More about HSIC-ANOVA indices…
What is hidden behind Sobolev kernels?

DE LA RECHERCHE À L'INDUSTRIE

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Summary

Introduction

1) From HSIC indices to HSIC-ANOVA indices

- Reminders on HSIC indices
- Towards an ANOVA decomposition in the HSIC paradigm
- Focus on Sobolev kernels

2) How to find a feature map for Sobolev kernels?

- **Approach 1:** kernel feature analysis
- **Approach 2:** transformation into a Cauchy problem
- **Approach 3:** series expansions of Bernoulli polynomials

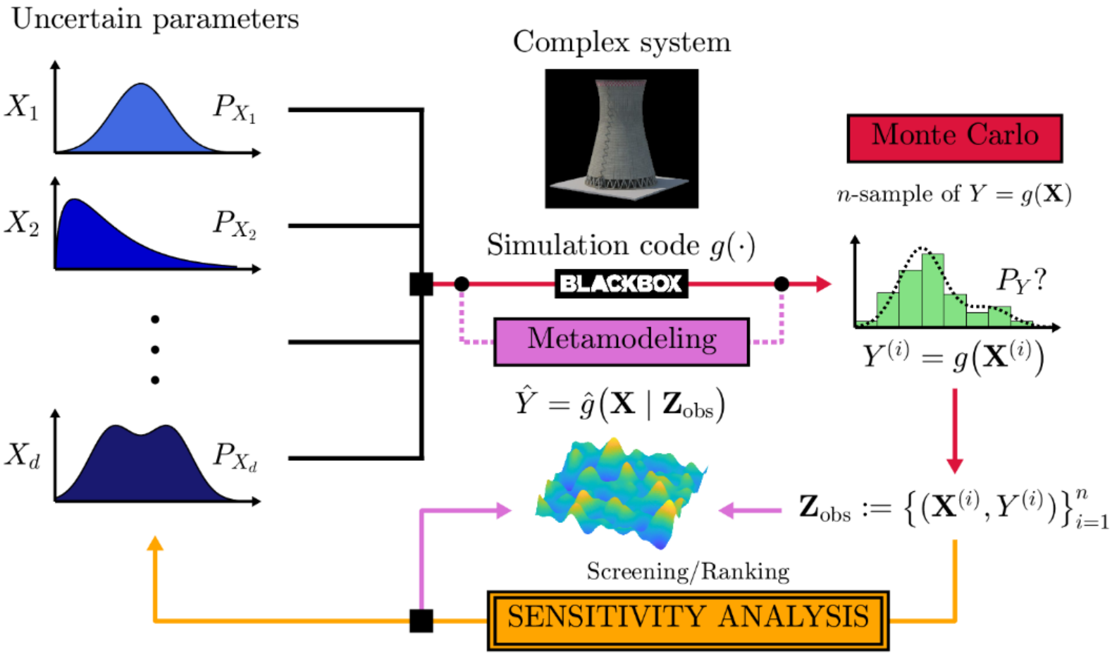
3) Are Sobolev kernels characteristic?

Conclusion

Introduction

→ Let $\boldsymbol{X} := [X_1, \dots, X_d]$ be a random vector with **independent** components ($d \approx 100$).

→ Let $Y := g(\boldsymbol{X})$ where $g: \mathbb{R}^d \to \mathbb{R}$ is a **computationally-expensive** simulation code.



→ Total-order Sobol' indices cannot be estimated from a small amount of input-output samples.

→ The HSIC indices of Gretton *et al.* (2005) have been inscreasingly used since Da Veiga (2014).

