Sensitivity to statistical estimation uncertainties and probabilistic model identification

ETICS 2022

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7th of October 2022

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2. Proposed approach
3. Sensitivity analysis
4. Illustration
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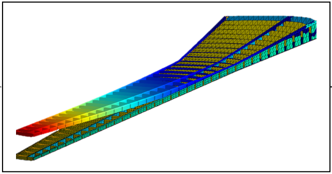
Context - Uncertainty Quantification

Simulation code of a mechanical structure:

d parameters
$(\mathrm{E}, \nu, \mathrm{L}, ...)$

→



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An output quantity
$(\sigma, \mathrm{u}, ...)$

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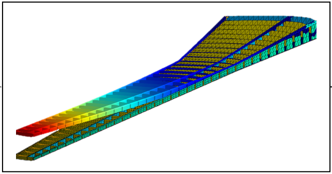

An output quantity
$(\sigma, \mathrm{u}, ...)$

In an uncertainty quantification context, those parameters are considered as an input continuous random vector :

$$\boldsymbol{X} \longrightarrow \boxed{\text{Black Box} \;\; \phi} \longrightarrow Y$$

with $\boldsymbol{X} = (X_1, ..., X_d)^t$ with values on the domain $\mathcal{X} \subseteq \mathbb{R}^d$ and defined by a given Probability Density Function (PDF) $f_{\boldsymbol{X}}$.

Context - 1^{st} uncertainty source

One could be interested in assessing the following expectation of a particular function τ of $Y = \phi(\boldsymbol{X})$ (e.g. a mean or a probability of failure):

$$\mathbb{E}_{f_{\boldsymbol{X}}}\left[\tau\left(\phi\left(\boldsymbol{X}\right)\right)\right] = \int_{\mathcal{X}} \tau\left(\phi\left(\boldsymbol{x}\right)\right) f_{\boldsymbol{X}}\left(\boldsymbol{x}\right) \mathrm{d}\boldsymbol{x}. \tag{1.1}$$

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Assuming $\tau = \mathrm{Id}$, the Monte Carlo (MC) estimator of this integral is given by:

$$\hat{\mu}^{MC} = \frac{1}{N_{\boldsymbol{X}}} \sum_{j=1}^{N_{\boldsymbol{X}}} \phi\left(\boldsymbol{X}^{(j)}\right), \tag{1.2}$$

with $\boldsymbol{X}^{(j)} \overset{i.i.d.}{\sim} f_{\boldsymbol{X}}$ and $N_{\boldsymbol{X}}$ the size of the MC sample.

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with $\boldsymbol{X}^{(j)} \overset{i.i.d.}{\sim} f_{\boldsymbol{X}}$ and $N_{\boldsymbol{X}}$ the size of the MC sample. A first uncertainty source is related to this sample, defined as $\widetilde{\boldsymbol{X}}$ in the following process:

$$\boxed{\widetilde{\boldsymbol{X}} = \{\boldsymbol{X}^{(j)}, j = 1, \dots, N_{\boldsymbol{X}}\}} \xrightarrow{\Sigma} \boxed{\hat{\mu}^{MC}}$$

Context - 2^{nd} uncertainty source

In a realistic context, the PDF $f_{\boldsymbol{X}}$ may be unknown [1]. Thus, the probabilistic model must be inferred from experimental tests:

$$\widetilde{\boldsymbol{D}} = \{\boldsymbol{D}^{(i)}, i = 1, \ldots, N_{\boldsymbol{D}}\}$$
with $\boldsymbol{D}^{(i)} \overset{i.i.d.}{\sim} f_{\boldsymbol{X}}$

$\hat{f}_{\boldsymbol{X}|\widetilde{\boldsymbol{D}}}$

with $N_{\boldsymbol{D}}$ the size of the database $\widetilde{\boldsymbol{D}}$. The estimation $\hat{f}_{\boldsymbol{X}|\widetilde{\boldsymbol{D}}}$ [2, 3] of the PDF $f_{\boldsymbol{X}}$ induces a second uncertainty source related to $\widetilde{\boldsymbol{D}}$.

[1] G Sarazin. Analyse de sensibilité fiabiliste en présence d'incertitudes épistémiques introduites par les données d'apprentissage, 2021.

