

# Sensitivity analysis for optimization under constraints and with uncertainties

Sensitivity analysis on (excursion) sets

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# System & black-box model

Input parameters :

- component size
- material
- swell height
- ...

inputs →

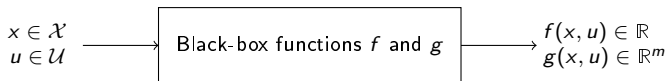
Complex system :  
Floating wind turbine

→ output

- Cost
- energy production
- environmental impact
- ...



# System & black-box model



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

# Optimization problem

## Robust optimization problem

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

## Deterministic strategy

$$\begin{aligned}
 x^* &= \arg \min_x F(x) \\
 \text{s.t. } &G(x) \leq 0
 \end{aligned} \tag{2}$$

- Goal Oriented Sensitivity Analysis to reduce the input dimension : Spagnol 2020
- Huge evaluation cost of  $F$  and  $G$
- What about the  $U$ ?

**How to quantify the impact of the uncertain inputs  $U$  on the optimization ?**

# Toy function

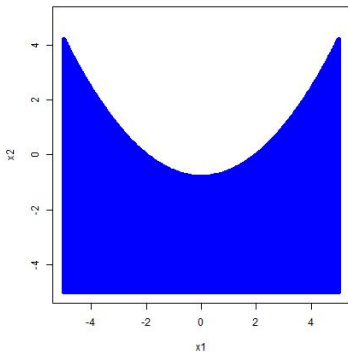
Toy function from [El-Amri et al. 2021]

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

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

$u_2$  fixé

$u_1 = -5 \quad u_2 = 0$



# Toy function

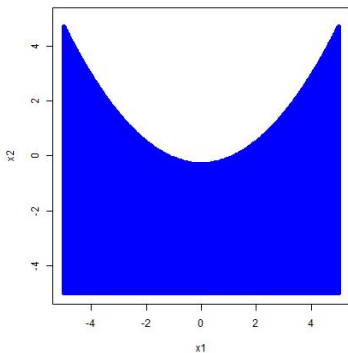
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$u_1 = -2.5 \quad u_2 = 0$



# Toy function

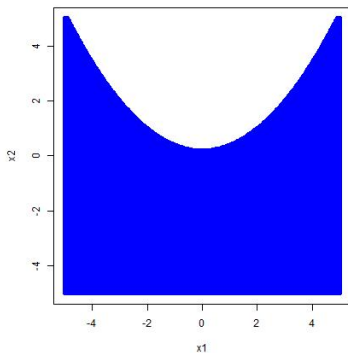
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$u_2$  fixé

$u_1 = 0 \quad u_2 = 0$



# Toy function

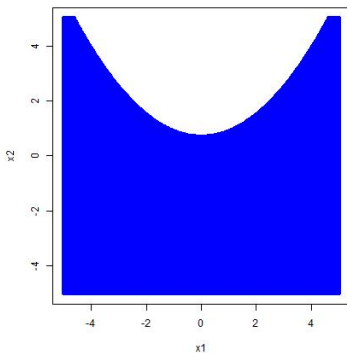
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$u_2$  fixé

$u_1 = 2.5 \quad u_2 = 0$





# Toy function

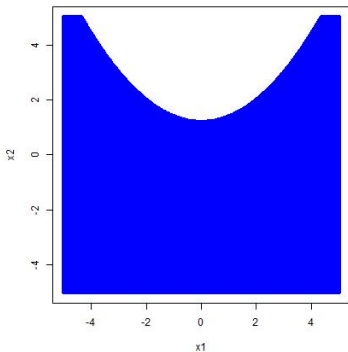
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$u_2$  fixé

$u_1 = 5 \quad u_2 = 0$



# Toy function

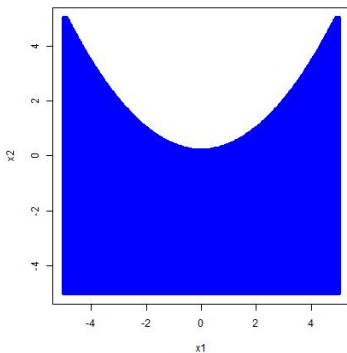
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$u_1$  fixé

$u_1 = 0 \quad u_2 = 0$



# Toy function

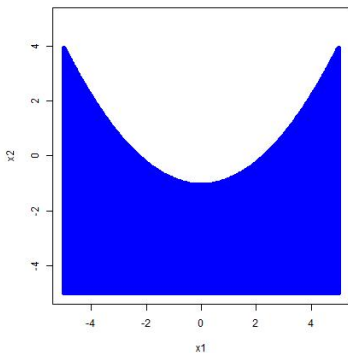
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$u_1$  fixé