Reminders on HSIC indices

- → Let $\mathbb{P}_{\boldsymbol{X}}$ and $\mathbb{P}_Y$ be the probability measures associated to $\boldsymbol{X}$ to Y.
- → A kernel $K_i : \mathcal{X}_i \times \mathcal{X}_i \to \mathbb{R}$ (with feature space $\mathcal{F}_i$ and feature map φ_i) is assigned to X_i.
- → A kernel $K_Y : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ (with feature space $\mathcal{G}$ and feature map φ_Y) is assigned to Y.

$$\forall 1 \leq i \leq d, \quad \boxed{K_i(x_i, x_i') = \langle \varphi_i(x_i'), \varphi_i(x_i) \rangle_{\mathcal{F}_i}} \quad \text{and} \quad \boxed{K_Y(y, y') = \langle \varphi_Y(y'), \varphi_Y(y) \rangle_{\mathcal{G}}}$$

- ➢ This allows to define the **Hilbert-Schmidt Independence Criterion (HSIC)**.
  - ✓ **Kernel-based dissimilarity measure** between $\mathbb{P}_{X_i Y}$ and $\mathbb{P}_{X_i} \otimes \mathbb{P}_Y$.

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- This allows to define the **Hilbert-Schmidt Independence Criterion (HSIC)**.
  - ✓ **Kernel-based dissimilarity measure** between $\mathbb{P}_{X_i Y}$ and $\mathbb{P}_{X_i} \otimes \mathbb{P}_Y$.
  - ✓ Norm of a **covariance-like operator** between the feature maps φ_i and φ_Y.

$$\mathrm{HSIC}(X_i, Y) = \|C_{X_i Y}\|^2_{\mathrm{HS}} \quad \text{with} \quad \begin{aligned} & C_{X_i Y} : \mathcal{G} \longrightarrow \mathcal{F}_i \\ & C_{X_i Y} = \mathbb{E}[\varphi_i(X_i) \otimes \varphi_Y(Y)] - \mathbb{E}[\varphi_i(X_i)] \otimes \mathbb{E}[\varphi_Y(Y)] \end{aligned}$$

- Explicit knowledge about the feature maps φ_i and φ_Y may help understand HSIC indices.

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- ✓ **Kernel-based dissimilarity measure** between $\mathbb{P}_{X_iY}$ and $\mathbb{P}_{X_i} \otimes \mathbb{P}_Y$.
- ✓ Norm of a **covariance-like operator** between the feature maps φ_i and φ_Y.

→ Let (X_i, Y) and (X_i', Y') be two independent copies of $\mathbb{P}_{X_iY}$.

$$\begin{aligned}\mathrm{HSIC}(X_i, Y) = \; & \mathbb{E}_{\substack{X_iY \\ X_i'Y'}}\left[K_i(X_i, X_i')\, K_Y(Y, Y')\right] + \mathbb{E}_{X_iX_i'}\left[K_i(X_i, X_i')\right] \mathbb{E}_{YY'}\left[K_Y(Y, Y')\right] \\ & -2\mathbb{E}_{X_iY}\left[\mathbb{E}_{X_i'}\left[K_i(X_i, X_i')\right] \mathbb{E}_{Y'}\left[K_Y(Y, Y')\right]\right]\end{aligned}$$

➢ The estimation of $\mathrm{HSIC}(X_i, Y)$ can be considered with either a **U-statistic** or a **V-statistic**.

Towards an ANOVA decomposition in the HSIC paradigm

Keynote 4 - Sébastien DA VEIGA
A kernel-based ANOVA decompositon: extending sensitivity analysis and Shapley effects with kernels

- Da Veiga (2021) → $\mathrm{HSIC}(\boldsymbol{X}, Y)$ may be apportioned between **independent** inputs.

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

- The **first-order and total-order HSIC-ANOVA indices** are then defined by:

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

- Each input kernel K_i must be an **ANOVA kernel**.
  - ✓ $K_i = 1 + k_i$ with k_i an **orthogonal kernel**.

$$\forall x_i \in \mathcal{X}_i, \quad \int_{\mathcal{X}_i} k_i(x_i, z)\, \mathrm{d}\mathbb{P}_{X_i}(z) = 0$$

Focus on Sobolev kernels

→ The input variables $X_1, \ldots, X_d$ need to be **independent** and **uniformly distributed** on $[0,1]$.

