

Sensitivity analysis for optimization under constraints and with uncertainties

Sensitivity analysis on excursion sets

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System

Input parameters :

- component size
- material
- swell height

-...

inputs

Complex system :
Floating wind turbine

output

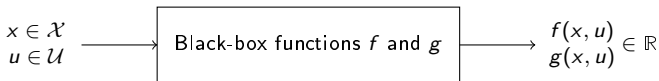
-Cost

- energy production
- environmental impact

-...



Black-box model & optimization problem



- The x are the deterministic inputs
- The u are uncertain inputs : $u = U(\omega)$ with U a random vector of density ρ_U
- f is the objective function to minimize
- g is the constraint function defining the constraint to respect : $g \leq 0$

Optimization problem

$$\begin{aligned} x^* &= \arg \min \mathbb{E}_U[f(x, U)] \\ \text{s.t. } &\mathbb{P}_U[g(x, U) \leq 0] \geq P_{target} \end{aligned} \quad (1)$$

Sensitivity analysis adapted to optimization

Sensitivity analysis (SA) = Studying the impact of each input on the variability of the output.

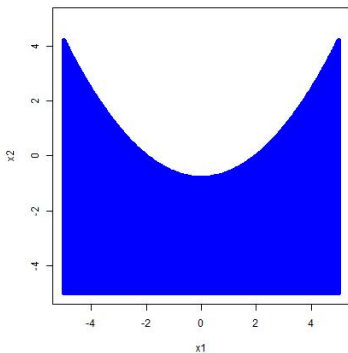
⇒ SA + Optimization : Studying the impact of each input on the minimization of the objective function and on the respect of the constraints.

Toy function

Toy function from [El-Amri et al. 2021]

$$\forall (x, u) \in [-5, 5]^4 \quad g(x, u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

 u_2 fixé $u_1 = -5 \quad u_2 = 0$ 

Toy function

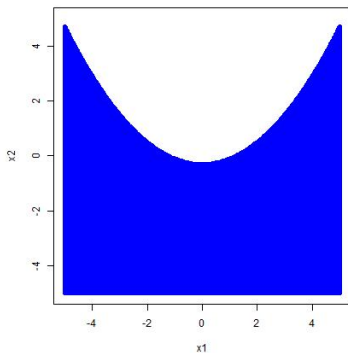
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

u_2 fixé

$u_1 = -2.5 \quad u_2 = 0$



Toy function

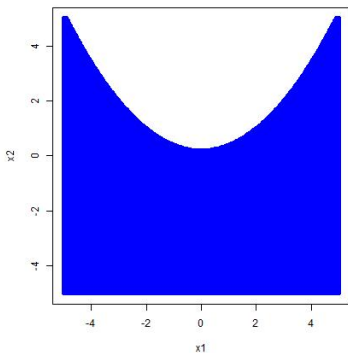
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

u_2 fixé

$u_1 = 0 \quad u_2 = 0$



Toy function

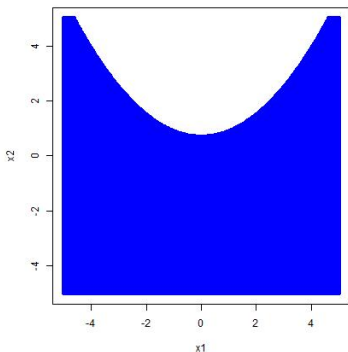
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

u_2 fixé

$u_1 = 2.5 \quad u_2 = 0$



Toy function

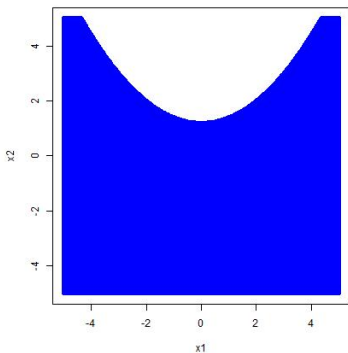
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

u_2 fixé

$u_1 = 5 \quad u_2 = 0$



Toy function

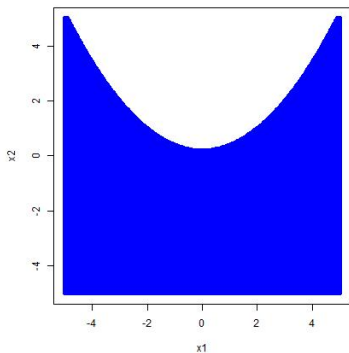
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u_1 fixé

