

Sensitivity Analysis on (excursion) sets based on kernel embedding of random sets

Christophette Blanchet

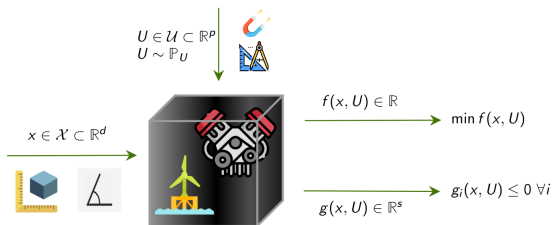
École Centrale de Lyon & ICJ

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Adrien Spagnol & Delphine Sinoquet (IFPEN)

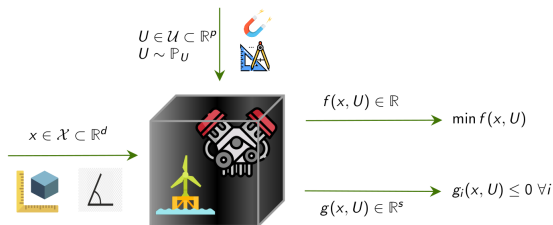
Gaussian Processes 7-9/07/25 ANR GAP-Toulouse



Robust conception of an electrical machine



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Robust optimization problem

$$x^* = \arg \min_{x \in \mathcal{K}} \mathbb{E}[f(x, U)] \text{ where } \mathcal{K} = \{x \in \mathcal{X}, \mathbb{P}[g(x, U) \leq 0] \geq 0.95\}$$

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- ▶ High Dimension for d and $p \implies$ Sensitivity analysis to reduce the space.

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- ▶ Uncertain inputs \implies How to quantify the impact

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Idea : Quantify the impact of U on excursion set

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

A toy excursion set

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

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

Excursion sets

New output :

$$\Gamma_U = \{x \in \mathcal{X}, f(x, U) \leq 0\}, \quad (1)$$

which is called a random excursion set.

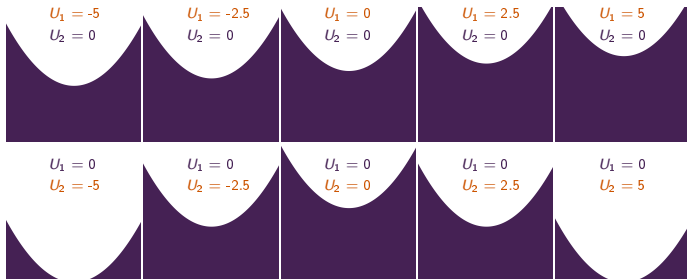


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- Robust conception of an electrical machine

Sensitivity analysis

Sensitivity analysis (SA)

$$(U_1, \dots, U_d) \xrightarrow{f} Y = f(U_1, \dots, U_d)$$

How can the uncertainty of Y be divided and allocated to the uncertainty of the inputs U_i ?

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- ▶ Sobol indices: $S_i = \frac{\text{Var } \mathbb{E}(Y|U_i)}{\text{Var } Y}$
- ▶ Dependence measures: $S_i = \|\mathbb{P}_{(U_i, Y)} - \mathbb{P}_{U_i} \otimes \mathbb{P}_Y\|$
 - ▶ Density-based indices (Borgonovo 2007)
 - ▶ Cramer von mises indices (Gamboa, Klein, and Lagnoux 2018)
 - ▶ Hilbert Schmidt Independence Criterion : [HSIC](#) (Gretton, Bousquet, et al. 2005)

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Problem: What if the output Y is set-valued?

Solution : Kernel-based Sensitivity Analysis

Distribution embedding into a RKHS

Dependence measures: $S_i = \|\mathbb{P}_{(U_i, Y)} - \mathbb{P}_{U_i} \otimes \mathbb{P}_Y\|$

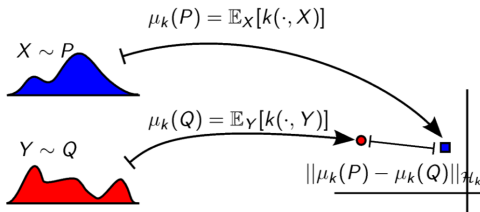


Figure: Kernel mean embedding

with k a (positive definite) kernel $k : (x, x') \in \mathcal{X}^2 \mapsto k(x, x') \in \mathbb{R}$.

