Towards more interpretable kernel-based sensitivity analysis

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SAMOURAI Final Workshop – Work Package 1

December 10-11, 2024, at Institut Henri Poincaré, Paris.

0. Introduction

GSA in support to metamodel construction

- In all four work packages, there is a need to construct **metamodels** for **high-dimensional design problems**.
  - Let $\boldsymbol{X} := [X_1, \dots, X_d]$ be a random vector with **independent** components ($d \approx 100$).
  - Let $Y := g(\boldsymbol{X})$ where $g: \mathcal{X}_1 \times \dots \times \mathcal{X}_d \to \mathcal{Y}$ is a **computationally-expensive** simulation code.
  - $\boldsymbol{Z} = (\boldsymbol{X}, Y)$ is the **augmented vector** containing the input and output variables.

⚠ **The design of experiments (DoE) consists of a number of input-output observations.**

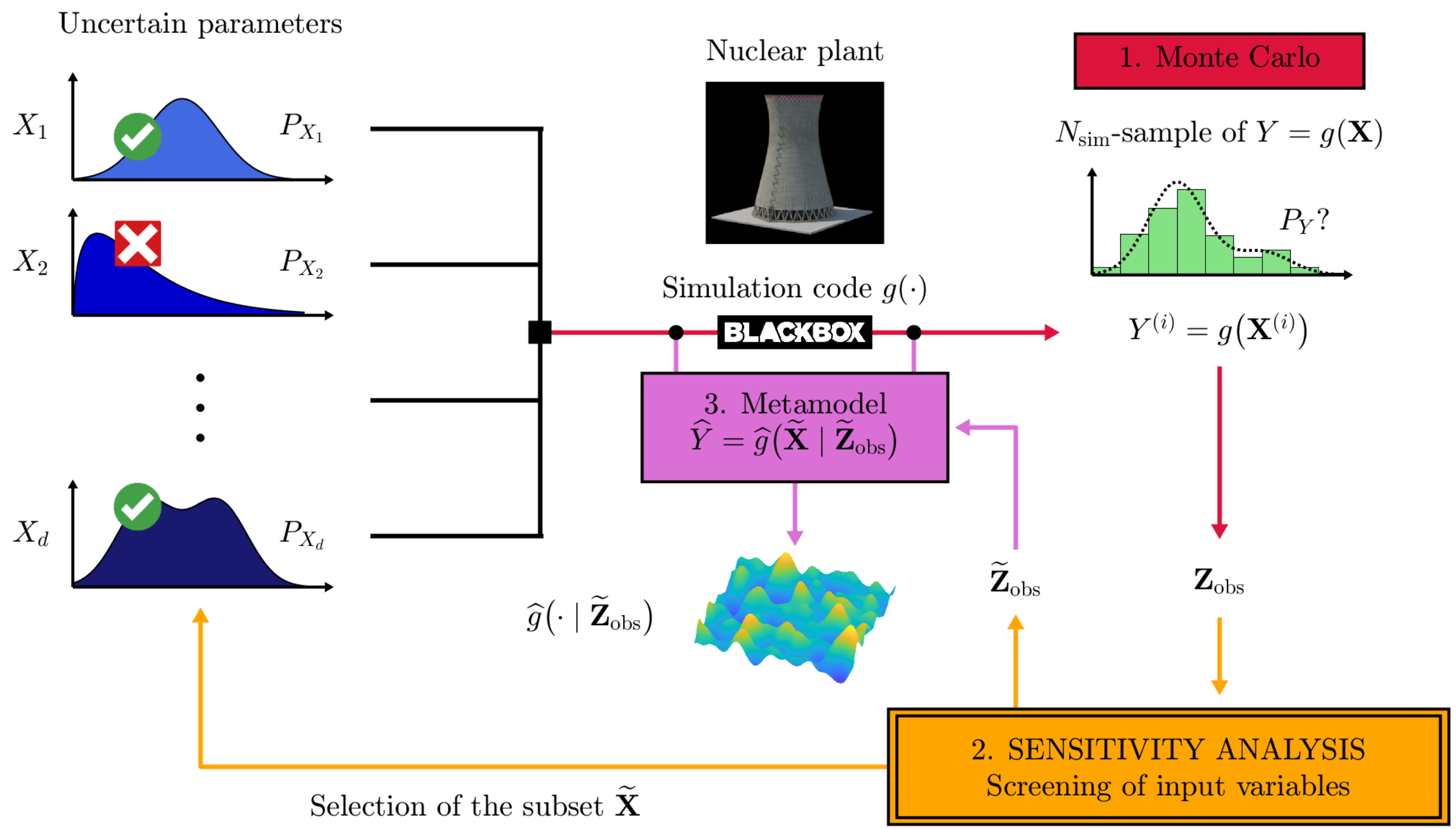
- The metamodel $\hat{g}$ is constructed from $\boldsymbol{Z}_{\text{obs}} := \left\{\left(\boldsymbol{X}^{(i)}, Y^{(i)}\right)\right\}_{1 \le i \le N_{\text{sim}}}$ with $N_{\text{sim}} \le 10d$ → **SMALL DATA**.
- For a nice coverage of the input domain of variation, the DoE must be space-filling → **GIVEN DATA**.

⚠ Classical metamodeling techniques (such as **GP regression**) cannot be used directly.
Curse of dimensionality → too many **GP hyperparameters** have to be optimized!

Many existing strategies (screening, additive and ANOVA models, linear and nonlinear embeddings).
→ Binois & Wycoff (2022) for a comprehensive review.

Focus on **SCREENING** → preliminary GSA for **variable selection** (and thus **dimension reduction**).

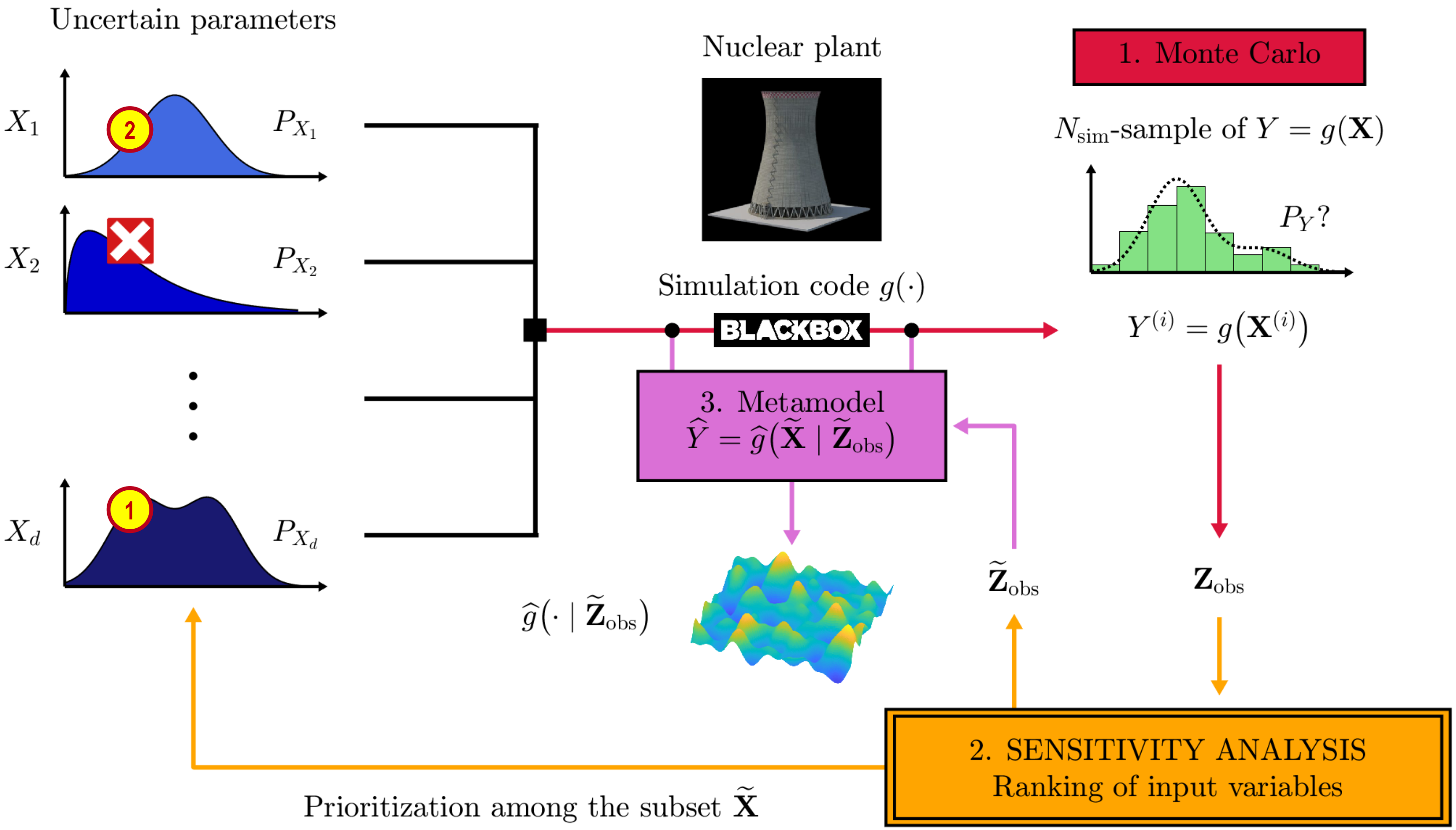
GSA in support to metamodel construction



- **Steps 2 and 3 of the ICSCREAM methodology** → Iooss & Marrel (2019) or Marrel *et al.* (2020)
  - ✓ **Identification of penalizing Configurations using SCREening And Metamodel**

- Performing a **preliminary GSA** has **two main advantages**.
  - **Screening-oriented GSA** → (crude) **dimension reduction** by discarding non-influential input variables.

GSA in support to metamodel construction



- ➢ **Steps 2 and 3 of the ICSCREAM methodology** → Iooss & Marrel (2019) or Marrel *et al.* (2020)
  - ✓ **Identification of penalizing Configurations using SCREening And Metamodel**
- ➢ Performing a **preliminary GSA** has **two main advantages**.
  - ▪ **Screening-oriented GSA** → (crude) **dimension reduction** by discarding non-influential input variables.
  - ▪ **Ranking-oriented GSA** → **sequential building process** of the GP metamodel.

