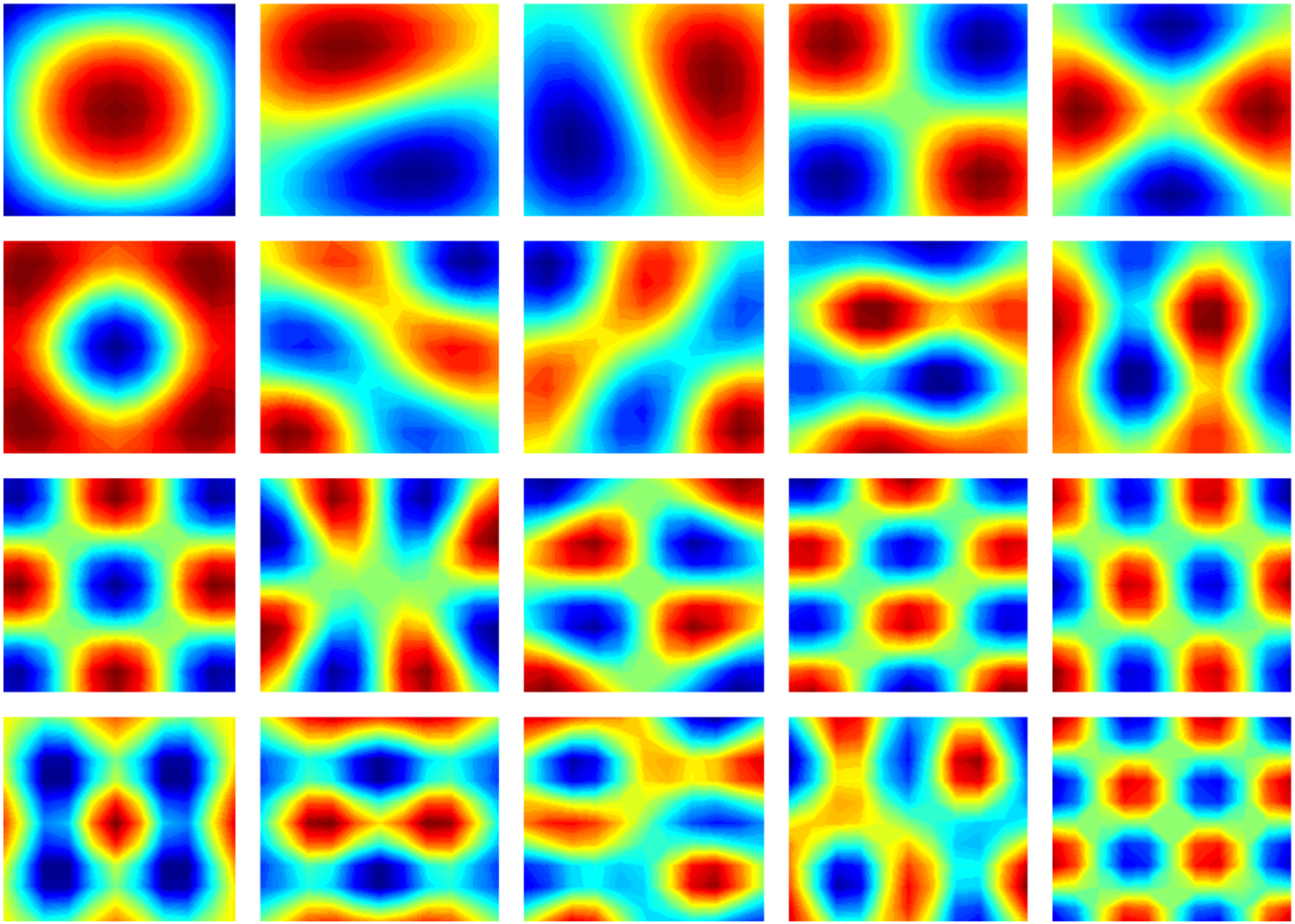
Li & Der Kiureghian (1993)

For an appropriately defined grid $\{\boldsymbol{\zeta}_1, \ldots, \boldsymbol{\zeta}_n\}$ in $D$:

$$\widehat{g}(\boldsymbol{z}) = \sum_{i=1}^{M} \frac{\xi_i}{\sqrt{l_i}} \boldsymbol{\phi}_i^{\mathrm{T}} \boldsymbol{C}_{\boldsymbol{z}\boldsymbol{\zeta}}$$

