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Aggregated test of independence based on HSIC measures

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Abstract

Dependence measures based on reproducing kernel Hilbert spaces, also known as Hilbert-Schmidt Independence Criterion and denoted HSIC, are widely used to statistically decide whether or not two random vectors are dependent. Recently, non-parametric HSIC-based statistical tests of independence have been performed. However, these tests lead to the question of prior choice of the kernels associated to HSIC, there is as yet no method to objectively select specific kernels. In order to avoid a particular kernel choice, we propose a new HSIC-based aggregated procedure allowing to take into account several Gaussian kernels. To achieve this, we first propose non-asymptotic single tests of level $\alpha \in (0, 1)$ and second type error controlled by $\beta \in (0, 1)$. We also provide a sharp upper bound of the uniform separation rate of the proposed tests. Thereafter, we introduce a multiple testing procedure in the case of Gaussian kernels, considering a set of various parameters. These aggregated tests are shown to be of level α and to overperform single tests in terms of uniform separation rates.

1 Introduction

In this paper, we study the problem of testing the independence of two random vectors $X = (X^{(1)}, \dots, X^{(p)}) \in \mathbb{R}^p$ and $Y = (Y^{(1)}, \dots, Y^{(q)}) \in \mathbb{R}^q$. Let us first introduce some notations and assumptions. The couple (X, Y) is assumed to have a joint density f w.r.t. Lebesgue measure on \mathbb{R}^{p+q} . The probability measure associated to this density is denoted P_f . The marginal densities of X and Y are respectively denoted f_1 and f_2 . We also denote by $f_1 \otimes f_2$, the product of the marginal densities f_1 and f_2 , defined as follows:

$$f_1 \otimes f_2 : (x, y) \in \mathbb{R}^p \times \mathbb{R}^q \mapsto f_1(x)f_2(y).$$

By analogy with the notation P_f , the notation $P_{f_1 \otimes f_2}$ designates the probability measure associated to $f_1 \otimes f_2$. The density f is assumed to be unknown as well as the marginales f_1 and f_2 . We also assume that we have a n -sample $(X_1, Y_1), \dots, (X_n, Y_n)$ of i.i.d random variables with common density f . We address here the question of testing the null hypothesis (\mathcal{H}_0) : “ X and Y are independent” against the alternative (\mathcal{H}_1) : “ X and Y are dependent”. That is equivalent to test

$$(\mathcal{H}_0): “f = f_1 \otimes f_2” \quad \text{against} \quad (\mathcal{H}_1): “f \neq f_1 \otimes f_2”.$$

Throughout this document, the densities f , f_1 and f_2 are assumed to be bounded and M_f denotes the maximum of their infinity norms: $M_f = \max\{\|f\|_\infty, \|f_1\|_\infty, \|f_2\|_\infty\}$.

Non parametric tests of independence. To test independence between X and Y , many approaches have been explored in the last few decades. Among them, [Hoeffding, 1948] proposes an independence test based on the difference between the distribution function of (X, Y) and the product of the marginal distribution functions. This test has good properties in the asymptotic framework: consistent and distribution-free under the null hypothesis. But, it is only designated to univariate random

variables ($p = q = 1$). Moreover, the statistic of this test is not practical to estimate. The authors of [Bergsma et al., 2014] propose an improvement of Hoeffding’s test, which is also applicable to discrete random variables. Besides, the statistic associated to this test is easier to estimate than Hoeffding’s one. Lately, [Weihs et al., 2018] propose to extend Hoeffding’s test to the case of multivariate random variables. The estimation of the associated statistic requires a prior partition of the sample $(X_i, Y_i)_{1 \leq i \leq n}$ space. Still, the chosen partition highly impacts the quality of the test, and there is no theoretical method to objectively choose this partition. Another classical method for testing independence between X and Y is based on comparing the joint density f and the product of the marginales $f_1 \otimes f_2$ [Ahmad and Li, 1997, Rosenblatt and Wahlen, 1992]. For this, an intermediate step is to estimate these densities using the kernel-based method of Parzen-Rosenblatt [Parzen, 1962]. The major drawback of this method is that the convergence is slow for high dimensions i.e. when $p + q$ is large (this fact is also called the *curse of dimensionality*, see e.g. [Scott, 2012]). This approach is therefore not feasible in the case of high dimensions with limited sample size. More recently, many approaches based on Reproducing Kernel Hilbert Spaces (RKHS, see [Aronszajn, 1950] for more details) have been developed. In particular, several RKHS-based dependence measures have been proposed. These measures have all the characteristic (under certain conditions on kernels) to be zero if and only if X and Y are independent. We mention the Kernel Canonical Correlation (KCC), first introduced in [Bach and Jordan, 2002]. It has been shown that this measure characterizes independence in the case of Gaussian kernels (see [Bach and Jordan, 2002] for more details). Unfortunately, the estimation of KCC requires an extra regularisation which is not practical. Other dependence measures, easier to estimate and characterizing independence for a largest class of RKHS kernels: *universal kernels* [Micchelli et al., 2006] have been proposed later. For instance, the Kernel Mutual Information (KMI) [Gretton et al., 2003, Gretton et al., 2005b] and the Constrained covariance (COCO) [Gretton et al., 2005c, Gretton et al., 2005b], which are relatively easy to interpret and implement, have been widely used. Last but not least, one of the most interesting kernel dependence measure is the Hilbert-Schmidt Independence Criterion (HSIC) [Gretton et al., 2005a]. The HSIC is very easy to compute and overperforms both analytically and numerically all previous kernel-based dependence measures [Gretton et al., 2005a]. Furthermore, beyond the good quality of a given dependence measure, a straightforward interpretation of its estimated value, may not be enough to discern the dependence from the independence. To further study the independence between X and Y , independence tests based on these measures can be used. The first RKHS-based statistical test for independence is proposed by [Gretton et al., 2008]. This statistical test was proposed in an asymptotic framework for HSIC measures using the distributions of HSIC estimators under (\mathcal{H}_0) and under (\mathcal{H}_1) . These tests remain by far the most commonly used kernel-based tests for independence. A generalisation of this test for the joint and mutual independence of several random variables is presented in [Pfister et al., 2018]. We also mention the RKHS-based test [Póczos et al., 2012], inspired from [Gretton et al., 2008]. This test is based on a new dependence measure called Copula-based kernel dependency measure. Yet, this measure seems more difficult to estimate than the HSIC. Lately, the distance covariance which is based on the difference between the characteristic function of (X, Y) and the product of the marginal characteristic functions has been introduced in [Székely et al., 2007]. The distance covariance has good properties and has been used to study the independence between random variables of high dimensions [Székely and Rizzo, 2013, Yao et al., 2018]. Furthermore, it has been shown that the distance covariance is not truly a new dependence measure. Indeed, this measure is none other than HSIC with specific choice of the kernels. We also mention the statistical test of independence based on the kernel mutual information recently proposed by [Berrett and Samworth, 2017]. This new statistical test seems to achieve comparable results with the classical tests based on HSIC. Still, the implementation of this test is more difficult and time-consuming. For all these reasons, we focus in this paper on HSIC measures to test independence between X and Y .

Review on HSIC measures. The definition of the HSIC is derived from the notion of cross-covariance operator [Fukumizu et al., 2004], which can be seen as a generalisation of the classical covariance, measuring many forms of dependence between X and Y (not only linear ones). For this, [Gretton et al., 2005a] associate to X a RKHS \mathcal{F} composed of fonctions mapping from \mathbb{R}^p to \mathbb{R} (\mathcal{F} is a set of transformations for X), and characterized a scalar product $\langle \cdot, \cdot \rangle_{\mathcal{F}}$. The same operation is carried out for Y , considering a RKHS denoted \mathcal{G} and a scalar product $\langle \cdot, \cdot \rangle_{\mathcal{G}}$. The cross-covariance operator $C_{X,Y}$ associated to RKHS \mathcal{F} and \mathcal{G} is the operator mapping from \mathcal{G} to \mathcal{F} and verifying for all

$(F, G) \in \mathcal{F} \times \mathcal{G}$,

$$\langle F, C_{X,Y}(G) \rangle_{\mathcal{F}} = \text{Cov}(F(X), G(Y)).$$

Designating by $(u_i)_i$ and $(v_j)_j$ respectively orthonormal bases of \mathcal{F} and \mathcal{G} , the HSIC between X and Y is the square of the operator's $C_{X,Y}$ Hilbert-Schmidt norm [Gretton et al., 2005a] defined as

$$\text{HSIC}(X, Y) = \|C_{X,Y}\|_{\text{HS}}^2 = \sum_{i,j} \langle u_i, C_{X,Y}(v_j) \rangle_{\mathcal{F}}^2 = \sum_{i,j} \text{Cov}(u_i(X), v_j(Y))^2.$$

The fundamental idea behind this definition is that $\text{HSIC}(X, Y)$ is zero if and only if $\text{Cov}(F(X), G(Y)) = 0$ for all $(F, G) \in \mathcal{F} \times \mathcal{G}$. Furthermore, we already know (see e.g. [Jacod and Protter, 2012]) that X and Y are independent if and only if $\text{Cov}(F(X), G(Y)) = 0$ for all bounded and continuous functions F and G . It follows that, for well chosen RKHS, the nullity of the HSIC characterizes independence. Before giving such a condition, we recall that [Gretton et al., 2005a] expressed $\text{HSIC}(X, Y)$ in a very convenient form, using kernels k and l respectively associated to \mathcal{F} and \mathcal{G} ,

$$\begin{aligned} \text{HSIC}(X, Y) &= \mathbb{E}[k(X, X')l(Y, Y')] + \mathbb{E}[k(X, X')] \mathbb{E}[l(Y, Y')] \\ &\quad - 2\mathbb{E}[\mathbb{E}[k(X, X') | X] \mathbb{E}[l(Y, Y') | Y]], \end{aligned} \quad (1)$$

where (X', Y') is an independent and identically distributed copy of (X, Y) . Note that $\text{HSIC}(X, Y)$ only depends on the density f of (X, Y) . We thus denote it $\text{HSIC}(f)$ in the following.

Authors of [Gretton et al., 2005a] showed that a sufficient condition so that the nullity of the associated HSIC is characteristic of independence is that the RKHS \mathcal{F} (resp. \mathcal{G}) induced by k and (resp. l) is dense in the space of bounded and continuous functions mapping from \mathbb{R}^p (resp. \mathbb{R}^q) to \mathbb{R} . These kernels are called universal [Michelli et al., 2006]. Among this class of kernels, the most commonly used are Gaussian kernels [Steinwart, 2001]. We consider in the rest of this paper Gaussian kernels. Let us introduce some notations. We denote by g_s the density of the standard Gaussian distribution on \mathbb{R}^s defined for all $x \in \mathbb{R}^s$ by

$$g_s(x) = \frac{1}{(2\pi)^{s/2}} \exp\left(-\frac{1}{2} \sum_{i=1}^s x_i^2\right). \quad (2)$$

For any bandwidths $\lambda = (\lambda_1, \dots, \lambda_p) \in (0, +\infty)^p$ and $\mu = (\mu_1, \dots, \mu_q) \in (0, +\infty)^q$, we define for any $x \in \mathbb{R}^p$ and $y \in \mathbb{R}^q$,

$$\varphi_\lambda(x) = \frac{1}{\lambda_1 \dots \lambda_p} g_p\left(\frac{x_1}{\lambda_1}, \dots, \frac{x_p}{\lambda_p}\right), \quad (3)$$

$$\phi_\mu(y) = \frac{1}{\mu_1 \dots \mu_q} g_q\left(\frac{y_1}{\mu_1}, \dots, \frac{y_q}{\mu_q}\right). \quad (4)$$

Finally, we define the Gaussian kernels, for $x, x' \in \mathbb{R}^p$ and $y, y' \in \mathbb{R}^q$,

$$k_\lambda(x, x') = \varphi_\lambda(x - x'), \quad l_\mu(y, y') = \phi_\mu(y - y').$$

We denote by $\text{HSIC}_{\lambda,\mu}(f)$ the HSIC measure defined in (1), where the kernels k and l are respectively the Gaussian kernels k_λ and l_μ .

In practice, the computation of $\text{HSIC}_{\lambda,\mu}(f)$ is not feasible, since it depends on the unknown density f . Given an i.i.d n -sample $(X_i, Y_i)_{1 \leq i \leq n}$ with common density f , $\text{HSIC}_{\lambda,\mu}(f)$ can be estimated by estimating each expectation of Equation (1). For this, we introduce the following U -statistics, respectively with order 2, 3 and 4,

$$\begin{aligned} \widehat{\text{HSIC}}_{\lambda,\mu}^{(2)} &= \frac{1}{n(n-1)} \sum_{(i,j) \in \mathbf{i}_2^n} k_\lambda(X_i, X_j) l_\mu(Y_i, Y_j), \\ \widehat{\text{HSIC}}_{\lambda,\mu}^{(3)} &= \frac{1}{n(n-1)(n-2)} \sum_{(i,j,r) \in \mathbf{i}_3^n} k_\lambda(X_i, X_j) l_\mu(Y_j, Y_r), \end{aligned}$$

and

$$\widehat{\text{HSIC}}_{\lambda,\mu}^{(4)} = \frac{1}{n(n-1)(n-2)(n-3)} \sum_{(i,j,q,r) \in \mathbf{i}_4^n} k_\lambda(X_i, X_j) l_\mu(Y_q, Y_r),$$

where \mathbf{i}_r^n is the set of all r -tuples drawn without replacement from the set $\{1, \dots, n\}$. We estimate $\text{HSIC}_{\lambda,\mu}(f)$ by the U -statistic

$$\widehat{\text{HSIC}}_{\lambda,\mu} = \widehat{\text{HSIC}}_{\lambda,\mu}^{(2)} + \widehat{\text{HSIC}}_{\lambda,\mu}^{(4)} - 2\widehat{\text{HSIC}}_{\lambda,\mu}^{(3)}. \quad (5)$$

Such estimators of the HSIC have been used to construct independence tests. A first asymptotic test of level $\alpha \in (0, 1)$ has been proposed by [Gretton et al., 2008]. For this, the authors show that under (\mathcal{H}_0) , the asymptotic distribution of the HSIC estimator can be approximated by a Gamma distribution with parameters which are easy to estimate. Furthermore, [Gretton and Györfi, 2010] also show the asymptotic consistency of the test (the convergence to one of the power under any reasonable alternative). However, there are two main disadvantages of this testing procedure. Firstly, it is purely asymptotic in the sense that the critical value of the test is obtained from an approximation of the asymptotic distribution under (\mathcal{H}_0) . In particular, the first kind error is controlled only in the asymptotic framework. Secondly, only an heuristic choice of the bandwidths λ and μ is proposed with no theoretical guarantees. In order to avoid such an arbitrary choice, we consider aggregated procedures which may lead to adaptive tests.

Towards adaptivity. To avoid the unjustified choice of the bandwidths λ and μ , a first step is to define a criterion allowing to compare the performances of the HSIC-tests associated to different bandwidths. For this, we consider the *uniform separation rate* as defined in [Baraud et al., 2003]. For any level- α test Δ_α with values in $\{0, 1\}$, rejecting independence when $\Delta_\alpha = 1$, the uniform separation rate $\rho(\Delta_\alpha, \mathcal{C}_\delta, \beta)$ of the test Δ_α , over a class \mathcal{C}_δ of alternatives f such that $f - f_1 \otimes f_2$ satisfies smoothness assumptions, with respect to the \mathbb{L}_2 -norm, is defined for all β in $(0, 1)$ by

$$\rho(\Delta_\alpha, \mathcal{C}_\delta, \beta) = \inf \left\{ \rho > 0, \sup_{f \in \mathcal{F}_\rho(\mathcal{C}_\delta)} \mathbb{P}_f(\Delta_\alpha = 0) \leq \beta \right\}, \quad (6)$$

where $\mathcal{F}_\rho(\mathcal{C}_\delta) = \{f, f - f_1 \otimes f_2 \in \mathcal{C}_\delta, \|f - f_1 \otimes f_2\|_{L_2} > \rho\}$.

The uniform separation rate is then the smallest value in the sense of the \mathbb{L}_2 -norm of $f - f_1 \otimes f_2$ (the difference between the joint density and the product of marginales) allowing to control the 2^{nd} -kind error of the test by β . This definition is naturally the non-asymptotic version of the *critical radius* defined and studied for several examples in a serie of Ingster papers (see e.g. [Ingster, 1993a, Ingster, 1996]). A test of level α having the optimal performances, should then have the smallest possible uniform separation rate (up to a multiplicative constant) over \mathcal{C}_δ . These tests are generally called *optimal in the minimax sense*. The problem of non-asymptotic minimax rate of testing was raised in many papers over the past years. Among them, we mention for example [Ingster and Suslina, 1998, Laurent et al., 2012] for minimax detection of signals and [Donoho et al., 1996, Kerkycharian and Picard, 1993] for minimax density estimation. However, only few works exist already for the problem of minimax independence testing. The notable works are those of Ingster [Ingster, 1989, Ingster, 1993b] and those of Yodé [Yodé, 2004, Yodé, 2011]. Still, these works are provided in the asymptotic framework. As far as we know, no minimax rate of testing independence was yet proved in the non-asymptotic framework. Furthermore, beyond the problem of minimax rate, the straightforward practical construction of a minimax test is impossible. Indeed, this construction depends on the unknown smoothness parameters defining the space \mathcal{C}_δ . The objective is then to construct a minimax test which does not need any smoothness property to be implemented. These tests are called *minimax adaptive* (or assumption free). It has been shown that a standard logarithmic price is sometimes inevitable for adaptivity [Spokoiny et al., 1996]. The problem of adaptivity has received a good attention in the literature. We mention for instance [Baraud et al., 2003] for testing a linear regression model with normal noise and [Butucea and Tribouley, 2006] for testing the equality of two samples densities. For the specific case of testing independence, the adaptive testing procedure proposed in [Yodé, 2011] seems to be the only currently existing. As mentioned above this test is

purely asymptotic, but we are interested here in the non-asymptotic framework. Recently, an interesting approach of testing proposed in [Fromont et al., 2013], consists on testing the equality of intensities of two poisson processes by aggregating several kernels in a unique testing procedure. It has been shown in [Fromont et al., 2013] that this testing procedure is adaptive over several regularity spaces. Inspired by these works, and following the work of [Gretton et al., 2008, Gretton and Györfi, 2010], we consider in this paper a procedure of testing independence based on HSIC measures and aggregating a given set of Gaussian-kernel HSIC tests. Firstly, this procedure allows to avoid a particular kernel for HSIC-tests. Secondly, we show in this paper that the rate of this testing procedure over particular Sobolev and Nikol'skii-Besov balls can be upper bounded by a rate which seems optimal compared to "classical" rates of testing in other frameworks. This suggests that this test may be adaptive over these spaces of regularity.