[2] K James, Lindsey and others. Parametric statistical inference. Oxford University Press, 1996.

[3] A J Izenman. Recent developments in nonparametric density estimation. Journal of the american statistical association, 1991.

Context - Small-Data

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$\downarrow$

Test-Simulation trade-off

Context - Conditioning on a given database

The expectation (1.1) and its estimator are thus written as following for a given database $\widetilde{\boldsymbol{D}} = \widetilde{\boldsymbol{d}}$:

$$\mathbb{E}_{\hat{f}_{\boldsymbol{X} \mid \widetilde{\boldsymbol{D}}=\widetilde{\boldsymbol{d}}}}\left[\phi\left(\boldsymbol{X}\right)\right] = \int_{\mathcal{X}} \phi\left(\boldsymbol{x}\right) \hat{f}_{\boldsymbol{X} \mid \widetilde{\boldsymbol{D}}=\widetilde{\boldsymbol{d}}}\left(\boldsymbol{x}\right) \mathrm{d}\boldsymbol{x} \qquad (1.3)$$

$$\approx \frac{1}{N_{\boldsymbol{X}}} \sum_{j=1}^{N_{\boldsymbol{X}}} \phi\left(\boldsymbol{X}^{(j)}\right), \qquad (1.4)$$

with $\boldsymbol{X}^{(j)} \overset{i.i.d.}{\sim} \hat{f}_{\boldsymbol{X} \mid \widetilde{\boldsymbol{D}}=\widetilde{\boldsymbol{d}}}$. The estimator (1.4) is now subject to the first uncertainty source conditioned on the database $\widetilde{\boldsymbol{D}} = \widetilde{\boldsymbol{d}}$.

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However, the uncertainty related to the database is not considered in the following variance :

$$\mathbb{V}_{\hat{f}_{\boldsymbol{X}|\widetilde{\boldsymbol{D}}=\widetilde{\boldsymbol{d}}}}\left[\hat{\mu}^{MC}\right] = \frac{1}{N_{\boldsymbol{X}}} \mathbb{V}_{\hat{f}_{\boldsymbol{X}|\widetilde{\boldsymbol{D}}=\widetilde{\boldsymbol{d}}}}\left[\phi\left(\boldsymbol{X}\right)\right]. \tag{1.5}$$

Context - Problems

$$\widetilde{\boldsymbol{D}} = \{\boldsymbol{D}^{(i)}, i = 1, \dots, N_{\boldsymbol{D}}\}$$

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Problem A

How to take into account the uncertainty of the database in the variance of the estimator?

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How to take into account the uncertainty of the database in the variance of the estimator?

Problem B

In order to improve efficiently the accuracy of the estimator, should the investment of data be made in the database or the MC sample?

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Proposed approach - Double integral expectation

Problem A

How to take into account the uncertainty of the database in the variance of the estimator?

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The following expectation takes into account the variation of the database:

$$\mathbb{E}_{f_{(\boldsymbol{X},\widetilde{\boldsymbol{D}})}}\left[\phi\left(\boldsymbol{X}\right)\right] = \int_{\mathcal{X}^{N_D}} \int_{\mathcal{X}} \phi\left(\boldsymbol{x}\right) f_{(\boldsymbol{X},\widetilde{\boldsymbol{D}})}(\boldsymbol{x},\widetilde{\boldsymbol{d}}) \mathrm{d}\boldsymbol{x} \; \mathrm{d}\widetilde{\boldsymbol{d}}. \tag{2.1}$$

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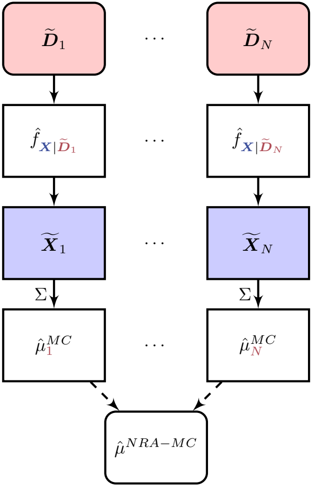
An estimator of this integral [4] is the following:

$$\hat{\mu}^{NRA-MC} = \frac{1}{N}\sum_{k=1}^{N}\frac{1}{N_{\boldsymbol{X}}}\sum_{j=1}^{N_{\boldsymbol{X}}}\phi\left(\boldsymbol{X}_k^{(j)}\right) = \frac{1}{N}\sum_{k=1}^{N}\hat{\mu}_k^{MC}, \tag{2.2}$$

with $\boldsymbol{X}_k^{(j)} \overset{i.i.d.}{\sim} \hat{f}_{\boldsymbol{X}|\widetilde{\boldsymbol{D}}_k}$ and N the number of databases of size $N_{\boldsymbol{D}}$.