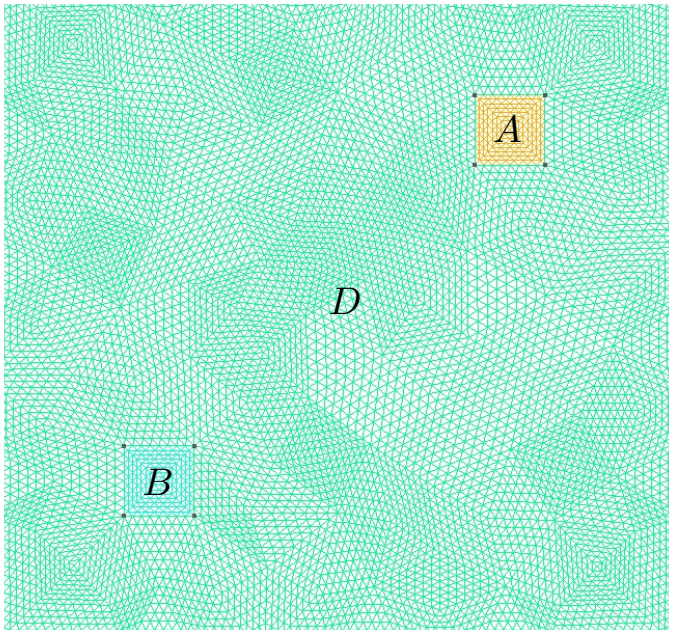
- $\xi_i \sim \mathcal{N}(0,1)$
- $(l_i, \boldsymbol{\phi}_i)$: (eigenvalues, eigenvectors) of matrix $\boldsymbol{C}_{\boldsymbol{\zeta}\boldsymbol{\zeta}}$ with $\boldsymbol{C}_{\boldsymbol{\zeta}\boldsymbol{\zeta}}^{(k,l)} = \rho(\boldsymbol{\zeta}_k, \boldsymbol{\zeta}_l)$, $k, l = 1, \ldots, n$
- $\boldsymbol{C}_{\boldsymbol{z}\boldsymbol{\zeta}}^{(k)} = \rho(\boldsymbol{z}, \boldsymbol{\zeta}_k)$, $k = 1, \ldots, n$
- **M=53 modes** are selected to represent $99\%$ of the spectrum

