A KERNEL-BASED ANOVA DECOMPOSITION

EXTENDING SENSITIVY INDICES AND SHAPLEY EFFECTS WITH KERNELS

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Outline

Context – Global Sensitivity Analysis (GSA)

Generalized GSA via kernel embedding of probability distributions

Conclusion & outlook

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CONTEXT

GLOBAL SENSITIVITY ANALYSIS

Sensitivity analysis: Sobol' indices arise from a functional ANOVA decomposition

Theorem 1 (ANOVA decomposition (Hoeffding, 1948; Antoniadis, 1984)). *Assume that* $\eta : \mathcal{X}_1 \times \ldots \times \mathcal{X}_d \to \mathcal{Y}$ *is a square integrable function of* d *independent random variables* $X_1, \ldots, X_d$. *Then* η *admits a decomposition*

$$Y = \eta(X_1, \ldots, X_d) = \sum_{A \subseteq \mathcal{P}_d} \eta_A(\mathbf{X}_A),$$

with η_A *depending only on the variables* $\mathbf{X}_A$ *and satisfying*

(a) $\eta_\emptyset = \mathbb{E}(Y)$,

(b) $\mathbb{E}_{X_l}(\eta_A(\mathbf{X}_A)) = 0$ *if* $l \in A$,

(c) $\eta_A(\mathbf{X}_A) = \sum_{B \subset A} (-1)^{|A|-|B|} \mathbb{E}(Y|\mathbf{X}_B)$.

Furthermore, (b) implies that all the terms η_A *in the decomposition are mutually orthogonal. As a consequence, the output variance can be decomposed as*

$$\operatorname{Var} Y = \sum_{A \subseteq \mathcal{P}_d} \operatorname{Var} \eta_A(\mathbf{X}_A) = \sum_{A \subseteq \mathcal{P}_d} V_A \qquad (1)$$

where

$$V_A = \sum_{B \subset A} (-1)^{|A|-|B|} \operatorname{Var} \mathbb{E}(Y|\mathbf{X}_B). \qquad (2)$$

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Sensitivity analysis: Sobol' indices arise from a functional ANOVA decomposition

Definition 1 (Sobol' indices (Sobol', 1993)). *Under the same assumptions of Theorem 1, the Sobol' sensitivity index associated to a subset A of input variables is defined as*

$$S_A = \frac{V_A}{\operatorname{Var} Y}, \quad (3)$$

A is a subset of input variables

while the total Sobol' index associated to A is

$$S_A^T = \sum_{B \subseteq \mathcal{P}_d,\, B \cap A \neq \emptyset} S_B. \quad (4)$$

In particular, the first-order Sobol' index of an input X_l writes

$$S_l = \frac{\operatorname{Var} \mathbb{E}(Y|X_l)}{\operatorname{Var} Y}$$

Impact of an input alone

and its total Sobol' index is given by

$$S_l^T = \sum_{B \subseteq \mathcal{P}_d, l \in B} S_B = 1 - \frac{\operatorname{Var} \mathbb{E}(Y|\mathbf{X}_{-l})}{\operatorname{Var} Y}.$$

Impact of an input through all its potential interactions with others

Finally, the ANOVA decomposition (1) readily provides an interpretation of Sobol' indices as a percentage of explained output variance, i.e.

$$\sum_{A \subseteq \mathcal{P}_d} S_A = 1. \quad (5)$$

Interpretation as percentage

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Sensitivity analysis: Sobol' indices

Sobol' indices

- The impact of each input can be quantitatively assessed
  - First-order effect
  - Total effect including also all possible interactions with other inputs
  - **Pure interactions can be properly defined**

$$S_{ll'} = \frac{\mathrm{Var}\,\mathbb{E}(Y|X_l,\, X_{l'}) - \mathrm{Var}\,\mathbb{E}(Y|X_l) - \mathrm{Var}\,\mathbb{E}(Y|X_{l'})}{\mathrm{Var}\,Y} = \frac{\mathrm{Var}\,\mathbb{E}(Y|X_l,\, X_{l'})}{\mathrm{Var}\,Y} - S_l - S_{l'}$$

First-order effects can be propertly subtracted

Sensitivity analysis: Sobol' indices

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Limitations

- **Assumption of independent inputs (more on this later)**
- **Impact on output variance only**
- **Outputs may not be scalars**

Sensitivity analysis: other indices

Going beyond the variance 1: goal-oriented sensitivity analysis

- Indices based on contrast functions (Fort et al. 2014), in particular quantile-oriented indices
- Reliability-based indices
- Many industrial applications

Going beyond the variance 2: moment-independent indices

- Principle: Quantify the impact of an input parameter on the **probability distribution of the output**

$$\mathcal{S}_l^{TV} = \int |p_Y(y) - p_{Y|X_l=x}(y)| p_{X_l}(x) dx dy$$

Borgonovo 2007

$$\mathcal{S}_l^{KL} = \int p_{Y|X_l=x}(y) \ln \left(\frac{p_{Y|X_l=x}(y)}{p_Y(y)} \right) p_{X_l}(x) dx dy$$

Kraskov et al. 2001

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Sensitivity analysis: general point of view

General framework for moment-independent indices

$$S_l = \mathbb{E}_{X_l}\left(d(\mathrm{P}_Y, \mathrm{P}_{Y|X_l})\right)$$

Baucells & Borgonovo 2013
D. 2015

- If the output probability distribution and the conditional one are « close », the input parameter has little influence
- Example: f-divergence (D. 2015, Rahman 2016), with particular cases TV & KL

Sensitivity analysis – Moment-independent indices

Pros

- They account for the whole effect of a parameter on the output distribution
- They are density-based
  - Many methods and packages for estimation
  - Several distances can be investigated without additional cost

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- Definition of higher-order indices means curse of dimensionality for density estimation
- No ANOVA-like decomposition
  - No access to a « natural » normalisation constant
  - No proper separation of interactions and main effects

Does this make sense ?

$$\mathcal{S}_{ll'}^{TV} = \int |p_Y(y)p_{X_l}(x)p_{X_{l'}}(x') - p_{X_l,X_{l'},Y}(x,x',y)|dxdx'dy - \mathcal{S}_l^{TV} - \mathcal{S}_{l'}^{TV}$$

