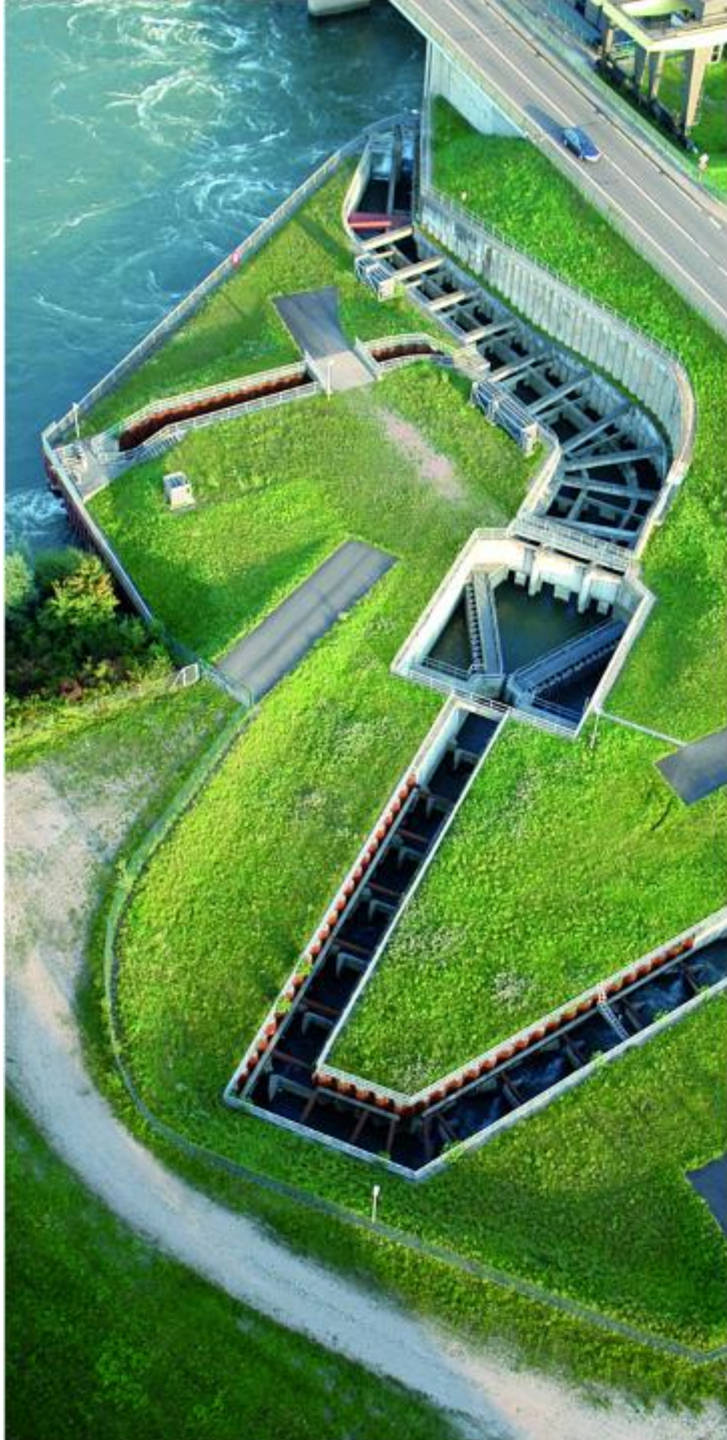
New practices in global sensitivity analysis and robustness analysis of model outputs



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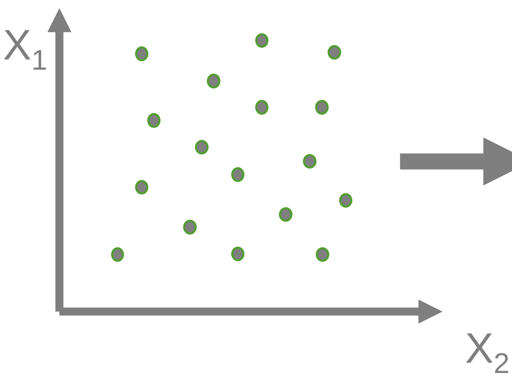
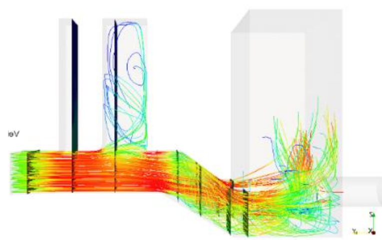
5th IPSMNA conference, October, 2024