# Random field discretization

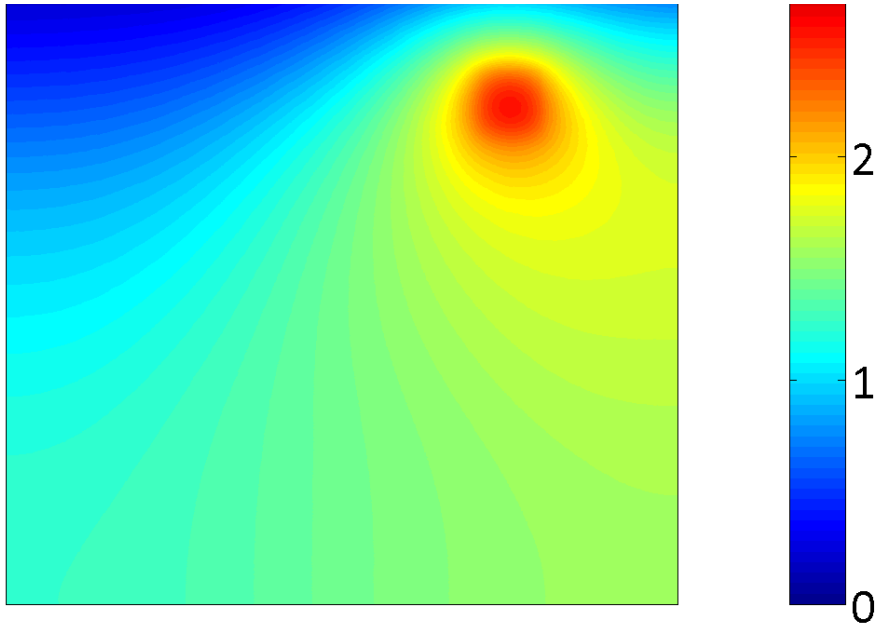


**Shapes of first 20 spatial functions in EOLE discretization**

# Stationary heat conduction - finite element model




**Finite element discretization**

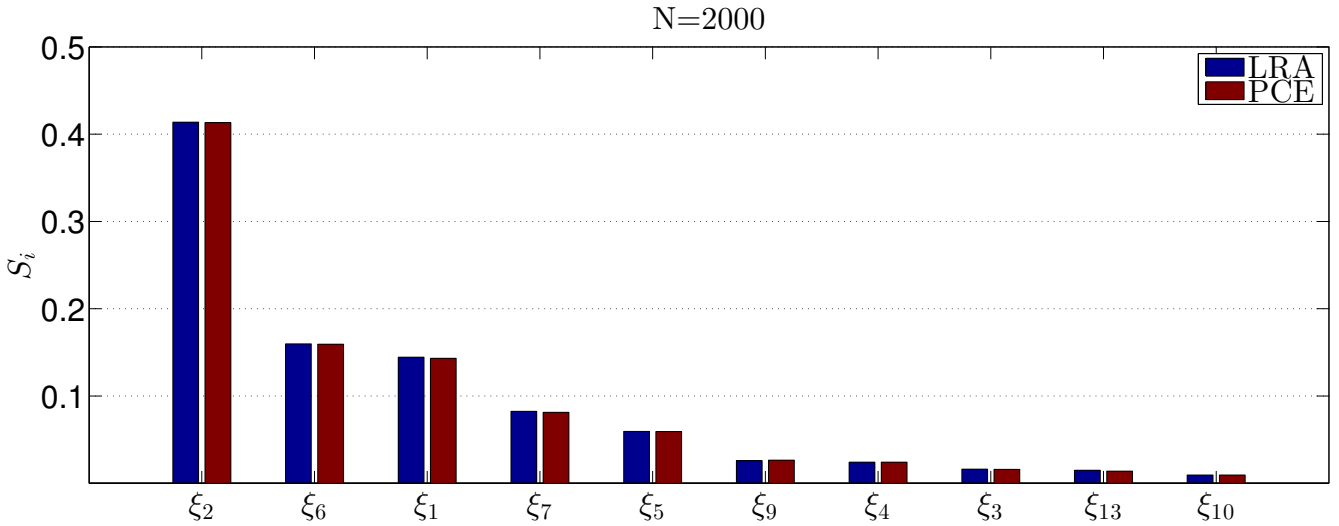



**Temperature field**

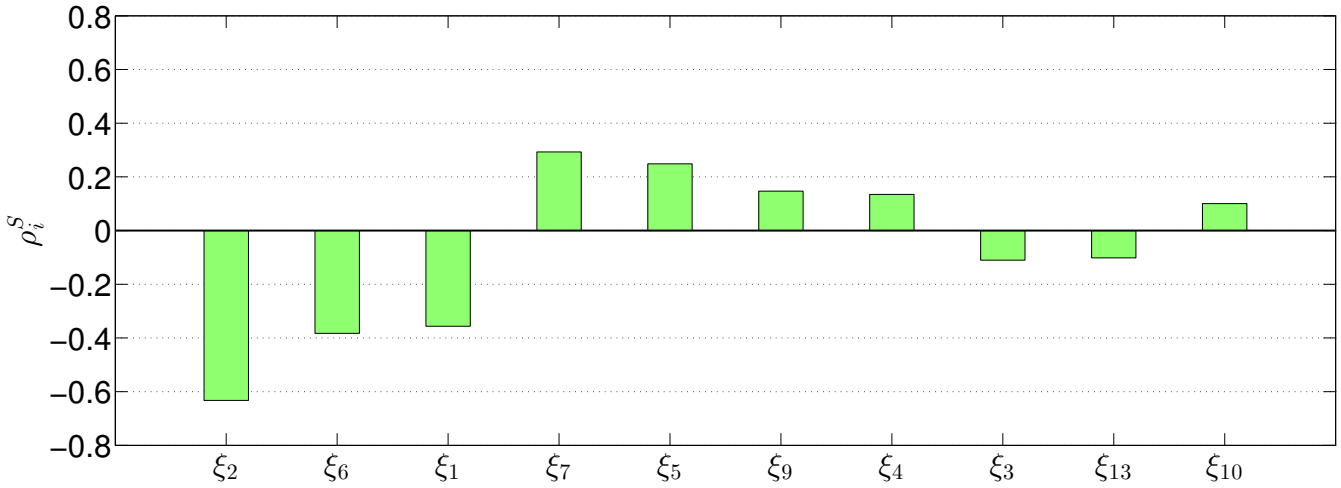
## Quantity of interest

$$\widetilde{T} = \frac{1}{|B|} \int_{\boldsymbol{z} \in B} T(\boldsymbol{z}) \, d\boldsymbol{z} \quad [^\circ\mathrm{C}]$$