Summary

1. A few concepts related to **kernels**
2. Sensitivity measures based on the **HSIC**
3. A bridge between two opposite worlds: **HSIC-ANOVA indices**
4. Is it relevant to talk about **interactions** for HSIC-ANOVA indices?
5. More about **Sobolev kernels** and their properties
6. Does all this benefit independence testing?

1. A few concepts related to kernels

Fundamentals of reproducing kernel theory

1 Kernel mean embeddings → Muandet *et al.* (2017)

→ Let $\mathcal{M}_1^+(\mathcal{Z})$ be the space of all probability measures defined on $\mathcal{Z} \subseteq \mathbb{R}^p$.
→ Let $K: \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ be a kernel and let $\mathcal{H}$ be the induced RKHS.

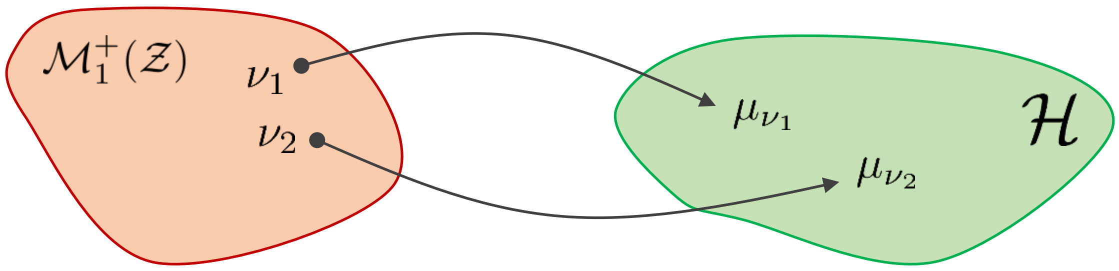
➢ Any probability measure $\nu \in \mathcal{M}_1^+(\mathcal{Z})$ can be represented by a (well-defined) function $\mu_\nu \in \mathcal{H}$.

$$\begin{aligned} \mu_\nu : \ & \mathcal{Z} \longrightarrow \mathbb{R} \\ & z \longmapsto \mu_\nu(z) = \mathbb{E}_\nu\left[K(z, Z)\right] = \int_{\mathcal{Z}} K(z,\zeta)\,\mathrm{d}\nu(\zeta) \end{aligned}$$

Assumptions

- K must be measurable
- $\mathbb{E}_\nu\left[\sqrt{K(Z,Z)}\right] < \infty$

➢ K is said to be a **characteristic kernel** if the map $\nu \mapsto \mu_\nu$ is **injective**.



Space of all probability distributions

RKHS

➢ The **dissimilarity** between ν_1 and ν_2 can be measured through the **distance** in $\mathcal{H}$ between μ_{ν_1} and μ_{ν_2}.
  ✓ Definition of a **kernel-based dissimilarity measure** on $\mathcal{M}_1^+(\mathcal{Z})$.

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2 Maximum Mean Discrepancy (MMD) → Gretton *et al.* (2006)

$$\begin{aligned} \mathrm{MMD}^2(\nu_1,\nu_2) &= \|\mu_{\nu_1} - \mu_{\nu_2}\|_{\mathcal{H}}^2 \\ &= \mathbb{E}_{\nu_1\otimes\nu_1}\left[K(Z,Z')\right] + \mathbb{E}_{\nu_2\otimes\nu_2}\left[K(Z,Z')\right] - 2\,\mathbb{E}_{\nu_1\otimes\nu_2}\left[K(Z,Z')\right] \end{aligned}$$

✓ **Definition resulting from the embedding mechanism**

✓ **Alternative formula paving the way to a simple estimation procedure**

Fundamentals of reproducing kernel theory

3 Feature maps → **Chapter 4** in Steinwart & Christmann (2008)

→ Let $K: \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ be a kernel and let $\mathcal{H}$ be the induced RKHS.

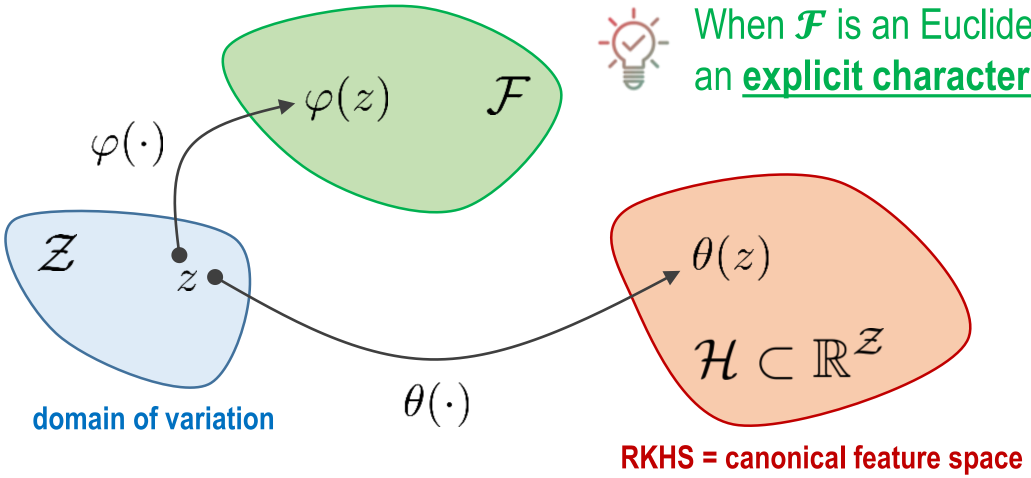
➢ Let us assume that there exist a **Hilbert space** $\mathcal{F}$ and a **map** $\varphi: \mathcal{Z} \to \mathcal{F}$ such that:

$$\forall z, z' \in \mathcal{Z},\ K(z, z') = \langle \varphi(z), \varphi(z') \rangle_{\mathcal{F}}$$

$\mathcal{F}$ is called a **feature space**. φ is called a **feature map**. Any object $\varphi(z)$ is called a **feature function**.

➢ Existence of at least one feature map.
  - ✓ The **canonical feature map** $\theta : \mathcal{Z} \to \mathcal{H}$ is thus defined by $\theta(z) := K(\cdot, z)$ for any $z \in \mathcal{Z}$.

➢ Non-unicity of the feature map.
  - ✓ There may exist a feature space where the kernel action is **much easier to understand**.



When $\mathcal{F}$ is an Euclidean space or a sequence space, an explicit characterization of the RKHS can be derived.

⚠ Most often, $\theta(\cdot)$ is **NOT informative!**

Fundamentals of reproducing kernel theory

4 Feature-based characterization of the RKHS → **Chapter 4** in Steinwart & Christmann (2008)

First, let us examine **two particular kernels!**

Example 1

- The **polynomial kernel** with position parameter $c \geq 0$ and exponent $m \in \mathbb{N}^*$.

initial definition

$$K_{\text{poly}}(x, x') := (xx' + c)^m = \sum_{k=0}^{m} \binom{m}{k} x^k (x')^k c^{m-k}$$

$$= \langle \varphi_{\text{poly}}(x), \varphi_{\text{poly}}(x') \rangle_{\mathbb{R}^{m+1}} \quad \text{with} \quad \varphi_{\text{poly}}(x) = \left[(\sqrt{c})^{m-k} \sqrt{\binom{m}{k}} x^k \right]_{0 \leq k \leq m}$$

finite number of polynomial features

✓ The **binomial theorem** reveals a feature map φ_{poly} from $\mathbb{R}$ to the **Euclidean** space $\mathbb{R}^{m+1}$.

Fundamentals of reproducing kernel theory

4 **Feature-based characterization of the RKHS** → **Chapter 4** in Steinwart & Christmann (2008)

First, let us examine **two particular kernels!**

Example 2 ➢ The **Gaussian kernel** with scale parameter $\gamma > 0$.

initial definition

$$K_\gamma(x,x') := e^{-\frac{1}{2}\left(\frac{x-x'}{\gamma}\right)^2} = e^{-\frac{1}{2}\left(\frac{x}{\gamma}\right)^2} e^{-\frac{1}{2}\left(\frac{x'}{\gamma}\right)^2} \sum_{k=0}^{\infty} \frac{1}{k!}\left(\frac{x}{\gamma}\right)^k \left(\frac{x'}{\gamma}\right)^k$$

$$= \langle \varphi_\gamma(x), \varphi_\gamma(x') \rangle_{\ell^2} \quad \text{with} \quad \varphi_\gamma(x) := e^{-\frac{1}{2}\left(\frac{x}{\gamma}\right)^2} \left[\frac{1}{\sqrt{k}}\left(\frac{x}{\gamma}\right)^k\right]_{k \geq 0}$$

infinite number of damped polynomial features

✓ The **Taylor series expansion** reveals a feature map φ_γ from $\mathbb{R}$ into the **Hilbert** space $\ell^2(\mathbb{N})$.

Fundamentals of reproducing kernel theory

4 Feature-based characterization of the RKHS → **Chapter 4** in Steinwart & Christmann (2008)

- As shown in these two examples, a **kernel expansion** allows to identify a **feature map.**
  - ✓ More importantly, it provides **all-in-one characterization** of the RKHS.

→ Let $K: \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$ be a kernel and let $\mathcal{H}$ be the induced RKHS.

- It is assumed that it can be expanded as a sum (or series) of **symmetric** and **separable** functions.

$$\forall\, z, z' \in \mathcal{Z}, \quad K(z, z') = \sum_{i \in I} g_i(z)\, g_i(z')$$

Polynomial kernel → $I = \{0, \dots, m\}$

Gaussian kernel → $I = \mathbb{N}$

✓ The functions $(g_i)_{i \in I}$ are the **features**. They must be **linearly independent** (in the ℓ^2-sense).

❶ $$\mathcal{H} = \left\{ h \in \mathbb{R}^{\mathcal{Z}} \;\middle|\; h(\cdot) = \sum_{i \in I} a_i\, g_i(\cdot) \;\text{ with }\; (a_i)_{i \in I} \in \ell^2(I, \mathbb{R}) \right\}$$

❷ $$\begin{array}{llcll} \langle \cdot, \cdot \rangle_{\mathcal{H}} : & \mathcal{H} & \times & \mathcal{H} & \longrightarrow \mathbb{R} \\ & \Big(h_1(\cdot) = \sum_{i \in I} a_i\, g_i(\cdot) & , & h_2(\cdot) = \sum_{i \in I} b_i\, g_i(\cdot) \Big) & \longmapsto \sum_{i \in I} a_i\, b_i \end{array}$$

❸ The functions $(g_i)_{i \in I}$ form an **orthonormal basis (ONB)** of $\mathcal{H}$.

