



Efficient estimation of multiple expectations with the same sample by adaptive importance sampling and control variates

Julien Demange-Chrst, PhD student

julien.demange-chrst@onera.fr

Ph.D. supervisors: Jérôme Morio¹, François Bachoc²

¹ ONERA/DTIS, University of Toulouse, ²Institut de Mathématiques de Toulouse, University Toulouse III - Paul Sabatier

Context

Uncertainty quantification

Numerical code

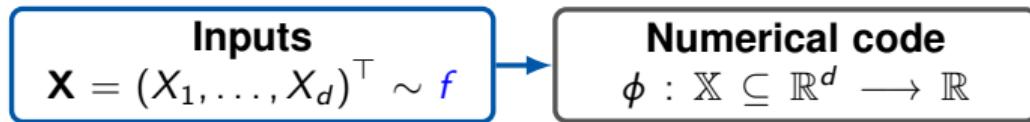
$$\phi : \mathbb{X} \subseteq \mathbb{R}^d \longrightarrow \mathbb{R}$$

Characteristics of the numerical code ϕ :

- black-box model
- deterministic
- expensive to evaluate
 \Rightarrow cost of an algorithm : number of calls to ϕ

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Uncertainty quantification

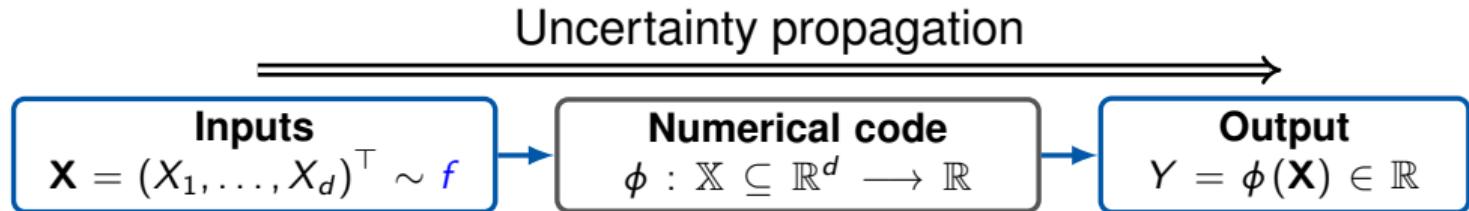


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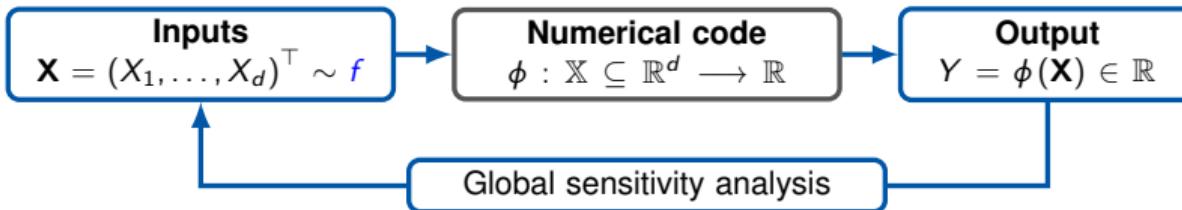


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Variance-based global sensitivity analysis

Introduction



Goal of global sensitivity analysis

Identify the most influential input variables of \mathbf{X} on the variability of the output Y

Some motivations of sensitivity analysis:

- input prioritisation
- factor fixing
- variance cutting

Independent inputs: Sobol' indices [1]

Definition, properties and estimation

With **independent** input variables, the functional variance decomposition (or ANOVA) is unique and leads to the Sobol' indices [1]:

First order Sobol' indices:

$$S_i = \frac{\mathbb{V} [\mathbb{E} (\phi(\mathbf{X}) | X_i)]}{\mathbb{V} (\phi(\mathbf{X}))}$$

Important properties:

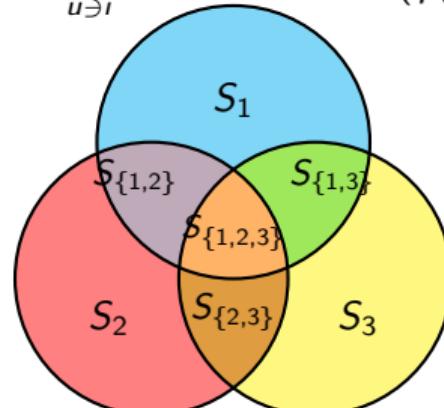
$$0 \leq S_i \leq S_{T_i} \leq 1 \text{ and } \sum_{u \in [1, d]} S_u = 1$$

Some estimation methods:

- Pick-Freeze [1]
- estimators based on rank statistics [3]
- surrogate-based methods (PCE) [4]

Total order Sobol' indices [2]:

$$S_{T_i} = \sum_{u \ni i} S_u = 1 - \frac{\mathbb{V} [\mathbb{E} (\phi(\mathbf{X}) | \mathbf{X}_{-i})]}{\mathbb{V} (\phi(\mathbf{X}))}$$



Estimation of multiple expectations

Problem presentation

For $J \geq 2$, the main goal is to **efficiently** and **commonly** estimate with the same N -sample the expectations:

$$\forall j \in \llbracket 1, J \rrbracket, I_j = \mathbb{E}_{f_j} (\phi_j (\mathbf{X}))$$

 The distributions $(f_j)_{j \in \llbracket 1, J \rrbracket}$ are OpenTURNS distributions and the computer models $(\phi_j)_{j \in \llbracket 1, J \rrbracket}$ are OpenTURNS PythonFunction.

Application examples :

- estimation of sensitivity indices
- sensitivity analysis under epistemic uncertainty
- estimation of covariance matrices

Estimation of multiple expectations

Problem presentation

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Criterion to minimise

The quality of the common estimation of a family of expectations is quantified by:

$$\sum_{j=1}^J w_j \mathbb{V} (\widehat{I}_j)$$

where $\widehat{I}_1, \dots, \widehat{I}_J$ are **unbiased** estimators based on the same N -sample.