# Sobol' indices obtained from the two surrogate models

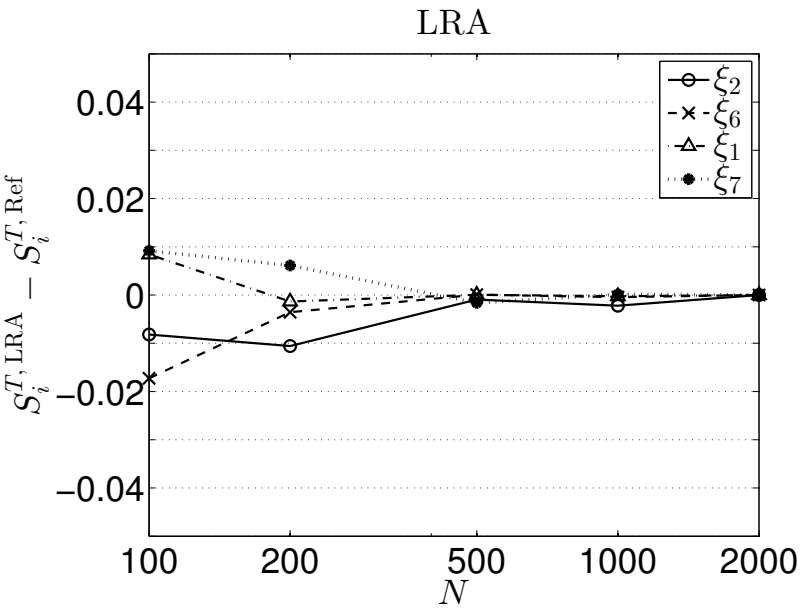



**First order Sobol' indices**

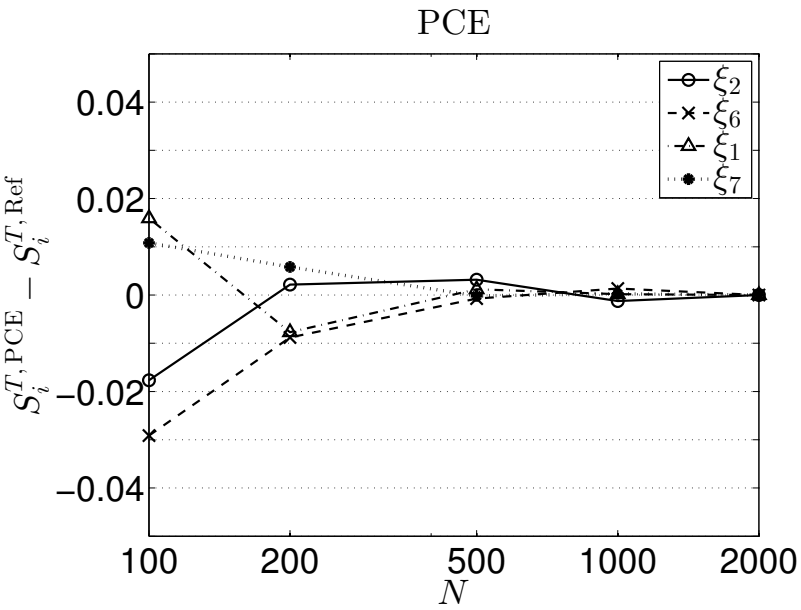



**I/O rank correlation**

# Heat transfer - convergence




**LRA surrogate**




**PCE surrogate**

- Only 10 out of 53 parameters influence the output
- From an experimental design size of 500 the results are accurate enough

# Outline

# Gaussian process modelling

Gaussian process modelling (*a.k.a.* Kriging) assumes that the map $y = \mathcal{M}(\boldsymbol{x})$ is a realization of a Gaussian process:

$$Y(\boldsymbol{x}, \omega) = \sum_{j=1}^{p} \beta_j \, f_j(\boldsymbol{x}) + \sigma \, Z(\boldsymbol{x}, \omega)$$

where:

- $\boldsymbol{f} = \{f_j, j = 1, \ldots, p\}^\mathsf{T}$ are predefined (*e.g.* polynomial) functions which form the trend or regression part
- $\boldsymbol{\beta} = \{\beta_1, \ldots, \beta_p\}^\mathsf{T}$ are the regression coefficients
- $\sigma^2$ is the variance of $Y(\boldsymbol{x}, \omega)$
- $Z(\boldsymbol{x}, \omega)$ is a stationary, zero-mean, unit-variance Gaussian process

$$\mathbb{E}\left[Z(\boldsymbol{x}, \omega)\right] = 0 \qquad \mathrm{Var}\left[Z(\boldsymbol{x}, \omega)\right] = 1 \qquad \forall \, \boldsymbol{x} \in \mathbb{X}$$

The Gaussian measure artificially introduced is different from the aleatory uncertainty on the model parameters $\boldsymbol{X}$

# Assumptions on the trend and the zero-mean process

Prior assumptions are made based on the existing knowledge on the model to surrogate (linearity, smoothness, etc.)

## Trend

- Simple Kriging: known constant $\beta$
- Ordinary Kriging: $p = 1$, unknown constant $\beta$
- Universal Kriging: $f_j$'s is a set of polynomial functions, *e.g.* $\left\{f_j(x) = x^{j-1},\, j = 1, \ldots, p\right\}$ in 1D

## Type of auto-correlation function of $Z(\boldsymbol{x})$

A family of auto-correlation function $R(\cdot;\, \boldsymbol{\theta})$ is selected:

$$\mathrm{Cov}\left[Z(\boldsymbol{x}), Z(\boldsymbol{x}')\right] = \sigma^2\, R(\boldsymbol{x}, \boldsymbol{x}';\, \boldsymbol{\theta})$$

*e.g.* Gaussian, generalized exponential, Matérn, etc.

# Matérn autocorrelation function (1D)

## Definition

$$R_1(x, x') = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left( \sqrt{2\,\nu}\, \frac{|x - x'|}{\ell} \right)^{\nu} \kappa_\nu \left( \sqrt{2\,\nu}\, \frac{|x - x'|}{\ell} \right)$$

where $\nu \geq 1/2$ is the shape parameter, $\ell$ is the scale parameter, $\Gamma(\cdot)$ is the Gamma function and $\kappa_\nu(\cdot)$ is the modified Bessel function of the second kind

## Properties

The values $\nu = 3/2$ and $\nu = 5/2$ are usually used $\left( h = \frac{|x - x'|}{\ell} \right)$:

$$R_1(h;\, \nu = 3/2) = (1 + \sqrt{3}\, h) \exp(-\sqrt{3}\, h)$$

$$R_1(h;\, \nu = 5/2) = (1 + \sqrt{5}\, h + \frac{5}{3}\, h^2) \exp(-\sqrt{5}\, h)$$

# Two approaches to Kriging

## Data

- Given is an experimental design $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ and the output of the computational model $\boldsymbol{y} = \{y_1 = \mathcal{M}(\boldsymbol{x}_1), \ldots, y_N = \mathcal{M}(\boldsymbol{x}_N)\}$
- We assume that $\mathcal{M}(\boldsymbol{x})$ is a realization of a Gaussian process $Y(\boldsymbol{x})$ such that the values $y_i = \mathcal{M}(\boldsymbol{x}_i)$ are known at the various points $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$
- Of interest is the prediction at a new point $\boldsymbol{x}_0 \in \mathbb{X}$, denoted by $\hat{Y}_0 \equiv \hat{Y}(\boldsymbol{x}_0, \omega)$, which will be used as a surrogate $\tilde{\mathcal{M}}(\boldsymbol{x}_0)$

