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# Aggregated tests of independence based on HSIC measures (part 2)

European Meeting of Statisticians, 2019

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# Outline

Introduction

The aggregated testing procedure

Simulation results

Conclusion and Prospect

# Introduction

- We recall that we **study the independence of two real random vectors**  $X = (X^{(1)}, \dots, X^{(p)})$  and  $Y = (Y^{(1)}, \dots, Y^{(q)})$  with marginal densities resp. denoted  $f_1$  and  $f_2$  and joint density  $f$ .
- We recall that we have an i.i.d. sample  $\mathbb{Z}_n = (X_i, Y_i)_{1 \leq i \leq n}$  of  $(X, Y)$ .
- We rely on HSIC-based independence tests with **Gaussian kernels**  $k_\lambda$  and  $l_\mu$  resp. associated to  $X$  and  $Y$ .
- **In the previous talk**, we first proposed for each couple of values  $(\lambda, \mu)$  a **theoretical** HSIC test of independence of level  $\alpha$  in  $(0, 1)$ , followed by a **non-asymptotic permutation-based** test, of the same level  $\alpha$ .
- The **power of the permuted test** is shown to be approximately the same as **theoretical power** if enough permutations are used.

# Introduction

- When  $f - f_1 \otimes f_2$  belongs to a **Sobolev ball** with regularity  $\delta$  in  $(0, 2]$ , **sharp upper bounds** of the uniform separation rate w.r.t. the values of  $\lambda$  and  $\mu$  are provided.
- The HSIC test with the **optimal upper bound** is shown to be **mini-max** over Sobolev balls.
- This optimal test is **not adaptive**, since it depends on the regularity  $\delta$ .
- **In this talk**, we provide an **adaptive procedure of testing independence** which doesn't depend on the regularity  $\delta$ .
- This procedure is based on the **aggregation** of a collection of HSIC-tests with a collection of different bandwidths  $\lambda$  and  $\mu$ .
- Numerical studies to **assess the performance** of the procedure and to **compare methodological choices** are then provided.

## The aggregated testing procedure

- Single HSIC-based test leads to the **question of the choice of kernel bandwidths**  $\lambda$  and  $\mu$ . **Heuristic choices are adopted in practice**, with no theoretical justifications.
- We propose here an **aggregated testing procedure** combining a **collection** of single tests based on different bandwidths.
- We consider a finite or countable collection  $\Lambda \times U$  of bandwidths in  $(0, +\infty)^p \times (0, +\infty)^q$  and a collection of positive weights  $\{\omega_{\lambda, \mu} / (\lambda, \mu) \in \Lambda \times U\}$  such that  $\sum_{(\lambda, \mu) \in \Lambda \times U} e^{-\omega_{\lambda, \mu}} \leq 1$ .

## The aggregated testing procedure

- For a given  $\alpha \in (0, 1)$ , we define the aggregated test  $\Delta_\alpha$  which rejects  $(\mathcal{H}_0)$  if there is at least one  $(\lambda, \mu) \in \Lambda \times U$  such that

$$\widehat{\text{HSIC}}_{\lambda, \mu} > q_{1-u_\alpha}^{\lambda, \mu} e^{-\omega_{\lambda, \mu}},$$

where  $u_\alpha$  is the less conservative value such that the test is of level  $\alpha$ , and is defined by

$$u_\alpha = \sup \left\{ u > 0 ; P_{f_1 \otimes f_2} \left( \sup_{(\lambda, \mu) \in \Lambda \times U} \left( \widehat{\text{HSIC}}_{\lambda, \mu} - q_{1-ue}^{\lambda, \mu} e^{-\omega_{\lambda, \mu}} \right) > 0 \right) \leq \alpha \right\}.$$

- The test function  $\Delta_\alpha$  associated to this aggregated test, takes values in  $\{0, 1\}$  and is defined by

$$\Delta_\alpha = 1 \iff \sup_{(\lambda, \mu) \in \Lambda \times U} \left( \widehat{\text{HSIC}}_{\lambda, \mu} - q_{1-u_\alpha}^{\lambda, \mu} e^{-\omega_{\lambda, \mu}} \right) > 0.$$