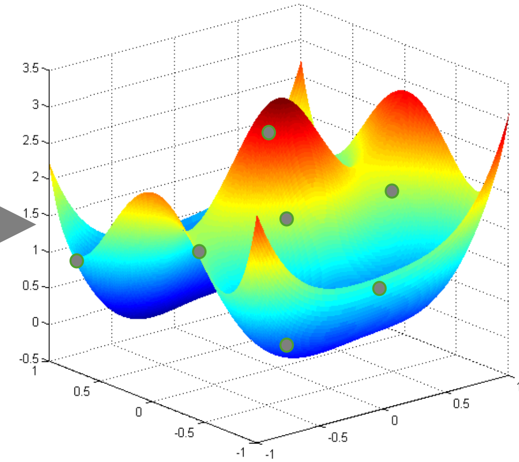
Computer experiments framework



Computer experiments

$Y = G(X_1, \ldots, X_d)$





Design

Minimize costs

Analysis

Understand & measure the inputs' effects

Modeling

Build fast emulators (surrogate/reduced models)

Optimization

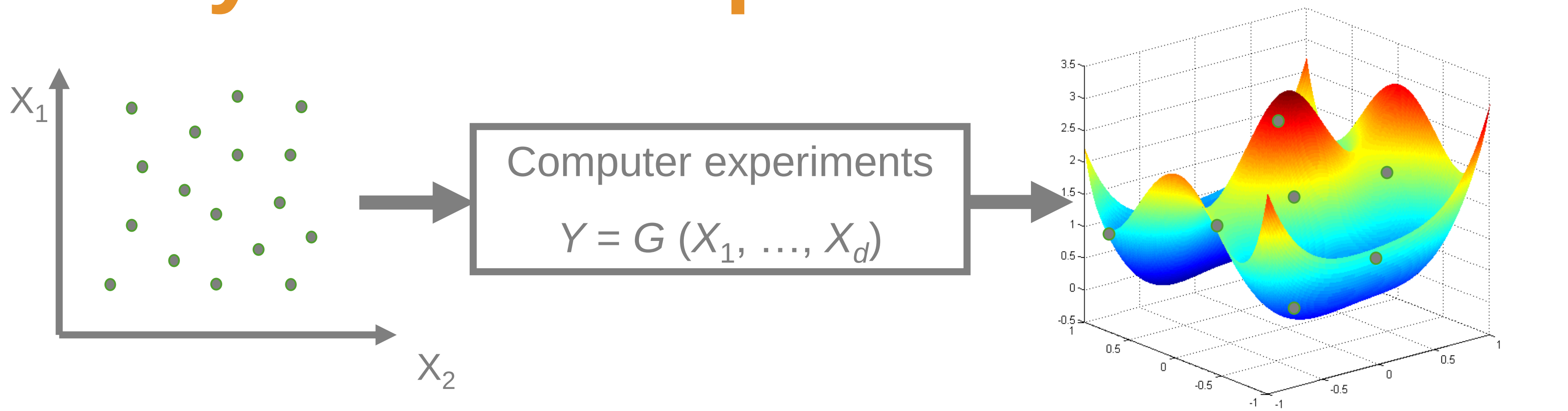
Find the right scenarios

Reliability

Evaluate the residual risks

Decision

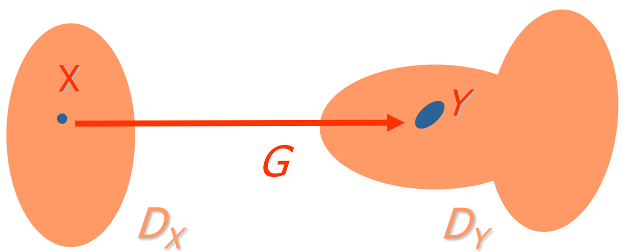
Analysis of computer experiments



Analysis: **From a (Monte Carlo) sample of runs: measure the inputs' effects**

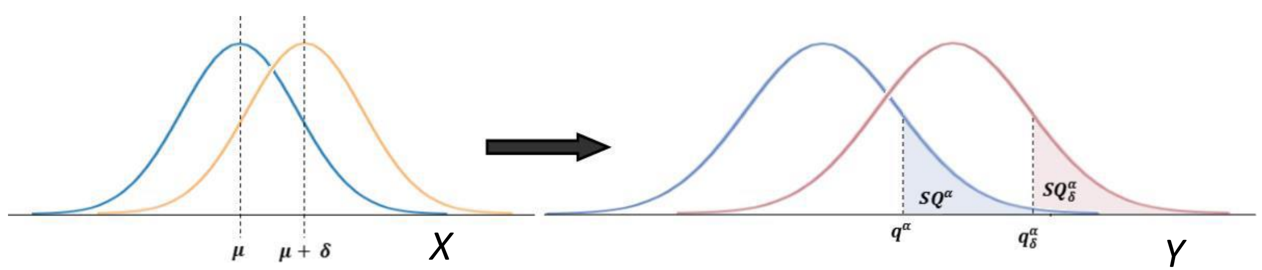
