Sensitivity analysis for optimization under constraints and with uncertainties

Kernel-based 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 ρ_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 ?

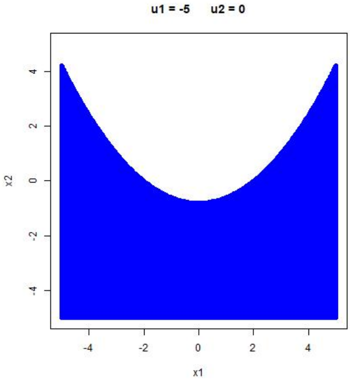
Toy function

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

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

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

u_2 fixé



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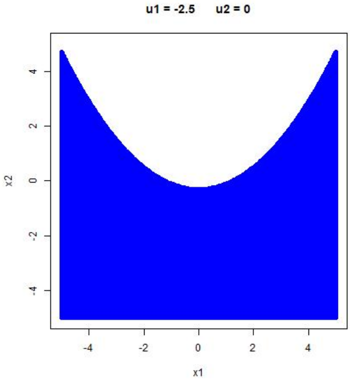

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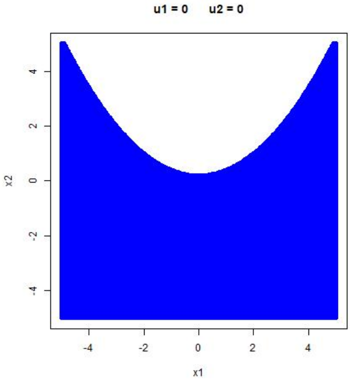

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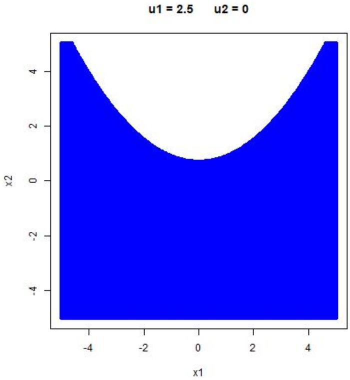

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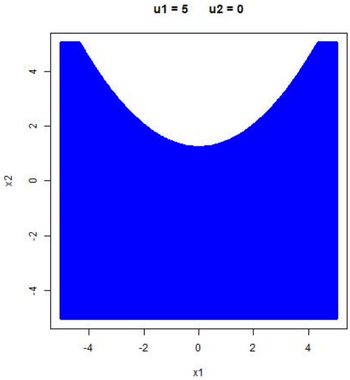

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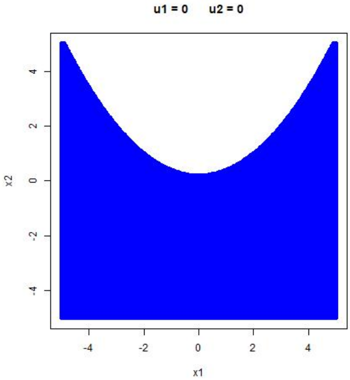
u_1 fixé



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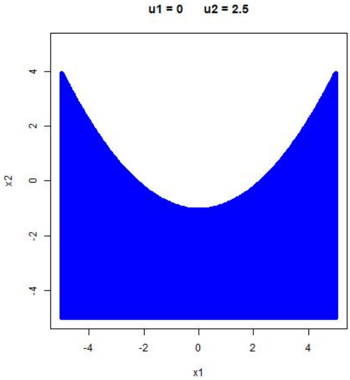

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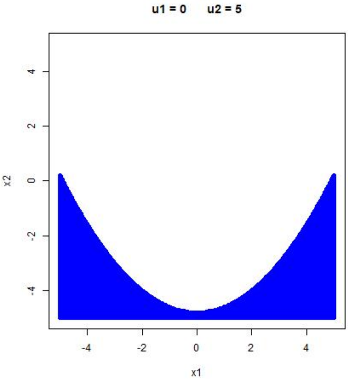

Subproblem : Excursion sets

Excursion sets

New output :

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

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 ?

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

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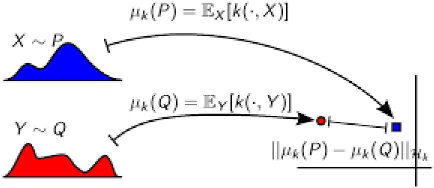
Distribution embedding into a RKHS



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

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

From a distance between distributions to sensitivity indices

MMD-based index, daVeiga 2021

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

HSIC-based index, Gretton et al. 2006

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

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

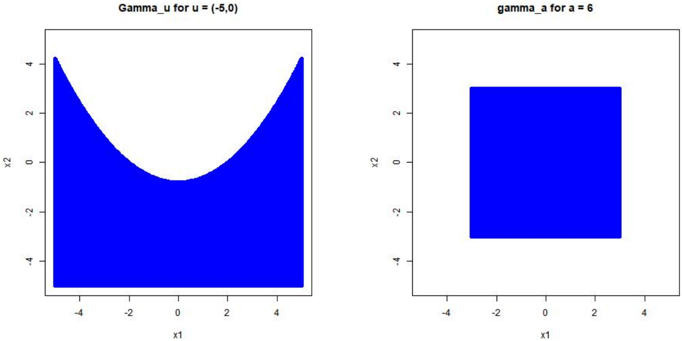
SA on sets : a kernel between sets

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

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

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

is positive definite for any positive scalars σ *and* λ.



