Sensitivity analysis for set-valued models. Application to pollutant concentration maps

Thesis: Sensitivity analysis for constrained robust optimization

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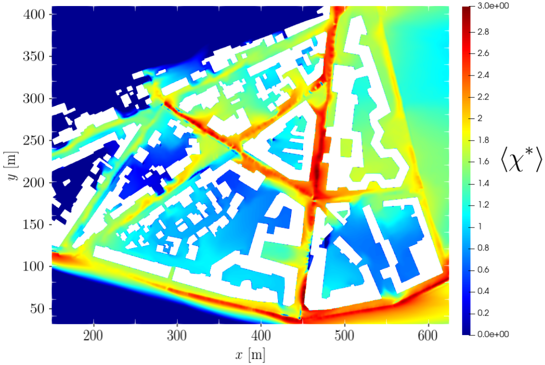
Model of pollutant concentration maps [M. Pasquier]

Input $\boldsymbol{U} = (\theta, U_\infty, q, \beta, \nu_{max})$ with,

- Wind direction $\theta \sim \mathcal{N}_{[5,10]}(0.7, 0.5^2)$ [rad]
- Wind speed $U_\infty \sim \mathcal{N}_{[-0.35;1.75]}(8, 2)$ [m/s]
- Traffic volume $q \sim \mathcal{SN}_{[100;500]}(450, 100, -3)$ [vehicle/h]
- Proportion of diesel and petrol engine $\beta \sim \mathcal{U}([0, 1])$ [-]
- Speed limit $\nu_{\text{max}} \sim \mathcal{U}([30; 50])$ [km/h]

Output : $(x, y) \mapsto \Phi_{\boldsymbol{U}}(x, y)$ a pollutant concentration map



Sensitivity Analysis of map-valued models

Map-valued model :

$$\Phi : \boldsymbol{U} \mapsto \Phi_{\boldsymbol{U}}$$

where

$$\Phi_{\boldsymbol{U}} : (x, y) \mapsto \Phi_{\boldsymbol{U}}(x, y) \in \mathbb{R}$$

Goal : Quantify the effect of the inputs $\boldsymbol{U}$ on the spatial output $\Phi_{\boldsymbol{U}}$

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Sensitivity analysis context

$$(U_1, ..., U_d) \overset{f}{\mapsto} Y = f(U_1, ..., U_d)$$

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

- Sobol indices : $S_i = \frac{\text{Var}\,\mathbb{E}(Y|U_i)}{\text{Var}\,Y}$
- Dependence measures : $S_i = ||\mathbb{P}_{(U_i,Y)} - \mathbb{P}_{U_i} \otimes \mathbb{P}_Y||$

Screening : $U_1, ..., U_k$ are influential and $U_{k+1}, ...U_d$ are not influential
Ranking : $U_1 \prec ... \prec U_d$

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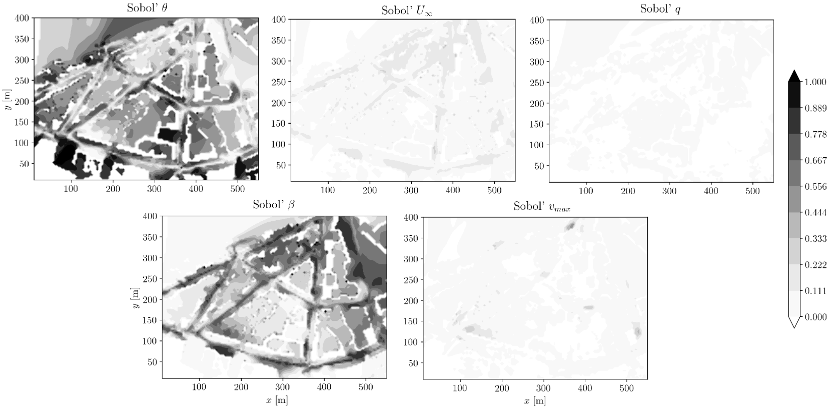
Sobol indices maps [M. Pasquier]

Sobol indices at the position (x_1, x_2) :

$$S_i(x_1, x_2) = \frac{\mathrm{Var}[\mathbb{E}[\Phi_{\boldsymbol{U}}(x_1, x_2) | U_i]]}{\mathrm{Var}[\Phi_{\boldsymbol{U}}(x_1, x_2)]}.$$



Generalized Sobol indices [M. Pasquier]

Generalized Sobol' indices (Gamboa, Janon et al. 2013) :

$$S_i^{\mathbf{gen}} := \sum_{j=1}^{m} w_j S_i(x_1^{(j)}, x_2^{(j)}) \quad \text{with} \qquad w_j = \frac{\mathrm{Var}[\Phi_{\boldsymbol{U}}(x_1^{(j)}, x_2^{(j)})]}{\sum_{k=1}^{m} \mathrm{Var}[\Phi_{\boldsymbol{U}}(x_1^{(k)}, x_2^{(k)})]}.$$