## Two visions

- $\hat{Y}_0$ is obtained as a linear combination of the observations: BLUP
- $\hat{Y}_0$ is considered as a conditional Gaussian process:

$$\hat{Y}_0 = Y\left(\boldsymbol{x}_0 \mid Y(\boldsymbol{x}_1) = y_1, \ldots, Y(\boldsymbol{x}_N) = y_N\right)$$

# Mean predictor

Santner, William & Notz (2003)

The prediction in a new point $\boldsymbol{x}_0 \in \mathcal{D}_{\boldsymbol{X}}$ is a Gaussian variable:

$$\widehat{Y}_0 \sim \mathcal{N}(\mu_{\widehat{Y}_0}, \sigma^2_{\widehat{Y}_0})$$

## Surrogate model: mean predictor

$$\mu_{\widehat{Y}_0} = \boldsymbol{f}_0^{\mathsf{T}}\,\widehat{\boldsymbol{\beta}} + \boldsymbol{r}_0^{\mathsf{T}}\mathbf{R}^{-1}\left(\boldsymbol{y} - \mathbf{F}\,\widehat{\boldsymbol{\beta}}\right)$$

where the regression coefficients $\widehat{\boldsymbol{\beta}}$ are obtained from the generalized least-square solution:

$$\widehat{\boldsymbol{\beta}} = \left(\mathbf{F}^{\mathsf{T}}\,\mathbf{R}^{-1}\,\mathbf{F}\right)^{-1}\,\mathbf{F}^{\mathsf{T}}\,\mathbf{R}^{-1}\,\boldsymbol{y}$$

## Properties

- The mean predictor has a regression part $\boldsymbol{f}_0^{\mathsf{T}}\,\widehat{\boldsymbol{\beta}} = \sum_{j=1}^{p}\widehat{\beta}_j\,f_j(\boldsymbol{x}_0)$ and a local correction
- It interpolates the experimental design:

$$\mu_{\widehat{Y}_i} \equiv \mu_{\widehat{Y}(\boldsymbol{x}_i)} = y_i \qquad \forall\,\boldsymbol{x}_i \in \mathcal{X}$$

# Kriging variance

- The Kriging variance reads:

$$\sigma^2_{\widehat{Y}_0} = \mathbb{E}\left[(\widehat{Y}_0 - Y_0)^2\right] = \sigma^2 \left(1 - \boldsymbol{r}_0^{\mathsf{T}} \mathbf{R}^{-1} \boldsymbol{r}_0 + \boldsymbol{u}_0^{\mathsf{T}} \left(\mathbf{F}^{\mathsf{T}} \mathbf{R}^{-1} \mathbf{F}\right)^{-1} \boldsymbol{u}_0\right)$$

with $\boldsymbol{u}_0 = \mathbf{F}^{\mathsf{T}} \mathbf{R}^{-1} \boldsymbol{r}_0 - \boldsymbol{f}_0$

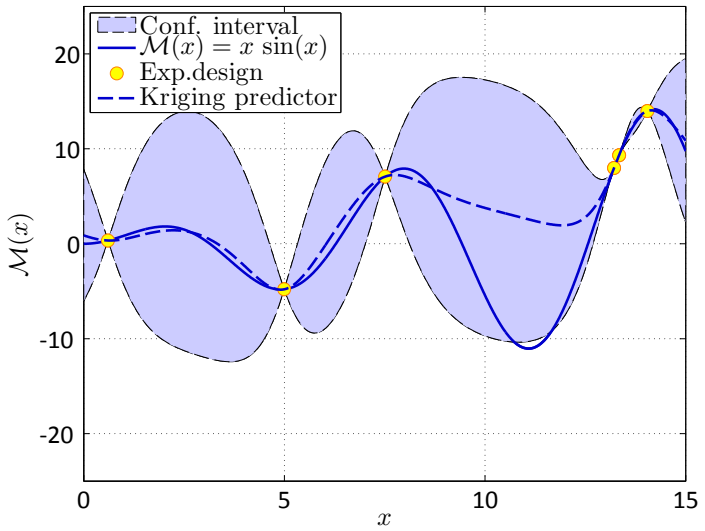
- The Kriging predictor is interpolating the data in the experimental design:

$$\sigma^2_{\widehat{Y}_i} \equiv \sigma^2_{\widehat{Y}(\boldsymbol{x}_i)} = 0 \qquad \forall\, \boldsymbol{x}_i \in \mathcal{X}$$

# Confidence intervals

- Due to Gaussianity of the predictor $\widehat{Y}_0 \sim \mathcal{N}(\mu_{\widehat{Y}_0}, \sigma^2_{\widehat{Y}_0})$, one can derive confidence intervals on the prediction

- With confidence level $(1-\alpha)$, *e.g.* 95%, one gets:




$$\mu_{\widehat{Y}_0} - 1.96\,\sigma_{\widehat{Y}_0} \leq \mathcal{M}(\boldsymbol{x}_0) \leq \mu_{\widehat{Y}_0} + 1.96\,\sigma_{\widehat{Y}_0}$$