Variance reduction methods

Method 1 : importance sampling

Principle of importance sampling

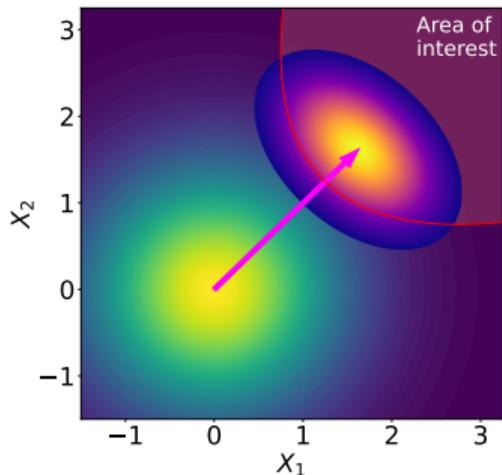
Consider an auxiliary sampling distribution g to draw more samples in interesting zones of the input domain \mathbb{X} .

Variance reduction methods

Method 1 : importance sampling

Principle of importance sampling

Consider an auxiliary sampling distribution g to draw more samples in interesting zones of the input domain \mathbb{X} .



Rewriting I according to g :

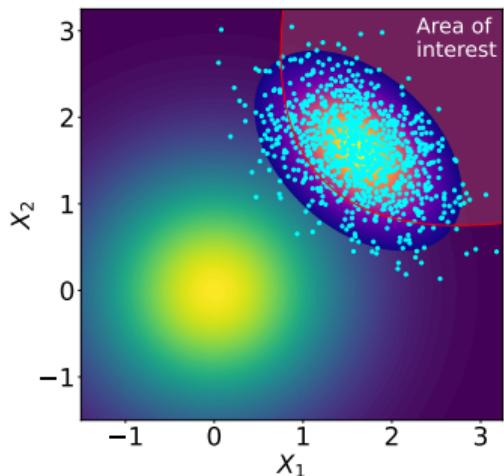
$$I = \mathbb{E}_f [\phi(\mathbf{X})] = \mathbb{E}_g \left[\phi(\mathbf{X}) \frac{f(\mathbf{X})}{g(\mathbf{X})} \right]$$

Variance reduction methods

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Importance sampling estimator of I :

$$\hat{I}_N^{\text{IS}} = \frac{1}{N} \sum_{n=1}^N \phi(\mathbf{X}^{(n)}) \frac{f(\mathbf{X}^{(n)})}{g(\mathbf{X}^{(n)})} \text{ with } (\mathbf{X}^{(n)})_{n \in [1, N]} \sim g$$

Variance reduction methods

Choice of the auxiliary distribution g

Variance of \hat{I}_N^{IS} :

$$\mathbb{V}_{\textcolor{red}{g}} \left(\hat{I}_N^{\text{IS}} \right) \propto \mathbb{V}_{\textcolor{red}{g}} \left(\phi(\mathbf{x}) \frac{f_{\mathbf{x}}(\mathbf{x})}{g(\mathbf{x})} \right)$$

$\implies \mathbb{V}_{\textcolor{red}{g}} \left(\hat{I}_N^{\text{IS}} \right)$ strongly depends on g

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Optimal IS auxiliary distribution [5]: $g_{\text{opt}}(\mathbf{x}) = \frac{\phi(\mathbf{x}) f_{\mathbf{x}}(\mathbf{x})}{I}$ when $\phi \geq 0$

\implies leads to zero-variance estimator

\implies impossible to use because it depends on I

Variance reduction methods

Choice of the auxiliary distribution g

Variance of \hat{I}_N^{IS} :

$$\mathbb{V}_g(\hat{I}_N^{\text{IS}}) \propto \mathbb{V}_g\left(\phi(\mathbf{x}) \frac{f_{\mathbf{x}}(\mathbf{x})}{g(\mathbf{x})}\right)$$

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Existing approximation techniques:

- parametric importance sampling [6]
- non-parametric importance sampling [7]

Variance reduction methods

Method 2 : Control variates [8]

Principle of control variates

Exploiting the known value of the integral of a **control function** h and a **control parameter** $\beta \in \mathbb{R}$ to control the variance of the corresponding estimator.

Variance reduction methods

Method 2 : Control variates [8]

Principle of control variates

Exploiting the known value of the integral of a **control function** h and a **control parameter** $\beta \in \mathbb{R}$ to control the variance of the corresponding estimator.

Estimator of I with control variates and importance sampling [8] :

$$\hat{I}_{N,g,h,\beta}^{\text{IS-CV}} = \frac{1}{N} \sum_{n=1}^N \frac{\phi(\mathbf{X}^{(n)}) f(\mathbf{X}^{(n)}) - \beta h(\mathbf{X}^{(n)})}{g(\mathbf{X}^{(n)})} + \beta \int_{\mathbb{X}} h(x) dx$$

where $(\mathbf{X}^{(n)})_{n \in [\![1, N]\!]} \sim g$ is an unbiased estimator of $I = \mathbb{E}_f(\phi(\mathbf{X}))$.

Variance reduction methods

Method 2 : Control variates [8]

Principle of control variates

Exploiting the known value of the integral of a **control function** h and a **control parameter** $\beta \in \mathbb{R}$ to control the variance of the corresponding estimator.

Minimisation of the variance of the estimator according to β :

$$\beta^* = \arg \min_{\beta \in \mathbb{R}} \mathbb{V}_g \left(\hat{I}_{N,g,h,\beta}^{\text{IS-CV}} \right) = \mathbb{V}_g \left(\frac{h(\mathbf{X})}{g(\mathbf{X})} \right)^{-1} \text{Cov}_g \left(\frac{\phi(\mathbf{X}) f(\mathbf{X})}{g(\mathbf{X})}, \frac{h(\mathbf{X})}{g(\mathbf{X})} \right)$$

$$\text{Then, } \mathbb{V} \left(\hat{I}_{N,g,h,\beta^*}^{\text{IS-CV}} \right) \leq \mathbb{V} \left(\hat{I}_{N,g}^{\text{IS}} \right).$$

Estimation of multiple expectations

Optimal estimator family

Theorem [9]