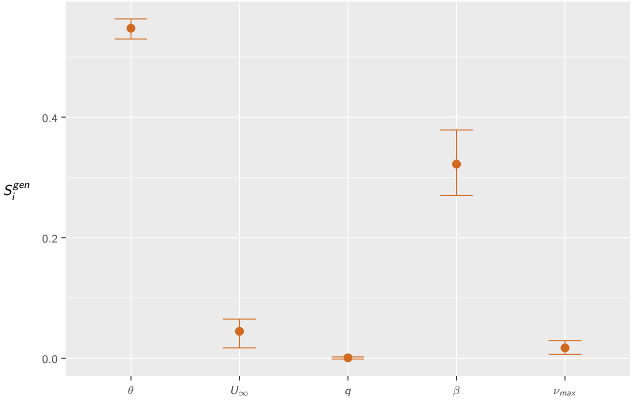
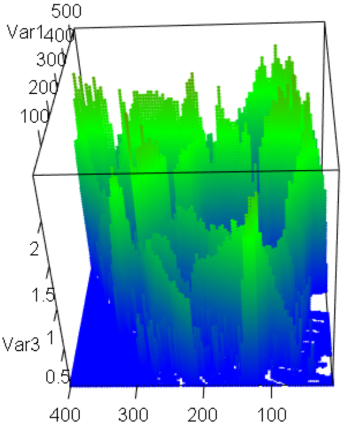


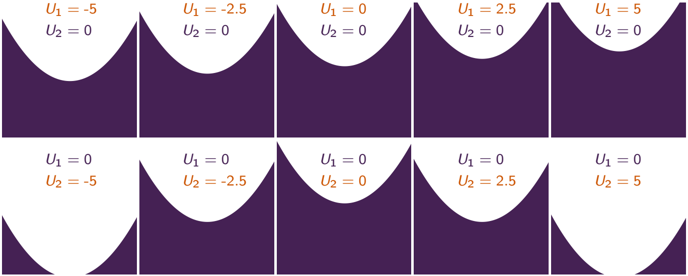
Figure – Estimated generalised first-order Sobol' indices with 2^{12} model evaluations.

From map-valued model to set-valued model

$$\Psi : \begin{array}{ccc} \mathcal{U} & \longrightarrow & \mathcal{L}(\mathcal{X}) \\ \boldsymbol{u} & \mapsto & \Gamma_{\boldsymbol{u}} = \{(x_1, x_2, c) \in \mathcal{D} \times [0, C_{max}],\ c \leq \Phi_{\boldsymbol{u}}(x_1, x_2)\} \end{array}$$



Sensitivity analysis of set-valued models ?



How to do sensitivity analysis of set-valued models ?

Sensitivity analysis on the volume

How to do sensitivity analysis of set-valued models ?

- Conduct sensitivity analysis on the volume : $U \to \lambda(\Gamma_U)$

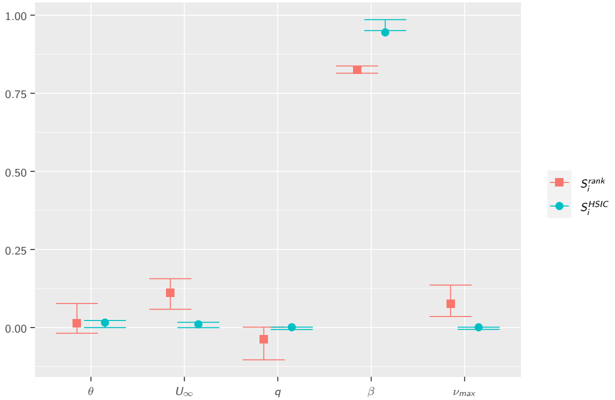


Figure – Estimation of Sobol indices (rank-method) and HSIC-based indices (rbf_anova kernel) of the volume of Γ_U. 1000 model evaluations are used and confidence interval are estimated with 100 bootstrap resamples.

Sensitivity analysis on the volume

How to do sensitivity analysis of set-valued models ?

- ~~Conduct sensitivity analysis on the volume : $U \to \lambda(\Gamma_U)$~~

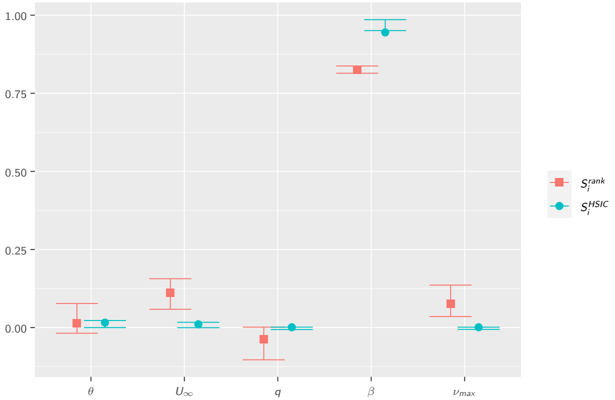


Figure – Estimation of Sobol indices (rank-method) and HSIC-based indices (rbf_anova kernel) of the volume of Γ_U. 1000 model evaluations are used and confidence interval are estimated with 100 bootstrap resamples.