- Realizations of the conditional random field may be obtained from those of the unconditional field

# Application to sensitivity analysis

Marrel *et al.* (2008,2009), Le Gratiet, Cannamela & Iooss (2014)

Le Gratiet, Marelli and Sudret, Handbook on Uncertainty Quantification (2016)

## Reformulation

$$S_{\mathbf{u}} = \frac{\mathrm{Var}\left[\mathbb{E}\left[Y|\boldsymbol{X}_{\mathbf{u}}\right]\right]}{\mathrm{Var}\left[Y\right]} = \frac{\mathrm{Cov}\left[Y,\, Y^{\mathbf{u}}\right]}{\mathrm{Var}\left[Y\right]}$$

where:

- The components of $\boldsymbol{X}$ are split into two groups $\boldsymbol{X} = (\boldsymbol{X}_{\mathbf{u}}, \boldsymbol{X}_{\sim\mathbf{u}})$
- $\boldsymbol{X}'$ is an independent copy of $\boldsymbol{X}$
- and:

$$Y \overset{\text{def}}{=} \mathcal{M}(\boldsymbol{X})$$

$$Y^{\mathbf{u}} \overset{\text{def}}{=} \mathcal{M}(\boldsymbol{X}_{\mathbf{u}}, \boldsymbol{X}'_{\sim\mathbf{u}})$$

# Monte Carlo estimators

Sobol' (1993, 2001)

Consider two sample sets $\boldsymbol{\chi} = \left\{\boldsymbol{x}^1, \ldots, \boldsymbol{x}^N\right\}$ and $\boldsymbol{\chi}' = \{\boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_N\}$ and define:

$$y_i = \mathcal{M}(\boldsymbol{x}^i) \qquad y_i^{\mathbf{u}} = \mathcal{M}(\boldsymbol{x}^i_{\mathbf{u}}, \boldsymbol{x}'^i_{\sim\mathbf{u}})$$

$$\bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i \qquad \bar{y}^{\mathbf{u}} = \frac{1}{N}\sum_{i=1}^{N} y_i^{\mathbf{u}}$$

- Homma-Saltelli:

$$\widehat{S_{\mathbf{u}}^{HS}} = \frac{\frac{1}{N}\sum_{i=1}^{N} y_i\, y_i^{\mathbf{u}} - \bar{y}\cdot\bar{y}^{\mathbf{u}}}{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - \bar{y}\right)^2}$$

- Janon:

$$\widehat{S_{\mathbf{u}}^{J}} = \frac{\frac{1}{N}\sum_{i=1}^{N} y_i\, y_i^{\mathbf{u}} - \left[(\bar{y}+\bar{y}^{\mathbf{u}})/2\right]^2}{\frac{1}{2N}\sum_{i=1}^{N}\left[(y_i)^2 + (y_i^{\mathbf{u}})^2\right] - \left[(\bar{y}+\bar{y}^{\mathbf{u}})/2\right]^2}$$

# Confidence intervals on Sobol' indices

## Plug-in estimators

- A Kriging surrogate model is calibrated
- Standard Monte Carlo estimators of the Sobol' indices can be computed straightforwardly using the surrogate

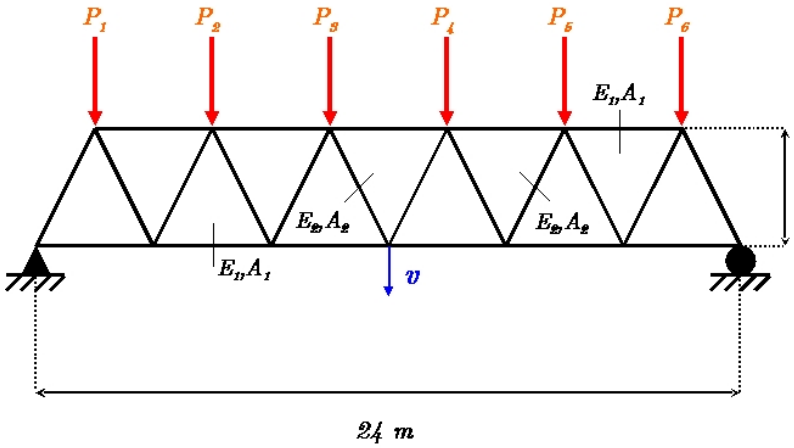
## Accounting for epistemic uncertainty

- Realizations of the conditional random process $\hat{Y}_0$ are sampled
- MCS estimates of the Sobol' indices are computed for each realization
- Summarizing statistics (mean, standard deviation) are obtained

# Application: elastic truss

## Structural model

Blatman & Sudret (2011)