[4] V Chabridon. Analyse de sensibilité fiabiliste avec prise en compte d'incertitudes sur le modèle probabiliste, 2018.

Proposed approach - Empirical variance



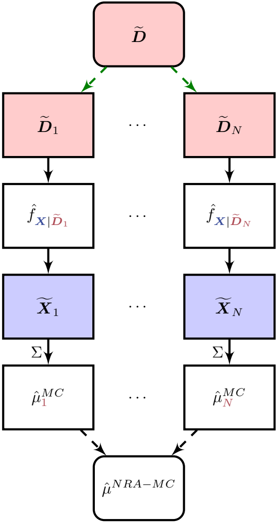
The process is repeated in order to estimate the variance with respect to the database.

Empirical variance:

$$\hat{\mathbb{V}}_{f_{(X,\widetilde{D})}}\left[\hat{\mu}^{MC}\right] = \frac{1}{N-1}\sum_{k=1}^{N}\left(\hat{\mu}_k^{MC} - \hat{\mu}^{NRA-MC}\right)^2 \quad (2.3)$$

(2.2)

Proposed approach - Small-data context



(2.3)

(2.2)

In a small-data context, only a database $\widetilde{\boldsymbol{D}}$ of limited size $N_{\boldsymbol{D}}$ is available.

Resampling method

Allows to generate N databases from the initial one. [5, 6] (e.g. Bootstrap)

Solution A

The nested estimator (2.2) is now conditioned on the initial database but the method allows to take into account the uncertainty related to it.

[5] C H Yu. Resampling methods: concepts, applications, and justification. Practical Assessment, Research, and Evaluation, 2002.

[6] B Efron. The jackknife, the bootstrap and other resampling plans. SIAM, 1982.

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Sensitivity analysis - ANOVA

Problem B

In order to improve efficiently the accuracy of the estimator, should the investment of data be made in the database or the MC sample?

Sensitivity analysis - ANOVA

Problem B

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An ANalysis Of VAriance [7, 8] is performed:

$$\begin{cases} S_{\widetilde{\boldsymbol{D}}} = \dfrac{\mathbb{V}\left[\mathbb{E}\left[\hat{\mu}^{MC} | \widetilde{\boldsymbol{D}}\right]\right]}{\mathbb{V}\left[\hat{\mu}^{MC}\right]} \\ S_{\widetilde{\boldsymbol{X}}} = \dfrac{\mathbb{V}\left[\mathbb{E}\left[\hat{\mu}^{MC} | \widetilde{\boldsymbol{X}}\right]\right]}{\mathbb{V}\left[\hat{\mu}^{MC}\right]} \end{cases} . \tag{3.1}$$

Interpretation of Sobol' indices:

- $S_{\widetilde{\boldsymbol{D}}} \to$ proportion of variance due to the database,
- $S_{\widetilde{\boldsymbol{X}}} \to$ proportion of variance due to the MC sample.

[7] Ilya M Sobol'. Sensitivity analysis for non-linear mathematical models. Mathematical modelling and computational experiment, 1993.
[8] F Gamboa and others. Statistical inference for sobol pick-freeze monte carlo method. Statistics, 50(4):881–902, 2016.