➢ Sobolev kernels $K^r_{Sob} = 1 + k^r_{Sob}$ (with r a smoothing parameter) are then **orthogonal**.

$$K^r_{\text{Sob}}(x,x') = 1 + \sum_{i=1}^{r} \frac{B_j(x)B_j(x')}{(j!)^2} + \frac{(-1)^{r+1}}{(2r)!} B_{2r}(|x-x'|)$$

$$= 1 + k^r_A(x,x') + k^r_B(x,x')$$

$$\langle \theta^r_{\text{Sob}}(x'), \theta^r_{\text{Sob}}(x) \rangle_{\mathcal{H}^r_{\text{Sob}}} = 1 + \langle \varphi^r_A(x'), \varphi^r_A(x) \rangle_{\mathbb{R}^r} + \langle \theta^r_B(x'), \theta^r_B(x) \rangle_{\mathcal{H}^r_B}$$

trivial feature map in $\mathbb{R}^r$ — **canonical feature map**

1. The definition is based on **Bernoulli polynomials** → $\int_0^1 B_k(t)dt = 0$ for all $k \geq 1$.
2. It is easy to see that $k^r_A(x,x') = \langle \varphi^r_A(x'), \varphi^r_A(x) \rangle_{\mathbb{R}^r}$ with $\varphi^r_A(x) = \left[\frac{B_j(x)}{j!}\right]_{1 \leq j \leq r}$.
3. Bochner's theorem cannot be applied because $k^r_B(x,x') = t^r_B(|x-x'|)$ with $t^r_B \notin L^2(\mathbb{R})$.

❑ **How to find a unified feature map φ^r_{Sob}?**

Approach 1: kernel feature analysis

→ Let $\mathbb{P}_X$ be a probability measure on a **compact** domain $\mathcal{X}$.

➢ The **kernel integral operator** is defined by:

$$\begin{aligned} T_K : L^2(\mathcal{X}, \mathbb{P}_X) &\longrightarrow L^2(\mathcal{X}, \mathbb{P}_X) \\ f &\longmapsto T_K f \end{aligned} \quad \text{with } [T_K f](x) := \int_{\mathcal{X}} K(x,z) f(z)\, d\mathbb{P}_X(z)$$

Mercer's theorem

There exists an **orthonormal basis** $\{\phi_i\}_{i\in I}$ of $L^2(\mathcal{X}, \mathbb{P}_X)$ consisting of **eigenfunctions** of T_K.
The associated eigenvalues $\{\lambda_i\}_{i\in I}$ are **non-negative**.
K admits the following representation:

$$K(x,x') = \sum_{i\in I} \lambda_i\, \phi_i(x)\phi_i(x') = \langle \varphi(x'), \varphi(x) \rangle_{\ell^2(I,\mathbb{R})}$$

and convergence is **absolute** and **uniform**. In addition, $\varphi(x) = \left[\sqrt{\lambda_i}\phi_i(x)\right]_{i\in I}$.

➢ An **infinite-dimensional eigenvalue problem** has to be solved → $T_K\phi = \lambda\phi$ with $\lambda > 0$

How to find a feature map for Sobolev kernels?

Approach 1: kernel feature analysis

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\end{aligned}
$$

Kernel Feature Analysis (KFA) / Kernel PCA

→ Let $\{x_j\}_{1 \le j \le n}$ be a n-sample of a random variable $X \sim \mathbb{P}_X$.

➢ Discretization leads to a **finite-dimensional eigenvalue problem**:

$$\mathbf{L}\mathbf{v} = (n\lambda)\mathbf{v} \quad \text{with} \quad \mathbf{L} = \left[K(x_i, x_j)\right]_{1 \le i,j \le n} \quad \text{and} \quad \mathbf{v} = \left[\phi(x_i)\right]_{1 \le i \le n}$$

➢ Computation of the **eigenvalues** and **eigenvectors** of the Gram matrix $\boldsymbol{L}$.

- ✓ Estimation of the n largest **eigenvalues** and **eigenfunctions** of T_K.

