

## DISTANCE-BASED AND RKHS-BASED DEPENDENCE METRICS IN HIGH DIMENSION

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In this paper, we study distance covariance, Hilbert-Schmidt covariance (aka Hilbert-Schmidt independence criterion [Gretton et al. (2008)]) and related independence tests under the high dimensional scenario. We show that the sample distance/Hilbert-Schmidt covariance between two random vectors can be approximated by the sum of squared componentwise sample cross-covariances up to an asymptotically constant factor, which indicates that the standard distance/Hilbert-Schmidt covariance based test can only capture linear dependence in high dimension. Under the assumption that the components within each high-dimensional vector are weakly dependent, the distance correlation based  $t$  test developed by Székely and Rizzo (2013) for independence is shown to have trivial limiting power when the two random vectors are nonlinearly dependent but component-wisely uncorrelated. This new and surprising phenomenon, which seems to be discovered and carefully studied for the first time, is further confirmed in our simulation study. As a remedy, we propose tests based on an aggregation of marginal sample distance/Hilbert-Schmidt covariances and show their superior power behavior against their joint counterparts in simulations. We further extend the distance correlation based  $t$  test to those based on Hilbert-Schmidt covariance and marginal distance/Hilbert-Schmidt covariance. A novel unified approach is developed to analyze the studentized sample distance/Hilbert-Schmidt covariance as well as the studentized sample marginal distance covariance under both null and alternative hypothesis. Our theoretical and simulation results shed light on the limitation of distance/Hilbert-Schmidt covariance when used jointly in the high dimensional setting and suggest the aggregation of marginal distance/Hilbert-Schmidt covariance as a useful alternative.

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**1. Introduction.** Testing for independence between two random vectors  $X \in \mathbb{R}^p$  and  $Y \in \mathbb{R}^q$  is a fundamental problem in statistics. There is a huge literature in the low dimensional context. Here we mention rank correlation coefficients based tests and nonparametric Cramér-von Mises type statistics in [Hoeffding \(1948\)](#), [Blum, Kiefer and Rosenblatt \(1961\)](#), [De Wet \(1980\)](#); tests based on signs or empirical characteristic functions, see [Sinha and Wieand \(1977\)](#), [Deheuvels \(1981\)](#), [Csörgő \(1985\)](#), [Hettmansperger and Oja \(1994\)](#), [Gieser and Randles \(1997\)](#), [Taskinen, Kankainen and Oja \(2003\)](#) among others; tests based on recently developed nonlinear dependence metrics that target at non-linear and non-monotone dependence include distance covariance [[Székely, Rizzo and Bakirov \(2007\)](#)], Hilbert-Schmidt independence criterion (HSIC) [[Gretton et al. \(2008\)](#)] (aka Hilbert-Schmidt covariance in this work) and sign covariance [[Bergsma and Dassios \(2014\)](#)]. Also see [Berrett and Samworth \(2019\)](#) for some recent work on independence testing via mutual information.

In the high dimensional setting, the literature is scarce. [Székely and Rizzo \(2013\)](#) extended the distance correlation proposed in [Székely, Rizzo and Bakirov \(2007\)](#) to the problem of testing independence of two random vectors under the setting that the dimensions  $p$  and  $q$  grow while sample size  $n$  is fixed. This setting is known as high dimension, low sample size (HDLSS) in the literature and has been adopted in [Hall, Marron and Neeman \(2005\)](#), [Ahn et al. \(2007\)](#), [Jung and Marron \(2009\)](#), and [Wei et al. \(2016\)](#) etc. A closely related asymptotic framework is the high dimension medium sample size (HDMSS) [[Aoshima et al. \(2018\)](#)], where  $n \wedge p \wedge q \rightarrow \infty$  with  $p, q$  growing more rapidly. Among the recent work that is related to independence testing in the high dimensional setting, [Pan, Gao and Yang \(2014\)](#) proposed tests of independence among a large number of high dimensional random vectors using insights from random matrix theory; [Yang and Pan \(2015\)](#) proposed a new statistic based on the sum of regularized sample canonical correlation coefficients of  $X$  and  $Y$ , which is limited to testing for uncorrelatedness due to the use of canonical correlation. [Leung and Drton \(2018\)](#) proposed to test for mutual independence of high dimensional vectors using sum of pairwise rank correlations and sign covariances; [Yao, Zhang and Shao \(2018\)](#) addressed the mutual independence testing problem in the high dimensional context by using sum of pairwise squared sample distance covariances; [Zhang et al. \(2018\)](#) proposed a  $L^2$  type test for conditional mean/quantile dependence of a univariate response variable given a high dimensional covariate vector based on martingale difference divergence [[Shao and Zhang \(2014\)](#)], which is an extension of distance covariance to quantify (conditional) mean dependence.

Distance covariance/correlation was first introduced in [Székely, Rizzo and Bakirov \(2007\)](#) and has received much attention since then. Owing to its notable ability to quantify any types of dependence including non-monotone, non-linear dependence and also the flexibility to be applicable to two random vectors in arbitrary, not necessarily equal dimensions, a lot of research work has been done to extend and apply distance covariance into many modern statistical problems; see e.g. [Kong et al. \(2012\)](#), [Li, Zhong and Zhu \(2012\)](#), [Zhou \(2012\)](#), [Lyons \(2013\)](#), [Székely and Rizzo \(2014\)](#), [Dueck et al. \(2014\)](#), [Shao and Zhang \(2014\)](#), [Park, Shao and Yao \(2015\)](#), [Matteson and Tsay \(2017\)](#), [Zhang et al. \(2018\)](#), [Edelmann, Richards and Vogel \(2017\)](#), [Yao, Zhang and Shao \(2018\)](#) among others. In this paper, we shall revisit the test proposed by [Székely and Rizzo \(2013\)](#), which seems to be the only test in the high dimensional setting that captures nonlinear and nonmonotonic dependence. Unlike the positive finding reported in [Székely and Rizzo \(2013\)](#), we obtained some negative results that show the limitation of distance covariance/correlation in the high dimensional context.

Specifically, we show that for two random vectors  $X = (x_1, \dots, x_p)^T \in \mathbb{R}^p$  and  $Y = (y_1, \dots, y_q)^T \in \mathbb{R}^q$  with finite component-wise second moments, as  $p, q \rightarrow \infty$  and  $n$  can either be fixed or grows to infinity at a slower rate,

$$(1) \quad \text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) \approx \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j),$$

where  $X_k \stackrel{d}{=} X$  and  $Y_k \stackrel{d}{=} Y$  are independent samples,  $\mathcal{X}_i$  and  $\mathcal{Y}_j$  are the component-wise samples,  $\mathbf{X} = (X_1, X_2, \dots, X_n)^T = (\mathcal{X}_1, \mathcal{X}_2, \dots, \mathcal{X}_p)$  and  $\mathbf{Y} = (Y_1, Y_2, \dots, Y_n)^T = (\mathcal{Y}_1, \mathcal{Y}_2, \dots, \mathcal{Y}_q)$  denote the sample matrices,  $\text{dCov}_n^2(\mathbf{X}, \mathbf{Y})$  is the unbiased sample distance covariance,  $\tau$  is a constant quantity depending on the marginal distributions of  $X$  and  $Y$  as well as  $p$  and  $q$ ,  $\text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j)$  is an unbiased sample estimate of  $\text{cov}^2(x_i, y_j)$  to be defined later. To the best of our knowledge, this is the first work in the literature uncovering the connection between sample distance covariance and sample covariance, the latter of which can only measure the linear dependence between two random variables. This approximation suggests that the distance covariance can only measure linear dependence in the high dimensional setting although it is well-known to be capable of capturing non-linear dependence in the fixed dimensional case.

[Gretton et al. \(2008\)](#) proposed Hilbert-Schmidt independence criterion (aka Hilbert-Schmidt covariance in this paper), which can be seen as a generalization of distance covariance by kernelizing the  $L^2$  distance as shown by [Sejdinovic et al. \(2013\)](#). Despite the kernelization process, we show that the

Hilbert-Schmidt covariance (hCov) enjoys similar approximation property under high dimension low/medium sample size setting, i.e.

$$(2) \quad \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) \approx A_p B_q \times \frac{1}{\tau^2} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j),$$

where  $\text{hCov}_n^2(\mathbf{X}, \mathbf{Y})$  is the unbiased sample Hilbert-Schmidt covariance,  $A_p$  and  $B_q$  both converge in probability to constants that depend on the pre-chosen kernels. This approximation also suggests that when the dimension is high, the standard Hilbert-Schmidt covariance (hCov) applied to the whole components of the vectors also exhibits the loss of power when  $X$  and  $Y$  are non-linearly dependent, but component-wisely uncorrelated or weakly correlated.

As a natural remedy, we propose a distance covariance based marginal test statistic, i.e.,

$$\text{mdCov}_n^2(\mathbf{X}, \mathbf{Y}) = \sqrt{\binom{n}{2}} \sum_{i=1}^p \sum_{j=1}^q \text{dCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j).$$

This test statistic is an aggregate of the componentwise sample distance covariances and captures the component by component nonlinear dependence. Similarly, the marginal Hilbert-Schmidt covariance (mhCov) is defined as

$$\text{mhCov}_n^2(\mathbf{X}, \mathbf{Y}) = \sqrt{\binom{n}{2}} \sum_{i=1}^p \sum_{j=1}^q \text{hCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j).$$

The distance covariance, Hilbert-Schmidt covariance, marginal distance covariance and marginal Hilbert-Schmidt covariance based tests can be carried out by standard permutation procedures. The superiority of mdCov and mhCov based tests over its joint counterparts in power is demonstrated in the simulation studies. On the other hand, [Székely and Rizzo \(2013\)](#) discussed the distance correlation (dCor) based  $t$ -test under HDLSS and derived the limiting null distribution of the test statistic under suitable assumptions. We consider the same  $t$ -test statistic and further extend to Hilbert-Schmidt covariance (hCov), marginal distance covariance (mdCov) and marginal Hilbert-Schmidt covariance (mhCov). To derive the asymptotic distribution of studentized version of dCov, hCov, mdCov and mhCov under both the null of independence (for HDLSS and HDMSS setting) and some specific alternative classes (for HDLSS setting), we develop a novel unified approach. In particular, we define a unified quantity (uCov) based

on the bivariate kernel  $k$  and show that under HDLSS setting, properly scaled  $\text{dCov}_n^2$ ,  $\text{hCov}_n^2$  and  $\text{mdCov}_n^2$  are all asymptotically equal to  $\text{uCov}_n^2$  up to different choices of kernels, i.e.