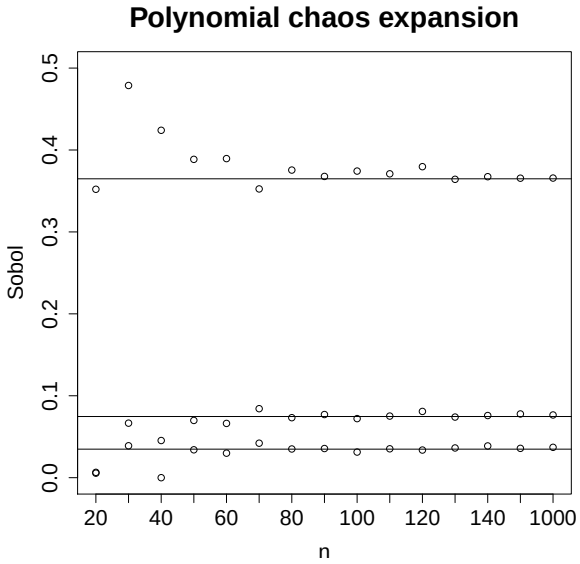


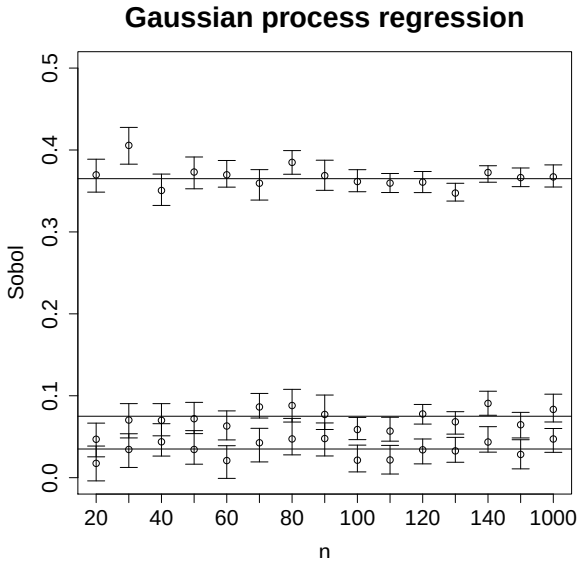

- Response quantity: maximum deflection $v$

## Probabilistic model

| Variable | Distribution | mean | CoV |
|---|---|---|---|
| Hor. bars cross section $A_1$ [m] | Lognormal | 0.002 | 0.10 |
| Oblique bars cross section $A_2$ [m] | Lognormal | 0.001 | 0.10 |
| Young's moduli $E_1, E_2$ [MPa] | Lognormal | 210,000 | 0.10 |
| Loads $P_1, \ldots, P_6$ [KN] | Gumbel | 50 | 0.15 |

# Sobol' first order indices




| Variable | Ref. | PCE | GP |
|---|---|---|---|
| $A_1$ | 0.365 | 0.366 | 0.384 |
| $E_1$ | 0.365 | 0.369 | 0.362 |
| $P_3$ | 0.075 | 0.078 | 0.075 |
| $P_4$ | 0.074 | 0.076 | 0.069 |
| $P_5$ | 0.035 | 0.036 | 0.029 |
| $P_2$ | 0.035 | 0.036 | 0.028 |
| $A_2$ | 0.011 | 0.012 | 0.015 |
| $E_2$ | 0.011 | 0.012 | 0.008 |
| $P_6$ | 0.003 | 0.005 | 0.002 |
| $P_1$ | 0.002 | 0.005 | 0.000 |

Le Gratiet, Marelli and Sudret, Handbook on Uncertainty Quantification (2016)

Confidence intervals can also be obtained from PCE by bootstrap

# Conclusions

- Surrogate models allow the analyst to replace complex computer codes by fast-to-evaluate functions, that can be sampled for global sensitivity analysis
- Polynomial chaos expansions and low-rank tensor approximations provide analytical expressions of the sensitivity indices at any order from the expansion coefficients
- These techniques allow to get accurate results with $\mathcal{O}(100)$ runs of the model up to dimension $M = 10 - 100)$
- Kriging allows one to account for epistemic uncertainty (associated with the surrogate model) by sampling conditional GPs, at a high cost though
- General purpose software implement the various approaches:
  - + R packages `sensitivity`, `CompModSA`, `DiceKriging`, `DiceDesign`, etc.
  - + UQLab


PUB

# UQLab

## The Framework for Uncertainty Quantification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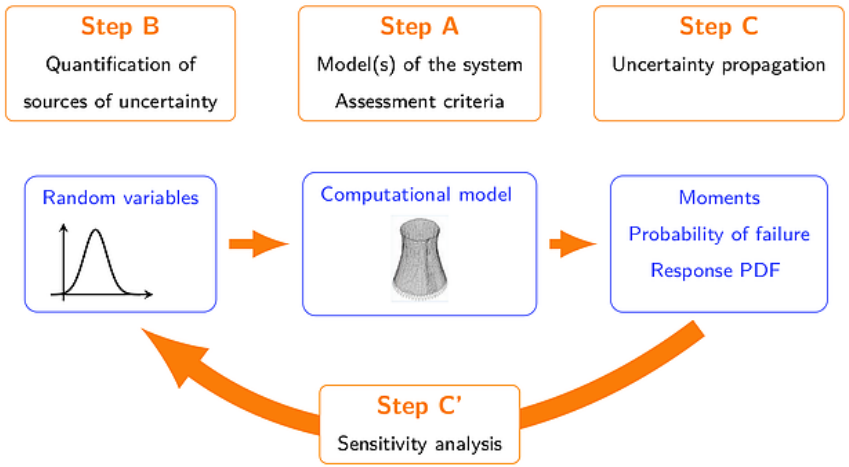
**"Make uncertainty quantification available for anybody, in any field of applied science and engineering"**




