# Introduction to sensitivity analysis

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Kolkata, December, 2018

### Using « Best-estimate » computer codes in engineering

Exploratory studies: <u>understand</u> a phenomenon, an experim/indust.process

**Safety studies:** <u>compute</u> a failure risk (margins, rare events) and prioritize the risk indicators, with validated computer models

**Design studies:** <u>optimize and manage</u> the system performances



# UQ methodology

#### Step C : Uncertainty propagation Design of experiments



# Example: Garonne flood risk (TELEMAC code Uncertainty analysis

#### **Global analysis**





# Industrial example: Garonne flood risk Sensitivity analysis

#### Global analysis : First order indices of Sobol





La Réole

Marmande

Fourgues sur Garon

- The flowrate input factor explains about 80% of the variance of the output variable
- Few interactions between the uncertain variables

### **Sensitivity analysis notions**

Sensitivity, for example  $\partial Z / \partial X_i$ 

The model :  $Z = G(X_1, ..., X_p)$ 

Answer to: how the output varies with respect to potential perturbations of the inputs?

Contribution = sensitivity x importance, for example  $\frac{\partial Z}{\partial X_i}\sigma(X_i)$ 

Gives the weight of an input (or group of inputs) on the uncertainty of the output



The input contributions are often called "importance measures", "sensitivity indices", ...

## Quadratic combination method Independent case

If the  $X_i$  (i = 1...p) are independent, by using the first-order Taylor decomposition of Z around  $\mu$  (linearization), we obtain:

$$\operatorname{Var}(Z) = \sum_{i=1}^{p} \left( \frac{\partial G}{\partial X_{j}} \Big|_{X=\mu} \right)^{2} \sigma_{i}^{2}$$

Quadratic summation formula

Contribution of each input variable to the uncertainty of the output variable

Computation of derivatives via finite differences, exact differentiation, or automatic differentiation

$$\eta_i^2 = \frac{1}{\operatorname{Var}(Z)} \left( \frac{\partial G}{\partial X_i} \Big|_{X=\mu} \right)^2 \sigma_i^2$$

Sensitivity indices (normalized)

#### Sensitivity analysis is directly obtained



# Main objectives of sensitivity analysis (SA)

- 1. Understand the behaviour of the model (decompose input-output relations)
- 2. Simplify the computer model (dimension reduction)
  - Determine the non-influent variables (that can be fixed)
  - Determine the non-influent phenomena (to skip in the analysis)
  - Build a simplified model, a metamodel

#### 3. Prioritize the uncertainty sources to reduce the model output uncertainty

Quantitative partitioning

- Variables to be fixed to obtain the **largest output uncert. reduction**
- Most influent variables in a given output domain

4. Analyze the robustness of the quantity of interest (QoI) with respect to the input uncertainty laws





**Screening** 

Methodology of SA (Qol= variability of the output)

#### Three types of answers:

- 1. <u>Screening (qualitative information: influent/non influent)</u>
  - classical design of experiments,
  - numerical design of experiments (Morris, sequential bifurcation)
- 2. <u>Quantitative measures of global influence</u>
  - correlation/regression on values/ranks,
  - functional variance decomposition (Sobol)

- 3. <u>Deep exploration of sensitivities</u>
  - smoothing techniques (param./non parametric)
  - metamodels









## Outline

- 1. Design of experiments
- 2. Global sensitivity analysis

### 2.1 Screening

2.2 Sampling-based approaches2.3 More advanced methods



### Screening without hypothesis on function: Morris' method





### Morris' method



• OAT design is repeated R times (total:  $n = R^*(p+1)$  experiments)

• It gives an *R*-sample for each elementary effect

 $\begin{cases} d_{X1}^i \\_{i=1...R} \\ d_{X2}^i \end{cases}_{i=1...R}$ 

• Sensitivity measures:

 $\mu_i^* = \mathbf{E}(|d_{X_i}|)$  $\sigma_i = \sigma(d_{X_i})$ 



### **Morris: Sensitivity measures**

•  $\mu_i^* = E(|d_{X_i}|)$  is a measure of the sensitivity:

Important value  $\rightarrow$  important effects (in mean)  $\rightarrow$  sensitive model to input variations

•  $\sigma_i = \sigma(d_{X_i})$  is a measure of the interactions and of the non linear effects:

important value → different effects in the *R*-sample
→ effects which depend on the value:
of the input X<sub>i</sub> => non linear effect
or of the other inputs => interaction

(the distinction between the two cases is impossible)



## **Morris: Example**



20 factors 210 simulations  $\rightarrow$  Graph ( $\mu^*, \sigma$ )

# Distinction between 3 groups:

- 1. Negligible effects
- 2. Linear effects
- 3. Non linear effects and/or with interactions

Test case: non monotonic funtion of Morris



## **Example : fuel irradiation computation in HTR**

Computer code ATLAS (CEA) : simulation of the HTR fuel (fuel particles) behaviour under irradiation

Noyau de matière fissile Carbone pyrolytique poreux Carbone pyrolytique dense Carbure de Silicium



Number of particles inside a reactor : 10<sup>9</sup> to 10<sup>10</sup> !