The family of estimator

$$\widehat{I}_{N, \mathbf{g}_\alpha, \mathbf{g}_j^*, \beta^*}^{\text{IS-CV}} = \frac{1}{N} \sum_{n=1}^N \frac{\phi_j(\mathbf{X}^{(n)}) \mathbf{f}_j(\mathbf{X}^{(n)}) - \beta_j^* \mathbf{g}_j^*(\mathbf{X}^{(n)})}{\mathbf{g}_\alpha(\mathbf{X}^{(n)})} + \beta_j^*$$

with $(\mathbf{X}^{(n)})_{n \in \llbracket 1, N \rrbracket} \sim \mathbf{g}_\alpha = \sum_{j=1}^J \alpha_j \mathbf{g}_j^*$ and $\beta_j^* = I_j$, satisfies

$$\sum_{j=1}^J w_j \mathbb{V} \left(\widehat{I}_{N, \mathbf{g}_\alpha, \mathbf{g}_j^*, \beta_j^*}^{\text{IS-CV}} \right) = 0.$$

These optimal estimators cannot be used in practice

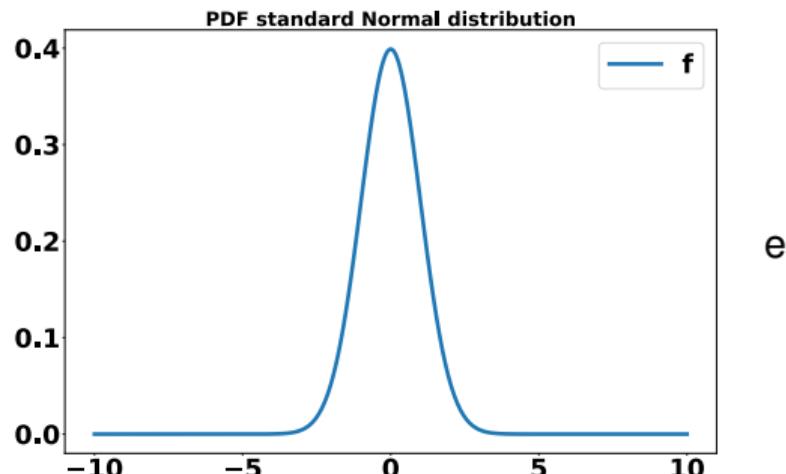
⇒ require a procedure to approach these optimal estimators: **ME-aISCV** algorithm [9]

ME-aISCV algorithm [9]

Example

Estimation of the first $J = 10$ even moments of the 1-dimensional standard Normal distribution $\mathcal{N}_1(0, 1)$:

$$\forall j \in \llbracket 1, J \rrbracket, \begin{cases} f_j &= f \equiv \mathcal{N}_1(0, 1) \\ I_j &= \mathbb{E}_f(X^{2j}) \end{cases}$$



ME-aISCV algorithm [9]

Description of the algorithm

Initialisation $k = 0$
Initial MC sample

Initialisation $k = 0$:

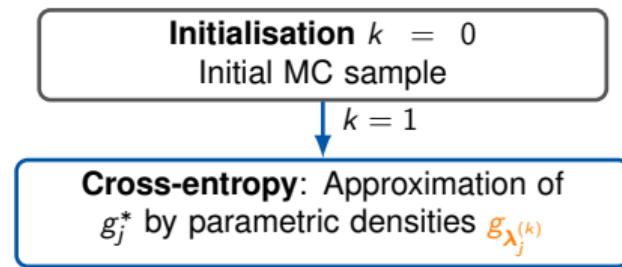
- Draw an initial MC sample
 $(\mathbf{X}^{(0,n)})_{n \in \llbracket 1, N_0 \rrbracket} \sim f$  and estimate :

$$\hat{I}_j^{(0)} = \frac{1}{N} \sum_{n=1}^N \phi_j(\mathbf{x}^{(0,n)})$$

- Initialisation of the coefficients $\alpha^{(0)}$ and $\beta_j^{(0)}$

ME-aISCV algorithm [9]

Description of the algorithm



Cross-entropy:

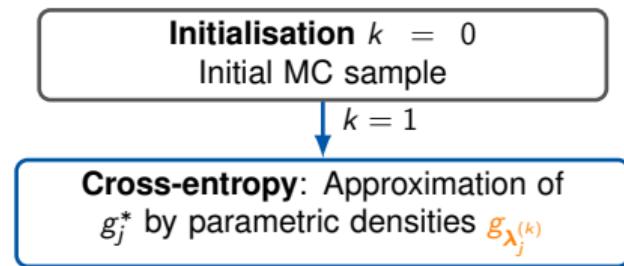
- Update $k = k + 1$
- Approaching the optimal distributions g_j^* within a parametric family of distributions $g_{\lambda_j^{(k)}}$ by solving the optimisation problem:

$$\lambda_j^{(k)} = \arg \min_{\lambda_j} D_{\text{KL}}(g_j^*, g_{\lambda_j})$$

In practice, g_{λ_j} is picked up in the Gaussian family or in the Gaussian mixture family.

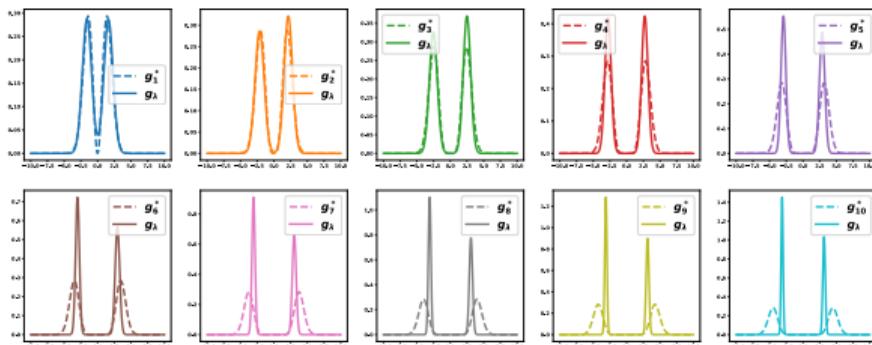
ME-aISCV algorithm [9]