$u_1 = 0 \quad u_2 = 0$



Toy function

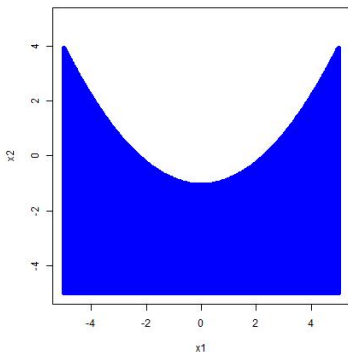
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

u_1 fixé

$u_1 = 0 \quad u_2 = 2.5$



Toy function

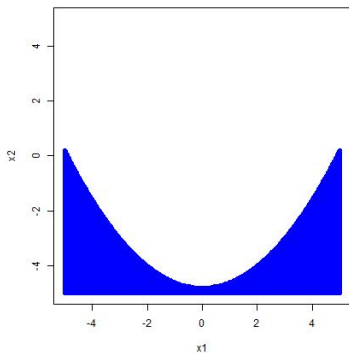
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

u_1 fixé

$u_1 = 0 \quad u_2 = 5$



Subproblem : Excursion sets

Excursion sets

New output :

$$\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}, \quad (2)$$

which is called a random excursion set.

Influence of the uncertain inputs U on Γ_U ? \Rightarrow SA on excursion sets.

Yet most SA techniques have scalar or vectorial outputs.

How then can we do sensitivity analysis on (excursion) sets?

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- 1 Sensitivity analysis on excursion sets through random set theory
 - Random set theory
 - Adaption of the Sobol indices for random sets
 - Results

- 2 Sensitivity analysis on excursion sets using universal indices from [Gamboa et al. 2021] and [Fort, Klein et Lagnoux 2021]
 - Definition of the universal index
 - Adaption and estimation
 - Results

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Random set theory [Molchanov 2005]

The natural definition of a random set is as a set-valued random variable X i.e. as a measurable function :

$$X : \begin{array}{ccc} (\Omega, \mathcal{F}) & \rightarrow & (\mathcal{K}(\mathcal{X}), \mathcal{B}(\mathcal{K}(\mathcal{X}))) \\ \omega & \mapsto & X(\omega) \end{array} . \quad (3)$$

The notion of measurability depends on the definition of $\mathcal{B}(\mathcal{K}(\mathcal{X}))$ which depends on the topology we choose for $\mathcal{K}(\mathcal{X})$.

From [Molchanov 2005], a notion of measurability can be written as :

$$\forall K \in \mathcal{K}(\mathcal{X}), X^- = \{\omega \in \Omega, X(\omega) \cap K \neq \emptyset\} \in \mathcal{F}. \quad (4)$$

With this definition of measurability, we can show that our sets $\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}$ are random compact sets (see 29).

Sobol indices on random sets ?

- We want to characterize the influence of the input U_i on the output $\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}$ which is a random set.
- Sobol indices on random sets : We would want to compute $S_i = \frac{\text{Var} \mathbb{E}[\Gamma|U_i]}{\text{Var} \Gamma} \rightarrow$
The difficulty lies in defining the (conditional) expectation and the variance of a random set.