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A promising candidate: kernel-embedding of probability distributions

$$S_l = \mathbb{E}_{X_l}\left(d(\mathrm{P}_Y, \mathrm{P}_{Y|X_l})\right)$$

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KERNEL-EMBEDDING OF PROBABILITY DISTRIBUTIONS

Kernel-embedding of probability distributions

The kernel mean embedding of a probability measure is defined as

$$\mu_{\mathrm{P}} = \mathbb{E}_{\xi\sim\mathrm{P}} k_{\mathcal{X}}(\xi,\cdot) = \int_{\mathcal{X}} k_{\mathcal{X}}(\xi,\cdot) d\mathrm{P}(\xi)$$

A distance between probability measures is then given by the Maximum Mean Discrepancy

$$\mathrm{MMD}(\mathrm{P}_1,\mathrm{P}_2) = \|\mu_{\mathrm{P}_1} - \mu_{\mathrm{P}_2}\|_{\mathcal{H}}$$

The reproducing property in the RKHS gives the central result

$$\mathrm{MMD}^2(\mathrm{P}_1,\mathrm{P}_2) = \mathbb{E}_{\xi,\xi'} k_{\mathcal{X}}(\xi,\xi') - 2\mathbb{E}_{\xi,\zeta} k_{\mathcal{X}}(\xi,\zeta) + \mathbb{E}_{\zeta,\zeta'} k_{\mathcal{X}}(\zeta,\zeta')$$

Smola et al. 2007, Song 2008, Song et al. 2009

Kernel-embedding of probability distributions

Other major use: testing independence of random vectors

$$\mathrm{MMD}^2(\mathrm{P}_{\mathbf{UV}}, \mathrm{P}_{\mathbf{U}} \otimes \mathrm{P}_{\mathbf{V}}) = \|\mu_{\mathrm{P}_{\mathbf{UV}}} - \mu_{\mathrm{P}_{\mathbf{U}}} \otimes \mu_{\mathrm{P}_{\mathbf{V}}}\|^2_{\mathcal{H}}$$

$$\begin{aligned}\mathrm{HSIC}(\mathbf{U}, \mathbf{V}) &= \mathrm{MMD}^2(\mathrm{P}_{\mathbf{UV}}, \mathrm{P}_{\mathbf{U}} \otimes \mathrm{P}_{\mathbf{V}}) \\ &= \mathbb{E}_{\mathbf{U},\mathbf{U}',\mathbf{V},\mathbf{V}'} k_{\mathcal{X}}(\mathbf{U}, \mathbf{U}') k_{\mathcal{Y}}(\mathbf{V}, \mathbf{V}') \\ &+ \mathbb{E}_{\mathbf{U},\mathbf{U}'} k_{\mathcal{X}}(\mathbf{U}, \mathbf{U}') \mathbb{E}_{\mathbf{V},\mathbf{V}'} k_{\mathcal{Y}}(\mathbf{V}, \mathbf{V}') \\ &- 2\mathbb{E}_{\mathbf{U},\mathbf{V}} \left[\mathbb{E}_{\mathbf{U}'} k_{\mathcal{X}}(\mathbf{U}, \mathbf{U}') \mathbb{E}_{\mathbf{V}'} k_{\mathcal{Y}}(\mathbf{V}, \mathbf{V}')\right]\end{aligned}$$

Gretton et al. 2005a,b

Many applications: goodness-of-fit, independence tests, feature selection, …

Kernel-embedding of probability distributions

Pros

- Thanks to the RKHS, only involves expectations of kernels
- Less prone to the curse of dimensionality
- **Can easily handle structured objects (curves, images, graphs, probability measures, …) by using specific kernels tailored at such tasks**

Cons

- Choice of kernel / kernel hyperparameters …

Kernel-embedding of probability distributions for GSA: MMD

Remember our general GSA setting ?

$$\mathcal{S}_l = \mathbb{E}_{X_l}\left(d(\mathrm{P}_Y, \mathrm{P}_{Y|X_l})\right)$$

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$$\mathcal{S}_l = \mathbb{E}_{X_l}\left(d(\mathrm{P}_Y, \mathrm{P}_{Y|X_l})\right)$$

Straightforward use of kernel-embeddings

First-order

$$\begin{aligned}
\mathcal{S}_l^{\mathrm{MMD}} &= \mathbb{E}_{X_l}\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|X_l}) \\
&= \mathbb{E}_{X_l}\mathbb{E}_{\xi,\xi'\sim\mathrm{P}_Y} k_{\mathcal{Y}}(\xi,\xi') - 2\mathbb{E}_{X_l}\mathbb{E}_{\xi\sim\mathrm{P}_Y,\zeta\sim\mathrm{P}_{Y|X_l}} k_{\mathcal{Y}}(\xi,\zeta) + \mathbb{E}_{X_l}\mathbb{E}_{\zeta,\zeta'\sim\mathrm{P}_{Y|X_l}} k_{\mathcal{Y}}(\zeta,\zeta') \\
&= \mathbb{E}_{X_l}\mathbb{E}_{\zeta,\zeta'\sim\mathrm{P}_{Y|X_l}} k_{\mathcal{Y}}(\zeta,\zeta') - \mathbb{E}_{\xi,\xi'\sim\mathrm{P}_Y} k_{\mathcal{Y}}(\xi,\xi')
\end{aligned}$$

D. 2016 & 2021, Barr & Rabitz 2022

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&= \mathbb{E}_{X_l}\mathbb{E}_{\zeta,\zeta'\sim\mathrm{P}_{Y|X_l}} k_{\mathcal{Y}}(\zeta,\zeta') - \mathbb{E}_{\xi,\xi'\sim\mathrm{P}_Y} k_{\mathcal{Y}}(\xi,\xi')
\end{aligned}$$

Group

$$\mathcal{S}_A^{\mathrm{MMD}} = \mathbb{E}_{\mathbf{X}_A}\left(\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_A})\right) = \mathbb{E}_{\mathbf{X}_A}\mathbb{E}_{\zeta,\zeta'\sim\mathrm{P}_{Y|\mathbf{X}_A}} k_{\mathcal{Y}}(\zeta,\zeta') - \mathbb{E}_{\xi,\xi'\sim\mathrm{P}_Y} k_{\mathcal{Y}}(\xi,\xi')$$