$$(3) \quad \left. \begin{aligned} \text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) &\approx a \times \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) \\ \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) &\approx A_p B_q \times \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) \end{aligned} \right\} \text{ when } k(x, y) = |x - y|^2,$$

$$\text{mdCov}_n^2(\mathbf{X}, \mathbf{Y}) = b \times \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) \quad \left. \right\} \text{ when } k(x, y) = |x - y|,$$

where  $a, b$  are constants and  $A_p, B_p$  both converge in probability to constants. Next, we show that

$$\left\{ \begin{aligned} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &\xrightarrow{d} \frac{2}{n(n-3)} \mathbf{c}^T \mathbf{M} \mathbf{d}, \quad \text{under HDLSS,} \\ C_{n,p,q} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &\xrightarrow{d} N(0, 1), \quad \text{under HDMSS,} \end{aligned} \right.$$

where  $\mathbf{c}, \mathbf{d}$  are jointly Gaussian,  $\mathbf{M}$  is a projection matrix and  $C_{n,p,q}$  is a normalizing constant. Thus, we can easily apply the above results to  $\text{dCov}$ ,  $\text{hCov}$  and  $\text{mdCov}$ -based  $t$ -test statistics using (3). The unified approach still works for  $\text{mhCov}$ -based  $t$ -test if we consider the bandwidth parameters appeared in the kernel distance to be fixed constants. However, we encounter technical difficulties if the bandwidth parameters along each dimension depends on the whole component-wise samples, since this makes the pair-wise sample distance correlated with each other and complicates the asymptotic analysis.

We obtain the same limiting null distribution as [Székely and Rizzo \(2013\)](#) and further show that this test statistic has a trivial power against the alternative where  $X$  and  $Y$  are non-linearly dependent, but component-wisely uncorrelated. This clearly demonstrates that the distance covariance/correlation based joint independence test (i.e., treating all components of a vector as a whole jointly) fails to capture the non-linear dependence in high dimension. This phenomenon is new and was not reported in [Székely and Rizzo \(2013\)](#). It shows that there might be some intrinsic difficulties for standard distance covariance to capture the non-linear dependence when the dimension is high and provide a cautionary note on the use of distance covariance/correlation directly to the whole components of high dimensional data. Besides, we have the following additional contributions relative to [Székely and Rizzo \(2013\)](#): (i) we relax the component-wise i.i.d. assumption used for asymptotic analysis; (ii) the limiting distributions are derived under both the null and certain classes of alternative hypothesis for the HDLSS framework; (iii) our unified approach holds for any bivariate kernel that has continuous second order derivative in a neighborhood containing 1; (iv) our approach is built on some new technical arguments which reveal some insights on  $\mathcal{U}$ -

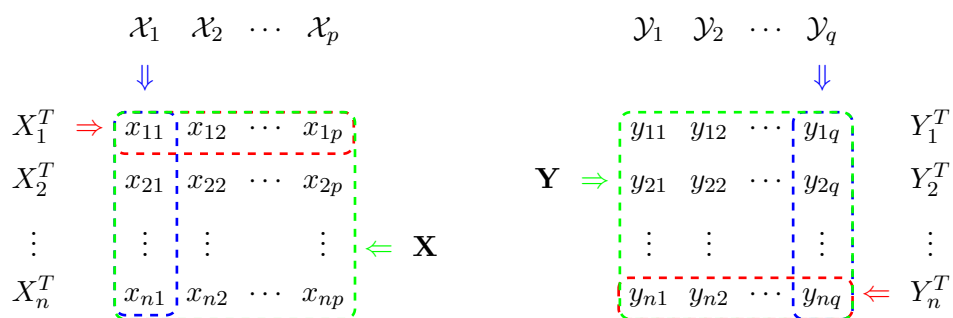
centering; (v) the limiting null distribution is also derived under the HDMSS setting.

As pointed out by a referee, there is an awareness of the importance of choosing the right kernel in the machine learning community and it may be clear to many researchers in this area that the standard distance covariance (or Hilbert-Schmidt covariance) is not the right choice when the dimension is moderate or high. It is worth noting that the phenomenon of decreasing power with higher dimension for Hilbert-Schmidt covariance (with Gaussian/Laplacian kernels) based independence test has been observed in [Ramdas et al. \(2015\)](#), but they did not provide a complete theoretical explanation. In this sense, our theory to a large extent settles their conjecture and offers a deeper understanding about the dimension's impact on the behavior of Hilbert-Schmidt covariance. In addition, the marginally aggregated distance/Hilbert-Schmidt covariance can be viewed as a kind of distance/Hilbert-Schmidt covariance with the Euclidean norm/kernel replaced by a new norm/kernel; see Remark 2.1.2. Therefore, our theory demonstrates the limitation of using Euclidean norm in distance/Hilbert-Schmidt covariance in the high dimensional setting and motivates the question of what is the optimal norm or kernel for independence testing in the high dimension, which is left for future research.

Standard Distance and Hilbert-Schmidt (with Gaussian kernel or Laplacian kernel) covariance have been frequently applied to testing dependence between high dimensional vectors in biological science, see [Kroupi et al. \(2014\)](#), [Kroupi et al. \(2012\)](#), [Hua and Ghosh \(2015\)](#), [Yang \(2017\)](#), etc. In particular, [Kroupi et al. \(2014\)](#) use Hilbert-Schmidt (with Gaussian or Laplacian kernel) covariance to test the dependence between EEG signals for the perception of pleasant and unpleasant odors across subjects, where the data are collected for 5 subjects, each with 18 trials and dimension 250. [Hua and Ghosh \(2015\)](#) use Hilbert-Schmidt covariance with Gaussian kernel to examine the association between phenotype variable and genotype variable. The Alzheimers Disease Neuroimaging Initiative (ADNI) data is used in their simulation studies, where phenotype variable has dimension 119 and genotype variable has dimension 141. Finally, Hilbert-Schmidt covariance with Gaussian kernel is used by [Yang \(2017\)](#) to conduct independence test between neural responses and visual features, where the dimensions are of several hundreds. In the machine learning community, the application of Hilbert-Schmidt (with linear, Gaussian or Laplacian kernel) covariance for high dimensional data involves multi-label dimension reduction [[Zhang and Zhou \(2010\)](#), [Xu et al. \(2016\)](#), [Mikalsen et al. \(2019\)](#) etc] and unsupervised feature selection [[Bedo \(2008\)](#)], among others. In all the above-mentioned

applications, the dimensions of the vectors involved are at hundreds or thousands.

1.1. *Notations.* In this paper, random data samples are denoted as, for each  $i = 1, 2, \dots, n$ ,  $X_i \stackrel{d}{=} X = (x_1, \dots, x_p)^T \in \mathbb{R}^p$ ,  $Y_i \stackrel{d}{=} Y = (y_1, \dots, y_q)^T \in \mathbb{R}^q$ . Next, let  $\mathbf{X} = (X_1, X_2, \dots, X_n)^T$  and  $\mathbf{Y} = (Y_1, Y_2, \dots, Y_n)^T$  denote the random sample matrices. In addition, the random component-wise samples are denoted as  $\mathcal{X}_1, \dots, \mathcal{X}_p$  and  $\mathcal{Y}_1, \dots, \mathcal{Y}_q$ , which are illustrated in the following table,



Furthermore, matrices are denoted by upper case boldface letters (e.g.  $\mathbf{A}$ ,  $\mathbf{B}$ ). For any matrix  $\mathbf{A} = (a_{st}) \in \mathbb{R}^{n \times n}$ , we use  $\tilde{\mathbf{A}} = (\tilde{a}_{st}) \in \mathbb{R}^{n \times n}$  to denote the  $\mathcal{U}$ -centered version of  $\mathbf{A}$ , i.e.,

$$\tilde{a}_{st} = \begin{cases} a_{st} - \frac{1}{n-2} \sum_{v=1}^n a_{sv} - \frac{1}{n-2} \sum_{u=1}^n a_{ut} + \frac{1}{(n-1)(n-2)} \sum_{u,v=1}^n a_{uv}, & s \neq t, \\ 0, & s = t. \end{cases}$$

Following Székely and Rizzo (2014), the inner product between two  $\mathcal{U}$ -centered matrices  $\tilde{\mathbf{A}} = (\tilde{a}_{st}) \in \mathbb{R}^{n \times n}$  and  $\tilde{\mathbf{B}} = (\tilde{b}_{st}) \in \mathbb{R}^{n \times n}$  is defined as

$$(\tilde{\mathbf{A}} \cdot \tilde{\mathbf{B}}) := \frac{1}{n(n-3)} \sum_{s \neq t} \tilde{a}_{st} \tilde{b}_{st}.$$

Next, we use  $\mathbf{1}_n$  to denote the  $n$  dimensional column vector whose entries are all equal to 1. Similarly, we use  $\mathbf{0}_n$  to denote the  $n$  dimensional column vector whose entries are all equal to 0. Finally, we use  $|\cdot|$  to denote the  $L^2$  norm of a vector,  $(X', Y')$  and  $(X'', Y'')$  to be independent copies of  $(X, Y)$  and  $X \perp Y$  to indicate that  $X$  and  $Y$  are independent.

We utilize the order in probability notations such as stochastic boundedness  $O_p$  (big O in probability), convergence in probability  $o_p$  (small o in

probability) and equivalent order  $\asymp_p$ , which is defined as follows: for a sequence of random variables  $\{Z_s\}_{s \in \mathbb{Z}}$  and a sequence of numbers  $\{a_s\}_{s \in \mathbb{Z}}$ ,  $Z_s \asymp_p a_s$  if and only if  $Z_s/a_s = O_p(1)$  and  $a_s/Z_s = O_p(1)$  as  $s \rightarrow \infty$ . For more details about these notations, please see [DasGupta \(2008\)](#).

**2. High Dimension Low Sample Size.** The analyses in this section are conducted under the HDLSS setting, i.e., the sample size  $n$  is fixed and the dimensions  $p \wedge q \rightarrow \infty$ .