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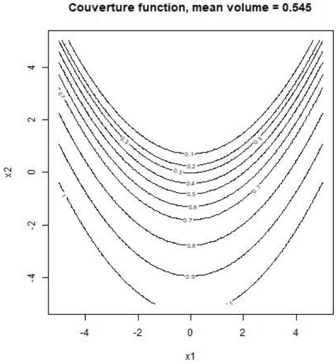
A little bit of random set theory (Molchanov 2005)

Sobol indices on sets ? Requires an expectation and a variance of random sets

Vorob'ev expectation

$$\mathbb{E}^V[\Gamma] = \{x \in \mathcal{X}, \mathbb{P}(x \in \Gamma) \geq \alpha^*\} = Q_{\alpha^*} \text{ with } \mathbb{E}[\lambda(\Gamma)] = \lambda(Q_{\alpha^*}) \quad (1)$$



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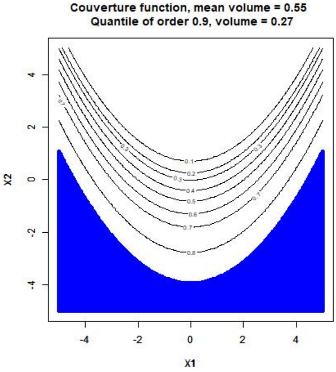

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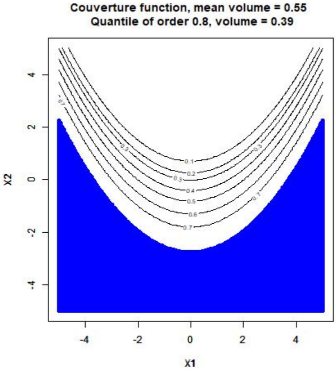

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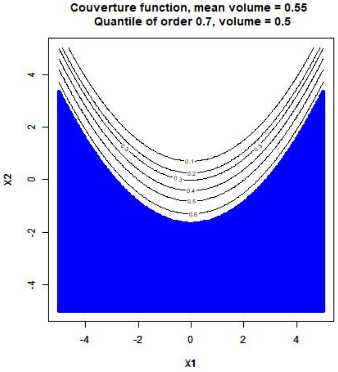

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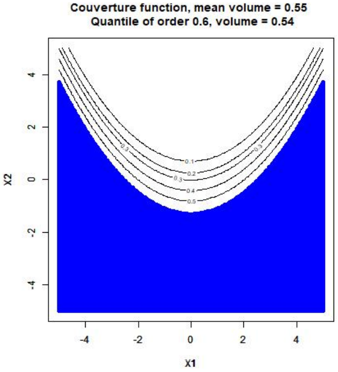

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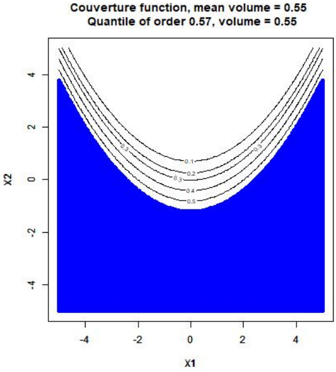

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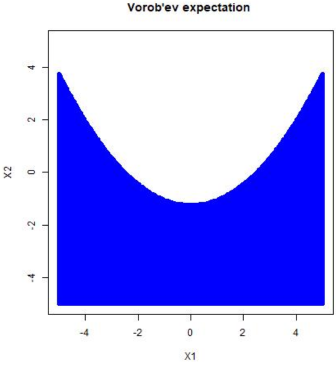

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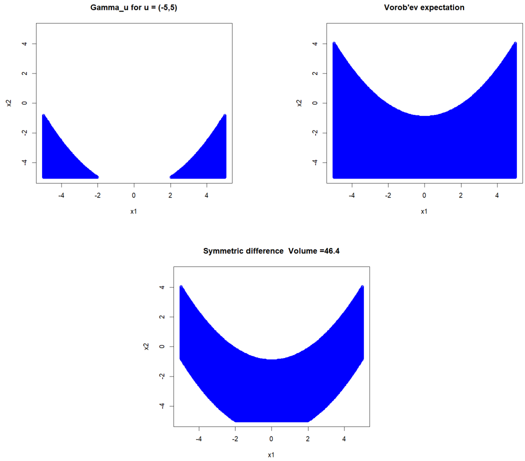
Vorob'ev deviation

$\mathrm{Var}^V(\Gamma) = \mathbb{E}[\lambda(\Gamma \Delta \mathbb{E}^V[\Gamma])]$, with $A \Delta B = A \bigcup B - A \bigcap B$ the symmetric difference