- Global Sensitivity Analysis (GSA)

How an input or a group of input apportion into the uncertainty of the output?



- Robustness Analysis (RA)

What is the impact on the QoI of the uncertainty on the probabilistic model of the inputs?



Safety motivation: Simulation of IB-LOCA accident

IB-LOCA: *Intermediate break loss of coolant accident*

Pressurized Water Reactor scenario:
Loss of primary coolant accident due to a break in cold leg

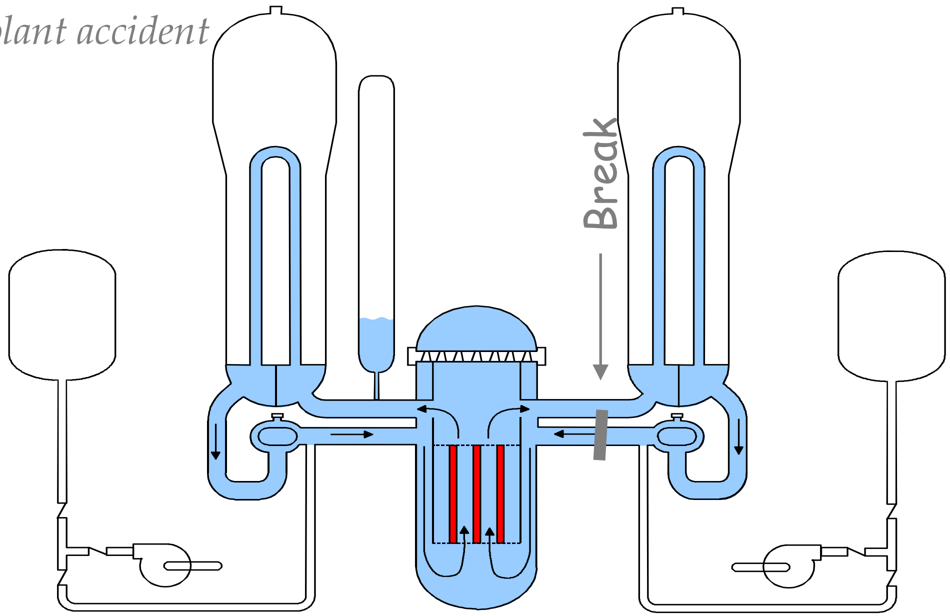
***d* (~ 100) uncertain input variables *X*:**
Critical flowrates, initial/boundary conditions, phys. eq. coef., …
Probabilistic modeling

