Shapley effect estimation in reliability-oriented sensitivity analysis with dependent inputs by importance sampling

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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
  $\Longrightarrow$ cost of an algorithm : number of calls to ϕ

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$\mathbf{X} = (X_1, \dots, X_d)^\top \sim f_{\mathbf{X}}$

→

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Characteristics of the random vector $\mathbf{X}$:

- $f_{\mathbf{X}}$ d-dimensional continuous distribution
- $f_{\mathbf{X}}$ fully known
- dependent components

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Uncertainty quantification

Uncertainty propagation $\Longrightarrow$

Inputs	**Numerical code**	**Output**
$\mathbf{X} = (X_1, \ldots, X_d)^\top \sim f_{\mathbf{X}}$	$\phi : \mathbb{X} \subseteq \mathbb{R}^d \longrightarrow \mathbb{R}$	$Y = \phi(\mathbf{X}) \in \mathbb{R}$

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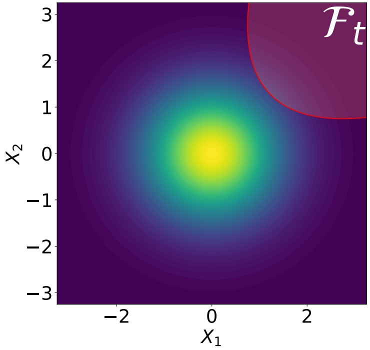
Reliability analysis

Introduction

Inputs $\mathbf{X} = (X_1, \ldots, X_d)^\top \sim f_{\mathbf{X}}$ → **Numerical code** $\phi : \mathbb{X} \subseteq \mathbb{R}^d \longrightarrow \mathbb{R}$ → **Output** $Y = \phi(\mathbf{X}) \in \mathbb{R}$ → **Quantity of interest** $\psi_t(\mathbf{X}) = \mathbf{1}(\phi(\mathbf{X}) > t)$



- $t \in \mathbb{R}$ is a **critical threshold**
- $\{\phi(\mathbf{X}) > t\}$ is the **failure event**
- the **failure domain** is $\mathcal{F}_t = \{\mathbf{x} \in \mathbb{X} / \phi(\mathbf{x}) > t\}$
- the **limit state** is $\{\mathbf{x} \in \mathbb{X} / \phi(\mathbf{x}) = t\}$

Failure probability:

$$p_t = \mathbb{P}(\phi(\mathbf{X}) > t) = \int_{\mathcal{F}_t} f_{\mathbf{X}}(\mathbf{x})\, d\mathbf{x} = \mathbb{E}[\mathbf{1}(\phi(\mathbf{X}) > t)]$$

Importance sampling

Estimator

Main idea of importance sampling

Consider an auxiliary sampling distribution g to draw more samples in $\mathcal{F}_t$ than $f_{\mathbf{X}}$

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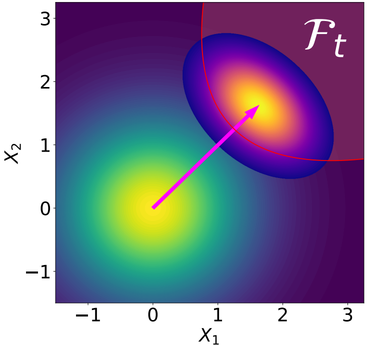

Rewriting p_t according to g:

$$p_t = \mathbb{E}_{f_{\mathbf{X}}}\left[\mathbf{1}\left(\phi\left(\mathbf{X}\right) > t\right)\right] = \mathbb{E}_g\left[\mathbf{1}\left(\phi\left(\mathbf{X}\right) > t\right)\frac{f_{\mathbf{X}}\left(\mathbf{X}\right)}{g\left(\mathbf{X}\right)}\right]$$

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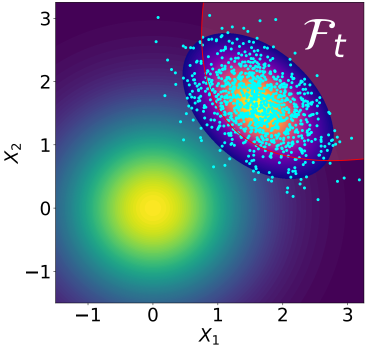