D. 2016 & 2021, Barr & Rabitz 2022

Kernel-embedding of probability distributions for GSA: MMD

Links with Sobol': if we use the vanilla dot product kernel $k_{\mathcal{Y}}(y, y') = yy'$

$$
\begin{aligned}
\mathcal{S}_A^{\mathrm{MMD}} &= \mathbb{E}_{\mathbf{X}_A}\left(\mathbb{E}_{\xi\sim\mathrm{P}_Y}(\xi) - \mathbb{E}_{\zeta\sim\mathrm{P}_{Y|\mathbf{X}_A}}(\zeta)\right)^2 \\
&= \mathbb{E}_{\mathbf{X}_A}\left(\mathbb{E}Y - \mathbb{E}(Y|\mathbf{X}_A)\right)^2 \\
&= \mathrm{Var}\,\mathbb{E}(Y|\mathbf{X}_A)
\end{aligned}
$$

Unnormalized Sobol'

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Kernel-embedding of probability distributions for GSA: MMD

Links with Sobol': if we use the vanilla dot product kernel $k_{\mathcal{Y}}(y, y') = yy'$

$$\begin{aligned}\mathcal{S}_A^{\text{MMD}} &= \mathbb{E}_{\mathbf{X}_A}\left(\mathbb{E}_{\xi\sim \mathrm{P}_Y}(\xi) - \mathbb{E}_{\zeta\sim \mathrm{P}_{Y|\mathbf{X}_A}}(\zeta)\right)^2 \\ &= \mathbb{E}_{\mathbf{X}_A}\left(\mathbb{E}Y - \mathbb{E}(Y|\mathbf{X}_A)\right)^2 \\ &= \mathrm{Var}\,\mathbb{E}(Y|\mathbf{X}_A) \quad \text{Unnormalized Sobol'}\end{aligned}$$

Links with Sobol': if Mercer's theorem holds

$$k_{\mathcal{Y}}(y, y') = \sum_{r=1}^{\infty} \phi_r(y)\phi_r(y') \Rightarrow$$

$$\begin{aligned}\mathcal{S}_A^{\text{MMD}} &= \sum_{r=1}^{\infty}\left\{\mathbb{E}_{\mathbf{X}_A}\mathbb{E}_{\xi,\xi'\sim \mathrm{P}_{Y|\mathbf{X}_A}}\left(\phi_r(\xi)\phi_r(\xi')\right) - \mathbb{E}_{\zeta,\zeta'\sim \mathrm{P}}\left(\phi_r(\zeta)\phi_r(\zeta')\right)\right\} \\ &= \sum_{r=1}^{\infty}\left\{\mathbb{E}_{\mathbf{X}_A}\mathbb{E}\left(\phi_r(Y)|\mathbf{X}_A\right)^2 - \mathbb{E}\left(\phi_r(Y)\right)^2\right\} \\ &= \sum_{r=1}^{\infty}\mathrm{Var}\,\mathbb{E}\left(\phi_r(Y)|\mathbf{X}_A\right).\end{aligned}$$

> **Aggregation of Sobol' indices on a (possibly) infinite number of nonlinear transformations of the output**

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Kernel-embedding of probability distributions for GSA: MMD

More importantly, we have an ANOVA-like decomposition !

Theorem 3 (ANOVA decomposition for MMD). *Under the same assumptions of Theorem 1 (in particular, the random vector* $\mathbf{X}$ *has independent components) and with Assumption 1, denote* $\mathrm{MMD}^2_{\mathrm{tot}} = \mathbb{E}k_{\mathcal{Y}}(Y, Y) - \mathbb{E}k_{\mathcal{Y}}(Y, Y')$ *where* Y' *is an independent copy of* Y*. Then the total MMD can be decomposed as*

$$\mathrm{MMD}^2_{\mathrm{tot}} = \sum_{A \subseteq \mathcal{P}_d} \mathrm{MMD}^2_A$$

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$$\mathrm{MMD}^2_{\mathrm{tot}} = \sum_{A \subseteq \mathcal{P}_d} \mathrm{MMD}^2_A$$

where each term is given by

$$\mathrm{MMD}^2_A = \sum_{B \subset A} (-1)^{|A|-|B|} \mathbb{E}_{\mathbf{X}_B} \left(\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_B}) \right).$$

- **So we can define properly normalized MMD-based sensitivity indices**
- Proof is straightforward with Mercer's theorem

Kernel-embedding of probability distributions for GSA: MMD

More importantly, we have an ANOVA-like decomposition !

Definition 2 (MMD-based sensitivity indices). *In the frame of Theorem 3, let $A \subseteq \mathcal{P}_d$. The normalized MMD-based sensitivity index associated to a subset A of input variables is defined as*

$$S_A^{\mathrm{MMD}} = \frac{\mathrm{MMD}_A^2}{\mathrm{MMD}_{\mathrm{tot}}^2},$$

Impact of a subset alone

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while the total MMD-based index associated to A is

$$S_A^{T,\mathrm{MMD}} = \sum_{B \subseteq \mathcal{P}_d,\, B \cap A \neq \emptyset} S_B^{\mathrm{MMD}} = 1 - \frac{\mathbb{E}_{\mathbf{X}_{-A}}\left(\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_{-A}})\right)}{\mathrm{MMD}_{\mathrm{tot}}^2}.$$

Impact of a subset alone

Impact of a subset through all its potential interactions with others

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Impact of a subset through all its potential interactions with others

From Theorem 3, we have the fundamental identity providing the interpretation of MMD-based indices as percentage of the explained generalized variance $\text{MMD}_{\text{tot}}^2$:

$$\sum_{A \subseteq \mathcal{P}_d} S_A^{\text{MMD}} = 1.$$

Interpretation as percentage

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Kernel-embedding of probability distributions for GSA: MMD

New MMD-based sensitivity index

- **First moment-independent index with a decomposition**
- Can handle easily structured outputs
- Close generalization of Sobol' index, which is obtained as a particular case

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Estimation

- We can easily recycle estimators proposed for Sobol' indices
- Monte-Carlo, Pick-freeze, Rank, k-NN
- See D. 2021 for details

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Going further by taking a step back

Kernel-embedding of probability distributions for GSA

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$$\mathcal{S}_l = \mathbb{E}_{X_l}\left(d(\mathrm{P}_Y, \mathrm{P}_{Y|X_l})\right)$$

Other point of view

$$\begin{aligned}
\mathcal{S}_l^{KL} &= \int p_{Y|X_l=x}(y) \ln\left(\frac{p_{Y|X_l=x}(y)}{p_Y(y)}\right) p_{X_l}(x) dx dy \\
&= \int \ln\left(\frac{p_{Y,X_l}(y,x)}{p_Y(y) p_{X_l}(x)}\right) p_{Y,X_l}(y,x) dx dy \\
&= \mathrm{MI}(X_l, Y)
\end{aligned}$$

> The KL-based index actually corresponds to the mutual information between one of the inputs and the output, i.e. a measure of their dependence

Kernel-embedding of probability distributions for GSA

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Other point of view

$$\mathcal{S}_l^{KL} = \int p_{Y|X_l=x}(y)\ln\left(p_{Y|} \ldots \right. \ldots xdy$$

$$= \int \ln\left(p \ldots \right. \ldots (y, x)dxdy$$

Why not use HSIC instead?