❑ **What about Sobolev kernels k_{Sob}^r?**

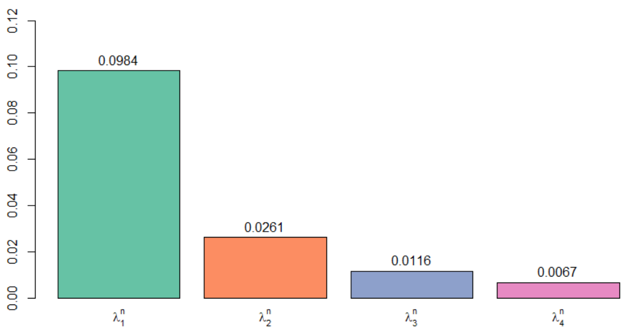
How to find a feature map for Sobolev kernels?

1 Sobolev kernel with $r = 1$

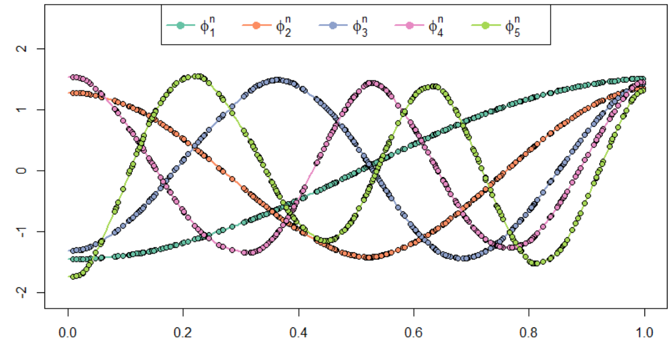
→ $\mathbb{P}_X = \mathcal{U}([0,1])$

→ $k^1_{Sob}(x, x') = B_1(x)B_1(x') + \frac{1}{2}B_2(|x - x'|)$

❑ **What do the eigenfunctions look like?**



Eigenvalues



Eigenfunctions

- **Conjecture**: $\forall k \geq 1, \phi_k(t) = \sqrt{2}\cos(k\pi t)$
- **Calculation by hand**:

$$[T_{k^1_{\mathrm{Sob}}}\phi_k](x_0) = \int_0^1 k^1_{\mathrm{Sob}}(x_0, z)\phi_k(z)\,\mathrm{d}z = \ldots = \overbrace{\frac{1}{(k\pi)^2}}^{\lambda_k}\phi_k(x_0)$$

- **Conclusion**: $K^1_{\mathrm{Sob}}(x, x') = 1 + 2\sum_{k=1}^{\infty}\frac{1}{(k\pi)^2}\cos(k\pi x)\cos(k\pi x')$

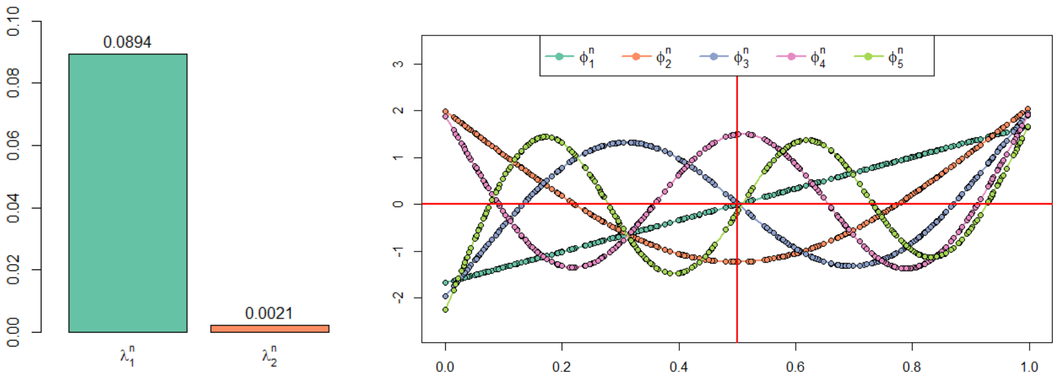
How to find a feature map for Sobolev kernels?