In this paper, we first study a theoretical test (in the sense the critical value depends on the unknown marginal densities f_1 and f_2) based on such estimators of the HSIC, for which we provide non-asymptotic conditions to control the second kind error. The study of this theoretical test allows us to introduce a new procedure based on the aggregation of these tests for various bandwidths avoiding the arbitrary choice of those parameters. We provide non-asymptotic theoretical guarantees for this aggregated procedure by proving that they satisfy a non-asymptotic oracle type condition for the uniform separation rate and outperform single tests. Notice that in practice, we consider a permutation approach allowing to implement the aggregated testing procedure, leading to a test with non-asymptotic prescribed level α . We complete this study by establishing non-asymptotic uniform separation rates over Sobolev balls and Nikol'skii-Besov balls. This document is organized as follows: in Section 2, we first give in Section 2.1 a non-asymptotic condition on f in terms of the theoretical value $\text{HSIC}_{\lambda,\mu}(f)$ so that the second error type of the single test associated to λ and μ is controlled. We then provide in Section 2.2 such condition w.r.t parameters λ , μ and the sample size n . Finally, we give in Section 2.4 a sharp upper bound of the separation rate of single tests. In Section 3, we present in Section 3.1 the aggregated testing procedure. Thereafter, we give in Section 3.2 an oracle type inequality of the separation rate of the aggregated test. In Section 3.3, we consider two particular classes of functions: Sobolev balls and Nikol'skii-Besov balls, showing that the uniform separation rate of a well chosen aggregated test is as the same order as the optimal single one, up to a small factor of $\log \log(n)$.

All along the paper, the generic notation $C(a, b, \dots)$ denotes a positive constant depending only on its arguments (a, b, \dots) and that may vary from line to line.

2 Single kernel-based tests

2.1 The testing procedures

A first theoretical test. Since Gaussian kernels are characteristic, testing independence between X and Y is equivalent to test

$$(\mathcal{H}_0) : \text{HSIC}_{\lambda,\mu}(f) = 0 \quad \text{against} \quad (\mathcal{H}_1) : \text{HSIC}_{\lambda,\mu}(f) > 0.$$

The statistic $\widehat{\text{HSIC}}_{\lambda,\mu}$ is then a natural choice to test independence between X and Y , since it is an unbiased estimator of $\text{HSIC}_{\lambda,\mu}(f)$. The corresponding test rejects independence if $\widehat{\text{HSIC}}_{\lambda,\mu}$ is significantly large. Specifically, for $\alpha \in]0, 1[$, we consider the statistical test which rejects (\mathcal{H}_0) if $\widehat{\text{HSIC}}_{\lambda,\mu} > q_{1-\alpha}^{\lambda,\mu}$, where $q_{1-\alpha}^{\lambda,\mu}$ denotes the $(1-\alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda,\mu}$ under $P_{f_1 \otimes f_2}$. The associated test function is defined by

$$\Delta_\alpha^{\lambda,\mu} = \mathbb{1}_{\widehat{\text{HSIC}}_{\lambda,\mu} > q_{1-\alpha}^{\lambda,\mu}}. \quad (7)$$

Then, the null hypothesis is rejected if and only if $\Delta_\alpha^{\lambda,\mu} = 1$. By definition of the quantile, this theoretical test is of non-asymptotic level α , that is if $f = f_1 \otimes f_2$,

$$P_f(\Delta_\alpha^{\lambda,\mu} = 1) \leq \alpha.$$

Note that the non-asymptotic test $\Delta_\alpha^{\lambda,\mu}$ is defined here using the quantiles as in [Albert et al., 2015] rather than the p-values

A permutation test of independence. The analytical computation of the quantile $q_{1-\alpha}^{\lambda,\mu}$ is not possible since its value depends on the unknown marginals f_1 and f_2 of the couple (X, Y) . In practice, a permutation method with a Monte Carlo approximation is applied to approach $q_{1-\alpha}^{\lambda,\mu}$ as follows. Denote $\mathbb{Z}_n = (X_i, Y_i)_{1 \leq i \leq n}$ the original sample and compute the test statistic $\widehat{\text{HSIC}}_{\lambda,\mu}(\mathbb{Z}_n)$ defined by Equation (5). Then, consider B independent and uniformly distributed random permutations of $\{1, \dots, n\}$, denoted τ_1, \dots, τ_B , independent of \mathbb{Z}_n . Define for each permutation τ_b the corresponding permuted sample $\mathbb{Z}_n^{\tau_b} = (X_i, Y_{\tau_b(i)})_{1 \leq i \leq n}$ and compute the permuted test statistic

$$\widehat{H}_{\lambda,\mu}^{*b} = \widehat{\text{HSIC}}_{\lambda,\mu}(\mathbb{Z}_n^{\tau_b})$$

on this new sample.

Under $P_{f_1 \otimes f_2}$, each permuted sample $\mathbb{Z}_n^{\tau_b}$ has the same distribution than the original sample \mathbb{Z}_n . Hence, the random variables $\widehat{H}_{\lambda,\mu}^{*b}$, $1 \leq b \leq B$, have the same distribution as $\widehat{\text{HSIC}}_{\lambda,\mu}$. We apply a trick, based on [Romano and Wolf, 2005, Lemma 1], which consists in adding the original sample to the Monte Carlo sample in order to obtain a test of non-asymptotic level α . To do so, denote

$$\widehat{H}_{\lambda,\mu}^{*B+1} = \widehat{\text{HSIC}}_{\lambda,\mu}, \quad \text{and} \quad \widehat{H}_{\lambda,\mu}^{*(1)} \leq \widehat{H}_{\lambda,\mu}^{*(2)} \leq \dots \leq \widehat{H}_{\lambda,\mu}^{*(B+1)}$$

the order statistic. Then, the permuted quantile with Monte Carlo approximation $\widehat{q}_{1-\alpha}^{\lambda,\mu}$ is thus defined as

$$\widehat{q}_{1-\alpha}^{\lambda,\mu} = \widehat{H}_{\lambda,\mu}^{*(\lceil (B+1)(1-\alpha) \rceil)}. \quad (8)$$

The permuted test with Monte Carlo approximation $\widehat{\Delta}_\alpha^{\lambda,\mu}$ performed in practice is then defined as

$$\widehat{\Delta}_\alpha^{\lambda,\mu} = \mathbb{1}_{\widehat{\text{HSIC}}_{\lambda,\mu} > \widehat{q}_{1-\alpha}^{\lambda,\mu}}. \quad (9)$$

Proposition 1.

Let α be in $]0, 1[$ and $\widehat{\Delta}_\alpha^{\lambda,\mu}$ the test defined by Equation (9). Then, under $P_{f_1 \otimes f_2}$, that is if $f = f_1 \otimes f_2$,

$$P_f \left(\widehat{\Delta}_\alpha^{\lambda,\mu} = 1 \right) \leq \alpha, \quad (10)$$

that is, this permuted test with Monte Carlo approximation is of prescribed non-asymptotic level α .

2.2 Control of the second kind error in terms of HSIC

For given $\beta \in (0, 1)$, we propose in the following lemma a first non-asymptotic condition on the alternative f ensuring that the probability of second kind error of the theoretical test under such f is at most equal to β . This condition is given for the value of $\text{HSIC}_{\lambda,\mu}(f)$. It involves the variance of the estimator $\widehat{\text{HSIC}}_{\lambda,\mu}$ which is finite since this estimator is a bounded random variable.

Lemma 1.

Let $(X_i, Y_i)_{1 \leq i \leq n}$ be an i.i.d. sample with distribution P_f and consider the test statistic $\widehat{\text{HSIC}}_{\lambda,\mu}$ defined by (5). Let α, β in $(0, 1)$, and $q_{1-\alpha}^{\lambda,\mu}$ be the $(1-\alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda,\mu}$ under $P_{f_1 \otimes f_2}$ as defined in Section 2.1. Then $P_f(\widehat{\text{HSIC}}_{\lambda,\mu} \leq q_{1-\alpha}^{\lambda,\mu}) \leq \beta$ as soon as

$$\text{HSIC}_{\lambda,\mu}(f) > \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} + q_{1-\alpha}^{\lambda,\mu}.$$

Lemma 1 gives a threshold for $\text{HSIC}_{\lambda,\mu}(f)$ from which the dependence between X and Y is detectable with probability at least $1-\beta$ using given Gaussian kernels k_λ and l_μ . Furthermore, it would be useful to give more explicit conditions w.r.t the bandwidths λ and μ and the sample size n . The objective of this section is to provide a condition w.r.t λ, μ and n on the theoretical value $\text{HSIC}_{\lambda,\mu}$, so that the test $\widehat{\Delta}_\alpha^{\lambda,\mu}$ has a second type error controlled by arbitrarily small $\beta \in (0, 1)$. For this, we already give in Lemma 1 a condition w.r.t $\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})$ and $q_{1-\alpha}^{\lambda,\mu}$. It is therefore necessary to provide sharp upper bounds for these two quantities w.r.t λ, μ and n . Propositions 2 and 3 give these upper bounds.

Proposition 2.

Let $(X_i, Y_i)_{1 \leq i \leq n}$ be an i.i.d. sample with distribution P_f and consider the test statistic $\widehat{\text{HSIC}}_{\lambda, \mu}$ defined by (5). Assume that the densities f , f_1 and f_2 are bounded. Then,

$$\text{Var}_f(\widehat{\text{HSIC}}_{\lambda, \mu}) \leq C(M_f, p, q) \left\{ \frac{1}{n} + \frac{1}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2} \right\},$$

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

Proposition 3.

Let $(X_i, Y_i)_{1 \leq i \leq n}$ be an i.i.d. sample with distribution P_f and consider the test statistic $\widehat{\text{HSIC}}_{\lambda, \mu}$ defined by (5). Let α in $(0, 1)$ and $q_{1-\alpha}^{\lambda, \mu}$ be the $(1 - \alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda, \mu}$ under $P_{f_1 \otimes f_2}$ as defined in Section 2.1. Assuming that the densities f_1 , f_2 are bounded,

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

Then,

$$q_{1-\alpha}^{\lambda, \mu} \leq \frac{C(\|f_1\|_\infty, \|f_2\|_\infty, p, q)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

Combining Lemma 1, Propositions 2 and 3, we can then give a sufficient condition on $\text{HSIC}_{\lambda, \mu}$ depending on the parameters λ , μ and the sample size n in order to control the second type error by β . This result is presented in the following corollary.

Corollary 1.

Let $(X_i, Y_i)_{1 \leq i \leq n}$ be an i.i.d. sample with distribution P_f and consider the test statistic $\widehat{\text{HSIC}}_{\lambda, \mu}$ defined by (5). Let α, β in $(0, 1)$, and $q_{1-\alpha}^{\lambda, \mu}$ be the $(1 - \alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda, \mu}$ under $P_{f_1 \otimes f_2}$ as defined in Section 2.1. Assume that the densities f , f_1 and f_2 are bounded, and that

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

Then, one has $P_f(\widehat{\text{HSIC}}_{\lambda, \mu} \leq q_{1-\alpha}^{\lambda, \mu}) \leq \beta$ as soon as

$$\text{HSIC}_{\lambda, \mu}(f) > C(M_f, p, q, \beta) \left\{ \frac{1}{\sqrt{n}} + \frac{1}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right) \right\},$$

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

Note that the right hand term given in Corollary 1 is not computable in practice since it depends on the unknown density f . However, this dependence is weak since it only depends on the infinite norm of f and its marginals.

For given $\beta \in (0, 1)$, Corollary 1 provides conditions on the value of $\text{HSIC}_{\lambda, \mu}(f)$ ensuring that the probability of second kind error of the theoretical test under such f is at most equal to β . We now want to express such conditions in terms of the \mathbb{L}_2 -norm of the function $f - f_1 \otimes f_2$, for the sake of interpretation, and in order to be able to determine separation rates with respect to this \mathbb{L}_2 -norm for our test.

2.3 Control of the second kind error in terms of \mathbb{L}_2 -norm

In order to express a condition on the \mathbb{L}_2 -norm of the function $f - f_1 \otimes f_2$ ensuring a probability of second kind error controlled by β , we first give in Lemma 2 a link between $\text{HSIC}_{\lambda, \mu}$ and $\|f - f_1 \otimes f_2\|_{L_2}^2$.

Lemma 2.

Let $\psi = f - f_1 \otimes f_2$. The HSIC measure $\text{HSIC}_{\lambda,\mu}(f)$ associated to kernels k_λ and l_μ and defined in Equation (1) can be written as

$$\text{HSIC}_{\lambda,\mu}(f) = \langle \psi, \psi * (\varphi_\lambda \otimes \phi_\mu) \rangle_{\mathbb{L}_2},$$

where φ_λ and ϕ_μ are the functions respectively defined in Equations (3) and (4). Moreover, the notation $\langle \cdot, \cdot \rangle_{\mathbb{L}_2}$ designates the usual scalar product in the space \mathbb{L}_2 . One can easily deduce the following Equation:

$$\text{HSIC}_{\lambda,\mu}(f) = \frac{1}{2} \left(\|\psi\|_{\mathbb{L}_2}^2 + \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 - \|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 \right). \quad (11)$$

The following proposition gives a sufficient condition on $\|f - f_1 \otimes f_2\|_{\mathbb{L}_2}^2$, for the test $\Delta_\alpha^{\lambda,\mu}$ to be β -powerful.

Theorem 1.

Let $(X_i, Y_i)_{1 \leq i \leq n}$ be an i.i.d. sample with distribution P_f and consider the test statistic $\widehat{\text{HSIC}}_{\lambda,\mu}$ defined by (5). Denote $\psi = f - f_1 \otimes f_2$. Let α, β in $(0, 1)$, and $q_{1-\alpha}^{\lambda,\mu}$ be the $(1 - \alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda,\mu}$ under $P_{f_1 \otimes f_2}$ as defined in Section 2.1. Assume that the densities f, f_1 and f_2 are bounded, and that

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

One has $P_f(\widehat{\text{HSIC}}_{\lambda,\mu} \leq q_{1-\alpha}^{\lambda,\mu}) \leq \beta$ as soon as

$$\|\psi\|_{\mathbb{L}_2}^2 > \|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 + \frac{C(M_f, p, q, \beta)}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log \left(\frac{1}{\alpha} \right).$$

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

In the condition given in Theorem 1, appears a compromise between a bias term $\|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2$ and a term induced by the square-root of the variance of the estimator $\widehat{\text{HSIC}}_{\lambda,\mu}$. Comparing the conditions on the HSIC given in Corollary 1 and on $\|f - f_1 \otimes f_2\|_{\mathbb{L}_2}^2$ given in Theorem 1, the meticulous reader may notice that the term in $1/\sqrt{n}$ has been removed. This suppression seems to be necessary to obtain optimal separation rates according to the literature in other testing frameworks. This derives from quite tricky computations that we point out here. By combining Lemmas 1 and 2, direct computations lead to the condition

$$\|\psi\|_{\mathbb{L}_2}^2 > \|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 - \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 + 2 \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} + 2q_{1-\alpha}^{\lambda,\mu}.$$

If one directly considers the upper bound of the variance $\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})$ given in Proposition 2, one would get the unwanted $1/\sqrt{n}$ term. The idea is to take advantage of the negative term $-\|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2$ to compensate such term. To do so, we need a more refined control of the variance given in the following technical proposition.

Proposition 4.

Let $(X_i, Y_i)_{1 \leq i \leq n}$ be an i.i.d. sample with distribution P_f and consider the test statistic $\widehat{\text{HSIC}}_{\lambda,\mu}$ defined by (5). Assume that the densities f, f_1 and f_2 are bounded. Then,

$$\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu}) \leq \frac{C(M_f) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2}{n} + \frac{C(M_f, p, q)}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2},$$

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

Finally, using standard inequalities such as $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ and $2\sqrt{ab} \leq \delta a + b/\delta$ for all positive a, b and δ , one can prove

$$2 \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} \leq \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 + \frac{C(M_f, \beta)}{n} + \frac{C(M_f, p, q, \beta)}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}},$$

which leads to Theorem 1. Notice that such trick is already present in [Fromont et al., 2013].

2.4 Uniform separation rate

The bias term in Theorem 1 comes from the fact that we do not estimate $\|f - f_1 \otimes f_2\|_{L_2}^2$ but $\text{HSIC}_{\lambda, \mu}(f)$. In order to have a control of the bias term w.r.t λ and μ , we assume that $f - f_1 \otimes f_2$ belongs some class of regular functions. We introduce the two following classes: Sobolev balls (isotropic case) and Nikol'skii-Besov balls (anisotropic case).

2.4.1 Case Sobolev balls

For $d \in \mathbb{N}^*$, $\delta > 0$ and $R > 0$, the Sobolev ball $\mathcal{S}_d^\delta(R)$ is the set defined by

$$\mathcal{S}_d^\delta(R) = \left\{ s : \mathbb{R}^d \rightarrow \mathbb{R} / s \in \mathbb{L}^1(\mathbb{R}^d) \cap \mathbb{L}^2(\mathbb{R}^d), \int_{\mathbb{R}^d} \|u\|_2^{2\delta} |\hat{s}(u)|^2 du \leq (2\pi)^d R^2 \right\}, \quad (12)$$

where \hat{s} denotes the Fourier transform of s defined by $\hat{s}(u) = \int_{\mathbb{R}^d} s(x) e^{i\langle x, u \rangle} dx$, $\langle \cdot, \cdot \rangle$ denotes the usual scalar product in \mathbb{R}^d and $\|\cdot\|_2$ the Euclidean norm in \mathbb{R}^d .

The following proposition gives an upper bound for the bias term in the case when $f - f_1 \otimes f_2$ belongs to particular Sobolev balls.

Lemma 3.

Let $\psi = f - f_1 \otimes f_2$. We assume that $\psi \in \mathcal{S}_{p+q}^\delta(R)$, where $\delta \in (0, 2]$ and $\mathcal{S}_d^\delta(R)$ is defined by (12). Let φ_λ and ϕ_μ be the functions respectively defined in Equations (3) and (4). Then we have the following inequality,

$$\|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{L_2}^2 \leq C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right].$$

One can deduce from Theorem 1 upper bounds for the uniform separation rates (defined in (6)) of the test $\Delta_\alpha^{\lambda, \mu}$ over Sobolev balls.

Theorem 2. Let $\alpha, \beta \in (0, 1)$ and consider the same notation and assumptions as in Theorem 1. Let $\delta \in (0, 2]$ and $R > 0$. Then, the uniform separation rate $\rho(\Delta_\alpha^{\lambda, \mu}, \mathcal{S}_{p+q}^\delta(R), \beta)$ defined in (6) over the Sobolev ball $\mathcal{S}_{p+q}^\delta(R)$ can be upper bounded as follows

$$\left[\rho(\Delta_\alpha^{\lambda, \mu}, \mathcal{S}_{p+q}^\delta(R), \beta) \right]^2 \leq C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right] + \frac{C(M_f, p, q, \beta)}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right), \quad (13)$$

where $M_f = \max(\|f\|_\infty, \|f_1\|_\infty, \|f_2\|_\infty)$, $C(M_f, p, q, \beta)$ and $C(R, \delta)$ are positive constants depending only on their arguments.

One can now determine optimal bandwidths (λ^*, μ^*) in order to minimize the right-hand side of Equation (13). To do so, the idea is to find for which (λ, μ) both terms in the right hand side of (13) are of the same order w.r.t. n . We also provide an upper bound for the uniform separation rate of the optimized test $\Delta_\alpha^{\lambda^*, \mu^*}$ on Sobolev balls.

Corollary 2.