- The KL-bas… esponds to the mutual information between one of the inputs and the output, i.e. a measure of th… nce

Kernel-embedding of probability distributions for GSA: HSIC

HSIC-based sensitivity index

$$\mathcal{S}_A^{HS} = \mathrm{HSIC}(\mathbf{X}_A, Y)$$

- Already proposed with a hand-made normalization in D. 2015
- Works very well for screening, with small sample size

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But it actually exhibits an ANOVA decomposition too

Assumption 3. *The reproducing kernel $k_{\mathcal{X}}$ of $\mathcal{F}$ is of the form*

$$k_{\mathcal{X}}(\mathbf{x}, \mathbf{x}') = \prod_{l=1}^{p} \left(1 + k_l(x_l, x_l')\right) \tag{10}$$

where for each $l = 1, \ldots, d$, $k_l(\cdot, \cdot)$ is the reproducing kernel of a RKHS $\mathcal{F}_l$ of real functions depending only on variable x_l and such that $1 \notin \mathcal{F}_l$.
In addition, for all $l = 1, \ldots, d$ and $\forall x_l \in \mathcal{X}_l$, we have

$$\int_{\mathcal{X}_l} k_l(x_l, x_l') d\mathrm{P}_{X_l}(x_l') = 0. \tag{11}$$

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Zero-mean kernel

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Needed to get orthogonality inside the RKHS

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$$k_{\mathcal{X}}(\mathbf{x}, \mathbf{x}') = \prod_{l=1}^{p} \left(1 + k_l(x_l, x_l')\right) \qquad (10)$$

Product kernel

where for each $l = 1, \ldots, d$, $k_l(\cdot, \cdot)$ is the reproducing kernel of a RKHS $\mathcal{F}_l$ of real functions depending only on variable x_l and such that $1 \notin \mathcal{F}_l$. **Without constant functions**

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Zero-mean kernel

Kernel-embedding of probability distributions for GSA: HSIC

ANOVA-like decomposition for HSIC

Theorem 4 (ANOVA decomposition for HSIC)**.** *Under the same assumptions of Theorem 1 (in particular, the random vector* $\mathbf{X}$ *has independent components) and with Assumptions 2 and 3, the HSIC dependence measure between* $\mathbf{X} = (X_1, \ldots, X_d)$ *and* Y *can be decomposed as*

$$\mathrm{HSIC}(\mathbf{X}, Y) = \sum_{A \subseteq \mathcal{P}_d} \mathrm{HSIC}_A$$

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where each term is given by

$$\mathrm{HSIC}_A = \sum_{B \subset A} (-1)^{|A|-|B|} \mathrm{HSIC}(\mathbf{X}_B, Y)$$

and $\mathrm{HSIC}(\mathbf{X}_B, Y)$ *is defined with a product RKHS* $\mathcal{H}_B = \mathcal{F}_B \times \mathcal{G}$ *with kernel* $k_B(\mathbf{x}_B, \mathbf{x}'_B) k_\mathcal{Y}(y, y') = \prod_{l \in B} (1 + k_l(x_l, x'_l))\, k_\mathcal{Y}(y, y')$ *as in (10).*

> So we can define properly normalized HSIC-based sensitivity indices

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- **So we can define properly normalized HSIC-based sensitivity indices**
- Proof relies on orthogonal decompositions in RKHS (see Appendix)

Kernel-embedding of probability distributions for GSA: HSIC

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Definition 3 (HSIC-based sensitivity indices). *In the frame of Theorem 4, let $A \subseteq \mathcal{P}_d$. The normalized HSIC-based sensitivity index associated to a subset A of input variables is defined as*

$$S_A^{\mathrm{HSIC}} = \frac{\mathrm{HSIC}_A}{\mathrm{HSIC}\left(\mathbf{X}, Y\right)},$$

Impact of a subset alone

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Impact of a subset alone

while the total HSIC-based index associated to A is

$$S_A^{T,\text{HSIC}} = \sum_{B \subseteq \mathcal{P}_d,\, B \cap A \neq \emptyset} S_B^{\text{HSIC}} = 1 - \frac{\text{HSIC}(\mathbf{X}_{-A}, Y)}{\text{HSIC}\,(\mathbf{X}, Y)}.$$

Impact of a subset through all its potential interactions with others

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Impact of a subset through all its potential interactions with others

From Theorem 4, we have the fundamental identity providing the interpretation of HSIC-based indices as percentage of the explained HSIC dependence measure between $\mathbf{X} = (X_1, \ldots, X_d)$ and Y:

$$\sum_{A \subseteq \mathcal{P}_d} S_A^{\mathrm{HSIC}} = 1.$$

Interpretation as percentage

Kernel-embedding of probability distributions for GSA: HSIC

New HSIC-based sensitivity index

- Also a decomposition
- Can handle easily structured outputs

Kernel-embedding of probability distributions for GSA: HSIC

New HSIC-based sensitivity index

- Also a decomposition
- Can handle easily structured outputs
- **Generalization of MMD-based index!**

Kernel more or less converging to a dirac

Proposition 2. *For all subset* $A \subseteq \mathcal{P}_d$*, let us define a product RKHS* $\mathcal{H}_A = \mathcal{F}_A \times \mathcal{G}$ *with kernel* $k_A(\mathbf{x}_A, \mathbf{x}'_A) k_{\mathcal{Y}}(y, y')$*. We further assume that* $\forall \mathbf{x}_A \in \mathcal{X}_A$*,* $p_{\mathbf{X}_A}(\mathbf{x}_A) > 0$ *and that*

$$k_A(\mathbf{x}_A, \mathbf{x}'_A) = \frac{1}{\sqrt{p_{\mathbf{X}_A}(\mathbf{x}_A)}\sqrt{p_{\mathbf{X}_A}(\mathbf{x}'_A)}} \prod_{l \in A} \frac{1}{h} K\left(\frac{x_l - x'_l}{h}\right) \tag{13}$$

where $K : \mathbb{R} \to \mathbb{R}$ *is a symmetric kernel function satisfying* $\int_u K(u)du = 1$*, and* $h > 0$*.*

