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KERNEL-BASED SENSITIVITY ANALYSIS ON EXCURSION SETS

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Introduction

Goal: Quantifying the influence of **uncertain inputs** on **feasible sets** associated to a constrained robust optimization problem.

$$\mathbf{x}^* = \arg \min_{\mathbf{x} \in \mathcal{X}} \mathbb{E}_{\mathbf{U}}[f(\mathbf{x}, \mathbf{U})] \text{ s.t. } \mathbb{P}_{\mathbf{U}}[g(\mathbf{x}, \mathbf{U}) \leq 0] \geq \alpha.$$

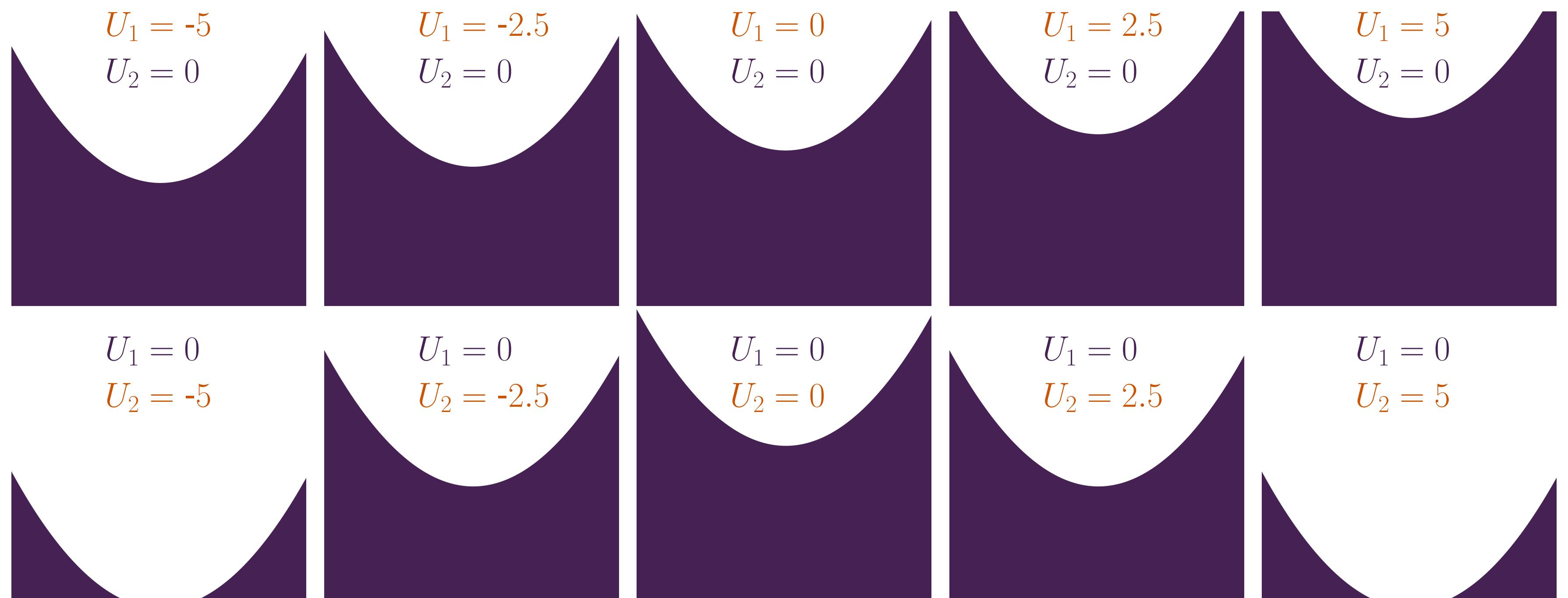
Answer: Performing **Sensitivity analysis** on **excursion sets** $\Gamma_{\mathbf{U}}$ using **kernel-based** methods. We propose a kernel k_{set} with which we compute **HSIC-ANOVA** indices.

$$(U_1, \dots, U_p) \mapsto \Gamma = \{\mathbf{x} \in \mathcal{X}, g(\mathbf{x}, \mathbf{U}) \leq 0\}$$

Example:

$$\Gamma = \{\mathbf{x} \in [-5, 5]^2, x_1^2 + 5x_2 - U_1 + U_2^2 - 1 \leq 0\}$$

→ U_2 seems more influential than U_1 on the feasible sets.