Sensitivity analysis - Interpretation

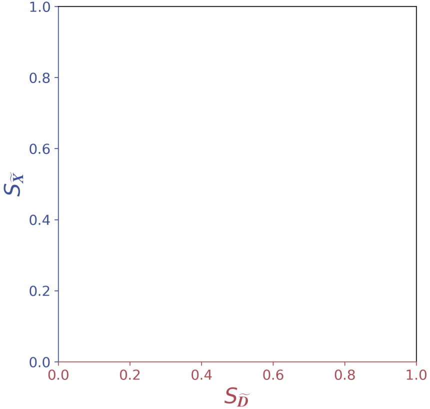
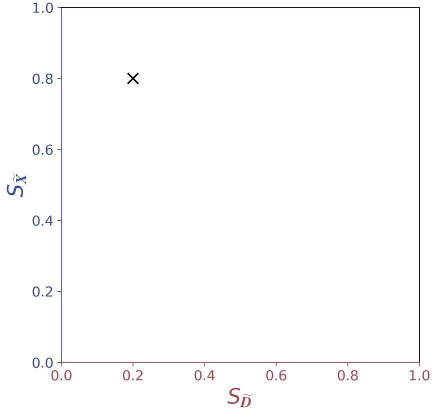


Figure 3.1: Interpretation of Sobol' indices associated to the database and the Monte Carlo sample.

Sensitivity analysis - Interpretation



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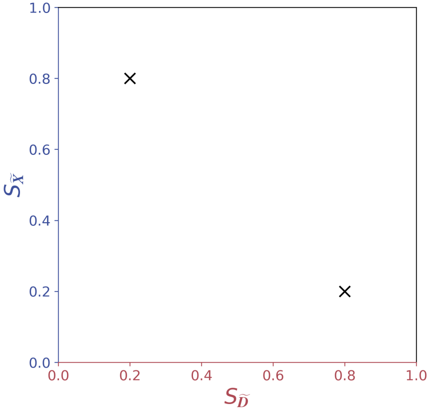

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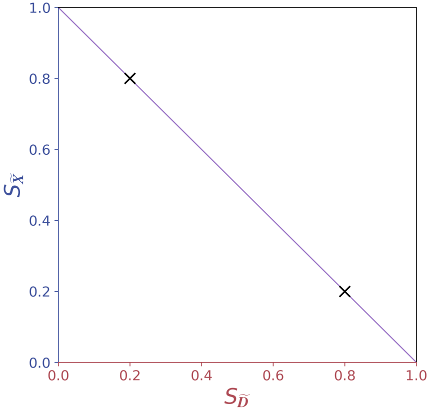

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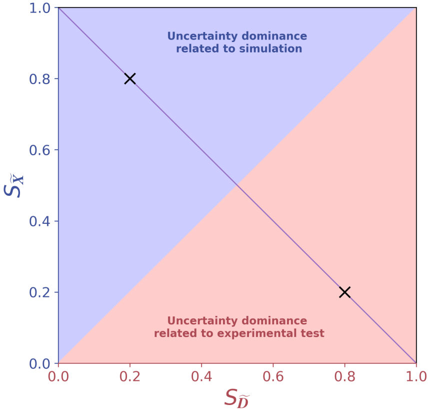

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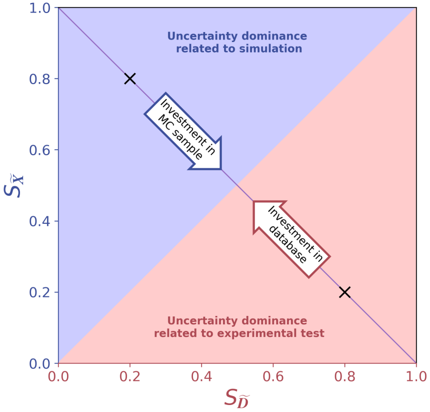

Figure 3.1: Interpretation of Sobol' indices associated to the database and the Monte Carlo sample.

Sensitivity analysis - Independance of inputs

However, the dependance of $\widetilde{X}$ to $\widetilde{D}$ is an issue for the sensitivity analysis.

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However, the dependance of $\widetilde{\boldsymbol{X}}$ to $\widetilde{\boldsymbol{D}}$ is an issue for the sensitivity analysis.

Isoprobabilistic transformation

The transformation $\mathcal{T}_{\boldsymbol{D}}$ [9, 10, 11] is performed here to work with an independent sample $\widetilde{\boldsymbol{U}} = \{\boldsymbol{U}^{(j)}, j = 1, ..., N_{\boldsymbol{X}}\}$:

$$\mathcal{T}_{\boldsymbol{D}} : \left| \begin{array}{ccc} [0,1]^d & \longrightarrow & \mathcal{X} \\ \boldsymbol{U} & \longmapsto & \boldsymbol{X} \end{array} \right. , \tag{3.2}$$

with $\boldsymbol{U}^{(j)} \overset{i.i.d.}{\sim} \mathcal{U}\,[0,1]^d$.

