Surrogate models for uncertainty quantification and design optimization

Surrogate models for uncertainty quantification and design optimization

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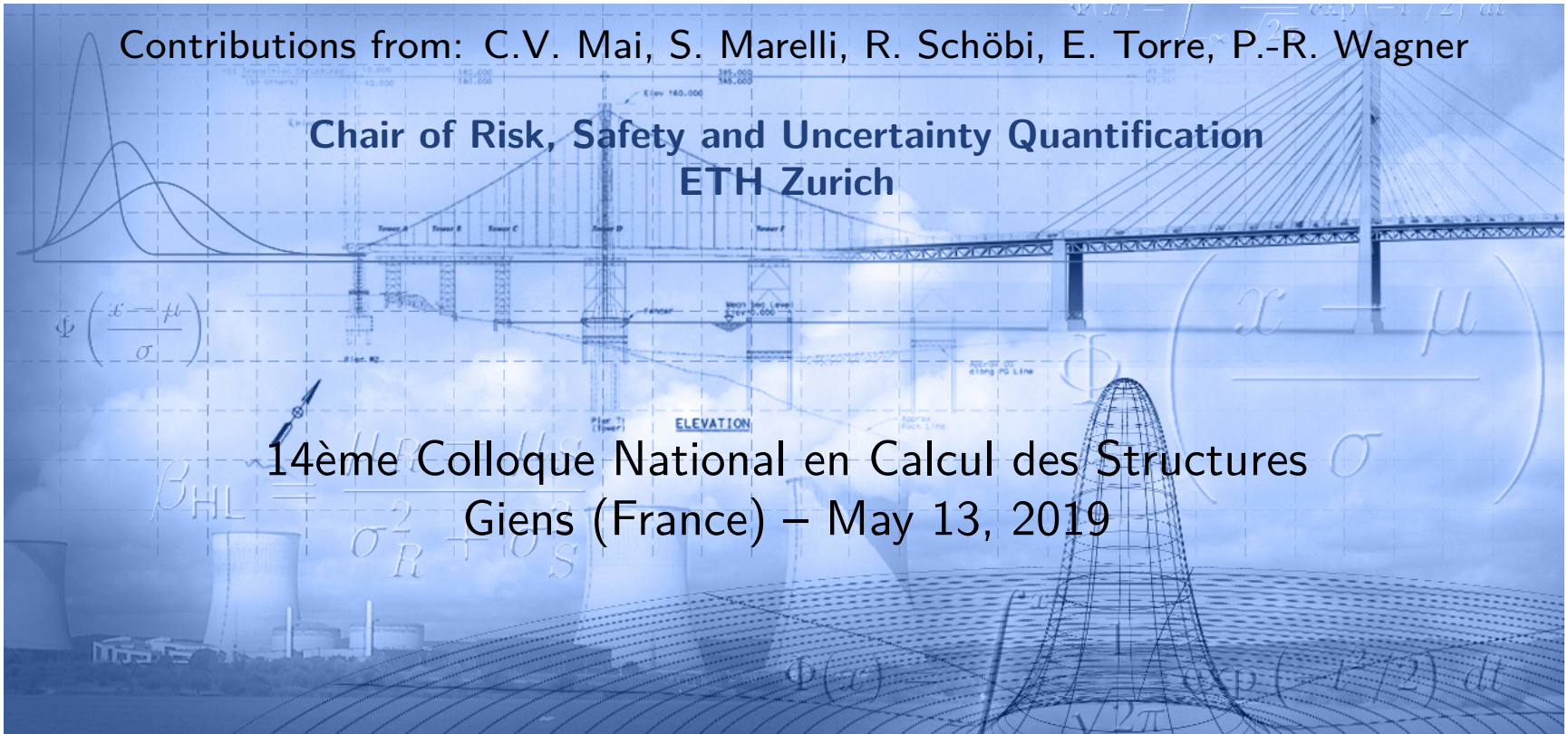
Chair of Risk, Safety and Uncertainty Quantification
ETH Zurich



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How to cite?

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Computational models in engineering

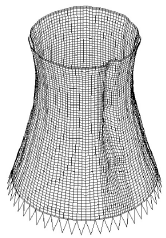
Complex engineering systems are designed and assessed using computational models, a.k.a simulators

A computational model combines:

- A mathematical description of the physical phenomena (governing equations), *e.g.* mechanics, electromagnetism, fluid dynamics, etc.

$$\begin{aligned} \operatorname{div} \boldsymbol{\sigma} + \boldsymbol{f} &= \mathbf{0} \\ \boldsymbol{\sigma} &= \mathbf{D} \cdot \boldsymbol{\varepsilon} \\ \boldsymbol{\varepsilon} &= \frac{1}{2}\left(\nabla \boldsymbol{u} + {}^{\mathsf{T}}\nabla \boldsymbol{u}\right) \end{aligned}$$

- Discretization techniques which transform continuous equations into linear algebra problems

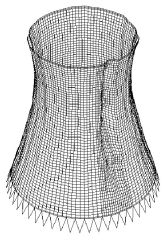


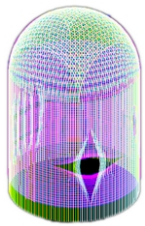
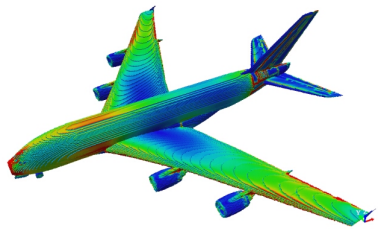
- Algorithms to solve the discretized equations

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

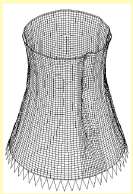
A computational model may be seen as a black box program that computes quantities of interest (QoI) (a.k.a. model responses) as a function of input parameters

Vector of input parameters $\boldsymbol{x} \in \mathbb{R}^M$

Computational model $\mathcal{M}$

Model response $\boldsymbol{y} = \mathcal{M}(\boldsymbol{x}) \in \mathbb{R}^Q$

- Geometry
- Material properties
- Loading

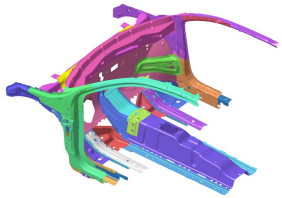


- Analytical formula
- Finite element model
- Comput. workflow

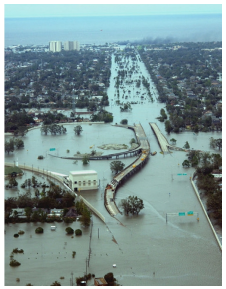
- Displacements
- Strains, stresses
- Temperature, etc.

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

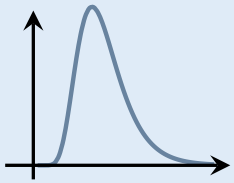
Global framework for uncertainty quantification

Step B
Quantification of sources of uncertainty

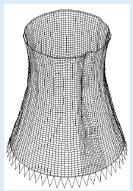
Step A
Model(s) of the system
Assessment criteria

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)*

Step B: Quantification of the sources of uncertainty

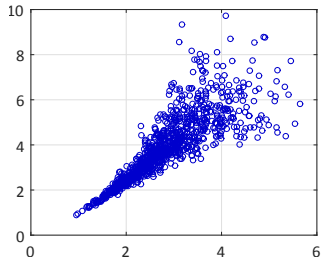
Goal: represent the uncertain parameters based on the available data and information

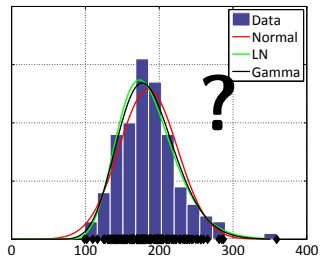
Probabilistic model $f_{\boldsymbol{X}}$

Experimental data is available

- What is the distribution of each parameter ?
- What is the dependence structure ?

Copula theory

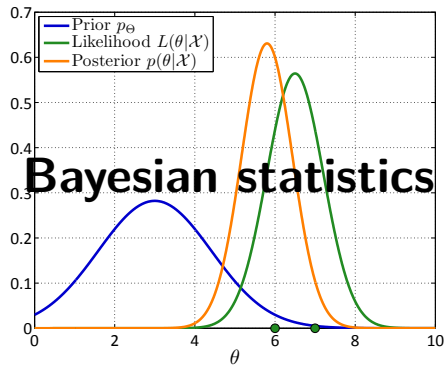




No data is available: expert judgment

- Engineering knowledge (*e.g.* reasonable bounds and uniform distributions)
- Statistical arguments and literature (*e.g.* extreme value distributions for climatic events)

Scarce data + expert information



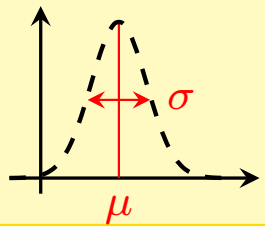
Step C: uncertainty propagation

Goal: estimate the uncertainty / variability of the quantities of interest (QoI) $Y = \mathcal{M}(\boldsymbol{X})$ due to the input uncertainty $f_{\boldsymbol{X}}$

- Output statistics, *i.e.* mean, standard deviation, etc.

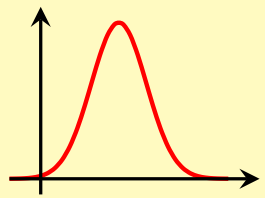
$$\mu_Y = \mathbb{E}_{\boldsymbol{X}}\left[\mathcal{M}(\boldsymbol{X})\right]$$
$$\sigma_Y^2 = \mathbb{E}_{\boldsymbol{X}}\left[\left(\mathcal{M}(\boldsymbol{X}) - \mu_Y\right)^2\right]$$

Mean/std. deviation



- Distribution of the QoI

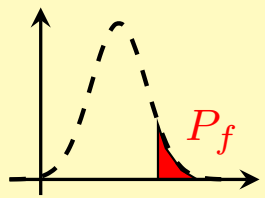
Response PDF



- Probability of exceeding an admissible threshold y_{adm}

$$P_f = \mathbb{P}\left(Y \geq y_{adm}\right)$$

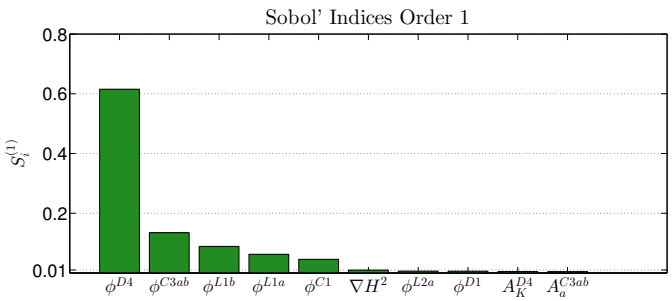
Probability of failure



Step C': sensitivity analysis

Goal: determine what are the input parameters (or combinations thereof) whose uncertainty explains the variability of the quantities of interest

- Screening: detect input parameters whose uncertainty has no impact on the output variability
- Feature setting: detect input parameters which allow one to best decrease the output variability when set to a deterministic value
- Exploration: detect interactions between parameters, *i.e.* joint effects not detected when varying parameters one-at-a-time