2. Sensitivity measures based on the HSIC

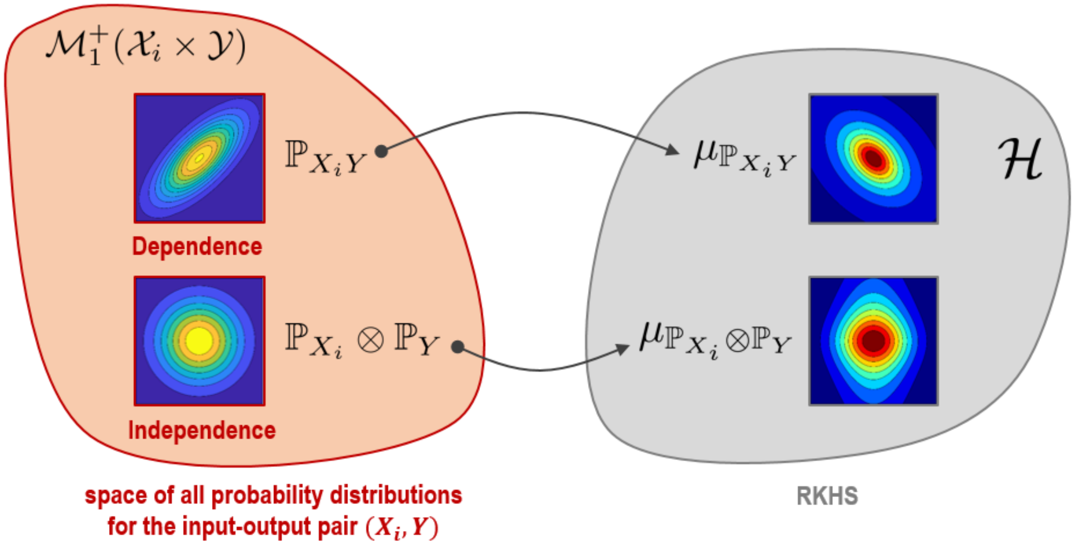
Several views on HSIC indices

1 Kernel-based dependences measures → Da Veiga (2015)

- $\mathbb{P}_{X_iY}$ → Joint distribution of (X_i, Y) → True influence of X_i on Y
- $\mathbb{P}_{X_i}\otimes\mathbb{P}_Y$ → Independence within (X_i, Y) → Hypothetical lack of influence

$$S_i^{\Delta} := \Delta\left(\mathbb{P}_{X_iY}, \mathbb{P}_{X_i} \otimes \mathbb{P}_Y\right)$$

How to measure the discrepancy?
What about using the MMD?



- $K_i : \mathcal{X}_i \times \mathcal{X}_i \to \mathbb{R}$ assigned to X_i
- $K_Y : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ assigned to Y
- $K_i \otimes K_Y$ used to handle (X_i, Y)
- $\mathcal{H} := \mathcal{H}_i \otimes \mathcal{H}_Y$ induced by $K_i \otimes K_Y$

$$\mathrm{HSIC}(X_i, Y) := \mathrm{MMD}^2\left(\mathbb{P}_{X_iY}, \mathbb{P}_{X_i} \otimes \mathbb{P}_Y\right) = \left\|\mu_{\mathbb{P}_{X_iY}} - \mu_{\mathbb{P}_{X_i}\otimes\mathbb{P}_Y}\right\|_{\mathcal{H}}^2$$

How to estimate HSIC indices from a given dataset?

Several views on HSIC indices

2 Efficient estimation → Gretton *et al.* (2005, 2007) and Serfling (2009)

➢ The **alternative formula of the MMD** allows to rewrite the HSIC only in terms of **kernel-based moments**.

$$\mathrm{HSIC}(X_i,Y) = \mathbb{E}\Big[K_i\left(X_i,X_i'\right)\,K_Y\left(Y,Y'\right)\Big] + \mathbb{E}\Big[K_i\left(X_i,X_i'\right)\,K_Y\left(Y'',Y'''\right)\Big] - 2\,\mathbb{E}\Big[K_i\left(X_i,X_i'\right)\,K_Y\left(Y,Y''\right)\Big]$$

⚠ $(X_i,Y) \perp (X_i',Y') \perp (X_i'',Y'') \perp (X_i''',Y''')$ follow the **joint input-output distribution** $\mathbb{P}_{X_iY}$.

➢ **U-statistics** and **V-statistics** are well-adapted to estimate HSIC indices from a given DoE.

$N_{\mathrm{sim}} = n$

$$\widehat{H}_i^U = \frac{1}{(n)_2}\sum_{1\le p\ne q\le n} K_i\left(X_i^{(p)},X_i^{(q)}\right)K_Y\left(Y^{(p)},Y^{(q)}\right) + \frac{1}{(n)_4}\sum_{1\le p\ne q\ne r\ne s\le n} K_i\left(X_i^{(p)},X_i^{(q)}\right)K_Y\left(Y^{(r)},Y^{(s)}\right) - \frac{2}{(n)_3}\sum_{1\le p\ne q\ne r\le n} K_i\left(X_i^{(p)},X_i^{(q)}\right)K_Y\left(Y^{(p)},Y^{(r)}\right) \quad \text{with} \quad (n)_p = p!\binom{n}{p}$$

- $\widehat{H}_i^U$ denotes the **U-statistic** estimator of $\mathrm{HSIC}(X_i,Y)$ → **no bias** BUT **no guarantee of positivity**.
- $\widehat{H}_i^V$ denotes the **V-statistic** estimator of $\mathrm{HSIC}(X_i,Y)$ → **positivity** BUT **bias**.
- **Consistency** and **existence of a CLT** → convergence at rate $1/\sqrt{n}$.
- **Low computational complexity** → only $\mathcal{O}(n^2)$ operations are required to compute estimates.

Several views on HSIC indices

3 Independence testing → Gretton *et al.* (2007)

→ The input kernel $K_i : \mathcal{X}_i \times \mathcal{X}_i \to \mathbb{R}$ is assumed to be **characteristic** to $\mathcal{M}_1^+(\mathcal{X}_i)$.

→ The output kernel $K_Y : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ is assumed to be **characteristic** to $\mathcal{M}_1^+(\mathcal{Y})$.

$$X_i \perp Y \iff \mathrm{HSIC}(X_i, Y) = 0$$

- **Testing independence** between X_i and Y is equivalent to **testing the nullity** of the HSIC.

$$(H_0) : \mathrm{HSIC}(X_i, Y) = 0 \quad \text{vs.} \quad (H_1) : \mathrm{HSIC}(X_i, Y) > 0$$

- **Test statistic** → either $\widehat{H}_i^U$ or $\widehat{H}_i^V$
- **Test procedure** → selected according to the **sample size** and the chosen **test statistic**
  - ✓ **Asymptotic test procedure** → Sejdinovic *et al.* (2013) and Zhang *et al.* (2018)
  - ✓ **Permutation-based test procedure** → De Lozzo & Marrel (2016)
  - ✓ **Sequential permutation-based test procedure** → El Amri & Marrel (2022)
  - ✓ **Non-asymptotic Gamma test procedure** → El Amri & Marrel (2024)
- **Theoretical guarantees** → control of the **type-I error** + minimization of the **type-II error**
  - ✓ **Type-I error** controlled even when n is small. → Albert *et al.* (2022)
  - ✓ **Type-II error** vanishing asymptotically. → Gretton *et al.* (2007) and Pfister *et al.* (2018)

Sobol' indices vs. HSIC indices

- HSIC indices perfectly meet the needs of **screening-oriented** GSA.
  - ✓ **The use of characteristic kernels allows to detect any type of input-output dependence.**
  - ✓ **Inference is an easy task (no need for specific data, big data or density estimation).**

GSA requirements	S_i	T_i	$\mathrm{HSIC}(X_i, Y)$
ANOVA decomposition → RANKING	✓	✓	✗
Characterize independence → SCREENING	✗	✓	✓
Estimation from GIVEN DATA	✓	✗	✓
Estimation from SMALL DATA	✓	✗	✓
Compatibility with DEPENDENT inputs	✗	✗	✓
INVARIANCE through monotonic transformations	✓	✓	✗

Still room to improve HSIC indices?

- HSIC indices **lack interpretability** and they are not tailored to perform **ranking-oriented** GSA.

⚠ **Sum not equal to 1.** ⚠ **No universal bound.** ⚠ **Different MMD scales.**

GSA requirements	S_i	T_i	$\mathrm{HSIC}(X_i, Y)$
ANOVA decomposition → RANKING	✓	✓	✗
Characterize independence → SCREENING	✗	✓	✓
Estimation from GIVEN DATA	✓	✗	✓
Estimation from SMALL DATA	✓	✗	✓
Compatibility with DEPENDENT inputs	✗	✗	✓
INVARIANCE through monotonic transformations	✓	✓	✗

How to do better on that point?