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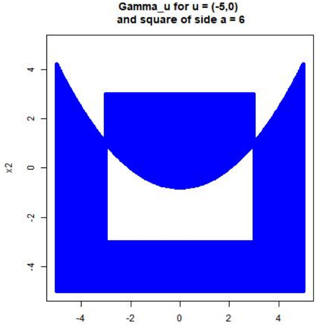

Estimation with set-valued outputs

$$\mathbb{E}k_{set}(\Gamma,\Gamma') = \mathbb{E}[e^{-\mu(\Gamma\Delta\Gamma')}] \quad (4)$$

$$= \mathbb{E}[e^{-\mathbb{E}[\mathbb{1}_{\Gamma\Delta\Gamma'}(X)]}] \text{ with } X \sim \mathcal{U}(\mathcal{X}) \quad (5)$$

$$\simeq \frac{1}{n}\sum_{j=1}^{n} e^{-\mu(\mathcal{X})\frac{1}{N_x}\sum_{i=1}^{N_x}\mathbb{1}_{\Gamma(j)_{\Delta\Gamma'(j)}}(X^i)} \quad (6)$$

Proposition (Quadratic error)

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

$$\mathbb{E}\left(\frac{1}{n}\sum_{j=1}^{n} e^{-\mu(\mathcal{X})\frac{1}{N_x}\sum_{i=1}^{N_x}\mathbb{1}_{\Gamma(j)_{\Delta\Gamma'(j)}}(X^i)} - \mathbb{E}k_{set}(\Gamma,\Gamma')\right)^2 = \mathcal{O}(\frac{1}{n}+\frac{1}{N_x}). \quad (7)$$

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Toy function, El-Amri et al. 2021

$$\forall x, u \in [-5,5]^2 \times [-5,5]^2 \quad g(x,u) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1. \tag{8}$$

$$\Gamma_U = \{x \in \mathcal{X}, g(x,U) \leq 0\}, \tag{9}$$

Index	HSIC-based index	MMD-based index
s_1	0.086	0.071
s_2	0.278	0.478
$1-(s_1+s_2)$		0.451

Table – Kernel-based indices on the toy function g

Test case : oscillator, Cousin 2021

$$g_1(\boldsymbol{x}, \boldsymbol{u}) = u_{r_1} - \max_{t \in [0,T]} \mathcal{Y}'(x_1 + u_1, x_2 + u_2, u_p; t), \quad (10)$$

$$g_2(\boldsymbol{x}, \boldsymbol{u}) = u_{r_2} - \max_{t \in [0,T]} \mathcal{Y}''(x_1 + u_1, x_2 + u_2, u_p; t), \quad (11)$$

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

$$(x_1 + u_1)\mathcal{Y}''(t) + u_p\mathcal{Y}'(t) + (x_2 + u_2)\mathcal{Y}(t) = \eta(t). \quad (12)$$

Constraints	Index	U_1	U_2	U_p	U_{r_1}	U_{r_2}
g_1	MMD	0.041	0.002	0.012	0.485	0.000
	MMD_T	0.427	0.153	0.340	0.932	0.000
g_2	MMD	0.056	0.000	0.000	0.000	0.450
	MMD_T	0.548	0.008	0.031	0.000	0.948
(g_1, g_2)	MMD	0.034	0.000	0.003	0.125	0.114
	MMD_T	0.538	0.115	0.248	0.587	0.581

Constraints \ Input	U_1	U_2	U_p	U_{r_1}	U_{r_2}
g_1	0.099	0.009	0.038	0.723	0.005
g_2	0.150	0.003	0.002	0.003	0.694
(g_1, g_2)	0.164	0.008	0.028	0.488	0.472

Table – MMD and HSIC-based indices on the oscillator case

To conclude

Future work

- Develop other sensitivity indices on sets
- Incorporate such method inside an optimization

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Random set distribution embedding

Proposition (Capacity functional)

The capacity functional of a random closed set Γ denoted T_Γ is defined by :

$$T_\Gamma : \begin{array}{ccc} \mathcal{K}(\mathcal{X}) & \to & [0,1] \\ K & \mapsto & \mathbb{P}(\Gamma \cap K \neq \emptyset). \end{array} \quad (13)$$

Proposition (Embedding of random sets distribution into a RKHS)

Let Γ be a random closed set on a topological space $\mathcal{X}$. Let T_Γ be its capacity functional. With k a measurable and bounded kernel on $\mathcal{F}(\mathcal{X})$, T_Γ can be embedded as

$$T_\Gamma \to \mu_\Gamma = \mathbb{E}[k(\Gamma, \cdot)]. \quad (14)$$