*2.1. Distance Covariance and Variants.* In this section, we introduce the following test statistics based on distance covariance (dCov), marginal distance covariance (mdCov), Hilbert-Schmidt covariance (hCov) and marginal Hilbert-Schmidt covariance (mhCov). In addition, their asymptotic behaviors under the HDLSS setting are derived. The following moment conditions will be used throughout the paper.

ASSUMPTION D1. *For any  $p, q$ , the variance and the second moment of any coordinate of  $X = (x_1, x_2, \dots, x_p)^T$  and  $Y = (y_1, y_2, \dots, y_q)^T$  is uniformly bounded below and above, i.e.,*

$$0 < a \leq \inf_i \text{var}(x_i) \leq \sup_i \text{E}(x_i^2) \leq b < \infty,$$

$$0 < a' \leq \inf_j \text{var}(y_j) \leq \sup_j \text{E}(y_j^2) \leq b' < \infty,$$

for some constants  $a, b, a', b'$ .

Next, denote  $\tau_X^2 = \text{E}|X - X'|^2$ ,  $\tau_Y^2 = \text{E}|Y - Y'|^2$  and  $\tau^2 := \tau_X^2 \tau_Y^2 = \text{E}|X - X'|^2 \text{E}|Y - Y'|^2$ . Notice that under Assumption D1, it can be easily seen that

$$\tau_X \asymp \sqrt{p}, \tau_Y \asymp \sqrt{q} \text{ and } \tau \asymp \sqrt{pq}.$$

The statistics we study in this work use the pair-wise  $L^2$  distance between data points. The following proposition presents an expansion formula on the normalized  $L^2$  distance when the dimension is high, which plays a key role in our theoretical analysis.

PROPOSITION 2.1.1. *Under Assumption D1, we have*

$$\frac{|X - X'|}{\tau_X} = 1 + \frac{1}{2}L_X(X, X') + R_X(X, X'),$$



where

$$L_X(X, X') := \frac{|X - X'|^2 - \tau_X^2}{\tau_X^2},$$

and  $R_X(X, X')$  is the remainder term. If we further assume that as  $p \wedge q \rightarrow \infty$ ,  $L_X(X, X') = o_p(1)$ , then  $R_X(X, X') = O_p(L_X(X, X')^2)$ . Similar result holds for  $Y$ .

In order for the approximations in equations (1) and (2) to work well, it is required that  $L_X(X_s, X_t)$  and  $L_Y(Y_s, Y_t)$  should decay relatively fast as  $p \wedge q \rightarrow \infty$ . The following assumption specifies the order of  $L_X(X_s, X_t)$  and  $L_Y(Y_s, Y_t)$ .

ASSUMPTION D2.  $L_X(X, X') = O_p(a_p)$  and  $L_Y(Y, Y') = O_p(b_q)$ , where  $a_p, b_q$  are sequences of numbers such that

$$\begin{aligned} a_p &= o(1), b_q = o(1), \\ \tau_X^2 a_p^3 &= o(1), \tau_Y^2 b_q^3 = o(1), \tau a_p^2 b_q = o(1), \tau a_p b_q^2 = o(1). \end{aligned}$$

REMARK 2.1.1. A sufficient condition for  $L_X(X, X') = o_p(1)$  is that  $E[L_X(X, X')^2] = o(1)$ . Let  $\Sigma_X = \text{cov}(X)$ . By a straightforward calculation, we obtain  $|X - X'|^2 = \sum_{j=1}^p (x_j - x'_j)^2$ ,  $E|X - X'|^2 = 2 \sum_{j=1}^p \text{var}(x_j) = 2\text{tr}(\Sigma_X)$ , and

$$E[L_X(X, X')^2] = \frac{\sum_{j,j'=1}^p [\text{cov}(x_j^2, x_{j'}^2) + 2\text{cov}^2(x_j, x_{j'})]}{2\text{tr}^2(\Sigma_X)}.$$

Therefore,  $E[L_X(X, X')^2] = o(1)$  holds if the component-wise dependence within  $X$  is not too strong. To illustrate this point, we consider the general multivariate model,

$$X_{p \times 1} = \mathbf{A}_{p \times s_1} U_{s_1 \times 1} + \mu_{p \times 1},$$

where  $\mathbf{A}$  is a constant matrix with  $s_1 \geq p$ ,  $\mu$  is the mean vector for  $X$ , and  $U = (u_1, \dots, u_{s_1})^T$  has i.i.d components with mean zero and variance one. Suppose

$$\frac{\text{tr}(\mathbf{A}\mathbf{A}^T\mathbf{A}\mathbf{A}^T)}{\text{tr}^2(\mathbf{A}\mathbf{A}^T)} = \frac{\text{tr}(\Sigma_X^2)}{\text{tr}^2(\Sigma_X)} = O(p^{-1})$$

and  $\sup_s E[u_s^4] < \infty$ . Then the multivariate model satisfies Assumption D2 with  $a_p = 1/\sqrt{p}$ , see Section C.2 of the Appendix for more details.

2.1.1. *Distance Covariance.* Distance covariance was first introduced by Székely, Rizzo and Bakirov (2007) to measure the dependence between two random vectors of arbitrary dimensions. For two random vectors  $X \in \mathbb{R}^p$  and  $Y \in \mathbb{R}^q$ , the (squared) distance covariance is defined as

$$\text{dCov}^2(X, Y) = \int_{\mathbb{R}^{p+q}} \frac{|\phi_{X,Y}(t, s) - \phi_X(t)\phi_Y(s)|^2}{c_p c_q |t|^{1+p} |s|^{1+q}} dt ds,$$

where  $c_p = \pi^{(1+p)/2} / \Gamma((1+p)/2)$ ,  $|\cdot|$  is the (complex) Euclidean norm defined as  $|x| = \sqrt{\bar{x}^T x}$  for any vector  $x$  in the complex vector space ( $\bar{x}$  denotes the conjugate of  $x$ ),  $\phi_X$  and  $\phi_Y$  are the characteristic functions of  $X$  and  $Y$  respectively,  $\phi_{X,Y}$  is the joint characteristic function. According to Theorem 7 of Székely and Rizzo (2009), an alternative definition of distance covariance is given by

$$(4) \quad \text{dCov}^2(X, Y) = \text{E}|X - X'| |Y - Y'| + \text{E}|X - X'| \text{E}|Y - Y'| - 2\text{E}|X - X'| |Y - Y''|,$$

where  $(X', Y')$  and  $(X'', Y'')$  are independent copies of  $(X, Y)$ . It has been shown that  $\text{dCov}^2(X, Y) = 0$  if and only if  $X$  and  $Y$  are independent. Therefore, it is able to measure any type of dependence including non-linear and non-monotonic dependence between  $X$  and  $Y$ , whereas the commonly used Pearson correlation can only measure the linear dependence and the rank correlation coefficients (Kendall's  $\tau$  and Spearman's  $\rho$ ) can only capture the monotonic dependence.

Notice that in the above setting,  $p, q$  are arbitrary positive integers. Therefore, distance covariance is applicable to the high dimensional setting, where we allow  $p, q \rightarrow \infty$ . However, it is unclear whether this metric can still retain the power to detect the nonlinear dependence or not when the dimension is high. Distance correlation ( $\text{dCor}$ ) is the normalized version of distance covariance, which is defined as

$$\text{dCor}^2(X, Y) = \begin{cases} \frac{\text{dCov}^2(X, Y)}{\sqrt{\text{dCov}^2(X, X)\text{dCov}^2(Y, Y)}}, & \text{dCov}^2(X, X)\text{dCov}^2(Y, Y) > 0, \\ 0, & \text{dCov}^2(X, X)\text{dCov}^2(Y, Y) = 0. \end{cases}$$

Following Székely and Rizzo (2014), we introduce the  $\mathcal{U}$ -centering based unbiased sample distance covariance ( $\text{dCov}_n^2$ ) as follows.

$$\text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = (\tilde{\mathbf{A}} \cdot \tilde{\mathbf{B}}),$$

where  $\tilde{\mathbf{A}}, \tilde{\mathbf{B}}$  are the  $\mathcal{U}$ -centered versions of  $\mathbf{A} = (a_{st})_{s,t=1}^n, \mathbf{B} = (b_{st})_{s,t=1}^n$  respectively and  $a_{st} = |X_s - X_t|, b_{st} = |Y_s - Y_t|$  for  $s, t = 1, \dots, n$ . Correspondingly, the sample distance correlation ( $\text{dCor}_n^2$ ) is given as

$$\text{dCor}_n^2(\mathbf{X}, \mathbf{Y}) = \begin{cases} \frac{\text{dCov}_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{\text{dCov}_n^2(\mathbf{X}, \mathbf{X})\text{dCov}_n^2(\mathbf{Y}, \mathbf{Y})}}, & \text{dCov}_n^2(\mathbf{X}, \mathbf{X})\text{dCov}_n^2(\mathbf{Y}, \mathbf{Y}) > 0, \\ 0, & \text{dCov}_n^2(\mathbf{X}, \mathbf{X})\text{dCov}_n^2(\mathbf{Y}, \mathbf{Y}) = 0. \end{cases}$$

Here, for  $s \neq t$ , we can apply the approximation in Proposition 2.1.1, that is

$$(5) \quad \frac{a_{st}}{\tau_X} = 1 + \frac{1}{2}L_X(X_s, X_t) + R_X(X_s, X_t),$$

$$(6) \quad \frac{b_{st}}{\tau_Y} = 1 + \frac{1}{2}L_Y(Y_s, Y_t) + R_Y(Y_s, Y_t),$$

where

$$L_X(X_s, X_t) = \frac{|X_s - X_t|^2 - \tau_X^2}{\tau_X^2}, \quad L_Y(Y_s, Y_t) = \frac{|Y_s - Y_t|^2 - \tau_Y^2}{\tau_Y^2},$$

and  $R_X, R_Y$  are the remainder terms from the approximation. The approximation of the pair-wise  $L^2$  distance in Equations (5) and (6) is our building block to decompose the unbiased sample (squared) distance covariance ( $\text{dCov}_n^2$ ) into a leading term plus a negligible remainder term under the HDLSS setting. The following main theorem summarizes the decomposition properties of sample distance covariance ( $\text{dCov}_n^2$ ).