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Importance sampling estimator of p_t:

$$\widehat{p}_{t,N}^{\text{IS}} = \frac{1}{N}\sum_{n=1}^{N}\mathbf{1}\left(\phi\left(\mathbf{X}^{(n)}\right) > t\right)\frac{f_{\mathbf{X}}\left(\mathbf{X}^{(n)}\right)}{g\left(\mathbf{X}^{(n)}\right)}$$

with $\left(\mathbf{X}^{(n)}\right)_{n\in[\![1,N]\!]} \sim g$

Importance sampling

Choice of the auxiliary distribution g

Variance of $\widehat{p}^{\text{IS}}_{t,N}$: $\mathbb{V}_g\left(\widehat{p}^{\text{IS}}_{t,N}\right) \propto \mathbb{V}_g\left(\mathbf{1}\left(\phi\left(\mathbf{X}\right) > t\right)\frac{f_{\mathbf{X}}\left(\mathbf{X}\right)}{g\left(\mathbf{X}\right)}\right)$

$\Longrightarrow \mathbb{V}_g\left(\widehat{p}^{\text{IS}}_{t,N}\right)$ strongly depends on g

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Optimal IS auxiliary distribution [BB04]: $g_{\text{opt}}\left(\mathbf{x}\right) = \dfrac{\mathbf{1}\left(\phi\left(\mathbf{x}\right) > t\right) f_{\mathbf{X}}\left(\mathbf{x}\right)}{p_t} = f_{\mathbf{X}|\mathbf{X}\in\mathcal{F}_t}\left(\mathbf{x}\right)$

$\Longrightarrow$ leads to zero-variance estimator

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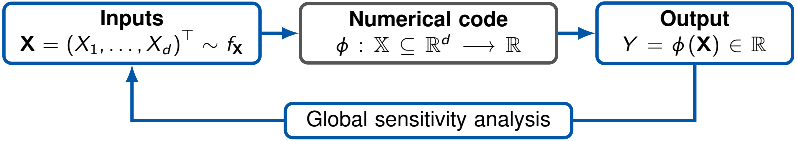
Existing approximation techniques:

- non-adaptive importance sampling based on the design point from FORM/SORM [Mel89]
- parametric adaptive importance sampling [RK04]
- non-parametric adaptive importance sampling [Mor11]

Variance-based global sensitivity analysis

Introduction



Goal of global sensitivity analysis

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

Some motivations of sensitivity analysis:

- input prioritisation
- factor fixing
- variance cutting

Independent inputs: Sobol' indices [Sob93]

Definition, properties and estimation

With **independent** inputs, the functional variance decomposition (or ANOVA) is unique and leads to the Sobol' indices [Sob93]:

First order Sobol' indices:

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

Important properties:

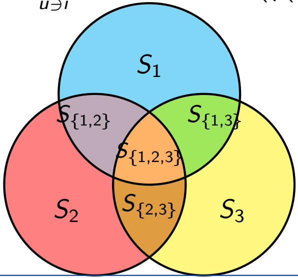
$$0 \leq S_i \leq S_{T_i} \leq 1 \text{ and } \sum_{u\in[\![1,d]\!]} S_u = 1$$

Some estimation methods of the Sobol' indices:

- Pick-Freeze [Sob93]
- estimators based on rank statistics [GGKL20]
- surrogate-based methods (PCE) [Sud08]

Total order Sobol' indices [HS96]:

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



Dependent inputs

Issues and existing approaches

When the input variables are **dependent**:

- the ANOVA representation is not unique
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Approaches for dealing with dependent inputs:

- generalized ANCOVA decomposition [LRY+10]
- methods based on an iso-probabilistic transformation to decorrelate the inputs [MT12]
- compute the Shapley effects for variance-based global sensitivity analysis [Owe14]

Dependent inputs: Shapley effects

Cooperative game theory

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Fairly allocate the gains resulting from a team effort to each player

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Consider a set of players $\mathcal{D} = [\![1, d]\!]$ and a cost function $c : \mathcal{P}\left(\mathcal{D}\right) \longrightarrow \mathbb{R}$, mapping every possible group of players to its common contribution.