Kernel-embedding of probability distributions for GSA: HSIC

New HSIC-based sensitivity index

- Also a decomposition
- Can handle easily structured outputs
- **Generalization of MMD-based index!**

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where $K : \mathbb{R} \to \mathbb{R}$ *is a symmetric kernel function satisfying* $\int_u K(u)du = 1$*, and* $h > 0$*. Then we have* $\forall A \subseteq \mathcal{P}_d$

$$\lim_{h \to 0} \mathrm{HSIC}(\mathbf{X}_A, Y) = \mathbb{E}_{\mathbf{X}_A}\left(\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_A})\right)$$

where $\mathrm{HSIC}(\mathbf{X}_A, Y)$ *is defined with the product RKHS* $\mathcal{H}_A = \mathcal{F}_A \times \mathcal{G}$ *and* $\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_A})$ *with the RKHS* $\mathcal{G}$*.*

Kernel-embedding of probability distributions for GSA: HSIC

New HSIC-based sensitivity index

- Also a decomposition
- Can handle easily structured outputs
- Generalization of MMD-based index !

Estimation

- Very easy, U-stat or V-stat, see Song et al. (2007); Gretton et al. (2008)

Kernel-embedding of probability distributions for GSA: HSIC

Wait a minute!

In addition, for all $l = 1, \ldots, d$ *and* $\forall x_l \in \mathcal{X}_l$, *we have*

$$\int_{\mathcal{X}_l} k_l(x_l, x_l')\mathrm{dP}_{X_l}(x_l') = 0. \qquad (11)$$

Zero-mean kernel

> **How do we build a kernel satisfying this?**

Kernel-embedding of probability distributions for GSA: HSIC

Zero-mean kernel

$$\int_{\mathcal{X}_l} k_l(x_l, x_l') d\mathrm{P}_{X_l}(x_l') = 0.$$

Easy case: inputs are uniform on [0,1]

- We can directly use famous Sobolev kernels (from SS-ANOVA, COSSO, ACOSSO, …)

$$k_l(x_l, x_l') = \frac{B_{2r}(|x_l - x_l'|)}{(-1)^{r+1}(2r)!} + \sum_{j=1}^{r} \frac{B_j(x_l)B_j(x_l')}{(j!)^2}$$

where B are Bernoulli polynomials.

- Always possible to transform independent inputs to end up with this case (via probability integral transform)
- But sensitivity index is not invariant via nonlinear transformations
- **See G. Sarazin’s talk on Wednesay (session 6A)**

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Kernel-embedding of probability distributions for GSA: HSIC

Zero-mean kernel

$$\int_{\mathcal{X}_l} k_l(x_l, x_l') d\mathrm{P}_{X_l}(x_l') = 0.$$

General case 1

- Kernels built by Durrande et al. (2012) in the context of GP models with ANOVA decomposition inside

$$k_0^D(x, x') = k(x, x') - \frac{\int k(x,t) d\mathrm{P}(t) \int k(x', t) d\mathrm{P}(t)}{\iint k(s,t) d\mathrm{P}(s) d\mathrm{P}(t)}$$

- Built from any initial kernel k
- Very nice theory, but needs numerical integration to compute the second term in general

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Kernel-embedding of probability distributions for GSA: HSIC

Zero-mean kernel

$$\int_{\mathcal{X}_l} k_l(x_l, x_l')d\mathrm{P}_{X_l}(x_l') = 0.$$

General case 2

- Kernels introduced in the context of Stein discrepancy in lieu of MMD

$$k_0^S(\mathbf{x}, \mathbf{x}') = \nabla_{\mathbf{x}}\nabla_{\mathbf{x}'}k(\mathbf{x}, \mathbf{x}') + \frac{\nabla_{\mathbf{x}}p(\mathbf{x})}{p(\mathbf{x})}\nabla_{\mathbf{x}'}k(\mathbf{x}, \mathbf{x}') + \frac{\nabla_{\mathbf{x}'}p(\mathbf{x}')}{p(\mathbf{x}')}\nabla_{\mathbf{x}}k(\mathbf{x}, \mathbf{x}') + \frac{\nabla_{\mathbf{x}}p(\mathbf{x})}{p(\mathbf{x})}\frac{\nabla_{\mathbf{x}'}p(\mathbf{x}')}{p(\mathbf{x}')}k(\mathbf{x}, \mathbf{x}')$$

- Built from any initial kernel k again, but must be differentiable this time
- Needs derivative of the log pdf of the inputs
- Means that we only need to know the pdf up to a constant
  - Trick extensively used lately (see Chris' talk)
  - **A potential interest for GSA problems where some inputs are obtained through Bayesian calibration**

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3

WHAT ABOUT DEPENDENT INPUTS ?

Shapley effects

Definition 4 (Shapley effects (Shapley, 1953)). *For any $l = 1 \ldots, d$, the Shapley effect of input X_l is given by*

$$Sh_l = \frac{1}{\operatorname{Var} Y} \frac{1}{p} \sum_{A \subseteq \mathcal{P}_d,\, A \not\ni l} \binom{p-1}{|A|}^{-1} \left\{ \operatorname{Var} \mathbb{E}\left(Y | \mathbf{X}_{A \cup \{l\}}\right) - \operatorname{Var} \mathbb{E}\left(Y | \mathbf{X}_A\right) \right\}. \tag{14}$$

This definition corresponds to the Shapley value (Shapley, 1953)

$$\phi_l = \frac{1}{p} \sum_{A \subseteq \mathcal{P}_d,\, A \not\ni l} \binom{p-1}{|A|}^{-1} \left\{ \operatorname{val}\left(A \cup \{l\}\right) - \operatorname{val}\left(A\right) \right\}$$

with value function $\operatorname{val} : \mathcal{P}_d \to \mathbb{R}_+$ *equal to* $\operatorname{val}(A) = \operatorname{Var} \mathbb{E}\left(Y | \mathbf{X}_A\right) / \operatorname{Var} Y$. *Moreover, we have the following decomposition*

$$\sum_{l=1}^{p} Sh_l = 1.$$

The only requirement is that the value function satisfies $\operatorname{val} : \mathcal{P}_d \to \mathbb{R}_+$ such that $\operatorname{val}(\emptyset) = 0$.