**THEOREM 2.1.1.** *Under Assumption D1, we can show that*

(i)

$$(7) \quad \text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n.$$

Here

$$\text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) = \frac{1}{\binom{n}{4}} \sum_{s < t < u < v} h(x_{si}, x_{ti}, x_{ui}, x_{vi}; y_{sj}, y_{tj}, y_{uj}, y_{vj}),$$

and the kernel  $h$  is defined as

$$\begin{aligned} h(x_{si}, x_{ti}, x_{ui}, x_{vi}; y_{sj}, y_{tj}, y_{uj}, y_{vj}) \\ = \frac{1}{4!} \sum_{*}^{(s,t,u,v)} \frac{1}{4} (x_{si} - x_{ti})(y_{sj} - y_{tj})(x_{ui} - x_{vi})(y_{uj} - y_{vj}), \end{aligned}$$

where the summation  $\sum_*^{(s,t,u,v)}$  is over all permutations of the 4-tuples of indices  $(s, t, u, v)$  and  $\mathcal{R}_n$  is the remainder term.  $\text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j)$  is a fourth-order  $U$ -statistic and is an unbiased estimator for the squared covariance between  $x_i$  and  $y_j$ , i.e.,  $\mathbb{E}[\text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j)] = \text{cov}^2(x_i, y_j)$ .

(ii) Further suppose Assumption D2 holds. Then

$$\frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) = O_p(\tau a_p b_q),$$

$$\mathcal{R}_n = O_p(\tau a_p^2 b_q + \tau a_p b_q^2) = o_p(1),$$

thus the remainder term is of smaller order compared to the leading term and therefore is asymptotically negligible.

Equation (7) in Theorem 2.1.1 shows that the leading term for sample distance covariance is the sum of all component-wise squared sample cross-covariances scaled by  $\tau$ , which depends on the marginal variances of  $X$  and  $Y$ . This theorem suggests that in the HDLSS setting, the sample distance covariance can only measure the component-wise linear dependence between the two random vectors.

As argued previously, sample distance covariance ( $\text{dCov}_n^2$ ) based tests suffer from power loss when  $X$  and  $Y$  are component-wisely non-linear dependent but uncorrelated. To remedy this drawback, we can consider the following aggregation of marginal sample distance covariances,

$$\text{mdCov}_n^2(\mathbf{X}, \mathbf{Y}) = \sqrt{\binom{n}{2}} \sum_{i=1}^p \sum_{j=1}^q \text{dCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j),$$

where  $\text{dCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) = (\tilde{\mathbf{A}}(i) \cdot \tilde{\mathbf{B}}(j))$ ,  $\tilde{\mathbf{A}}(i)$  and  $\tilde{\mathbf{B}}(j)$  are the  $\mathcal{U}$ -centered versions of  $\mathbf{A}(i) = (a_{st}(i))_{s,t=1}^n$ ,  $\mathbf{B}(j) = (b_{st}(j))_{s,t=1}^n$  respectively and  $a_{st}(i) = |x_{si} - x_{ti}|$ ,  $b_{st}(j) = |y_{sj} - y_{tj}|$ .

Note that  $\text{mdCov}_n^2$  captures the pairwise low dimensional nonlinear dependence, which can be viewed as the main effects of the dependence between two high dimensional random vectors. It is natural in many fields of statistics to test for main effects first before proceeding to high order interactions. See Chakraborty and Zhang (2018) for some discussions on main effects and high order effects in the context of joint dependence testing. In the testing of mutual independence of a high dimensional vector, Yao, Zhang and Shao (2018) also approached the problem by testing the pairwise independence using distance covariance and demonstrated that there may be intrinsic difficulty to capture the effects beyond main effects (pairwise dependence in

the mutual independence testing problem), as the tests that target joint dependence do not perform well in the high dimensional setting.

2.1.2. *Hilbert-Schmidt Covariance.* A generalization of the Distance Covariance (dCov) is Hilbert-Schmidt Covariance (hCov), first proposed and aka Hilbert-Schmidt independence criterion (*HSIC*) by [Gretton et al. \(2008\)](#). In particular, the (squared) Hilbert-Schmidt Covariance (hCov) is obtained by kernelizing the Euclidean distance in equation (4), i.e.,

$$\begin{aligned} \text{hCov}^2(X, Y) &= \mathbb{E}[K(X, X')L(Y, Y')] \\ &\quad + \mathbb{E}[K(X, X')]\mathbb{E}[L(Y, Y')] - 2\mathbb{E}[K(X, X')L(Y, Y'')], \end{aligned}$$

where  $(X', Y')$ ,  $(X'', Y'')$  are independent copies of  $(X, Y)$  and  $K, L$  are user specified kernels. Following the literature, we consider the following widely used kernels

$$\begin{aligned} \text{Gaussian kernel: } K(x, y) &= \exp\left(-\frac{|x-y|^2}{2\gamma^2}\right), \\ \text{Laplacian kernel: } K(x, y) &= \exp\left(-\frac{|x-y|}{\gamma}\right), \end{aligned}$$

where  $\gamma$  is a bandwidth parameter. For later convenience, we focus on the kernels that can be represented compactly as  $K(x, y) = f(|x-y|/\gamma)$  for some continuously differentiable function  $f$ . For example, the Gaussian and Laplacian kernel can be defined by choosing different function  $f$ ,

$$\begin{aligned} \text{Gaussian kernel: } K(x, y) &= f\left(\frac{|x-y|}{\gamma}\right), f(a) = \exp\left(-\frac{a^2}{2}\right), \\ \text{Laplacian kernel: } K(x, y) &= f\left(\frac{|x-y|}{\gamma}\right), f(a) = \exp(-a). \end{aligned}$$

In practice, the bandwidth parameter is usually set as the median of pairwise sample  $L^2$  distance. Thus, a natural estimator for  $\text{hCov}^2(X, Y)$  is defined as

$$\text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) = (\tilde{\mathbf{R}} \cdot \tilde{\mathbf{H}}),$$

where  $\tilde{\mathbf{R}}$  and  $\tilde{\mathbf{H}}$  are the  $\mathcal{U}$ -centered versions of  $\mathbf{R} = (r_{st})_{s,t=1}^n$ ,  $\mathbf{H} = (h_{st})_{s,t=1}^n$  respectively and  $r_{st} = h_{st} = 0$  if  $s = t$ , otherwise

$$\begin{cases} r_{st} = K(X_s, X_t, \mathbf{X}) = f\left(\frac{|X_s - X_t|}{\gamma_{\mathbf{X}}}\right), \gamma_{\mathbf{X}} = \text{median}\{|X_s - X_t|, s \neq t\}, \\ h_{st} = L(Y_s, Y_t, \mathbf{Y}) = g\left(\frac{|Y_s - Y_t|}{\gamma_{\mathbf{Y}}}\right), \gamma_{\mathbf{Y}} = \text{median}\{|Y_s - Y_t|, s \neq t\}. \end{cases}$$

Similar to the definition of distance correlation, the Hilbert-Schmidt Correlation (hCor) is defined as

$$\text{hCor}^2(X, Y) = \begin{cases} \frac{\text{hCov}^2(X, Y)}{\sqrt{\text{hCov}^2(X, X)\text{hCov}^2(Y, Y)}}, & \text{hCov}^2(X, X)\text{hCov}^2(Y, Y) > 0, \\ 0, & \text{hCov}^2(X, X)\text{hCov}^2(Y, Y) = 0, \end{cases}$$

and the sample Hilbert-Schmidt Correlation ( $\text{hCor}_n^2$ ) is defined in the same way by replacing  $\text{hCov}^2$  with the corresponding sample version.

Next, we can extend the decomposition results for sample distance covariance ( $\text{dCov}_n^2$ ) to sample Hilbert-Schmidt covariance ( $\text{hCov}_n^2$ ) as shown in the following theorem. Throughout the paper, we use  $f^{(1)}$  and  $f^{(2)}$  to denote the first and second derivative of the function  $f$ .

**THEOREM 2.1.2.** *Under Assumption D1, we have*

(i)

$$(8) \quad \begin{aligned} & \tau \times \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) \\ &= f^{(1)}\left(\frac{\tau_X}{\gamma_{\mathbf{X}}}\right) g^{(1)}\left(\frac{\tau_Y}{\gamma_{\mathbf{Y}}}\right) \frac{\tau_X}{\gamma_{\mathbf{X}}} \frac{\tau_Y}{\gamma_{\mathbf{Y}}} \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n, \end{aligned}$$

where  $\text{cov}_n^2$  is defined the same as in Theorem 2.1.1 and  $\mathcal{R}_n$  is the remainder term.

(ii) Further suppose Assumption D2 holds. Then

$$\begin{aligned} & f^{(1)}\left(\frac{\tau_X}{\gamma_{\mathbf{X}}}\right) g^{(1)}\left(\frac{\tau_Y}{\gamma_{\mathbf{Y}}}\right) \frac{\tau_X}{\gamma_{\mathbf{X}}} \frac{\tau_Y}{\gamma_{\mathbf{Y}}} \asymp_p 1, \\ & \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) = O_p(\tau a_p b_q), \\ & \mathcal{R}_n = O_p(\tau a_p^2 b_q + \tau a_p b_q^2) = o_p(1). \end{aligned}$$

Thus the remainder term is of smaller order compared to the leading term and is therefore asymptotically negligible.

Notice that different from the decomposition of  $\text{dCov}_n^2(\mathbf{X}, \mathbf{Y})$  as in Theorem 2.1.1, here we decompose  $\text{hCov}_n^2$  multiplied by  $\tau = \tau_X \tau_Y$ . This is expected, since in  $\text{hCov}_n^2$ , each pair-wise distance is normalized by  $\gamma_{\mathbf{X}}$  or  $\gamma_{\mathbf{Y}}$ , which has asymptotically the same magnitude as  $\tau_X$ ,  $\tau_Y$  respectively. In the high dimensional case, the expansion (8) suggests that hCov-based tests also suffer from power loss when  $X$  and  $Y$  are component-wisely uncorrelated but nonlinearly dependent.