Consider the assumptions of Theorem 2, and define for all i in $\{1, \dots, p\}$ and for all j in $\{1, \dots, q\}$,

$$\lambda_i^* = \mu_j^* = n^{-\frac{2}{4\delta + (p+q)}}.$$

The uniform separation rate of the test $\Delta_\alpha^{\lambda^*, \mu^*}$ over the Sobolev ball $\mathcal{S}_{p+q}^\delta(R)$ is controlled as follows

$$\rho\left(\Delta_\alpha^{\lambda^*, \mu^*}, \mathcal{S}_{p+q}^\delta(R), \beta\right) \leq C(M_f, p, q, \alpha, \beta, \delta) n^{-\frac{2\delta}{4\delta + (p+q)}}. \quad (14)$$

Note that, in the definition of the Sobolev ball $\mathcal{S}_{p+q}^\delta(R)$, we have the same regularity parameter $\delta > 0$ for all the directions in \mathbb{R}^{p+q} . This corresponds to isotropic regularity conditions. We now introduce other classes of functions allowing to take into account possible anisotropic regularity properties.

2.4.2 Case of Nikol'skii-Besov balls

For $d \in \mathbb{N}^*$, $\delta = (\delta_1, \dots, \delta_d) \in (0, +\infty)^d$ and $R > 0$, we consider the anisotropic Nikol'skii-Besov ball $\mathcal{N}_{2,d}^\delta(R)$ defined by

$$\mathcal{N}_{2,d}^\delta(R) = \left\{ s : \mathbb{R}^d \rightarrow \mathbb{R}/s \text{ has continuous partial derivatives } D_i^{[\delta_i]} \text{ of order } [\delta_i] \text{ w.r.t } u_i, \text{ and } \forall i = 1, \dots, d, \right. \\ \left. u_1, \dots, u_d, v \in \mathbb{R}, \|D_i^{[\delta_i]} s(u_1, \dots, u_i + v, \dots, u_d) - D_i^{[\delta_i]} s(u_1, \dots, u_d)\|_{\mathbb{L}_2} \leq R|v|^{\delta_i - [\delta_i]} \right\}, \quad (15)$$

where $[\delta_i]$ denotes the floor function of δ_i if δ_i is not integer and $[\delta_i] = \delta_i - 1$ if δ_i is an integer. We give in the following proposition an upper bound of the bias term, similar to that of Lemma 3, in the case when $f - f_1 \otimes f_2$ belongs to particular Nikol'skii-Besov balls.

Lemma 4.

We assume that $\psi \in \mathcal{N}_{2,p+q}^\delta(R)$, where $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q) \in (0, 2]^{p+q}$. Then, we have the following inequality,

$$\|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{L_2}^2 \leq C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\nu_i} + \sum_{j=1}^q \mu_j^{2\gamma_j} \right].$$

As in Section 2.4.1, one can deduce from Theorem 1 upper bounds for the uniform separation rates of the test $\Delta_\alpha^{\lambda, \mu}$ over Nikol'skii-Besov balls.

Theorem 3. Let $\alpha, \beta \in (0, 1)$ and consider the same notation and assumptions as in Theorem 1. Let $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q) \in (0, 2]^{p+q}$ and $R > 0$. Then, the uniform separation rate $\rho(\Delta_\alpha^{\lambda, \mu}, \mathcal{N}_{2,p+q}^\delta(R), \beta)$ defined in (6) over the Nikol'skii-Besov ball $\mathcal{N}_{2,p+q}^\delta(R)$ can be upper bounded as follows

$$[\rho(\Delta_\alpha^{\lambda, \mu}, \mathcal{N}_{2,p+q}^\delta(R), \beta)]^2 \leq C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\nu_i} + \sum_{j=1}^q \mu_j^{2\gamma_j} \right] + \frac{C(M_f, p, q, \beta)}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log \left(\frac{1}{\alpha} \right). \quad (16)$$

where $M_f = \max(\|f\|_\infty, \|f_1\|_\infty, \|f_2\|_\infty)$, $C(M_f, p, q, \beta)$ and $C(R, \delta)$ are positive constants depending only on their arguments.

As in Section 2.4.1, we now determine optimal bandwidths (λ^*, μ^*) which minimize the right-hand side of Equation (16) and compute an upper bound for the uniform separation rate of the optimized test $\Delta_\alpha^{\lambda^*, \mu^*}$ on Nikol'skii-Besov balls.

Corollary 3.

Consider the assumptions of Theorem 3, and define for all i in $\{1, \dots, p\}$ and for all j in $\{1, \dots, q\}$,

$$\lambda_i^* = n^{-\frac{2\eta}{\nu_i(1+4\eta)}} \text{ and } \mu_j^* = n^{-\frac{2\eta}{\gamma_j(1+4\eta)}},$$

where η is defined by $\frac{1}{\eta} = \sum_{i=1}^p \frac{1}{\nu_i} + \sum_{j=1}^q \frac{1}{\gamma_j}$,

The uniform separation rate of the test $\Delta_\alpha^{\lambda^*, \mu^*}$ over the Nikol'skii-Besov ball $\mathcal{N}_{2,p+q}^\delta(R)$ is controlled as follows

$$\rho(\Delta_\alpha^{\lambda^*, \mu^*}, \mathcal{N}_{2,p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) n^{-\frac{2\eta}{(1+4\eta)}}. \quad (17)$$

Notice that the upper bound obtained for Nikol'skii-Besov balls in Corollary 3 is analogue to that obtained for Sobolev balls in Corollary 2. Indeed, if we consider the same regularities in all directions in the case of Nikol'skii-Besov balls: $\nu_1 = \dots = \nu_p = \gamma_1 = \dots = \gamma_q$, we obtain a similar upper bound. These upper bounds obtained in Corollaries 2 and 3 remind the asymptotic minimax separation rate of testing independence w.r.t. the \mathbb{L}_2 -norm over Hölder spaces [Ingster, 1989, Yodé, 2004]. However, the test having a rate with the smallest upper bound is not adaptive, it depends on the regularity parameter δ . In the next section, for the purpose of adaptivity, we build an aggregated testing procedure taking into account a collection of bandwidths $(\lambda, \mu) \in \Lambda \times U$. In particular, this avoids the delicate choice of arbitrary bandwidths. We then prove that the uniform separation rate of this aggregated procedure is of the same order as the smallest uniform separation rate of the chosen collection, up to a logarithmic term.

3 Multiple non-asymptotic kernel-based test

In Section 2, we consider single tests based on Gaussian kernels associated to a particular choice of the bandwidths (λ, μ) . However, applying such a procedure leads to the question of the choice of these parameters. There is as yet no justified method to choose λ and μ . In many cases, authors choose these parameters w.r.t the available data $(X_i, Y_i)_{1 \leq i \leq n}$ by taking for example λ (resp. μ) as the empirical median or standard deviation of the X_i 's (resp. the Y_i 's), which is not necessarily an optimal choice. To avoid this delicate choice, we propose in this section an aggregated testing procedure combining a collection of single tests based on different bandwidths.

3.1 The aggregated testing procedure

Consider now a collection of Gaussian kernels $\{(k_\lambda, l_\mu) / (\lambda, \mu) \in \Lambda \times U\}$, where Λ and U are finite or countable subsets of $(0, +\infty)^p$ and $(0, +\infty)^q$ respectively. Consider a collection of positive weights $\{\omega_{\lambda, \mu} / (\lambda, \mu) \in \Lambda \times U\}$ such that $\sum_{(\lambda, \mu) \in \Lambda \times U} e^{-\omega_{\lambda, \mu}} \leq 1$.

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

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

where u_α is the less conservative value such that the test is of level α , and is defined by

$$u_\alpha = \sup \left\{ u > 0 ; P_{f_1 \otimes f_2} \left(\sup_{(\lambda, \mu) \in \Lambda \times U} \left(\widehat{\text{HSIC}}_{\lambda, \mu} - q_{1-ue^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) > 0 \right) \leq \alpha \right\}. \quad (18)$$

We should mention here that the supremum in Equation (18) exists. Indeed, for all (λ, μ) in $\Lambda \times U$: $0 < 1 - u \exp(-\omega_{\lambda, \mu})$, this leads to, $u < \inf_{(\lambda, \mu) \in \Lambda \times U} (\exp(\omega_{\lambda, \mu})) < +\infty$. Then, u_α is well defined and verify: $u_\alpha < \inf_{(\lambda, \mu) \in \Lambda \times U} (\exp(\omega_{\lambda, \mu}))$.

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

$$\Delta_\alpha = 1 \iff \sup_{(\lambda, \mu) \in \Lambda \times U} \left(\widehat{\text{HSIC}}_{\lambda, \mu} - q_{1-u_\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) > 0. \quad (19)$$

It is easy to check that the test Δ_α is of level α , this is directly derived from the definitions of u_α .

For implementational limitations, the collections Λ and U are finite in practice. Moreover, note that, as for the quantile, the correction u_α of the level is not analytically computable since it depends on the unknown marginals f_1 and f_2 . In practice, it can also be approached by a permutation method with Monte Carlo approximation, as done in [Albert et al., 2015], by

$$\hat{u}_\alpha = \sup \left\{ u > 0 ; \frac{1}{B} \sum_{b=1}^B \mathbf{1}_{\max_{(\lambda, \mu) \in \Lambda \times U} \left\{ \widehat{\text{HSIC}}_{\lambda, \mu}^{[b]} - \hat{q}_{1-ue^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right\} > 0} \leq \alpha \right\}.$$

In the next section, we will provide a uniform separation rate similar to that of Corollaries 2 and 3 for the test Δ_α . This uniform separation rate will be given in the two cases mentioned earlier in Section 2.4 where $f - f_1 \otimes f_2$ belongs to isotropic Sobolev balls or to anisotropic Nikol'skii-Besov balls.

3.2 Oracle type conditions for the second kind error

As a reminder, our target is to construct a testing procedure with a uniform separation rate as small as possible and, whose implementation does not require any information about the regularity of f . For this, we will first show in the following lemma that the second kind error of the aggregated procedure proposed in the previous section is of the same order of the smallest error over the chosen collection of parameters.

Lemma 5. *Let α, β in $(0, 1)$, and consider the aggregated test Δ_α defined in (19). Then,*

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

In particular, if there exists at least one $(\lambda, \mu) \in \Lambda \times U$ such that the associated single test $\Delta_{\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu}$ has a probability of second kind error at most equal to β , then the probability of the second kind error of the aggregated test Δ_α is at most equal to β .

We now give an oracle inequality for the uniform separation rate of the aggregation procedure Δ_α . This inequality given in the following theorem shows the interest of this testing procedure.

Theorem 4. *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 also assume that all bandwidths (λ, μ) in $\Lambda \times U$ verify the conditions given in Theorem 1, and that f, f_1 and f_2 are bounded. Then, the test Δ_α of level α defined in Equation (19) has a uniform separation rate $\rho(\Delta_\alpha, C_\delta, \beta)$ which can be upper bounded as follows*

- If $C_\delta = \mathcal{S}_{p+q}^\delta(R)$, where $\delta \in (0, 2]$ and $R > 0$, then

$$\left[\rho(\Delta_\alpha, \mathcal{S}_{p+q}^\delta(R), \beta) \right]^2 \leq C(M_f, p, q, \beta, \delta) \inf_{(\lambda, \mu) \in \Lambda \times U} \left\{ \frac{1}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \left(\log \left(\frac{1}{\alpha} \right) + \omega_{\lambda, \mu} \right) + \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right] \right\}, \quad (20)$$

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.

- If $C_\delta = \mathcal{N}_{2, p+q}^\delta(R)$, where $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q) \in (0, 2]^{p+q}$ and $R > 0$, then

$$\left[\rho(\Delta_\alpha, \mathcal{N}_{2, p+q}^\delta(R), \beta) \right]^2 \leq C(M_f, p, q, \beta, \delta) \inf_{(\lambda, \mu) \in \Lambda \times U} \left\{ \frac{1}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \left(\log \left(\frac{1}{\alpha} \right) + \omega_{\lambda, \mu} \right) + \left[\sum_{i=1}^p \lambda_i^{2\nu_i} + \sum_{j=1}^q \mu_j^{2\gamma_j} \right] \right\}, \quad (21)$$

where $C(M_f, p, q, \beta, \delta)$ is a positive constant depending only on its arguments.

According to Theorem 4, the uniform separation rate of the aggregated testing procedure Δ_α is the infimum of all $(\lambda, \mu) \in \Lambda \times U$, up to the additional term $\omega_{\lambda, \mu}$. This theorem can also be interpreted as an oracle type condition for the second kind error of the test Δ_α . Indeed, without knowing $f - f_1 \otimes f_2$, we prove that the uniform separation rate of Δ_α is of the same order of the smallest uniform separation rate over $(\lambda, \mu) \in \Lambda \times U$, up to $\omega_{\lambda, \mu}$.

3.3 Uniform separation rate over Sobolev balls and Nikol'skii-Besov balls

In this section, we provide an upper bound of the uniform separation rate $\rho(\Delta_\alpha, C_\delta, \beta)$ of the multiple testing procedure Δ_α over the classes of Sobolev balls and Nikol'skii-Besov balls. For this, we consider the sets Λ and U respectively of parameters λ and μ , defined by

$$\Lambda = \{(2^{-m_{1,1}}, \dots, 2^{-m_{1,p}}) ; (m_{1,1}, \dots, m_{1,p}) \in (\mathbb{N}^*)^p\}, \quad (22)$$

and

$$U = \{(2^{-m_{2,1}}, \dots, 2^{-m_{2,q}}) ; (m_{2,1}, \dots, m_{2,q}) \in (\mathbb{N}^*)^q\}. \quad (23)$$

In addition, 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

$$\omega_{\lambda,\mu} = 2 \sum_{i=1}^p \log \left(m_{1,i} \times \frac{\pi}{\sqrt{6}} \right) + 2 \sum_{j=1}^q \log \left(m_{2,j} \times \frac{\pi}{\sqrt{6}} \right), \quad (24)$$

so that $\sum_{(\lambda,\mu) \in \Lambda \times U} e^{-\omega_{\lambda,\mu}} = 1$. The following corollary gives these upper bounds.

Corollary 4. *Assuming that $\log \log(n) > 1$, $\alpha, \beta \in (0, 1)$ and Δ_α the test defined in (19), with the particular choice of Λ , U and the weights $(\omega_{\lambda,\mu})_{(\lambda,\mu) \in \Lambda \times U}$ defined in (22), (23) and (24). Then, the uniform separation rate $\rho(\Delta_\alpha, C_\delta, \beta)$ of the aggregated test Δ_α can be upper bounded as follows.*

- If $C_\delta = \mathcal{S}_{p+q}^\delta(R)$, where $\delta \in (0, 2]$ and $R > 0$, then,

$$\rho(\Delta_\alpha, \mathcal{S}_{p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) \left(\frac{\log \log(n)}{n} \right)^{\frac{2\delta}{4\delta + (p+q)}}, \quad (25)$$

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

- If $C_\delta = \mathcal{N}_{2,p+q}^\delta(R)$, where $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q) \in (0, 2]^{p+q}$ and $R > 0$, then,

$$\rho(\Delta_\alpha, \mathcal{N}_{2,p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) \left(\frac{\log \log(n)}{n} \right)^{\frac{2\eta}{(1+4\eta)}}, \quad (26)$$

where $\frac{1}{\eta} = \sum_{i=1}^p \frac{1}{\nu_i} + \sum_{j=1}^q \frac{1}{\gamma_j}$ and $M_f = \max(\|f\|_\infty, \|f_1\|_\infty, \|f_2\|_\infty)$.

Comment. *According to Corollary 4, the rate of the aggregation procedure over the classes of Sobolev balls and Nikol'skii-Besov balls is in the same order of the best rate of single tests (given in Theorem 1), up to a $\log \log(n)$ factor.*

4 Proofs

All along the proofs, we set $Z = (X, Y)$ and $Z_i = (X_i, Y_i)$ for all i in $\{1, \dots, n\}$. We also denote by A, B and C positive universal constants whose values may change from line to line. Furthermore, for all n in \mathbb{N}^* and r in $\{1, \dots, n\}$, we denote:

$$(n)_r = \frac{n!}{(n-r)!}. \quad (27)$$

4.1 Proof of Proposition 1

Let α be in $(0, 1)$. In order to prove that the permuted test with Monte Carlo approximation $\widehat{\Delta}_\alpha^{\lambda,\mu}$ is of prescribed level α , we use the following lemma of [Romano and Wolf, 2005].

Lemma 6 ([Romano and Wolf, 2005, Lemma 1]). *Let R_1, \dots, R_{B+1} be $(B+1)$ exchangeable random variables. Then, for all u in $(0, 1)$*

$$\mathbb{P} \left(\frac{1}{B+1} \left(1 + \sum_{b=1}^B \mathbb{1}_{R_b \geq R_{B+1}} \right) \leq u \right) \leq u.$$

Recall that for all $1 \leq b \leq B$,

$$\widehat{H}_{\lambda,\mu}^{\star b} = \widehat{\text{HSIC}}_{\lambda,\mu}(\mathbb{Z}_n^{\tau_b}) \quad \text{and} \quad \widehat{H}_{\lambda,\mu}^{\star B+1} = \widehat{\text{HSIC}}_{\lambda,\mu}(\mathbb{Z}_n) = \widehat{\text{HSIC}}_{\lambda,\mu}(\mathbb{Z}_n^{\tau_{B+1}}),$$

where $\tau_{B+1} = \text{id}$ is the identity permutation of $\{1, \dots, B+1\}$ (deterministic).

Assume that $f = f_1 \otimes f_2$. Then the random variables $\widehat{H}_{\lambda,\mu}^{\star 1}, \dots, \widehat{H}_{\lambda,\mu}^{\star B}$ and $\widehat{H}_{\lambda,\mu}^{\star B+1}$ are exchangeable. Indeed, let π be a (deterministic) permutation of $\{1, \dots, B+1\}$ and let us prove that

$$\left(\widehat{H}_{\lambda,\mu}^{\star 1}, \dots, \widehat{H}_{\lambda,\mu}^{\star B}, \widehat{H}_{\lambda,\mu}^{\star B+1} \right) \quad \text{and} \quad \left(\widehat{H}_{\lambda,\mu}^{\star \pi(1)}, \dots, \widehat{H}_{\lambda,\mu}^{\star \pi(B+1)} \right) \quad \text{have the same distribution.} \quad (28)$$

1st case: if $\pi(B+1) = B+1$. Then, since the permutations $(\tau_b)_{1 \leq b \leq B}$ are i.i.d., they are exchangeable. Hence, $(\tau_{\pi(1)}, \dots, \tau_{\pi(B)})$ is an i.i.d. sample of uniform permutations of $\{1, \dots, n\}$, independent of \mathbb{Z}_n and (28) holds by construction.