3. A bridge between two opposite worlds: HSIC-ANOVA indices

Taking inspiration from standard ANOVA…

- **ANOVA decomposition for Sobol' indices** → Sobol' (1993)
  - ✓ The output variance $\mathbb{V}(Y)$ is apportioned between **all subsets of inputs**.

$$\mathbb{V}(Y) = \sum_{\boldsymbol{u} \subseteq \{1,\dots,d\}} V_{\boldsymbol{u}} = \sum_{\boldsymbol{u} \subseteq \{1,\dots,d\}} \sum_{\boldsymbol{v} \subseteq \boldsymbol{u}} (-1)^{|\boldsymbol{u}|-|\boldsymbol{v}|} \mathbb{V}\Big(\mathbb{E}\big[Y \mid X_{\boldsymbol{u}}\big]\Big)$$

⚠ $X_1 \perp \cdots \perp X_d$

- **First-order and total-order Sobol' indices**
  - ✓ **First-order** Sobol' indices $(S_i)_{1 \le i \le d}$ → **main effects** only!
  - ✓ **Total-order** Sobol' indices $(T_i)_{1 \le i \le d}$ → **main effects + interactions**.

$$\forall\, 1 \le i \le d, \quad S_i = \frac{\mathbb{V}(\mathbb{E}[Y \mid X_i])}{\mathbb{V}(Y)} \quad \text{and} \quad T_i = 1 - \frac{\mathbb{V}(\mathbb{E}[Y \mid \boldsymbol{X}_{-i}])}{\mathbb{V}(Y)}$$

- **Constraints imposed on the sub-functions of the Sobol'-Hoeffding decomposition**

$$g(\boldsymbol{x}) = \sum_{\boldsymbol{u} \subseteq \{1,\dots,d\}} \eta_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}}) \quad \text{such that} \quad \forall\, i \in \boldsymbol{u}, \quad \int_{\mathcal{X}_i} \eta_{\boldsymbol{u}}(\boldsymbol{x}_{\boldsymbol{u}})\, \mathrm{d}\mathbb{P}_{X_i}(x_i) = 0$$

… and bringing ANOVA into the HSIC paradigm

- **HISC-ANOVA decomposition** → Da Veiga (2021)
  - ✓ The quantity $\mathrm{HSIC}(\boldsymbol{X}, Y)$ is apportioned between **all subsets of inputs**.

$$\mathrm{HSIC}(\boldsymbol{X}, Y) = \sum_{\boldsymbol{u} \subseteq \{1,\dots,d\}} H_{\boldsymbol{u}} = \sum_{\boldsymbol{u} \subseteq \{1,\dots,d\}} \sum_{\boldsymbol{v} \subseteq \boldsymbol{u}} (-1)^{|\boldsymbol{u}|-|\boldsymbol{v}|} \mathrm{HSIC}(\boldsymbol{X}_{\boldsymbol{v}}, Y)$$

⚠ $X_1 \perp \cdots \perp X_d$

- **First-order and total-order HSIC-ANOVA indices**
  - ✓ **First-order** HSIC-ANOVA indices $\left(S_i^{\mathrm{HSIC}}\right)_{1 \le i \le d}$ → **main effects** only!
  - ✓ **Total-order** HSIC-ANOVA indices $\left(T_i^{\mathrm{HSIC}}\right)_{1 \le i \le d}$ → **main effects + interactions**.

$$\forall\, 1 \le i \le d, \quad S_i^{\mathrm{HSIC}} := \frac{\mathrm{HSIC}(X_i, Y)}{\mathrm{HSIC}(\mathbf{X}, Y)} \quad \text{and} \quad T_i^{\mathrm{HSIC}} := 1 - \frac{\mathrm{HSIC}(\mathbf{X}_{-i}, Y)}{\mathrm{HSIC}(\mathbf{X}, Y)}$$

- **Constraints imposed on the input kernels**
  - ✓ Each input kernel K_i must be an **ANOVA** kernel (≈ a **constant** kernel + an **orthogonal** kernel).

$$K_i(x_i, x_i') = 1 + k_i(x_i, x_i') \quad \text{with} \quad \forall\, x_i \in \mathcal{X}_i, \quad \int_{\mathcal{X}_i} k_i(x_i, x_i')\, \mathrm{d}\mathbb{P}_{X_i}(x_i') = 0$$

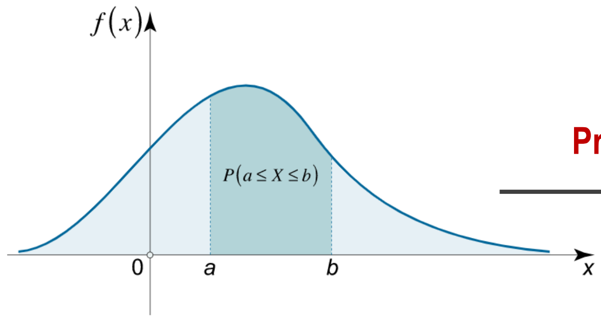
  - ✓ $\boldsymbol{\mathcal{H}}_i = \mathbb{R} \oplus \boldsymbol{\mathcal{G}}_i$ where $\boldsymbol{\mathcal{G}}_i$ is only composed of **zero-mean functions** (with respect to $\mathbb{P}_{X_i}$).

How to find ANOVA kernels?

For most **parametric families of distributions**, there is no well-known **characteristic ANOVA** kernel.

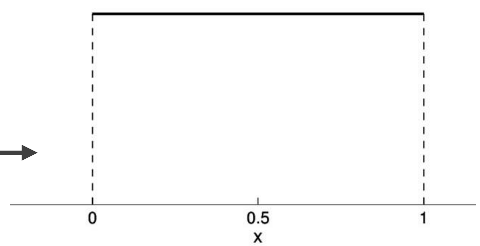
How to implement the HSIC-ANOVA decomposition in practice?

1. Transform each input distribution $\mathbb{P}_{X_i}$ into a standard uniform distribution $\mathcal{U}([0,1])$.



$$U_i = F_{X_i}(X_i)$$

Probability Integral Transform (PIT)



Density of the i-th input variable

Density of the uniform distribution

2. Assign a **Sobolev kernel** K^r_{Sob} to each new input variable $U_i := F_{X_i}(X_i)$.

$$\forall\, u, u' \in [0,1], \quad K^r_{\text{Sob}}(u,u') := 1 + \sum_{i=1}^{r} \frac{B_i(u)\, B_i(u')}{(i!)^2} + \frac{(-1)^{r+1}}{(2r)!} B_{2r}(|u-u'|)$$

- ✓ $r \in \mathbb{N}^*$ is an **integer parameter** indicating the **degree of smoothness** of the RKHS.
- ✓ The functions $(B_i)_{i\geq 1}$ are the **Bernoulli polynomials** → $\int_0^1 B_i(u)\, du = 0$.

A grey area around HSIC-ANOVA indices?

1. How do they measure sensitivity? How to distinguish between main effects and interactions?
2. Are they able to characterize independence?

GSA requirements	T_i	$\mathrm{HSIC}(X_i, Y)$	S_i^{HSIC}	? T_i^{HSIC}
ANOVA decomposition → RANKING	✓	✗	?	?
Characterize independence → SCREENING	✓	✓	? ?	? ?
Estimation from GIVEN DATA	✗	✓	✓	✓
Estimation from SMALL DATA	✗	✓	✓	✓
Compatibility with DEPENDENT inputs	✗	✓	✗	✗
INVARIANCE through monotonic transformations	✓	✗	✗	✗

4. Is it relevant to talk about interactions for HSIC-ANOVA indices?

Focus on HSIC-ANOVA interactions

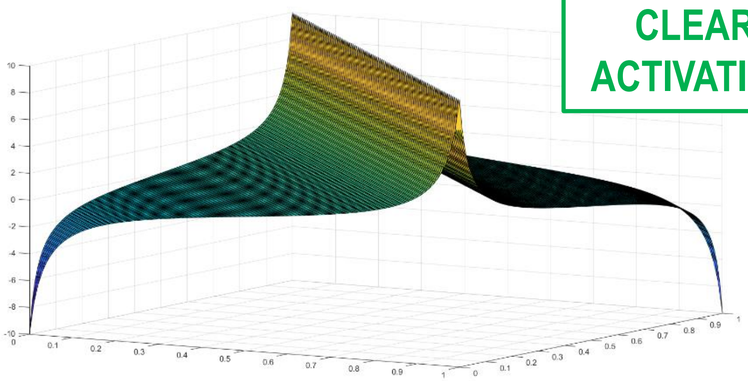
For most benchmark test cases, HSIC-ANOVA interactions are not significant.

Example → the **Ishigami** function

$$Y = g(X_1, X_2, X_3) = \sin(X_1) + \sin^2(X_2) + X_3^4 \sin(X_1) \quad \text{with} \quad X_i \sim \mathcal{U}([-\pi, \pi])$$

- Strong interaction between X_1 and X_3 in the **variance-based ANOVA** framework.
- No interaction between X_1 and X_3 in the **HSIC-ANOVA** framework.

Counterexample → Hand-made **pathological functions** (only for $d \approx 2$)



CLEAR ACTIVATION

Hull function

$$g(x_1, x_2) = -\tan\left[(2\sqrt{2})a\left|\frac{x_1 + x_2 - 1}{\sqrt{2}}\right| - a\right]$$

$$S_1^{\text{HSIC}} = S_2^{\text{HSIC}} = 17\%$$

$$T_1^{\text{HSIC}} = T_2^{\text{HSIC}} = 83\%$$

No clear explanation on why those functions lead to strong HSIC-ANOVA interactions.

The feature-based viewpoint on the HSIC allows to break the deadlock.

A detour through cross-covariance operators

1 HSIC indices → Gretton *et al.* (2005)

- Let $K_i : \mathcal{X}_i \times \mathcal{X}_i \to \mathbb{R}$ be the i-th input kernel (with RKHS denoted by $\mathcal{H}_i$).
- Let $K_Y : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ be the output kernel (with RKHS denoted by $\mathcal{H}_Y$).

➢ The knowledge of $\mathcal{H}_i$ and $\mathcal{H}_Y$ allows to rewrite $\mathrm{HSIC}(X_i, Y)$ as a kind of generalized covariance.

$$\mathrm{HSIC}(X_i, Y) = \sum_k \sum_l \left|\mathrm{Cov}\left(v_{ik}(X_i), w_l(Y)\right)\right|^2 \quad \text{with} \quad \begin{cases} (v_{ik})_k & \text{an ONB of } \mathcal{H}_i \\ (w_l)_l & \text{an ONB of } \mathcal{H}_Y \end{cases}$$

sum of covariances for different patterns **catalogues of transformations**

✓ **Aggregation of covariance terms** obtained after applying sequences of **preliminary basis transformations**.

✓ Each **pair of non-linear functions** $(v_{ik}(\cdot), w_l(\cdot))$ corresponds to a **non-linear dependence pattern**.