2 Sobolev kernel with $r = 2$

→ $\mathbb{P}_X = \mathcal{U}([0,1])$

→ $k_{Sob}^2(x,x') = B_1(x)B_1(x') + \frac{1}{4}B_2(x)B_2(x') - \frac{1}{24}B_4(|x-x'|)$

❑ **What do the eigenfunctions look like?**



Eigenvalues   Eigenfunctions

- **Conjecture**: $\forall k \geq 1, \phi_k(t) = \sqrt{2k+1}\, L_k(2t-1)$ with L_k the k-th Legendre polynomial
- **Calculation by hand**: this is a numerical illusion!
  - ✓ $\lambda_1 \gg \lambda_2$ and ϕ_1 pseudo-linear → $K_{Sob}^2(x,x') \approx 1 + 12\,\lambda_1 \left(x - \frac{1}{2}\right)\left(x' - \frac{1}{2}\right)$
- **Conclusion**: K_{Sob}^2 is very close to the **dot-product kernel**.

Approach 2: transformation into a Cauchy problem

- Any eigenfunction ϕ of $T_{k^r_{Sob}}$ is **infinitely differentiable** on $[0,1]$. We proved that:

$$T_{k^r_{\mathrm{Sob}}}\phi = \lambda\phi$$

$$\Updownarrow$$

$$\lambda\phi^{[2r]} + (-1)^{r+1}\phi = 0 \quad \text{with} \quad \begin{cases} \phi^{[r]}(0) = \phi^{[r]}(1) = 0 \\ \forall 0 \le p \le r-2, (-1)^{r+p}\left(\phi^{[p]}(1) - \phi^{[p]}(0)\right) = \phi^{[2r-p-1]}(0) \\ \forall 0 \le p \le r-2, \phi^{[2r-p-1]}(0) = \phi^{[2r-p-1]}(1) \end{cases}$$

- For k^r_{Sob}, the eigenvalue problem is equivalent to a Cauchy problem $(\mathcal{C}_r)$ comprised of:
  - ✓ An homogeneous linear ODE of order $2r$ with constant coefficients.
  - ✓ $2r$ boundary conditions on ϕ and its following derivatives (up to order $2r-1$).

1 Sobolev kernel with $r = 1$

$$(\mathcal{C}_1): \;\; \lambda\phi''(t) + \phi(t) = 0 \;\; \text{with} \;\; \phi'(0) = 0 \;\; \text{and} \;\; \phi'(1) = 0$$

- There are solutions to $(\mathcal{C}_1)$ if and only if $\lambda \in \left(\frac{1}{(k\pi)^2}\right)_{k\geq 1}$.
- Analytical resolution yields $\phi_k(t) = \sqrt{2}\cos(k\pi t)$ → consistent with KFA!

Approach 2: transformation into a Cauchy problem

- Any eigenfunction ϕ of $T_{k^r_{Sob}}$ is **infinitely differentiable** on $[0,1]$. We proved that:

$$T_{k^r_{\mathrm{Sob}}}\phi = \lambda\phi$$

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  - ✓ $2r$ boundary conditions on ϕ and its following derivatives (up to order $2r-1$).

2 **Sobolev kernel with $r = 2$**

$$(\mathcal{C}_2): \;\; \lambda\phi^{[4]}(t) - \phi(t) = 0 \;\; \text{with} \;\; \begin{cases} \phi''(0) = \phi''(1) = 0 \\ \phi(1) - \phi(0) = \phi^{[3]}(0) = \phi^{[3]}(1) \end{cases}$$

- The eigenfunctions are actually **not polynomials**.
- We cannot go further! There is **no closed-form expression** for these eigenvalues.

How to find a feature map for Sobolev kernels?