Kernel-based Sensitivity Analysis

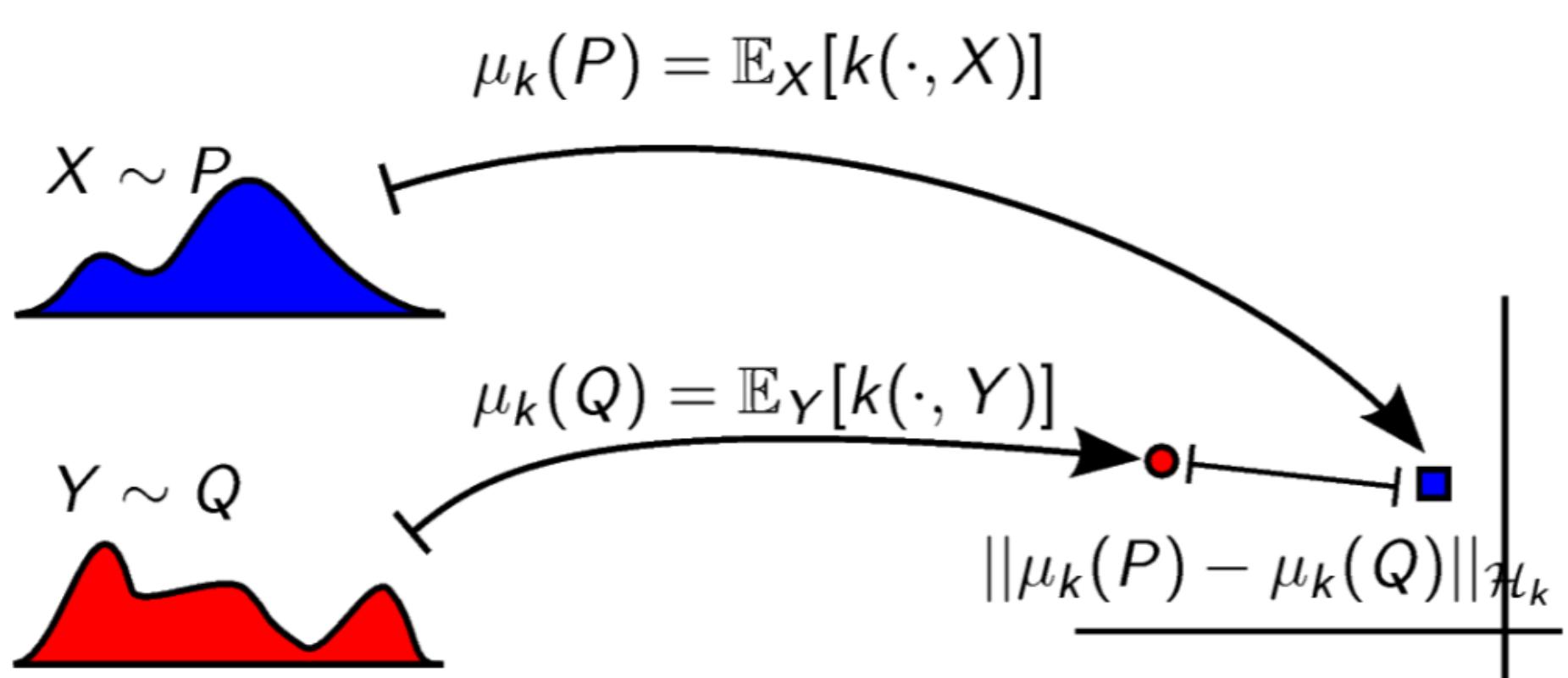


Fig. 1: Kernel mean embedding [6]