Example ➢ **HSIC indices** computed with **Gaussian kernels** → $K_i = K_Y = K_\gamma$

$$K_\gamma(z, z') = e^{-\frac{1}{2}\left(\frac{z-z'}{\gamma}\right)^2} = \sum_{k=0}^{\infty} g_k(z)\, g_k(z') \quad \text{with} \quad g_k(z) \propto e^{-\frac{1}{2}\left(\frac{z}{\gamma}\right)^2} z^k$$

damped polynomial feature

$$\mathrm{HSIC}(X_i, Y) = \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} \left|\mathrm{Cov}\left(g_k(X_i), g_l(Y)\right)\right|^2$$

✅ **Infinitely many damped polynomial transformations are applied to both X_i and Y.**

A detour through cross-covariance operators

2 HSIC-ANOVA indices

$$S_1^{\text{HSIC}} + S_2^{\text{HSIC}} + \Delta_{12}^{\text{HSIC}} = 1$$

- For the sake of clarity, it is assumed that $d = 2$.
  - ✓ **No loss of generality. Everything remains true in higher dimension!**

A detour through cross-covariance operators

2 HSIC-ANOVA indices

$$S_1^{\mathrm{HSIC}} + S_2^{\mathrm{HSIC}} + \Delta_{12}^{\mathrm{HSIC}} = 1$$

$$S_1^{\mathrm{HSIC}} \propto \sum_i \sum_k \left|\mathrm{Cov}\left(u_{1i}(X_1), w_k(Y)\right)\right|^2$$

with

$$\begin{cases} (u_{1i})_i & \text{an ONB of } \mathcal{G}_1 \\ (w_k)_k & \text{an ONB of } \mathcal{H}_Y \end{cases}$$

dependence patterns captured by k_1 and K_Y

$$\Delta_{12}^{\mathrm{HSIC}} \propto \sum_i \sum_j \sum_k \left|\mathrm{Cov}\left(u_{1i}(X_1)\, u_{2j}(X_2), w_k(Y)\right)\right|^2$$

with

$$\begin{cases} (u_{1i})_i & \text{an ONB of } \mathcal{G}_1 \\ (u_{2j})_j & \text{an ONB of } \mathcal{G}_2 \\ (w_k)_k & \text{an ONB of } \mathcal{H}_Y \end{cases}$$

dependence patterns captured by $k_1 \otimes k_2$ and K_Y

A detour through cross-covariance operators

2 HSIC-ANOVA indices

$$S_1^{\mathrm{HSIC}} + S_2^{\mathrm{HSIC}} + \Delta_{12}^{\mathrm{HSIC}} = 1$$

$$S_1^{\mathrm{HSIC}} \propto \sum_i \sum_k \left|\mathrm{Cov}\left(u_{1i}(X_1), w_k(Y)\right)\right|^2$$

with $\begin{cases} (u_{1i})_i & \text{an ONB of } \mathcal{G}_1 \\ (w_k)_k & \text{an ONB of } \mathcal{H}_Y \end{cases}$?

dependence patterns captured by k_1 and K_Y

$$\Delta_{12}^{\mathrm{HSIC}} \propto \sum_i \sum_j \sum_k \left|\mathrm{Cov}\left(u_{1i}(X_1)\, u_{2j}(X_2), w_k(Y)\right)\right|^2$$

with $\begin{cases} (u_{1i})_i & \text{an ONB of } \mathcal{G}_1 \\ (u_{2j})_j & \text{an ONB of } \mathcal{G}_2 \\ (w_k)_k & \text{an ONB of } \mathcal{H}_Y \end{cases}$?

dependence patterns captured by $k_1 \otimes k_2$ and K_Y

- Remember the **simplest solution** to compute HSIC-ANOVA indices.
  - ✓ **Uniform inputs** → $U_1 \perp U_2 \sim \mathcal{U}([0,1])$
  - ✓ **Sobolev kernels for the inputs** → $K_1 = K_2 = K_{\mathrm{Sob}}^r$
  - ✓ **Gaussian kernel for the output** → $K_Y = K_\gamma$

$$\forall\, u, u' \in [0,1], \quad K_{\mathrm{Sob}}^r(u,u') := 1 + \sum_{k=1}^{r} \frac{B_k(u)\,B_k(u')}{(k!)^2} + \frac{(-1)^{r+1}}{(2r)!} B_{2r}\left(|u-u'|\right)$$

🤔 **What are the basis functions in the case of Sobolev kernels?**

5. More about Sobolev kernels and their properties

Sobolev kernels and their feature maps

Many questions at the beginning of this work…

1. What is the RKHS $\mathcal{H}^r_{\mathrm{Sob}}$ induced by K^r_{Sob}?
2. Is K^r_{Sob} a characteristic kernel?
3. Is there an explicit and easily interpretable feature map $\varphi^r_{\mathrm{Sob}} : [0,1] \to \mathcal{F}^r_{\mathrm{Sob}}$?
4. How to identify an ONB of $\mathcal{H}^r_{\mathrm{Sob}}$? Is there a link with feature maps?
5. How to choose r in practice?

Sobolev kernels and their feature maps

Many questions at the beginning of this work…

1. What is the RKHS $\mathcal{H}^r_{\text{Sob}}$ induced by K^r_{Sob}? → see Gu (2013) or Kuo *et al.* (2010)

- **A standard function space:** the Sobolev space of order r defined on $[0,1]$ for the L^2-norm.

$$H^r([0,1]) := \left\{ h \in \mathbb{R}^{[0,1]} \,\middle|\, \forall 0 \le k \le r, \quad D^k h \in L^2([0,1]) \right\}$$

- **A specific inner product:**

$$\langle f, g \rangle_{\mathcal{H}^r_{\text{Sob}}} := \sum_{k=0}^{r-1} \left(\int_0^1 D^k f(x)\,\mathrm{d}x \right) \left(\int_0^1 D^k g(x)\,\mathrm{d}x \right) + \int_0^1 D^r f(x)\, D^r g(x)\,\mathrm{d}x$$

Sobolev kernels and their feature maps

Many questions at the beginning of this work…

1. What is the RKHS $\mathcal{H}^r_{\mathrm{Sob}}$ induced by K^r_{Sob}?

2. Is K^r_{Sob} a characteristic kernel?

- **YES!** Simply because $H^r([0,1])$ is **uniformly dense** in $C([0,1])$.

- **Major consequence**
  - ✓ The **HSIC-ANOVA indices** based on **Sobolev kernels** are able to characterize independence.

$$X_i \perp Y \iff S_i^{\mathrm{HSIC}} = 0 \iff T_i^{\mathrm{HSIC}} = 0$$

⚠ This is different from what happens for **Sobol' indices**.

$$S_i = 0 \not\Longrightarrow X_i \perp Y \quad \text{while} \quad X_i \perp Y \iff T_i = 0$$

Sobolev kernels and their feature maps

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2. Is K^r_{Sob} a characteristic kernel?
3. Is there an explicit and easily interpretable feature map $\varphi^r_{\text{Sob}} : [0,1] \to \mathcal{F}^r_{\text{Sob}}$?

$$K^r_{\text{Sob}}(x,x') = \left\langle \varphi^r_{\text{Sob}}(x), \varphi^r_{\text{Sob}}(x') \right\rangle_{\mathcal{F}^r_{\text{Sob}}}$$

- For $r = 1$, the **Mercer expansion** of K^1_{Sob} is actually known. → Dick *et al.* (2014, 2015)

$$K^1_{\text{Sob}}(x,x') := 1 + \sum_{k=1}^{\infty} \frac{1}{(k\pi)^2} c_k(x)\, c_k(x') \quad \text{with} \quad c_k(x) := \sqrt{2}\cos(k\pi x)$$

- For $r \geq 2$, a **series expansion** of K^r_{Sob} is also mentioned in the literature. → Baldeaux *et al.* (2009)

$$K^r_{\text{Sob}}(x,x') := 1 + \sum_{k=1}^{r} \frac{B_k(x)\, B_k(x')}{(k!)^2} + \sum_{k=1}^{\infty} \frac{1}{(2k\pi)^{2r}} \left[c_{2k}(x)\, c_{2k}(x') + s_{2k}(x)\, s_{2k}(x') \right] \quad \text{with} \quad \begin{cases} c_{2k}(x) := \sqrt{2}\cos(2k\pi x) \\ s_{2k}(x) := \sqrt{2}\sin(2k\pi x) \end{cases}$$

Sobolev kernels and their feature maps

🤔 Many questions at the beginning of this work…

1. What is the RKHS $\mathcal{H}^r_{\text{Sob}}$ induced by K^r_{Sob}?
2. Is K^r_{Sob} a characteristic kernel?
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4. How to identify an ONB of $\mathcal{H}^r_{\text{Sob}}$? Is there a link with feature maps?

- **Mercer expansion** of K^1_{Sob} → $$K^1_{\text{Sob}}(x,x') := 1 + \sum_{k=1}^{\infty} \frac{1}{(k\pi)^2} c_k(x)\, c_k(x')$$
- **ONB** of the **RKHS** $\mathcal{H}^1_{\text{Sob}}$ → $$\left\{ 1 ; \left(\frac{c_k(\cdot)}{k\pi} \right)_{k \geq 1} \right\}$$
- **Series expansion** of K^r_{Sob} → $$K^r_{\text{Sob}}(x,x') := 1 + \sum_{k=1}^{r} \frac{B_k(x)\, B_k(x')}{(k!)^2} + \sum_{k=1}^{\infty} \frac{1}{(2k\pi)^{2r}} \left[c_{2k}(x)\, c_{2k}(x') + s_{2k}(x)\, s_{2k}(x') \right]$$
- **ONB** of the **RKHS** $\mathcal{H}^r_{\text{Sob}}$ → $$\left\{ 1 ; \left(\frac{B_k(\cdot)}{k!} \right)_{1 \leq k \leq r} ; \left(\frac{c_{2k}(\cdot)}{(2k\pi)^r} \right)_{k \geq 1} ; \left(\frac{s_{2k}(\cdot)}{(2k\pi)^r} \right)_{k \geq 1} \right\}$$

Sobolev kernels and their feature maps

Many questions at the beginning of this work…

1. What is the RKHS $\mathcal{H}^r_{\text{Sob}}$ induced by K^r_{Sob}?
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4. How to identify an ONB of $\mathcal{H}^r_{\text{Sob}}$? Is there a link with feature maps?
5. How to choose r in practice?

- Taking $r = 1$ is recommended!
- For $r \geq 2$, $K^r_{\text{Sob}}(x, x') \approx 1 + k_{\text{lin}}(x, x')$ → **poor numerical performance** for screening!