Vorob'ev expectation and deviation [Molchanov 2005]

The Vorob'ev expectation of a random set Γ is defined as the Vorob'ev quantile which volume is equal (or closer) to the mean volume of Γ :

$$\mathbb{E}^V[\Gamma] = \{x \in \mathcal{X}, \mathbb{P}(x \in \Gamma) \geq \alpha^*\} = Q_{\alpha^*}, \quad (5)$$

with α^* defined by :

$$\mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*}). \quad (6)$$

Or if the previous equation has no solution, from :

$$\mu(Q_\alpha) \leq \mathbb{E}[\mu(\Gamma)] \leq \mu(Q_{\alpha^*}) \quad \forall \alpha > \alpha^*. \quad (7)$$

Then, the Vorob'ev deviation is defined by :

$$\text{Var}^V(\Gamma) = \mathbb{E}[\mu(\Gamma \Delta \mathbb{E}^V[\Gamma])], \quad (8)$$

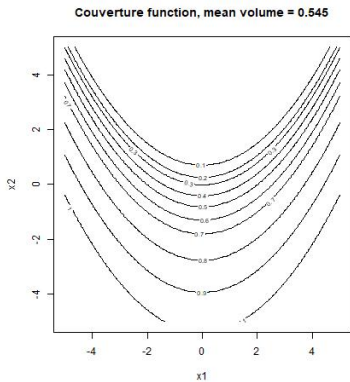
with the symmetric difference Δ defined by $A \Delta B = (A \cup B) \setminus (A \cap B)$.

Example of Vorob'ev expectation

Vorob'ev expectation

$$\mathbb{E}^V[\Gamma] = \{x \in \mathcal{X}, \mathbb{P}(x \in \Gamma) \geq \alpha^*\} = Q_{\alpha^*}$$

$$\mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*})$$

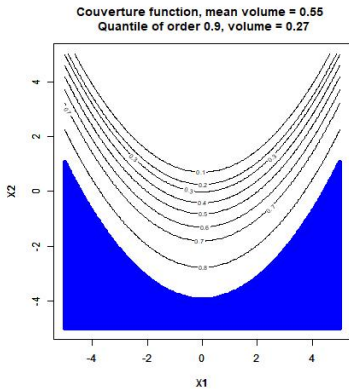


Example of Vorob'ev expectation

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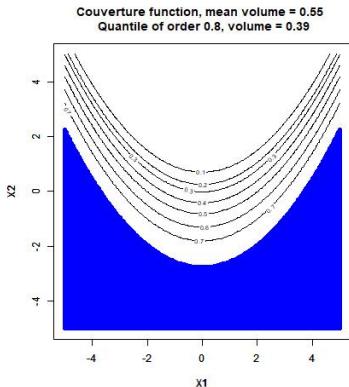


Example of Vorob'ev expectation

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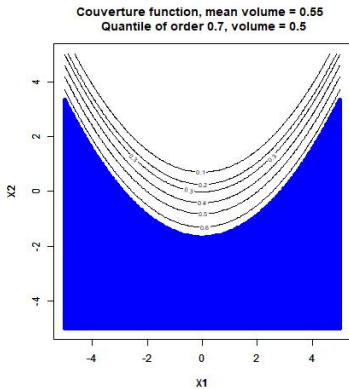


Example of Vorob'ev expectation

Vorob'ev expectation

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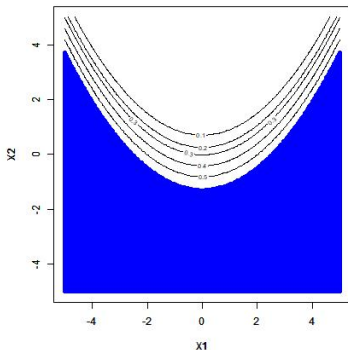
Example of Vorob'ev expectation

Vorob'ev expectation

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$$\mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*})$$

Couverture function, mean volume = 0.55
Quantile of order 0.6, volume = 0.54



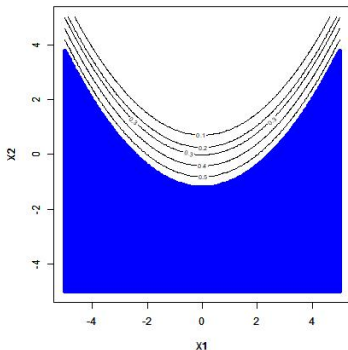
Example of Vorob'ev expectation

Vorob'ev expectation

$$\mathbb{E}^V[\Gamma] = \{x \in \mathcal{X}, \mathbb{P}(x \in \Gamma) \geq \alpha^*\} = Q_{\alpha^*}$$

$$\mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*})$$

Couverture function, mean volume = 0.55
Quantile of order 0.57, volume = 0.55



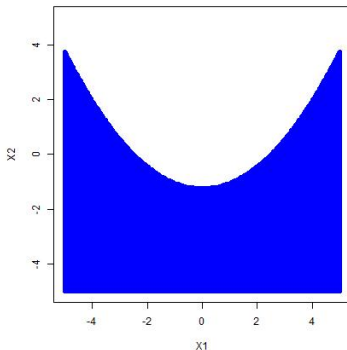
Example of Vorob'ev expectation

Vorob'ev expectation

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$$\mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*})$$