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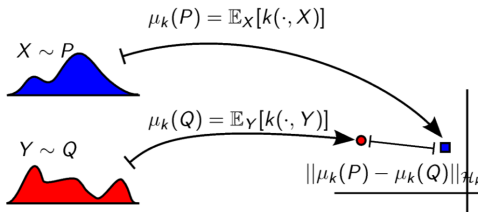


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Hilbert Schmidt Independence Criterion (HSIC), Gretton, Borgwardt, et al. 2006

With a kernel $K = k_{\mathcal{U}_i} \otimes k_Y$, the HSIC is given by:

$$\text{HSIC}_K(U_i, Y) = ||\mu_K(U_i, Y) - \mu_{k_{\mathcal{U}_i}}(U_i) \otimes \mu_{k_Y}(Y)||_{\mathcal{H}_K}^2$$

HSIC-based indices

- ▶ When K is **characteristic** (injectivity of the mean embedding),

$$\text{HSIC}_K(U_i, Y) = 0 \text{ iff } U_i \perp Y \rightarrow \text{screening}.$$

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$$\text{HSIC}(\mathbf{U}, Y) = \sum_{A \subseteq \{1, \dots, d\}} \sum_{B \subseteq A} (-1)^{|A|-|B|} \text{HSIC}(\mathbf{U}_B, Y)$$

$$\left. \begin{aligned} S_i^{\text{HSIC}} &:= \frac{\text{HSIC}(U_i, Y)}{\text{HSIC}(\mathbf{U}, Y)} \\ S_{T_i}^{\text{HSIC}} &:= 1 - \frac{\text{HSIC}(\mathbf{U}_{-i}, Y)}{\text{HSIC}(\mathbf{U}, Y)} \end{aligned} \right\} \rightarrow \text{ranking}$$

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- ▶ Easy to estimate in ANOVA case

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- ▶ Only require (characteristic) kernels on the inputs and on the output (whatever the type of inputs/outputs you have)

SA on sets: a kernel between sets

With $A \Delta B = A \cup B - B \cap A$ and λ the Lebesgue measure, we define a kernel on the Lebesgue σ -algebra $\mathcal{B}(\mathcal{X})$ by:

$$\forall \Gamma_1, \Gamma_2 \in \mathcal{B}(\mathcal{X}), \quad k_{set}(\Gamma_1, \Gamma_2) = \exp \left(-\frac{\lambda(\Gamma_1 \Delta \Gamma_2)}{2\sigma^2} \right).$$

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Proposition (A kernel between sets)

k_{set} is a kernel [Balança and Herbin 2012] and is characteristic.

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For a given random excursion set $\Gamma_U = \{x \in \mathcal{X}, g(x, U) \leq 0\}$, we can define HSIC-based indices on sets:

$$S_i^{\text{H}_{\text{set}}} := \frac{\text{HSIC}_{k_{\text{set}}}(U_i, \Gamma_U)}{\text{HSIC}_{k_{\text{set}}}(\mathbf{U}, \Gamma_U)},$$

which quantifies how much U_i impacts the excursion set Γ .

k_{set} is characteristic, sketch of proof

- $\mathcal{B}(\mathcal{X}) \rightarrow \mathcal{B} = \mathcal{B}(\mathcal{X}) / \sim_\delta$ where δ is the volume of the symmetric difference and \sim_δ the equivalent relation $A \sim_\delta B$ iif $\delta(A, B) = 0$ i.e. A and B are equal except on a λ -negligible set.
- We show that (\mathcal{B}, δ) is a Polish space (separable completely metrizable topological space). (\mathcal{B}, δ) is a metric space so we just need separability and completeness. Separability holds as "it's a subspace of $L_2(\mathcal{X})$ " and we show that it's closed.
- We use a Proposition from Ziegel, Ginsbourger, and Dümbgen 2022,

Proposition (Ziegel, Ginsbourger, and Dümbgen 2022)

Let \mathcal{B} be a Polish space, H a separable Hilbert space, T a measurable and injective mapping from \mathcal{B} to H , and $\varphi \in \Phi_\infty^+$. Then, the kernel k on \mathcal{B} defined by

$$k(\gamma, \gamma') := \varphi \left(\|T(\gamma) - T(\gamma')\|_H^2 \right), \quad \gamma, \gamma' \in \mathcal{B}$$

is integrally strictly positive definite with respect to $\mathcal{M}(\mathcal{B})$ (which implies that it is characteristic).

with $H = L_2(\mathcal{X})$, $\varphi = \exp(-\frac{\cdot}{2\sigma^2})$ and T defined by $T(\gamma) := x \mapsto \mathbb{K}_\gamma(x)$ for any $\gamma \in \mathcal{B}$ so that $\|T(\gamma) - T(\gamma')\|_H^2 = \lambda(\gamma \Delta \gamma')$.