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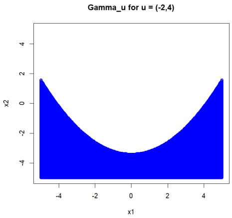

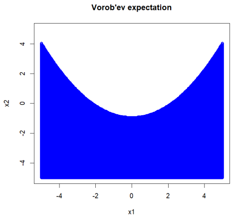

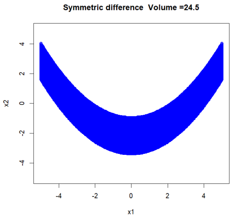

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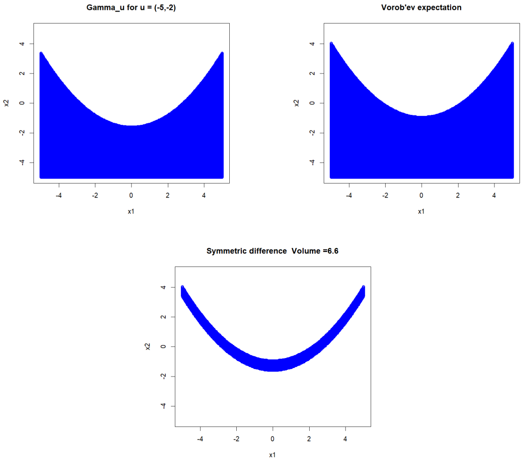

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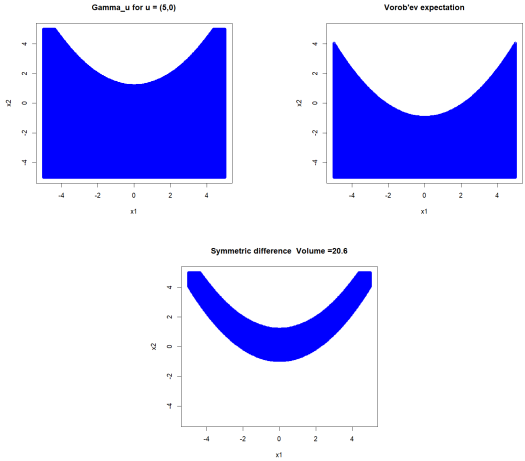

Definition of indices based on random set theory

Sobol indices :

$$S_i = 1 - \frac{\mathbb{E}\,\mathrm{Var}[Y|U_i]}{\mathrm{Var}\ Y}.$$

$$\begin{array}{lcl} \mathbb{E} & \longleftrightarrow & Q_{0.5} = \{x \in \mathcal{X},\ \mathbb{P}(x \in \Gamma) \geq 0.5\} \\ \mathrm{Var} & \longleftrightarrow & \mathbb{E}(\lambda(\Gamma \Delta Q_{0.5})) \\ \mathrm{Var}(\Gamma|U_i) & \longleftrightarrow & \mathbb{E}(\lambda(\Gamma \Delta Q^i_{0.5})|U_i) \\ \mathbb{E}\mathrm{Var}(\Gamma|U_i) & \longleftrightarrow & \mathbb{E}(\lambda(\Gamma \Delta Q^i_{0.5})) \end{array}$$

where $Q^i_{0.5} = \{\boldsymbol{x} \in \mathcal{X}, \mathbb{P}(\boldsymbol{x} \in \Gamma|U_i) \geq 0.5\}$.
"Sobol indices" on random sets :

$$S_i^V = 1 - \frac{\mathbb{E}[\lambda(\Gamma \Delta Q^i_{0.5})]}{\mathbb{E}[\lambda(\Gamma \Delta Q_{0.5})]}$$

Proposition

$0 \leq S_i^V \leq 1$

Estimation

$$\tilde{S}_i^V = 1 - \frac{\sum_{j=1}^{n} \hat{\lambda}_m(\Gamma^{(j)} \Delta \hat{Q}^i_{0.5}(U_i^{(j)}))}{\sum_{j=1}^{n} \hat{\lambda}_m(\Gamma^{(j)} \Delta \hat{Q}_{0.5})}.$$

where

- $\Gamma^{(j)} = \Psi(U^{(j)})$
- $\Gamma_l(U_i^{(j)}) = \Psi(U_i^{(j)}, U_{-i}^{(j,l)})$
- $\hat{Q}^i_{0.5}(U_i^{(j)}) := \{x \in \mathcal{X}, \frac{1}{n} \sum_{l=1}^{n} \mathbb{1}_{\Gamma_l(U_i^{(j)})}(x) \geq 0.5\}$
- $\hat{\lambda}_m(A) = \frac{1}{m} \sum_{k=1}^{m} \mathbb{1}_A(\boldsymbol{x}^{(l)})$.