Vorob'ev expectation



Definition of the proposed indices & estimation

Using the previous definitions, we still need a definition of conditional Vorob'ev expectation. We propose the following :

$$\mathbb{E}^V(\Gamma|U_1) = \omega \mapsto \mathbb{E}^V(\Gamma|U_1(\omega)) \quad \text{where} \quad \Gamma|U_1(\omega) = \{x \in \mathcal{X}, g(x, U_1(\omega), U_2) \leq 0\}.$$

With this definition, the first order Vorob'ev index is :

$$\begin{aligned} S_i^V &= \frac{\text{Var}^V(\mathbb{E}^V(\Gamma|U_i))}{\text{Var}^V(\Gamma)} \\ &= \frac{\mathbb{E}[\mu(\mathbb{E}^V(\Gamma|U_i)\Delta\mathbb{E}^V[\mathbb{E}^V(\Gamma|U_i)])]}{\mathbb{E}[\mu(\Gamma\Delta\mathbb{E}^V(\Gamma))]} \end{aligned}$$

Estimation

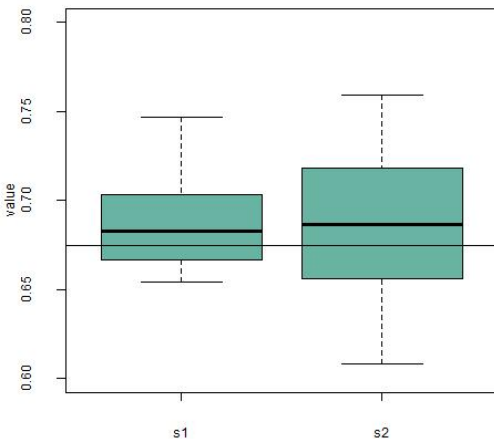
- Monte Carlo estimation
- Issue : $\mathbb{E}^V[\mathbb{E}^V(\Gamma|U_i)] \neq \mathbb{E}^V(\Gamma) \rightarrow$ Costly estimation

Results

Toy function 1

$$\forall (x, u_1, u_2) \in [0, 1]^3 \quad g(x, u) = x - u_1 - u_2$$

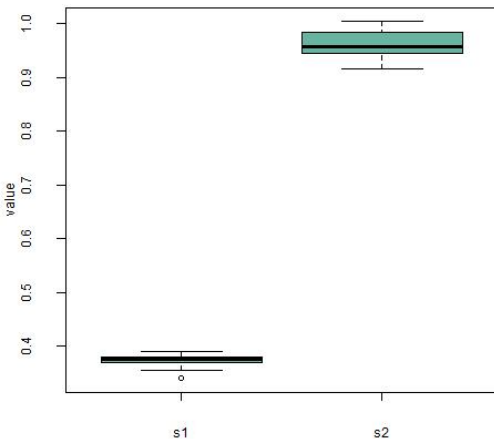
Vorob'ev indices for $N_x=N_U=400$



Results

Toy function 2

$$\forall (x, u) \in [-5, 5]^4 \quad g(x, u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