$u_1 = 0 \quad u_2 = 2.5$



# Toy function

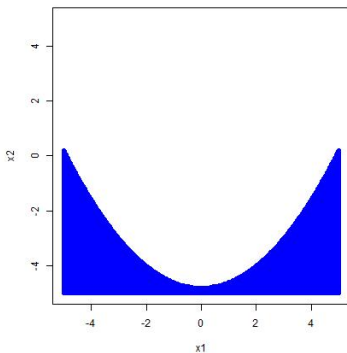
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$$\Gamma_u = \{x \in [-5, 5]^2, g(x, u) \leq 0\}$$

$u_1$  fixé

$u_1 = 0 \quad u_2 = 5$



## Subproblem : Excursion sets

### Excursion sets

New output :

$$\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}, \quad (3)$$

which is called a random excursion set.

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

Yet most SA techniques have scalar or vectorial outputs.

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

- SA on sets using random set theory notably Vorob'ev expectation and deviation
- SA on sets using universal indices from Gamboa et al. 2021
- **SA on sets using RKHS theory**

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## Sobol indices on random sets ?

- How to quantify 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 :

$$S_i = \frac{\text{Var } \mathbb{E}[\Gamma|U_i]}{\text{Var } \Gamma}$$

→ Expectation and Variance of a random set ?



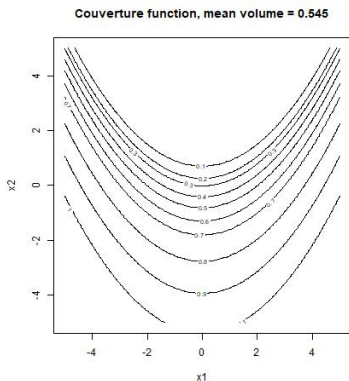
# Vorob'ev expectation and deviation (Molchanov 2005)

## Vorob'ev expectation

$$\mathbb{E}^V[\Gamma] = \{x \in \mathcal{X}, \mathbb{P}(x \in \Gamma) \geq \alpha^*\} = Q_{\alpha^*} \text{ with } \mathbb{E}[\mu(\Gamma)] = \mu(Q_{\alpha^*}) \quad (4)$$

## Vorob'ev deviation

$$\text{Var}^V(\Gamma) = \mathbb{E}[\mu(\Gamma \Delta \mathbb{E}^V[\Gamma])], \quad (5)$$



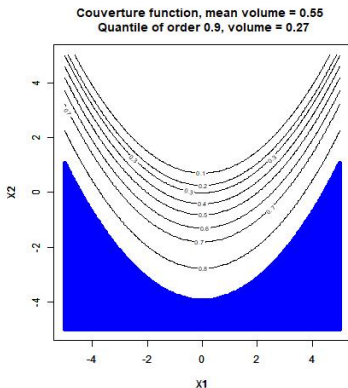
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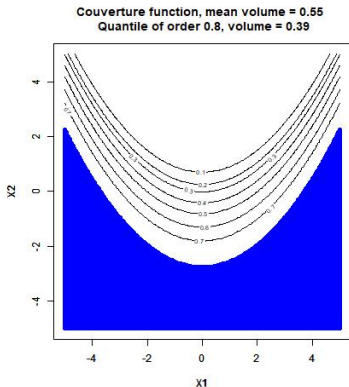
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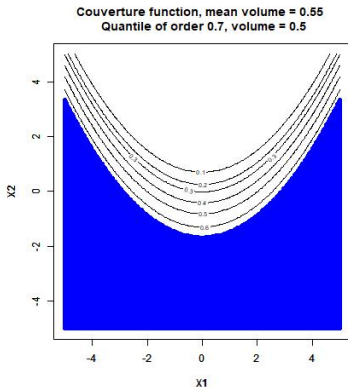
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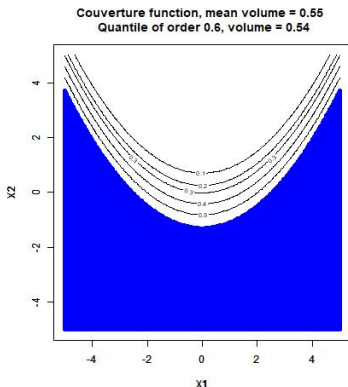
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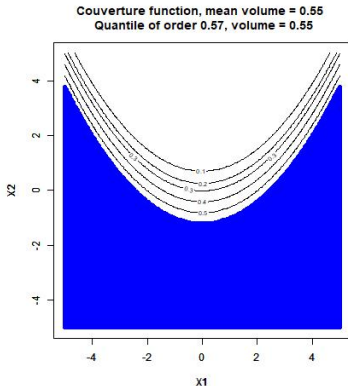
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# Vorob'ev expectation and deviation (Molchanov 2005)