## Oracle type conditions for the second kind error

- The aggregated testing procedure  $\Delta_\alpha$  is of **level**  $\alpha$ .
- The **second kind** error of the aggregated testing procedure  $\Delta_\alpha$  verifies the inequality

$$\mathbb{P}_f(\Delta_\alpha = 0) \leq \inf_{(\lambda, \mu) \in \Lambda \times U} \left\{ \mathbb{P}_f \left( \Delta_{\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} = 0 \right) \right\},$$

where  $\Delta_{\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu}$  is the single test of level  $\alpha e^{-\omega_{\lambda, \mu}}$  associated to the bandwidths  $(\lambda, \mu)$

- The aggregated testing procedure has a **second kind at most equal to**  $\beta$ , if there exists at least one  $(\lambda, \mu) \in \Lambda \times U$  such that the test  $\Delta_{\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu}$  has a probability of second kind error at most equal to  $\beta$ .



# Oracle type conditions for the second kind error

## THEOREM

*Let  $\alpha, \beta \in (0, 1)$ ,  $\{(k_\lambda, l_\mu) / (\lambda, \mu) \in \Lambda \times U\}$  a collection of Gaussian kernels and  $\{\omega_{\lambda, \mu} / (\lambda, \mu) \in \Lambda \times U\}$  a collection of positive weights, such that  $\sum_{(\lambda, \mu) \in \Lambda \times U} e^{-\omega_{\lambda, \mu}} \leq 1$ .*

*We assume that  $f$ ,  $f_1$  and  $f_2$  are bounded. We also assume that all bandwidths  $(\lambda, \mu)$  in  $\Lambda \times U$  verify the following conditions*

$$\max(\lambda_1 \dots \lambda_p, \mu_1 \dots \mu_q) < 1 \text{ and } n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} > \log \left( \frac{1}{\alpha} \right) > 1.$$

*Then, the uniform separation rate  $\rho(\Delta_\alpha, S_{p+q}^\delta(R), \beta)$ , where  $\delta \in (0, 2]$  and  $R > 0$  can be upper bounded as follows*

## Oracle type conditions for the second kind error

$$[\rho(\Delta_\alpha, \mathcal{S}_{p+q}^\delta(R), \beta)]^2 \leq C(M_f, p, q, \beta, \delta) \inf_{(\lambda, \mu) \in \Lambda \times U} \left\{ \frac{1}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \left( \log\left(\frac{1}{\alpha}\right) + \omega_{\lambda, \mu} \right) + \left[ \sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right] \right\}$$

where  $M_f = \max(\|f\|_\infty, \|f_1\|_\infty, \|f_2\|_\infty)$  and  $C(M_f, p, q, \beta, \delta)$  is a positive constant depending only on its arguments.

- This theorem gives an **oracle type condition** of the uniform separation rate. Indeed, without knowing the regularity of  $f - f_1 \otimes f_2$ , we prove that the uniform separation rate of  $\Delta_\alpha$  is of the same order as the smallest uniform separation rate over  $(\lambda, \mu) \in \Lambda \times U$ , up to  $\omega_{\lambda, \mu}$ .

# Adaptive procedure of testing independence

- We consider the bandwidth collections  $\Lambda$  and  $U$  defined by

$$\Lambda = \{(2^{-m_{1,1}}, \dots, 2^{-m_{1,p}}) ; (m_{1,1}, \dots, m_{1,p}) \in (\mathbb{N}^*)^p\}, \quad (1)$$

$$U = \{(2^{-m_{2,1}}, \dots, 2^{-m_{2,q}}) ; (m_{2,1}, \dots, m_{2,q}) \in (\mathbb{N}^*)^q\}. \quad (2)$$

- We associate to every  $\lambda = (2^{-m_{1,1}}, \dots, 2^{-m_{1,p}})$  in  $\Lambda$  and  $\mu = (2^{-m_{2,1}}, \dots, 2^{-m_{2,q}})$  in  $U$  the positive weights

$$\omega_{\lambda, \mu} = 2 \sum_{i=1}^p \log \left( m_{1,i} \times \frac{\pi}{\sqrt{6}} \right) + 2 \sum_{j=1}^q \log \left( m_{2,j} \times \frac{\pi}{\sqrt{6}} \right), \quad (3)$$

so that  $\sum_{(\lambda, \mu) \in \Lambda \times U} e^{-\omega_{\lambda, \mu}} = 1$ .