Vorob'ev indices for $N_x=20, N_u=500$ 

Results

With $N_x = 20$ and $N_u = 500$

g function	Index	Results
$-x_1^2 + 5x_2 - u_1 + u_2^2 - 1$	s_1	0.366
	s_2	0.949
	$s_1 + s_2$	1.314
$-x_1^2 + 5x_2 + u_1^2 + u_2^2 - 1$	s_1	0.721
	s_2	0.715
	$s_1 + s_2$	1.436
$-x_1^2 + 5x_2 + u_1^2 + u_2^2 + u_1u_2 - 1$	s_1	0.598
	s_2	0.547
	$s_1 + s_2$	1.146
$-x_1^2 + 5x_2 + u_1^2 - 1$	s_1	1.00
	s_2	0.00
	$s_1 + s_2$	1.00
$-x_1^2 + 5x_2 + u_1^2 + u_1u_2 - 1$	s_1	0.721
	s_2	0.034
	$s_1 + s_2$	0.755

Conclusion on SA through random sets

- The index quantifies an influence of the inputs on the excursion set
- Very costly estimation
- No variance decomposition

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Definition of the universal index

Index introduced in [Gamboa et al. 2021] and [Fort, Klein et Lagnoux 2021] which generalizes many existing indices, and only requires the output space to be a metric space.

With $Z = f(U_1, \dots, U_p) \in \mathcal{Z}$, the universal sensitivity index with respect to U_i is defined as

$$S_{2, \text{Univ}}^i(T_\cdot, \mathbb{Q}) := \frac{\int_{\mathcal{A}} \text{Var}(\mathbb{E}[T_a(Z) | U_i]) d\mathbb{Q}(a)}{\int_{\mathcal{A}} \text{Var}(T_a(Z)) d\mathbb{Q}(a)}, \quad (9)$$

where (T_a) are tests functions defined by :

$$\begin{aligned} \mathcal{A} \times \mathcal{Z} &\rightarrow \mathbb{R} \\ (a, z) &\mapsto T_a(z), \end{aligned} \quad (10)$$

and \mathcal{A} is some measurable space endowed with a probability measure \mathbb{Q} .

Generalization of existing indices :

- Sobol index : $S^i = S_{2, \text{Univ}}^i(\text{Id}, \mathbb{Q})$ with Id being the indicator function :
 $T_a(z) = z$.
- Cramér-von Mises index : $T_a(z) = \mathbb{1}_{x \leq a}$, $\mathbb{Q} = \mathbb{P}$ with $\mathcal{A} = \mathcal{X}$.

Interpretation of the universal index on random sets

With $Z = \Gamma_U$, the index is :

$$S_{2, \text{Univ}}^i(T, \mathbb{Q}) := \frac{\int_{\mathcal{A}} \text{Var}(\mathbb{E}[T_a(\Gamma_U) | U_i]) d\mathbb{Q}(a)}{\int_{\mathcal{A}} \text{Var}(T_a(\Gamma_U)) d\mathbb{Q}(a)},$$

Interpretation :

- Let $a \in \mathcal{A}$, it defines a random variable $T_a(\Gamma_U)$ which contains a part of information on Γ_U : for instance $T_a(\Gamma_U) = a\mu(\Gamma_U)$.
- $\text{Var}(T_a(\Gamma_U)) = \text{Var}(\mathbb{E}[T_a(\Gamma_U) | U_i]) + \mathbb{E}(\text{Var}[T_a(\Gamma_U) | U_i])$.
- $\int_{\mathcal{A}} \text{Var}(T_a(\Gamma_U)) = \int_{\mathcal{A}} \text{Var}(\mathbb{E}[T_a(\Gamma_U) | U_i]) + \int_{\mathcal{A}} \mathbb{E}(\text{Var}[T_a(\Gamma_U) | U_i])$.

Influence of T_a and \mathbb{Q}

What are the impact of the choices of T_a and \mathbb{Q} , how to choose them ?

Adaptation of the universal index on random sets

$$S_{2, \text{Univ}}^i(T_a, \mathbb{Q}) := \frac{\int_{\mathcal{A}} \text{Var}(\mathbb{E}[T_a(\Gamma_U) | U_i]) d\mathbb{Q}(a)}{\int_{\mathcal{A}} \text{Var}(T_a(\Gamma_U)) d\mathbb{Q}(a)}$$