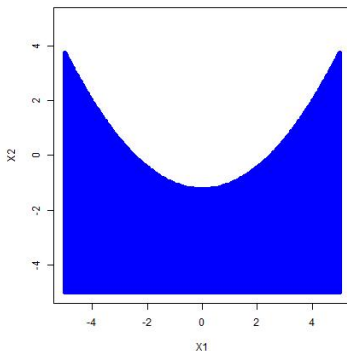
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## Vorob'ev deviation

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Vorob'ev expectation



## Definition of the proposed indices & estimation

First order Vorob'ev index :

$$S_i^V = \frac{\text{Var}^V(\mathbb{E}^V(\Gamma|U_i))}{\text{Var}^V(\Gamma)}$$

$$= \frac{\mathbb{E}[\mu(\mathbb{E}^V(\Gamma|U_i)\Delta\mathbb{E}^V[\mathbb{E}^V(\Gamma|U_i)])]}{\mathbb{E}[\mu(\Gamma\Delta\mathbb{E}^V(\Gamma))]}.$$

But :

$$\mathbb{E}^V[\mathbb{E}^V(\Gamma|U_i)] \neq \mathbb{E}^V(\Gamma)$$

which has two mains issues :

- Very costly Monte Carlo estimation
- No variance decomposition

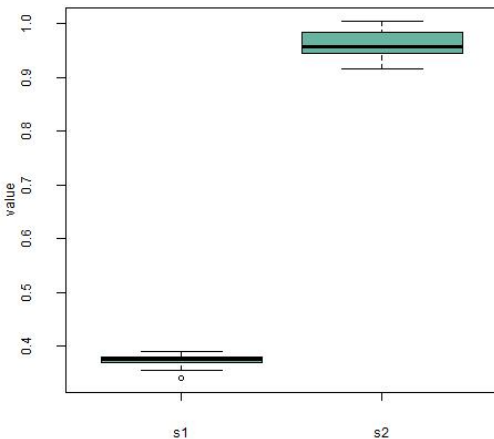


# Results

## Toy function

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

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



# 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 :

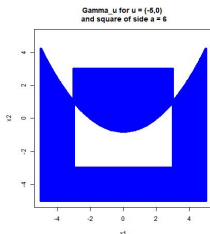
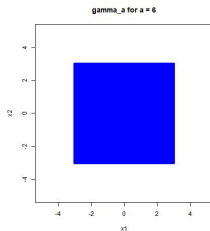
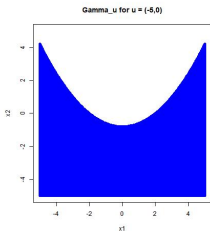
$$T_a(\Gamma) = \mu(\gamma_a \Delta \Gamma), \quad (6)$$

with :

- the symmetric difference  $\Delta$  defined by  $A\Delta B = A \cup B - A \cap B$ .
- The volume  $\mu$  defined by  $\mu(\Gamma) = \int_{\mathcal{X}} \mathbb{1}_{x \in \Gamma} dx$ .
- $\mathbb{Q}$  is taken uniform on  $\mathcal{A}$ .
- the  $\gamma_a$ , 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  $a$ .

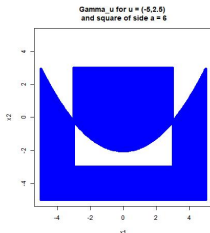
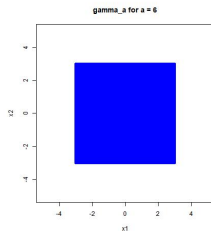
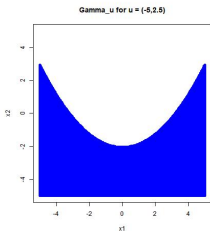
# Idea of the universal index

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



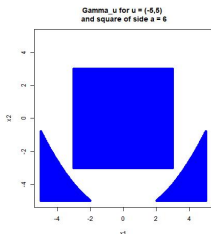
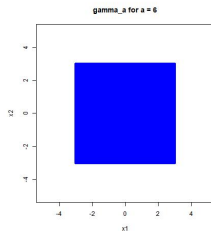
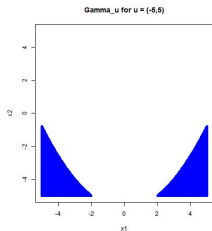
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# Conclusion on universal indices on sets

## Issues

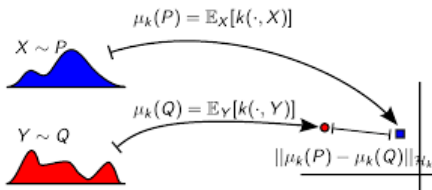
- Choice of  $\mathcal{T}$  (the symmetric difference)
- Choice of  $\mathbb{Q}$
- Choice of the test sets : we used squares and circles.