2nd case: if $\pi(B+1) \neq B+1$. Then,

$$\widehat{H}_{\lambda, \mu}^{\star \pi(B+1)} = \widehat{\text{HSIC}}_{\lambda, \mu}(\mathbb{Z}_n^{\tau_{\pi(B+1)}}) = \widehat{\text{HSIC}}_{\lambda, \mu}(\tilde{\mathbb{Z}}_n), \quad \text{where } \tilde{\mathbb{Z}}_n = \mathbb{Z}_n^{\tau_{\pi(B+1)}}.$$

In particular, for all b in $\{1, \dots, B\}$,

$$\begin{cases} \widehat{H}_{\lambda, \mu}^{\star \pi(b)} = \widehat{\text{HSIC}}_{\lambda, \mu}(\mathbb{Z}_n^{\tau_{\pi(b)}}) = \widehat{\text{HSIC}}_{\lambda, \mu}(\tilde{\mathbb{Z}}_n^{\tau_{\pi(b)} \circ \tau_{\pi(B+1)}^{-1}}) & \text{if } \pi(b) \neq B+1, \\ \widehat{H}_{\lambda, \mu}^{\star \pi(b)} = \widehat{\text{HSIC}}_{\lambda, \mu}(\mathbb{Z}_n) = \widehat{\text{HSIC}}_{\lambda, \mu}(\tilde{\mathbb{Z}}_n^{\text{id} \circ \tau_{\pi(B+1)}^{-1}}) & \text{if } \pi(b) = B+1. \end{cases}$$

Therefore, in order to prove (28), it is sufficient to prove that $\{\tau_{\pi(1)} \circ \tau_{\pi(B+1)}^{-1}, \dots, \tau_{\pi(B)} \circ \tau_{\pi(B+1)}^{-1}\}$ is an i.i.d. sample of uniform permutations of $\{1, \dots, n\}$ independent of $\tilde{\mathbb{Z}}_n$.

Let A be a measurable set, and $\sigma_1, \dots, \sigma_B$ be (fixed) permutations of $\{1, \dots, n\}$. Then

$$\begin{aligned} & \mathbb{P}(\tilde{\mathbb{Z}}_n \in A, \tau_{\pi(1)} \circ \tau_{\pi(B+1)}^{-1} = \sigma_1, \dots, \tau_{\pi(B)} \circ \tau_{\pi(B+1)}^{-1} = \sigma_B) \\ &= \mathbb{P}(\mathbb{Z}_n^{\tau_{\pi(B+1)}} \in A, \tau_{\pi(1)} = \sigma_1 \circ \tau_{\pi(B+1)}, \dots, \tau_{\pi(B)} = \sigma_B \circ \tau_{\pi(B+1)} = \sigma_B) \\ &= \mathbb{E}[\mathbb{P}(\mathbb{Z}_n^{\tau_{\pi(B+1)}} \in A, \tau_{\pi(1)} = \sigma_1 \circ \tau_{\pi(B+1)}, \dots, \tau_{\pi(B)} = \sigma_B \circ \tau_{\pi(B+1)} | \tau_{\pi(B+1)})] \\ &= \mathbb{E} \left[\mathbb{P}(\mathbb{Z}_n \in A) \times \left(\prod_{\substack{b=1 \\ b \neq \pi^{-1}(B+1)}}^{B+1} \mathbb{P}(\tau_{\pi(b)} = \sigma_b \circ \tau_{\pi(B+1)} | \tau_{\pi(B+1)}) \right) \times \mathbb{P}(\text{id} = \sigma_{\pi^{-1}(B+1)} \circ \tau_{\pi(B+1)} | \tau_{\pi(B+1)}) \right], \tag{29} \\ &= \mathbb{E} \left[\mathbb{P}(\mathbb{Z}_n \in A) \left(\frac{1}{n!} \right)^{B-1} \mathbb{P}(\text{id} = \sigma_{\pi^{-1}(B+1)} \circ \tau_{\pi(B+1)} | \tau_{\pi(B+1)}) \right], \\ &= \mathbb{P}(\mathbb{Z}_n \in A) \left(\frac{1}{n!} \right)^{B-1} \mathbb{P}(\tau_{\pi(B+1)} = \sigma_{\pi^{-1}(B+1)}^{-1}), \\ &= \mathbb{P}(\mathbb{Z}_n \in A) \left(\frac{1}{n!} \right)^B, \end{aligned}$$

where (29) holds by independence of all permutations τ_b and of \mathbb{Z}_n and since, if $f = f_1 \otimes f_2$, $\mathbb{Z}_n^{\tau_{\pi(B+1)}}$ and \mathbb{Z}_n have the same distribution. This ends the proof of the exchangeability of the $(\widehat{H}_{\lambda, \mu}^{\star b})_{1 \leq b \leq B+1}$.

Then, by applying Lemma 6 to the $(\widehat{H}_{\lambda,\mu}^{*b})_{1 \leq b \leq B+1}$, we obtain

$$\begin{aligned}
P_{f_1 \otimes f_2} \left(\widehat{\Delta}_\alpha^{\lambda,\mu} = 1 \right) &= P_{f_1 \otimes f_2} \left(\widehat{\text{HSIC}}_{\lambda,\mu} > \widehat{q}_{1-\alpha}^{\lambda,\mu} \right) \\
&= P_{f_1 \otimes f_2} \left(\widehat{H}_{\lambda,\mu}^{*B+1} > \widehat{H}_{\lambda,\mu}^{* \lceil (B+1)(1-\alpha) \rceil} \right) \\
&= P_{f_1 \otimes f_2} \left(\sum_{b=1}^{B+1} \mathbb{1}_{\widehat{H}_{\lambda,\mu}^{*b} < \widehat{H}_{\lambda,\mu}^{*B+1}} \geq \lceil (B+1)(1-\alpha) \rceil \right) \\
&= P_{f_1 \otimes f_2} \left(\sum_{b=1}^{B+1} \mathbb{1}_{\widehat{H}_{\lambda,\mu}^{*b} \geq \widehat{H}_{\lambda,\mu}^{*B+1}} \leq \lfloor \alpha(B+1) \rfloor \right) \\
&= P_{f_1 \otimes f_2} \left(\sum_{b=1}^{B+1} \mathbb{1}_{\widehat{H}_{\lambda,\mu}^{*b} \geq \widehat{H}_{\lambda,\mu}^{*B+1}} \leq \alpha(B+1) \right) \\
&= P_{f_1 \otimes f_2} \left(\frac{1}{B+1} \left(1 + \sum_{b=1}^B \mathbb{1}_{\widehat{H}_{\lambda,\mu}^{*b} \geq \widehat{H}_{\lambda,\mu}^{*B+1}} \right) \leq \alpha \right) \\
&\leq \alpha,
\end{aligned} \tag{30}$$

where (30) comes from the fact that

$$B+1 - \lceil (B+1)(1-\alpha) \rceil = \lfloor \alpha(B+1) \rfloor,$$

and (31) is obtained from Lemma 6.

4.2 Proof of Lemma 1

Let α and β be in $(0, 1)$. We aim here to give a condition on $\text{HSIC}_{\lambda,\mu}(f)$ w.r.t. the variance $\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})$ and the quantile $q_{1-\alpha}^{\lambda,\mu}$, so that the statistical test $\widehat{\Delta}_\alpha^{\lambda,\mu}$ has a second type error controlled by β . For this, we use Chebyshev's inequality. Since $\widehat{\text{HSIC}}_{\lambda,\mu}$ is an unbiased estimator of $\text{HSIC}_{\lambda,\mu}(f)$,

$$P_f \left(\left| \widehat{\text{HSIC}}_{\lambda,\mu} - \text{HSIC}_{\lambda,\mu}(f) \right| \geq \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} \right) \leq \beta.$$

We then have the following inequality:

$$P_f \left(\widehat{\text{HSIC}}_{\lambda,\mu} \leq \text{HSIC}_{\lambda,\mu}(f) - \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} \right) \leq \beta.$$

Consequently, one has $P_f \left(\widehat{\text{HSIC}}_{\lambda,\mu} \leq q_{1-\alpha}^{\lambda,\mu} \right) \leq \beta$, as soon as

$$\text{HSIC}_{\lambda,\mu}(f) > \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} + q_{1-\alpha}^{\lambda,\mu}.$$

4.3 Proof of Proposition 2

In order to provide an upper bound of the variance $\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})$ w.r.t. the bandwidths λ, μ and the sample-size n , let us first give the following lemma for a general U -statistic of any order r in $\{1, \dots, n\}$.

Lemma 7. *Let h be a symmetric function with $r \leq n$ inputs, V_1, \dots, V_n be independent and identically distributed random variables and U_n be the U -statistic defined by*

$$U_n = \frac{1}{\binom{n}{r}} \sum_{(i_1, \dots, i_r) \in \mathbf{i}_r^n} h(V_{i_1}, \dots, V_{i_r}),$$

where $(n)_r$ is defined in (27). The following inequality gives an upper bound of the variance of U_n ,

$$\text{Var}(U_n) \leq C(r) \left(\frac{\sigma^2}{n} + \frac{s^2}{n^2} \right), \quad (32)$$

where $\sigma^2 = \text{Var}(\mathbb{E}[h(V_1, \dots, V_r) | V_1])$ and $s^2 = \text{Var}(h(V_1, \dots, V_r))$.

Proof. First, using Hoeffding's decomposition (see e.g. [Serfling, 2009]), the variance of U_n can be decomposed as

$$\text{Var}(U_n) = \binom{n}{r}^{-1} \sum_{c=1}^r \binom{r}{c} \binom{n-r}{r-c} \zeta_c,$$

where $\zeta_c = \text{Var}(\mathbb{E}[h(V_1, \dots, V_r) | V_1, \dots, V_c])$.

Let us now prove that, for all $n \in \mathbb{N}^*$, $r \in \{1, \dots, n\}$ and $c \in \{1, \dots, r\}$,

$$\binom{n}{r}^{-1} \binom{r}{c} \binom{n-r}{r-c} \leq \frac{C(r, c)}{n^c}. \quad (33)$$

We first write

$$\begin{aligned} \binom{n}{r}^{-1} \binom{r}{c} \binom{n-r}{r-c} &= \binom{r}{c} \times \frac{(n-r)!}{(r-c)!(n+c-2r)!} \times \frac{r!(n-r)!}{n!} \\ &= \binom{r}{c} \times \frac{r!}{(r-c)!} \times \frac{(n-r)!}{(n+c-2r)!} \times \frac{(n-r)!}{n!}. \end{aligned} \quad (34)$$

Moreover,

$$\begin{aligned} n! &= (n-r)! \times (n-r+1) \times \dots \times (n-r+r) \\ &\geq (n-r)! \times (n-r+1)^r, \end{aligned}$$

and

$$\begin{aligned} (n-r)! &= (n-2r+c)! \times (n-2r+c+1) \times \dots \times (n-2r+c+r-c) \\ &\leq (n-2r+c)! \times (n-r+1)^{r-c}. \end{aligned}$$

Then, we have

$$\frac{(n-r)!}{(n+c-2r)!} \times \frac{(n-r)!}{n!} \leq \frac{1}{(n-r+1)^c}.$$

Furthermore, using that $n \geq r$, one can write

$$\begin{aligned} \frac{n-r+1}{n} &= 1 - \frac{r-1}{n} \\ &\geq 1 - \frac{r-1}{r} \\ &= \frac{1}{r}. \end{aligned}$$

This leads to, $n-r+1 \geq \frac{n}{r}$. Finally, using Equation (34) we have (33).

By upper bounding each term in Hoeffding's decomposition of the variance of U_n according to Inequation (33), we obtain the following inequality:

$$\text{Var}(U_n) \leq C(r) \sum_{c=1}^r \frac{\zeta_c}{n^c} \quad (35)$$

On the other hand, using the law of total variance (see e.g. [Weiss, 2006]), for all c in $\{2, \dots, r\}$: $\zeta_c \leq s^2$. By injecting this last inequality in Equation (35), we obtain for all n in \mathbb{N}^* :

$$\text{Var}(U_n) \leq C(r) \left(\frac{\sigma^2}{n} + \frac{s^2}{n^2} \right),$$

which achieves the proof of Lemma 7. \square

Let us now apply Lemma 7 in order to control the variance of $\widehat{\text{HSIC}}_{\lambda, \mu}$ w.r.t λ , μ and n . For this, we first recall that $\widehat{\text{HSIC}}_{\lambda, \mu}$ can be written as a single U -statistic of order 4 [Gretton et al., 2008] as

$$\widehat{\text{HSIC}}_{\lambda, \mu} = \frac{1}{(n)_4} \sum_{(i,j,q,r) \in \mathfrak{I}_4^n} h_{i,j,q,r},$$

where the general term $h_{i,j,q,r}$ of $\widehat{\text{HSIC}}_{\lambda, \mu}$ is defined as

$$h_{i,j,q,r} = \frac{1}{4!} \sum_{(t,u,v,w) \in \mathfrak{I}_4^n}^{(i,j,q,r)} (k_{t,u} l_{t,u} + k_{t,u} l_{v,w} - 2k_{t,u} l_{t,v}). \quad (36)$$

where $k_{t,u}$ (resp. $l_{t,u}$) is defined for all t, u in $\{1, \dots, n\}$ as $k_{t,u} = k(X_t, X_u)$ (resp. $l_{t,u} = l(Y_t, Y_u)$) and the sum represents all ordered quadruples (t, u, v, w) drawn without replacement from (i, j, q, r) .

Thus, using Lemma 7, the variance of $\widehat{\text{HSIC}}_{\lambda, \mu}$ can be upper bounded as follows:

$$\text{Var}_f \left(\widehat{\text{HSIC}}_{\lambda, \mu} \right) \leq C \left(\frac{\sigma^2(\lambda, \mu)}{n} + \frac{s^2(\lambda, \mu)}{n^2} \right), \quad (37)$$

where $\sigma^2(\lambda, \mu) = \text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1])$ and $s^2(\lambda, \mu) = \text{Var}_f(h_{1,2,3,4})$.

4.3.1 Upper bound of $\sigma^2(\lambda, \mu)$

By now, we upper bound $\sigma^2(\lambda, \mu)$ defined in Equation (37) w.r.t. λ and μ . For this, we first notice that in the cases when $k_\lambda(X_a, X_b)l_\mu(Y_c, Y_d)$ is independent from Z_1 , the variance of its expectation conditionally on Z_1 equals 0. That are the cases when a, b, c and d are all different from 1. We then have the following inequality:

$$\sigma^2(\lambda, \mu) \leq C \sum_{i=1}^6 \sigma_i^2(\lambda, \mu),$$

where

$$\begin{aligned} \sigma_1^2(\lambda, \mu) &= \text{Var}_f(\mathbb{E}[k_\lambda(X_1, X_2)l_\mu(Y_1, Y_2) | Z_1]), & \sigma_2^2(\lambda, \mu) &= \text{Var}_f(\mathbb{E}[k_\lambda(X_1, X_2)l_\mu(Y_3, Y_4) | X_1]), \\ \sigma_3^2(\lambda, \mu) &= \text{Var}_f(\mathbb{E}[k_\lambda(X_3, X_4)l_\mu(Y_1, Y_2) | Y_1]), & \sigma_4^2(\lambda, \mu) &= \text{Var}_f(\mathbb{E}[k_\lambda(X_1, X_2)l_\mu(Y_1, Y_3) | Z_1]), \\ \sigma_5^2(\lambda, \mu) &= \text{Var}_f(\mathbb{E}[k_\lambda(X_2, X_1)l_\mu(Y_2, Y_3) | X_1]), & \sigma_6^2(\lambda, \mu) &= \text{Var}_f(\mathbb{E}[k_\lambda(X_2, X_3)l_\mu(Y_2, Y_1) | Y_1]). \end{aligned}$$

Case 1. Upper bound of $\sigma_1^2(\lambda, \mu)$

$$\begin{aligned} \sigma_1^2(\lambda, \mu) &\leq \mathbb{E} \left[\left(\mathbb{E}[k_\lambda(X_1, X_2)l_\mu(Y_1, Y_2) | Z_1] \right)^2 \right] \\ &\leq \mathbb{E} [k_\lambda(X_1, X_2)l_\mu(Y_1, Y_2)k_\lambda(X_1, X_3)l_\mu(Y_1, Y_3)]. \end{aligned}$$

Moreover, we have

$$\begin{aligned} &\mathbb{E} [k_\lambda(X_1, X_2)k_\lambda(X_1, X_3)l_\mu(Y_1, Y_2)l_\mu(Y_1, Y_3)] \\ &= \int k_\lambda(x_1, x_2)k_\lambda(x_1, x_3)l_\mu(y_1, y_2)l_\mu(y_1, y_3) \prod_{k=1}^3 f(x_k, y_k) dx_k dy_k. \end{aligned}$$

By upper bounding $f(x_2, y_2)$ and $f(x_3, y_3)$ by $\|f\|_\infty$, we have

$$\begin{aligned}\sigma_1^2(\lambda, \mu) &\leq \|f\|_\infty^2 \int k_\lambda(x_1, x_2) k_\lambda(x_1, x_3) l_\mu(y_1, y_2) l_\mu(y_1, y_3) f(x_1, y_1) \prod_{k=1}^3 dx_k dy_k \\ &= \|f\|_\infty^2 \int \left[\int k_\lambda(x_1, x_2) dx_2 \right] \left[\int k_\lambda(x_1, x_3) dx_3 \right] \left[\int l_\mu(y_1, y_2) dy_2 \right] \left[\int l_\mu(y_1, y_3) dy_3 \right] f(x_1, y_1) dx_1 dy_1.\end{aligned}$$

Finally, using that $\int k_\lambda(x, \cdot) dx = \int l_\mu(\cdot, y) dy = 1$, we write

$$\sigma_1^2(\lambda, \mu) \leq \|f\|_\infty^2. \quad (38)$$

Case 2. Upper bound of $\sigma_2^2(\lambda, \mu)$

$$\begin{aligned}\sigma_2^2(\lambda, \mu) &\leq \mathbb{E} \left[\left(\mathbb{E} [k_\lambda(X_1, X_2) l_\mu(Y_3, Y_4) \mid X_1] \right)^2 \right] \\ &\leq \mathbb{E} \left[\left(\mathbb{E} [k_\lambda(X_1, X_2) \mid X_1] \right)^2 \right] \left(\mathbb{E} [l_\mu(Y_3, Y_4)] \right)^2 \\ &\leq \mathbb{E} [k_\lambda(X_1, X_2) k_\lambda(X_1, X_3)] \left(\mathbb{E} [l_\mu(Y_3, Y_4)] \right)^2.\end{aligned}$$

Moreover, it is easy to see that by upper bounding $f_1(x_2)$ and $f_1(x_3)$ by $\|f_1\|_\infty$, and recalling that $\int k_\lambda(x_1, x) dx = 1$, we have,

$$\begin{aligned}\mathbb{E} [k_\lambda(X_1, X_2) k_\lambda(X_1, X_3)] &= \int \left[\int k_\lambda(x_1, x_2) f_1(x_2) dx_2 \right] \left[\int k_\lambda(x_1, x_3) f_1(x_3) dx_3 \right] f_1(x_1) dx_1 \\ &\leq \|f_1\|_\infty^2.\end{aligned}$$