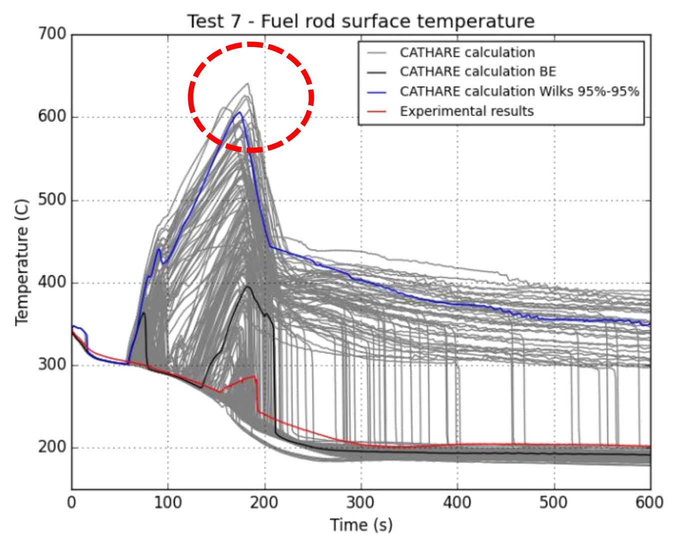
<u>Modelled using **CATHARE2 code**:</u>
(thermal-hydraulic phenomena)

CPU cost for one code run > 1 hour
In industrial studies: *N* ~ O(1000) runs

Variables of Interest *Y* :
Cladding temperature (fct of time)
Peak Cladding Temperature (PCT)

Quantity of Interest (QoI) :
high-order (e.g. 95%) quantile of *Y*, …





100 output transients corresponding to 100 (Monte Carlo) runs

Global sensitivity indices

Standard practice in the independent inputs' case

? Linear relation ?

Yes

Linear regression between *Y* and ***X***

$$Y = Y(\boldsymbol{X}) = \sum_{i=1}^{d} \beta_i X_i + \epsilon$$

Regression coefficients β_i
=> Standard Regr. Coef. (SRC)

No

Sobol' indices

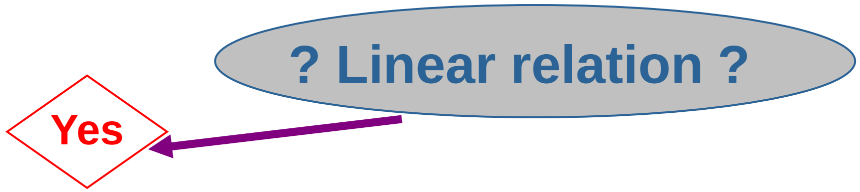
Sensitivity Indices (variance decomposition)

$$\mathrm{SRC}_i^2 = \beta_i^2 \frac{\mathrm{Var}(X_i)}{\mathrm{Var}(Y)}$$

$$S_i = \frac{\mathrm{Var}[\mathrm{E}(Y|X_i)]}{\mathrm{Var}(Y)}$$

Global sensitivity indices

How to deal with the dependent (correlated) inputs' case?



The SRC² do not decompose the variance anymore and the inputs effects have to be decorrelated.
Standard practice: Use the partial correlation coefficient: $\mathrm{PCC}(X_i) = \rho\left(X_i - \widehat{X_{-i}}, Y - \widehat{Y_{-i}}\right)$

<u>This practice has to be banned</u>: PCC(X_i) only measures the linearity between X_i and Y

The right formulation consists in averaging all the R^2-contributions of X_i wrt all the other inputs' combinations (R^2 is the explained variance by the linear model)

Sensitivity Indices (variance decomposition)

$$\mathrm{LMG}_i = \frac{1}{d}\sum_{u\subseteq\{-i\}} \binom{d-1}{|u|}^{-1} \left[R^2_{Y(\boldsymbol{X}_{u\cup\{i\}})} - R^2_{Y(\boldsymbol{X}_u)}\right]$$