$\rightarrow$ double loop estimation

Results

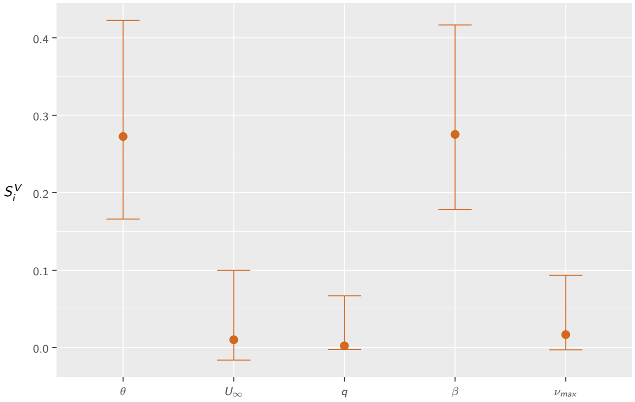

Figure – Estimation of S_V^i for each input with 1024 model evaluations and a confidence interval estimated with 100 bootstrap resamples.

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Definition of the universal index [Fort, Klein et Lagnoux 2021]

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

$$S^i_{2,\text{ Univ}}\left(T_\cdot, \mathbb{Q}\right) := \frac{\int_{\mathcal{A}} \text{Var}\left(\mathbb{E}\left[T_a(Z) \mid U_i\right]\right) d\mathbb{Q}(a)}{\int_{\mathcal{A}} \text{Var}\left(T_a(Z)\right) d\mathbb{Q}(a)}, \tag{2}$$

where (T_a) are tests functions defined by :

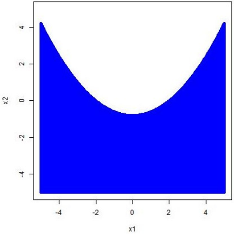
$$\begin{array}{ccc} \mathcal{A} \times \mathcal{Z} & \to & \mathbb{R} \\ (a, z) & \mapsto & T_a(z), \end{array} \tag{3}$$

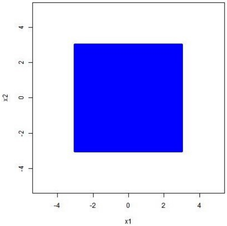
and $\mathcal{A}$ is some measurable space endowed with a probability measure $\mathbb{Q}$.

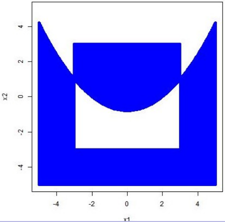
- Generalization of existing indices :
  - Sobol index : $S^i = S^i_{2,\text{ Univ}}\left(Id, \mathbb{Q}\right)$ with Id beeing the indicator function : $T_a(z) = z$.
  - Cramér-von Mises index : $T_a(z) = \mathbb{1}_{x \leq a}$, $\mathbb{Q} = \mathbb{P}$ with $\mathcal{A} = \mathcal{X}$.
- Defined for any **metric** output space

Adaptation of the universal indices to sets

$$S_i^{\text{Univ}}(\gamma, \mathbb{Q}) = \frac{\int_0^1 \text{Var}\,\mathbb{E}\left[\lambda(\Gamma \Delta \gamma_a) \mid U_i\right] d\mathbb{Q}(a)}{\int_0^1 \text{Var}\left(\lambda(\Gamma \Delta \gamma_a)\right) d\mathbb{Q}(a)}$$ with γ_a a square with side length a







Definition of the indices

Definition (adaptation of the universal indices from Fort, Klein et Lagnoux 2021)

$$S_i^{\text{Univ}}(\gamma, \mathbb{Q}) = \frac{\int_0^1 \text{Var}\, \mathbb{E}\left[\lambda(\Gamma \Delta \gamma_a) \mid U_i\right] d\mathbb{Q}(a)}{\int_0^1 \text{Var}\left(\lambda(\Gamma \Delta \gamma_a)\right) d\mathbb{Q}(a)}.$$

where $(\gamma_a)_{a \in [0,1]} \subset \mathcal{X}$ is a collection of test sets parameterised by $a \in [0,1]$ and $\mathbb{Q}$ is a probability distribution on $[0,1]$ to choose.

- Centered balls : $\gamma_a = B(x^0, a)$ with $\mathbb{Q} \sim \mathcal{U}([0, \frac{1}{2}])$
- Centered squares : $\gamma_a = \{x \in [0,1]^3, ||x - x^0||_\infty \leq a\}$ with $\mathbb{Q} \sim \mathcal{U}([0, \frac{1}{2}])$
- Slices along the i-th dimension : $\gamma_a^i = \{x \in [0,1]^3, x^i \leq a\}$ with $\mathbb{Q} \sim \mathcal{U}([0,1])$
- Vorob'ev quantiles : $\gamma_a = \{x \in [0,1]^3, \mathbb{P}(x \in \Gamma) \geq a\}$ with $\mathbb{Q} \sim \mathcal{N}(\frac{1}{2}, 0.05^2)$

Estimation (rank-based estimation)