Besides, upper bounding $f_2(y_3)$ by $\|f_2\|_\infty$ in the integral form of $\mathbb{E} [l_\mu(Y_3, Y_4)]$ gives

$$\mathbb{E} [l_\mu(Y_3, Y_4)] \leq \|f_2\|_\infty.$$

By combining these inequalities, we obtain

$$\sigma_2^2(\lambda, \mu) \leq \|f_1\|_\infty^2 \|f_2\|_\infty^2. \quad (39)$$

Case 3. Upper bound of $\sigma_3^2(\lambda, \mu)$

This case is similar to case 2 by exchanging X by Y and k_λ by l_μ . Thus, we have the inequality

$$\sigma_3^2(\lambda, \mu) \leq \|f_1\|_\infty^2 \|f_2\|_\infty^2. \quad (40)$$

Case 4. Upper bound of $\sigma_4^2(\lambda, \mu)$

$$\begin{aligned}\sigma_4^2(\lambda, \mu) &\leq \mathbb{E} \left[\left(\mathbb{E} [k_\lambda(X_1, X_2) l_\mu(Y_1, Y_3) \mid Z_1] \right)^2 \right] \\ &\leq \mathbb{E} [k_\lambda(X_1, X_2) k_\lambda(X_1, X_4) l_\mu(Y_1, Y_3) l_\mu(Y_1, Y_5)].\end{aligned}$$

By upper bounding $f_1(x_2)$, $f_1(x_4)$ by $\|f_1\|_\infty$ and $f_2(y_3)$, $f_2(y_5)$ by $\|f_2\|_\infty$ in the integral form of $\mathbb{E} [k_\lambda(X_1, X_2) k_\lambda(X_1, X_4) l_\mu(Y_1, Y_3) l_\mu(Y_1, Y_5)]$, we obtain

$$\sigma_4^2(\lambda, \mu) \leq \|f_1\|_\infty^2 \|f_2\|_\infty^2. \quad (41)$$

Case 5. Upper bound of $\sigma_5^2(\lambda, \mu)$

$$\begin{aligned}\sigma_5^2(\lambda, \mu) &\leq \mathbb{E} \left[\left(\mathbb{E} [k_\lambda(X_2, X_1) l_\mu(Y_2, Y_3) \mid X_1] \right)^2 \right] \\ &\leq \mathbb{E} [k_\lambda(X_2, X_1) k_\lambda(X_4, X_1) l_\mu(Y_2, Y_3) l_\mu(Y_4, Y_5)].\end{aligned}$$

By upper bounding $f(x_2, y_2)$ and $f(x_4, y_4)$ by $\|f\|_\infty$ in the integral form of the last expectation, we have

$$\sigma_5^2(\lambda, \mu) \leq \|f\|_\infty^2. \quad (42)$$

Case 6. Upper bound of $\sigma_6^2(\lambda, \mu)$

This case is similar to case 5 by exchanging X by Y and k_λ by l_μ . We have then the inequality

$$\sigma_6^2(\lambda, \mu) \leq \|f\|_\infty^2. \quad (43)$$

Finally, by combining inequalities (38), (39), (40), (41), (42) and (43), we have the following inequality

$$\sigma^2(\lambda, \mu) \leq C(M_f). \quad (44)$$

4.3.2 Upper bound of $s^2(\lambda, \mu)$

Let us first recall that the general term of the U -statistic $\widehat{\text{HSIC}}_{\lambda, \mu}$ is written as

$$h_{1,2,3,4}(Z_1, Z_2, Z_3, Z_4) = \frac{1}{4!} \sum_{(u,v,w,t)}^{(1,2,3,4)} k_\lambda(X_u, X_v) [l_\mu(Y_u, Y_v) + l_\mu(Y_w, Y_t) - 2l_\mu(Y_u, Y_w)].$$

Moreover, all the terms of the last sum have the same distribution. We then have:

$$\text{Var}_f(h_{1,2,3,4}(Z_1, Z_2, Z_3, Z_4)) \leq C \text{Var}_f(k_\lambda(X_1, X_2) [l_\mu(Y_1, Y_2) + l_\mu(Y_3, Y_4) - 2l_\mu(Y_1, Y_3)]),$$

It follows that,

$$\begin{aligned} \text{Var}_f(h_{1,2,3,4}(Z_1, Z_2, Z_3, Z_4)) &\leq C [\text{Var}_f(k_\lambda(X_1, X_2)l_\mu(Y_1, Y_2)) + \text{Var}_f(k_\lambda(X_1, X_2)l_\mu(Y_3, Y_4)) \\ &\quad + \text{Var}_f(k_\lambda(X_1, X_2)l_\mu(Y_1, Y_3))] \\ &\leq C (\mathbb{E}[k_\lambda^2(X_1, X_2)l_\mu^2(Y_1, Y_2)] + \mathbb{E}[k_\lambda^2(X_1, X_2)l_\mu^2(Y_3, Y_4)] \\ &\quad + \mathbb{E}[k_\lambda^2(X_1, X_2)l_\mu^2(Y_1, Y_3)]), \end{aligned}$$

In order to bring back to multivariate normal densities, we express k_λ^2 and l_μ^2 as

$$k_\lambda^2 = \frac{k_{\lambda'}}{(4\pi)^{\frac{p}{2}} \lambda_1 \dots \lambda_p} \quad \text{and} \quad l_\mu^2 = \frac{l_{\mu'}}{(4\pi)^{\frac{q}{2}} \mu_1 \dots \mu_q},$$

where $\lambda' = \frac{\lambda}{\sqrt{2}}$ and $\mu' = \frac{\mu}{\sqrt{2}}$.

Consequently, the expectation $\mathbb{E}[k_\lambda^2(X_1, X_2)l_\mu^2(Y_1, Y_2)]$ can be expressed as

$$\begin{aligned} \mathbb{E}[k_\lambda^2(X_1, X_2)l_\mu^2(Y_1, Y_2)] &= \frac{1}{(4\pi)^{\frac{p+q}{2}} \lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} \mathbb{E}[k_{\lambda'}(X_1, X_2)l_{\mu'}(Y_1, Y_2)] \\ &= \frac{1}{(4\pi)^{\frac{p+q}{2}} \lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} \int k_{\lambda'}(x_1, x_2)l_{\mu'}(y_1, y_2)f(x_1, y_1)f(x_2, y_2)dx_1 dx_2 dy_1 dy_2. \end{aligned}$$

By upper bounding $f(x_2, y_2)$ by $\|f\|_\infty$ in the last integral, we have

$$\begin{aligned} &\int k_{\lambda'}(x_1, x_2)l_{\mu'}(y_1, y_2)f(x_1, y_1)f(x_2, y_2)dx_1 dx_2 dy_1 dy_2 \\ &\leq \|f\|_\infty \int \left[\int k_{\lambda'}(x_1, x_2)dx_2 \right] \left[\int l_{\mu'}(y_1, y_2)dy_2 \right] f(x_1, y_1)dx_1 dy_1 \\ &= \|f\|_\infty. \end{aligned}$$

This leads to,

$$\mathbb{E}[k_\lambda^2(X_1, X_2)l_\mu^2(Y_1, Y_2)] \leq \frac{\|f\|_\infty}{(4\pi)^{\frac{p+q}{2}} \lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}. \quad (45)$$

We can easily show by similar argument that

$$\mathbb{E} [k_\lambda^2(X_1, X_2)l_\mu^2(Y_3, Y_4)] \leq \frac{\|f_1\|_\infty \|f_2\|_\infty}{(4\pi)^{\frac{p+q}{2}} \lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}. \quad (46)$$

and

$$\mathbb{E} [k_\lambda^2(X_1, X_2)l_\mu^2(Y_1, Y_3)] \leq \frac{\|f\|_\infty}{(4\pi)^{\frac{p+q}{2}} \lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}. \quad (47)$$

From Equations (45), (46) and (47), we have

$$s^2(\lambda, \mu) \leq \frac{C(M_f)}{(4\pi)^{\frac{p+q}{2}} \lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}. \quad (48)$$

From Equations (44) and (48) we obtain the following inequality for $\text{Var}_f(\widehat{\text{HSIC}}_{\lambda, \mu})$

$$\text{Var}_f(\widehat{\text{HSIC}}_{\lambda, \mu}) \leq C(M_f, p, q) \left\{ \frac{1}{n} + \frac{1}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2} \right\}.$$

4.4 Proof of Proposition 3

To give an upper bound for the quantile $q_{1-\alpha}^{\lambda, \mu}$ w.r.t λ and μ , we use concentration inequalities for general U -statistics. However, sharp upper bounds are obtained only for degenerate U -statistics (see e.g. [Houdré and Reynaud-Bouret, 2003]). We recall that, an U -statistic $U_n = U_n(V_1, \dots, V_r)$ is degenerate if $\mathbb{E}[U_n | V_1, \dots, V_i] = 0$ for all i in $\{1, \dots, r-1\}$. The first step to upper bound $q_{1-\alpha}^{\lambda, \mu}$ is then to write $\widehat{\text{HSIC}}_{\lambda, \mu}$ as a sum of degenerate U -statistics. For this, we rely on ANOVA-decomposition (ANOVA for ANalyse Of VAriance, see e.g. [Sobol, 2001]) of the symmetrical function $h_{i,j,q,r}$ introduced in Equation (36). We then write:

$$h_{i,j,q,r} = \frac{1}{2} \sum_{(t,u)}^{(i,j,q,r)} h_{t,u} + \frac{1}{6} \sum_{(t,u,v)}^{(i,j,q,r)} h_{t,u,v} + \tilde{h}_{i,j,q,r}, \quad (49)$$

where the first (resp. the second) sum represents all ordered pairs (t, u) (resp. triplets (t, u, v)) drawn without replacement from (i, j, q, r) and the terms $h_{t,u}$, $h_{t,u,v}$ and $\tilde{h}_{i,j,q,r}$ are defined as

$$\begin{aligned} h_{t,u} &= \mathbb{E}[h_{i,j,q,r} | Z_t, Z_u], \\ h_{t,u,v} &= \mathbb{E}[h_{i,j,q,r} | Z_t, Z_u, Z_v] - \frac{1}{2} \sum_{(t',u')}^{(t,u,v)} h_{t',u'}, \\ \tilde{h}_{i,j,q,r} &= h_{i,j,q,r} - \frac{1}{6} \sum_{(t,u,v)}^{(i,j,q,r)} h_{t,u,v} - \frac{1}{2} \sum_{(t,u)}^{(i,j,q,r)} h_{t,u}. \end{aligned}$$

Hence, by summing all terms $h_{i,j,q,r}$ for (i, j, q, r) in \mathbf{i}_4^n and then dividing by $(n)_4$, we have:

$$\widehat{\text{HSIC}}_{\lambda, \mu} = 6\widehat{\text{HSIC}}_{\lambda, \mu}^{(2,D)} + 4\widehat{\text{HSIC}}_{\lambda, \mu}^{(3,D)} + \widehat{\text{HSIC}}_{\lambda, \mu}^{(4,D)}, \quad (50)$$

where

$$\begin{aligned} \widehat{\text{HSIC}}_{\lambda, \mu}^{(2,D)} &= \frac{1}{(n)_2} \sum_{(i,j) \in \mathbf{i}_2^n} h_{i,j}, \quad \widehat{\text{HSIC}}_{\lambda, \mu}^{(3,D)} = \frac{1}{(n)_3} \sum_{(i,j,q) \in \mathbf{i}_3^n} h_{i,j,q} \\ \widehat{\text{HSIC}}_{\lambda, \mu}^{(4,D)} &= \frac{1}{(n)_4} \sum_{(i,j,q,r) \in \mathbf{i}_4^n} \tilde{h}_{i,j,q,r}. \end{aligned}$$

Lemma 8. *Let us assume that $f = f_1 \otimes f_2$. Then, the U -statistics $\widehat{\text{HSIC}}_{\lambda, \mu}^{(2,D)}$, $\widehat{\text{HSIC}}_{\lambda, \mu}^{(3,D)}$ and $\widehat{\text{HSIC}}_{\lambda, \mu}^{(4,D)}$ are degenerated.*

Proof. According to Theorem 2 of [Gretton et al., 2008], if $f = f_1 \otimes f_2$, we have:

$$\mathbb{E}[h_{i,j,q,r} | Z_i] = 0.$$

We then easily show that $\widehat{\text{HSIC}}_{\lambda,\mu}^{(2,D)}$ is degenerated by writing

$$\mathbb{E}[h_{i,j} | Z_i] = \mathbb{E}[h_{i,j,q,r} | Z_i] = 0. \quad (51)$$

Moreover, to prove that $\widehat{\text{HSIC}}_{\lambda,\mu}^{(3,D)}$ is degenerated, we have

$$\begin{aligned} \mathbb{E}[h_{i,j,q} | Z_i, Z_j] &= \mathbb{E}[h_{i,j,q,r} | Z_i, Z_j] - \mathbb{E}[h_{i,j} | Z_i, Z_j] - \mathbb{E}[h_{i,q} | Z_i] - \mathbb{E}[h_{j,q} | Z_j] \\ &= h_{i,j} - h_{i,j} \quad (\text{by definition of } h_{i,j} \text{ and Equation (51)}) \\ &= 0. \end{aligned} \quad (52)$$

Finally, to show that $\widehat{\text{HSIC}}_{\lambda,\mu}^{(4,D)}$ is degenerated, we write

$$\begin{aligned} \mathbb{E}[\tilde{h}_{i,j,q,r} | Z_i, Z_j, Z_q] &= \mathbb{E}[h_{i,j,q,r} | Z_i, Z_j, Z_q] - h_{i,j,q} - h_{i,j} - h_{i,q} - h_{j,q} \\ &= 0. \end{aligned} \quad (53)$$

□

Once we have upper bounds of the $(1 - \alpha)$ -quantiles of $\widehat{\text{HSIC}}_{\lambda,\mu}^{(r,D)}$ with r in $\{2, 3, 4\}$ under the assumption $f = f_1 \otimes f_2$, an upper bound of the quantile $q_{1-\alpha}^{\lambda,\mu}$ is naturally obtained. In fact, we can easily show that,

$$q_{1-\alpha}^{\lambda,\mu} \leq 6q_{1-\alpha/3,2}^{\lambda,\mu} + 4q_{1-\alpha/3,3}^{\lambda,\mu} + q_{1-\alpha/3,4}^{\lambda,\mu}$$

where $q_{1-\alpha,r}^{\lambda,\mu}$ is the $(1 - \alpha)$ -quantiles of $\widehat{\text{HSIC}}_{\lambda,\mu}^{(r,D)}$ under the assumption $f = f_1 \otimes f_2$.

4.4.1 Upper bound of $q_{1-\alpha,2}^{\lambda,\mu}$

In this part, we give an upper bound of $q_{1-\alpha,2}^{\lambda,\mu}$. For this, we use the concentration Inequality 3.5, page 15 of [Giné et al., 2000], given for degenerated U-statistics of order 2. We write for all $t > 0$:

$$\mathbb{P}\left(\left|\sum_{i,j} h_{i,j}\right| > t\right) \leq A \exp\left(-\frac{1}{A} \min\left[\frac{t}{M}, \left(\frac{t}{L}\right)^{2/3}, \left(\frac{t}{K}\right)^{1/2}\right]\right), \quad (54)$$

where

$$\begin{aligned} K &= \max_{i,j} \|h_{i,j}\|_\infty, \quad M^2 = \sum_{i,j} \mathbb{E}[h_{i,j}^2] \\ L^2 &= \max\left[\left\|\sum_i \mathbb{E}[h_{i,j}^2(Z_i, y)]\right\|_\infty, \left\|\sum_j \mathbb{E}[h_{i,j}^2(x, Z^{(j)})]\right\|_\infty\right]. \end{aligned}$$

By setting $\varepsilon = \frac{t}{n^2}$, and using Equation (54), we obtain

$$\mathbb{P}\left(\frac{1}{n^2} \left|\sum_{i,j} h_{i,j}\right| > \varepsilon\right) \leq A \exp\left(-\frac{1}{A} \min\left[\frac{n^2\varepsilon}{M}, \left(\frac{n^2\varepsilon}{L}\right)^{2/3}, \left(\frac{n^2\varepsilon}{K}\right)^{1/2}\right]\right).$$

Therefore, we have for all $\varepsilon > 0$,

$$\begin{aligned} \mathbb{P}\left(\frac{1}{n^2} \left|\sum_{i,j} h_{i,j}\right| > \varepsilon\right) &\leq A \exp\left(-\frac{1}{A} \min\left[\frac{n^2\varepsilon}{M}, \left(\frac{n^2\varepsilon}{L}\right)^{2/3}, \left(\frac{n^2\varepsilon}{K}\right)^{1/2}\right]\right) \\ &= A \max\left[\exp\left(-\frac{n^2\varepsilon}{AM}\right), \exp\left(-\frac{n^{4/3}\varepsilon^{2/3}}{AL^{2/3}}\right), \exp\left(-\frac{n\varepsilon^{1/2}}{AK^{1/2}}\right)\right]. \end{aligned}$$

By adjusting the constant A , we can replace in the last inequality $\frac{1}{n^2} \sum_{i,j} h_{i,j}$ by $\widehat{\text{HSIC}}_{\lambda,\mu}^{(2,D)}$,

$$\mathbb{P} \left(\left| \widehat{\text{HSIC}}_{\lambda,\mu}^{(2,D)} \right| > \varepsilon \right) \leq A \max \left[\exp \left(-\frac{n^2 \varepsilon}{AM} \right), \exp \left(-\frac{n^{4/3} \varepsilon^{2/3}}{AL^{2/3}} \right), \exp \left(-\frac{n \varepsilon^{1/2}}{AK^{1/2}} \right) \right].$$

Furthermore, if ε_α is a positif number verifying

$$\alpha = A \max \left[\exp \left(-\frac{n^2 \varepsilon_\alpha}{AM} \right), \exp \left(-\frac{n^{4/3} \varepsilon_\alpha^{2/3}}{AL^{2/3}} \right), \exp \left(-\frac{n \varepsilon_\alpha^{1/2}}{AK^{1/2}} \right) \right].$$

Then, we can easily show the following inequality

$$q_{1-\alpha,2}^{\lambda,\mu} \leq \varepsilon_\alpha. \quad (55)$$

By now, we upper bound ε_α (and consequently $q_{1-\alpha,2}^{\lambda,\mu}$), in the 3 following cases.