To analyze the asymptotic property of sample Hilbert-Schmidt covariance, most literature would assume the bandwidth parameters to be fixed constants, see e.g. Gretton et al. (2008). In contrast, our approach can handle the case where these bandwidth parameters are selected to be the median of pairwise sample distance, which is random and whose magnitude increases with dimension.

Similar to the marginal distance covariance introduced in Section 2.1.1, we can also aggregate the marginal Hilbert-Schmidt Covariance (mhCov), which is defined as

$$\text{mhCov}_n^2(\mathbf{X}, \mathbf{Y}) = \sqrt{\binom{n}{2}} \sum_{i=1}^p \sum_{j=1}^q \text{hCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j)$$

where  $\text{hCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) = (\tilde{\mathbf{R}}(i) \cdot \tilde{\mathbf{H}}(j))$ ,  $\tilde{\mathbf{R}}(i)$  and  $\tilde{\mathbf{H}}(j)$  are  $\mathcal{U}$ -centered version of  $\mathbf{R}(i) = (r_{st}(i))_{s,t=1}^n$ ,  $\mathbf{H}(j) = (h_{st}(j))_{s,t=1}^n$  respectively and  $r_{st}(i) = h_{st}(j) = 0$  if  $s = t$ , otherwise

$$\begin{cases} r_{st}(i) = K(x_{si}, x_{ti}, \mathcal{X}_i) = f\left(\frac{|x_{si} - x_{ti}|}{\gamma_{\mathcal{X}_i}}\right), \gamma_{\mathcal{X}_i} = \text{median}\{|x_{si} - x_{ti}|, s \neq t\}, \\ h_{st}(j) = L(y_{sj}, y_{tj}, \mathcal{Y}_j) = g\left(\frac{|y_{sj} - y_{tj}|}{\gamma_{\mathcal{Y}_j}}\right), \gamma_{\mathcal{Y}_j} = \text{median}\{|y_{sj} - y_{tj}|, s \neq t\}. \end{cases}$$

REMARK 2.1.2. *By the multi-linearity of the operator  $(\tilde{\cdot}, \tilde{\cdot})$ , it can be easily seen that  $\text{mdCov}_n^2(\mathbf{X}, \mathbf{Y})$  is equal to (up to a constant)  $\text{dCov}_n^2(\mathbf{X}, \mathbf{Y})$  equipped with  $L^1$ -distance and  $\text{mhCov}_n^2(\mathbf{X}, \mathbf{Y})$  is equal to (up to a constant)  $\text{hCov}_n^2(\mathbf{X}, \mathbf{Y})$  equipped with kernels*

$$K'(X_s, X_t, \mathbf{X}) = \sum_{i=1}^p K(x_{si}, x_{ti}, \mathcal{X}_i) \text{ and } L'(Y_s, Y_t, \mathbf{Y}) = \sum_{j=1}^q L(y_{sj}, y_{tj}, \mathcal{Y}_j).$$

2.2. *Studentized Test Statistics.* In this section, we provide studentized version of the statistics introduced in Section 2.1. It is worth mentioning that we provide a unified approach to the asymptotic analysis of studentized dCov, mdCov and further extend them to the analysis of studentized hCov.

2.2.1. *Unified Approach.* Firstly, we will present results that will be useful for deriving the studentized version of the interested statistics, i.e. distance covariance (dCov), marginal distance covariance (mdCov), Hilbert-Schmidt Covariance (hCov), marginal Hilbert-Schmidt Covariance (mhCov). It can be shown later that many previously mentioned statistics are asymptotically equal to the unified quantity  $\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})$  multiplied by some normalizing factor. Here,  $\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})$  is defined as

$$\text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q (\tilde{\mathbf{K}}(i) \cdot \tilde{\mathbf{L}}(j)),$$

where  $\tilde{\mathbf{K}}(i)$  and  $\tilde{\mathbf{L}}(j)$  are the  $\mathcal{U}$ -centered versions of  $\mathbf{K}(i) = (k_{st}(i))_{s,t=1}^n$ ,  $\mathbf{L}(j) = (l_{st}(j))_{s,t=1}^n$  respectively and  $k_{st}(i) = l_{st}(j) = 0$  if  $s = t$ , otherwise  $k_{st}(i)$ ,

$l_{st}(j)$  are the double centered kernel distances, i.e., for bivariate kernels  $k$  and  $l$ ,

$$\begin{aligned} k_{st}(i) &= k(x_{si}, x_{ti}) - \mathbb{E}[k(x_{si}, x_{ti})|x_{si}] - \mathbb{E}[k(x_{si}, x_{ti})|x_{ti}] + \mathbb{E}[k(x_{si}, x_{ti})], \\ l_{st}(i) &= l(y_{si}, y_{ti}) - \mathbb{E}[l(y_{si}, y_{ti})|y_{si}] - \mathbb{E}[l(y_{si}, y_{ti})|y_{ti}] + \mathbb{E}[l(y_{si}, y_{ti})]. \end{aligned}$$

The advantage of using the double centering kernel distance is that we can have 0 covariance between  $k_{st}(i)$  and  $k_{uv}(j)$  ( $l_{st}(i)$  and  $l_{uv}(j)$ ) for  $\{s, t\} \neq \{u, v\}$  as shown in the following proposition.

**PROPOSITION 2.2.1.** *For all  $1 \leq i, i' \leq p, 1 \leq j, j' \leq q$ , if  $\{s, t\} \neq \{u, v\}$ , then*

$$\mathbb{E}[k_{st}(i)k_{uv}(i')] = \mathbb{E}[l_{st}(j)l_{uv}(j')] = \mathbb{E}[k_{st}(i)l_{uv}(j)] = 0.$$

To derive the limiting distribution of the unified quantity, we need the following assumptions.

**ASSUMPTION D3.** *For fixed  $n$ , as  $p \wedge q \rightarrow \infty$ ,*

$$\begin{pmatrix} p^{-1/2} \sum_{i=1}^p k_{st}(i) \\ q^{-1/2} \sum_{j=1}^q l_{uv}(j) \end{pmatrix}_{s < t, u < v} \xrightarrow{d} \begin{pmatrix} c_{st} \\ d_{uv} \end{pmatrix}_{s < t, u < v},$$

where  $\{c_{st}, d_{uv}\}_{s < t, u < v}$  are jointly Gaussian. Naturally, we further assume the existence of the following constants that show up in the covariance matrix of  $\{c_{st}, d_{uv}\}$ ,

$$\begin{aligned} \text{var}[c_{st}] &:= \sigma_x^2 = \lim_p \frac{1}{p} \sum_{i,j=1}^p \text{cov}[k_{st}(i), k_{st}(j)] \\ &= \begin{cases} \lim_p \frac{\sum_{i,j=1}^p \text{dCov}^2(x_i, x_j)}{p}, & \text{if } k(x, y) = l(x, y) = |x - y|, \\ \lim_p \frac{\sum_{i,j=1}^p 4\text{cov}^2(x_i, x_j)}{p}, & \text{if } k(x, y) = l(x, y) = |x - y|^2, \end{cases} \\ \text{var}[d_{st}] &:= \sigma_y^2 = \lim_q \frac{1}{q} \sum_{i,j=1}^q \text{cov}[l_{st}(i), l_{st}(j)] \\ &= \begin{cases} \lim_q \frac{\sum_{i,j=1}^q \text{dCov}^2(y_i, y_j)}{q}, & \text{if } k(x, y) = l(x, y) = |x - y|, \\ \lim_q \frac{\sum_{i,j=1}^q 4\text{cov}^2(y_i, y_j)}{q}, & \text{if } k(x, y) = l(x, y) = |x - y|^2, \end{cases} \end{aligned}$$



$$\begin{aligned} \text{cov}[c_{st}, d_{st}] &:= \sigma_{xy}^2 = \lim_{p,q} \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q \text{cov}[k_{st}(i), l_{st}(j)] \\ &= \begin{cases} \lim_{p,q} \frac{\sum_{i=1}^p \sum_{j=1}^q \text{dCov}^2(x_i, y_j)}{\sqrt{pq}}, & \text{if } k(x, y) = l(x, y) = |x - y|, \\ \lim_{p,q} \frac{\sum_{i=1}^p \sum_{j=1}^q 4\text{cov}^2(x_i, y_j)}{\sqrt{pq}}, & \text{if } k(x, y) = l(x, y) = |x - y|^2. \end{cases} \end{aligned}$$

REMARK 2.2.1. Notice that when  $\{s, t\} \neq \{u, v\}$ , we do not assume the form of  $\text{cov}[c_{st}, c_{uv}]$ ,  $\text{cov}[d_{st}, d_{uv}]$ ,  $\text{cov}[c_{st}, d_{uv}]$  in Assumption D3, since it follows easily from Proposition 2.2.1 that  $\text{cov}[c_{st}, c_{uv}] = 0$ ,  $\text{cov}[d_{st}, d_{uv}] = 0$  and  $\text{cov}[c_{st}, d_{uv}] = 0$  if  $\{s, t\} \neq \{u, v\}$ .

REMARK 2.2.2. The above Central Limit Theorem (CLT) result can be derived under suitable moment and weak dependence assumptions for the components of  $X$  and  $Y$  and the weak dependence assumptions can be satisfied by a broad range of time series models such as ARMA models. We refer the reader to [Doukhan and Neumann \(2008\)](#) for a relatively recent survey of weak dependence notions and the CLT results under such weak dependence. It is worth noting that the commonly used weak dependence assumptions in time series analysis, such as  $\alpha$ -mixing,  $\beta$ -mixing and variants [[Bradley \(2007\)](#)], near epoch dependence [[Gallant and White \(1988\)](#), [Davidson \(1994\)](#)] and physical dependence measure [[Wu \(2005\)](#)], all require the components have a natural time ordering. In our setting, the components do not necessarily have a natural ordering but our results still hold as long as there exists a permutation of components that satisfy the weak dependence assumption. Furthermore we remark that the weak dependence assumption typically rules out long range dependence and local strong dependence, under which we might have non-Gaussian limit and different norming rate. We shall examine the validity of our tests in these two scenarios via simulations.

The following theorem is our main result, which shows that the unified quantity converges in distribution to a quadratic form of random variables.