With $K = k_{\mathcal{X}} \otimes k_{\mathcal{Y}}$, the Hilbert Schmidt Independence Criterion (HSIC) is given by:

$$\begin{aligned} \text{HSIC}_{k_{\mathcal{X}}, k_{\mathcal{Y}}}(X, Y) &= \| \mu_K(X, Y) - \mu_{k_{\mathcal{X}}}(X) \otimes \mu_{k_{\mathcal{Y}}}(Y) \|_{\mathcal{H}_K}^2 \\ &= \mathbb{E}[k_{\mathcal{X}}(X, X') k_{\mathcal{Y}}(Y, Y')] \\ &\quad + \mathbb{E}[k_{\mathcal{X}}(X, X')] \mathbb{E}[k_{\mathcal{Y}}(Y, Y') | Y] \\ &\quad - 2 \mathbb{E}[k_{\mathcal{X}}(X, X') | X] \mathbb{E}[k_{\mathcal{Y}}(Y, Y') | Y]. \end{aligned}$$

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

$$\text{HSIC}_{k_{\mathcal{X}}, k_{\mathcal{Y}}}(X, Y) = 0 \text{ iff } X \perp Y.$$

→ **screening**

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

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

HSIC-ANOVA indices [3] are then defined as:

$$\begin{aligned} S_i^{\text{HSIC}} &:= \frac{\text{HSIC}(X_i, Y)}{\text{HSIC}(\mathbf{X}, Y)}, \\ S_{T_i}^{\text{HSIC}} &:= 1 - \frac{\text{HSIC}(\mathbf{X}_{-i}, Y)}{\text{HSIC}(\mathbf{X}, Y)} \end{aligned}$$

and are suited for **ranking** (and screening [5]).

HSIC for set-valued outputs

With $A \Delta B = A \cup B - B \cap A$ and μ the Lebesgue measure, we define a kernel on closed sets by:

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

Proposition 1
 k_{set} is a kernel [1] and is characteristic.

Given an input U_l and an associated ANOVA kernel k_l , the HSIC on sets that we call H_{set} is defined by:

$$\begin{aligned} H_{set}(U_l, \Gamma) &:= \text{HSIC}_{k_l, k_{set}}(U_l, \Gamma) \\ &= \mathbb{E}[(k_l(U_l, U_l') - 1) k_{set}(\Gamma, \Gamma')]. \end{aligned}$$

It can be estimated with its U-statistic:

$$\widehat{H}_{set}(U_l, \Gamma) = \frac{2}{n(n-1)} \sum_{i < j}^n \left(k_l(U_l^{(i)}, U_l^{(j)}) - 1 \right) k_{set}(\Gamma^{(i)}, \Gamma^{(j)}).$$

k_{set} is rarely exactly known and requires to be estimated. Given $X^{(1)}, \dots, X^{(m)}$ an iid sample of $X \sim \mathcal{U}(\mathcal{X})$, we propose the estimator:

$$\widehat{k}_{set}(\Gamma^{(i)}, \Gamma^{(j)}) = e^{-\frac{\mu(\mathcal{X})}{2\sigma^2} \frac{1}{m} \sum_{k=1}^m \mathbb{1}_{\Gamma^{(i)} \Delta \Gamma^{(j)}}(X^{(k)})},$$

leading finally to the **nested** H_{set} estimator:

$$\widehat{\widehat{H}}_{set}(U_l, \Gamma) = \frac{2}{n(n-1)} \sum_{i < j}^n \left(k_l(U_l^{(i)}, U_l^{(j)}) - 1 \right) e^{-\frac{\mu(\mathcal{X})}{2\sigma^2} \frac{1}{m} \sum_{k=1}^m \mathbb{1}_{\Gamma^{(i)} \Delta \Gamma^{(j)}}(X^{(k)})}.$$