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GSA with dependent inputs: Shapley effects

But we have flexibility in the choice of the value function

- Reliability-oriented value function (Idrissi et al. 2021 – session 5A on Wednesday)
- **Why not plugging our kernel-based indices ?**

GSA with dependent inputs: Shapley effects

But we have flexibility in the choice of the value function

- Reliability-oriented value function (Idrissi et al. 2021 – session 5A on Wednesday)
- **Why not plugging our kernel-based indices ?**

Definition 5 (Kernel-embedding Shapley effects)**.** *For any $l = 1 \dots, d$, we define*

(a) The MMD-Shapley effect

$$Sh_l^{\mathrm{MMD}} = \frac{1}{\mathrm{MMD}^2_{\mathrm{tot}}} \frac{1}{p} \sum_{A \subseteq \mathcal{P}_d,\, A \not\ni l} \binom{p-1}{|A|}^{-1} \Big\{ \mathbb{E}_{\mathbf{X}_{A\cup\{l\}}} \left(\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_{A\cup\{l\}}}) \right) - \mathbb{E}_{\mathbf{X}_A} \left(\mathrm{MMD}^2(\mathrm{P}_Y, \mathrm{P}_{Y|\mathbf{X}_A}) \right) \Big\} \quad (15)$$

provided Assumption 1 holds.

(b) The HSIC-Shapley effect

$$Sh_l^{\mathrm{HSIC}} = \frac{1}{\mathrm{HSIC}\,(\mathbf{X}, Y)} \frac{1}{p} \sum_{A \subseteq \mathcal{P}_d,\, A \not\ni l} \binom{p-1}{|A|}^{-1} \Big\{ \mathrm{HSIC}\,(\mathbf{X}_{A\cup\{l\}}, Y) - \mathrm{HSIC}\,(\mathbf{X}_A, Y) \Big\} \quad (16)$$

provided Assumptions 2 and 3 hold.

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4

EXAMPLES

Examples

Obviously kernel indices can be used in standard GSA studies

But we believe their true potential lies in how they can handle more complex cases

- Stochastic simulators
  - Meaning the model output is a probability distribution (molecular dynamics, predictive maintenance, …)
- Functional simulators (curves, images, …)
- Multi-class outputs
  - Goal-oriented for different output regimes, or intrinsic categorical models

Examples: stochastic simulator

$$Y = (X_1 + 2X_2 + U_1)\sin(3X_3 - 4X_4 + N) + U_2 + 5X_5 B + \sum_{i=1}^{5} iX_i$$

Input variables

« Internal » random variables responsible for code stochasticity

$$X_1, \ldots, X_5 \sim \mathcal{U}(0,1)$$

$$U_1 \sim \mathcal{U}(0,1),\ U_2 \sim \mathcal{U}(1,2),\ N \sim \mathcal{N}(0,1)\quad B \sim \text{Bernoulli}(1/2)$$

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Examples: stochastic simulator

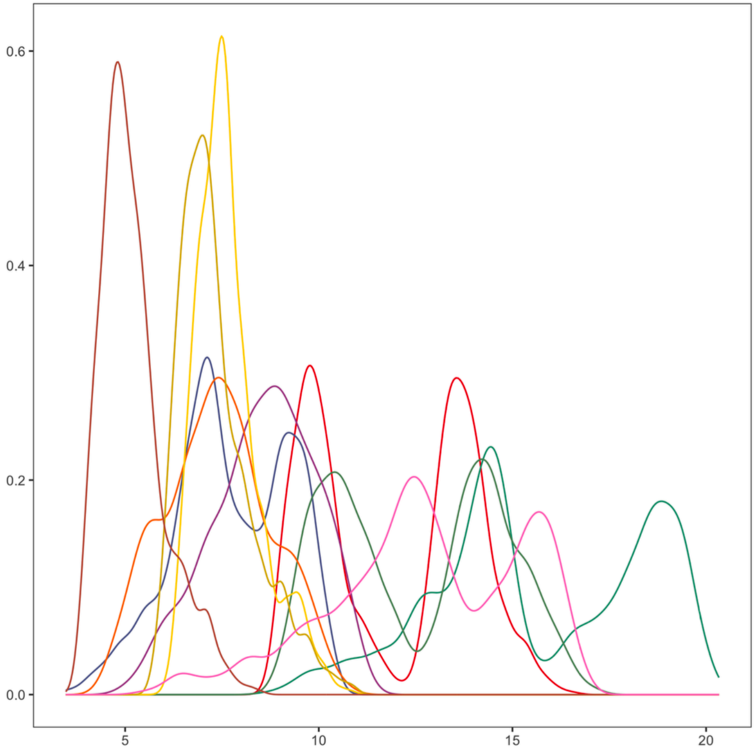


Figure 3: Stochastic simulator test case. Output probability distribution for 20 values of the input variables chosen at random. The distribution is estimated with a kernel-density estimator.

Examples: stochastic simulator

Kernel-based indices: we need to define a kernel on probability distributions

- Several options
- Histogram kernel, Wasserstein kernel, **MMD-kernel** $k_{\mathcal{Y}}(\mathrm{P},\mathrm{Q}) = \sigma^2 e^{-\lambda \mathrm{MMD}^2(\mathrm{P},\mathrm{Q})}$