Approach 3: series expansions of Bernoulli polynomials

$$K^r_{\mathrm{Sob}}(x,x') = 1 + k^r_A(x,x') + k^r_B(x,x') \quad \text{with} \quad k^r_B(x,x') = \frac{(-1)^{r+1}}{(2r)!} B_{2r}(|x-x'|)$$

$$\forall n \geq 2, \quad \forall\, 0 \leq x \leq 1, \quad B_n(x) = (-2) \times n! \sum_{k=1}^{\infty} \frac{\cos\left(2k\pi x - \frac{n\pi}{2}\right)}{(2k\pi)^n}$$

- With this in mind, it is straighforward to see that:

$$\begin{aligned} k^r_B(x,x') &= 2\sum_{k=1}^{\infty} \frac{1}{(2k\pi)^{2r}} \left[\cos(2k\pi x)\cos(2k\pi x') + \sin(2k\pi x)\sin(2k\pi x')\right] \\ &= \sum_{k=1}^{\infty} \lambda_k c_k(x) c_k(x') + \sum_{k=1}^{\infty} \lambda_k s_k(x) s_k(x') \quad \text{with} \quad \begin{cases} \lambda_k & := \frac{1}{(2k\pi)^{2r}} \\ c_k(t) & := \sqrt{2}\cos(2k\pi t) \\ s_k(t) & := \sqrt{2}\sin(2k\pi t) \end{cases} \end{aligned}$$

1. Explicit feature map φ^r_B of k^r_B in $\ell^2(\mathbb{N},\mathbb{R})$. It can be combined with φ^r_A which arrives in $\mathbb{R}^r$.
2. The functions $(c_k)_{k\geq 1}$ and $(s_l)_{l\geq 1}$ are orthonormal. This is the Mercer decomposition of k^r_B.
3. For $j \geq 1$, (c_j, s_j) is one orthonormal basis for the 2-dimensional eigenspace of λ_j.

How to find a feature map for Sobolev kernels?

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- **Global feature map** from $[0{,}1]$ in $\ell^2(\mathbb{N},\mathbb{R})$ that explicits feature functions:

$$K^r_{\mathrm{Sob}}(x,x') = 1 + \sum_{k=1}^{r} \frac{B_k(x)B_k(x')}{(k!)^2} + 2\sum_{k=1}^{\infty} \frac{1}{(2k\pi)^{2r}} \left[\cos(2k\pi x)\cos(2k\pi x') + \sin(2k\pi x)\sin(2k\pi x')\right]$$

$$K^r_{\mathrm{Sob}}(x,x') = \left\langle \varphi^r_{\mathrm{Sob}}(x'), \varphi^r_{\mathrm{Sob}}(x) \right\rangle_{\ell^2(\mathbb{N},\mathbb{R})} \quad \text{with:}$$

$$\varphi^r_{\mathrm{Sob}}(x) = \left[1, \left(\frac{B_k(x)}{k!}\right)_{1\leq k\leq r}, \left(\frac{\sqrt{2}\cos(2k\pi x)}{(2k\pi)^r}\right)_{k\geq 1}, \left(\frac{\sqrt{2}\sin(2k\pi x)}{(2k\pi)^r}\right)_{k\geq 1}\right]$$

Are Sobolev kernels characteristic?

	constant features		polynomial features		sinusoidal features
$K^r_{\text{Sob}} =$	$\boxed{1}$	$+$	$\boxed{k^r_A}$	$+$	$\boxed{k^r_B}$
$\downarrow$	$\downarrow$		$\downarrow$		$\downarrow$
$\mathcal{H}^r_{\text{Sob}} =$	$\text{Span}(\{1\})$	$\oplus$	$\mathcal{H}^r_A$	$\oplus$	$\mathcal{H}^r_B$
	constant functions		zero-mean functions		

$$\mathcal{H}^r_{\text{Sob}} = \left\{ f \in \mathbb{R}^{[0,1]} \;\middle|\; \begin{array}{l} f(\cdot) = \boxed{\gamma_0} + \boxed{\sum_{i=1}^{r} \beta_i B_i(\cdot)} + \boxed{\sum_{k=1}^{\infty} \frac{a_k}{(2k\pi)^r} c_k(\cdot) + \sum_{k=1}^{\infty} \frac{b_k}{(2k\pi)^r} s_k(\cdot)} \\ \text{with } \gamma_0 \in \mathbb{R}, \;\; (\beta_i)_{1 \le i \le r} \in \mathbb{R}^r \;\text{ and }\; (a_k)_{k\ge1}, (b_k)_{k\ge1} \in \ell^2(\mathbb{N}^*, \mathbb{R}) \end{array} \right\}$$