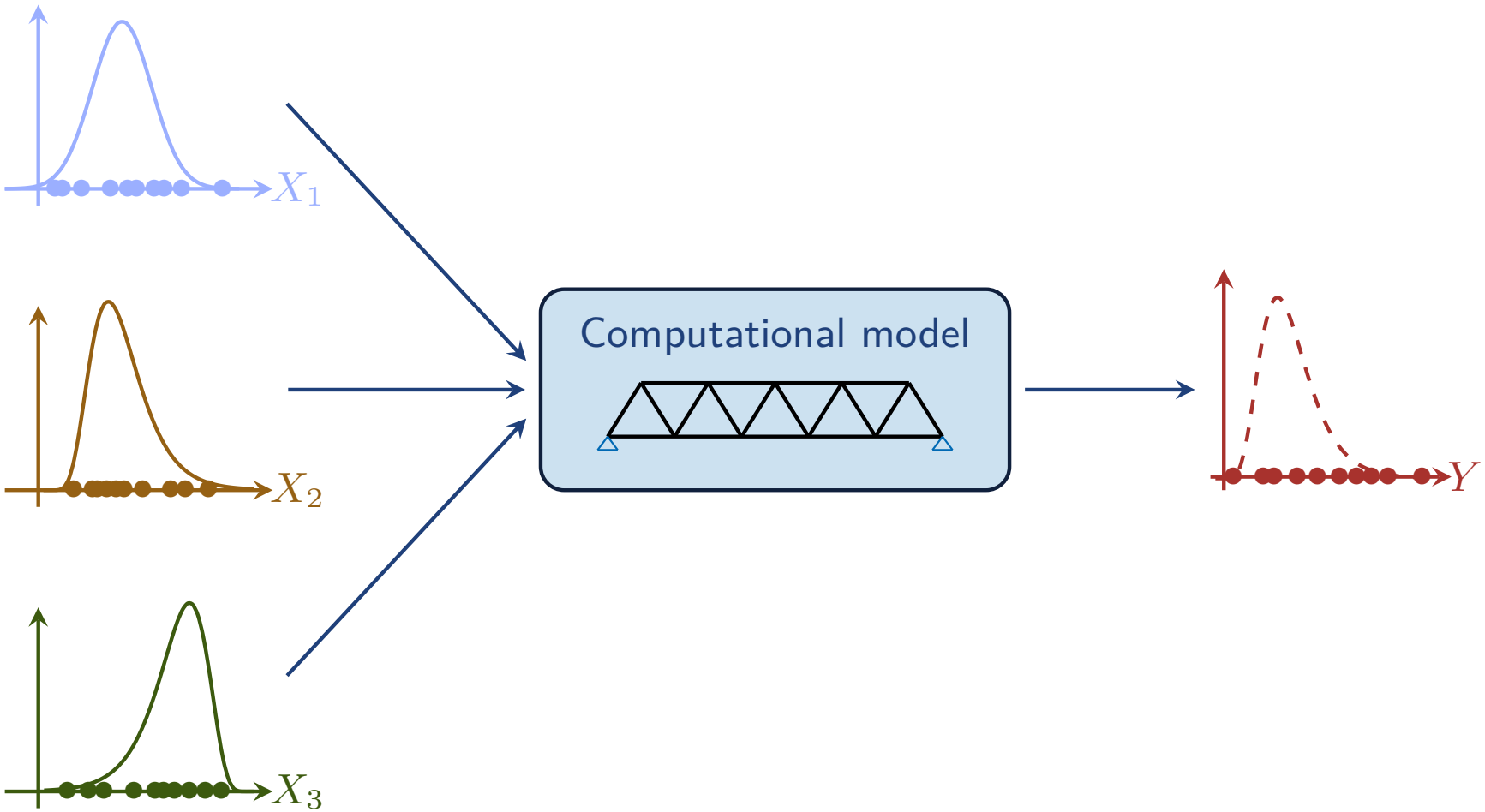
Variance decomposition (Sobol' indices)

Uncertainty propagation using Monte Carlo simulation

Principle: Generate virtual prototypes of the system using random numbers

- A sample set $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is drawn according to the input distribution $f_{\boldsymbol{X}}$
- For each sample the quantity of interest (resp. performance criterion) is evaluated, say $\mathcal{Y} = \{\mathcal{M}(\boldsymbol{x}_1), \ldots, \mathcal{M}(\boldsymbol{x}_n)\}$
- 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 $n \to \infty$
- 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 $\propto n^{-1/2}$

Monte Carlo for reliability analysis

To compute $P_f = 10^{-k}$ with an accuracy of $\pm 10\%$ (coef. of variation of 5%), $4 \cdot 10^{k+2}$ runs are required

Surrogate models for uncertainty quantification

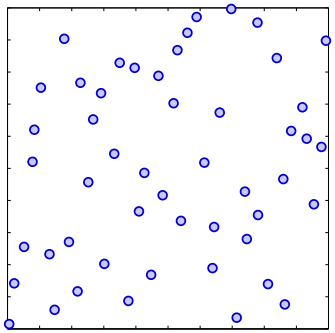
A surrogate model $\tilde{\mathcal{M}}$ is an approximation of the original computational model $\mathcal{M}$ with the following features:

- 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
- 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; 2003); 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

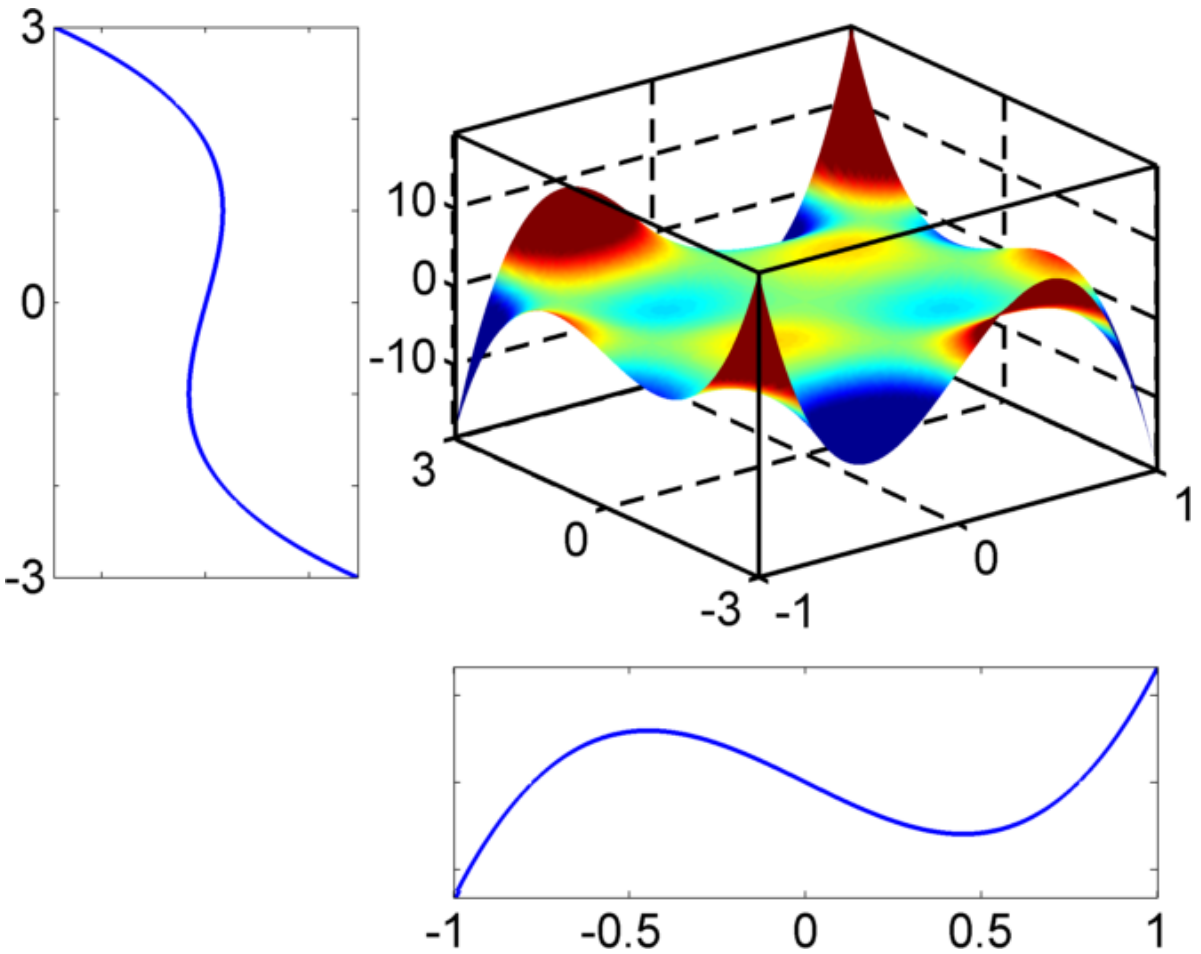
$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \overset{\text{def}}{=} \prod_{i=1}^{M} \Psi_{\alpha_i}^{(i)}(x_i) \qquad \mathbb{E}\left[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})\Psi_{\boldsymbol{\beta}}(\boldsymbol{X})\right] = \delta_{\boldsymbol{\alpha}\boldsymbol{\beta}}$$

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

Dealing with complex input distributions

Independent variables

Input parameters with given marginal CDFs $X_i \sim F_{X_i}, \quad i = 1, \ldots, M$

- Arbitrary PCE: orthogonal polynomial computed numerically on-the-fly
- Isoprobabilistic transform through a one-to-one mapping to reduced variables, *e.g.* :

$$X_i = F_{X_i}^{-1}\left(\frac{\xi_i + 1}{2}\right) \qquad \text{if } \xi_i \sim \mathcal{U}(-1\,,\,1)$$

$$X_i = F_{X_i}^{-1}\left(\Phi(\xi_i)\right) \qquad \text{if } \xi_i \sim \mathcal{N}(0,1)$$

General case: addressing dependence

Sklar's theorem (1959)

- The joint CDF is defined through its marginals and copula

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

- Rosenblatt or Nataf isoprobabilistic transform is used

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 coefficients)

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

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

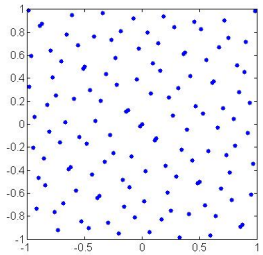
An estimate of the mean square error (sample average) is minimized:

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

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

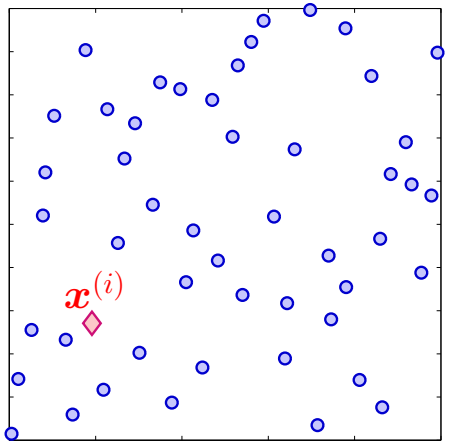
$$E_{emp} = \frac{1}{n}\sum_{i=1}^{n}\left(\mathcal{M}(\boldsymbol{x}^{(i)}) - \mathcal{M}^{\mathsf{PC}}(\boldsymbol{x}^{(i)})\right)^2$$

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

$$R^2 = 1 - \frac{E_{emp}}{\mathrm{Var}\left[\mathcal{Y}\right]} \qquad \mathrm{Var}\left[\mathcal{Y}\right] = \frac{1}{n}(\mathcal{M}(\boldsymbol{x}^{(i)}) - \bar{\mathcal{Y}})^2$$

R^2 is a poor estimator of the accuracy of the PCE when there is overfitting

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 $\mathbf{A}(\mathbf{A}^\mathsf{T}\mathbf{A})^{-1}\mathbf{A}^\mathsf{T}$