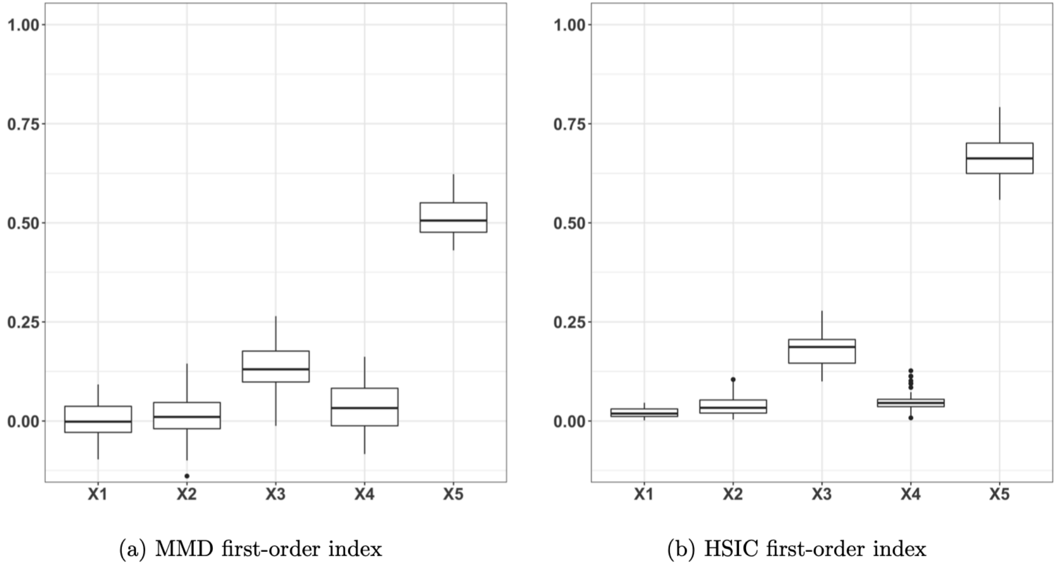
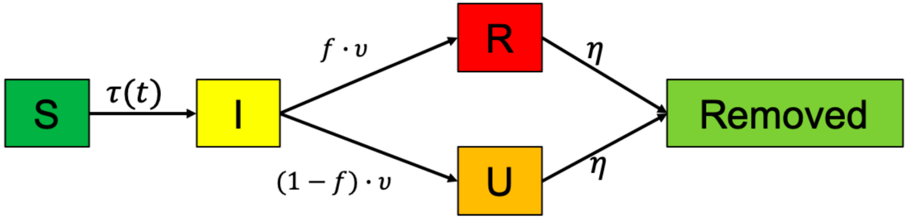


Figure 5: Stochastic simulator test case. First-order MMD (a) and HSIC (b) indices of the output distribution with rank and V-statistic estimators, respectively, $n = 200$, 50 replicates.

Examples: functional outputs

We consider a simple modified SIR model for COVID-19



$$\begin{aligned}\frac{dS}{dt} &= -\tau S(I+U)\\ \frac{dI}{dt} &= \tau S(I+U) - \nu I\\ \frac{dR}{dt} &= f\nu I - \eta R\\ \frac{dU}{dt} &= (1-f)\nu I - \eta U\end{aligned}$$

Incertain input parameters

$$CR(t) = \chi_1 \exp(\chi_2 t) - 1$$

$$I_0 = \frac{\chi_2}{f\nu},\ \ U_0 = \frac{(1-f)\nu}{\eta + \chi_2} I_0,\ \ R_0 = 1$$

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Examples: functional outputs

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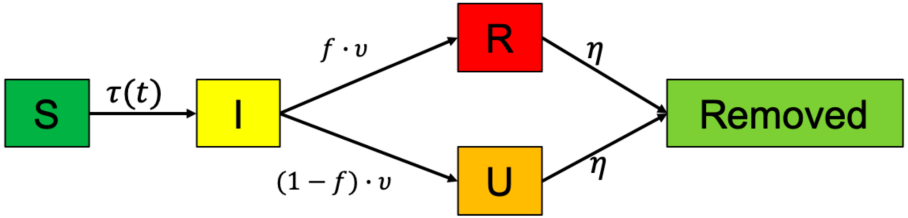

$$
\begin{aligned}
\frac{dS}{dt} &= -\tau S(I+U) \\
\frac{dI}{dt} &= \tau S(I+U) - \nu I \\
\frac{dR}{dt} &= f\nu I - \eta R \\
\frac{dU}{dt} &= (1-f)\nu I - \eta U
\end{aligned}
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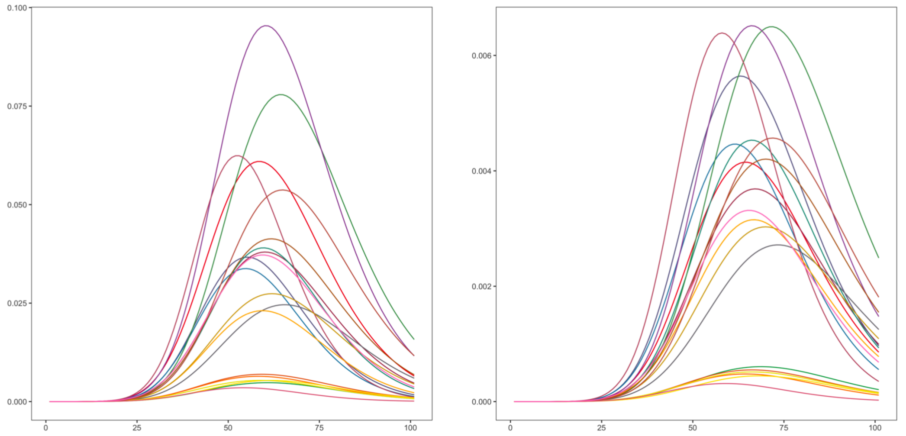


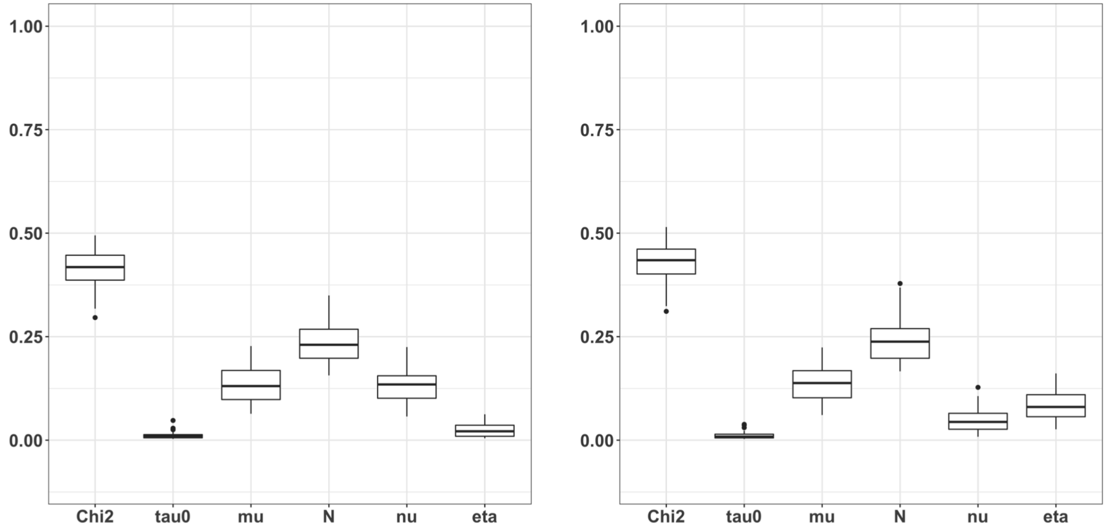
(a) Infectious cases (b) Reported cases

Figure 7: Functional simulator test case. Output dynamics over time for compartment I (left) and R (right) for 20 values of the input variables chosen at random. They are both normalized by the total population S_0.