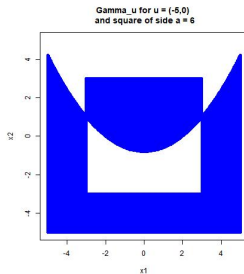
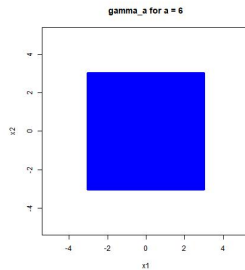
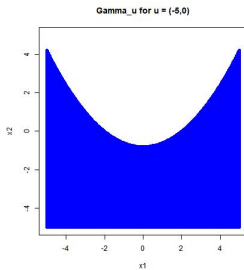
We use $T_a(\Gamma)$ defined by :

$$T_a(\Gamma) = \mu(\gamma_a \Delta \Gamma), \quad (11)$$

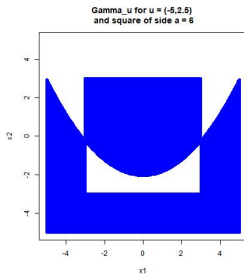
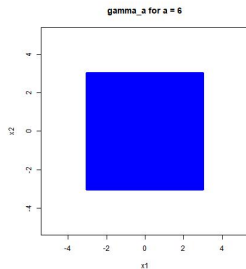
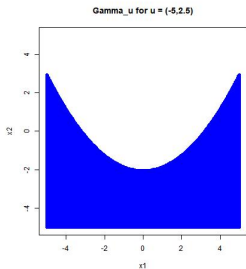
with :

- the symmetric difference Δ defined by $A \Delta B = A \cup B - A \cap B$.
- The volume μ defined by $\mu(\Gamma) = \int_{\mathcal{X}} \mathbb{1}_{x \in \Gamma} dx$.
- \mathbb{Q} is taken uniform on \mathcal{A} .
- the γ_a , called test sets, defined through the scalar (or real valued vector) $a \in \mathbb{R}^m$:
For instance concentric disks of radius a or concentric squares of side a .

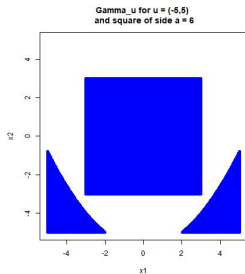
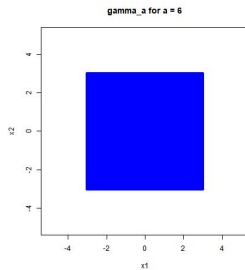
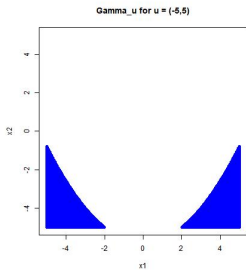
Symmetric difference



Symmetric difference



Symmetric difference



Estimation

Pick and freeze method : U' independent copy of U ,

$$U = (U_1 \quad \cdots \quad U_i \quad \cdots \quad U_p), \quad \tilde{U} = (U_1 \quad \cdots \quad U'_i \quad \cdots \quad U_p)$$

We have then : $\text{Var}(\mathbb{E}[T_a(\Gamma_U) \mid U_i]) = \text{Cov}(T_a(\Gamma_U), T_a(\Gamma_{\tilde{U}}))$.

Estimation $\mu(\mathcal{X}) = 1$

Using $T_a(\Gamma_U) = \mu(\Gamma_U \Delta \gamma_a) = \mathbb{E}_X(\mathbb{1}_{X \in \Gamma_U \Delta \gamma_a})$ with X uniform on \mathcal{X} , we have then