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Fairly allocate the gains resulting from a team effort to each player

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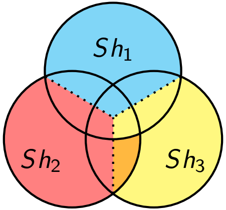
An acceptable allocation must satisfy 4 axioms [Sha53]
$\implies$ unique allocation possible:

Shapley effects

$$\forall i \in [\![1, d]\!],\ Sh_i = \frac{1}{d} \sum_{u \subseteq -i} \binom{d-1}{|u|}^{-1} \left(c\left(u \cup \{i\}\right) - c\left(u\right)\right)$$



Dependent inputs: Shapley effects

Back to sensitivity analysis

By an analogy between **players** and **inputs**, the Shapley effects are adapted to variance-based global sensitivity analysis [Owe14]

Shapley effects for global sensitivity analysis

$$\forall i \in [\![1, d]\!],\ Sh_i = \frac{1}{d\mathbb{V}(\phi(\mathbf{X}))} \sum_{u \subseteq -i} \binom{d-1}{|u|}^{-1} \left(S^c_{u\cup\{i\}} - S^c_u \right)$$

where $S^c_u = \mathbb{V}[\mathbb{E}(\phi(\mathbf{X})|\mathbf{X}_u)]$ [Owe14] or $S^c_u = \mathbb{E}[\mathbb{V}(\phi(\mathbf{X})|\mathbf{X}_{-u})]$ [SNS16]

Properties:

- $\forall i \in [\![1, d]\!],\ 0 \leq Sh_i \leq 1$
- $\sum_{i=1}^{d} Sh_i = 1$

Advantage and drawback:

- allow for an easy interpretation of the decomposition of the variance
- not possible to split dependence and interaction

Dependent inputs: Shapley effects

Estimation

Shapley effects for global sensitivity analysis

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Estimation scheme of the Shapley effects:

1. estimation of the closed Sobol indices S^c_u for some $u \subseteq [\![1, d]\!]$
   - double Monte-Carlo
   - Pick-Freeze
2. aggregation procedure
   - subset procedure [BBD20]
   - random permutation procedure [SNS16]

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Estimation costs	double Monte-Carlo	Pick-Freeze
Subset procedure	$N_{\mathbb{V}} + (2^d - 2)N_I N_O$	$N_{\mathbb{V}} + (2^d - 2) \times 2N_O$
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with
- N_I : size of the inner loop — $N_{\mathbb{V}}$: number of points to estimate $\mathbb{V}(\phi(\mathbf{X}))$
- N_O : size of the outer loop — m : number of permutations

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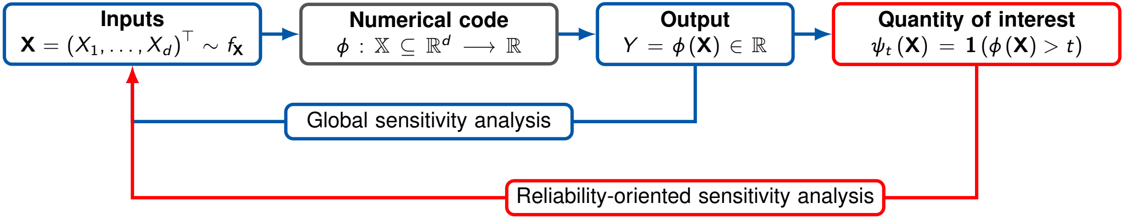
Important improvement: the **nearest-neighbour approximation** can be used to approximate the conditional distributions and leads to a significant cost reduction since it only requires an i.i.d. input/output N-sample [BBD20]: this is the **given-data** framework

Reliability-oriented sensitivity analysis

Introduction

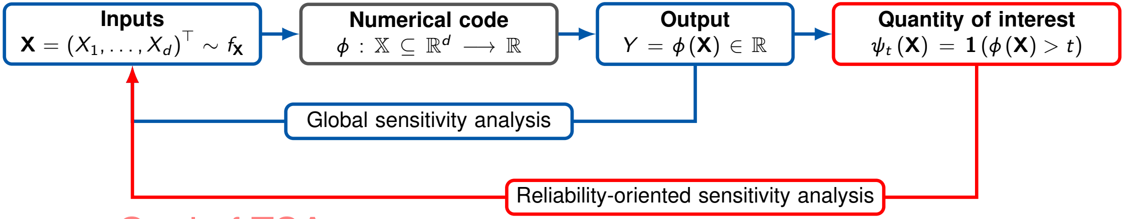


2 types of reliability-oriented sensitivity analyses [MC21]:

- conditional sensitivity analysis (CSA)
- target sensitivity analysis (TSA)

Reliability-oriented sensitivity analysis

Introduction



Goal of TSA

Identify the most influential input variables of $\mathbf{X}$ on the occurrence of the failure

Methodology of TSA

Estimate the sensitivity indices applied on the quantity of interest $\psi_t(\mathbf{X}) = \mathbf{1}(\phi(\mathbf{X}) > t)$

Methodology of TSA with dependent inputs

Estimate the Shapley effects applied on the quantity of interest $\psi_t(\mathbf{X}) = \mathbf{1}(\phi(\mathbf{X}) > t)$

Target Shapley effects T-Sh$_i$ and first estimation schemes are introduced in [ICI21]:

- estimation of T-S$_u^c$ by double Monte Carlo
- use of both subset and random permutation aggregation procedures
- extension to the case when only an i.i.d input/output N-sample from $f_{\mathbf{X}}$ is available using the nearest-neighbour approximation

Target sensitivity analysis with dependent inputs

Existing approach

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Main problem

Existing estimators of T-Sh$_i$ require too many calls to ϕ to be accurate when $p_t \ll 1$

Target Shapley effects with importance sampling

Introduction of importance sampling in T-S_u^c

Methodology [DCBM22]

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1. estimate T-S_u^c by importance sampling
   - double Monte Carlo

$$\mathbb{E}_{f_{\mathbf{X}}}\left[\mathbb{V}_{f_{\mathbf{X}}}\left(\psi_t\left(\mathbf{X}\right)|\mathbf{X}_{-u}\right)\right] = p_t - \mathbb{E}_{f_{\mathbf{X}}}\left[\mathbb{E}_{f_{\mathbf{X}}}\left(\psi_t(\mathbf{X})|\mathbf{X}_{-u}\right)^2\right] = p_t - \mathbb{E}_{g}\left[\mathbb{E}_{g}\left(\psi_t(\mathbf{X})\frac{f_{\mathbf{X}}\left(\mathbf{X}_u\right)}{g\left(\mathbf{X}_u\right)}\middle|\mathbf{X}_{-u}\right)^2 \frac{g_{\mathbf{X}_{-u}}\left(\mathbf{X}_{-u}\right)}{f_{\mathbf{X}_{-u}}\left(\mathbf{X}_{-u}\right)}\right]$$

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   - Pick-Freeze

$$\mathbb{V}_{f_{\mathbf{X}}}\left[\mathbb{E}_{f_{\mathbf{X}}}\left(\psi_t\left(\mathbf{X}\right)|\mathbf{X}_u\right)\right] = \mathbb{E}_{f_{\mathbf{X}}}\left(\psi_t(\mathbf{X})\psi_t(\mathbf{X}^u)\right) - p_t^2 = \mathbb{E}_{g}\left(\psi_t\left(\mathbf{X}\right)\psi_t\left(\mathbf{X}^u\right)\frac{f_{\mathbf{X}}(\mathbf{X})f_{\mathbf{X}}(\mathbf{X}^u)g_{\mathbf{X}_u}(\mathbf{X}_u)}{g(\mathbf{X})g(\mathbf{X}^u)f_{\mathbf{X}_u}(\mathbf{X}_u)}\right) - p_t^2$$

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2. aggregation procedure: subset or random permutation

From reliability analysis to TSA

Use of the available sample

In practice, a target sensitivity analysis always comes after a prior reliability analysis $\Longrightarrow$ we have at our disposal an i.i.d. N-sample input/output $\left(\mathbf{X}^{(n)}, \psi_t\left(\mathbf{X}^{(n)}\right)\right)_{n\in[\![1,N]\!]}$ distributed according to g close to g_{opt}