We could compare realizations to each other  $\rightarrow$  Kernel-based sensitivity analysis.

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# Distribution embedding into a RKHS



Distance between distributions as expectation of kernels, Gretton et al. 2006

$$\gamma_k^2(\mathbb{P}, \mathbb{Q}) := \|\mu_{\mathbb{P}} - \mu_{\mathbb{Q}}\|_{\mathcal{H}_k}^2 = \mathbb{E}_{\substack{X, X' \sim \mathbb{P} \\ Y, Y' \sim \mathbb{Q}}} [k(X, X') + k(Y, Y') - 2k(X, Y)]$$

→ is a distance between distribution iff  $k$  is *characteristic* (i.e. injectivity of the embedding)



# MMD-based index

## MMD-based index

$$\begin{aligned} S_i &:= \mathbb{E}_{X_i} [\gamma_k^2(\mathbb{P}_Y, \mathbb{P}_{Y|X_i})] \\ &= \mathbb{E}_{X_i} \mathbb{E}_{\xi \sim \mathbb{P}_{Y|X_i}} \mathbb{E}_{\xi' \sim \mathbb{P}_{Y|X_i}} [k(\xi, \xi')] - \mathbb{E}_{Y \sim \mathbb{P}_Y} \mathbb{E}_{Y' \sim \mathbb{P}_Y} [k(Y, Y')]. \end{aligned}$$

→ has a ANOVA decomposition (daVeiga 2021) : can be used to rank the inputs by influence.

## Estimation

- Pick & freeze estimation
- Rank-based estimation

## HSIC-based index Gretton et al. 2006

## HSIC-based index

$$\begin{aligned}HSIC_k(X_i, Y) &:= \gamma_k^2(\mathbb{P}_{X_i, Y}, \mathbb{P}_{X_i} \otimes \mathbb{P}_Y) \\ &= \mathbb{E}_{X_i, X'_i, Y, Y'} k_{\mathcal{X}}(X_i, X'_i) k(Y, Y') \\ &\quad + \mathbb{E}_{X_i, X'_i} k_{\mathcal{X}}(X_i, X'_i) \mathbb{E}_{Y, Y'} k(Y, Y') \\ &\quad - 2 \mathbb{E}_{X_i, Y} [\mathbb{E}_{X'_i} k_{\mathcal{X}}(X_i, X'_i) \mathbb{E}_{Y'} k(Y, Y')]\end{aligned}$$

with  $(X'_i, Y')$  an independent copy of  $(X_i, Y)$ .

$HSIC_k(X_i, Y) = 0$  iff  $X_i \perp Y$  (when  $k$  characteristic)  $\rightarrow$  suited to identify the negligible inputs through independence testing.

## Estimation

- Biased or unbiased classic estimators of  $HSIC_k(X_i, Y)$
- p-values computable through asymptotic results or bootstrap methods

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# SA on sets : a kernel between sets

Proposition (A kernel between sets, Balança et Herbin 2012)

The function  $k_{\text{set}} : \mathcal{F}(\mathcal{X}) \times \mathcal{F}(\mathcal{X}) \rightarrow \mathbb{R}$  defined by

$$\forall \Gamma, \Gamma' \in \mathcal{F}(\mathcal{X}), \quad k_{\text{set}}(\Gamma, \Gamma') = \frac{\sigma^2}{2\lambda} e^{-\lambda\mu(\Gamma\Delta\Gamma')},$$

is positive definite for any positive scalars  $\sigma$  and  $\lambda$ .

Moore-Aronszajn theorem (Aronszajn (1950)) gives then the existence of a unique RKHS  $\mathcal{H} \subset \mathcal{F}(\mathcal{X})^{\mathbb{R}}$  of reproducing kernel  $k_{\text{set}}$ .