Examples: functional outputs

Kernel-based indices: we need to define a kernel on timeseries

- Several options
- We use the **global-alignment kernel** of Cuturi (2011) inspired by dynamic-time warping



(a) First-order HSIC index for compartment I (b) First-order HSIC index for compartment R

Figure 8: Functional simulator test case. First-order HSIC index for compartments I (left) and R (right) with V-statistics estimator, $n = 200$, 50 replicates.

Conclusion & outlook

Introduction of new kernel-based sensitivity indices

- Generalizations of Sobol' indices
- But moment-independent or distributional indices
- Can easily handle more complex output types
- **With an ANOVA-like decomposition**
- More details on proofs, estimators and test cases in D. 2021 and example use in D. et al. 2021

Still room for improvement

- Theory: we heavily rely on Mercer's theorem, we will investigate if decompositions still holds without it
- Theory: CLT for our estimators would be useful to test if indices are zero
- **Practice: choice of kernels and hyperparameters**

Thank you for your attention

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5

APPENDIX

Proof outline for ANOVA decomposition of HSIC (1/2)

First assume that Mercer's theorem holds $k_{\mathcal{Y}}(y, y') = \sum_{r=1}^{\infty} \phi_r(y)\phi_r(y')$

Then write HSIC as

$$\mathrm{HSIC}(\mathbf{X}, Y) = \sum_{r=1}^{\infty} \|g^{[r]}\|_{\mathcal{F}}^2 \qquad g^{[r]}(\mathbf{x}) = \int_{\mathcal{X}} \int_{\mathcal{Y}} k_{\mathcal{X}}(\mathbf{x}, \mathbf{x}')\phi_r(y') \left[p_{\mathbf{X}Y}(\mathbf{x}', y') - p_{\mathbf{X}}(\mathbf{x}')p_Y(y')\right] d\mathbf{x}' dy'$$

Key part: orthogonal decomposition of each g function thanks to Kuo et al. (2010)

> This is where we need the strong assumptions on the input kernels

$$g^{[r]} = \sum_{A \subseteq \mathcal{P}_d} g_A^{[r]}$$

$$g_A^{[r]} = \sum_{B \subseteq A} (-1)^{|A|-|B|} P_{-B}(g^{[r]})$$

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Proof outline for ANOVA decomposition of HSIC (2/2)

We then plug the decompositions inside HSIC

$$\begin{aligned}
\mathrm{HSIC}(\mathbf{X}, Y) &= \sum_{r=1}^{\infty} \|g^{[r]}\|_{\mathcal{F}}^2 \\
&= \sum_{A \subseteq \mathcal{P}_d} \sum_{r=1}^{\infty} \|g_A^{[r]}\|_{\mathcal{F}}^2 \\
&= \sum_{A \subseteq \mathcal{P}_d} \sum_{B \subseteq A} (-1)^{|A|-|B|} \sum_{r=1}^{\infty} \|P_{-B}(g^{[r]})\|_{\mathcal{F}}^2
\end{aligned}$$

And the final result comes from rewriting the projections

$$\begin{aligned}
\sum_{r=1}^{\infty} \|P_{-B}(g^{[r]})\|_{\mathcal{F}}^2 &= \sum_{r=1}^{\infty} \int_{\mathcal{X}_B \times \mathcal{X}_B} \int_{\mathcal{Y} \times \mathcal{Y}} k_B(\mathbf{x}_B, \mathbf{x}'_B) \phi_r(y) \phi_r(y') \left[p_{\mathbf{X}_B Y}(\mathbf{x}_B, y) - p_{\mathbf{X}_B}(\mathbf{x}_B) p_Y(y)\right] \\
&\quad \left[p_{\mathbf{X}_B Y}(\mathbf{x}'_B, y') - p_{\mathbf{X}_B}(\mathbf{x}'_B) p_Y(y')\right] d\mathbf{x}_B d\mathbf{x}'_B dy dy' \\
&= \int_{\mathcal{X}_B \times \mathcal{X}_B} \int_{\mathcal{Y} \times \mathcal{Y}} k_B(\mathbf{x}_B, \mathbf{x}'_B) \left(\sum_{r=1}^{\infty} \phi_r(y) \phi_r(y') \right) \left[p_{\mathbf{X}_B Y}(\mathbf{x}_B, y) - p_{\mathbf{X}_B}(\mathbf{x}_B) p_Y(y)\right] \\
&\quad \left[p_{\mathbf{X}_B Y}(\mathbf{x}'_B, y') - p_{\mathbf{X}_B}(\mathbf{x}'_B) p_Y(y')\right] d\mathbf{x}_B d\mathbf{x}'_B dy dy' \\
&= \int_{\mathcal{X}_B \times \mathcal{X}_B} \int_{\mathcal{Y} \times \mathcal{Y}} k_B(\mathbf{x}_B, \mathbf{x}'_B) k_{\mathcal{Y}}(y, y') \left[p_{\mathbf{X}_B Y}(\mathbf{x}_B, y) - p_{\mathbf{X}_B}(\mathbf{x}_B) p_Y(y)\right] \\
&\quad \left[p_{\mathbf{X}_B Y}(\mathbf{x}'_B, y') - p_{\mathbf{X}_B}(\mathbf{x}'_B) p_Y(y')\right] d\mathbf{x}_B d\mathbf{x}'_B dy dy' \\
&= \mathrm{HSIC}(\mathbf{X}_B, Y).
\end{aligned}$$