Case 1. $\alpha = A \exp \left(-\frac{n^2 \varepsilon_\alpha}{AM} \right)$

In this case, ε_α is expressed as

$$\varepsilon_\alpha = \frac{AM}{n^2} \left(\log \left(\frac{1}{\alpha} \right) + \log(A) \right).$$

We can then upper bound ε_α as

$$\varepsilon_\alpha \leq \frac{CM}{n^2} \left(\log \left(\frac{1}{\alpha} \right) + 1 \right).$$

Furthermore, considering the values of α such that $\log \left(\frac{1}{\alpha} \right) > 1$ and by changing constant C value, we obtain

$$\varepsilon_\alpha \leq \frac{CM}{n^2} \log \left(\frac{1}{\alpha} \right). \quad (56)$$

Let us upper bound M w.r.t λ , μ and n . For this, we first write

$$M^2 = \sum_{i,j} \mathbb{E}[h_{i,j}^2] = n^2 \mathbb{E}[h_{1,2}^2].$$

Moreover, using the law of total variance, we have under the hypothesis $f = f_1 \otimes f_2$,

$$\begin{aligned} \mathbb{E}[h_{1,2}^2] &= \text{Var}(\mathbb{E}[h_{1,2,3,4} | Z_1, Z_2]) \\ &\leq \text{Var}(h_{1,2,3,4}). \end{aligned}$$

Furthermore, we have shown in Annexe 4.3.2 that,

$$\text{Var}(h_{1,2,3,4}) \leq \frac{C(M_f, p, q)}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}.$$

Hence, we can upper bound M as follows,

$$M \leq \frac{C(M_f, p, q) n}{\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}}. \quad (57)$$

Consequently, by combining Equations (56) and (57), we obtain

$$q_{1-\alpha,2}^{\lambda,\mu} \leq \frac{C(M_f, p, q)}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log \left(\frac{1}{\alpha} \right). \quad (58)$$

Case 2. $\alpha = A \exp \left(-\frac{n^{4/3} \varepsilon_\alpha^{2/3}}{AL^{2/3}} \right)$

In this case, ε_α verify that,

$$\varepsilon_\alpha^{2/3} = \frac{AL^{2/3}}{n^{4/3}} \left(\log \left(\frac{1}{\alpha} \right) + \log(A) \right).$$

Thus, ε_α can be upper bounded as

$$\varepsilon_\alpha \leq \frac{CL}{n^2} \log \left(\frac{1}{\alpha} \right)^{3/2}, \quad (59)$$

Let us upper bound L w.r.t n , λ and μ . For this, knowing that $h_{i,j}$ is symmetrical we write

$$L^2 = \left\| \sum_i \mathbb{E}[h_{i,j}^2(Z_i, y)] \right\|_\infty.$$

Moreover, according to [Gretton et al., 2008] page 10, we have under the hypothesis $f = f_1 \otimes f_2$,

$$h_{i,j}(Z_i, Z_j) = \frac{1}{6} [k_\lambda(X_i, X_j) + (k_\lambda)_{..} - (k_\lambda)_{i.} - (k_\lambda)_{.j}] [l_\mu(Y_i, Y_j) + (l_\mu)_{..} - (l_\mu)_{i.} - (l_\mu)_{.j}],$$

where $(k_\lambda)_{..} = \mathbb{E}[k_\lambda(X_i, X_j)]$, $(k_\lambda)_{i.} = \mathbb{E}[k_\lambda(X_i, X_j) \mid X_i]$, $(k_\lambda)_{.j} = \mathbb{E}[k_\lambda(X_i, X_j) \mid X_j]$ and $(l_\mu)_{..}$, $(l_\mu)_{i.}$, $(l_\mu)_{.j}$ are defined in a similar way.

Hence, we write for all $y = (y_1, y_2) \in \mathbb{R}^2$,

$$\begin{aligned} h_{i,j}^2(Z_i, y) &= \frac{1}{36} \left[k_\lambda(X_i, y_1) + (k_\lambda)_{..} - \mathbb{E}[k_\lambda(X_i, X_j) \mid X_i] - \mathbb{E}[k_\lambda(X_i, y_1)] \right]^2 \\ &\quad \times \left[l_\mu(Y_i, y_2) + (l_\mu)_{..} - \mathbb{E}[l_\mu(Y_i, Y_j) \mid Y_i] - \mathbb{E}[l_\mu(Y_i, y_2)] \right]^2. \end{aligned}$$

Therefore, we have the following inequality for $h_{i,j}^2(Z_i, y)$,

$$\begin{aligned} h_{i,j}^2(Z_i, y) &\leq C \left[k_\lambda(X_i, y_1)^2 + (k_\lambda)_{..}^2 + \mathbb{E}[k_\lambda(X_i, X_j) \mid X_i]^2 + \mathbb{E}[k_\lambda(X_i, y_1)]^2 \right] \\ &\quad \times \left[l_\mu(Y_i, y_2)^2 + (l_\mu)_{..}^2 + \mathbb{E}[l_\mu(Y_i, Y_j) \mid Y_i]^2 + \mathbb{E}[l_\mu(Y_i, y_2)]^2 \right]. \end{aligned}$$

Using that (X_1, \dots, X_n) and (Y_1, \dots, Y_n) are independent, we write

$$\begin{aligned} L^2 &\leq C (M_f) n \mathbb{E} \left[k_\lambda(X_i, y_1)^2 + (k_\lambda)_{..}^2 + \mathbb{E}[k_\lambda(X_i, X_j) \mid X_i]^2 + \mathbb{E}[k_\lambda(X_i, y_1)]^2 \right] \\ &\quad \times \mathbb{E} \left[l_\mu(Y_i, y_2)^2 + (l_\mu)_{..}^2 + \mathbb{E}[l_\mu(Y_i, Y_j) \mid Y_i]^2 + \mathbb{E}[l_\mu(Y_i, y_2)]^2 \right]. \end{aligned}$$

Each term can be upper bounded by similar arguments as 4.3.2, we then have

$$L^2 \leq C (M_f) n \left(1 + \frac{1}{\lambda_1 \dots \lambda_p} \right) \left(1 + \frac{1}{\mu_1 \dots \mu_q} \right).$$

Thus, using that $\lambda_1 \dots \lambda_p < 1$ and $\mu_1 \dots \mu_q < 1$, we obtain:

$$L \leq \frac{C (M_f) \sqrt{n}}{\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}}. \quad (60)$$

By combining Equations (59) and (60), we have

$$\varepsilon_\alpha \leq \frac{C (M_f)}{\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} n^{3/2}} \left[\log \left(\frac{1}{\alpha} \right) \right]^{3/2}.$$

Moreover, knowing that $\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q < 1$, we obtain

$$\varepsilon_\alpha \leq \frac{C (M_f)}{(n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q})^{3/2}} \left[\log \left(\frac{1}{\alpha} \right) \right]^{3/2}. \quad (61)$$

Case 3. $\alpha = A \exp\left(-\frac{n\varepsilon_\alpha^{1/2}}{AK^{1/2}}\right)$

In this case, ε_α is expressed as

$$\varepsilon_\alpha^{1/2} = \frac{AK^{1/2}}{n} \left(\log\left(\frac{1}{\alpha}\right) + \log(A) \right).$$

Using that $\log\left(\frac{1}{\alpha}\right) > 1$ and by adjusting the value of A , we upper bound ε_α as

$$\varepsilon_\alpha \leq \frac{AK}{n^2} \left[\log\left(\frac{1}{\alpha}\right) \right]^2. \quad (62)$$

Moreover, we can easily show that

$$K \leq \frac{4}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}. \quad (63)$$

By combining Equations (62) and (63), we obtain:

$$q_{1-\alpha,2}^{\lambda,\mu} \leq \frac{C}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2} \left[\log\left(\frac{1}{\alpha}\right) \right]^2. \quad (64)$$

using (58), (61) and (64) and the fact that $\frac{1}{\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n}} \log\left(\frac{1}{\alpha}\right) < 1$, we have the following inequality

$$q_{1-\alpha,2}^{\lambda,\mu} \leq \frac{C(\|f_1\|_\infty, \|f_2\|_\infty, p, q)}{n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right). \quad (65)$$

4.4.2 Upper bound of $q_{1-\alpha,3}^{\lambda,\mu}$

In this part, we give an upper bound for the $(1-\alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda,\mu}^{(3,D)}$. For this, we propose to use the concentration inequality (c), page 1501 of [Arcones and Gine, 1993]. We write for all $t > 0$,

$$\mathbb{P}\left(n^{-3/2} \left| \sum_{i,j,q} h_{i,j,q} \right| > t\right) \leq A \exp\left[-\frac{Bt^{2/3}}{M^{2/3} + K^{1/2}t^{1/6}n^{-1/4}}\right], \quad (66)$$

where $K = \|h_{i,j,q}\|_\infty$, $M^2 = \mathbb{E}[h_{1,2,3}^2]$ and B an absolute positive constant.

By setting $\varepsilon = \frac{t}{n^{3/2}}$ and using Equation (66), we have

$$\mathbb{P}\left(\frac{1}{n^3} \left| \sum_{i,j,q} h_{i,j,q} \right| > \varepsilon\right) \leq A \exp\left[-\frac{Bn\varepsilon^{2/3}}{M^{2/3} + K^{1/2}\varepsilon^{1/6}}\right].$$

Moreover, by adjusting the value of B , we can write

$$\mathbb{P}\left(\left|\widehat{\text{HSIC}}_{\lambda,\mu}^{(3,D)}\right| > \varepsilon\right) \leq A \exp\left[-\frac{Bn\varepsilon^{2/3}}{M^{2/3} + K^{1/2}\varepsilon^{1/6}}\right]. \quad (67)$$

Furthermore, if ε_α is a positive number verifying

$$A \exp\left[-\frac{Bn\varepsilon_\alpha^{2/3}}{M^{2/3} + K^{1/2}\varepsilon_\alpha^{1/6}}\right] = \alpha, \quad (68)$$

then, we have the following inequality

$$q_{1-\alpha,3}^{\lambda,\mu} \leq \varepsilon_\alpha.$$

In order to upper bound ε_α in (68), we set $\gamma_\alpha = \varepsilon_\alpha^{1/6}$ and we obtain

$$Bn\gamma_\alpha^4 = K^{1/2} \log\left(\frac{A}{\alpha}\right) \gamma_\alpha + M^{2/3} \log\left(\frac{A}{\alpha}\right). \quad (69)$$

The polynomial Equation (69) is not resolvable. However, it's possible to give an upper bound of its roots. Indeed,

$$Bn\gamma_\alpha^4 \leq 2 \max\left[K^{1/2}\gamma_\alpha + M^{2/3}\right] \log\left(\frac{A}{\alpha}\right).$$

Case 1. $\max\left[K^{1/2}\gamma_\alpha + M^{2/3}\right] = K^{1/2}\gamma_\alpha$

In this case, γ_α verify the following inequality,

$$\gamma_\alpha^3 \leq \frac{BK^{1/2}}{n} \left(\log\left(\frac{1}{\alpha}\right) + \log(A) \right).$$

Hence,

$$\varepsilon_\alpha \leq \frac{BK}{n^2} \left(\log\left(\frac{A}{\alpha}\right) \right)^2.$$

Since $K \leq \frac{4}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}$, $\frac{1}{\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} n} \log\left(\frac{1}{\alpha}\right) < 1$ and $\log\left(\frac{1}{\alpha}\right) > 1$, we write

$$\varepsilon_\alpha \leq \frac{C}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

Case 2. $\max\left[K^{1/2}\gamma_\alpha + M^{2/3}\right] = M^{2/3}$

In this case,

$$\gamma_\alpha^4 \leq \frac{BM^{2/3}}{n} \left[\log\left(\frac{A}{\alpha}\right) \right].$$

Therefore, ε_α can be upper bounded as

$$\varepsilon_\alpha \leq \frac{BM}{n^{3/2}} \left[\log\left(\frac{A}{\alpha}\right) \right]^2.$$

Moreover, using the law of total variance, it's easy to see that under the hypothesis $f = f_1 \otimes f_2$,

$$M^2 = \text{Var}(h_{1,2,3}) \leq C \text{Var}(h_{1,2,3,4}). \quad (70)$$

Hence, according to Annexe 4.3.2, M can be upper bounded as

$$M \leq \frac{C(M_f, p, q)}{\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}}.$$

To conclude, in all cases we have the following inequality for $q_{1-\alpha,3}^{\lambda,\mu}$

$$q_{1-\alpha,3}^{\lambda,\mu} \leq \frac{C(\|f_1\|_\infty, \|f_2\|_\infty, p, q)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

4.4.3 Upper bound of $q_{1-\alpha,4}^{\lambda,\mu}$

In this part, we give an upper bound for the $(1 - \alpha)$ -quantile of $\widehat{\text{HSIC}}_{\lambda,\mu}^{(4,D)}$. For this, we use the concentration inequality (d), page 1501 of [Arcones and Gine, 1993]. We have for all $t > 0$:

$$\mathbb{P}\left(\frac{1}{n^2} \left| \sum_{i,j,q,r} \tilde{h}_{i,j,q,r} \right| > t\right) \leq A \exp\left(-B\sqrt{\frac{t}{K}}\right),$$

where, $K = \|\tilde{h}_{1,2,3,4}\|_\infty$.

By setting $\varepsilon = \frac{t}{n^2}$, we have

$$\mathbb{P}\left(\frac{1}{n^4} \left| \sum_{i,j,q,r} \tilde{h}_{i,j,q,r} \right| > \varepsilon\right) \leq A \exp\left(-Bn\sqrt{\frac{\varepsilon}{K}}\right).$$

Furthermore, by adjusting the constant B , we replace $\frac{1}{n^4} \sum_{i,j,q,r} \tilde{h}_{i,j,q,r}$ by $\widehat{\text{HSIC}}_{\lambda,\mu}^{(4,D)}$. We write

$$\mathbb{P}\left(\left|\widehat{\text{HSIC}}_{\lambda,\mu}^{(4,D)}\right| > \varepsilon\right) \leq A \exp\left(-Bn\sqrt{\frac{\varepsilon}{K}}\right). \quad (71)$$

Moreover, if ε_α is a positive number verifying

$$A \exp\left(-Bn\sqrt{\frac{\varepsilon_\alpha}{K}}\right) = \alpha, \quad (72)$$

then,

$$q_{1-\alpha,4}^{\lambda,\mu} \leq \varepsilon_\alpha.$$

By resolving Equation (72), we obtain the following equality

$$\varepsilon_\alpha = \frac{BK}{n^2} \left[\log\left(\frac{A}{\alpha}\right) \right]^2.$$

Therefore, we can easily show that

$$\varepsilon_\alpha \leq \frac{CK}{n^2} \left[\log\left(\frac{1}{\alpha}\right) \right]^2.$$

Moreover, by using the Inequality $K \leq \frac{4}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}$ we have

$$q_{1-\alpha,4}^{\lambda,\mu} \leq \frac{C}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2} \log\left(\frac{1}{\alpha}\right)^2.$$

Consequently,

$$q_{1-\alpha,4}^{\lambda,\mu} \leq \frac{C}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} n} \log\left(\frac{1}{\alpha}\right). \quad (73)$$

To conclude, the quantile $q_{1-\alpha}^{\lambda,\mu}$ can be upper bounded under the hypothesis $f = f_1 \otimes f_2$ as follows,

$$q_{1-\alpha}^{\lambda,\mu} \leq \frac{C(\|f_1\|_\infty, \|f_2\|_\infty, p, q)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right). \quad (74)$$

4.5 Proof of Corollary 1

The proof of this corollary is immediately obtained from Lemma 1, Proposition 2 and Proposition 3.

4.6 Proof of Lemma 2

Recalling the formulation of $\text{HSIC}_{\lambda,\mu}(f)$ given in Equation (1) with $k = k_\lambda$ and $l = l_\mu$, we obtain

$$\begin{aligned} \text{HSIC}_{\lambda,\mu}(f) &= \int k_\lambda(x, x') l_\mu(y, y') f(x, y) f(x', y') dx dy dx' dy' \\ &\quad - 2 \int k_\lambda(x, x') l_\mu(y, y') f(x, y) f_1(x') f_2(y') dx dy dx' dy' \\ &\quad + \int k_\lambda(x, x') l_\mu(y, y') f_1(x) f_2(y) f_1(x') f_2(y') dx dy dx' dy'. \end{aligned}$$

This expression can be compacted using the symmetry of the kernels k_λ and l_μ :

$$\begin{aligned} \text{HSIC}_{\lambda,\mu}(f) &= \int k_\lambda(x, x') l_\mu(y, y') \left[f(x, y) - f_1(x) f_2(y) \right] \left[f(x', y') - f_1(x') f_2(y') \right] dx dy dx' dy' \\ &= \int k_\lambda(x, x') l_\mu(y, y') \psi(x, y) \psi(x', y') dx dy dx' dy', \end{aligned}$$

where $\psi(x, y) = f(x, y) - f_1(x) f_2(y)$.

Thereafter, we reformulate this equation by replacing $k_\lambda(x, x')$ with $\varphi_\lambda(x - x')$ and replacing $l_\mu(y, y')$ with $\phi_\mu(y - y')$, where φ_λ and ϕ_μ are respectively the functions defined in Equations (3) and (4):

$$\begin{aligned} \text{HSIC}_{\lambda,\mu}(f) &= \int \psi(x, y) \left[\int \psi(x', y') \varphi_\lambda(x - x') \phi_\mu(y - y') dx' dy' \right] dx dy \\ &= \int \int \psi(x, y) [\psi * (\varphi_\lambda \otimes \phi_\mu)](x, y) dx dy \\ &= \langle \psi, \psi * (\varphi_\lambda \otimes \phi_\mu) \rangle_{\mathbb{L}_2} \end{aligned}$$

4.6.1 Proof of Proposition 4

First notice that according to Equations (37) and (48), one can write:

$$\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu}) \leq \frac{C}{n} \text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1]) + \frac{C(M_f, p, q)}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2}, \quad (75)$$

where $h_{1,2,3,4}$ is defined in Equation (36).

To prove the intended result from the last equation, we aim now to upper bound $\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1])$ by $\|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2$ up to a positive constant which depends only on M_f . The following lemma gives such an upper bound.

Lemma 9. *For all λ in $(0, +\infty)^p$ and μ in $(0, +\infty)^q$, we have*

$$\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1]) \leq C(M_f) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2.$$

Proof. The first step to upper bound $\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1])$ is to rewrite $h_{1,2,3,4}$ by isolating all the terms depending on Z_1 .

$$\begin{aligned} h_{1,2,3,4} &= \frac{1}{4!} \sum_{(t,u,v,w)}^{(1,2,3,4)} [k_{t,u} l_{t,u} + k_{t,u} l_{v,w} - 2k_{t,u} l_{t,v}] \\ &= \frac{2}{4!} \sum_{(u,v,w)}^{(2,3,4)} [k_{1,u} l_{1,u} + k_{1,u} l_{v,w} + k_{u,v} l_{1,w} - k_{w,v} l_{w,1} - k_{u,1} l_{u,v} - k_{1,u} l_{1,v}] + R(Z_2, Z_3, Z_4), \end{aligned}$$

where the last sum represents all triplets (u, v, w) drawn without replacement from $(2, 3, 4)$ and $R(Z_2, Z_3, Z_4)$ is a random variable depending only on Z_2, Z_3 and Z_4 .

Then,

$$h_{1,2,3,4} = R(Z_2, Z_3, Z_4) + \frac{1}{12} \sum_{(u,v,w)}^{(2,3,4)} [k_{1,u}(l_{1,u} - l_{1,v}) - k_{u,1}(l_{u,v} - l_{v,w}) - (k_{w,v} - k_{u,v})l_{1,w}].$$

The random variable $R(Z_2, Z_3, Z_4)$ being independent from Z_1 , the variance of its expectation conditionally to Z_1 is equal to 0. It is then easy to see that $\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1])$ can be upper bounded as follows:

$$\begin{aligned} \text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1]) &\leq C \left[\text{Var}_f(\mathbb{E}[k_{1,2}(l_{1,2} - l_{1,3}) | Z_1]) + \text{Var}_f(\mathbb{E}[k_{2,1}(l_{2,3} - l_{3,4}) | X_1]) \right. \\ &\quad \left. + \text{Var}_f(\mathbb{E}[(k_{2,3} - k_{4,3})l_{1,2} | Y_1]) \right], \end{aligned} \quad (76)$$

By now, we reformulate the function $\psi * (\varphi_\lambda \otimes \phi_\mu)$ in a simpler form in order to link its \mathbb{L}_2 -norm with the upper bound given in Equation (76). For notational convenience, we denote $G_{\lambda,\mu} = \psi * (\varphi_\lambda \otimes \phi_\mu)$. We then write

$$\begin{aligned} G_{\lambda,\mu}(x, y) &= \int \psi(x', y') k_\lambda(x, x') l_\mu(y, y') dx' dy' \\ &= \text{Cov}(k_\lambda(x, X'), l_\mu(y, Y')), \end{aligned}$$

where the random couple (X', Y') has f as distribution.