Sobolev kernels and their feature maps

Many questions at the beginning of this work…

1. What is the RKHS $\mathcal{H}^r_{\text{Sob}}$ induced by K^r_{Sob}?
2. Is K^r_{Sob} a characteristic kernel?
3. Is there an explicit and easily interpretable feature map $\varphi^r_{\text{Sob}} : [0,1] \to \mathcal{F}^r_{\text{Sob}}$?
4. How to identify an ONB of $\mathcal{H}^r_{\text{Sob}}$? Is there a link with feature maps?
5. How to choose r in practice?

What is the point of these theoretical results?

- Remember the pure interaction term $\Delta^{\text{HSIC}}_{12}$.
- Apply with $K_1 = K_2 = K^1_{\text{Sob}}$ now that an ONB of $\mathcal{H}^1_{\text{Sob}}$ is explicitly known.

$$\Delta^{\text{HSIC}}_{12} \propto \sum_i \sum_j \sum_k \left|\text{Cov}\big(u_{1i}(X_1)\, u_{2j}(X_2), w_k(Y)\big)\right|^2 = \boxed{\sum_i^{\infty} \sum_j^{\infty} \sum_k \frac{1}{ij\,\pi^2} \left|\text{Cov}\big(c_i(X_1)\, c_j(X_2), w_k(Y)\big)\right|^2}$$

✓ **This provides the hint to design a toy case.**

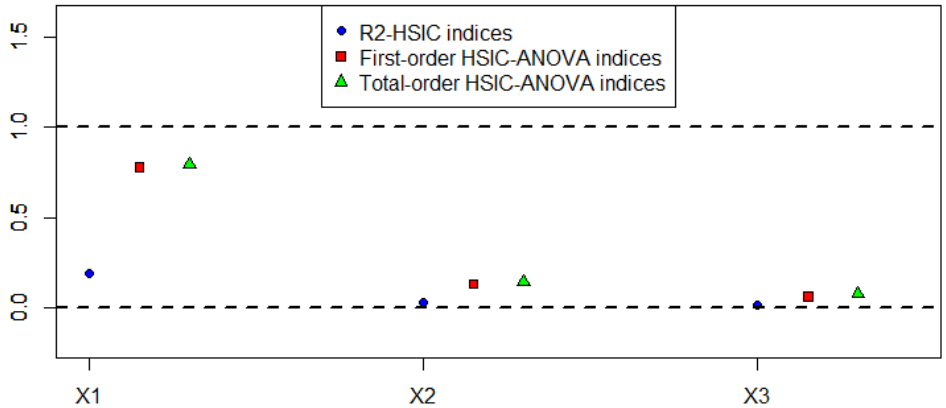
How to exacerbate HSIC-ANOVA interactions?

- Back to the Ishigami function
  - ✓ **Additional term** chosen to boost HSIC-ANOVA interactions.

$$Y = g(U_1, U_2, U_3) = \text{ishigami}(X_1, X_2, X_3) + \boldsymbol{\gamma} \cos(\pi U_1) \cos(\pi U_2) \quad \text{with} \quad \begin{array}{c} U_i \sim \mathcal{U}([0,1]) \\ X_i = \pi(2U_i - 1) \end{array}$$

- Design parameter
  - ✓ $\boldsymbol{\gamma = 0}$

- Estimation of sensitivity measures
  - ✓ Sample size $n = 500$
  - ✓ R^2-HSIC indices + HSIC-ANOVA indices



	U_1	U_2	U_3
R^2-HSIC	0.19	0.03	0.01
First-order	0.77	0.13	0.07
Total-order	0.79	0.14	0.08

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- Design parameter
  - ✓ $\boldsymbol{\gamma = 10}$

- Estimation of sensitivity measures
  - ✓ Sample size $n = 500$
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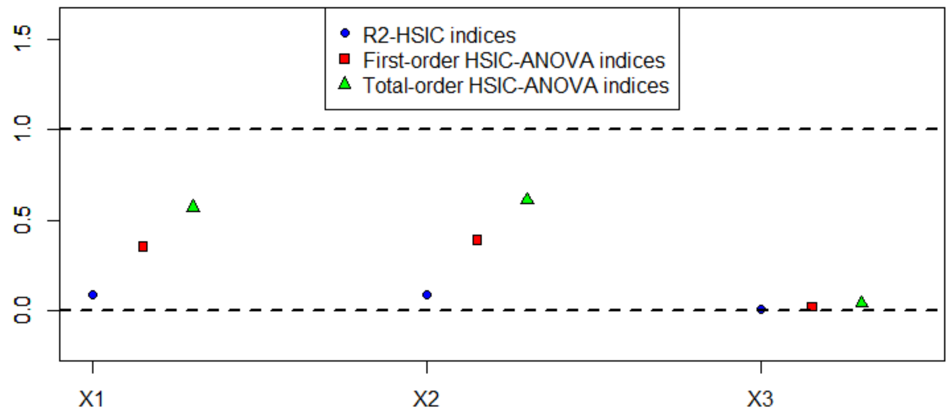

	U_1	U_2	U_3
R^2-HSIC	0.05	0.08	0.01
First-order	0.25	0.40	0.02
Total-order	0.56	0.71	0.04

How to exacerbate HSIC-ANOVA interactions?

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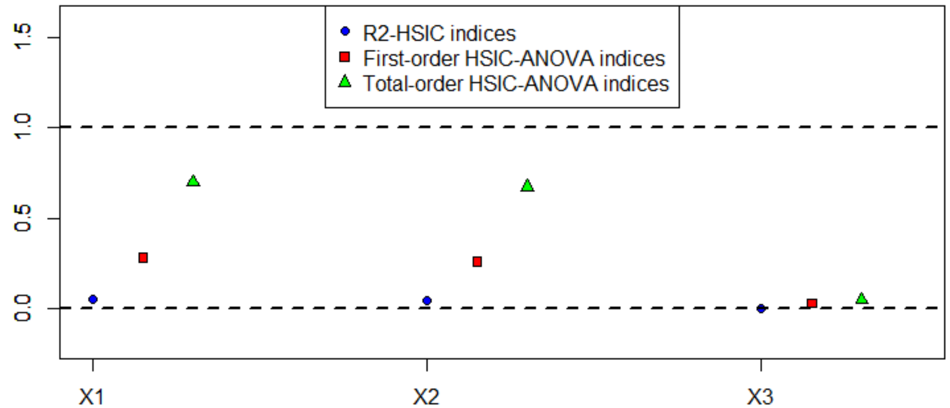
- **Design parameter**
  - ✓ $\boldsymbol{\gamma = 100}$

- **Estimation of sensitivity measures**
  - ✓ Sample size $n = 500$
  - ✓ R^2-HSIC indices + HSIC-ANOVA indices



	U_1	U_2	U_3
R^2-HSIC	0.05	0.05	0.01
First-order	0.28	0.23	0.04
Total-order	0.72	0.66	0.05

How to use HSIC-ANOVA in practice?

1. How to build a test of independence? How to extend to the existing test procedures?
2. Is there any advantage to using the total-order HSIC-ANOVA index?

GSA requirements	T_i	$\mathrm{HSIC}(X_i, Y)$	S_i^{HSIC}	T_i^{HSIC}
ANOVA decomposition → RANKING	✓	✗	✓	✓
Characterize independence → SCREENING	✓	✓	✓ ?	✓ ?
Estimation from GIVEN DATA	✗	✓	✓	✓
Estimation from SMALL DATA	✗	✓	✓	✓
Compatibility with DEPENDENT inputs	✗	✓	✗	✗
INVARIANCE through monotonic transformations	✓	✗	✗	✗

6. Does all this benefit independence testing?

Testing independence with HSIC-ANOVA indices

➢ A **test of independence** consists in testing the **null hypothesis** $(H_0^i) : X_i \perp Y$.

$$X_i \perp Y \iff S_i^{\text{HSIC}} = 0 \iff T_i^{\text{HSC}} = 0$$

$$\iff \boxed{\begin{array}{c}\text{HSIC}(X_i, Y) = 0 \\ \text{with } K^1_{\text{Sob}} \otimes K_Y\end{array}} \iff \boxed{\begin{array}{c}\text{HSIC}(\boldsymbol{X}, Y) - \text{HSIC}(\boldsymbol{X}_{-i}, Y) = 0 \\ \text{with } K^1_{\text{Sob}} \otimes \ldots \otimes K^1_{\text{Sob}} \otimes K_Y\end{array}}$$

Numerator of the first-order index

Numerator of the total-order index

Testing independence with HSIC-ANOVA indices

- A **test of independence** consists in testing the **null hypothesis** $(H_0^i): X_i \perp Y$.

$$X_i \perp Y \iff S_i^{\text{HSIC}} = 0 \iff T_i^{\text{HSC}} = 0$$

$$\iff \text{HSIC}(X_i, Y) = 0 \text{ with } K_{\text{Sob}}^1 \otimes K_Y \iff \text{HSIC}(\boldsymbol{X}, Y) - \text{HSIC}(\boldsymbol{X}_{-i}, Y) = 0 \text{ with } K_{\text{Sob}}^1 \otimes \ldots \otimes K_{\text{Sob}}^1 \otimes K_Y$$

Numerator of the first-order index

Numerator of the total-order index

V-statistic estimator

$$\widehat{S}_i(\boldsymbol{Z}_{\text{obs}}) = \widehat{\text{HSIC}}_v(X_i, Y)$$

Apply existing test procedures with $K_i = K_{\text{Sob}}^1$

Is there a reason to hope for higher statistical power?

Actually, NO!

Testing independence with HSIC-ANOVA indices

➢ A **test of independence** consists in testing the **null hypothesis** $(H_0^i) : X_i \perp Y$.

$$X_i \perp Y \iff S_i^{\text{HSIC}} = 0 \iff T_i^{\text{HSC}} = 0$$

$$\iff \begin{array}{c} \text{HSIC}(X_i, Y) = 0 \\ \text{with } K_{\text{Sob}}^1 \otimes K_Y \end{array} \iff \begin{array}{c} \text{HSIC}(\boldsymbol{X}, Y) - \text{HSIC}(\boldsymbol{X}_{-i}, Y) = 0 \\ \text{with } K_{\text{Sob}}^1 \otimes \ldots \otimes K_{\text{Sob}}^1 \otimes K_Y \end{array}$$

Numerator of the first-order index

Numerator of the total-order index

V-statistic estimator

$$\widehat{S}_i(\boldsymbol{Z}_{\text{obs}}) = \widehat{\text{HSIC}}_v(X_i, Y)$$

Apply existing test procedures with $K_i = K_{\text{Sob}}^1$

Is there a reason to hope for higher statistical power?