THEOREM 2.2.1. Fixing  $n$  and letting  $p \wedge q \rightarrow \infty$ , under Assumptions

*D1 and D3,*

$$\begin{aligned} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &\xrightarrow{d} \frac{1}{v} \mathbf{c}^T \mathbf{M} \mathbf{d}, \\ \text{uCov}_n^2(\mathbf{X}, \mathbf{X}) &\xrightarrow{d} \frac{1}{v} \mathbf{c}^T \mathbf{M} \mathbf{c} \stackrel{d}{=} \frac{\sigma_x^2}{v} \chi_v^2, \\ \text{uCov}_n^2(\mathbf{Y}, \mathbf{Y}) &\xrightarrow{d} \frac{1}{v} \mathbf{d}^T \mathbf{M} \mathbf{d} \stackrel{d}{=} \frac{\sigma_y^2}{v} \chi_v^2, \end{aligned}$$

where  $v := n(n-3)/2$ ,  $\mathbf{M}$  is a projection matrix of rank  $v$  and

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} \stackrel{d}{=} N \left( \mathbf{0}, \begin{pmatrix} \sigma_x^2 \mathbf{I}_{n(n-1)/2} & \sigma_{xy}^2 \mathbf{I}_{n(n-1)/2} \\ \sigma_{xy}^2 \mathbf{I}_{n(n-1)/2} & \sigma_y^2 \mathbf{I}_{n(n-1)/2} \end{pmatrix} \right).$$

For the exact form of  $\mathbf{M}$ , see the proof of Theorem 2.2.1 in the Appendix. Next, we define the quantity  $T_u$  as

$$T_u = \sqrt{v-1} \frac{\text{uCor}_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{1 - (\text{uCor}_n^2(\mathbf{X}, \mathbf{Y}))^2}},$$

where

$$\text{uCor}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{\text{uCov}_n^2(\mathbf{X}, \mathbf{X}) \text{uCov}_n^2(\mathbf{Y}, \mathbf{Y})}}.$$

We then define the constants  $v$  and  $\phi$  that appear in the limiting distribution of  $T_u$ . Set  $v = n(n-3)/2$  and  $\phi = \sigma_{xy}^2 / \sqrt{\sigma_x^2 \sigma_y^2}$  such that

$$\phi = \phi_1 \mathbb{I}_{\{k(x,y)=l(x,y)=|x-y|\}} + \phi_2 \mathbb{I}_{\{k(x,y)=l(x,y)=|x-y|^2\}},$$

where

$$\begin{aligned} \phi_1 &:= \lim_{p,q} \frac{\sum_{i=1}^p \sum_{j=1}^q \text{dCov}^2(x_i, y_j)}{\sqrt{\sum_{i,j=1}^p \text{dCov}^2(x_i, x_j) \sum_{i,j=1}^q \text{dCov}^2(y_i, y_j)}}, \\ \phi_2 &:= \lim_{p,q} \frac{\sum_{i=1}^p \sum_{j=1}^q \text{cov}^2(x_i, y_j)}{\sqrt{\sum_{i,j=1}^p \text{cov}^2(x_i, x_j) \sum_{i,j=1}^q \text{cov}^2(y_i, y_j)}}. \end{aligned}$$

The limiting distribution of  $T_u$  is derived under both null ( $H_0$ ) and alternative ( $H_A$ ) hypothesis, i.e.,

$$\begin{aligned} \text{null hypothesis : } & H_0 = \{(X, Y) \mid X \perp Y\}, \\ \text{alternative hypothesis : } & H_A = \{(X, Y) \mid X \not\perp Y\}. \end{aligned}$$

In addition, we also consider the local alternative hypothesis  $H_{A_l} \subset H_A$ , i.e.,

$$H_{A_l} = \left\{ (X, Y) \mid X \not\perp Y, \phi = \frac{\phi_0}{\sqrt{v}} \right\},$$

where  $v = n(n-3)/2$ ,  $\phi_0 = \phi_{0,1} \mathbb{I}_{\{k(x,y)=l(x,y)=|x-y|\}} + \phi_{0,2} \mathbb{I}_{\{k(x,y)=l(x,y)=|x-y|^2\}}$  and  $0 < \phi_{0,1}, \phi_{0,2} < \infty$  are constants with respect to  $n$ . It is also interesting to compare the asymptotic power under the following class of alternatives  $H_{A_s} \subset H_A$ , i.e.,

$$H_{A_s} = \{(X, Y) \mid x_i \not\perp y_j, \text{cov}(x_i, y_j) = 0 \text{ for all } 1 \leq i \leq p, 1 \leq j \leq q\}.$$

In summary, the following table illustrates the value of  $\phi$  under different cases we are considering,

$\phi$	$H_0$	$H_A$	$H_{A_l}$	$H_{A_s}$
$k(x, y) = l(x, y) =  x - y $	0	$\phi_1$	$\frac{\phi_{0,1}}{\sqrt{v}}$	$\phi_1$
$k(x, y) = l(x, y) =  x - y ^2$	0	$\phi_2$	$\frac{\phi_{0,2}}{\sqrt{v}}$	0

Next, denote by  $t_a$  the student  $t$ -distribution with degrees of freedom  $a$ . Let  $t_a^{(\alpha)}$  be the  $(1 - \alpha)$ th percentile of  $t_a$  and  $t_{a,b}$  be the non-central  $t$ -distribution with degrees of freedom  $a$  and non-central parameter  $b$ . The asymptotic distribution of  $T_u$  is stated in the following proposition.

**PROPOSITION 2.2.2.** *Fix  $n$  and let  $p \wedge q \rightarrow \infty$ . If Assumptions [D1](#) and [D3](#) hold, then for any fixed  $t \in \mathbb{R}$ ,*

$$\begin{aligned} P_{H_0}(T_u \leq t) &\rightarrow P(t_{v-1} \leq t), \\ P_{H_A}(T_u \leq t) &\rightarrow \mathbb{E}[P(t_{v-1,W} \leq t)], \end{aligned}$$

where  $W \sim \sqrt{\frac{\phi^2}{1-\phi^2}} \chi_v^2$  and  $\chi_v^2$  is the chi-square distribution with degrees of freedom  $v$ .

**REMARK 2.2.3.** *For the explicit form of  $\mathbb{E}[P(t_{v-1,W} \leq t)]$ , see [Lemma 3](#) in the [Appendix](#).*

Below we derive the large sample approximation of the limiting distribution  $\mathbb{E}[P(t_{v-1,W} \leq t)]$  under the local alternative hypothesis ( $H_{A_l}$ ).

**PROPOSITION 2.2.3.** *Under  $H_{A_l}$ , if we allow  $n$  to grow and  $t$  is bounded as  $n \rightarrow \infty$ ,  $\mathbb{E}[P(t_{v-1,W} \leq t)]$  can be approximated as*

$$\mathbb{E}_{H_{A_l}}[P(t_{v-1,W} \leq t)] = P(t_{v-1,\phi_0} \leq t) + O\left(\frac{1}{v}\right),$$

where  $\phi_0 = \phi_{0,1}\mathbb{I}_{\{k(x,y)=l(x,y)=|x-y|\}} + \phi_{0,2}\mathbb{I}_{\{k(x,y)=l(x,y)=|x-y|^2\}}$ . In particular, the result still holds if we replace  $t$  with  $t_{v-1}^{(\alpha)}$ .

**2.2.2. Studentized Tests.** For testing the null, permutation test can be used to determine the critical value of the distance covariance (dCov), Hilbert-Schmidt covariance (hCov), marginal distance covariance (mdCov) and marginal Hilbert-Schmidt covariance (mhCov) respectively. If  $\text{dCov}_n^2$ ,  $\text{hCov}_n^2$ ,  $\text{mdCov}_n^2$  or  $\text{mhCov}_n^2$  is larger than the corresponding critical value, which can be determined by the empirical permutation distribution function, we reject the null. Alternatively, similar to the construction of  $T_u$ , we transform each of  $\text{dCov}_n^2$ ,  $\text{hCov}_n^2$ ,  $\text{mdCov}_n^2$  and  $\text{mhCov}_n^2$  into a statistic that has asymptotic  $t$ -distribution under the null. Thus, instead of using permutation test, which can be quite computationally expensive, we can determine the critical value using this asymptotic  $t$ -distribution. For each  $R \in \{\text{dCov}, \text{hCov}, \text{mdCov}, \text{mhCov}\}$ , the studentized test statistic  $T_R$  is defined as

$$T_R = \sqrt{v-1} \frac{R^*(\mathbf{X}, \mathbf{Y})}{\sqrt{1 - (R^*(\mathbf{X}, \mathbf{Y}))^2}},$$

where

$$R^*(\mathbf{X}, \mathbf{Y}) = \frac{R_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{R_n^2(\mathbf{X}, \mathbf{X})R_n^2(\mathbf{Y}, \mathbf{Y})}}.$$

The way to derive the asymptotic distribution of  $T_R$  is to show that for each  $R \in \{\text{dCov}, \text{hCov}, \text{mdCov}\}$ ,  $R_n^2(\mathbf{X}, \mathbf{Y})$  and  $\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})$  are asymptotically equal up to an asymptotically constant factor, as shown below.

**PROPOSITION 2.2.4.** *Under Assumption D1,*

(i) *When  $k(x, y) = l(x, y) = |x - y|^2$ ,*

$$\text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{4} \frac{\sqrt{pq}}{\tau} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) + \mathcal{R}'_n,$$

$$\tau \times \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{\sqrt{pq}}{4\gamma_{\mathbf{X}}\gamma_{\mathbf{Y}}} f^{(1)}\left(\frac{\tau_{\mathbf{X}}}{\gamma_{\mathbf{X}}}\right) g^{(1)}\left(\frac{\tau_{\mathbf{Y}}}{\gamma_{\mathbf{Y}}}\right) \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) + \mathcal{R}''_n,$$

where  $\mathcal{R}'_n, \mathcal{R}''_n$  are the remainder terms. Further suppose Assumption D2 holds. Then

$$\text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) = O_p(\tau a_p b_q),$$

$$\mathcal{R}'_n = O_p(\tau a_p^2 b_q + \tau a_p b_q^2) = o_p(1),$$

$$\mathcal{R}''_n = O_p(\tau a_p^2 b_q + \tau a_p b_q^2) = o_p(1).$$

Thus the remainder term is of smaller order compared to the leading term and therefore is asymptotically negligible.