Thereafter, the conditional expectations in Equation (76) can all be expressed as follows:

$$\begin{aligned} \mathbb{E}[k_{1,2}(l_{1,2} - l_{1,3}) | Z_1] &= G_{\lambda,\mu}(X_1, Y_1), \\ \mathbb{E}[k_{2,1}(l_{2,3} - l_{3,4}) | X_1] &= \mathbb{E}[G_{\lambda,\mu}(X_1, Y_3) | X_1], \\ \mathbb{E}[(k_{2,3} - k_{4,3})l_{1,2} | Y_1] &= \mathbb{E}[G_{\lambda,\mu}(X_3, Y_1) | Y_1]. \end{aligned}$$

Thus, using the law of total variance [Weiss, 2006], we have the following upper bound for $\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1])$:

$$\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1]) \leq C \left[\text{Var}_f(G_{\lambda,\mu}(X_1, Y_1)) + \text{Var}_f(G_{\lambda,\mu}(X_1, Y_3)) + \text{Var}_f(G_{\lambda,\mu}(X_3, Y_1)) \right].$$

On the other hand, it is straightforward to upper bound the three variances in the last equation as

$$\begin{aligned} \text{Var}_f(G_{\lambda,\mu}(X_1, Y_1)) &\leq \|f\|_\infty \|G_{\lambda,\mu}\|_{\mathbb{L}_2}^2, \\ \text{Var}_f(G_{\lambda,\mu}(X_1, Y_3)) &\leq \|f_1 \otimes f_2\|_\infty \|G_{\lambda,\mu}\|_{\mathbb{L}_2}^2, \\ \text{Var}_f(G_{\lambda,\mu}(X_3, Y_1)) &\leq \|f_1 \otimes f_2\|_\infty \|G_{\lambda,\mu}\|_{\mathbb{L}_2}^2. \end{aligned}$$

Consequently, combining the three last Equations with Equation (76) gives us the following upper bound of $\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1])$:

$$\text{Var}_f(\mathbb{E}[h_{1,2,3,4} | Z_1]) \leq C(M_f) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2.$$

□

We then obtain as a result of Equation (75) and Lemma 9:

$$\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu}) \leq \frac{C(M_f) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2}{n} + \frac{C(M_f, p, q)}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q n^2}.$$

4.7 Proof of Theorem 1

We aim here to give a condition on the \mathbb{L}_2 -norm of $\psi = f - f_1 \otimes f_2$ so that the second type error of the test $\Delta_\alpha^{\lambda,\mu}$ is controlled by a given β in $(0, 1)$. For this, we first recall that Lemma 1 gives such a condition on the theoretical value $\text{HSIC}_{\lambda,\mu}(f)$. More specifically, $P_f(\widehat{\text{HSIC}}_{\lambda,\mu} \leq q_{1-\alpha}^{\lambda,\mu}) \leq \beta$ as soon as

$$\text{HSIC}_{\lambda,\mu}(f) > \sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} + q_{1-\alpha}^{\lambda,\mu}.$$

On the other hand, using the upper bound given in Proposition 3 for the quantile $q_{1-\alpha}^{\lambda,\mu}$ and the upper bound of the variance $\text{Var}(\widehat{\text{HSIC}}_{\lambda,\mu})$ provided by Proposition 4, one can easily deduce that if

$$\max(\lambda_1 \dots \lambda_p, \mu_1 \dots \mu_q) < 1 \quad \text{and} \quad n \sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} > \log\left(\frac{1}{\alpha}\right) > 1, \quad (77)$$

then we have the following inequality:

$$\sqrt{\frac{\text{Var}_f(\widehat{\text{HSIC}}_{\lambda,\mu})}{\beta}} + q_{1-\alpha}^{\lambda,\mu} \leq \frac{C(M_f, \beta) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}}{\sqrt{n}} + \frac{C(M_f, p, q, \beta)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

Under the conditions given in (77), a sufficient for the test $\Delta_\alpha^{\lambda,\mu}$ to have a second error at most equal to β is then

$$\text{HSIC}_{\lambda,\mu}(f) > \frac{C(M_f, \beta) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}}{\sqrt{n}} + \frac{C(M_f, p, q)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

On the other hand, according to Lemma 2, we have

$$\text{HSIC}_{\lambda,\mu}(f) = \frac{1}{2} \left(\|\psi\|_{\mathbb{L}_2}^2 + \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 - \|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 \right).$$

We can then convert the condition on $\text{HSIC}_{\lambda,\mu}(f)$ in a condition in terms of $\|\psi\|_{\mathbb{L}_2}^2$. Indeed, under the conditions given in (77), $P_f(\widehat{\text{HSIC}}_{\lambda,\mu} \leq q_{1-\alpha}^{\lambda,\mu}) \leq \beta$ as soon as

$$\|\psi\|_{\mathbb{L}_2}^2 > \|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 + \frac{C(M_f, p, q, \beta)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right) + R(M_f, \beta, \lambda, \mu, n),$$

$$\text{where } R(M_f, \beta, \lambda, \mu, n) = \frac{C(M_f, \beta) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}}{\sqrt{n}} - \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2.$$

By now, let us show that $R(M_f, \beta, \lambda, \mu, n)$ can be upper bounded by $1/n$ up to a positive constant depending only on M_f and β . For this, we simply use that for all $a > 0$ and $b > 0$, we have the inequality: $2ab < a^2 + b^2$. We then write

$$\frac{C(M_f, \beta) \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}}{\sqrt{n}} \leq \frac{C(M_f, \beta)}{n} + \|\psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2.$$

We then obtain the following inequality:

$$R(M_f, \beta, \lambda, \mu, n) \leq \frac{C(M_f, \beta)}{n}.$$

Consequently, under the conditions given in (77), $P_f(\widehat{\text{HSIC}}_{\lambda,\mu} \leq q_{1-\alpha}^{\lambda,\mu}) \leq \beta$ as soon as

$$\|\psi\|_{\mathbb{L}_2}^2 > \|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 + \frac{C(M_f, p, q, \beta)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

4.8 Proof of Lemma 3

The objective here is to provide an upper bound of the bias term $\|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2$ w.r.t λ and μ , when $\psi \in \mathcal{S}_{p+q}^\delta(R)$, where $\delta \in (0, 2]$. We first set $b = \psi * (\varphi_\lambda \otimes \phi_\mu) - \psi$, using that $b \in \mathbb{L}^1(\mathbb{R}^{p+q}) \cap \mathbb{L}^2(\mathbb{R}^{p+q})$, Plancherel's theorem gives that

$$\begin{aligned} (2\pi)^{p+q} \|b\|_{\mathbb{L}_2}^2 &= \|\hat{b}\|_{\mathbb{L}_2}^2 \\ &= \|(1 - \widehat{\varphi_\lambda \otimes \phi_\mu})\hat{\psi}\|_{\mathbb{L}_2}^2. \end{aligned} \tag{78}$$

Let us denote g_1 as in Equation (2), the real function defined for all $z \in \mathbb{R}$ as $g_1(z) = \frac{1}{\sqrt{2\pi}} \exp(-z^2/2)$.

We then obviously have the following equation:

$$\varphi_\lambda \otimes \phi_\mu(x, y) = \prod_{i=1}^p \frac{1}{\lambda_i} g_1\left(\frac{x_i}{\lambda_i}\right) \prod_{j=1}^q \frac{1}{\mu_j} g_1\left(\frac{y_j}{\mu_j}\right).$$

Moreover, it is quite known that $\hat{g}_1 = \sqrt{2\pi}g_1$, and that the Fourier transform of the product of functions with separate variables is the product of Fourier transform of each of these functions. We also recall that if G is a real function and $a > 0$ then, the Fourier transform of $z \mapsto 1/a \cdot G(z/a)$ is $u \mapsto \widehat{G}(au)$. We then obtain

$$\begin{aligned}\widehat{\varphi_\lambda \otimes \phi_\mu}(\xi, \zeta) &= (2\pi)^{\frac{p+q}{2}} \prod_{i=1}^p g_1(\lambda_i \xi_i) \prod_{j=1}^q g_1(\mu_j \zeta_j) \\ &= \exp\left(-(\lambda_1^2 \xi_1^2 + \dots + \lambda_p^2 \xi_p^2 + \mu_1^2 \zeta_1^2 + \dots + \mu_q^2 \zeta_q^2)/2\right).\end{aligned}$$

Thereafter, using Equation (78), the bias term $\|b\|_{\mathbb{L}_2}^2$ can then expressed as follows

$$\begin{aligned}\|b\|_{\mathbb{L}_2}^2 &= \frac{1}{(2\pi)^{p+q}} \int \left(1 - \exp\left(-(\lambda_1^2 \xi_1^2 + \dots + \lambda_p^2 \xi_p^2 + \mu_1^2 \zeta_1^2 + \dots + \mu_q^2 \zeta_q^2)/2\right)\right)^2 |\hat{\psi}(\xi, \zeta)|^2 d\xi d\zeta \\ &= \frac{1}{(2\pi)^{p+q}} \int \frac{\left(1 - \exp\left(-(\lambda_1^2 \xi_1^2 + \dots + \lambda_p^2 \xi_p^2 + \mu_1^2 \zeta_1^2 + \dots + \mu_q^2 \zeta_q^2)/2\right)\right)^2}{\|(\xi, \zeta)\|_2^{2\delta}} \|(\xi, \zeta)\|_2^{2\delta} |\hat{\psi}(\xi, \zeta)|^2 d\xi d\zeta.\end{aligned}\tag{79}$$

In order to upper bound the last integral, one can first notice that for all λ, ξ in $(0, +\infty)^p$ and μ, ζ in $(0, +\infty)^q$, we have: $\lambda_1^2 \xi_1^2 + \dots + \lambda_p^2 \xi_p^2 + \mu_1^2 \zeta_1^2 + \dots + \mu_q^2 \zeta_q^2 \leq \|(\lambda, \mu)\|_2^2 \|(\xi, \zeta)\|_2^2$. We then obtain:

$$\begin{aligned}& \sup_{(\xi, \zeta) \in \mathbb{R}^{p+q} \setminus \{0\}} \frac{1 - \exp\left(-(\lambda_1^2 \xi_1^2 + \dots + \lambda_p^2 \xi_p^2 + \mu_1^2 \zeta_1^2 + \dots + \mu_q^2 \zeta_q^2)/2\right)}{\|(\xi, \zeta)\|_2^\delta} \\ & \leq \sup_{(\xi, \zeta) \in \mathbb{R}^{p+q} \setminus \{0\}} \frac{1 - \exp\left(-\|(\lambda, \mu)\|_2^2 \|(\xi, \zeta)\|_2^2 / 2\right)}{\|(\xi, \zeta)\|_2^\delta} \\ & = \|(\lambda, \mu)\|_2^\delta \sup_{H > 0} \frac{1 - \exp(-H/2)}{H^{\delta/2}}.\end{aligned}$$

For δ in $(0, 2]$, the function $H \rightarrow \frac{1 - \exp(-H/2)}{H^{\delta/2}}$ is bounded in $(0, +\infty)$. Indeed, it is continuous on $(0, +\infty)$, tends to 0 in $+\infty$ and has a finite limit at 0 ($1/2$ if $\delta = 2$ and 0 else). Hence, we obtain the following inequality:

$$\sup_{(\xi, \zeta) \in \mathbb{R}^{p+q} \setminus \{0\}} \frac{\left(1 - \exp\left(-(\lambda_1^2 \xi_1^2 + \dots + \lambda_p^2 \xi_p^2 + \mu_1^2 \zeta_1^2 + \dots + \mu_q^2 \zeta_q^2)/2\right)\right)^2}{\|(\xi, \zeta)\|_2^{2\delta}} \leq C(\delta) \|(\lambda, \mu)\|_2^{2\delta}.$$

Thereafter, using Hölder's inequality, it is straightforward to see that

$$\|(\lambda, \mu)\|_2^{2\delta} \leq C(\delta) \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right].$$

Hence, combining the two last inequalities gives

$$\|b\|_{\mathbb{L}_2}^2 \leq C(\delta) \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right] \int \|(\xi, \zeta)\|_2^{2\delta} |\hat{\psi}(\xi, \zeta)|^2 d\xi d\zeta.$$

Recalling that ψ belongs to the Sobolev ball $\mathcal{S}_{p+q}^\delta(R)$, we obtain

$$\|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2 \leq C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right].$$

4.9 Proof of Theorem 2

We easily deduce from Theorem 1 and Lemma 3 that if ψ belongs to the Sobolev balls $\mathcal{S}_d^\delta(R)$ with δ in $(0, 2]$, $P_f(\widehat{\text{HSIC}}_{\lambda, \mu} \leq q_{1-\alpha}^{\lambda, \mu}) \leq \beta$ as soon as

$$\|\psi\|_{\mathbb{L}_2}^2 > C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\delta} + \sum_{j=1}^q \mu_j^{2\delta} \right] + \frac{C(M_f, p, q, \beta)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

It now follows from the definition (6) of the uniform separation rate that

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

4.10 Proof of Corollary 2

The objective here is to give the uniform separation rate having the smallest upper bound w.r.t. the sample-size n , when ψ belongs to a Sobolev ball $\mathcal{S}_d^\delta(R)$ with δ in $(0, 2]$. For this, we recall that according to Theorem 2, we have:

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

In order to have the smallest behaviour of the right side of the last inequality w.r.t. n , one has then to choose bandwidths $\lambda^* = (\lambda_1^*, \dots, \lambda_p^*)$ and $\mu^* = (\mu_1^*, \dots, \mu_q^*)$ w.r.t. n in such a way that

$$\sum_{i=1}^p \lambda_i^{*2\delta} + \sum_{j=1}^q \mu_j^{*2\delta} \quad \text{and} \quad \frac{1}{n\sqrt{\lambda_1^* \dots \lambda_p^* \mu_1^* \dots \mu_q^*}}$$

have the same behaviour in n . Thereafter, it is clear that all λ_i^* 's and μ_j^* 's have the same behaviour w.r.t. n . It obviously follows than for all i in $\{1, \dots, p\}$ and all j in $\{1, \dots, q\}$, we have:

$$\lambda_i^* = \mu_j^* = n^{-\frac{2}{4\delta + (p+q)}}.$$

Consequently, the separation rate $\rho(\Delta_\alpha^{\lambda^*, \mu^*}, \mathcal{S}_{p+q}^\delta(R), \beta)$ can be upper bound as

$$\rho(\Delta_\alpha^{\lambda^*, \mu^*}, \mathcal{S}_{p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) n^{-\frac{2\delta}{4\delta + (p+q)}}.$$

4.11 Proof of Lemma 4

The objective here is to give an upper bound of the bias term $\|\psi - \psi * (\varphi_\lambda \otimes \phi_\mu)\|_{\mathbb{L}_2}^2$ w.r.t. λ and μ , when ψ belongs to a Nikol'skii-Besov ball $\mathcal{N}_{2, p+q}^\delta(R)$, with $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q)$ in $(0, 2]^{p+q}$. We first set $b = \psi * (\varphi_\lambda \otimes \phi_\mu) - \psi$ and we write

$$\begin{aligned} b(x, y) &= \psi * (\varphi_\lambda \otimes \phi_\mu)(x, y) - \psi(x, y) \\ &= \int \psi(x', y') \varphi_\lambda(x - x') \phi_\mu(y - y') dx' dy' - \psi(x, y). \end{aligned}$$

Moreover, using Equations (3) and (4), the fonction b can be written in terms of the functions g_p and g_q defined in Equation (2):

$$\begin{aligned} b(x, y) &= \frac{1}{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q} \int \psi(x', y') g_p\left(\frac{x_1 - x'_1}{\lambda_1}, \dots, \frac{x_p - x'_p}{\lambda_p}\right) g_q\left(\frac{y_1 - y'_1}{\mu_1}, \dots, \frac{y_q - y'_q}{\mu_p}\right) dx' dy' - \psi(x, y) \\ &= \int \psi(x_1 + \lambda_1 u_1, \dots, x_p + \lambda_p u_p, y_1 + \mu_1 v_1, \dots, y_q + \mu_q v_q) g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) dudv - \psi(x, y). \end{aligned}$$

Thereafter, using that $\int_{\mathbb{R}^p} g_p = \int_{\mathbb{R}^q} g_q = 1$, the function b can be expressed as

$$b(x, y) = \int g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left[\psi(x_1 + \lambda_1 u_1, \dots, x_p + \lambda_p u_p, y_1 + \mu_1 v_1, \dots, y_q + \mu_q v_q) - \psi(x, y) \right] dudv.$$

Let us from now define for all i in $\{1, \dots, p\}$ and j in $\{1, \dots, q\}$, the functions $b_{1,i}$ and $b_{2,j}$ by

$$\begin{aligned} b_{1,i}(x, y) &= \int g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \omega_{1,i}(x, y, u_1, \dots, u_i) dudv \\ b_{2,j}(x, y) &= \int g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \omega_{2,j}(x, y, u_1, \dots, u_p, v_1, \dots, v_j) dudv, \end{aligned}$$

where the function $\omega_{1,i}$ is defined as

$$\omega_{1,i}(x, y, u_1, \dots, u_i) = \psi(x_1 + \lambda_1 u_1, \dots, x_i + \lambda_i u_i, x_{i+1}, \dots, x_p, y) - \psi(x_1 + \lambda_1 u_1, \dots, x_{i-1} + \lambda_{i-1} u_{i-1}, x_i, \dots, x_p, y),$$

while the function $\omega_{2,j}$ is defined as

$$\begin{aligned} \omega_{2,j}(x, y, u_1, \dots, u_p, v_1, \dots, v_j) &= \psi(x_1 + \lambda_1 u_1, \dots, x_p + \lambda_p u_p, y_1 + \mu_1 v_1, \dots, y_j + \mu_j v_j, y_{j+1}, \dots, y_q) \\ &\quad - \psi(x_1 + \lambda_1 u_1, \dots, x_p + \lambda_p u_p, y_1 + \mu_1 v_1, \dots, y_{j-1} + \mu_{j-1} v_{j-1}, y_j, \dots, y_q). \end{aligned}$$

It is then easy to see that the function b is the sum of all the functions $b_{1,i}$ and $b_{2,j}$:

$$b(x, y) = \sum_{i=1}^p b_{1,i}(x, y) + \sum_{j=1}^q b_{2,j}(x, y).$$

One can then deduce that it would be sufficient for the control of the \mathbb{L}_2 -norm of b , to control the \mathbb{L}_2 -normes of all the functions $b_{1,i}$ and $b_{2,j}$. Using the triangular inequality, we have:

$$\|b\|_{\mathbb{L}_2} \leq \sum_{i=1}^p \|b_{1,i}\|_{\mathbb{L}_2} + \sum_{j=1}^q \|b_{2,j}\|_{\mathbb{L}_2}. \quad (80)$$

By now, let us upper bound $\|b_{1,i}\|_{\mathbb{L}_2}^2$ and $\|b_{2,j}\|_{\mathbb{L}_2}^2$ for all i in $\{1, \dots, p\}$ and j in $\{1, \dots, q\}$. We distinguish two cases:

Case 1. $0 < \nu_i \leq 1$

We first recall that $\|b_{1,i}\|_{\mathbb{L}_2}^2$ can be written as

$$\|b_{1,i}\|_{\mathbb{L}_2}^2 = \int \left[\int g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \omega_{1,i}(x, y, u_1, \dots, u_i) dudv \right]^2 dx dy.$$

We use the following lemma from page 13 of [Tsybakov, 2009].