Description of the algorithm



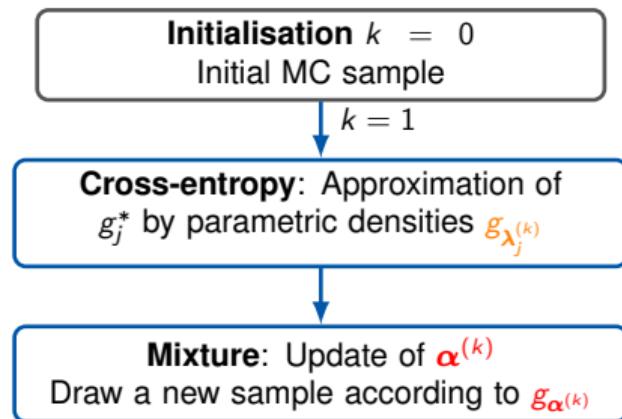
Cross-entropy:

Approximation of the g_j^* by parametric densities at iteration 1



ME-aISCV algorithm [9]

Description of the algorithm



Mixture:

- Update the weights α and create the new mixture $g_{\alpha^{(k)}} = \sum_{j=1}^J \alpha_j^{(k)} g_{\lambda_j^{(k)}}$ by solving the optimisation problem:

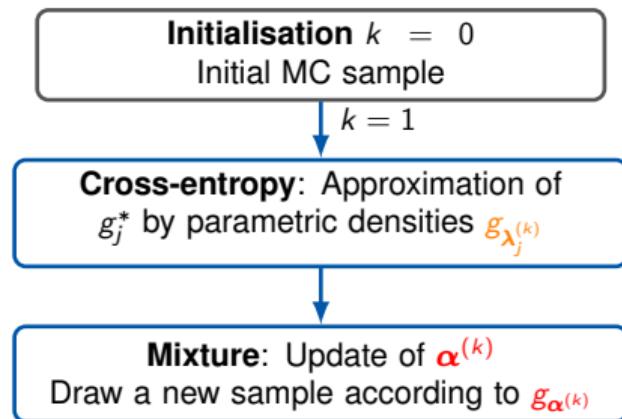
$$\alpha^{(k)} = \arg \min_{\sum_{j=1}^J \alpha_j = 1} \sum_{j=1}^J w_j \mathbb{V}_{g_{\alpha}} \left(\frac{\phi_j(\mathbf{x}) f_j(\mathbf{x}) - \beta_j^{(k-1)} g_{\lambda_j^{(k)}}(\mathbf{x})}{g_{\alpha^{(k)}}(\mathbf{x})} \right)$$

- Draw a new sample $(\mathbf{x}^{(k,n)})_{n \in \llbracket 1, N_k \rrbracket} \sim g_{\alpha^{(k)}}$

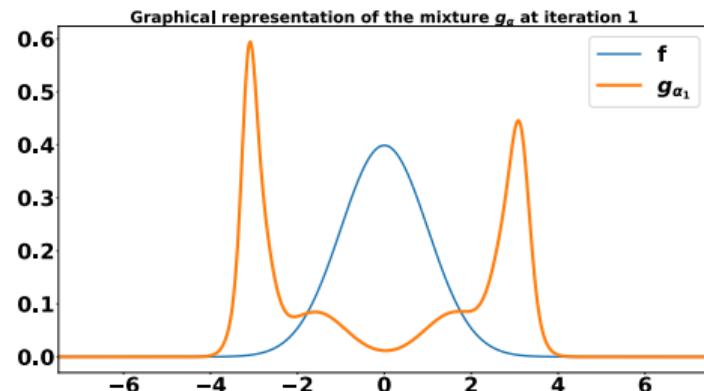


ME-aISCV algorithm [9]

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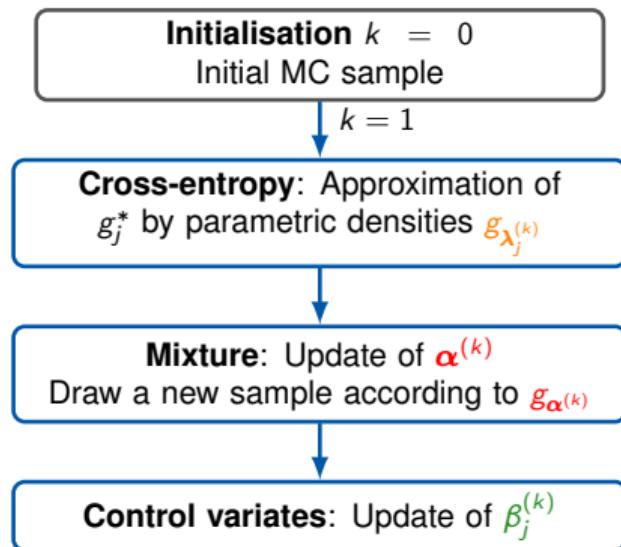


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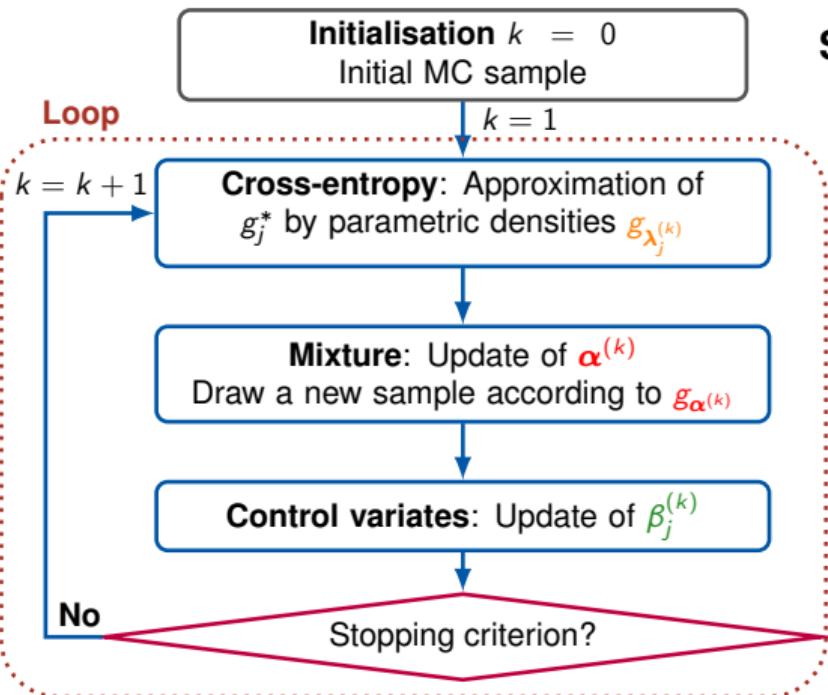
Control variates:

Update the control parameters β_j by estimating:

$$\beta_j^{(k)} \approx \frac{\text{Cov}_{g_{\alpha^{(k)}}} \left(\frac{\phi_j(\mathbf{X}) f_j(\mathbf{X})}{g_{\alpha^{(k)}}(\mathbf{X})}, \frac{g_{\lambda_j^{(k)}}(\mathbf{X})}{g_{\alpha^{(k)}}(\mathbf{X})} \right)}{\mathbb{V}_{g_{\alpha^{(k)}}} \left(\frac{g_{\lambda_j^{(k)}}(\mathbf{X})}{g_{\alpha^{(k)}}(\mathbf{X})} \right)}$$

ME-aISCV algorithm [9]

Description of the algorithm



Stopping criterion:

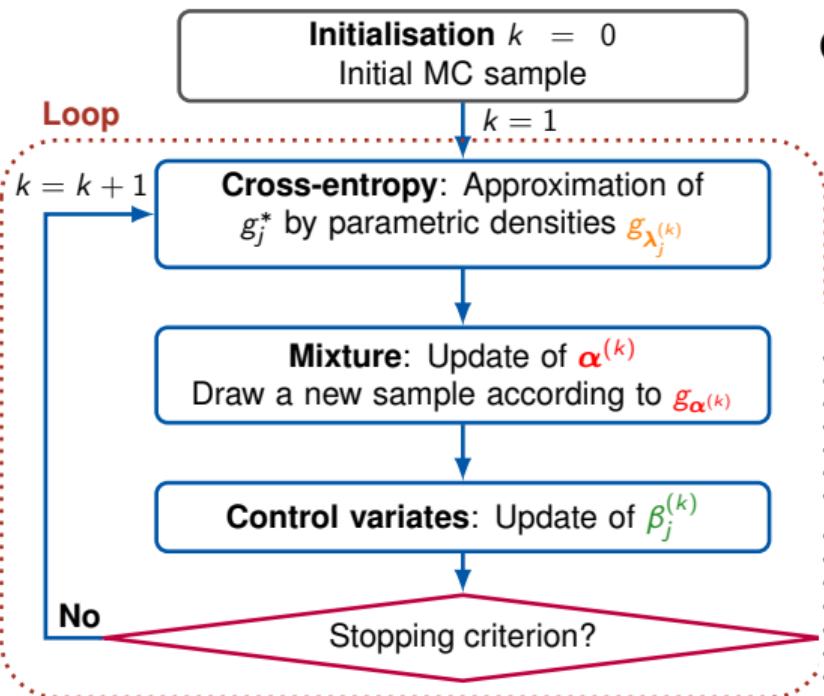
Quality of the approximation of the optimal parameters λ_j , α and β_j



Budget left N_f for the final estimates

ME-aISCV algorithm [9]

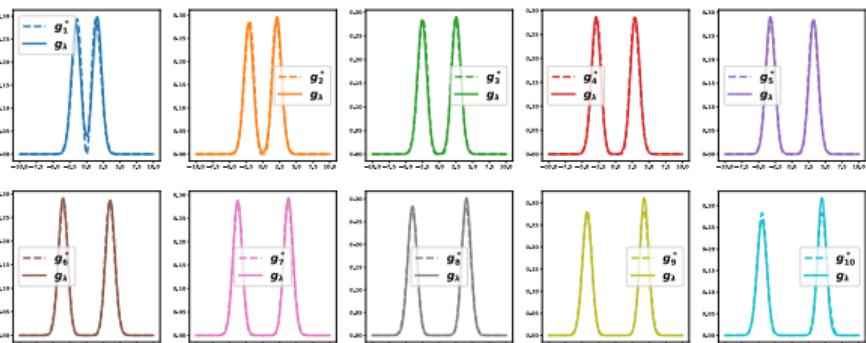
Description of the algorithm



Cross-entropy:

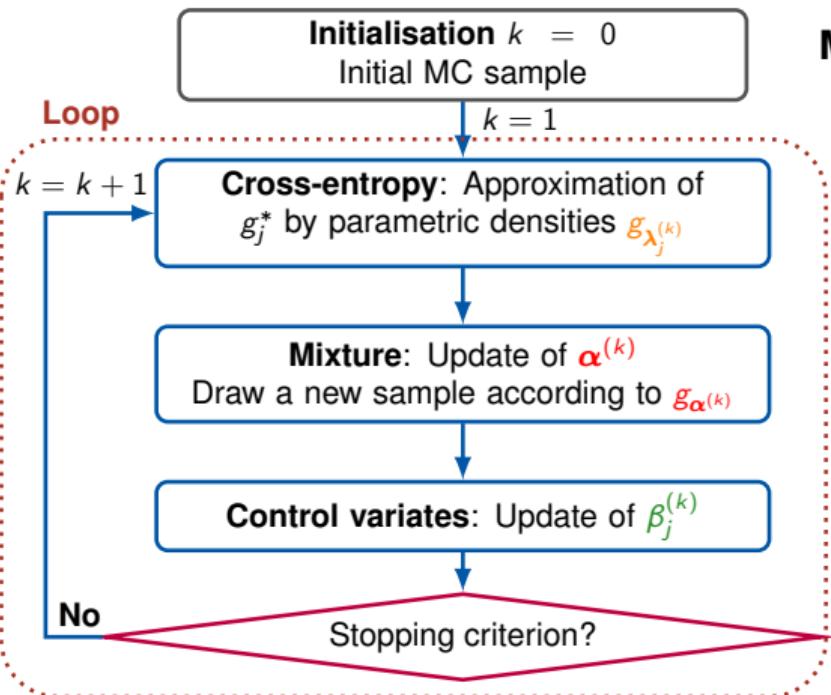
- Update $k = k + 1$
- Approaching the optimal distributions g_j^* by parametric densities $g_{\lambda_j^{(k)}}$

Approximation of the g_j^* by parametric densities at iteration 4



ME-aISCV algorithm [9]