Proposition 2

The quadratic risk of the nested estimator $\widehat{\widehat{H}}_{set}$ verifies:

$$\mathbb{E} \left(\widehat{\widehat{H}}_{set}(U_l, \Gamma) - H_{set}(U_l, \Gamma) \right)^2 \leq 2 \left(\frac{2\sigma_1^2}{n(n-1)} + \frac{4(n-2)\sigma_2^2}{n(n-1)} + \frac{K^2\sigma_3^2}{m} \right).$$

HSIC-ANOVA indices on sets are then denoted $S_i^{\widehat{\widehat{H}}_{set}}$ and $S_{T_i}^{\widehat{\widehat{H}}_{set}}$.

Toy case 1 [4]

$$\forall x, u \in [-5, 5]^2 \times [-5, 5]^3 \quad g_1(x_1, x_2, u_1, u_2, u_3) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

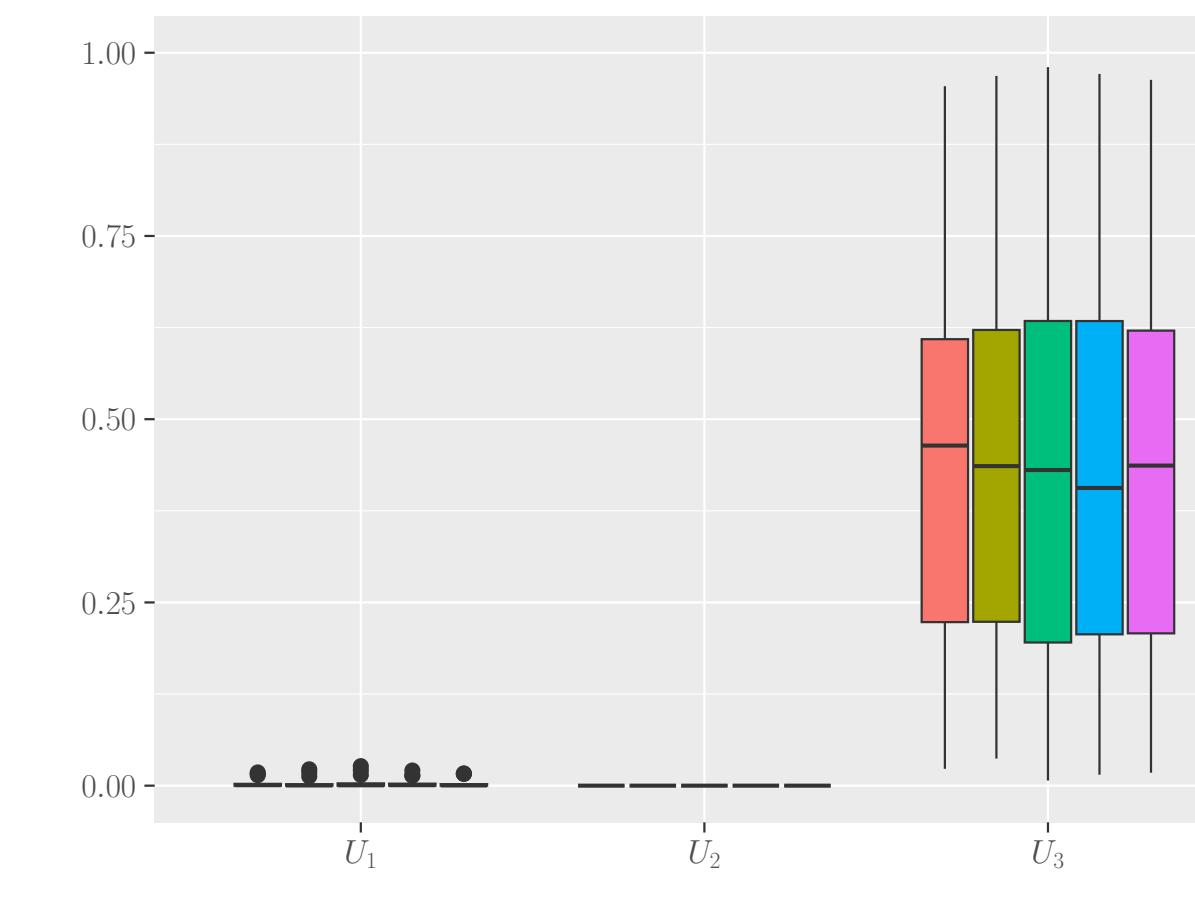


Fig. 2: p-value of \widehat{H}_{set} for $n = m = 100$

Fig. 3: $S_{T_i}^{\widehat{\widehat{H}}_{set}}$ for $n = m = 100$

Toy case 2 [2]

$$g_2(x_1, x_2, u_1, u_2, u_p, u_{r1}, u_{r2}) = u_{r2} - \max_{t \in [0, T]} \mathcal{Y}(x_1 + u_1, x_2 + u_2, u_p; t),$$

with $\mathcal{Y}(x_1 + u_1, x_2 + u_2, u_p; t)$ the solution of the harmonic oscillator defined by:

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

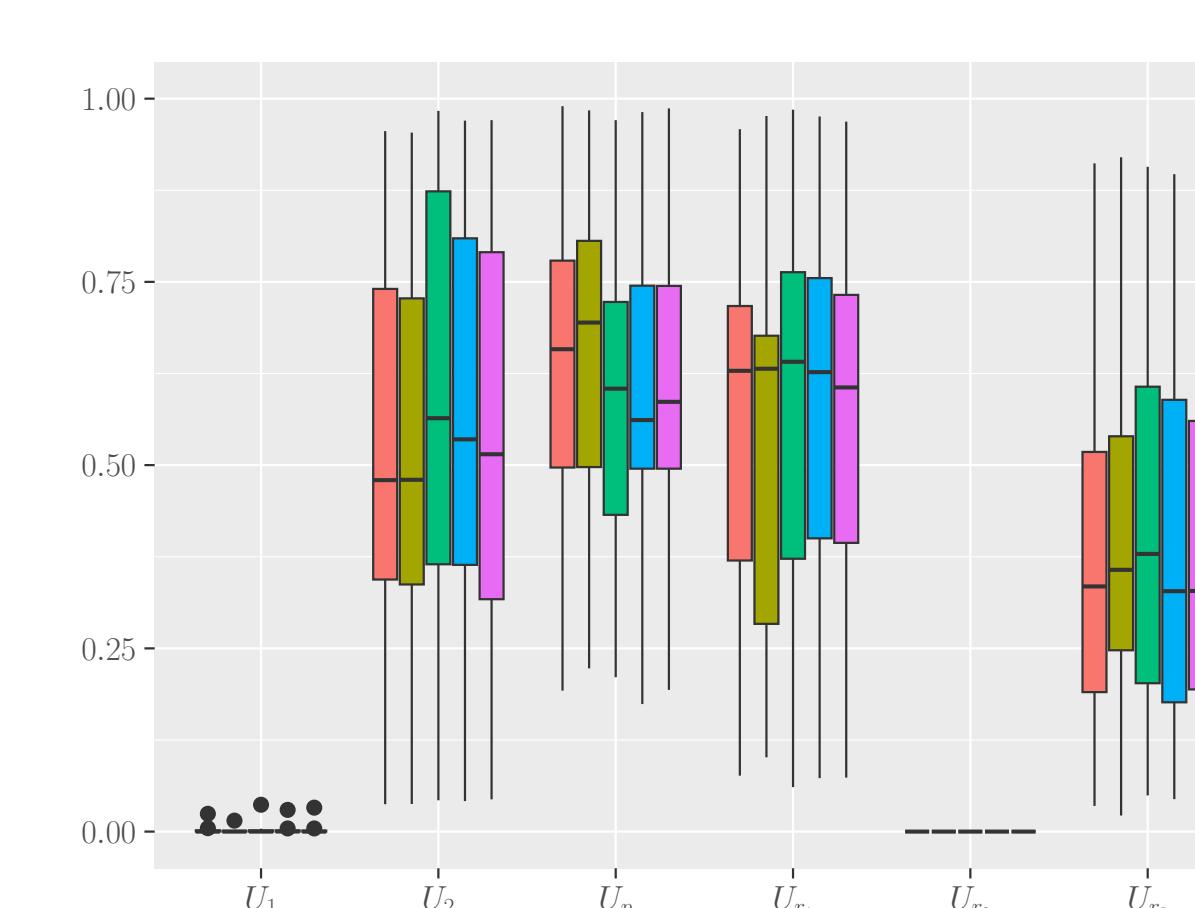


Fig. 4: p-value of \widehat{H}_{set} for $n = m = 100$

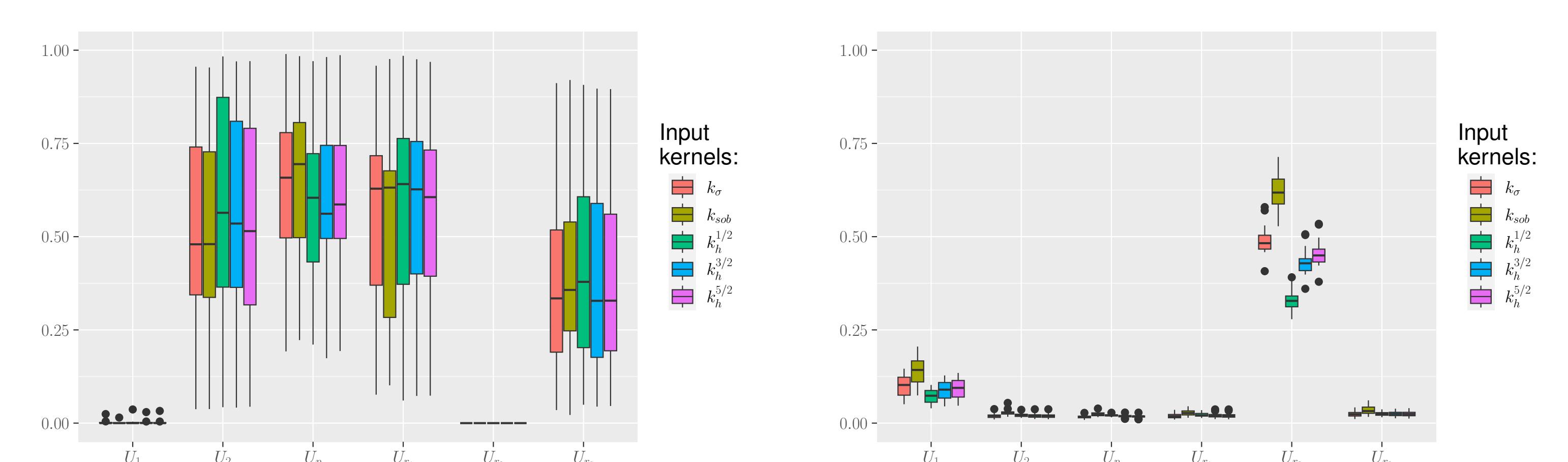


Fig. 5: $S_i^{\widehat{\widehat{H}}_{set}}$ for $n = m = 100$

Outlook

► Testing the indices on **industrial applications** (as viability kernels, or air pollutant concentration maps) and compared to other indices defined for set-valued output models.

► Incorporating this method inside a **robust optimization** methodology: reducing the uncertain input space dimension to get cheaper meta-models.

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