Now we need to embed "random sets distributions" in  $\mathcal{H}$

# Random set distribution embedding

## Definition (Capacity functional)

The capacity functional of a random closed set  $\Gamma$  denoted  $T_\Gamma$  is defined by :

$$T_\Gamma : \begin{array}{l} \mathcal{K}(\mathcal{X}) \rightarrow [0, 1] \\ K \mapsto \mathbb{P}(\Gamma \cap K \neq \emptyset). \end{array} \quad (7)$$

## Definition (Mean embedding of a capacity functional)

The mean embedding of  $T_\Gamma$  is defined as

$$\mu_\Gamma = \mathbb{E}[k_{\text{set}}(\Gamma, \cdot)]. \quad (8)$$

## Estimation with set-valued outputs

In the MMD- and HSIC-based indices expressions, we need to estimate quantities of the form  $\mathbb{E}k_{\text{set}}(\Gamma_1, \Gamma_2)$ .

With sets,  $k_{\text{set}}(\Gamma_1, \Gamma_2)$  also require an estimation.

$$k_{\text{set}}(\Gamma_1, \Gamma_2) = e^{-\mu(\Gamma_1 \Delta \Gamma_2)} \quad (9)$$

$$= e^{-\mathbb{E}[\mathbb{1}_{\Gamma \Delta \Gamma'}(X)]} \text{ with } X \sim \mathcal{U}(\mathcal{X}) \quad (10)$$

$$\simeq e^{-\mu(\mathcal{X}) \frac{1}{N_x} \sum_{i=1}^{N_x} \mathbb{1}_{\Gamma_1 \Delta \Gamma_2}(X^i)} \quad (11)$$

$$= \widehat{k_{\text{set}}}(\Gamma_1, \Gamma_2) \quad (12)$$

Then we inject it in the indices estimators. For instance the normalized MMD-based index estimated through pick and freeze method is :

$$\widehat{S_{A,p.f}^{MMD}} = \frac{\sum_{i=1}^n \widehat{k_{\text{set}}}(\Gamma^{(i)}, \tilde{\Gamma}^{A,(i)}) - \widehat{k_{\text{set}}}(\Gamma^{(i)}, \Gamma'^{(i)})}{\sum_{i=1}^n \widehat{k_{\text{set}}}(\Gamma^{(i)}, \Gamma^{(i)}) - \widehat{k_{\text{set}}}(\Gamma^{(i)}, \Gamma'^{(i)})}. \quad (13)$$

# Asymptotic behaviour of the indices on sets

## Proposition (Quadratic error of a nested Monte Carlo estimator)

With the previous notations, using Rainforth et al. 2018, we have

$$\mathbb{E} \left( \frac{1}{n} \sum_{j=1}^n \widehat{k_{\text{set}}}(\Gamma_1^{(j)}, \Gamma_2^{(j)}) - \mathbb{E}k_{\text{set}}(\Gamma_1, \Gamma_2) \right)^2 = \mathcal{O}\left(\frac{1}{n} + \frac{1}{N_x^2}\right). \quad (14)$$

With this result, we can show that each quadratic error of our indices on sets has the same asymptotic behavior with rate  $\mathcal{O}\left(\frac{1}{n} + \frac{1}{N_x^2}\right)$

## Toy function, El-Amri et al. 2021

$$\forall x, u \in [-5, 5]^2 \times [-5, 5]^2 \quad g(x, u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1. \quad (15)$$

$$\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}, \quad (16)$$

Toy function	Index	$U_1$	$U_2$
$g = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$	$\widehat{S}_{i,p.f}^{MMD}$	0.074	0.458
	$\widehat{S}_{i,p.f}^{T,MMD}$	0.545	0.935

Table – MMD-based indices

Toy function	Index	$U_1$	$U_2$
$g = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$	$\widehat{S}_i^{HSIC_u}$	0.072	0.284
	p-value	$4.70e - 03$	$5.97e - 10$

Table – HSIC-based indices



## Test case : oscillator, Cousin 2021

$$g_1(\mathbf{x}, \mathbf{u}) = u_{r_1} - \max_{t \in [0, T]} \mathcal{Y}'(x_1 + u_1, x_2 + u_2, u_p; t), \quad (17)$$

$$g_2(\mathbf{x}, \mathbf{u}) = u_{r_2} - \max_{t \in [0, T]} \mathcal{Y}''(x_1 + u_1, x_2 + u_2, u_p; t), \quad (18)$$