Estimation with set-valued outputs

In HSIC-based indices expressions, we need to estimate quantities of the form ;

$$S_i^{\text{H}_{\text{set}}} = \frac{\text{HSIC}(U_i, \Gamma)}{\text{HSIC}(\mathbf{U}, \Gamma)} = \frac{\mathbb{E} [(k_{\mathcal{U}_i}(U_i, U_i') - 1)k_{\text{set}}(\Gamma, \Gamma')]}{\mathbb{E} [(k_{\mathcal{U}}(\mathbf{U}, \mathbf{U}') - 1)k_{\text{set}}(\Gamma, \Gamma')]}$$

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Estimation:

$$\widehat{\text{HSIC}}(U_i, \Gamma) = \frac{2}{n(n-1)} \sum_{l < j}^n \left(k_{\mathcal{U}_i}(U_i^{(l)}, U_i^{(j)}) - 1 \right) k_{\text{set}}(\Gamma^{(l)}, \Gamma^{(j)}),$$

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

$$\widehat{k_{set}}(\Gamma^{(l)}, \Gamma^{(j)}) = \exp \left(-\frac{\text{vol}(\mathcal{X})}{2\sigma^2} \frac{1}{m} \sum_{k=1}^m 1_{\Gamma^{(l)} \Delta \Gamma^{(j)}}(\mathbf{X}^{(k)}) \right).$$

To reduce the computational cost we use the same samples of \mathbf{X} .

Asymptotic behaviour of the indices on sets

Then we inject it in the indices estimators. $\widehat{\widehat{\text{HSIC}}}(U_i, \Gamma)$: nested Monte Carlo estimator

Proposition (Quadratic risk)

$$\mathbb{E} \left(\widehat{\widehat{\text{HSIC}}}(U_A, \Gamma) - \text{HSIC}(U_A, \Gamma) \right)^2 = \mathcal{O} \left(\frac{1}{n} + \frac{1}{m} \right)$$

In the case of the classic NMC estimator, corresponding here to not reusing the same samples of X , the rate is $\mathcal{O} \left(\frac{1}{n} + \frac{1}{m^2} \right)$.

Toy function 1

From El-Amri et al. 2021,

$$\forall x, u \in [-5, 5]^2 \times [-5, 5]^3 \quad g(x_1, x_2, u_1, u_2, u_3) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

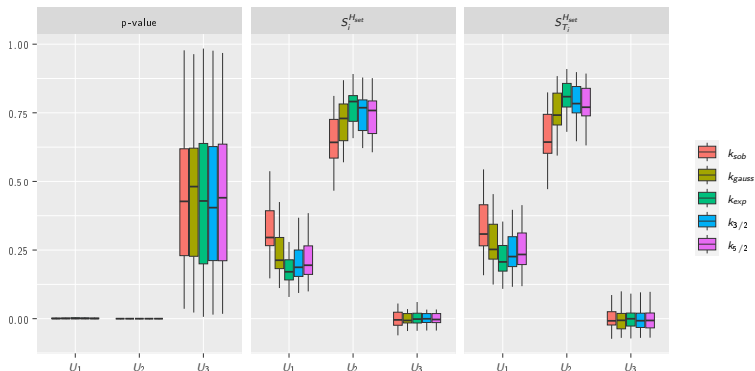


Figure: Estimation of the p-values, $\hat{S}_i^{H_{set}}$ and $\hat{S}_{T_i}^{H_{set}}$ for the excursion set defined by the constraint $g \leq 0$ computed for 5 Anova input kernels with $n = 100$, $m = 100$ and repeated 20 times

Convergence Results

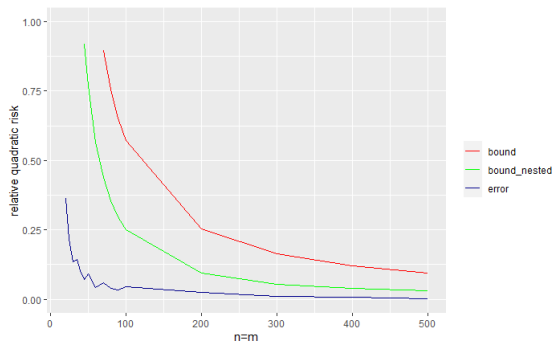
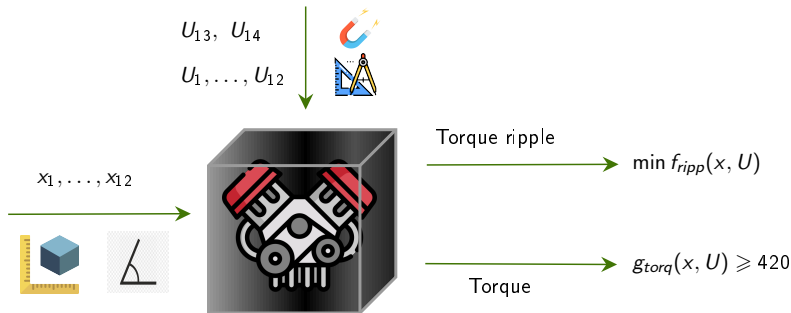