The estimator $\widehat{S}_i^{\text{Univ}}$ of S_i^{Univ} is given by the ratio between

$$\widehat{S}_{num} = \frac{1}{N_a}\sum_{l=1}^{N_a}\left[\frac{1}{n}\sum_{j=1}^{n}\left(\hat{\lambda}_m(\Gamma^{(j)}\Delta\gamma_{A_l})\right)\left(\hat{\lambda}_m(\Gamma^{(N_i(j))}\Delta\gamma_{a_l})\right)\right] - \frac{1}{N_a}\sum_{l=1}^{N_a}\left[\frac{1}{n}\sum_{j=1}^{n}\left(\hat{\lambda}_m(\Gamma^{(j)}\Delta\gamma_{a_l})\right)\right]^2$$

and,

$$\widehat{S}_{den} = \frac{1}{N_a}\sum_{l=1}^{N_a}\left[\frac{1}{n}\sum_{j=1}^{n}\left(\hat{\lambda}_m(\Gamma^{(j)}\Delta\gamma_{a_l})\right)^2\right] - \frac{1}{N_a}\sum_{l=1}^{N_a}\left[\frac{1}{n}\sum_{j=1}^{n}\left(\hat{\lambda}_m(\Gamma^{(j)}\Delta\gamma_{a_l})\right)\right]^2,$$

where (a_l) is an iid sample of the law $\mathbb{Q}$ and $N_i(j)$ is the index in the sample (U_i^l) that comes after U_i^j when (U_i^l) is sorted in ascending order (see Gamboa, Gremaud et al. 2022 for details).

Results

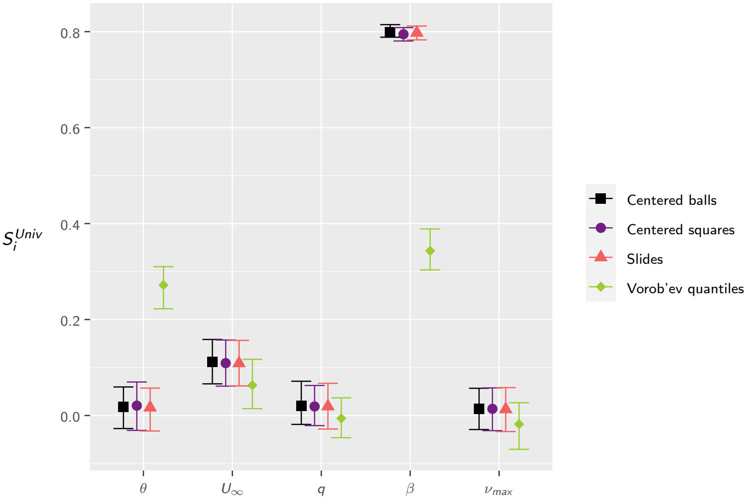
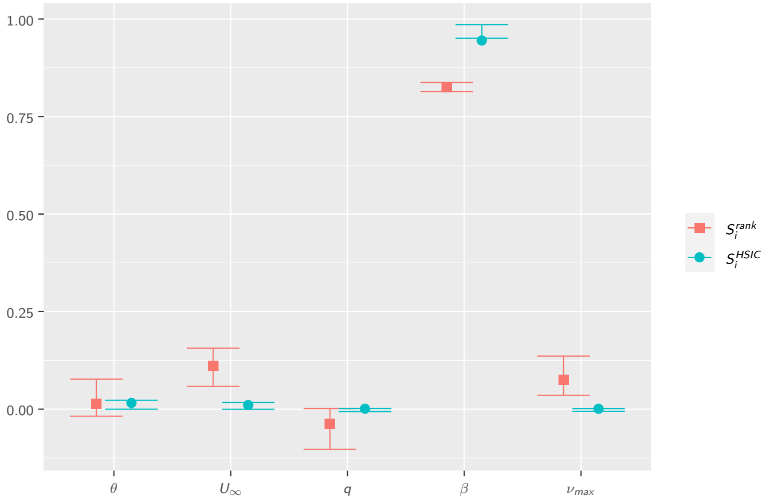


Figure – Estimation of the universal indices $S_i^{\mathbf{Univ}}$ for each input and for four different test sets and $N_a = 100$, with 1000 model evaluations. Confidence intervals are obtained with 100 bootstrap samples

Results



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Distribution embedding into a RKHS

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

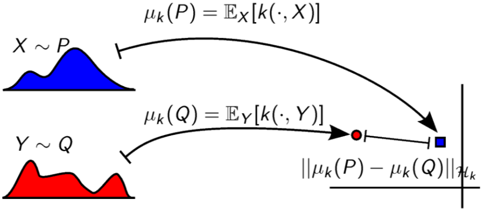

Figure – Kernel mean embedding

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

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

With $K = k_{\mathcal{X}_i} \otimes k_{\mathcal{Y}}$, the HSIC is given by :

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

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

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

HSIC-ANOVA index [daVeiga 2021]