Lemma 10. *Let $\rho : \mathbb{R}^d \times \mathbb{R}^{d'} \rightarrow \mathbb{R}$ be a Borel function, then we have the following inequality:*

$$\int \left(\int \rho(\theta, z) d\theta \right)^2 dz \leq \left[\int \left(\int \rho^2(\theta, z) dz \right)^{1/2} d\theta \right]^2.$$

By applying Lemma 10 to the function $((u, v), (x, y)) \mapsto g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \omega_{1,i}(x, y, u_1, \dots, u_i)$, we obtain:

$$\begin{aligned} \|b_{1,i}\|_{\mathbb{L}_2}^2 &\leq \left[\int \left(\int g_p^2(u_1, \dots, u_p) g_q^2(v_1, \dots, v_q) \omega_{1,i}^2(x, y, u_1, \dots, u_i) dx dy \right)^{1/2} dudv \right]^2 \\ &= \left[\int g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left(\int \omega_{1,i}^2(x, y, u_1, \dots, u_i) dx dy \right)^{1/2} dudv \right]^2. \end{aligned} \quad (81)$$

On the other hand, since ψ belongs to the Nikol'skii-Besov ball $\mathcal{N}_{2,p+q}^\delta(R)$, we have:

$$\left(\int \omega_{1,i}^2(x, y, u_1, \dots, u_i) dx dy \right)^{1/2} \leq R \lambda_i^{\nu_i} |u_i|^{\nu_i}.$$

We then have by injecting this last inequation in Equation (81), that

$$\|b_{1,i}\|_{\mathbb{L}_2}^2 \leq C(R, \nu_i) \lambda_i^{2\nu_i}.$$

Case 2. $1 < \nu_i \leq 2$

In this case the function ψ has continuous first-order partial derivatives. Using Taylor expansion with integral form of the remainder w.r.t. the i^{th} variable of ψ , we have:

$$\omega_{1,i}(x, y, u_1, \dots, u_i) = \lambda_i u_i \int_0^1 (1-\tau) D_i^1 \psi(x_1 + \lambda_1 u_1, \dots, x_i + \tau \lambda_i u_i, x_{i+1}, \dots, y) d\tau.$$

where D_i^1 denotes the first-order partial derivative of ψ w.r.t. the i^{th} variable.

Thereafter, by injecting the last equation in the expression of $b_{1,i}$, we obtain:

$$b_{1,i}(x, y) = \int \lambda_i u_i g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left[\int_0^1 (1-\tau) D_i^1 \psi(x_1 + \lambda_1 u_1, \dots, x_i + \tau \lambda_i u_i, x_{i+1}, \dots, y) d\tau \right] dudv.$$

Furthermore, using the fact that g_p is the density function of the multivariate normal distribution with mean 0 and covariance matrix equals identity, we have that $\int u_i g_p(u_1, \dots, u_p) du_i = 0$. The function $b_{1,i}$ can then be written as

$$b_{1,i}(x, y) = \int \lambda_i u_i g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left[\int_0^1 (1-\tau) D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i) d\tau \right] dudv.$$

We have then the following equation for the \mathbb{L}_2 -norm of $b_{1,i}$:

$$\|b_{1,i}\|_{\mathbb{L}_2}^2 = \int \left[\int \lambda_i u_i g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left(\int_0^1 (1-\tau) D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i) d\tau \right) dudv \right]^2 dx dy.$$

By now, we use as in case 1 Lemma 10 in order to upper bound $\|b_{1,i}\|_{\mathbb{L}_2}^2$. We then obtain:

$$\begin{aligned} \|b_{1,i}\|_{\mathbb{L}_2}^2 &\leq \left(\int \left[\int \left(\lambda_i u_i g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \int_0^1 (1-\tau) D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i) d\tau \right)^2 dx dy \right]^{1/2} dudv \right)^2 \\ &= \left(\int \lambda_i u_i g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left[\int \left(\int_0^1 (1-\tau) D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i) d\tau \right)^2 dx dy \right]^{1/2} dudv \right)^2. \end{aligned}$$

We apply a second time Lemma 10. For this, consider the function $\rho((x, y), \tau) = (1-\tau) D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i)$, we then have:

$$\|b_{1,i}\|_{\mathbb{L}_2}^2 \leq \left(\int \lambda_i u_i g_p(u_1, \dots, u_p) g_q(v_1, \dots, v_q) \left[\int_0^1 (1-\tau) \left(\int (D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i))^2 dx dy \right)^{1/2} d\tau \right] dudv \right)^2. \quad (82)$$

On the other hand, using that ψ belongs to the Nikol'skii-Besov ball $\mathcal{N}_{2,p+q}^\delta(R)$:

$$\left(\int (D_i^1 \omega_{1,i}(x, y, u_1, \dots, \tau u_i))^2 dx dy \right)^{1/2} \leq R \lambda_i^{\nu_i-1} |\tau u_i|^{\nu_i-1}.$$

We then obtain by injecting this last inequation in Equation (82), that

$$\|b_{1,i}\|_{\mathbb{L}_2}^2 \leq C(R, \nu_i) \lambda_i^{2\nu_i}.$$

Besides, for all j in $\{1, \dots, q\}$, by similar arguments:

$$\|b_{2,j}\|_{\mathbb{L}_2}^2 \leq C(R, \gamma_j) \mu_j^{2\gamma_j}.$$

Consequently, according to Equation (80), we have the following upper bound of $\|b\|_{\mathbb{L}_2}^2$:

$$\|b\|_{\mathbb{L}_2}^2 \leq C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\nu_i} + \sum_{j=1}^q \mu_j^{2\gamma_j} \right].$$

4.12 Proof of Theorem 3

The proof of this theorem is similar to that of Theorem 2. Indeed, assuming the conditions of Theorem 1, we have according to this theorem and Lemma 4 that if ψ belongs to $\mathcal{N}_{2,p+q}^\delta(R)$, with $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q)$ in $(0, 2]^{p+q}$: $P_f(\widehat{\text{HSIC}}_{\lambda, \mu} \leq q_{1-\alpha}^{\lambda, \mu}) \leq \beta$ as soon as

$$\|\psi\|_{\mathbb{L}_2}^2 > C(R, \delta) \left[\sum_{i=1}^p \lambda_i^{2\nu_i} + \sum_{j=1}^q \mu_j^{2\gamma_j} \right] + \frac{C(M_f, p, q, \beta)}{n\sqrt{\lambda_1 \dots \lambda_p \mu_1 \dots \mu_q}} \log\left(\frac{1}{\alpha}\right).$$

One can then conclude from the definition (6) of the uniform separation rate that

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

4.13 Proof of Corollary 3

We aim here to give the uniform separation rate having the smallest upper bound w.r.t. the sample-size n , when ψ belongs to a Nikol'skii-Besov ball $\mathcal{N}_{2,p+q}^\delta(R)$, with $\delta = (\nu_1, \dots, \nu_p, \gamma_1, \dots, \gamma_q)$ in $(0, 2]^{p+q}$. We first recall that Theorem 3 shows that:

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

So as to minimize the right side of the last inequality w.r.t. n , we have to choose bandwidths $\lambda^* = (\lambda_1^*, \dots, \lambda_p^*)$ and $\mu^* = (\mu_1^*, \dots, \mu_q^*)$ w.r.t. n such as

$$\left[\sum_{i=1}^p \lambda_i^{*2\nu_i} + \sum_{j=1}^q \mu_j^{*2\gamma_j} \right] \quad \text{and} \quad \frac{1}{n\sqrt{\lambda_1^* \dots \lambda_p^* \mu_1^* \dots \mu_q^*}}$$

have the same behaviour in n . Let us set for all i in $\{1, \dots, p\}$ and all j in $\{1, \dots, q\}$, $\lambda_i^* = n^{a_i}$ and $\mu_j^* = n^{b_j}$. It is then clear that for all i and all j :

$$2a_i\nu_i = 2b_j\gamma_j = -\frac{1}{2} \left[\sum_{r=1}^p a_r + \sum_{s=1}^q b_s \right] - 1. \quad (83)$$

One can first express all a_i 's and all b_j 's w.r.t a_1 as

$$a_i = a_1 \frac{\nu_1}{\nu_i} \quad \text{and} \quad b_j = a_1 \frac{\nu_1}{\gamma_j}.$$

Thereafter, using Equation (83) we have the following:

$$2a_1\nu_1 = \frac{-a_1\nu_1}{2\eta} - 1.$$

We then first write that $a_1 = \frac{-2\eta}{\nu_1(4\eta+1)}$. We next obtain for all i and for all j that:

$$a_i = \frac{-2\eta}{\nu_i(4\eta+1)} \quad \text{and} \quad b_j = \frac{-2\eta}{\gamma_j(4\eta+1)}.$$

Consequently, the separation rate $\rho(\Delta_\alpha^{\lambda^*, \mu^*}, \mathcal{N}_{2,p+q}^\delta(R), \beta)$ can be upper bound as

$$\rho(\Delta_\alpha^{\lambda^*, \mu^*}, \mathcal{N}_{2,p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) n^{-\frac{2\eta}{(1+4\eta)}}.$$

4.14 Proof of Lemma 5

Let α be in $(0, 1)$, we first prove that $u_\alpha \geq \alpha$. For this, we apply Bonferroni's Inequality:

$$\begin{aligned} & P_{f_1 \otimes f_2} \left(\sup_{(\lambda, \mu) \in \Lambda \times U} \left(\widehat{\text{HSIC}}_{\lambda, \mu} - q_{1-\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) > 0 \right) \\ &= P_{f_1 \otimes f_2} \left(\bigcup_{(\lambda, \mu) \in \Lambda \times U} \left\{ \widehat{\text{HSIC}}_{\lambda, \mu} > q_{1-\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right\} \right) \\ &\leq \sum_{(\lambda, \mu) \in \Lambda \times U} P_{f_1 \otimes f_2} \left(\widehat{\text{HSIC}}_{\lambda, \mu} > q_{1-\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) \\ &\leq \sum_{(\lambda, \mu) \in \Lambda \times U} \alpha e^{-\omega_{\lambda, \mu}} \\ &\leq \alpha. \end{aligned}$$

Then, by definition of u_α we have: $u_\alpha \geq \alpha$. Thereafter, we obtain:

$$\begin{aligned} P_f(\Delta_\alpha = 0) &= P_f \left(\bigcap_{(\lambda, \mu) \in \Lambda \times U} \left\{ \widehat{\text{HSIC}}_{\lambda, \mu} \leq q_{1-u_\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right\} \right) \\ &\leq \inf_{(\lambda, \mu) \in \Lambda \times U} P_f \left(\widehat{\text{HSIC}}_{\lambda, \mu} \leq q_{1-u_\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) \\ &\leq \inf_{(\lambda, \mu) \in \Lambda \times U} P_f \left(\widehat{\text{HSIC}}_{\lambda, \mu} \leq q_{1-\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} \right) \\ &= \inf_{(\lambda, \mu) \in \Lambda \times U} \left\{ P_f \left(\Delta_{\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} = 0 \right) \right\}, \end{aligned}$$

which concludes the proof.

4.15 Proof of Theorem 4

Let α and β be in $(0, 1)$. According to Lemma 5, $P_f(\Delta_\alpha = 0) \leq \beta$ as soon as there exists (λ, μ) in $\Lambda \times U$ such that

$$P_f \left(\Delta_{\alpha e^{-\omega_{\lambda, \mu}}}^{\lambda, \mu} = 0 \right) \leq \beta.$$

Then, according to Theorem 2 (resp. Theorem 3) if ψ belongs to $\mathcal{N}_{2,p+q}^\delta(R)$ (resp. ψ belongs to $\mathcal{S}_{p+q}^\delta(R)$): we take the infimum of the upper bounds for the uniform separation rates of the single tests over $\Lambda \times U$ while replacing $\log\left(\frac{1}{\alpha}\right)$ by $\log\left(\frac{1}{\alpha}\right) + \omega_{\lambda, \mu}$.

4.16 Proof of Corollary 4

Let us start with the case where ψ belongs to $\mathcal{N}_{2,p+q}^\delta(R)$. In this case, using Theorem 4, we have the following inequality for $\rho(\Delta_\alpha, \mathcal{N}_{2,p+q}^\delta(R), \beta)$,

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

Let us take $\lambda^* = (2^{-m_{1,1}^*}, \dots, 2^{-m_{1,p}^*})$ and $\mu^* = (2^{-m_{2,1}^*}, \dots, 2^{-m_{2,q}^*})$, where the integers $m_{1,1}^*, \dots, m_{1,p}^*, m_{2,1}^*, \dots, m_{2,q}^*$ are defined as follows

$$m_{1,i}^* = \left\lfloor \log_2 \left(\left(\frac{n}{\log \log(n)} \right)^{\frac{2\eta}{\nu_i(1+4\eta)}} \right) \right\rfloor \quad \text{and} \quad m_{2,j}^* = \left\lfloor \log_2 \left(\left(\frac{n}{\log \log(n)} \right)^{\frac{2\eta}{\gamma_j(1+4\eta)}} \right) \right\rfloor.$$

where $\frac{1}{\eta} = \sum_{i=1}^p \frac{1}{\nu_i} + \sum_{j=1}^q \frac{1}{\gamma_j}$.

Then, we obviously have

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

Besides, using the inequalities

$$m_{1,i}^* \leq \log_2 \left(\left(\frac{n}{\log \log(n)} \right)^{\frac{2\eta}{\nu_i(1+4\eta)}} \right) \quad \text{and} \quad m_{2,j}^* \leq \log_2 \left(\left(\frac{n}{\log \log(n)} \right)^{\frac{2\eta}{\gamma_j(1+4\eta)}} \right),$$

we upper bound $(\lambda_i^*)^{-1/2}$ and $(\mu_j^*)^{-1/2}$ by

$$(\lambda_i^*)^{-1/2} = 2^{m_{1,i}^*/2} \leq \left(\frac{n}{\log \log(n)} \right)^{\frac{\eta}{\nu_i(1+4\eta)}} \quad \text{and} \quad \mu_j^* = 2^{m_{2,j}^*} \leq \left(\frac{n}{\log \log(n)} \right)^{\frac{\eta}{\gamma_j(1+4\eta)}}.$$

Therefore, we obtain

$$(\lambda_1^* \dots \lambda_p^* \mu_1^* \dots \mu_q^*)^{-1/2} \leq \left(\frac{n}{\log \log(n)} \right)^{\frac{1}{(1+4\eta)}}. \quad (84)$$

Let us now upper bound $\omega_{\lambda^*, \mu^*}$, we first write

$$\begin{aligned} \omega_{\lambda^*, \mu^*} &= 2 \sum_{i=1}^p \log(m_{1,i}^* \times \pi/\sqrt{6}) + 2 \sum_{j=1}^q \log(m_{2,j}^* \times \pi/\sqrt{6}) \\ &= 2 \log(m_{1,1}^* \dots m_{1,p}^* m_{2,1}^* \dots m_{2,q}^*) + 2(p+q) \log(\pi/\sqrt{6}). \end{aligned}$$

Moreover, it is easy to see that

$$m_{1,i}^* \leq \frac{2\eta}{\nu_i(1+4\eta)} \log(n) \quad \text{and} \quad \mu_j^* \leq \frac{2\eta}{\gamma_j(1+4\eta)} \log(n).$$

Then,

$$\log(m_{1,1}^* \dots m_{1,p}^* m_{2,1}^* \dots m_{2,q}^*) \leq C(\delta) \log \log(n).$$

Thereafter, $\omega_{\lambda^*, \mu^*}$ can be upper bound as

$$\omega_{\lambda^*, \mu^*} \leq C(\delta) \log \log(n). \quad (85)$$

From Equations (84) and (85), we have

$$\frac{1}{n \sqrt{\lambda_1^* \dots \lambda_p^* \mu_1^* \dots \mu_q^*}} \left(\log \left(\frac{1}{\alpha} \right) + \omega_{\lambda^*, \mu^*} \right) \leq C(\alpha, \delta) \left(\frac{\log \log(n)}{n} \right)^{\frac{4\eta}{(1+4\eta)}}. \quad (86)$$

We aim now to upper bound $\sum_{i=1}^p (\lambda_i^*)^{2\nu_i} + \sum_{j=1}^q (\mu_j^*)^{2\gamma_j}$. For this, we first write

$$m_{1,i}^* \geq \log_2 \left(\left(\frac{n}{\log \log(n)} \right)^{\frac{2\eta}{\nu_i(1+4\eta)}} \right) - 1 \quad \text{and} \quad m_{2,j}^* \geq \log_2 \left(\left(\frac{n}{\log \log(n)} \right)^{\frac{2\eta}{\gamma_j(1+4\eta)}} \right) - 1.$$

We then have the following inequalities for $(\lambda_i^*)^{2\nu_i}$ and $(\mu_j^*)^{2\gamma_j}$,

$$(\lambda_i^*)^{2\nu_i} \leq 2^{2\nu_i} \left(\frac{\log \log(n)}{n} \right)^{\frac{4\eta}{(1+4\eta)}} \quad \text{and} \quad (\mu_j^*)^{2\gamma_j} \leq 2^{2\gamma_j} \left(\frac{\log \log(n)}{n} \right)^{\frac{4\eta}{(1+4\eta)}}.$$

Therefore, we obtain

$$\sum_{i=1}^p (\lambda_i^*)^{2\nu_i} + \sum_{j=1}^q (\mu_j^*)^{2\gamma_j} \leq C(\delta) \left(\frac{\log \log(n)}{n} \right)^{\frac{4\eta}{(1+4\eta)}}. \quad (87)$$

Consequently, from Equations (86) and (87),

$$\rho(\Delta_\alpha, \mathcal{N}_{2,p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) \left(\frac{\log \log(n)}{n} \right)^{\frac{2\eta}{(1+4\eta)}}.$$

In the case where ψ belongs to $\mathcal{S}_{p+q}^\delta(R)$, the same arguments above is applied by taking $\delta_1 = \dots = \delta_p = \gamma_1 = \dots = \gamma_q = \delta$, lead to

$$\rho(\Delta_\alpha, \mathcal{S}_{p+q}^\delta(R), \beta) \leq C(M_f, p, q, \alpha, \beta, \delta) \left(\frac{\log \log(n)}{n} \right)^{\frac{2\eta}{(1+4\eta)}},$$

where $\frac{1}{\eta} = (p+q)\frac{1}{\delta}$.

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