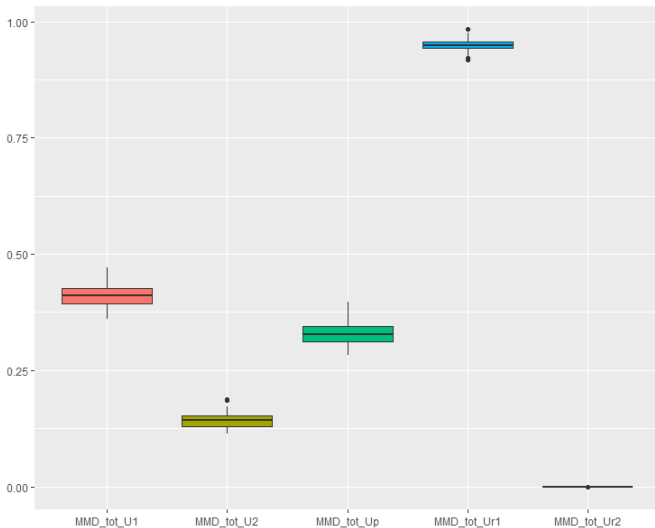
with  $\mathcal{Y}$  the solution of the harmonic oscillator defined by :

$$(x_1 + u_1)\mathcal{Y}''(t) + u_p\mathcal{Y}'(t) + (x_2 + u_2)\mathcal{Y}(t) = \eta(t). \quad (19)$$

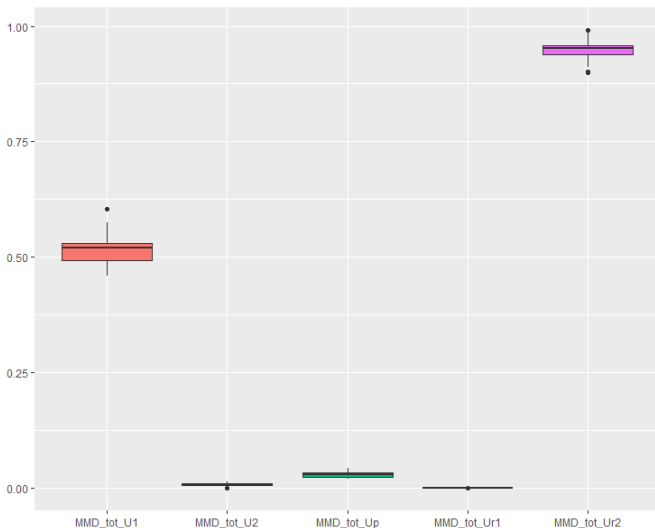
Uncertainty	Distribution	Uncertainty	Distribution
$U_1$	$\mathcal{U}[-0.3, 0.3]$	$U_{r_1}$	$\mathcal{N}(1, 0.1^2)$
$U_2$	$\mathcal{U}[-1, 1]$	$U_{r_2}$	$\mathcal{N}(2.5, 0.25^2)$
$U_p$	$\mathcal{U}[0.5, 1.5]$	$U_{r_3}$	$\mathcal{N}(15, 3^2)$

Table – Definition of the uncertain inputs

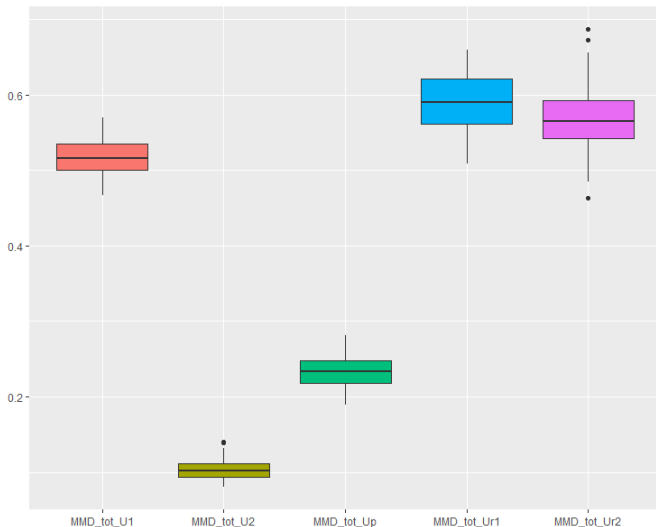
## Results on the oscillator case : MMD-based index

Figure – MMD-based total index for the constraint  $g_1 \leq 0$

## Results on the oscillator case : MMD-based index

Figure – MMD-based total index for the constraint  $g_2 \leq 0$

## Results on the oscillator case : MMD-based index

Figure – MMD-based total index for the constraint  $g_1 \leq 0$  and  $g_2 \leq 0$