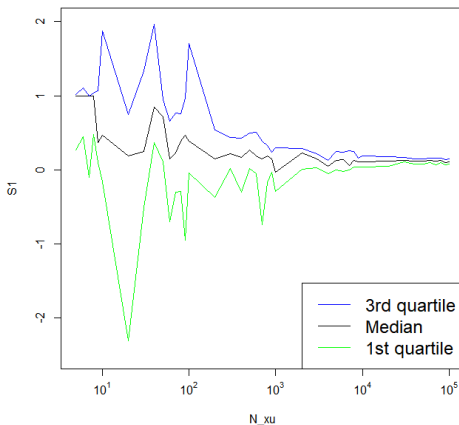
$$\begin{aligned} \text{Cov}_{U, \tilde{U}}(T_a(\Gamma_U), T_a(\Gamma_{\tilde{U}})) &= \mathbb{E}_{U, \tilde{U}}[\mathbb{E}_X(\mathbb{1}_{X \in \Gamma_U \Delta \gamma_a}) \mathbb{E}_X(\mathbb{1}_{X \in \Gamma_{\tilde{U}} \Delta \gamma_a})] \\ &\quad - \mathbb{E}_U[\mathbb{E}_X(\mathbb{1}_{X \in \Gamma_U \Delta \gamma_a})] \mathbb{E}_{\tilde{U}}[\mathbb{E}_X(\mathbb{1}_{X \in \Gamma_{\tilde{U}} \Delta \gamma_a})] \\ &= \mathbb{E}_{X, X', U, \tilde{U}}[\mathbb{1}_{X \in \Gamma_U \Delta \gamma_a} \mathbb{1}_{X' \in \Gamma_{\tilde{U}} \Delta \gamma_a}] \\ &\quad - \mathbb{E}_{X, U}[\mathbb{1}_{X \in \Gamma_U \Delta \gamma_a}] \mathbb{E}_{X', \tilde{U}}[\mathbb{1}_{X' \in \Gamma_{\tilde{U}} \Delta \gamma_a}] \\ &= \frac{1}{N_{xu}} \sum_{j=1}^{N_{xu}} [\mathbb{1}_{X^j \in \Gamma_{U^j} \Delta \gamma_a} \mathbb{1}_{X'^j \in \Gamma_{\tilde{U}^j} \Delta \gamma_a}] \\ &\quad - \frac{1}{N_{xu}} \sum_{j=1}^{N_{xu}} [\mathbb{1}_{X^j \in \Gamma_{U^j} \Delta \gamma_a}] \frac{1}{N_{xu}} \sum_{j=1}^{N_{xu}} [\mathbb{1}_{X'^j \in \Gamma_{\tilde{U}^j} \Delta \gamma_a}]. \end{aligned}$$

Results

Toy function

$$\forall (x, u) \in [-5, 5]^4 \quad g(x, u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

Influence of N_{xu} on $S1$ averaged on 20 realizations
with cubes test functions and $N_a=1000$

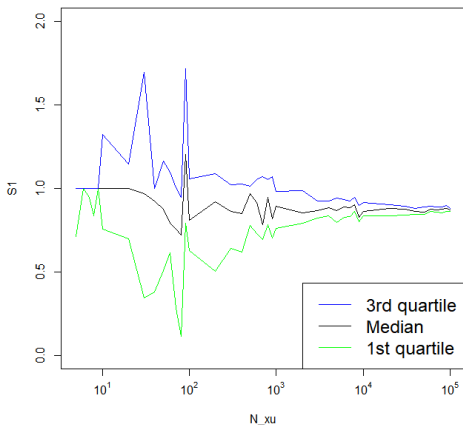


Results

Toy function

$$\forall (x, u) \in [-5, 5]^4 \quad g(x, u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

Influence of N_{xu} on S_2 averaged on 20 realizations
with cubes test functions and $N_a=1000$



Results

With $N_{xu} = 10^6$ and $N_a = 1000$

g function	Index	Results with squares	Results with disks
$-x_1^2 + 5x_2 - u_1 + u_2^2 - 1$	s_1	0.114	0.113
	s_2	0.868	0.864
	$s_1 + s_2$	0.982	0.978
$-x_1^2 + 5x_2 + u_1^2 + u_2^2 - 1$	s_1	0.468	0.450
	s_2	0.461	0.461
	$s_1 + s_2$	0.929	0.911
$-x_1^2 + 5x_2 + u_1^2 + u_2^2 + u_1 u_2 - 1$	s_1	0.286	0.263
	s_2	0.283	0.271
	$s_1 + s_2$	0.570	0.535
$-x_1^2 + 5x_2 + u_1^2 - 1$	s_1	1.00	1.00
	s_2	-0.022	0.031
	$s_1 + s_2$	0.977	1.031
$-x_1^2 + 5x_2 + u_1^2 + u_1 u_2 - 1$	s_1	0.426	0.412
	s_2	0.011	-0.000
	$s_1 + s_2$	0.438	0.412
$-x_1^2 + 5x_2 + u_1 + u_2 - 1$	s_1	0.473	0.445
	s_2	0.500	0.438
	$s_1 + s_2$	0.974	0.884