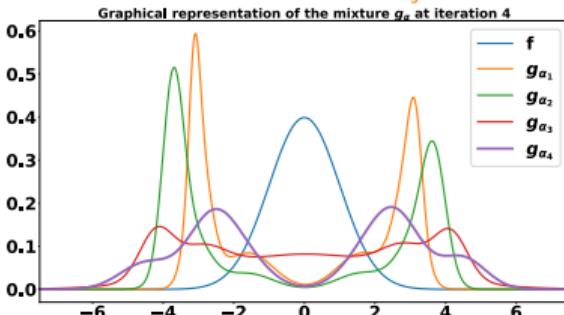
Description of the algorithm



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- Update the weights α and create the new mixture $g_{\alpha^{(k)}} = \sum_{j=1}^J \alpha_j^{(k)} g_{\lambda_j^{(k)}}$

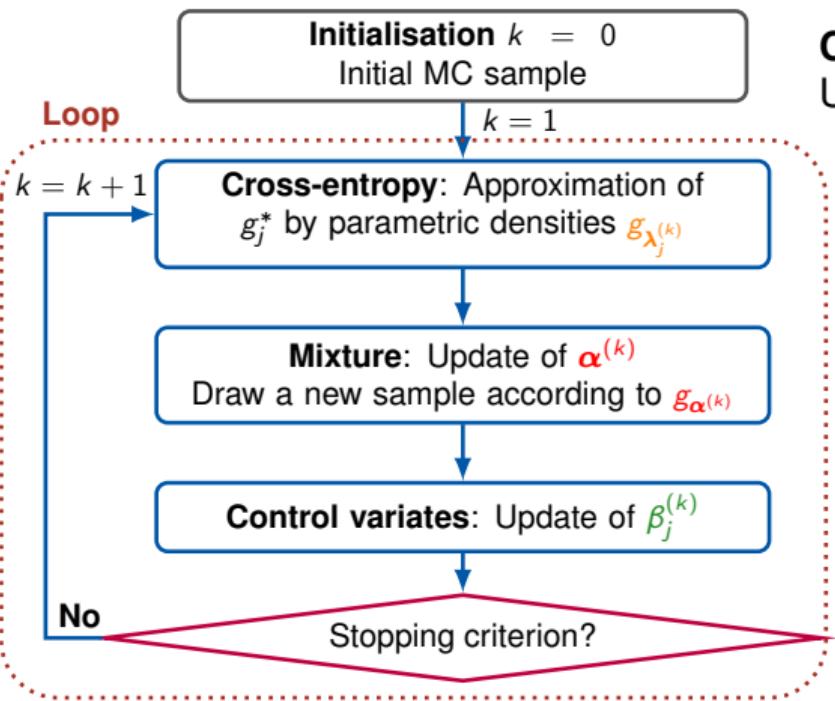
$$g_{\alpha^{(k)}} = \sum_{j=1}^J \alpha_j^{(k)} g_{\lambda_j^{(k)}}$$



- Draw a new sample $(\mathbf{X}^{(k,n)})_{n \in [1, N_k]} \sim g_{\alpha^{(k)}}$



ME-aISCV algorithm [9]

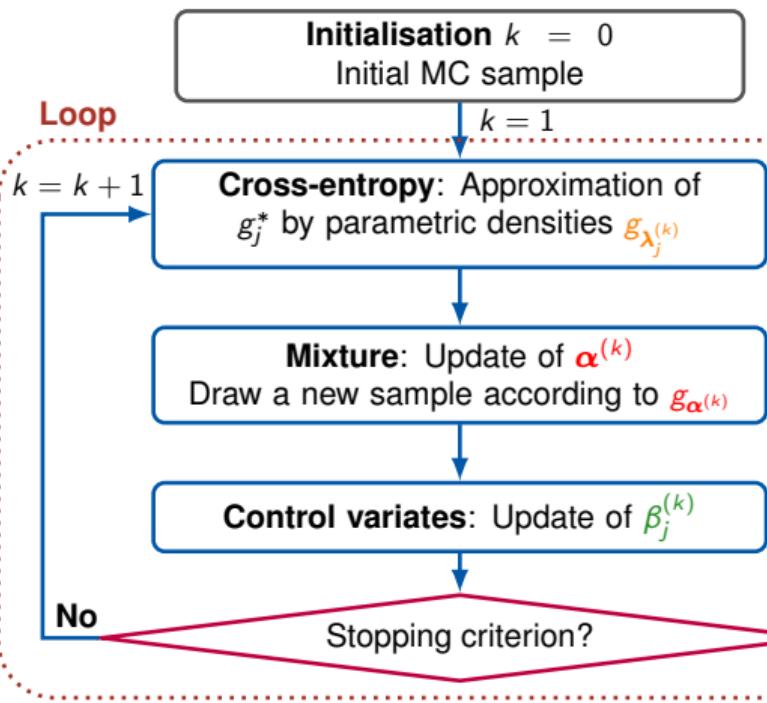


Control variates:

Update the control parameters β_j by estimating:

$$\beta_j^{(k)} \approx \frac{\text{Cov}_{g_{\alpha^{(k)}}} \left(\frac{\phi_j(\mathbf{X}) f_j(\mathbf{X})}{g_{\alpha^{(k)}}(\mathbf{X})}, \frac{g_{\lambda_j^{(k)}}(\mathbf{X})}{g_{\alpha^{(k)}}(\mathbf{X})} \right)}{\mathbb{V}_{g_{\alpha^{(k)}}} \left(\frac{g_{\lambda_j^{(k)}}(\mathbf{X})}{g_{\alpha^{(k)}}(\mathbf{X})} \right)}$$

ME-aISCV algorithm [9]



End :