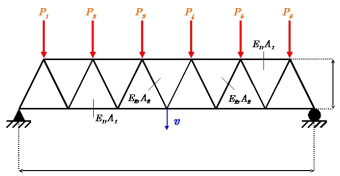
Outline

Curse of dimensionality

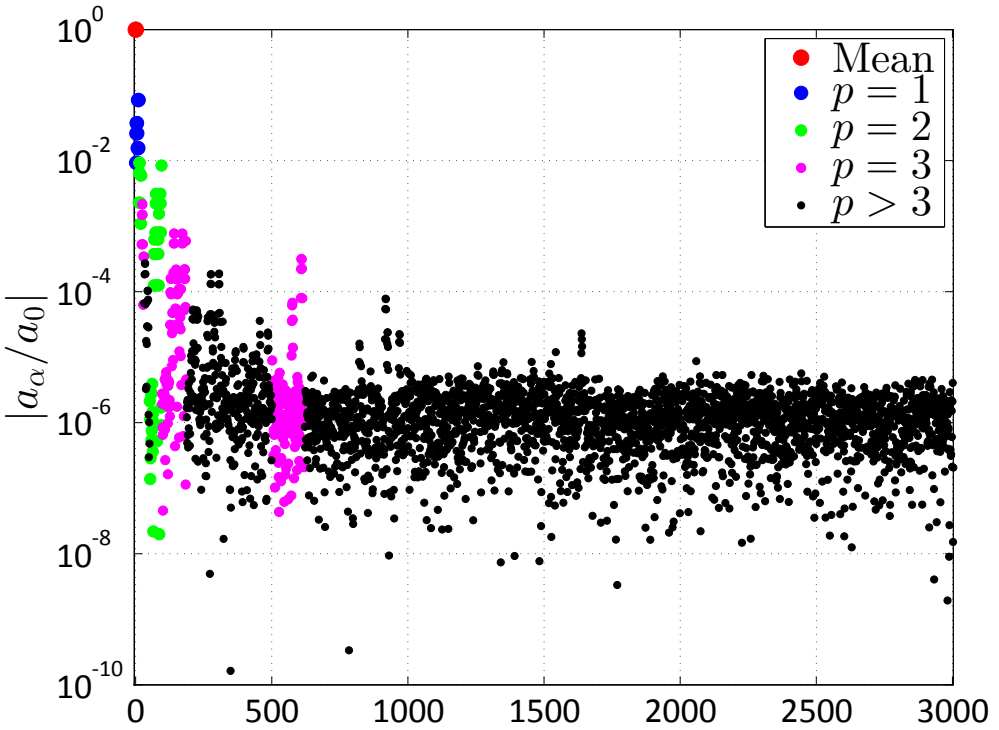
- The cardinality of the truncation scheme $\mathcal{A}^{M,p}$ is $P = \dfrac{(M+p)!}{M!\,p!}$
- Typical computational requirements: $n = OSR \cdot P$ where the oversampling rate is $OSR = 2 - 3$

However ... most coefficients are close to zero !

Example



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



Hyperbolic truncation sets

Sparsity-of-effects principle

Blatman & Sudret, Prob. Eng. Mech (2010); J. Comp. Phys (2011)

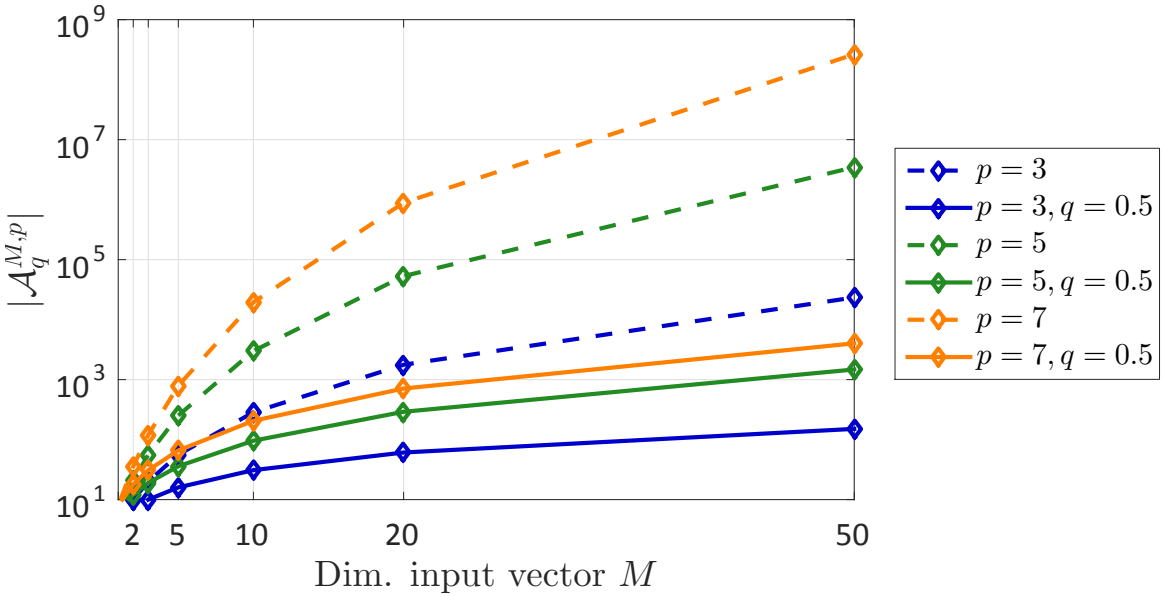
In most engineering problems, only low-order interactions between the input variables are relevant

- $q-$norm of a multi-index $\boldsymbol{\alpha}$:

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

- Hyperbolic truncation sets:

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



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:

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

- 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 inversion
- Leave-one-out cross validation error allows one to select the best model

Sparse PCE: wrap up

Algorithm 1: LAR-based Polynomial chaos expansion

Input: Computational budget n
Initialization
  Sample experimental design $\mathcal{X} = \{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)}\}$
  Evaluate model response $\mathcal{Y} = \{\mathcal{M}(\boldsymbol{x}^{(1)}), \ldots, \mathcal{M}(\boldsymbol{x}^{(n)})\}$
PCE construction
  for $p = p_{\min} : p_{\max}$ **do**
    for $q \in \mathcal{Q}$ **do**
      Select candidate basis $\mathcal{A}_q^{M,p}$
      Run LAR for extracting the optimal sparse basis $\mathcal{A}^*(p,q)$
      Compute coefficients $\{y_{\boldsymbol{\alpha}},\ \boldsymbol{\alpha} \in \mathcal{A}^*(p,q)\}$ by OLS
      Compute $e_{\text{LOO}}(p,q)$
    end
  end
  $(p^*, q^*) = \arg\min e_{\text{LOO}}(p,q)$
Return Optimal sparse basis $\mathcal{A}^*(p,q)$, PCE coefficients, $e_{\text{LOO}}(p^*,q^*)$

Outline

Post-processing sparse PC expansions

Statistical moments

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

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

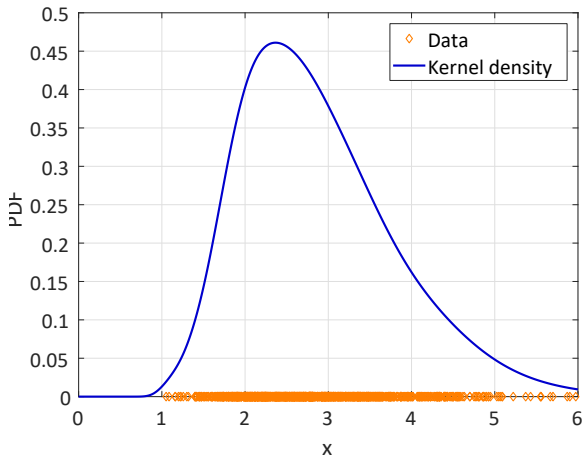
$$\text{Variance:} \qquad \hat{\sigma}_Y^2 = \sum_{\boldsymbol{\alpha}\in\mathcal{A}\setminus\mathbf{0}} y_{\boldsymbol{\alpha}}^2$$

Distribution of the QoI

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

$$\mathfrak{y}_j = \sum_{\boldsymbol{\alpha}\in\mathcal{A}} y_{\boldsymbol{\alpha}}\, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{x}_j) \quad j = 1, \ldots, n_{big}$$

- 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

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

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

$$= \mathcal{M}_0 + \sum_{\mathbf{u} \subset \{1, \ldots, M\}} \mathcal{M}_{\mathbf{u}}(\boldsymbol{x}_{\mathbf{u}}) \qquad (\boldsymbol{x}_{\mathbf{u}} \overset{\text{def}}{=} \{x_{i_1}, \ldots, x_{i_s}\})$$

- The summands satisfy the orthogonality condition:

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

Sobol' indices

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

- Sobol' indices:
$$S_{\mathbf{u}} \overset{\text{def}}{=} \frac{\mathrm{Var}\left[\mathcal{M}_{\mathbf{u}}(\boldsymbol{X}_{\mathbf{u}})\right]}{D}$$
- First-order Sobol' indices:
$$S_i = \frac{D_i}{D} = \frac{\mathrm{Var}\left[\mathcal{M}_i(X_i)\right]}{D}$$
Quantify the additive effect of each input parameter separately
- Total Sobol' indices:
$$S_i^T \overset{\text{def}}{=} \sum_{\mathbf{u} \supset i} S_{\mathbf{u}}$$
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

$\mathcal{M}^{\text{PC}}(\boldsymbol{X}) \overset{\text{def}}{=} \sum_{\boldsymbol{\alpha} \in \mathcal{A}} y_{\boldsymbol{\alpha}} \, \Psi_{\boldsymbol{\alpha}}(\boldsymbol{X})$

Interaction sets

For a given $\mathbf{u} \overset{\text{def}}{=} \{i_1, \ldots, i_s\}$: $\quad \mathcal{A}_{\mathbf{u}} = \{\boldsymbol{\alpha} \in \mathcal{A} : \; k \in \mathbf{u} \Leftrightarrow \alpha_k \neq 0\}$

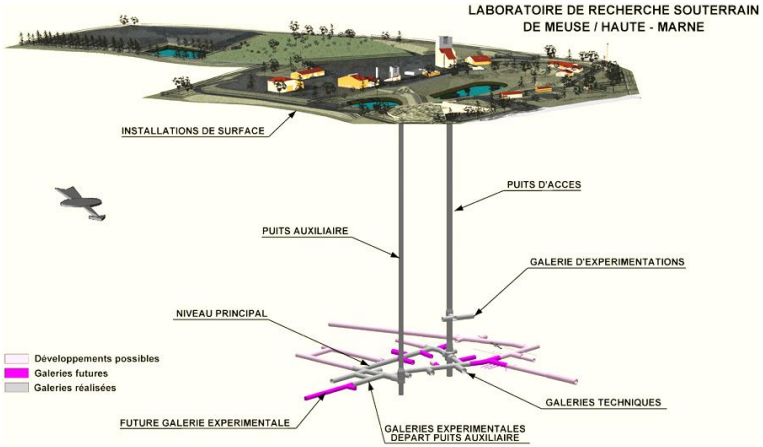
$$\mathcal{M}^{\text{PC}}(\boldsymbol{x}) = \mathcal{M}_0 + \sum_{\mathbf{u} \subset \{1, \ldots, M\}} \mathcal{M}_{\mathbf{u}}(\boldsymbol{x}_{\mathbf{u}}) \qquad \text{where} \qquad \mathcal{M}_{\mathbf{u}}(\boldsymbol{x}_{\mathbf{u}}) \overset{\text{def}}{=} \sum_{\boldsymbol{\alpha} \in \mathcal{A}_{\mathbf{u}}}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