Remark for the non-linear case: replace R² by Sobol' indices => Shapley effects

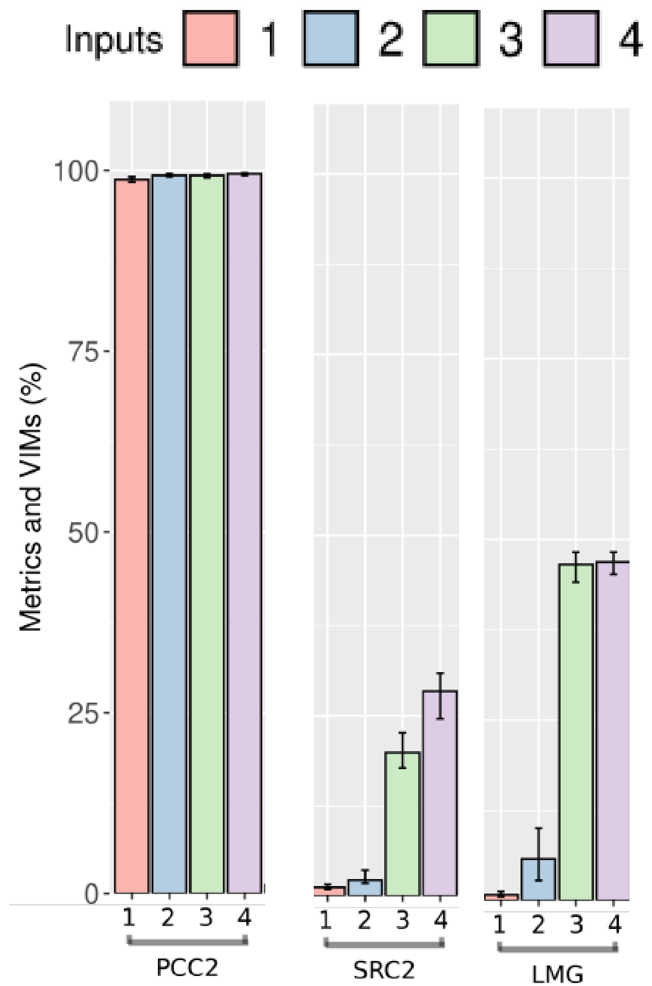
Simple example

$$G(X) = X_1^2 + X_2 + X_3 + X_4$$

$\mathcal{U}[0.5,1.5]$ $\mathcal{U}[1.5,4.5]$ $\mathcal{U}[4.5,13.5]$ $X_4 = X_3 + \mathcal{N}(0,1)$

We simulate a 100-size monte Carlo sample

We perform the linear regression on this sample and obtain: $R^2 = 1$



[Clouvel et al. 2024]

Robustness analysis using PLI (Perturbed Law-based Indices)

[Lemaître et al., 2015]
[Iooss et al. 2022]

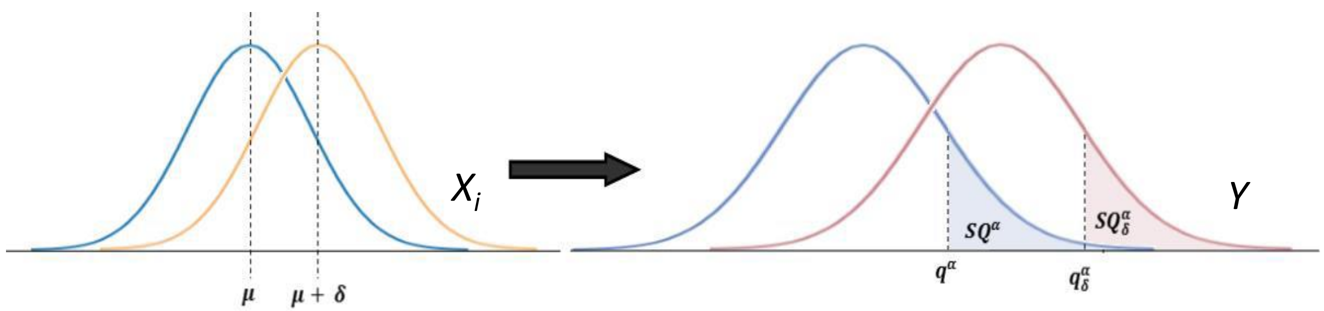
We aim at quantifying the impact on the QoI of a perturbation of the pdf of X_i

For example, what happens if we replace $E(X_i) = \mu_i$ by $E(X_i) = \mu_i + \delta$?