(ii) When  $k(x, y) = l(x, y) = |x - y|$ ,

$$\text{mdCov}_n^2(\mathbf{X}, \mathbf{Y}) = \sqrt{pq} \sqrt{\binom{n}{2}} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}).$$

As shown in Proposition 2.2.4,  $k(x, y) = l(x, y) = |x - y|$  would correspond to the mdCov-based  $t$ -test and  $k(x, y) = l(x, y) = |x - y|^2$  would correspond to the {dCov, hCov}-based  $t$ -tests. Then, for each  $R \in \{\text{dCov}, \text{hCov}, \text{mdCov}\}$  the asymptotic distribution of  $T_R$  is given in the following Corollary.

COROLLARY 2.2.1. *If Assumptions D1, D2 and D3 hold, for any fixed  $t$  and each  $R \in \{\text{dCov}, \text{hCov}, \text{mdCov}\}$ , we have*

$$P_{H_0}(T_R \leq t) \rightarrow P(t_{v-1} \leq t),$$

$$P_{H_A}(T_R \leq t) \rightarrow \mathbb{E}[P(t_{v-1, W} \leq t)], \text{ where } W \sim \sqrt{\frac{\phi^2}{1 - \phi^2}} \chi_v^2.$$

After knowing the asymptotic distribution of  $T_R$  under the null, i.e.  $t$ -distribution with degrees of freedom  $v - 1$ , we can set critical value as  $t_{v-1}^{(\alpha)}$ . Then, from Proposition 2.2.2, under the alternative, the asymptotic power of testing the null can be written as a function of  $\phi$ , i.e.,

$$\text{Power}_n(\phi) := \mathbb{E}[P(t_{v-1, W} > t_{v-1}^{(\alpha)})],$$

and under  $H_{A_t}$ , if we allow  $n$  to grow

$$\text{Power}_\infty(\phi_0) := \lim_{n \rightarrow \infty} \text{Power}_n\left(\frac{\phi_0}{\sqrt{v}}\right) = \lim_{n \rightarrow \infty} P(t_{v-1, \phi_0} > t_{v-1}^{(\alpha)}).$$

Next, we can actually bound the ratio of  $\phi_1$  and  $\phi_2$  for standard normal random variables.

PROPOSITION 2.2.5. *Suppose that*

$$\begin{pmatrix} X \\ Y \end{pmatrix} \stackrel{d}{=} N\left(\mathbf{0}, \begin{pmatrix} \mathbf{I}_p & \boldsymbol{\Sigma}_{XY} \\ \boldsymbol{\Sigma}_{XY}^T & \mathbf{I}_q \end{pmatrix}\right),$$

where  $\boldsymbol{\Sigma}_{XY} = \text{cov}(X, Y)$ . We have

$$0.89^2 \phi_2 \leq \phi_1 \leq \phi_2.$$

It will be shown later that  $\phi_1$  corresponds to the mdCov-based test, whereas  $\phi_2$  corresponds to the dCov and hCov-based tests. Thus considering models described in Proposition 2.2.5, we expect a power loss for the mdCov-based test comparing to the dCov and hCov-based tests. On the other hand, since  $\phi_1$  is bounded below by  $0.89^2\phi_2$ , the power loss is expected to be moderate.

Using Corollary 2.2.1, we can theoretically compare the power of these  $t$ -tests under different cases and the results are summarized in the following table

<i>Power</i>	$T_{\text{mdCov}}$	$T_{\text{dCov}}, T_{\text{hCov}}$
under $H_A$	$Power_n(\phi_1)$	$Power_n(\phi_2)$
under $H_{A_l}$ , allow $n$ growing to infinity	$Power_\infty(\phi_{0,1})$	$Power_\infty(\phi_{0,2})$
under $H_{A_s}$	$Power_n(\phi_1)$	$\alpha$

For the studentized version of mhCov, if we consider the bandwidth parameters to be fixed constants, then we can use the unified approach to get the limiting  $t$ -distribution of the transformed  $\text{mhCov}_n^2$ . On the other hand, if  $\gamma_{\mathcal{X}_i}$  and  $\gamma_{\mathcal{Y}_j}$  are treated to be median of sample distance along each dimension and are thus random, we encounter technical difficulties to derive the limiting distribution, as in this case the kernelized pair-wise distance along each dimension are correlated with each other. This is due to the choice of the bandwidth parameter and the high dimensional approximation used for  $\text{hCov}_n^2$  can not be directly applied, since  $\gamma_{\mathcal{X}_i}$  and  $\gamma_{\mathcal{Y}_j}$  are calculated component-wisely. Nevertheless, we shall examine the testing efficiency using  $t$ -distribution approximation when the bandwidth parameters are chosen to be the median of sample distance in simulation.

REMARK 2.2.4. *An anonymous referee inquired about the applicability of our tests to the setting when the  $p$ -dimensional data vector  $X = (x_1, \dots, x_p)^T$  is a growth curve and thus can be viewed as a stochastic process or random function evaluated at time points  $\{t_i\}_{i=1}^p$ , say  $0 \leq t_1 < t_2 < \dots < t_p \leq 1$ . Under suitable conditions, one can show that the Euclidean norm of  $X$  after proper scaling converges to the  $L_2$  norm of the random function when the number of sampling points goes to infinity. It is known that the Hilbert space  $L_2([0, 1])$  is of strong negative type [Lyons (2013)], and thus the HSIC or the distance covariance based on the  $L_2$  norm completely characterizes dependence. Therefore, the Euclidean norm is a proper norm to use if  $X$  is considered to be an element in  $L_2([0, 1])$  and we want to use the  $L_2$  norm to construct our distance metrics. However, the setting we are considering in this paper assumed the components of  $X$  and  $Y$  have weak dependence and*

the above growth curve example falls into the very strong dependent case, and thus our theoretical phenomenon does not apply. In practice, both strongly componentwise correlated high dimensional data and weakly componentwise dependent high dimensional data can be collected depending on the nature of data generating process. We shall illustrate the usefulness of our theory and proposed tests using an earthquake dataset in Section 3.

Our theory demonstrates the limitation of  $dCov$  and  $hCov$  in the high dimensional environment, which is intimately related to the use of Euclidean norm in their definitions. Similar phenomenon has been discovered for energy distance [Szekely and Rizzo (2004)] and maximum mean discrepancy [Gretton et al. (2012)] in the two sample testing problem recently; see Zhu and Shao (2019) and Chakraborty and Zhang (2019). It is natural to ask what norm would be desirable to use in the high dimensional setting and in what sense? We shall leave these questions for future study.

**3. Numerical Results.** Here, we consider some numerical examples to compare the “joint” tests, where the distance/Hilbert-Schmidt covariance is applied to whole components of data jointly, with the “marginal” tests, where distance/Hilbert-Schmidt covariance is applied to one dimensional components and then being aggregated. To this end, we consider the following statistics

$$\begin{array}{l} \text{“Joint”} \\ \text{“Marginal”} \end{array} \left\{ \begin{array}{l} dCov : \text{distance covariance (permutation)} \\ T_{dCov} : \text{studentized distance covariance} \\ hCov : \text{Hilbert-Schmidt covariance (permutation)} \\ T_{hCov} : \text{studentized Hilbert-Schmidt covariance} \\ \\ mdCov : \text{marginal distance covariance (permutation)} \\ T_{mdCov} : \text{studentized marginal distance covariance,} \\ mhCov : \text{marginal Hilbert-Schmidt covariance (permutation)} \\ T_{mhCov} : \text{studentized marginal Hilbert-Schmidt covariance} \end{array} \right.$$

In the above display,  $dCov_n^2$  and  $hCov_n^2$  are the two “joint” test statistics to measure the overall dependence between  $X$  and  $Y$ ,  $mdCov_n^2$  and  $mhCov_n^2$  are the “marginal” test statistics, and these four test statistics are implemented as permutation tests;  $T_{dCov}$  from Székely and Rizzo (2013) is the studentized version of  $dCov$ , our proposed  $t$ -tests  $T_{hCov}$ ,  $T_{mdCov}$ ,  $T_{mhCov}$  are the studentized versions of  $hCov$ ,  $mdCov$ ,  $mhCov$  respectively. All these four tests are implemented using the  $t$ -distribution based critical value. We examine both the Gaussian kernel and Laplacian kernel for the Hilbert-Schmidt covariance based tests.

For the permutation-based tests, we randomly shuffle the samples  $\{X_1, \dots, X_n\}$  and get  $(X_{\pi(1)}, \dots, X_{\pi(n)})$ , where  $\pi$  is the permutation map from  $\{1, \dots, n\}$  to  $\{1, \dots, n\}$ . Then we calculate the test statistic based on the permuted sample  $\{(X_{\pi(1)}, \dots, X_{\pi(n)}), (Y_1, \dots, Y_n)\}$ . The  $p$ -value for permutation-based test is defined as the proportion of times that the test statistic based on the permuted samples is greater than the one based on the original sample. All the numerical results from permutation-based tests are based on 200 permutations and the empirical rejection rate of the tests are based on 5000 Monte Carlo repetitions.

We first examine the size of the afore-mentioned tests.

EXAMPLE 3.1. *Generate i.i.d. samples from the following models for  $i = 1, \dots, n$ .*

- (i)  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \mathbf{I}_p), Y_i = (y_{i1}, \dots, y_{ip})^T \sim N(\mathbf{0}, \mathbf{I}_p)$ .
- (ii) Let  $AR(1)$  denotes the Gaussian autoregressive model of order 1 with parameter  $\phi, X_i \sim AR(1), \phi = 0.5, Y_i \sim AR(1), \phi = -0.5$ .
- (iii) Let  $\Sigma = (\sigma_{ij}) \in \mathbb{R}^{p \times p}$  and  $\sigma_{ij} = 0.7^{|i-j|}$ ,  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \Sigma), Y_i = (y_{i1}, \dots, y_{ip})^T \sim N(\mathbf{0}, \Sigma)$ .

From Table 1, we can see that all the tests have quite accurate size. Although the  $t$ -tests are derived under the high dimensional scenario, they still have pretty accurate size even for relatively low dimension (e.g.,  $p = 5$ ).