PC-based Sobol' indices

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

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

Example: sensitivity analysis in hydrogeology



Source: http://www.futura-sciences.com/

Source: http://lexpansion.lexpress.fr/

- When assessing a nuclear waste repository, the Mean Lifetime Expectancy MLE(x) is the time required for a molecule of water at point x to get out of the boundaries of the system
- Computational models have numerous input parameters (in each geological layer) that are difficult to measure, and that show scattering

Geological model

Joint work with University of Neuchâtel

Deman, Konakli, Sudret, Kerrou, Perrochet & Benabderrahmane, Reliab. Eng. Sys. Safety (2016)

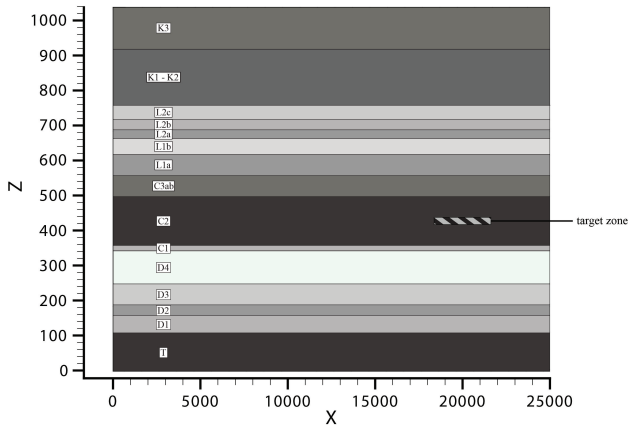
- Two-dimensional idealized model of the Paris Basin (25 km long / 1,040 m depth) with 5×5 m mesh (10^6 elements)
- Steady-state flow simulation with Dirichlet boundary conditions:

$$\nabla \cdot (\mathbf{K} \cdot \nabla H) = 0$$

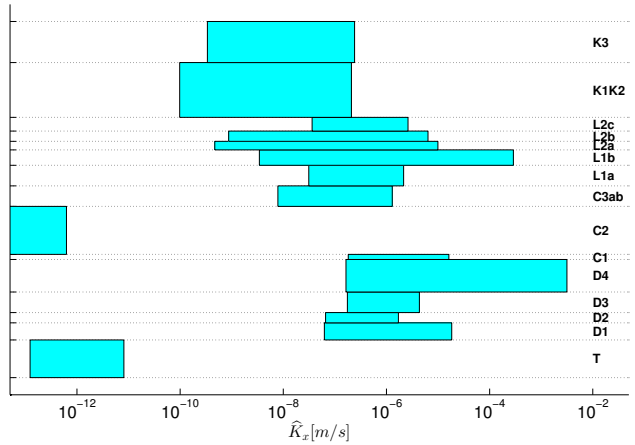
- 15 homogeneous layers with uncertainties in:
  - Porosity (resp. hydraulic conductivity)
  - Anisotropy of the layer properties (inc. dispersivity)
  - Boundary conditions (hydraulic gradients)

78 input parameters

Sensitivity analysis



Geometry of the layers



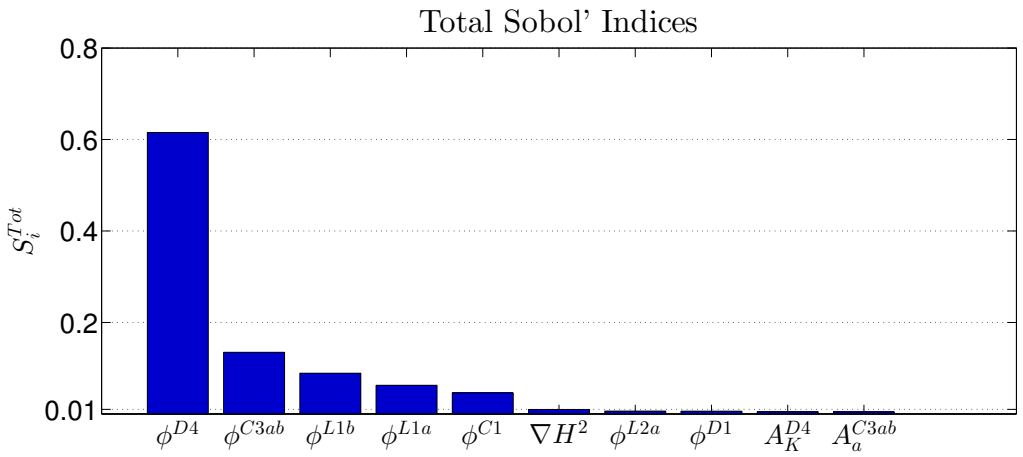
Conductivity of the layers

Question

What are the parameters (out of 78) whose uncertainty drives the uncertainty of the prediction of the mean life-time expectancy?

Sensitivity analysis: results

Technique: Sobol'indices computed from polynomial chaos expansions



Parameter	$\sum_j S_j$
ϕ (resp. K_x)	0.8664
A_K	0.0088
θ	0.0029
α_L	0.0076
A_α	0.0000
∇H	0.0057

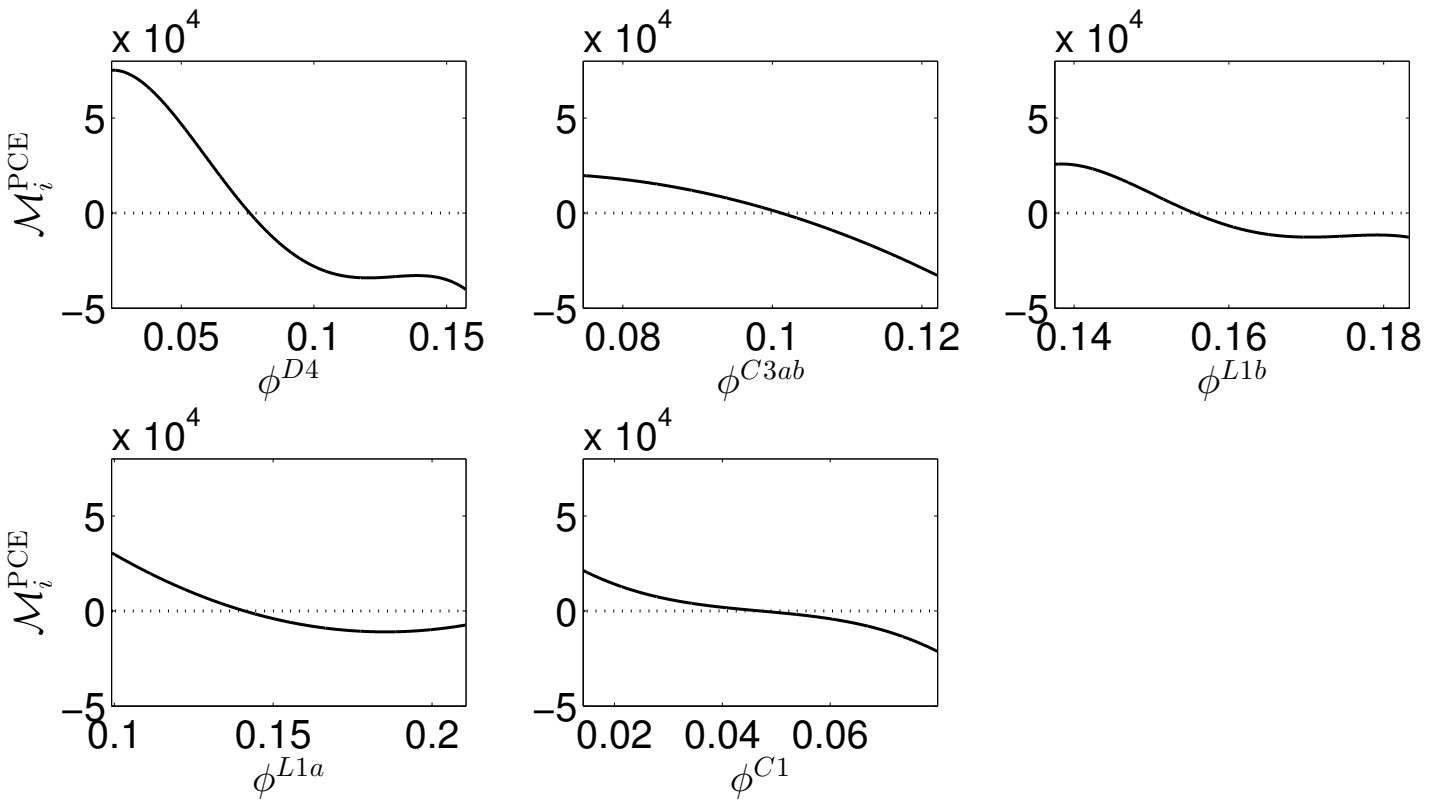
Conclusions

- Only 200 model runs allow one to detect the 10 important parameters out of 78
- Uncertainty in the porosity/conductivity of 5 layers explain 86% of the variability
- Small interactions between parameters detected

Bonus: univariate effects

The univariate effects of each variable are obtained as a straightforward post-processing of the PCE

$$\mathcal{M}_i(x_i) \overset{\text{def}}{=} \mathbb{E}\left[\mathcal{M}(\boldsymbol{X})|X_i = x_i\right], \; i = 1, \ldots, M$$



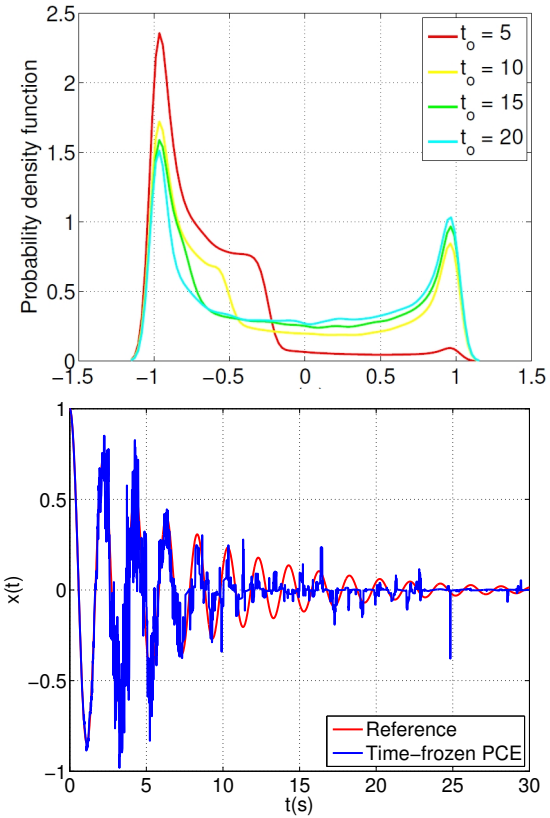
Outline

Polynomial chaos expansions in structural dynamics

Spiridonakos et al. (2015); Mai, Spiridonakos, Chatzi & Sudret, IJUQ (2016); Mai & Sudret, SIAM JUQ (2017)

Premise

- For dynamical systems, the complexity of the map $\boldsymbol{\xi} \mapsto \mathcal{M}(\boldsymbol{\xi}, t)$ increases with time.
- Time-frozen PCE does not work beyond first time instants



PC-NARX

- Use of non linear autoregressive with exogenous input models (NARX) to capture the dynamics:

$$y(t) = \mathcal{F}\left(x(t), \ldots, x(t-n_x), y(t-1), \ldots, y(t-n_y)\right) + \epsilon_t \equiv \mathcal{F}\left(\boldsymbol{z}(t)\right) + \epsilon_t$$