We define the PLI-quantiles as : $S_{i\delta} = \left(\frac{q_{i\delta}^{\alpha}}{q^{\alpha}} - 1\right)$ (with q^{α} and $q_{i\delta}^{\alpha}$ the α-quantile of Y and the perturbed quantile)

- It gives results in terms of percentage of perturbations
- $S_{i\delta} = 0$ when $q_{i\delta}^{\alpha} = q^{\alpha}$ i.e. when f_i has no impact on the quantile
- The sign of $S_{i\delta}$ indicates how the perturbation modifies the quantile

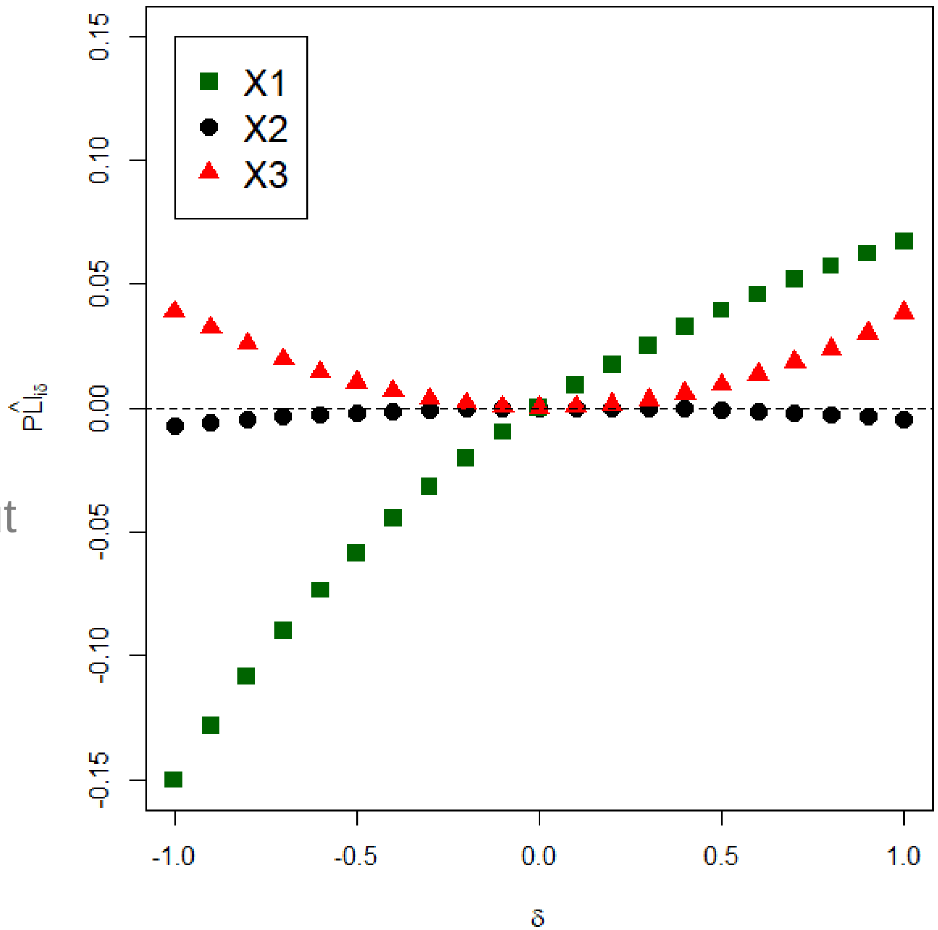
Example



Perturbation of the mean of the pdf of the input X_i

Computation of the deviation of the QoI (quantile of the output Z, ...)

Example on an analytical 3D function



100000-size Monte Carlo sample

Perturbations of the mean of each input

PLI on the 95%-quantile (QoI) of the output

Such elements can be used to assess the robustness of the QoI facing some lack of confidence on the probabilistic model of some inputs (epistemic uncertainties)

=> Useful to discuss with safety authorities

References

On GSA:

S. Da Veiga, F. Gamboa, B. Iooss and C. Prieur. *Basics and trends in sensitivity analysis: Theory and practice in R*, SIAM, 2021

L. Clouvel, V. Chabridon, B. Iooss, M. Il Idrissi and F. Robin, An overview of variance-based importance measures in the linear regression context: comparative analyses and numerical tests, Preprint

On RA:

B. Iooss, V. Vergès and V. Larget, BEPU robustness analysis via perturbed-law based sensitivity indices, *Proceedings of the Institution of Mechanical Engineers, Part O: Journal of Risk and Reliability*, 236:855-865, 2022

P. Lemaître, E. Sergienko, A. Arnaud, N. Bousquet, F. Gamboa and B. Iooss. Density modification-based reliability sensitivity analysis. *Journal of Statistical Computation and Simulation*, 85 :1200-1223, 2015

Software:

sensitivity package of R