Contamination sources: failure of particles Reliability studies are needed

The failure of a particle can be caused by the failure of the external thick layers (IPyC, SiC, OPyC)

Output variables are representative of failure phenomena: maximal orthoradial strains in external layers



### 3 uncertainty types for the inputs

- 5 parameters of irradiation (temperature, ...) Interval [min,max] uniform distributions
- 28 behaviour laws (functions of temperature, flux, ...) Expert judgment multiplicative constants (~ U[0.95,1.05])



### **Results of Morris**

p = 43 inputs, 20 repetitions, n = 860 runs, unitary cost ~ 1 mn => total=14h



#### Conclusion:

Morris method provides qualitative information about output variations due to potential variations of inputs

Useful in order to identify the potential influent inputs



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### The sampling-based approaches

Sample (  $X \in \Re^p$ ,  $Z(X) \in \Re$  ) of size N > p [..., Saltelli et al. 2000, Helton et al. 2006, ...]

Monte Carlo sample, space filling design, ...

Preliminary step : graphical visualization (for ex: scatterplots, but also cobweb...)



Example of the OpenTURNS graphical interface



## **First visualization: scatterplots**



4 : absence de liaison

### Example: Flood model - Scatterplots – Output S



Q = river flowrate ~ Gumbel on [500,3000]

Ks = friction coefficient ~ normal on [15,50]

Zv = downstream river bed heigth ~ triangular on [49,51]

Hd = dyke heigth ~ triangular on [7,9]

Cb = bank heigth ~ triangular on [55,56]

$$S = Z_v + H - H_d - C_b \text{ avec } H = \left(\frac{Q}{BK_s\sqrt{\frac{Z_m - Z_v}{L}}}\right)^{0.6}$$

Monte Carlo sample – N = 100



### Example: Flood model - Scatterplots – Output Cp

$$\begin{split} C_p &= \ \ \mathbbm{1}_{S>0} + \left\{ 0.2 + 0.8 \left[ 1 - \exp\left( -\frac{1000}{S^4} \right) \right] \right\} \ \mathbbm{1}_{S\leq 0} & \text{Monte Carlo sample} - \textit{N} = 100 \\ &+ \ \ \frac{1}{20} \left( H_d \mathbbm{1}_{H_d>8} + 8\mathbbm{1}_{8\leq H_d} \right) \ , \end{split}$$



<u>Major drawback</u>: only first order relations between inputs are analyzed and not their interactions (=> needs of other data anlysis tools)



## Second visualization: the cobweb plot





#### Interactive use with the OpenTURNS graphical interface



### Sensitivity indices in case of linear inputs/output relation

Independent inputs  $\mathbf{X} = (X_1, \dots, X_p)$ 

<u>Sample:</u> *n* realizations of  $(\mathbf{X}, Y)$ 

Linear regression model:  $Z = \beta_0 + \sum_{i=1}^{p} \beta_i X_i$ 

Standard Regression Coefficients (SRC):  $SRC(X_i) := \beta_i \sqrt{\frac{Var(X_i)}{Var(Z)}}$ 

Sign of  $\beta_i$  gives the direction of variation of  $Z / X_i$ 

- Similar to the linear correlation coefficient (Pearson)
- Validity of the linear model via regression diagnostics and *P*<sup>2</sup>:

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (\hat{Y}_{i} - Y_{i})^{2}}{\sum_{i=1}^{n} (Y_{i} - \overline{Y})^{2}}$$

Theoretically, we have  $R^2 = \sum_{i=1}^{p} SRC^2(X_i)$ , useful to interpret SRC



### A classical view on the « Sampling-based approaches »

Sample (  $X \in \Re^p$ ,  $Z(X) \in \Re$  ) of size N > p [..., Saltelli et al. 2000, Helton et al. 2006, ...]





## Application on the flood model – Output S



#### ⇒ SRC are valid sensitivity indices; global sensitivity analysis is achieved



=> linear model is not sufficiently valid



### Industrial example: Nuclear PWR severe accident study

#### Important issue for the safety core of the industrial operator



#### Main questions after a severe accident (PSA level 2):

- Is there some radionuclide release outside the containment (and what is the time of this release)?
- What is the efficiency of mitigation actions?
- Influence of the large parameter uncertainties on the failure probability?