Earthquake engineering – Bouc-Wen oscillator

Governing equations

Kafali & Grigoriu (2007), Spiridonakos & Chatzi (2015)

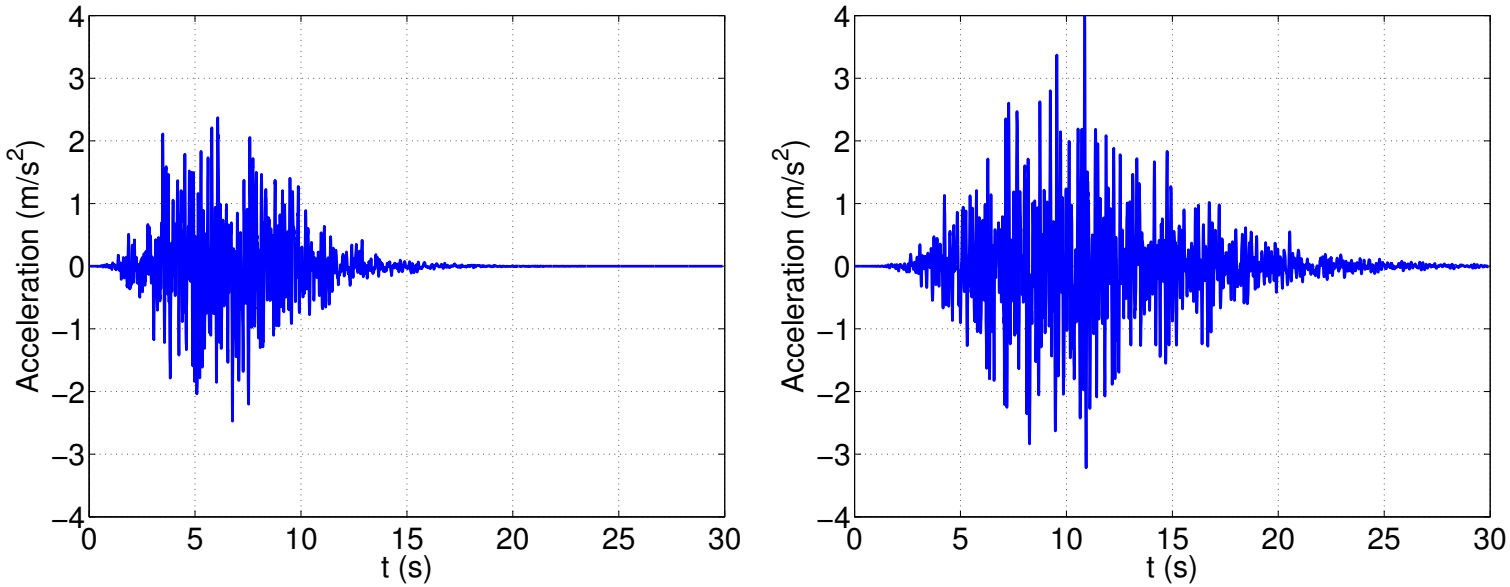
$$\ddot{y}(t) + 2\,\zeta\,\omega\,\dot{y}(t) + \omega^2(\rho\,y(t) + (1-\rho)\,z(t)) = -x(t),$$
$$\dot{z}(t) = \gamma\dot{y}(t) - \alpha\,|\dot{y}(t)|\,|z(t)|^{n-1}\,z(t) - \beta\,\dot{y}(t)\,|z(t)|^{n},$$

Excitation

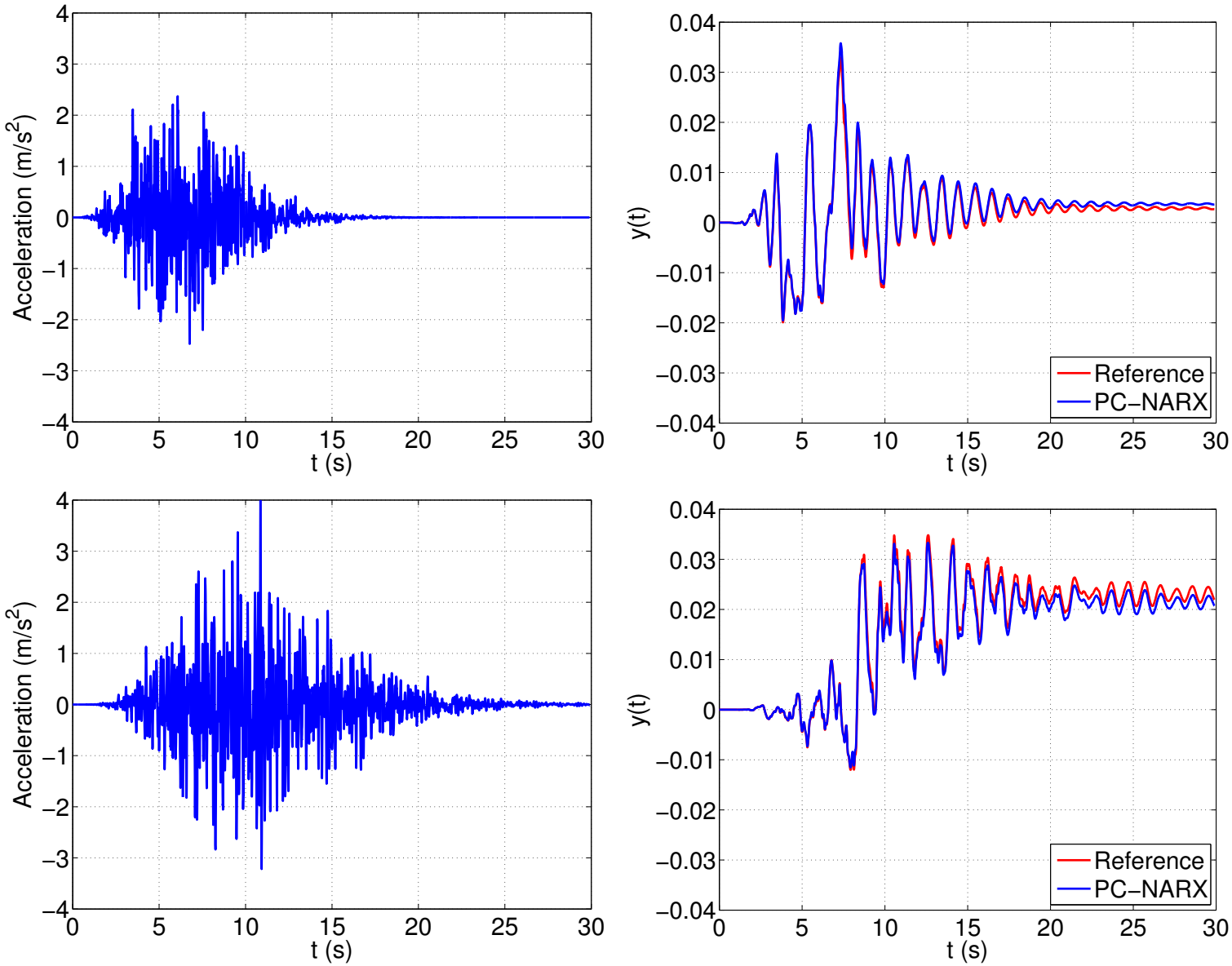
$x(t)$ is generated by a probabilistic ground motion model

Rezaeian & Der Kiureghian (2010)

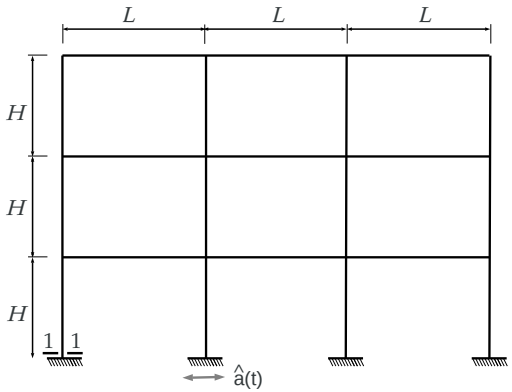
$$x(t) = q(t,\boldsymbol{\alpha}) \sum_{i=1}^{n} s_i\left(t, \boldsymbol{\lambda}(t_i)\right)\,U_i$$



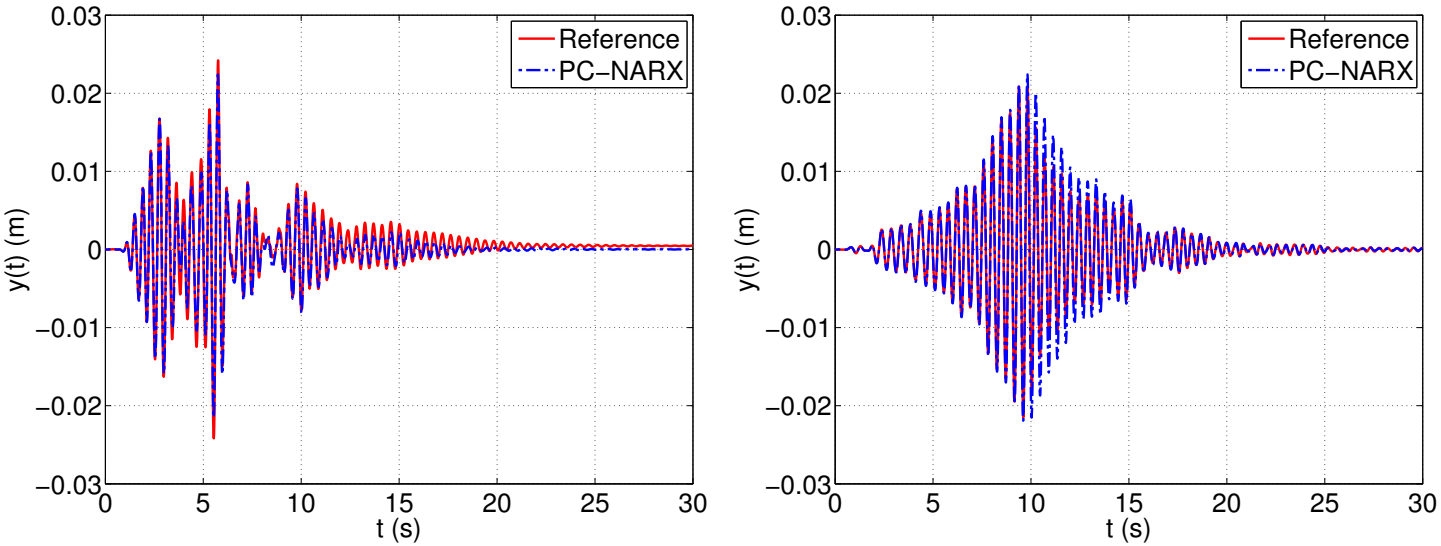
Bouc-Wen model: prediction



Earthquake engineering – frame structure



- 2D steel frame with uncertain properties submitted to synthetic ground motions
- Experimental design of size 300