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Question: Is it beneficial to reuse the same sample to estimate the T-Sh$_i$? YES

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Theorem [DCBM22]

$$\mathbb{V}_{g_{\text{opt}}}\left(\widehat{\text{T-S}}^{\text{IS}}_{u,\text{PF}}\right) \leq \frac{p_t^2}{N_u} \underset{p_t \to 0}{\leq} \mathbb{V}_{f_{\mathbf{X}}}\left(\widehat{\text{T-S}}_{u,\text{PF}}\right)$$

where $\widehat{\text{T-S}}_{u,\text{PF}}$ is the existing Pick-Freeze estimator of T-S_u^c and
where $\widehat{\text{T-S}}^{\text{IS}}_{u,\text{PF}}$ is the Pick-Freeze estimator with importance sampling of T-S_u^c.

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Additional costs	double Monte-Carlo	Pick-Freeze
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$\Longrightarrow N_{\mathbb{V}} + (2^d-2)N_O$ (resp. $N_{\mathbb{V}} + m(d-1)N_O$) calls saved with the subset (resp. random permutation) procedure

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- **given-data framework**: we can not draw additional points

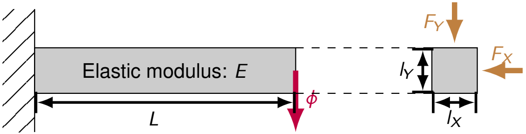
$\Longrightarrow$ extension of the proposed importance sampling estimators to the given-data framework with the nearest neighbour approximation

$\Longrightarrow$ allow to estimate the T-Sh$_i$ without additional calls to ϕ after the estimation of p_t by importance sampling

Cantilever beam

Non given-data

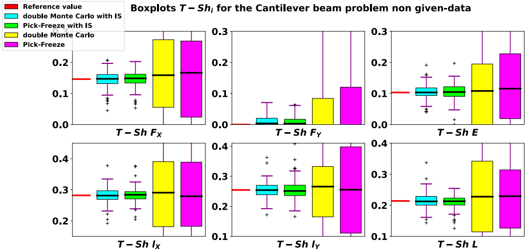
	Input	Distribution	Mean	C.o.V.
1	F_X	LogNormal	556.8 N	0.08
2	F_Y	LogNormal	453.6 N	0.08
3	E	LogNormal	200.10^9 Pa	0.06
4	l_X	Normal	0.062 m	0.1
5	l_Y	Normal	0.0987 m	0.1
6	L	Normal	4.29 m	0.1



Maximal displacement of the tip section:

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

Failure threshold: $t = 0.066$m s.t. $p_t = 0.015$



Cantilever beam

Given-data

	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
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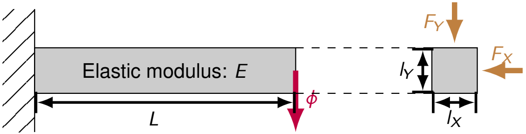

Maximal displacement of the tip section:

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

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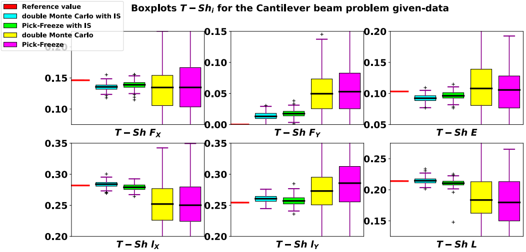

Conclusion and perspectives

What is new?

- unbiased importance sampling estimators of the target Shapley effects
- theoretical proof that $g_{\text{opt}} = f_{\mathbf{X}|\mathbf{X}\in\mathcal{F}_t}$ is a good auxiliary density to estimate the T-Sh$_i$
- procedure to reuse a sample stemming from a prior reliability analysis in both non given-data and given-data frameworks

Conclusion and perspectives

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- unbiased importance sampling estimators of the target Shapley effects
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- procedure to reuse a sample stemming from a prior reliability analysis in both non given-data and given-data frameworks

Perspectives:

- Is there an optimal distribution to estimate the T-S$_u^c$?
- Make the nearest neighbour approximation more accurate when the dimension increase
- Adapt the work of [PD19] to the Shapley effects

Thank you for your attention!

Any question?

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