Actually, NO!

Much more appealing!

V-statistic estimator

$$\widehat{T}_i = \widehat{\text{HSIC}}_v(\mathbf{X}, Y) - \widehat{\text{HSIC}}_v(\boldsymbol{X}_{-i}, Y)$$

Computing this test statistic is slightly more expensive.

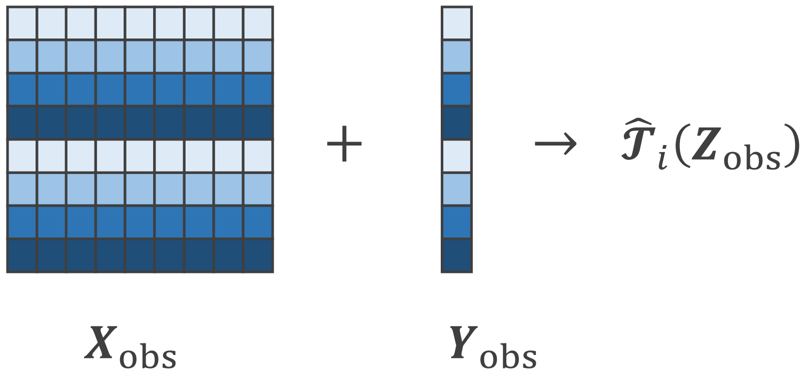
Is there a reason to hope for higher statistical power?

Let us see!

Testing independence with the total-order index

- The distribution of $\widehat{\mathcal{T}}_i(\boldsymbol{Z}_{\mathrm{obs}})$ under (H_0^i) can be **simulated from the available data**.

  ⚠ **All the columns of the DoE are required to compute the test statistic.**



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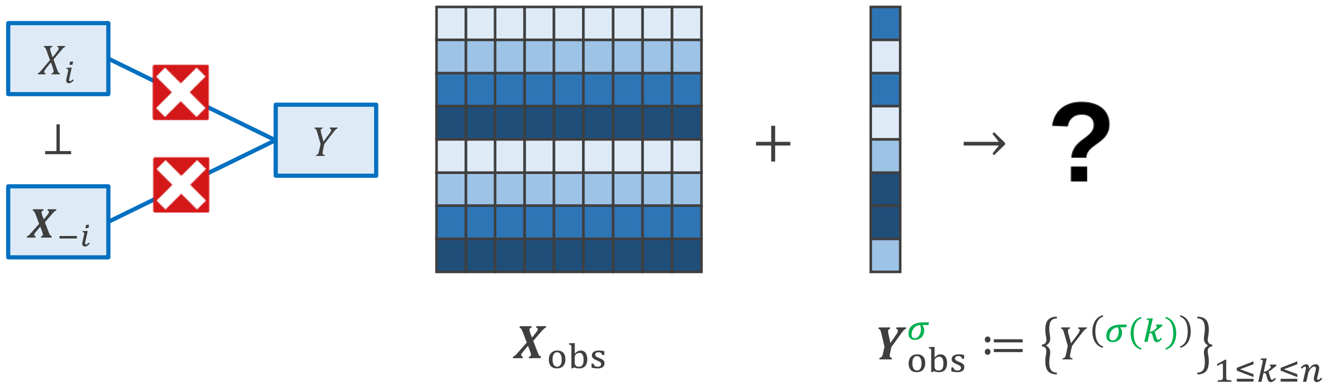
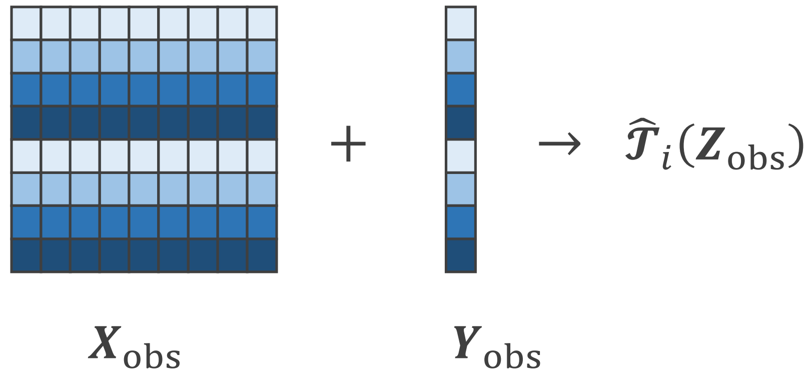


- Permuting $\mathbf{Y}_{\text{obs}}$ leads to **eliminate dependence** between the joint observations $(\mathbf{X}^{(k)}, Y^{(k)})$.
  - ✓ This boils down to testing $(H_0) : \mathbf{X} \perp Y$ and this is not what is desired!

Testing independence with the total-order index

- The distribution of $\widehat{\mathcal{T}}_i(\boldsymbol{Z}_{\mathrm{obs}})$ under (H_0^i) can be **simulated from the available data**.

Instead, the trick is to permute the observations of the input variable.



Testing independence with the total-order index

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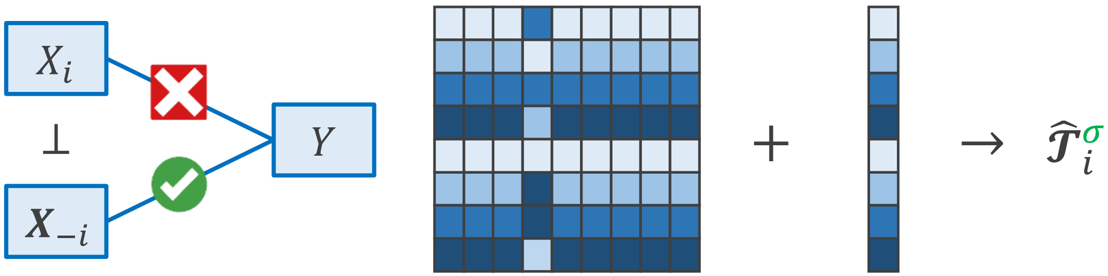


$$\boldsymbol{X}_{\text{obs}}^{\sigma} := \left\{\left(X_i^{(\sigma(k))}, \boldsymbol{X}_{-i}^{(k)}\right)\right\}_k \qquad \boldsymbol{Y}_{\text{obs}}$$

Testing independence with the total-order index

- The distribution of $\widehat{\mathcal{T}}_i(\boldsymbol{Z}_{\text{obs}})$ under (H_0^i) can be **simulated from the available data**.

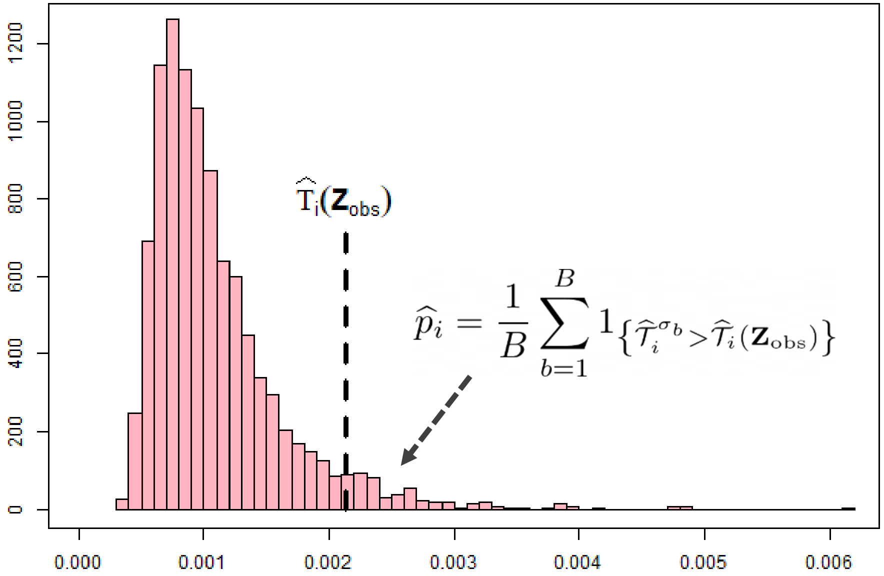
Instead, the trick is to permute the observations of the input variable.

Permutation-based test procedure

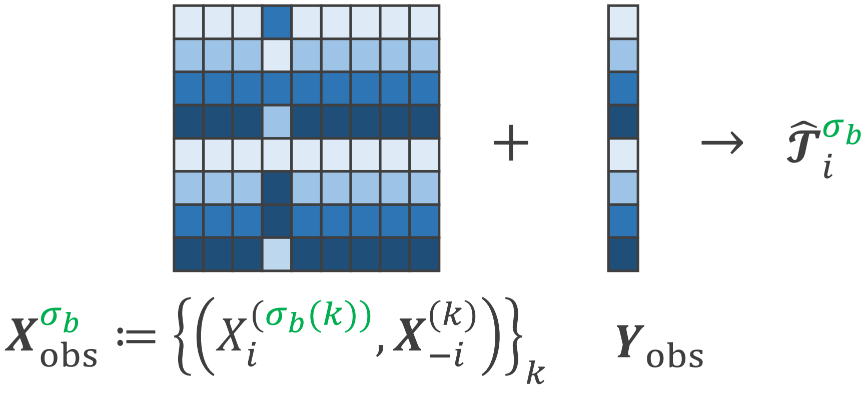
- **Step A** → Perform a sequence $\{\sigma_b\}_{1\le b\le B}$ of **random permutations** on the i-th column of $\boldsymbol{X}_{\text{obs}}$.
- **Step B** → Compute the value $\widehat{\mathcal{T}}_i^{\sigma_b}$ of the test statistic for each permuted design.
- **Step C** → Derive a **non-parametric estimate** of the p-value $p_i := \mathbb{P}\big(\widehat{\mathcal{T}}_i > \widehat{\mathcal{T}}_i(\boldsymbol{Z}_{\text{obs}})\big)$.

- **Default value:** $B \approx 10^3$
- **Complexity:** $(d^2 + 7Bd)\, n^2$

Simulation of the test statistic under the null hypothesis



Permutation scheme



Numerical study of the statistical power

- **Back to the Ishigami function**
  - ✓ <u>Additional term</u> chosen to boost HSIC-ANOVA interactions.