Assuming that the inputs are independent and that the input kernels are ANOVA,

$$\mathrm{HSIC}(\boldsymbol{X}, Y) = \sum_{A \subseteq \{1,\dots,d\}} \sum_{B \subseteq A} (-1)^{|A|-|B|} \, \mathrm{HSIC}\left(\boldsymbol{X}_B, Y\right).$$

HSIC-ANOVA indices are then defined as :

$$S_i^{\mathrm{HSIC}} := \frac{\mathrm{HSIC}(X_i, Y)}{\mathrm{HSIC}(\boldsymbol{X}, Y)},$$

$$S_{T_i}^{\mathrm{HSIC}} := 1 - \frac{\mathrm{HSIC}(\boldsymbol{X}_{-i}, Y)}{\mathrm{HSIC}(\boldsymbol{X}, Y)}$$

and are suited for ranking (and screening).

- Easy to estimate :

$$\begin{aligned} \mathrm{HSIC}_{k_{\mathcal{X}}, k_{\mathcal{Y}}}(X, Y) = {} & \mathbb{E}[k_{\mathcal{X}}(X, X') k_{\mathcal{Y}}(Y, Y')] \\ & + \mathbb{E}[k_{\mathcal{X}}(X, X')] \mathbb{E}[k_{\mathcal{Y}}(Y, Y')] \\ & - 2\mathbb{E}[\mathbb{E}[k_{\mathcal{X}}(X, X')|X] \mathbb{E}[k_{\mathcal{Y}}(Y, Y')|Y]]. \end{aligned}$$

- Only requirement : to have kernels on the inputs and on the output

HSIC ANOVA indices for sets, definition of the indices

Given an input kernel K_i and an output kernel k_{set},

$$HSIC_{K_i \otimes k_{set}}(U_i, \Gamma) = ||\mu_{K_i \otimes k_{set}}(\mathbb{P}_{(U_i,\Gamma)}) - \mu_{K_i \otimes k_{set}}(\mathbb{P}_{U_i} \otimes \mathbb{P}_\Gamma)||^2_{\mathcal{H}_{K_i \otimes k_{set}}}$$

If $K_i \otimes k_{set}$ is characteristic (injectivity of the mean embedding), then,

$$HSIC_{K_i \otimes k_{set}}(U_i, \Gamma) = 0 \text{ iif } U_i \perp \Gamma.$$

Proposition (Fellmann et al. 2023)

The kernel k_{set} defined by :

$$k_{set}(\gamma_1, \gamma_2) = \exp\left(-\frac{\lambda(\gamma_1 \Delta \gamma_2)}{2\sigma^2}\right)$$

is characteristic.

$$S_i^{\mathrm{H}_{set}} := \frac{\mathrm{HSIC}^{ANOVA}(U_i, \Gamma)}{\mathrm{HSIC}^{ANOVA}(\boldsymbol{U}, \Gamma)} = \frac{\mathbb{E}\left[(K_i(U_i, U_i') - 1)k_{set}(\Gamma, \Gamma')\right]}{\mathbb{E}\left[(K(\boldsymbol{U}, \boldsymbol{U}') - 1)k_{set}(\Gamma, \Gamma')\right]}$$

HSIC ANOVA indices for sets, definition of the indices

The indices can be estimated using :

$$\widehat{\mathrm{H}_{set}}\,(U_i, \Gamma) = \frac{2}{n(n-1)} \sum_{j<l}^{n} \left(K_i \left(U_i^{(j)}, U_i^{(l)} \right) - 1 \right) \exp(-\frac{\lambda(\mathcal{X})}{2\sigma^2} \hat{\lambda}_m(\Gamma^{(j)} \Delta \Gamma^{(l)})).$$

Input kernels :

- the Sobolev kernel of order 1,
  $k_{sob}(x, y) = 1 + (x - \frac{1}{2})(y - \frac{1}{2}) + \frac{1}{2}[(x-y)^2 - |x-y| + \frac{1}{6}]$
- the Gaussian kernel, $k_{rbf}(x, y) = e^{-\frac{1}{2}\left(\frac{x-y}{\sigma}\right)^2}$ with $\sigma > 0$,
- the Laplace kernel, $k_{exp}(x, y) = e^{-\frac{|x-y|}{h}}$ with $h > 0$,
- the Matérn 3/2, $k_{3/2}(x, y) = \left(1 + \sqrt{3}\frac{|x-y|}{h}\right) e^{-\sqrt{3}\frac{|x-y|}{h}}$ with $h > 0$,
- the Matérn 5/2, $k_{5/2}(x, y) = \left(1 + \sqrt{5}\frac{|x-y|}{h} + \frac{5}{3}\frac{|x-y|}{h^2}\right) e^{-\sqrt{5}\frac{|x-y|}{h}}$ with $h > 0$.