> Development of a soft simulating severe accident scenarios (corium behavior)



### Main objectives of these uncertainty studies

Complex and coupled numerical models which require sensitivity analysis to:

- Identify the main sources of uncertainties
- Understand the relations between uncertain inputs and interest outputs



<u>Additional problem</u>: provide tools for engineers knowing nothing little about stats



### 3 use levels of the soft – 1) Precise and punctual needs

<u>Example: relative study about the failure probability</u>

<u>Goal:</u> understand the influence of water injection in the vessel and/or in the reactor pit during the accident

Random var. X : 22 uniform - 1 binary (for the water presence/absence) N = 500 random simulations (LHS design)

Failure probability is estimated by Monte-Carlo method P(failure without water injection)/ P(failure with water injection) = 2.5 This kind of result could help the definition of management strategies



Sensitivity analysis via boxplots

No failure Failure



No failure Failure



### 3 use levels – 2) Detailed analyses for confirmed users

<u>Example: sensitivity analysis related to an output variable (corium mass)</u> with 22 inputs

<u>Goal:</u> understand which input variables strongly affect the corium mass





### 3 use levels – 3) Help to physical model developers

### Example: detection of anomalies

500 MC simulations

Corium mass in the vessel bottom

It has allowed to detect that important phenomena related to the corium transfer were not included in the physical model



Limit factor of the critical flux



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## **Issues in sensitivity analysis**

#### Numerical model' issues

P1) G(.) is complex: interactions, non linear, discontinuous, ...

#### => Sobol indices, moment-independent measures

P2) G(.) is costly (several minutes - days to compute one evaluation)

=> Metamodel

#### Model inputs' issues

P3) p is large : p > 10 ... 100 ... => Quantitative screening (HSIC, DGSM)
P4) Dependence between inputs => Shapley indices
P5) Uncertainty on inputs' pdfs (epistemic) => Robustness analysis (PLI)

#### Model outputs' issues

- P6) Z is not a single scalar, but a high-dimensional vector, a temporal function, a spatial field, ...
  => Ubiquitous and aggregated indices
- P7) Inputs or outputs are too voluminous

#### => Iterative sensitivity analysis

**P8)** The Quantity of Interest (QoI) is not the variance (e.g. a quantile)

=> GOSA (Goal-Oriented Sensitivity Analysis)



### P1) Sensitivity analysis for one scalar output

Sample (X, Z(X)) of size n > p, preferably n >> p Preliminary step: graphical vizualisation (for ex: scatterplots)

Quantitative sensitivity analysis methodology





## P1) Sensitivity indices without model hypotheses

**Functional ANOVA** [Efron & Stein 81] (hyp. of independence between  $X_i$ , i=1...p):

$$Var(Z) = \sum_{i=1}^{p} V_i(Z) + \sum_{i < j}^{p} V_{ij}(Z) + \dots + V_{12\dots p}(Z)$$
  
where  $V_i(Z) = Var[E(Z|X_i)]$   
 $V_{ij} = Var[E(Z|X_iX_j)] - V_i - V_j, \dots$ 

#### Sobol indices definition:

First order sensitivity indices:  $S_i = \frac{V_i}{Var(Z)}$ 

Second order sensitivity indices:

$$S_{ij} = \frac{V_{ij}}{\operatorname{Var}(Z)}$$





## **P1) Graphical interpretation**

First order Sobol' indices measure the variability of conditional expectations (mean trend curves in the scatterplots)





## P1) Sobol' indices properties

$$\begin{split} 1 &= \sum_{i=1}^{p} S_{i} + \sum_{i} \sum_{j} S_{ij} + \sum_{i} \sum_{j} \sum_{k} S_{ijk} \dots + S_{1,2,\dots,k} \\ &\sum_{i} S_{i} \leq 1 \qquad \text{Always} \\ &\sum_{i} S_{i} = 1 \qquad \text{Additive model} \\ &1 - \sum_{i} S_{i} \qquad \text{Measure the degree of interactions between variables} \end{split}$$

Examples : p = 4 gives 4 indices  $S_{i}$ , 6 indices  $S_{ij}$ , 4 indices  $S_{ijk}$ , 1 indice  $S_{ijkl}$ 

General case : 2<sup>*p*</sup>-1 indices to be estimated

Total sensitivity index:

$$S_{Ti} = S_i + \sum_j S_{ij} + \sum_{j,k} S_{ijk} + \dots = 1 - S_{-i}$$

[Homma & Saltelli 1996]

### **Come-back to the flood model example**

Overflow S



edf

Cost C<sub>p</sub>

### P1) The sampling-based approaches

Sample (  $X \in \Re^{p}$ ,  $Z(X) \in \Re$  ) of size N > p



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### P2) Sensitivity analysis by metamodels

- Mathematical function (polynomial, polyn. chaos, neural network, kriging, ...) representative of the computer model with negigible cpu cost (ex: 1 ms)
- Approximation from a design of experiments : N simulations ( $N \sim 10 p$ )
- Important: control the approximation and prediction capabilities