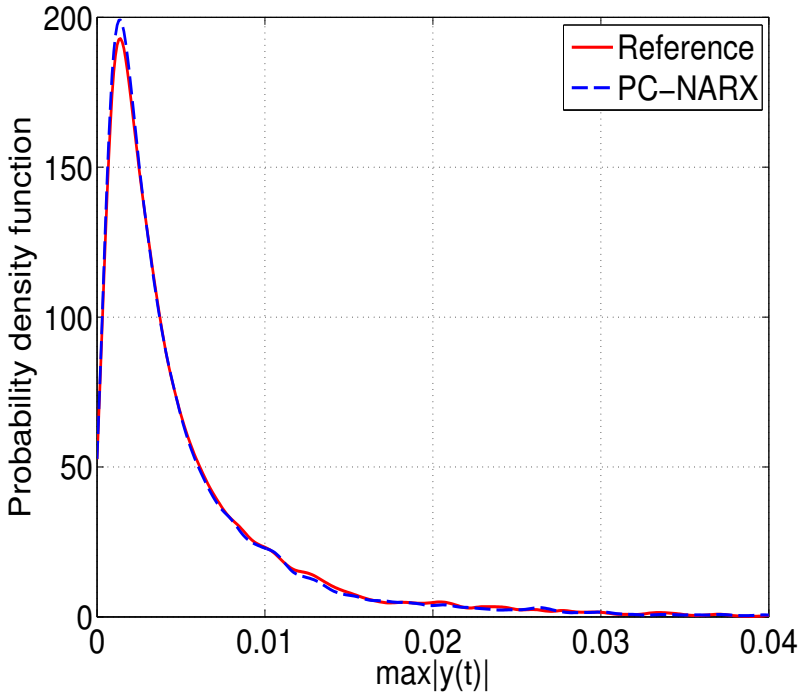


Surrogate model of single trajectories

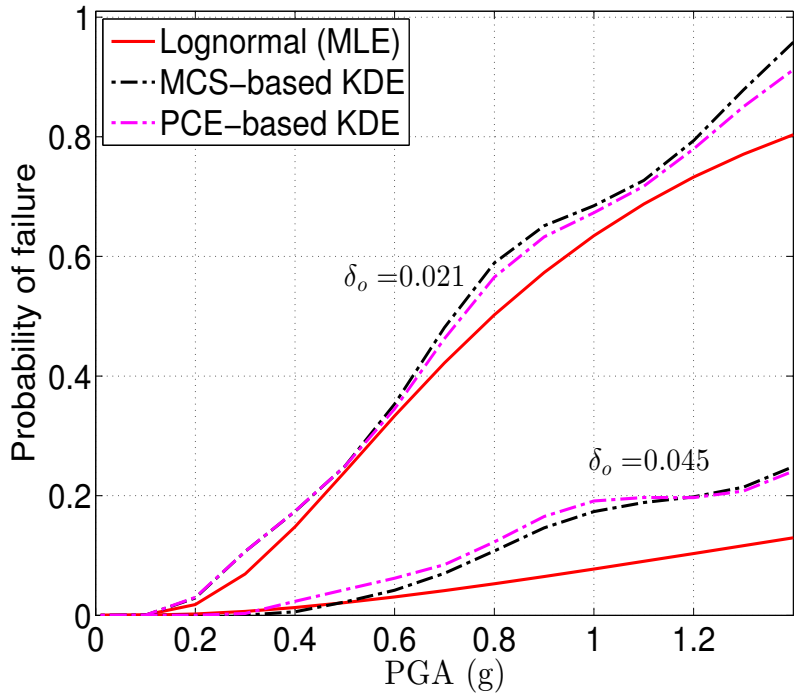
Frame structure – fragility curves

First-storey drift

- PC-NARX calibrated based on 300 simulations
- Reference results obtained from 10,000 Monte Carlo simulations



PDF of max. drift



Fragility curves for two drift thresholds

Outline

Gaussian process modelling (a.k.a Kriging)

Santner, Williams & Notz (2003)

Kriging assumes that $\mathcal{M}(\boldsymbol{x})$ is a trajectory of an underlying Gaussian process

$$\mathcal{M}(\boldsymbol{x}) \approx \mathcal{M}^{(\mathsf{K})}(\boldsymbol{x}) = \boldsymbol{\beta}^{\mathsf{T}} \boldsymbol{f}(\boldsymbol{x}) + \sigma^2 \, Z(\boldsymbol{x}, \omega)$$

where:

- $\boldsymbol{\beta}^{\mathsf{T}} \boldsymbol{f}(\boldsymbol{x})$: trend
- $Z(\boldsymbol{x}, \omega)$: zero mean, unit variance Gaussian process with autocorrelation function, *e.g.* :

$$R\left(\boldsymbol{x}, \boldsymbol{x}'\right) = \exp\left(\sum_{k=1}^{M} - \left(\frac{x_k - x'_k}{\theta_k}\right)^2\right)$$

- σ^2: variance

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

Kriging prediction

Unknown parameters

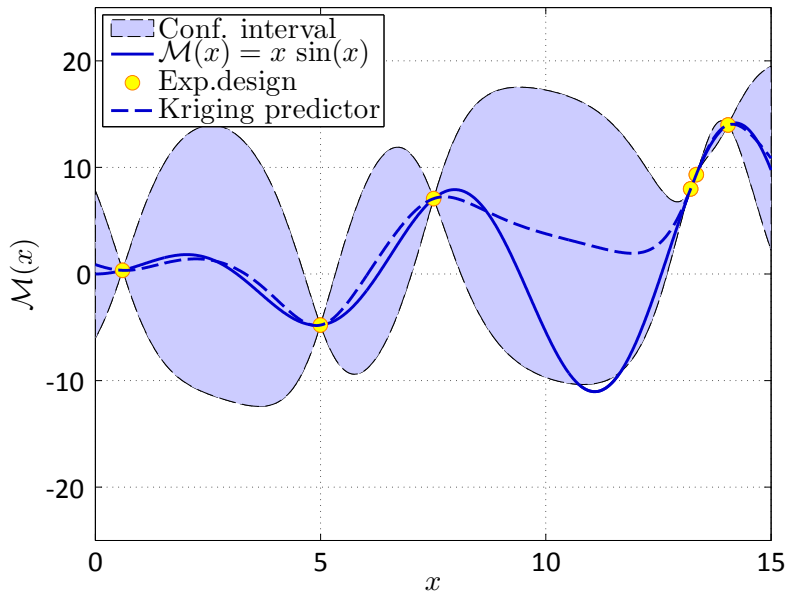
- Parameters $\{\boldsymbol{\theta},\, \boldsymbol{\beta},\, \sigma^2\}$ are estimated from the experimental design $\mathcal{Y} = \{y_i = \mathcal{M}(\boldsymbol{\chi}_i)\,,\, i = 1,\, \ldots\,,\, n\}$ by maximum likelihood estimation, cross validation or Bayesian calibration

Mean predictor

$$\mu_{\hat{g}}(\boldsymbol{x}) = \boldsymbol{f}\,(\boldsymbol{x})^{\mathsf{T}}\ \hat{\boldsymbol{\beta}} + \boldsymbol{r}\,(\boldsymbol{x})^{\mathsf{T}}\,\boldsymbol{R}^{-1}\left(\mathcal{Y} - \boldsymbol{F}\,\hat{\boldsymbol{\beta}}\right)$$

where:

$$\begin{aligned} r_i(\boldsymbol{x}) &= R\left(\boldsymbol{x} - \boldsymbol{x}^{(i)},\, \boldsymbol{\theta}\right) \\ \boldsymbol{R}_{ij} &= R\left(\boldsymbol{x}^{(i)} - \boldsymbol{x}^{(j)},\, \boldsymbol{\theta}\right) \\ \boldsymbol{F}_{ij} &= f_j\left(\boldsymbol{x}^{(i)}\right) \end{aligned}$$



Kriging variance

$$\sigma^2_{\widehat{Y}}(\boldsymbol{x}) = \sigma^2_Y\left(1 - \left\langle\ \boldsymbol{f}\,(\boldsymbol{x})^{\mathsf{T}} \quad \boldsymbol{r}\,(\boldsymbol{x})^{\mathsf{T}}\ \right\rangle \begin{bmatrix} \boldsymbol{0} & \boldsymbol{F}^{\mathsf{T}} \\ \boldsymbol{F} & \boldsymbol{R} \end{bmatrix}^{-1} \begin{bmatrix} \boldsymbol{f}\,(\boldsymbol{x}) \\ \boldsymbol{r}\,(\boldsymbol{x}) \end{bmatrix}\right)$$

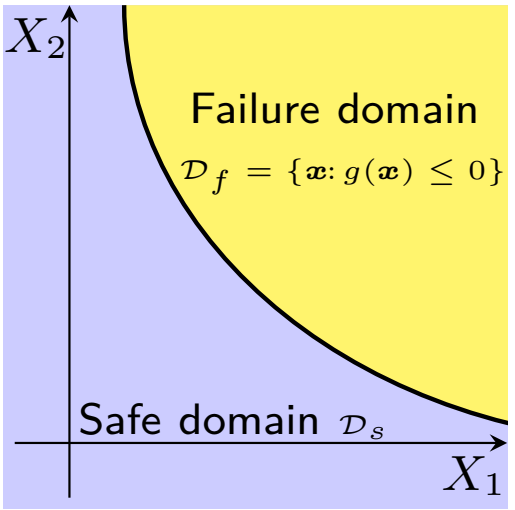
Structural reliability

Problem statement

- A limit state function g : $\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}} \subset \mathbb{R}^M \mapsto \mathbb{R}$ that describes the performance of the system:

  + $g(\boldsymbol{x}) > 0$ means "safe configuration"
  + $g(\boldsymbol{x}) \leq 0$ means "failure"

  e.g. Elastic behaviour is defined by: $g(\boldsymbol{x}) = \sigma_Y - \max_{\text{Structure}} \sigma_{VM}(\boldsymbol{x})$



- A probabilistic model (PDF) of the uncertainties: $\boldsymbol{X} \sim f_{\boldsymbol{X}}$

The probability of failure is defined by:

$$P_f = \mathbb{P}\left(g(\boldsymbol{X}) \leq 0\right) = \int_{\{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}} :\, g(\boldsymbol{x}) \leq 0\}} f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x}$$

Use of Kriging for structural reliability analysis

- From a given experimental design $\mathcal{X} = \left\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)}\right\}$, Kriging yields a mean predictor $\mu_{\hat{g}}(\boldsymbol{x})$ and the Kriging variance $\sigma_{\hat{g}}(\boldsymbol{x})$

- The mean predictor is substituted for the "true" limit state function, defining the surrogate failure domain

$$\mathcal{D}_f{}^0 = \{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}} \ : \ \mu_{\hat{g}}(\boldsymbol{x}) \leq 0\}$$

- The probability of failure is approximated by: Kaymaz, Struc. Safety (2005)

$$P_f^0 = \mathbb{P}\left[\mu_{\hat{g}}(\boldsymbol{X}) \leq 0\right] = \int_{\mathcal{D}_f^0} f_{\boldsymbol{X}}(\boldsymbol{x})\, d\boldsymbol{x} = \mathbb{E}\left[\mathbf{1}_{\mathcal{D}_f^0}(\boldsymbol{X})\right]$$

- Monte Carlo simulation can be used on the surrogate model:

$$\widehat{P_f^0} = \frac{1}{N} \sum_{k=1}^{N} \mathbf{1}_{\mathcal{D}_f^0}(\boldsymbol{x}_k)$$

Confidence bounds on the probability of failure

Shifted failure domains

Dubourg *et al.* , Struct. Mult. Opt. (2011)

- Let us define a confidence level $(1-\alpha)$ and $k_{1-\alpha} = \Phi^{-1}(1-\alpha/2)$, *i.e.* 1.96 if $1-\alpha = 95\%$, and:

$$\mathcal{D}_f^- = \{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}} \ : \ \mu_{\hat{g}}(\boldsymbol{x}) + k_{1-\alpha}\,\sigma_{\hat{g}}(\boldsymbol{x}) \leq 0\}$$

$$\mathcal{D}_f^+ = \{\boldsymbol{x} \in \mathcal{D}_{\boldsymbol{X}} \ : \ \mu_{\hat{g}}(\boldsymbol{x}) - k_{1-\alpha}\,\sigma_{\hat{g}}(\boldsymbol{x}) \leq 0\}$$