## Results on the oscillator case : MMD-based index

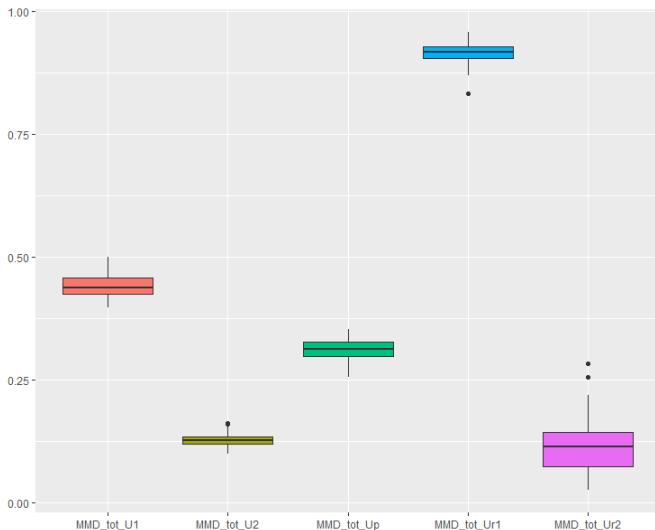
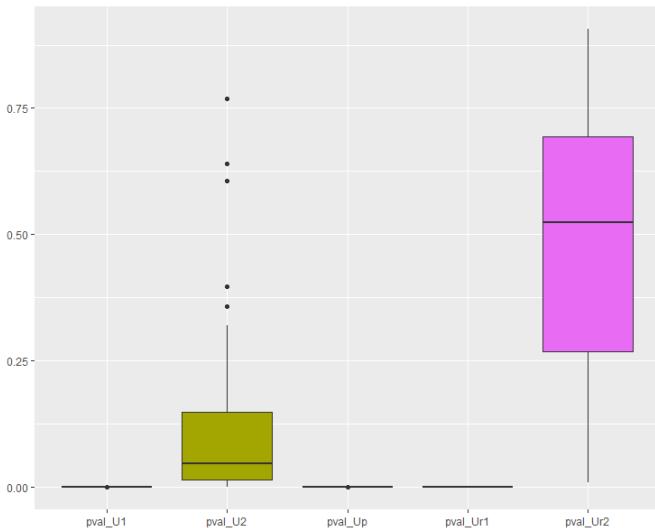
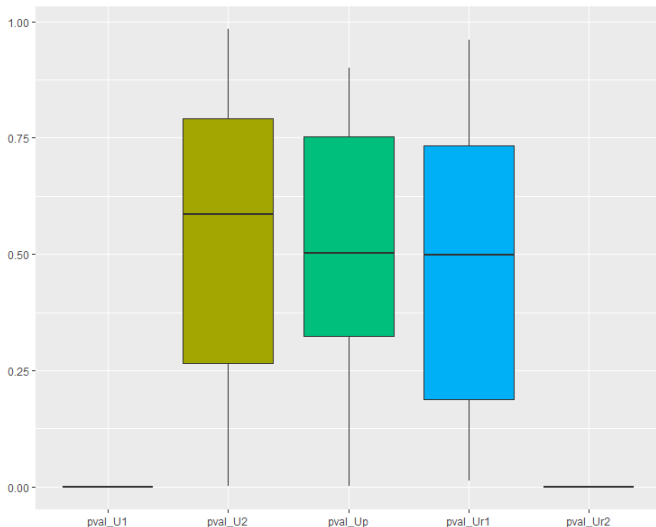


Figure – MMD-based total index for the couple ( $g_1 \leq 0, g_2 \leq 0$ )

## Results on the oscillator case : HSIC-based index

Figure – p-value of the HSIC-based index for the constraint  $g_1 \leq 0$

## Results on the oscillator case : HSIC-based index

Figure – p-value of the HSIC-based index for the constraint  $g_2 \leq 0$

## Results on the oscillator case : HSIC-based index

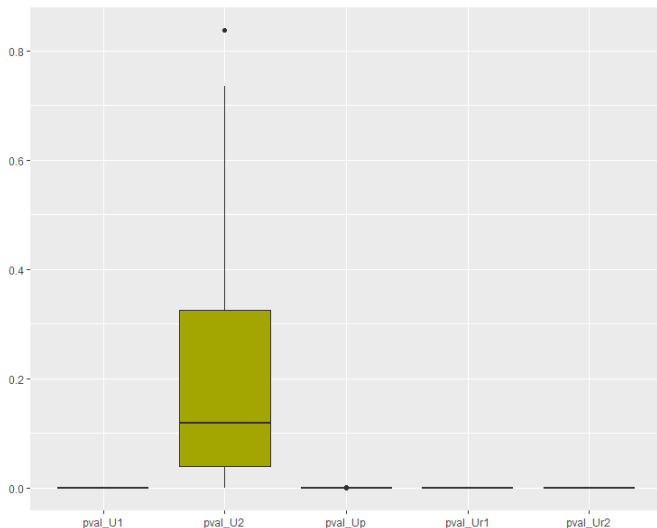


Figure – p-value of the HSIC-based index for the constraint  $g_1 \leq 0$  and  $g_2 \leq 0$