[9] M Rosenblatt. Remarks on a multivariate transformation. The annals of mathematical statistics, 1952.

[10] AE Brockwell. Universal residuals: A multivariate transformation. Statistics probability letters, 2007.

[11] R Lebrun and others. Do rosenblatt and nataf isoprobabilistic transformations really differ? Probabilistic Engineering Mechanics, 2009.

Sensitivity analysis - Solution

Solution B

The investment of data is guided by the highest index:

- $S_{\widetilde{\boldsymbol{D}}} > S_{\widetilde{\boldsymbol{U}}}$ $\longrightarrow$ Investment in the database (experimental tests),
- $S_{\widetilde{\boldsymbol{D}}} < S_{\widetilde{\boldsymbol{U}}}$ $\longrightarrow$ Investment in the MC sample (simulation).

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Illustration - Cantilever Beam

Mean deflection of the free end of a cantilever beam:

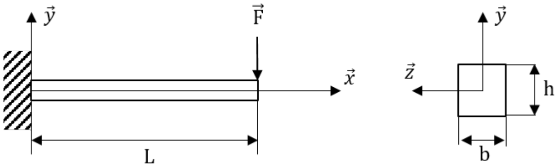


Figure 4.1: Representation of a cantilever beam where F is the transverse load applied on the free end of the beam of length L, Young's modulus E and cross-section bh.

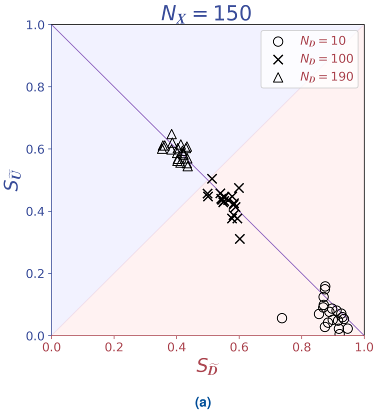
$$\phi\left(F, L, E, b, h\right) = \frac{4FL^3}{Ebh^3}$$

Table 4.1: Probabilistic models associated to independent input variables for a cantilever beam toy-case. [12]

Input variable	Distribution	Mean	Coefficient of variation
F	LogNormal	556.8 [N]	0.08
L	Normal	4290 [mm]	0.1
E	LogNormal	2.10^5 [MPa]	0.06
b	Normal	62 [mm]	0.1
h	Normal	98.7 [mm]	0.1

[12] L Baoyu and others. Reliability analysis based on a novel density estimation method for structures with correlations, 2017.

Illustration - Results



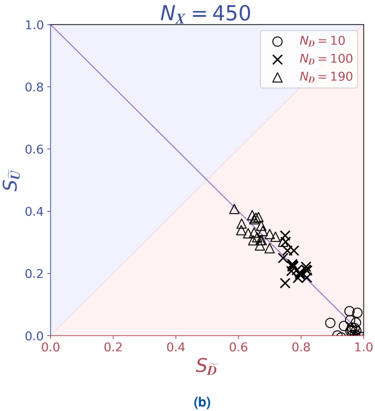


Figure 4.2: Evolution of Sobol' indices for the cantilever beam toy-case at $N_{\boldsymbol{D}} = [10, 100, 190]$ and (a) $N_{\boldsymbol{X}} = 150$ (b) $N_{\boldsymbol{X}} = 450$. Estimation of $n = 20$ indices for each combination.

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Conclusion

Framework

- The probabilistic model is **unknown** and is inferred from experimental tests,
- A **small-data context** is imposed by costly experimental tests and a costly black box function.

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Current method

A) Takes into account the database uncertainty in the variance of the estimator,

B) Answers the test-simulation trade-off by guiding the investment of data in the driving source of uncertainty.

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A) Takes into account the database uncertainty in the variance of the estimator,

B) Answers the test-simulation trade-off by guiding the investment of data in the driving source of uncertainty.

Perspectives

- Reduction of the computational burden with importance sampling methods, [13]
- Quantification of the amount of data to invest while considering cost differences.

[13] A Owen, Y Zhou. Safe and effective importance sampling. Journal of the American Statistical Association, 2000.

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