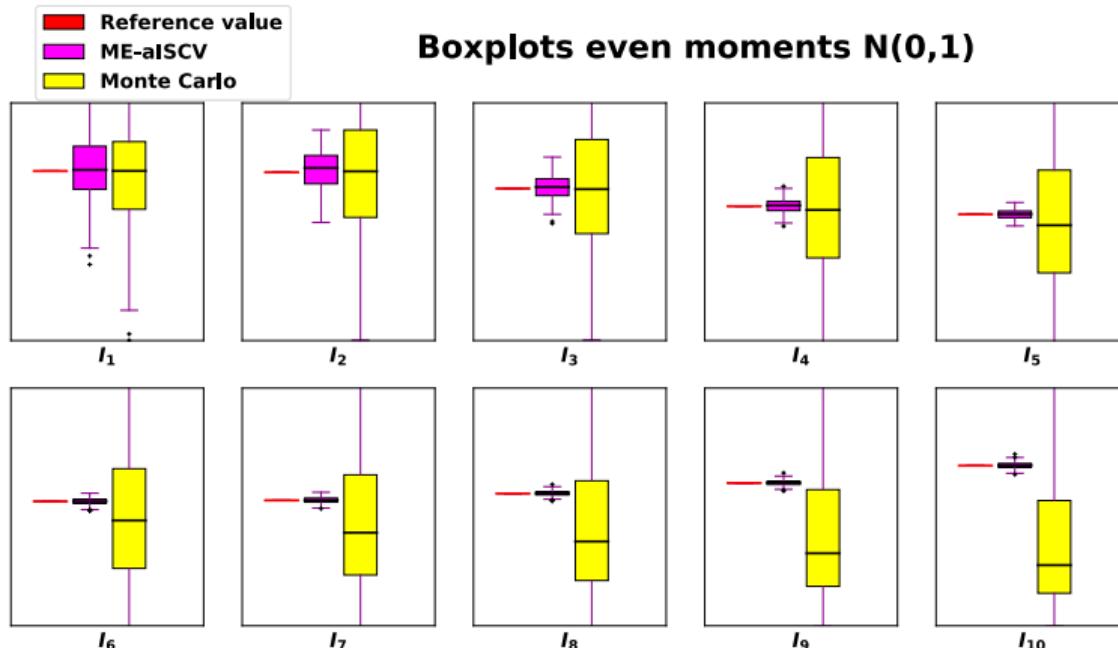
Draw a new sample independent $\textcolor{red}{\circlearrowleft}$ from the previous ones $(\mathbf{X}^{(n)})_{n \in [1, N_f]} \sim g_{\alpha^{(k)}}$ and return:

$$\hat{I}_{N_f, g_{\alpha^{(k)}}, g_{\lambda_j^{(k)}}, \beta_j^{(k)}} = \frac{1}{N_f} \sum_{n=1}^{N_f} \frac{\phi_j(\mathbf{X}^{(n)}) f_j(\mathbf{X}^{(n)}) - \beta_j^{(k)} g_{\lambda_j^{(k)}}(\mathbf{X}^{(n)})}{g_{\alpha^{(k)}}(\mathbf{X}^{(n)})} + \beta_j^{(k)}$$

End : Draw a new sample according to $g_{\alpha^{(k)}}$
Final estimates $\hat{I}_{N_f, g_{\alpha^{(k)}}, g_{\lambda_j^{(k)}}, \beta_j^{(k)}}$

ME-aISCV algorithm [9]

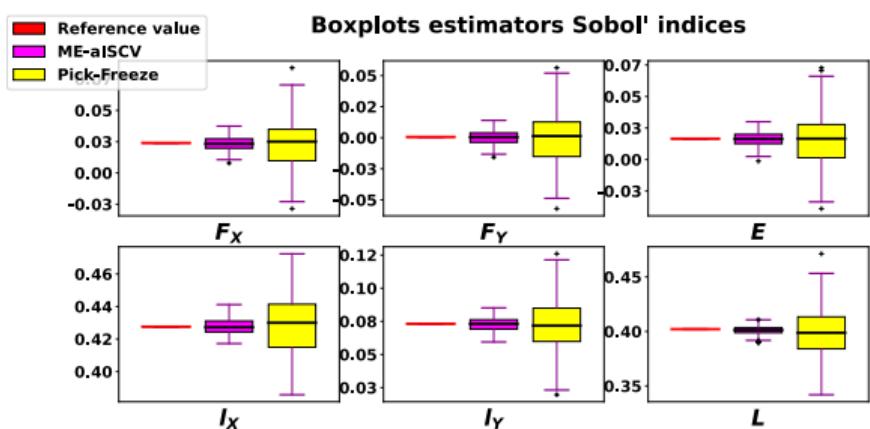
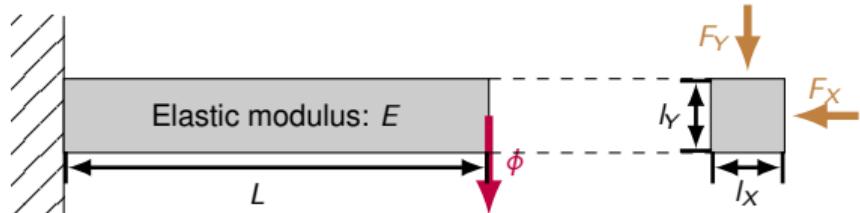
Results on the example



Results

Estimation of the first order Sobol' indices for the cantilever beam problem

	Input	Distribution	Mean	C.o.V.
1	F_x	LogNormal	556.8 N	0.08
2	F_y	LogNormal	453.6 N	0.08
3	E	LogNormal	200.10^9 Pa	0.06
4	l_x	Normal	0.062 m	0.1
5	l_y	Normal	0.0987 m	0.1
6	L	Normal	4.29 m	0.1



Maximal displacement of the tip section:

$$\phi(F_x, F_y, E, l_x, l_y, L) = \frac{4L^3}{EI_x l_y} \sqrt{\left(\frac{F_x}{l_x^2}\right)^2 + \left(\frac{F_y}{l_y^2}\right)^2}$$

Results

Epistemic uncertainty on the input distribution for the cantilever beam problem

	Input	Distribution	Mean	C.o.V.
1	F_X	LogNormal	m_1	0.08
2	F_Y	LogNormal	m_2	0.08
3	E	LogNormal	m_3	0.06
4	I_X	Normal	m_4	0.1
5	I_Y	Normal	m_5	0.1
6	L	Normal	m_6	0.1

Correlation between some inputs:

$$\rho_{I_X, I_Y} = m_7 \text{ and } \rho_{L, I_X} = m_8 \text{ and } \rho_{L, I_Y} = m_9.$$

Maximal displacement of the tip section:

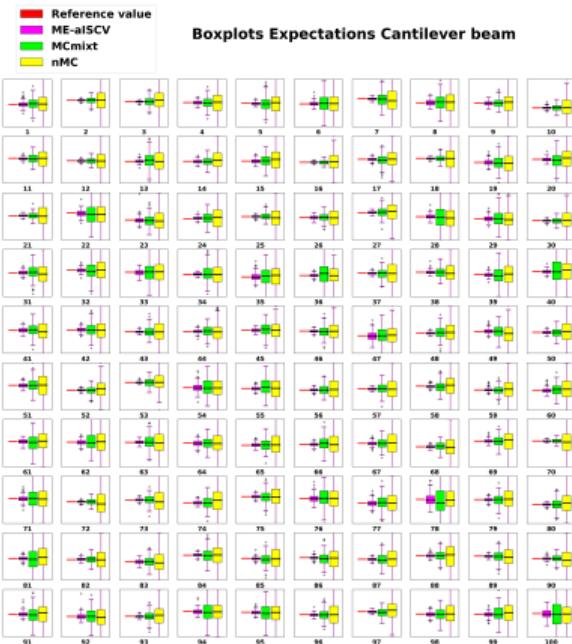
$$\phi(F_X, F_Y, E, I_X, I_Y, L) = \frac{4L^3}{EI_XI_Y} \sqrt{\left(\frac{F_X}{I_X^2}\right)^2 + \left(\frac{F_Y}{I_Y^2}\right)^2}$$

Goal of the test case: commonly estimate the family of expectations $\left(\mathbb{E}_{f_{m^{(j)}}}(\phi(\mathbf{X}))\right)_{j \in [1, J]}$ where

- $J = 100$ (!)
- each component of the vector $\mathbf{m}^{(j)} = (m_i)_{i \in [1, 9]}$ is drawn according to a Uniform distribution centered on the "true" value.

Results

Epistemic uncertainty on the input distribution for the cantilever beam problem



Final results:

	ME-aISCV	MC	MC mixture
$\sum_{j=1}^{100} \mathbb{V}(\widehat{I}_j)$	4.379×10^{-6}	1.309×10^{-4}	6.103×10^{-5}

Conclusion

What is new?

- introduction of the problem of the estimation of multiple expectations with the same N -sample
- definition of a criterion to quantify the quality of the common estimation
- ME-aISCV algorithm to reduce as much as possible the previous criterion

Accepted paper [9] and [codes](#) to reproduce the results are available online !

Efficient estimation of multiple expectations with the
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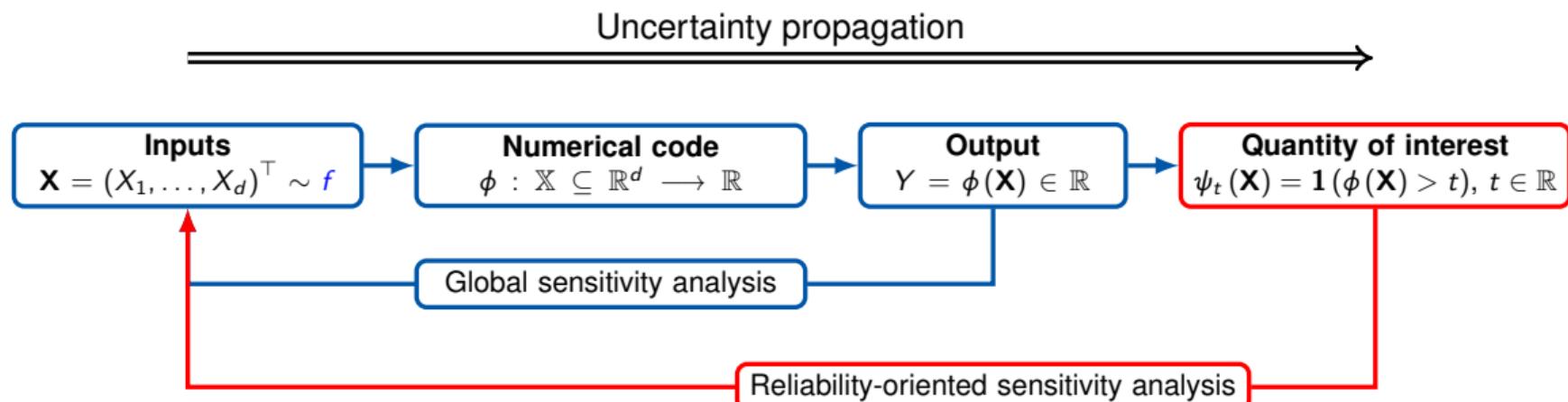
Julien DEMANGE-CHRYST^{a,b,*}, François BACHOC^b, Jérôme MORIO^a

^aONERA/DTIS, Université de Toulouse, F-31055 Toulouse, France

^bInstitut de Mathématiques de Toulouse, UMR5219 CNRS, 31062 Toulouse, France

Estimation of the target Shapley effects by IS

Uncertainty quantification and reliability analysis



Question

With correlated inputs, which components of \mathbf{X} are most likely to lead to the failure of the system ?

Estimation of the target Shapley effects by IS

Importance sampling and the use of OpenTURNS

Reliability-oriented Shapley effects

$$T\text{-Sh}_i = \frac{1}{d} \frac{1}{\mathbb{V}(\psi_t(\mathbf{X}))} \sum_{u \subseteq \{-i\}} \binom{d-1}{|u|}^{-1} \left(T\text{-S}_{u \cup \{i\}}^c - T\text{-S}_u^c \right) \text{ with } T\text{-S}_u^c = \begin{cases} \mathbb{V}[\mathbb{E}(\psi_t(\mathbf{X}) | \mathbf{X}_u)] & \text{or} \\ \mathbb{E}[\mathbb{V}(\psi_t(\mathbf{X}) | \mathbf{X}_{-u})] \end{cases}$$

Estimation process of $T\text{-Sh}_i$:

- ① estimation of $T\text{-S}_u^c$ for $u \subseteq [1, d]$
⇒ IS here
- ② aggregation procedure

Estimation of the $T\text{-S}_u^c$ with importance sampling:

- requires the likelihood ratios f/g , but also the marginal likelihood ratios $f_{\mathbf{X}_u}/g_{\mathbf{X}_u}$ for every subset $u \subseteq [1, d]$
-  OpenTURNS allows me to quickly compute all these ratios, even for complex distributions f or g !

Published article [10] and codes to reproduce the results are available online !

References

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