- MATLAB-based Uncertainty Quantification framework
- State-of-the art, highly optimized algorithms
- Easy to use and deploy
- Designed to be extended by users

http://www.uqlab.com

## Probabilistic input description

Define, transform and sample random distributions

**Key features:**

- Usual and custom marginals
- Dependence modelling through copulas
- Monte Carlo & Latin Hypercube sampling, low-discrepancy sequences

## Modelling

Connect your own simulation models to UQLab

**Key features:**

- Strings and inline function handles for analytical models
- MATLAB m-files
- Easy plugging of third party codes through wrappers

## Polynomial chaos expansions

Compute fast surrogate models using polynomial chaos expansions

**Key features:**

- Full and sparse PC expansions
- Quadrature, sparse grids, least-squares and least-angle regression
- Advanced truncation schemes, custom basis specification

## Kriging/Gaussian Processes

Compute robust surrogate models using Gaussian processes

**Key features:**

- Highly customizable trend and correlation functions
- Maximum likelihood and cross-validation for estimating hyperparameters
- Gradient-based and global optimizers

## Sensitivity analysis

Identify the important input variables and their interactions

**Key features:**

- Screening (Morris method)
- Linear measures: Taylor series expansion (perturbation), standard regression coefficients
- ANOVA: Sobol' indices through Monte Carlo and polynomial chaos expansions

## Reliability analysis/Rare events

NEW!

Estimate probabilities of failure and distribution tails

**Key features:**

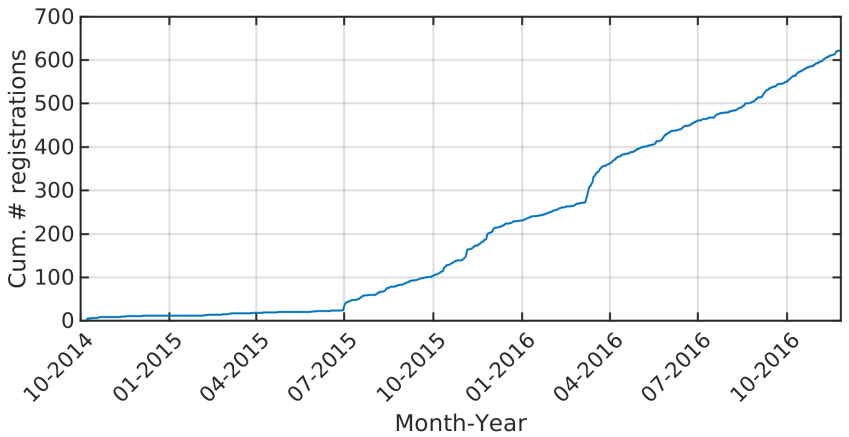
- FORM/SORM approximation methods
- Sampling methods (Monte Carlo, importance sampling, subset simulation)
- Kriging-based adaptive methods (AK-MCS)

http://www.uqlab.com

# UQLab: Facts and figures

http://www.uqlab.com

- Release of V0.9 on July 1st, 2015
- Release of V0.92 on March 1st, 2016
- **600$^+$ licences** in **48 countries**




| Country | # licences |
|---|---|
| United States | 91 |
| France | 64 |
| Switzerland | 54 |
| China | 31 |
| Germany | 30 |
| United Kingdom | 26 |
| Italy | 19 |
| India | 19 |
| Belgium | 15 |
| Brazil | 15 |

Open source version available in January 2017

# UQLab users


Finland
Iceland
Sweden
Norway
Russia
United Kingdom
Canada
Poland
Ukraine
Kazakhstan
Mongolia
Germany
Spain
Italy
Turkey
China
Japan
South Korea
United States
North Atlantic Ocean
Afghanistan
Iraq
Iran
Pakistan
Algeria
Libya
Egypt
Saudi Arabia
India
Thailand
Mexico
Mali
Niger
Sudan
Chad
Nigeria
Ethiopia
Venezuela
Colombia
Kenya
DR Congo
Indonesia
Papua New Guinea
Tanzania
Brazil
Peru
Angola
Bolivia
Namibia
Madagascar
Indian Ocean
Botswana
Australia
Chile
South Atlantic Ocean
South Africa
Argentina
Southern

# Online Sobol' indices calculator

**Quoting T. Mara, B. Belfort, V. Fontaine, A. Younes**, *"Addressing factors fixing setting from given data: A comparison of different methods"*, Env. Model. Software (2016):

> *This paper deals with global sensitivity analysis of computer model output. [...] we show that it is possible to evaluate the following global sensitivity measures: (i) the Sobol' indices, (ii) the Borgonovo's density-based sensitivity measure, and (iii) the derivative-based global sensitivity measure of Sobol' and Kucherenko. [...] The results show that the polynomial chaos expansion for estimating Sobol' indices is the most efficient approach.*

`http://uqlab1.wixsite.com/sobolindices`

# Questions ?

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**Chair of Risk, Safety & Uncertainty Quantification**

www.rsuq.ethz.ch

**The Uncertainty Quantification Laboratory**

www.uqlab.com

Thank you very much for your attention !