Are Sobolev kernels characteristic?

constant features | polynomial features | sinusoidal features

$$K^r_{\text{Sob}} = \boxed{1} + \boxed{k^r_A} + \boxed{k^r_B}$$

$$\downarrow \qquad \downarrow \qquad \downarrow \qquad \downarrow$$

$$\mathcal{H}^r_{\text{Sob}} = \boxed{\text{Span}(\{1\})} \oplus \boxed{\mathcal{H}^r_A \oplus \mathcal{H}^r_B}$$

constant functions | zero-mean functions

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- The RKHS contains all Bernoulli polynomials, hence all polynomials:

$$\boxed{B_0 = 1 \in \text{Span}(\{1\})} \ ; \ \boxed{B_1, \dots, B_r \in \mathcal{H}^r_A} \ ; \ \boxed{(B_k)_{k \ge r+1} \in \mathcal{H}^r_B}$$

- Stone-Weierstrass theorem → the polynomials are dense in $C([0,1])$.

K^r_{Sob} UNIVERSAL ⇔ K^r_{Sob} CHARACTERISTIC

Are Sobolev kernels characteristic?

constant features — polynomial features — sinusoidal features

$$K^r_{\text{Sob}} = \boxed{1} + \boxed{k^r_A} + \boxed{k^r_B}$$

$$\downarrow \qquad \downarrow \qquad \downarrow \qquad \downarrow$$

$$\mathcal{H}^r_{\text{Sob}} = \boxed{\text{Span}(\{1\})} \oplus \boxed{\mathcal{H}^r_A \oplus \mathcal{H}^r_B}$$

constant functions — zero-mean functions

$$\mathcal{H}^r_{\text{Sob}} = \left\{ f \in \mathbb{R}^{[0,1]} \,\middle|\, \begin{array}{l} f(\cdot) = \boxed{\gamma_0} + \boxed{\sum_{i=1}^{r} \beta_i B_i(\cdot)} + \boxed{\sum_{k=1}^{\infty} \frac{a_k}{(2k\pi)^r} c_k(\cdot) + \sum_{k=1}^{\infty} \frac{b_k}{(2k\pi)^r} s_k(\cdot)} \\ \text{with } \gamma_0 \in \mathbb{R}, \ (\beta_i)_{1 \le i \le r} \in \mathbb{R}^r \text{ and } (a_k)_{k \ge 1}, (b_k)_{k \ge 1} \in \ell^2(\mathbb{N}^*, \mathbb{R}) \end{array} \right\}$$

- Sobolev kernels K^r_{Sob} are **characteristic.**
  - ✓ First-order **HSIC-ANOVA indices** allow to detect independence:

$$S_i^{\text{HSIC}} = 0 \iff \text{HSIC}(X_i, Y) = 0 \iff X_i \perp Y$$

What must be remembered about Sobolev kernels?

$$K^r_{\text{Sob}}(x,x') = 1 + k^r_{\text{Sob}}(x,x') = 1 + k^r_A(x,x') + k^r_B(x,x')$$

- $\mathbb{P}_X = \mathcal{U}([0,1])$ → $K^r_{\text{Sob}}(x,x')$
- $k^r_{\text{Sob}}(x,x')$: orthogonality constraint → HSIC-ANOVA
- $k^r_A(x,x')$: sum of separable functions → polynomial features
- $k^r_B(x,x')$: translation invariance → sinusoidal features

➢ They are **CHARACTERISTIC** and they therefore can be used to build **tests of independence**.

1 Sobolev kernel with $r = 1$

➢ The joint effect of k_A^1 and k_B^1 results in sinusoidal features.

2 Sobolev kernel with $r = 2$ → It behaves like the **dot-product kernel**.

➢ The eigenvalues of $T_{k_B^2}$ have a faster decay speed ($1/k^4$ instead of $1/k^2$).

➢ The sinusoidal features vanish. They are replaced by polynomial-like features.

MUST NOT BE USED

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