# Adaptive procedure of testing independence

## COROLLARY

*Assuming that  $\log \log(n) > 1$ ,  $\alpha, \beta \in (0, 1)$  and  $\Delta_\alpha$  the aggregated testing procedure, with the particular choice of  $\Lambda$ ,  $U$  and the weights  $(\omega_{\lambda, \mu})_{(\lambda, \mu) \in \Lambda \times U}$  defined in (1), (2) and (3). Then, the uniform separation rate  $\rho(\Delta_\alpha, \mathcal{S}_{p+q}^\delta(R), \beta)$  of the aggregated test  $\Delta_\alpha$  over Sobolev spaces where  $\delta$  in  $(0, 2]$ , can be upper bounded as follows*

$$\rho(\Delta_\alpha, \mathcal{S}_{p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) \left( \frac{\log \log(n)}{n} \right)^{\frac{2\delta}{4\delta + (p+q)}},$$

where  $M_f = \max(\|f\|_\infty, \|f_1\|_\infty, \|f_2\|_\infty)$ .

- The rate of the aggregation procedure over the classes of Sobolev balls is in the **same order of the smallest rate of single tests**, up to a  $\log \log(n)$  factor. This combined with the result on the **lower bound over Sobolev** shows that the **aggregated test is adaptive** over these regularity classes.

## Implementation of the aggregated procedure

- The collections  $\Lambda$  and  $U$  are finite in practice.
- The correction  $u_\alpha$  defined as

$$u_\alpha = \sup \left\{ u > 0 ; P_{f_1 \otimes f_2} \left( \sup_{(\lambda, \mu) \in \Lambda \times U} \left( \widehat{\text{HSIC}}_{\lambda, \mu} - q_{1-ue^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) > 0 \right) \leq \alpha \right\}.$$

can be approached by a permutation method with Monte Carlo approximation, as done in [Albert et al., 2015](#).

- **To compute the quantiles**  $\hat{q}_{1-ue^{-\omega_{\lambda, \mu}}}^{\lambda, \mu}$ , we generate uniformly  $B_1$  independent random permutations  $\tau_1, \dots, \tau_{B_1}$ , independent of  $\mathbb{Z}_n$ . We then compute for each  $(\lambda, \mu) \in \Lambda \times U$  and each  $u > 0$  the permuted quantile **with Monte Carlo approximation**  $\hat{q}_{1-ue^{-\omega_{\lambda, \mu}}}^{\lambda, \mu}$ .

## Implementation of the aggregated procedure

- **To compute the probability  $P_{f_1 \otimes f_2}$** , we generate uniformly  **$B_2$**  independent random permutations  $\kappa_1, \dots, \kappa_{B_2}$ , independent of  $\mathbb{Z}_n$ . Denote for all permutation  $\kappa_b$ , the corresponding permuted statistic

$$\widehat{H}_{\lambda, \mu}^{\kappa_b} = \widehat{\text{HSIC}}_{\lambda, \mu}(\mathbb{Z}_n^{\kappa_b}).$$

- Then, the correction  $u_\alpha$  is approached by

$$\hat{u}_\alpha = \sup \left\{ u > 0 ; \frac{1}{B_2} \sum_{b=1}^{B_2} \mathbb{1}_{\max_{(\lambda, \mu) \in \Lambda \times U} \left\{ \widehat{H}_{\lambda, \mu}^{\kappa_b} - \hat{q}_{1-ue^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right\} > 0} \leq \alpha \right\}. \quad (4)$$

- The supremum in Equation (4) is estimated by **dichotomy**.
- **Simulation result:** the powers of the implemented and the theoretical procedures are **approximately the same if enough permutation** are used.

## Analytical examples

Dependence forms from [Berrett and Samworth., 2017](#):

**(i).** Defining the joint density  $f_l, l = 1, \dots, 10$  of  $(X, Y)$  on  $[-\pi, \pi]$  by

$$f_l(x, y) = \frac{1}{4\pi^2} \{1 + \sin(lx) \sin(ly)\}.$$

**(ii).** Considering  $X$  and  $Y$  as

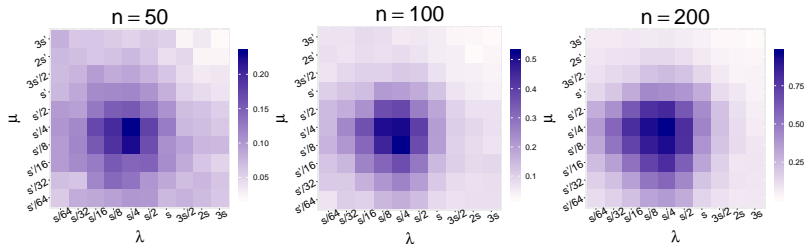
$$X = L \cos \Theta + \frac{\varepsilon_1}{4}, \quad Y = L \sin \Theta + \frac{\varepsilon_2}{4},$$