Comments on the results

Toy function

$$\forall (x, u) \in [-5, 5]^4 \quad g(x, u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

$$\Gamma_U = \{x \in [-5, 5]^2, -x_1^2 + 5x_2 \leq u_1 - u_2^2 + 1\}$$

- S^1 and S^2 don't sum to 1 because there are interactions between u_1 and u_2 in Γ_U :
Indeed, two admissible sets are equals if $u_1 - u_2^2 + 1$ is constant which links u_1 and u_2 .
- Use of the universal index and the choice of T_a as the symmetric difference gives an index which seems to quantify the influence of the input as observed initially.

Conclusion on the universal index on sets

Choices of T_a and \mathbb{Q} ?

Choice of T_a

T_a should be chosen so that the $(T_a(\Gamma_U)_{a \in \mathcal{A}})$ characterizes the most Γ_U .

- Choice of T : could be on other distance between sets or a function of a distance.
- Choice of the test sets : We want that the test sets cover the whole space of sets. For instance taking $a \in \mathbb{R}^2$ to defined rectangles could be better than squares.
- The best choice of the test sets could depend on the function g .

Choice of \mathbb{Q}

- uniform to cover the whole space of sets.

Conclusion





Vorob'ev index

- Sensitivity indices with sets output : Sobol indices with the Vorob'ev expectation and deviation
- Very costly to estimate and no variance decomposition

⇒ Meta-models adapted to the index

Universal sensitivity indices on sets

- Sensitivity indices with sets outputs : Variance of the transformation of the set output explained by an input averaged on a family of test functions
- Choices of the test function, the probability \mathbb{Q} and their influence on the index

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Excursion sets are random sets

For K compact, $h(U) = X = \{x \in \mathcal{X}, g(x, U) \leq 0\}$

$$\begin{aligned} \{K \cap X \neq \emptyset\} &=^c \{\omega, K \cap X(\omega) = \emptyset\} \\ &=^c \{\omega, \forall x \in K \ g(x, U(\omega)) > 0\} \\ &=^c \{\omega, \inf_{x \in K} g(x, U(\omega)) > 0\} \text{ as } K \text{ compact and } g \text{ continuous in } x \\ &=^c U^{-1}(\inf_{x \in K} g(x, \cdot)^{-1}(]0, +\infty[)) \in \mathcal{F} \end{aligned}$$

Universal index on random sets

Expectation of $T_a(\Gamma_U)$

As the randomness of Γ_U only depend on U , we have

$$\mathbb{E}[T_a(\Gamma_U)] = \int_{\mathcal{U}} T_a(\Gamma_U) du. \quad (12)$$

Theorem (Robbins' theorem Molchanov 2005)

Let Γ be a random closed set in a Polish space \mathcal{X} . If μ is a locally finite measure on Borel sets, then $\mu(\Gamma)$ is a random variable and :

$$\mathbb{E}(\mu(\Gamma)) = \int_{\mathcal{X}} \mathbb{P}(x \in \Gamma) \mu(dx). \quad (13)$$

$$\begin{aligned} \mathbb{E}(T_a(\Gamma_U)) &= \mathbb{E}(\mu(\Gamma_U \Delta \gamma_a)) = \int_{\mathcal{X}} \mathbb{P}(x \in \Gamma_U \Delta \gamma_a) \mu(dx) = \int_{\mathcal{X}} \mathbb{P}_U(x \in \Gamma_U \Delta \gamma_a) \mu(dx) \\ &= \int_{\mathcal{X}} \int_{\mathcal{U}} \mathbb{1}_{x \in \Gamma_U \Delta \gamma_a} \mu(dx) \\ &= \int_{\mathcal{U}} T_a(\Gamma_u) du. \end{aligned}$$