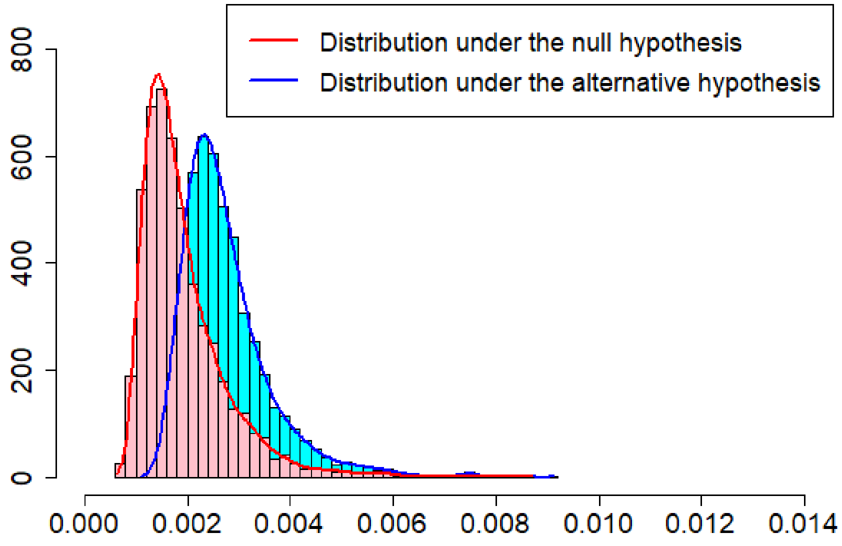
$$Y = g(U_1, U_2, U_3) = \text{ishigami}(X_1, X_2, X_3) + \boldsymbol{\gamma} \cos(\pi U_1) \cos(\pi U_2) \quad \text{with} \quad \begin{matrix} U_i \sim \mathcal{U}([0,1]) \\ X_i = \pi(2U_i - 1) \end{matrix}$$

- **Design parameter**
  - ✓ $\boldsymbol{\gamma = 0}$

- **Study of the statistical power**
  - ✓ Sample size $n = 50$
  - ✓ Number of replicates $M = 200$

	$\boldsymbol{U_1}$	$\boldsymbol{U_2}$	$\boldsymbol{U_3}$
HSIC	0.88	0.07	0.22
Total-order	0.87	0.19	0.19

- **Separation rate**
  - ✓ Distributions of $\widehat{\mathcal{T}}_i(\boldsymbol{Z}_{\text{obs}})$ under (H_0^i) et (H_1^i)



Numerical study of the statistical power

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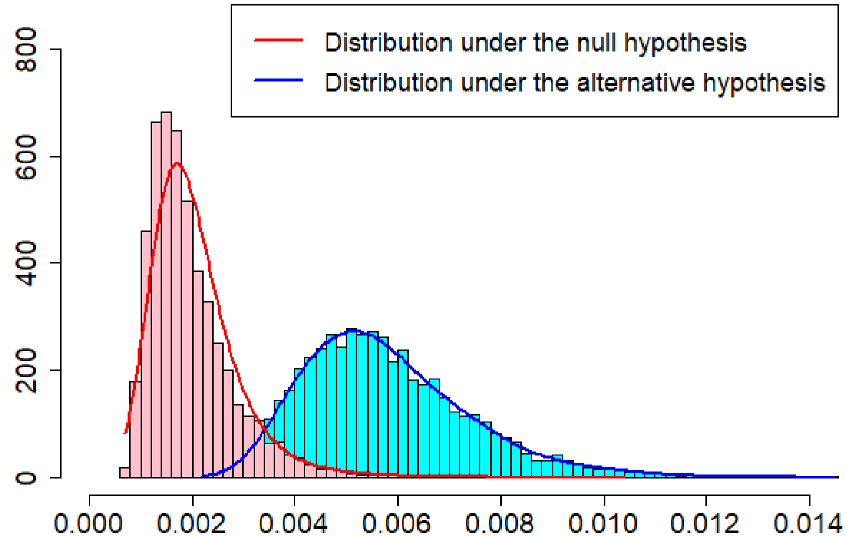
- **Design parameter**
  - ✓ $\boldsymbol{\gamma = 10}$

- **Study of the statistical power**
  - ✓ Sample size $n = 50$
  - ✓ Number of replicates $M = 200$

	U_1	U_2	U_3
HSIC	0.59	0.63	0.05
Total-order	0.92	0.94	0.07

- **Increased power** when $S_i^{\text{HSIC}} \ll T_i^{\text{HSIC}}$
- **Same power** when $S_i^{\text{HSIC}} \approx T_i^{\text{HSIC}}$

- **Separation rate**
  - ✓ Distributions of $\widehat{\mathcal{T}}_i(\boldsymbol{Z}_{\text{obs}})$ under (H_0^i) et (H_1^i)



Numerical study of the statistical power

- Back to the Ishigami function
  - ✓ **Additional term** chosen to boost HSIC-ANOVA interactions.

$$Y = g(U_1, U_2, U_3) = \text{ishigami}(X_1, X_2, X_3) + \gamma \cos(\pi U_1)\cos(\pi U_2) \quad \text{with} \quad \begin{array}{c} U_i \sim \mathcal{U}([0,1]) \\ X_i = \pi(2U_i - 1) \end{array}$$

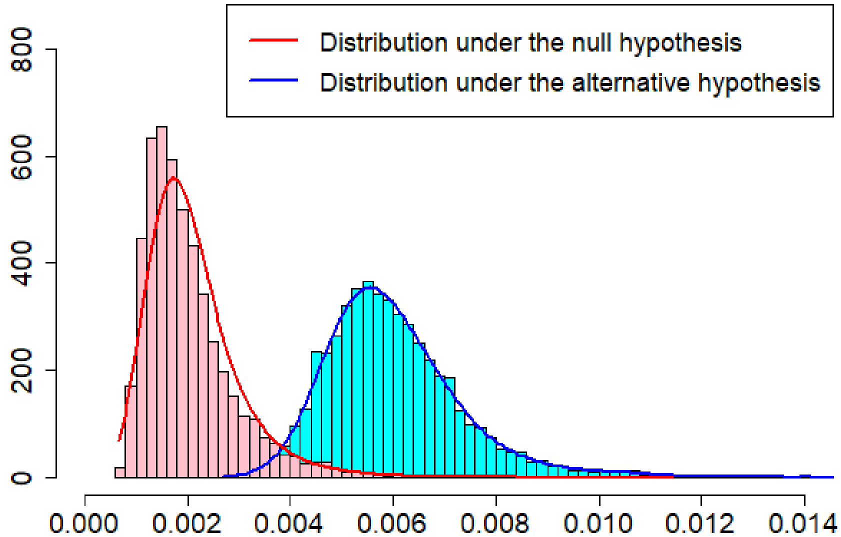
- Design parameter
  - ✓ $\gamma = 100$

- Study of the statistical power
  - ✓ Sample size $n = 50$
  - ✓ Number of replicates $M = 200$

	U_1	U_2	U_3
HSIC	0.65	0.70	0.07
Total-order	1.00	1.00	0.06

- Increased power when $S_i^{\text{HSIC}} \ll T_i^{\text{HSIC}}$
- Same power when $S_i^{\text{HSIC}} \approx T_i^{\text{HSIC}}$

- Separation rate
  - ✓ Distributions of $\widehat{\mathcal{T}}_i(\mathbf{Z}_{\text{obs}})$ under (H_0^i) et (H_1^i)



Benefits brought by HSIC-ANOVA indices in GSA

- HSIC-ANOVA indices are **fully transparent** sensitivity measures **able to perform screening and ranking!**
- In many situations, the test of independence based on T_i^{HSIC} is **more powerful!**

GSA requirements	T_i	$\mathrm{HSIC}(X_i, Y)$	S_i^{HSIC}	T_i^{HSIC}
ANOVA decomposition → RANKING	✔	✘	✔	✔
Characterize independence → SCREENING	✔	✔	✔	✔ ✔
Estimation from GIVEN DATA	✘	✔	✔	✔
Estimation from SMALL DATA	✘	✔	✔	✔
Compatibility with DEPENDENT inputs	✘	✔	✘	✘
INVARIANCE through monotonic transformations	✔	✘	✘	✘

7. Conclusion

Conclusion

- The very recent **HSIC-ANOVA indices** have enabled **significant progress in GSA** since they combine the advantages of **Sobol' indices** (variance-based GSA) and those of **HSIC indices** (kernel-based GSA).
- The **HSIC-ANOVA decomposition** requires the use of **characteristic ANOVA kernels** for the input variables.
- The way sensitivity is measured by HSIC-ANOVA indices is driven by the kernel feature maps.
- **Variable selection** can be performed with **test procedures** based on HSIC-ANOVA indices.
- Using the total-order HSIC-ANOVA indices leads to **more powerful** test procedures.

Traditional benchmarks

- ✓ **Ishigami, Friedman, Morris…**

$$S_i^{HSIC} \lesssim T_i^{HSIC}$$

$$\text{Power}\left(\widehat{\mathcal{S}}_i\right) \approx \text{Power}\left(\widehat{\text{HSIC}}_{\mathcal{N}}\right) \approx \text{Power}\left(\widehat{\mathcal{T}}_i\right)$$

Specific benchmarks

- ✓ **Hand-made use cases.**
- ✓ **Test functions in optimization.**
- ✓ **Flexible metafunction framework.**

$$S_i^{HSIC} \ll T_i^{HSIC}$$

$$\text{Power}\left(\widehat{\mathcal{S}}_i\right) \ll \text{Power}\left(\widehat{\text{HSIC}}_{\mathcal{N}}\right) \ll \text{Power}\left(\widehat{\mathcal{T}}_i\right)$$

Conclusion

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Publications

- **Preprint** → https://cea.hal.science/cea-04320711/document
- **Conference paper** → https://cea.hal.science/cea-03701170v1/document

Codes

- **Two dedicated routines the R package sensitivity**
  - ✓ **sensiHSIC** → https://rdrr.io/cran/sensitivity/man/sensiHSIC.html
  - ✓ **testHSIC** → https://rdrr.io/cran/sensitivity/man/testHSIC.html

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