- Interpretation ($1-\alpha = 95\%$):
  - If $\boldsymbol{x} \in \mathcal{D}_f^0$ it belongs to the true failure domain with a 50% chance
  - If $\boldsymbol{x} \in \mathcal{D}_f^+$ it belongs to the true failure domain with 95% chance: conservative estimation

Bounds on the probability of failure

$$\mathcal{D}_f^- \subset \mathcal{D}_f^0 \subset \mathcal{D}_f^+ \qquad \Leftrightarrow \qquad P_f^- \leq P_f^0 \leq P_f^+$$

Adaptive designs for reliability analysis

Premise

- When using high-fidelity computational models for assessing structural reliability, the goal is to minimize the number of runs
- Adaptive experimental designs allow one to start from a small ED and enrich it with new points in suitable regions (*i.e.* close to to the limit state surface)

Enrichment (infill) criterion

Bichon *et al.* , (2008, 2011); Echard *et al.* (2011); Bect *et al.* (2012), Balesdent *et al.* (2013), Morio & Balesdent (2015-16)

The following learning function is used:

$$LF(\boldsymbol{x}) = \frac{|\mu_{\hat{g}}(\boldsymbol{x})|}{\sigma_{\hat{g}}(\boldsymbol{x})}$$

- Small if $\mu_{\hat{g}}(\boldsymbol{x}) \approx 0$ ($\boldsymbol{x}$ close to the limit state surface) and/or $\sigma_{\hat{g}}(\boldsymbol{x}) >> 0$ (poor local accuracy)
- The probability of misclassification is $\Phi(-LF(\boldsymbol{x}))$
- At each iteration, the new point is: $\boldsymbol{\chi}^* = \arg\min LF(\boldsymbol{x})$

Adaptive Kriging for reliability analysis

Algorithm 2: Adaptive Kriging for reliability analysis

Initialization
  Initial experimental design $\mathcal{ED} = \{\boldsymbol{\chi}^{(1)}, \ldots, \boldsymbol{\chi}^{(n)}\}$
  Monte Carlo sample $\mathcal{X} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$
while *NotConverged* **do**
  Train a Kriging model $\widehat{\mathcal{M}}$ on the current experimental design
  Compute the probability of failure $\hat{P}_f^0$, and its bounds $[\hat{P}_f^-, \hat{P}_f^+]$ using $\widehat{\mathcal{M}}$
  if $(\hat{P}_f^+ - \hat{P}_f^-)/\hat{P}_f^0 \leq TOL$ **then**
    NotConverged = FALSE
  else
    Evaluate the learning function LF on $\mathcal{X}$
    Compute the next ED point: $\boldsymbol{\chi}^* = \arg\min_{\boldsymbol{x} \in \mathcal{X}} LF(\boldsymbol{x})$
    Update the experimental design: $\mathcal{ED} \leftarrow \mathcal{ED} \cup \{\boldsymbol{\chi}^*\}$
  end
end
Return Probability of failure $\hat{P}_f^0$ and confidence interval $[\hat{P}_f^-, \hat{P}_f^+]$

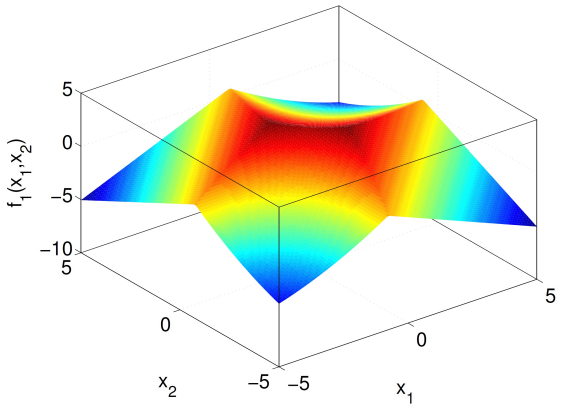
Series system

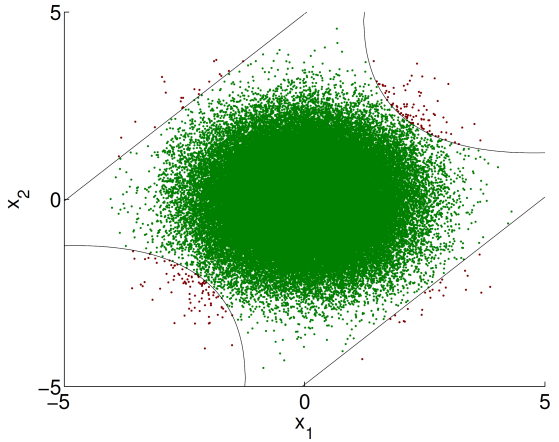
Schöbi, Sudret & Marelli, ASCE J. Risk Unc. (2016)

Consider the system reliability analysis defined by:

$$g(\boldsymbol{x}) = \min \begin{pmatrix} 3 + 0.1\,(x_1 - x_2)^2 - \frac{x_1+x_2}{\sqrt{2}} \\ 3 + 0.1\,(x_1 - x_2)^2 + \frac{x_1+x_2}{\sqrt{2}} \\ (x_1 - x_2) + \frac{6}{\sqrt{2}} \\ (x_2 - x_1) + \frac{6}{\sqrt{2}} \end{pmatrix}$$

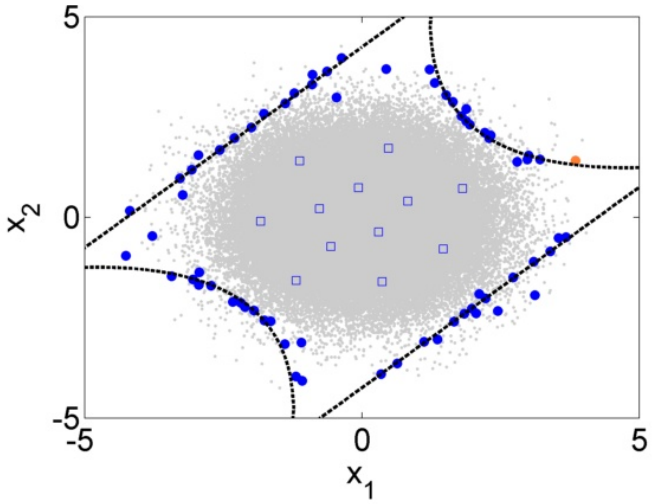
where $X_1, X_2 \sim \mathcal{N}(0,1)$

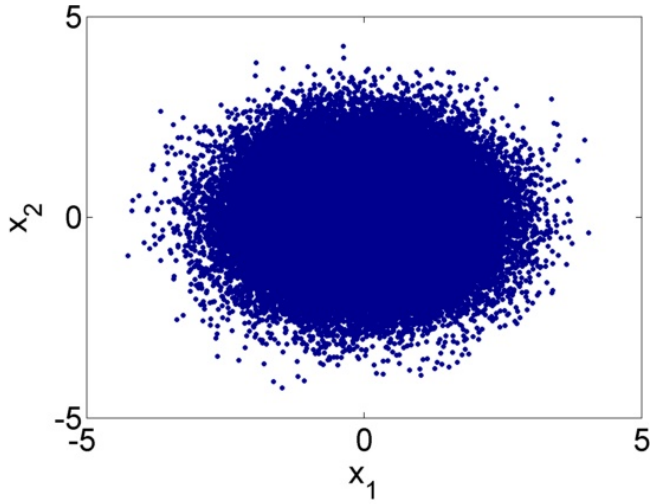


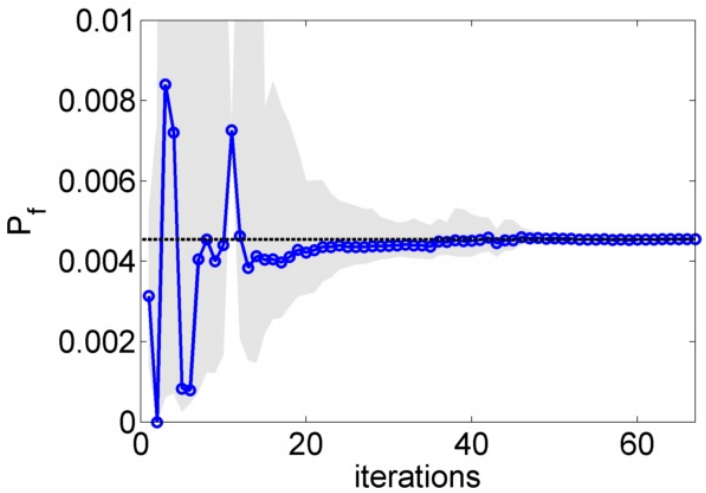


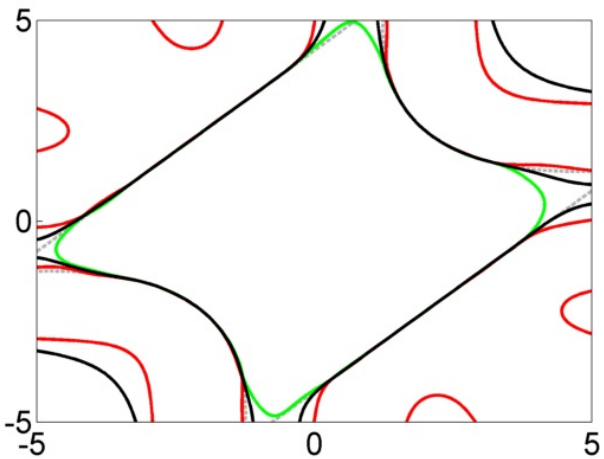
- Initial design: LHS of size 12 (transformed into the standard normal space)
- In each iteration, one point is added (maximize the probability of missclassification)

Results with PC Kriging









Conclusions

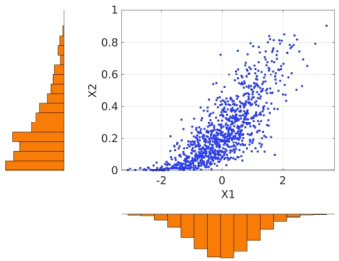
- Surrogate models are unavoidable for solving uncertainty quantification problems involving costly computational models (*e.g.* finite element models)
- Depending on the analysis, specific surrogates are most suitable: polynomial chaos expansions for distribution- and sensitivity analysis, Kriging (and low-rank tensor approximations) for reliability analysis
- Kriging and PC-Kriging are suitable for adaptive algorithms (enrichment of the experimental design)
- All these techniques are non-intrusive: they rely on experimental designs, the size of which is a user's choice
- They are versatile, general-purpose and field-independent
- All the presented algorithms are available in the general-purpose uncertainty quantification software UQLab

UQLab: The Uncertainty Quantification Software

www.uqlab.com

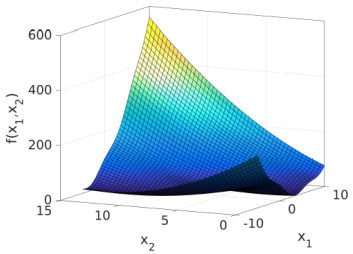
Probabilistic Input Modelling

- Common marginals
- Support for user-defined marginals
- Support for bounds on all distributions (including user-defined)
- Gaussian copula