## Results on the oscillator case : HSIC-based index

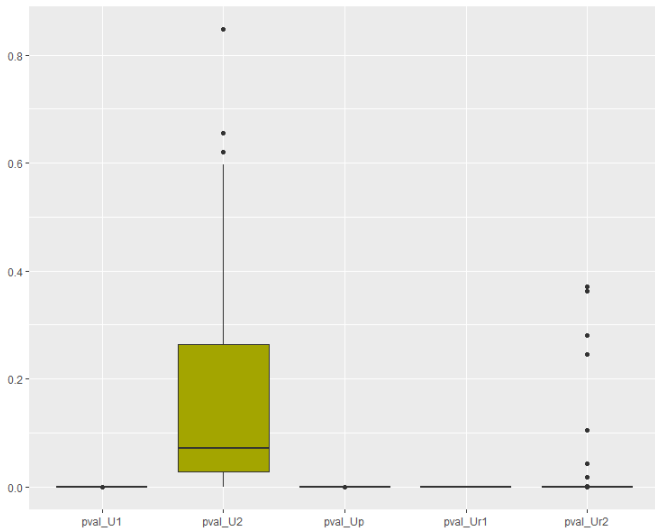


Figure – p-value of the HSIC-based index for the couple ( $g_1 \leq 0, g_2 \leq 0$ )





# Conclusion





## Kernel-based SA on set-valued outputs (paper "soon")

- A way to do SA on set-valued outputs
- On excursion sets : An answer to "How to do SA on the uncertain inputs in the context of robust optimization?"

## Future work

- Test the three methods on a real test case (of Adan Reyes Reyes from IFPEN)
- Use it inside an optimization

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## Excursion sets are random sets

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

$$\{K \cap X \neq \emptyset\} =^c \{\omega, K \cap X(\omega) = \emptyset\}$$

$$=^c \{\omega, \forall x \in K \ g(x, U(\omega)) > 0\}$$

$$=^c \{\omega, \inf_{x \in K} g(x, U(\omega)) > 0\} \text{ as } K \text{ compact and } g \text{ continuous in } x$$

$$=^c U^{-1}(\inf_{x \in K} g(x, \cdot)^{-1}(]0, +\infty[)) \in \mathcal{F}$$

## Indices estimation

$$S_{A,p.f}^{MMD} = \frac{\sum_{i=1}^n k_{\text{set}}(\Gamma^{(i)}, \tilde{\Gamma}^{A,(i)}) - k_{\text{set}}(\Gamma^{(i)}, \Gamma'^{(i)})}{\sum_{i=1}^n k_{\text{set}}(\Gamma^{(i)}, \Gamma^{(i)}) - k_{\text{set}}(\Gamma^{(i)}, \Gamma'^{(i)})}. \quad (20)$$

$$S_{I,\text{rank}}^{MMD} = \frac{\frac{1}{n} \sum_{i=1}^n k_{\text{set}}(\Gamma^{(i)}, \Gamma^{\sigma_n^l(i)}) - \frac{1}{n^2} \sum_{i,j=1}^n k_{\text{set}}(\Gamma^{(i)}, \Gamma^{(j)})}{\frac{1}{n} \sum_{i=1}^n k_{\text{set}}(\Gamma^{(i)}, \Gamma^{(i)}) - \frac{1}{n^2} \sum_{i,j=1}^n k_{\text{set}}(\Gamma^{(i)}, \Gamma^{(j)})}. \quad (21)$$

$$\text{HSIC}_u(U_A, \Gamma) = \frac{1}{n(n-1)} \sum_{i,j=1, i \neq j}^n \left( k_{\mathcal{U}_A}(U_A^{(i)}, U_A^{(j)}) - 1 \right) k_{\text{set}}(\Gamma^{(i)}, \Gamma^{(j)}), \quad (22)$$

$$\text{HSIC}_b(U_A, \Gamma) = \frac{1}{n^2} \sum_{i,j=1}^n \left( k_{\mathcal{U}_A}(U_A^{(i)}, U_A^{(j)}) - 1 \right) k_{\text{set}}(\Gamma^{(i)}, \Gamma^{(j)}). \quad (23)$$