where  $L, \Theta, \varepsilon_1$  and  $\varepsilon_2$  are independent, with  $L \sim \mathcal{U}\{1, \dots, l\}$  for  $l = 1, \dots, 10$ ,  $\Theta \sim \mathcal{U}[0, 2\pi]$  and  $\varepsilon_1, \varepsilon_2 \sim \mathcal{N}(0, 1)$ .

**(iii).** Defining  $X \sim \mathcal{U}[-1, 1]$ . For a given  $\rho = 0.1, 0.2, \dots, 1$ ,  $Y$  is defined as  $Y = |X|^\rho \varepsilon$ , where  $\varepsilon \sim \mathcal{N}(0, 1)$  independent with  $X$ .

# Collection of bandwidths

- **Choice of collections  $\Lambda$  and  $U$ :** recommendation of dyadic collection, multiple and dividers by powers of 2 of the  $X$  and  $Y$  standard deviations (respectively noted  $s$  and  $s'$  in Figure 1).

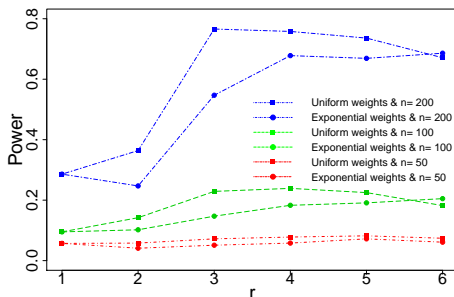


**FIGURE 1:** Analytical example (ii),  $l = 2$ . Power map of single HSIC test w.r.t. to kernel widths  $\lambda$  and  $\mu$  respectively associated to  $X$  and  $Y$ , for sample sizes  $n = 50, 100$  and  $200$ .



## Weights associated to the collection

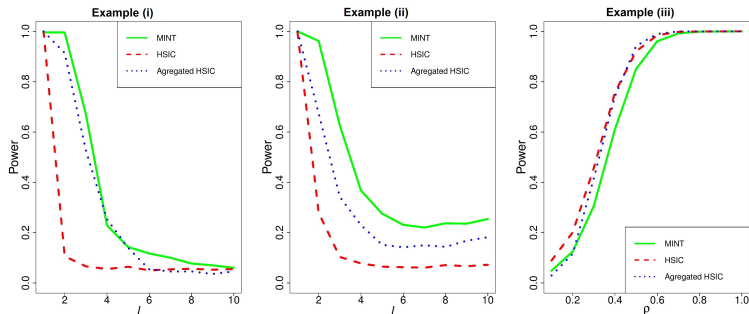
- **Choice of weights:** comparison of **uniform** and **exponential decreasing** weights in Figure 2.



**FIGURE 2:** Analytical example (ii),  $l = 2$ . Power of aggregated procedures with uniform and exponential weights, w.r.t. the number  $r$  of aggregated widths in each direction, for sample sizes  $n = 50, 100$  and  $200$ .

## Comparison with other independence tests

- **Comparison with** Single HSIC using the permutation method (De Lozzo et Marrel, 2016; Meynaoui et al., 2019) and the Mutual Information Test (MINT, Berrett et Samworth, 2017).



**FIGURE 3:** Power curves of MINT, single HSIC test and aggregated procedure for the mechanisms of dependence (i), (ii) and (iii).

## Conclusion and Prospect

- Proposition of a test procedure based on **aggregating single HSIC tests** with different choices of bandwidths.
- Procedure **adaptive over Sobolev balls**, i.e. achieving the optimal uniform separation rate and does not depend on any regularity parameter.
- Encouraging results (on terms of test power) on some analytical examples.

### Some possible improvements:

- **Extend** the aggregation procedure to **other characteristic kernels** and **other types of random variables** (e.g. discrete variables).
- **Extend** the aggregation procedure to **other types of experimental designs** such as Quasi-Monte Carlo and Space Filling Designs.
- A confrontation of the methodology to a **real data case** is in progress. Data stem from an **industrial case simulating a severe nuclear reactor accidental scenario**.

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