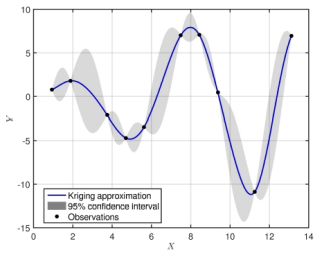
Modelling facilities

- Simple text strings
- MATLAB m-files
- MATLAB handles
- UQLink: easily connect UQLab to third party modelling software



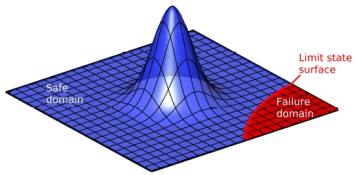
Advanced metamodelling

- Sparse degree-adaptive Polynomial Chaos Expansions
- Gaussian process modelling (Kriging)
- Polynomial-Chaos Kriging
- Low-rank tensor approximations
- Support vector machines



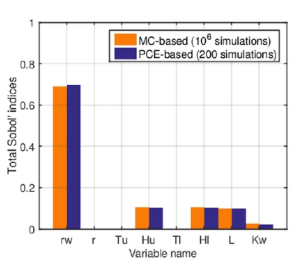
Reliability Analysis (Rare Event Estimation)

- FORM/SORM approximation
- Monte Carlo Simulation (MCS)
- Importance Sampling
- Subset Simulation
- Adaptive Kriging (AK-MCS)



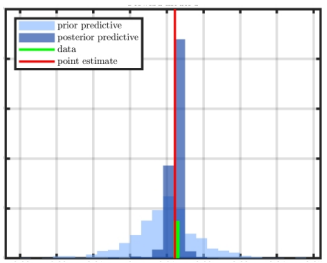
Sensitivity Analysis

- Correlation-based indices
- Standard Regression Coefficients
- Cotter measure
- Morris indices
- Sampling-based Sobol' indices
- PCE- and LRA-based Sobol' indices
- Borgonovo δ indices
- Support for dependent inputs



Bayesian inversion

- Intuitive problem statement
- Advanced MCMC algorithms
- Multi-model support (joint inversion)
- Support for custom likelihood



UQLab: The Uncertainty Quantification Software

http://www.uqlab.com

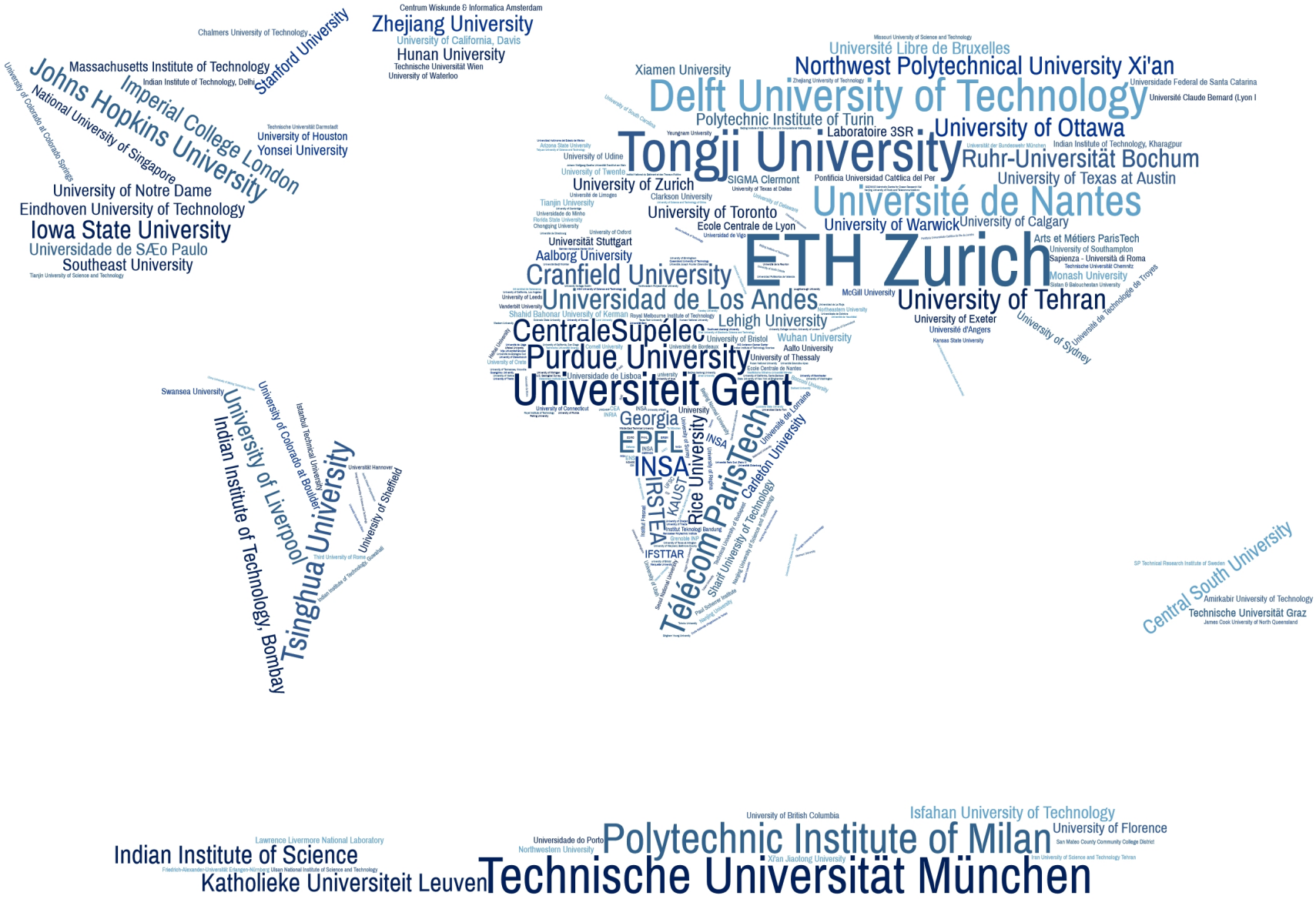
- **1,900 downloads**
- **950^{+} active users from 77 countries**

- Release of V0.9 on July 1st, 2015 (beta version)
- V1.0 on April 28th, 2017
  UQLabCore + modules (PCE, Kriging, Sensitivity, Rare events)
- V1.1 on July 1st, 2018
  Support vector machines, UQLink
- V1.2 on February 22nd, 2019
  Bayesian inversion, UQLib

Country	# Users
United States	343
China	217
France	214
Switzerland	177
Germany	130
United Kingdom	89
Italy	70
India	56
Brazil	50
Canada	50

As of April 23, 2019

UQLab users


Chalmers University of Technology
Stanford University
Massachusetts Institute of Technology
Indian Institute of Technology, Delhi
Johns Hopkins University
Imperial College London
National University of Singapore
University of Colorado at Colorado Springs
Technische Universität Darmstadt
University of Houston
Yonsei University
University of Notre Dame
Eindhoven University of Technology
Iowa State University
Universidade de SÆo Paulo
Southeast University
Tianjin University of Science and Technology
Centrum Wiskunde & Informatica Amsterdam
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ETH Zurich
Technische Universität Chemnitz
Monash University
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McGill University
University of Tehran
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University of Sydney
Université de Technologie de Troyes
CentraleSupélec
University of Bristol
Wuhan University
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Aalto University
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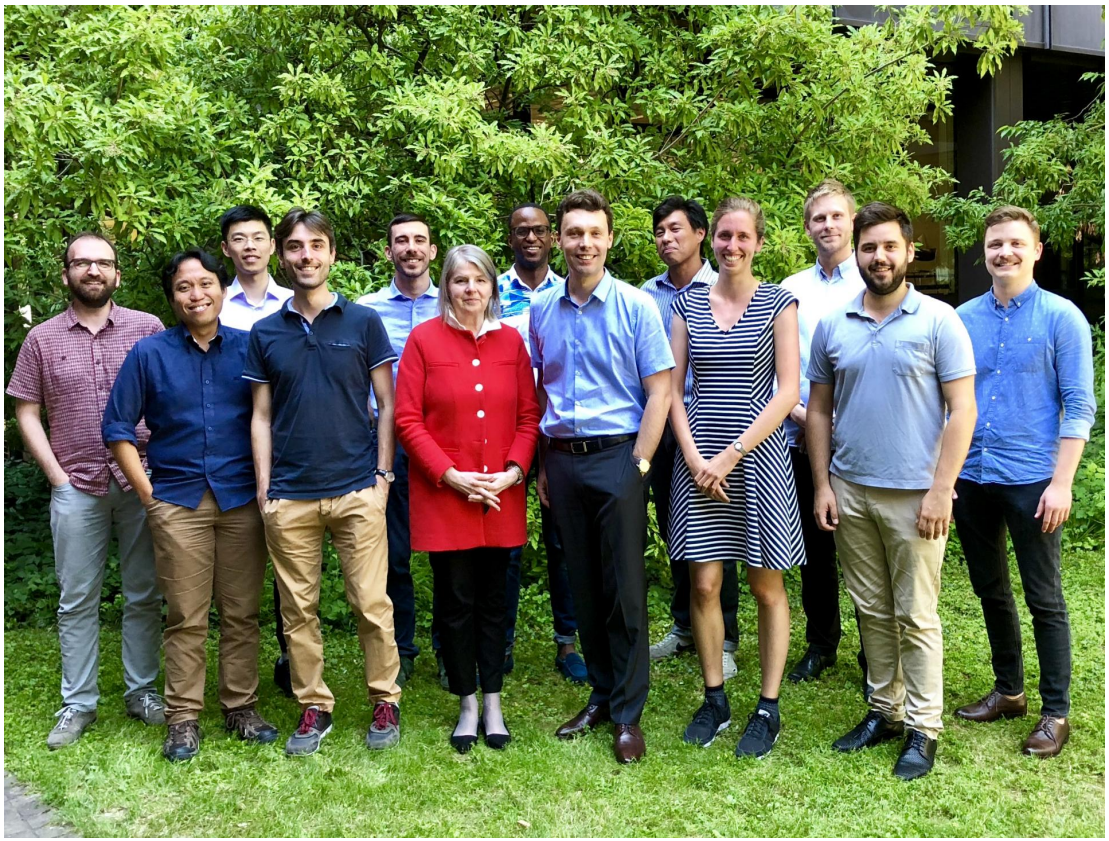
Ecole Centrale de Nantes
Universiteit Gent
University of Connecticut
Georgia
Université de Lorraine
Carleton University
EPFL
INSA
Rice University
KAUST
ParisTech
Télécom
IFSTTAR
Shanghai University of Technology
Swansea University
University of Liverpool
Istanbul Technical University
University of Colorado at Boulder
Indian Institute of Technology, Bombay
Tsinghua University
Universität Hannover
University of Sheffield
Third University of Rome
Central South University
SP Technical Research Institute of Sweden
Amirkabir University of Technology
Technische Universität Graz
James Cook University of North Queensland
Lawrence Livermore National Laboratory
Indian Institute of Science
Friedrich-Alexander-Universität Erlangen-Nürnberg
Ulsan National Institute of Science and Technology
Katholieke Universiteit Leuven
University of British Columbia
Universidade do Porto
Northwestern University
Isfahan University of Technology
Polytechnic Institute of Milan
University of Florence
San Mateo County Community College District
Xi'an Jiaotong University
Iran University of Science and Technology Tehran
Technische Universität München

Questions ?



Chair of Risk, Safety & Uncertainty Quantification

www.rsuq.ethz.ch

The Uncertainty Quantification Laboratory

www.uqlab.com

Thank you very much for your attention !

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