Results

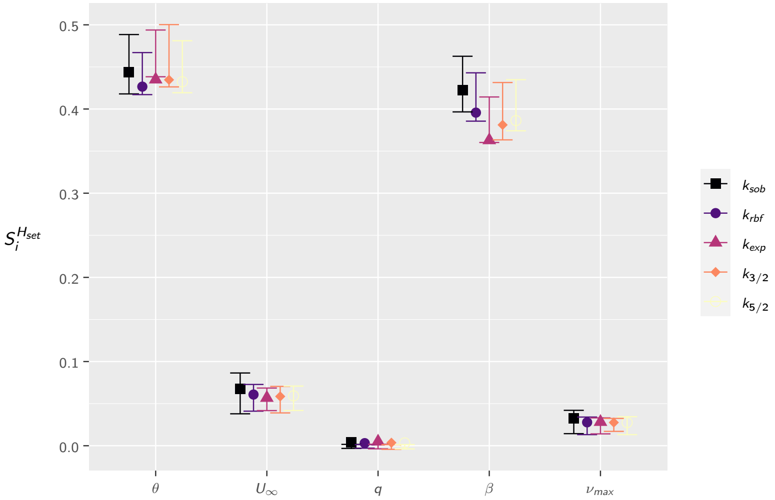

Figure – Estimation of $S_i^{\mathrm{H}set}$ for five input kernels, 1000 model evaluations. Confidence intervals are obtained by bootstrap with 100 resamples

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Comparison

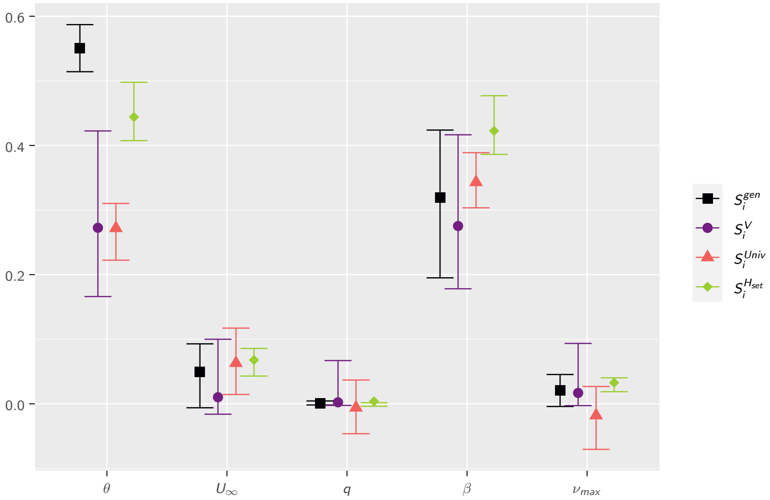

Figure – Comparison of the four indices with a total budget of $n = 1000$ model evaluations. 100 bootstrap sample are used to estimate confidence intervals

Comparison

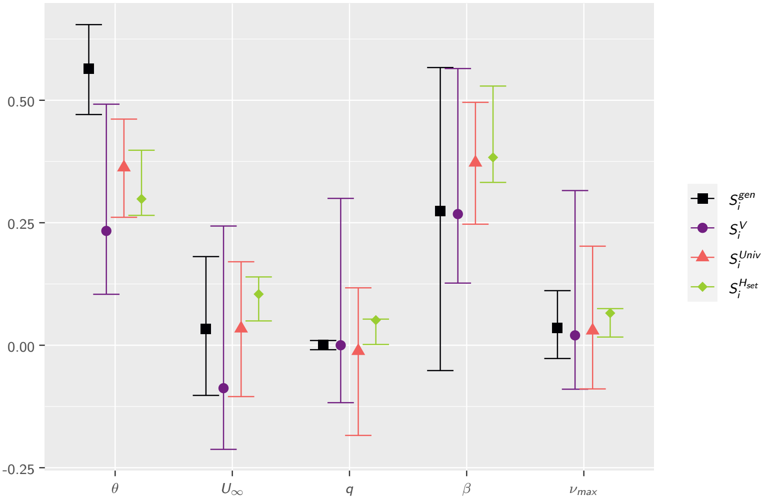

Figure – Comparison of the four indices with a total budget of $n = 100$ model evaluations. 100 bootstrap sample are used to estimate confidence intervals

Comparison and conclusion

	Ranking	**Screening**	**Evaluations**	**Limitations**
S_i^{gen}	✓ ANOVA	$\sim$ threshold	$\sim (p+1)n$	✗ pointwise influence
S_i^V	✗ no decomposition	✗ no screening method	✗ n^2 (double loop)	✓ no choice to be made
S_i^{Univ}	✓ ANOVA	$\sim$ threshold	$\sim$ n but big confidence intervals	✗ choice of the test sets
$S_i^{H_{set}}$	✓ ANOVA	✓ independence test	✓ n and small confidence intervals	$\sim$ choice of kernel ✗ Interactions interpretations

- HSIC-based indices seem to be the most efficient except if we are interested in the interactions between the inputs
- Methodology presented for map-valued outputs but can be used for any set-valued outputs

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