Figure: Evolution of $\widehat{\widehat{\mathcal{R}}}(\widehat{\text{HSIC}}(U_1, \Gamma_g))$ and of the associated upper bounds for the excursion set Γ_g

The "true" value of HSIC, used to compute the quadratic risk, and the constants in the bound are computed for $n = m = 3000$.

Application : excursion sets on the optimisation of the electric machine Meta-models form [Reyes Reyes et al. 2024]



$$x^* = \arg \min_{x \in \mathcal{K}} \mathbb{E}[f_{ripp}(x, U)] \text{ où } \mathcal{K} = \{x \in \mathcal{X}, \mathbb{P}[420 - g_{torq}(x, U) \leq 0] \geq 0.95\}.$$

$$U_1, \dots, U_{14} \mapsto \Gamma = \{x \in \mathcal{X}, f_{ripp}(x, U) \leq 7, g_{torq}(x, U) \geq 420\}$$

What is the impact of the input variables U_i on Γ ?

Robust conception of an electrical machine

Optimization problem

- f and g are defined on $\mathcal{X} \subset \mathbb{R}^{12}$ and $\mathcal{U} \subset \mathbb{R}^{14}$.
- 12 of the 14 uncertain inputs are manufacturing tolerances on each x ,
- U_{13} and U_{14} , describe the magnetic material properties, describe the magnetic material properties and follow uniform distributions on $[-1, 1]$.

Input parameters	Lower bound x_{\min}	Upper bound x_{\max}	Manufacturing Tolerance U
Slot angle	2.47°	3.27°	$\pm 0.1^\circ$
β_{L1P1}	27.03°	29.66°	$\pm 0.33^\circ$
β_{L1P2}	37.03°	39.66°	$\pm 0.33^\circ$
β_{L2P1}	31.03°	33.66°	$\pm 0.33^\circ$
β_{L2P2}	47.03°	49.66°	$\pm 0.33^\circ$
β_{L3P1}	33.7°	37°	$\pm 0.33^\circ$
β_{L3P2}	59.7°	63°	$\pm 0.33^\circ$
Airgap	0.55 mm	0.65 mm	± 0.03 mm
Bridge _{L1}	2.6 mm	2.98 mm	± 0.05 mm
Bridge _{L2}	0.9 mm	1.18 mm	± 0.05 mm
Bridge _{L3}	0.5 mm	0.62 mm	± 0.03 mm
Bridge _{tang}	0.4 mm	0.6 mm	± 0.05 mm

Table: Geometrical variables (see Reyes Reyes et al. (2024) for more details)

Application : sensibility analysis of some excursion sets on the optimisation of the electric machine

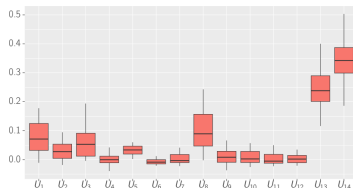


Figure: Estimation des HSIC-ANOVA ($n = m = 100$)

U_1	U_2	U_3	U_4	U_5	U_6	U_7	U_8	U_9	U_{10}	U_{11}	U_{12}	U_{13}	U_{14}
0.3	0.6	0.45	0.85	0.65	1	0.9	0.2	0.85	0.8	0.95	0.85	0	0







Table: Acceptance rates (%) over 20 independence tests with a risk of 5% for the excursion





Conclusion

Kernel-based SA on set-valued outputs

- ▶ A way to do SA on set-valued outputs
- ▶ On excursion sets: An answer to "Which variables is the most influent" => apply on concentration maps of pollutant.
- ▶ On robust optimization : Use it inside an Bayesian optimization (BO) to reduce the dimension
 - ▶ before the BO to reduce the dimension of the meta-model
 - ▶ inside the BO to reduce the dimension of acquisition function

Thanks for your attention !

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