Example: Kriging metamodel, which propagates the metamodel error on sens. indices



### **Come-back to the flood model example – Output Cp**

From the 100-size Monte Carlo sample, a Gaussian process metamodel is fitted

Predictivity of the Gp metamodel :  $Q_2 = 99\%$ 

The previously shown formula are applied on the metamodel predictor

	Indices (en %)	Q	$K_s$	$Z_v$	$H_d$	$C_b$
N=1e5 100 replicates	$S_i$ modèle	35.5	15.9	18.3	12.5	3.8
	$S_i$ métamodèle	38.9	16.8	18.8	13.9	3.7
	$S_{T_i}$ modèle	48.2	25.3	22.9	18.1	3.8
	$S_{T_i}$ métamodèle	45.5	21.0	21.3	16.8	4.3

N x (p+2) x 100 = 7 x 10<sup>7</sup> metamodel evaluations



# P3) Large *p* - Quantitative screening with HSIC

Generalized sensitivity indices (HSIC) which not limit SA to a single metric to compare change in the distribution of the output when there an input varies







X1 fixed

[ Da Veiga 2015 ]

X1 fixed

A dependence measure is used to compare the joint

distribution between Z and  $X_i$  and the product of marginals of Z and  $X_i$  with an infinity of metrics (kernel trick) => HSIC( $X_i$ , Z), which is computed with a single sample

high-dimensional SA

Rem: classical indices (SRC, Sobol) only use the « mean » metric



### P3) Large *p* - Quantitative screening with DGSM (Derivative-based Global Sensitivity Measures)

$$\nu_i = \int_{\text{Supp}(\mathbf{X})} \left( \frac{\partial G(\mathbf{X})}{\partial X_i} \right)^2 \, \mu_{\mathbf{X}} d\mathbf{X}$$

[Kucherenko et al. 2009]

- Mix stochastic and deterministic approaches as global and local approaches
- Inequality between DGSM and Sobol' indices:

$$0 \leq S_{Ti} \leq \frac{C(f_{X_i})}{\operatorname{Var}(Z)} \nu_i \qquad C(f_{X_i}) : \text{ constant} \qquad [Lamboni et al. 2013] \\ Roustant et al. 2017]$$

- Cost (empirical) of evaluating the integral: N ~ 100 (smaller than for Sobol' indices)
- Cost of evaluating the derivatives:
  - p + 1 by finite differences
  - Independent of p if the adjoint models of f is available

high-dimensional SA



### P5) Robustness analysis : PLI (Perturbed-Law based indices)

The idea is to pertub the pdf (prob. measure  $\mu_i$ ) of  $X_i$  by a statistics (e.g. the mean, variance, ...). With a  $\delta$  perturbation, it gives the perturbed measure  $\mu_{i\delta}$ 

[Lemaître et al. 2015]

#### Sensitivity indices on the Qol (e.g. a probability of failure P):

$$\mathbf{S}_{\mathbf{i}\delta} = \left(\frac{P_{\mathbf{i}\delta}}{P} - 1\right) \mathbf{1}_{P_{\mathbf{i}\delta} \geq P} + \left(1 - \frac{P}{P_{\mathbf{i}\delta}}\right) \mathbf{1}_{P_{\mathbf{i}\delta} < P}$$

- Two main technical ingredients:
  - Minimisation of the Kullback-Leibler divergence
  - Reverse importance sampling to estimate P and  $P_{i\delta}$  using the same model outputs



## P5) Examples of perturbed probability laws





## P5) Quantile-PLI – Analytical example

[Sueur et al. 2017]

 $G(X) = sin(X_1) + 7 * sin^2(X_2) + 0, 1 * X_3^4 * sin(X_1); X_i \sim U(-\pi, \pi)$  independent



The provided information are different

=> Robustness analysis for BEPU methodolology

## P6) Ubiquitous and aggregated indices



#### Synthesize the information on sensitivity indices:

#### Aggregated sensitivity indices:

 $GSI_{i} = \sum_{k=1}^{q} \frac{I_{k}}{I} S_{i}(t_{k})$ Total output variance

[Lamboni et al. 2009; Gamboa et al. 2014]





## **Conclusion: choosing the right method?**

- Requested information (qualitative/quantitative)
- Number of inputs
- Regularity of the model (linearity/monotony/continuity)
- Cpu cost of one model evaluation
- Number of outputs
- Additional constraints, for example :
  - Uncertainty/sensitivity joint analysis,
  - Dependency between inputs, …



## **Recall: Main objectives of sensitivity analysis**

- 1. Understand the behaviour of the model (decompose input-output relations)
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**Screening** 

## **Recall: Methodology of SA**

(Qol= variability of the output)

#### Three types of answers:

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### **Classification of methods**



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