As demonstrated in Theorem 2.1.1 and 2.1.2, the leading term in (7) and (8) can only measure the linear dependence as  $p \wedge q \rightarrow \infty$ , therefore we expect the “joint” test based on  $dCov_n^2(\mathbf{X}, \mathbf{Y})$  or  $hCov_n^2(\mathbf{X}, \mathbf{Y})$  may fail to capture the non-linear dependence in high dimension. On the other hand, we consider the “marginal” test where we take the sum of pairwise sample distance/Hilbert-Schmidt covariances to measure the low dimensional dependence for all the pairs as the test proposed in Sections 2.1.1 and 2.1.2. The “marginal” test statistic measures the dependence marginally in a low-dimensional fashion so that it can preserve the ability to capture component-wise non-linear dependence. In the following two examples, we demonstrate the superiority of “marginal” tests.

EXAMPLE 3.2. *Generate i.i.d. samples from the following models for  $i = 1, \dots, n$ .*

- (i)  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \mathbf{I}_p), Y_i = (y_{i1}, \dots, y_{ip})^T$ , where  $y_{ij} = x_{ij}^2$  for  $j = 1, \dots, p$ .
- (ii) Let  $\Sigma = (\sigma_{ij}) \in \mathbb{R}^{p \times p}$  and  $\sigma_{ij} = 0.7^{|i-j|}$ ,  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \Sigma), Y_i = (y_{i1}, \dots, y_{ip})^T$ , where  $y_{ij} = x_{ij}^2$  for  $j = 1, \dots, p$ .



TABLE 1  
Size comparison from Example 3.1

	n	p	α	dCov	mdCov	T <sub>dCov</sub>	T <sub>mdCov</sub>	Gaussian Kernel				Laplacian Kernel				
								hCov	mhCov	T <sub>hCov</sub>	T <sub>mhCov</sub>	hCov	mhCov	T <sub>hCov</sub>	T <sub>mhCov</sub>	
(i)	10	5	0.010	0.017	0.014	0.020	0.014	0.016	0.015	0.020	0.014	0.014	0.014	0.017	0.013	
	10	5	0.050	0.055	0.055	0.062	0.061	0.055	0.060	0.062	0.061	0.055	0.050	0.064	0.050	
	10	5	0.100	0.105	0.107	0.110	0.110	0.110	0.103	0.106	0.109	0.109	0.102	0.099	0.105	0.101
	10	30	0.010	0.015	0.015	0.013	0.011	0.015	0.016	0.012	0.012	0.014	0.014	0.011	0.011	
	10	30	0.050	0.054	0.053	0.050	0.053	0.053	0.054	0.050	0.052	0.052	0.052	0.059	0.050	0.054
	10	30	0.100	0.102	0.104	0.099	0.102	0.102	0.105	0.100	0.103	0.102	0.102	0.107	0.101	0.105
	30	5	0.010	0.014	0.016	0.019	0.018	0.016	0.016	0.020	0.017	0.016	0.015	0.019	0.015	
	30	5	0.050	0.052	0.053	0.062	0.059	0.052	0.057	0.061	0.059	0.054	0.055	0.061	0.058	
	30	5	0.100	0.105	0.104	0.105	0.107	0.103	0.107	0.106	0.106	0.105	0.104	0.109	0.104	
	30	30	0.010	0.014	0.014	0.011	0.012	0.014	0.017	0.010	0.013	0.014	0.017	0.011	0.013	
	30	30	0.050	0.051	0.053	0.052	0.051	0.051	0.056	0.052	0.053	0.051	0.058	0.051	0.052	
	30	30	0.100	0.097	0.105	0.096	0.103	0.097	0.105	0.095	0.101	0.099	0.104	0.100	0.102	
	60	5	0.010	0.013	0.015	0.018	0.016	0.014	0.013	0.019	0.016	0.014	0.015	0.017	0.015	
	60	5	0.050	0.052	0.055	0.061	0.057	0.054	0.061	0.060	0.064	0.053	0.057	0.058	0.058	
	60	5	0.100	0.103	0.104	0.109	0.104	0.107	0.108	0.110	0.110	0.102	0.101	0.103	0.102	
	60	30	0.010	0.019	0.017	0.016	0.012	0.019	0.015	0.015	0.013	0.020	0.016	0.015	0.014	
	60	30	0.050	0.060	0.063	0.057	0.058	0.060	0.058	0.057	0.058	0.061	0.058	0.058	0.055	
	60	30	0.100	0.113	0.112	0.110	0.107	0.113	0.109	0.111	0.105	0.110	0.111	0.107	0.107	
	(ii)	10	5	0.010	0.015	0.015	0.023	0.023	0.014	0.016	0.023	0.019	0.015	0.017	0.022	0.021
		10	5	0.050	0.051	0.054	0.064	0.066	0.053	0.058	0.064	0.066	0.054	0.058	0.066	0.062
		10	5	0.100	0.101	0.105	0.107	0.111	0.100	0.109	0.105	0.113	0.102	0.110	0.106	0.109
		10	30	0.010	0.014	0.018	0.013	0.016	0.014	0.017	0.014	0.013	0.017	0.018	0.017	0.013
		10	30	0.050	0.060	0.061	0.061	0.061	0.061	0.056	0.062	0.056	0.059	0.060	0.059	0.056
		10	30	0.100	0.105	0.105	0.110	0.107	0.105	0.105	0.109	0.099	0.106	0.108	0.111	0.104
30		5	0.010	0.012	0.011	0.022	0.023	0.012	0.014	0.021	0.020	0.013	0.013	0.019	0.016	
30		5	0.050	0.046	0.048	0.055	0.056	0.046	0.052	0.055	0.059	0.047	0.053	0.051	0.059	
30		5	0.100	0.094	0.096	0.094	0.096	0.096	0.100	0.097	0.100	0.093	0.107	0.097	0.104	
30		30	0.010	0.016	0.016	0.017	0.015	0.017	0.015	0.017	0.011	0.017	0.015	0.017	0.012	
30		30	0.050	0.061	0.058	0.060	0.059	0.061	0.055	0.060	0.054	0.058	0.052	0.060	0.051	
30		30	0.100	0.109	0.105	0.110	0.107	0.111	0.101	0.110	0.098	0.111	0.102	0.113	0.097	
60		5	0.010	0.015	0.013	0.026	0.022	0.016	0.014	0.024	0.020	0.013	0.015	0.020	0.018	
60		5	0.050	0.055	0.052	0.062	0.061	0.055	0.053	0.061	0.059	0.055	0.052	0.061	0.054	
60		5	0.100	0.101	0.100	0.103	0.100	0.102	0.100	0.104	0.099	0.101	0.097	0.103	0.099	
60		30	0.010	0.013	0.014	0.013	0.014	0.013	0.016	0.014	0.013	0.014	0.015	0.013	0.012	
60		30	0.050	0.055	0.051	0.058	0.051	0.054	0.054	0.057	0.053	0.058	0.053	0.053	0.052	
60		30	0.100	0.105	0.102	0.105	0.100	0.106	0.103	0.105	0.102	0.107	0.105	0.107	0.104	
(iii)		10	5	0.010	0.012	0.013	0.025	0.024	0.012	0.014	0.024	0.022	0.016	0.013	0.025	0.019
		10	5	0.050	0.051	0.051	0.068	0.069	0.053	0.051	0.068	0.062	0.053	0.049	0.067	0.056
		10	5	0.100	0.100	0.099	0.107	0.103	0.100	0.098	0.105	0.102	0.100	0.098	0.104	0.101
		10	30	0.010	0.014	0.015	0.016	0.014	0.014	0.015	0.016	0.013	0.015	0.015	0.017	0.013
		10	30	0.050	0.055	0.057	0.061	0.058	0.053	0.056	0.061	0.056	0.057	0.057	0.064	0.059
		10	30	0.100	0.104	0.105	0.105	0.107	0.103	0.105	0.104	0.107	0.106	0.110	0.106	0.112
	30	5	0.010	0.015	0.014	0.028	0.029	0.015	0.014	0.025	0.024	0.014	0.014	0.024	0.019	
	30	5	0.050	0.052	0.054	0.060	0.062	0.051	0.052	0.062	0.062	0.048	0.052	0.058	0.059	
	30	5	0.100	0.103	0.103	0.098	0.099	0.101	0.101	0.101	0.098	0.099	0.099	0.097	0.098	
	30	30	0.010	0.017	0.015	0.019	0.017	0.016	0.015	0.019	0.015	0.013	0.016	0.018	0.012	
	30	30	0.050	0.054	0.055	0.058	0.058	0.055	0.055	0.059	0.057	0.056	0.057	0.063	0.056	
	30	30	0.100	0.102	0.105	0.105	0.103	0.101	0.099	0.103	0.102	0.104	0.107	0.105	0.105	
	60	5	0.010	0.012	0.012	0.029	0.027	0.014	0.012	0.028	0.024	0.016	0.011	0.023	0.021	
	60	5	0.050	0.052	0.052	0.063	0.064	0.050	0.048	0.063	0.059	0.050	0.052	0.059	0.061	
	60	5	0.100	0.100	0.101	0.098	0.095	0.098	0.099	0.097	0.099	0.099	0.098	0.100	0.094	
	60	30	0.010	0.017	0.015	0.020	0.019	0.016	0.017	0.020	0.017	0.016	0.015	0.019	0.014	
	60	30	0.050	0.052	0.053	0.058	0.060	0.055	0.057	0.061	0.059	0.057	0.056	0.062	0.059	
	60	30	0.100	0.103	0.106	0.107	0.103	0.102	0.106	0.107	0.105	0.103	0.102	0.106	0.101	

(iii)  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \mathbf{I}_p), Y_i = (y_{i1}, \dots, y_{ip})^T$ , where  $y_{ij} = \log|x_{ij}|$  for  $j = 1, \dots, p$ .

TABLE 2  
Power comparison under  $H_{A_s}$  from Example 3.2

	$n$	$p$	$\alpha$	dCov	mdCov	$T_{dCov}$	$T_{mdCov}$	Gaussian Kernel				Laplacian Kernel			
								hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	hCov	mhCov	$T_{hCov}$	$T_{mhCov}$
(i)	10	5	0.010	0.113	0.285	0.144	0.321	0.110	0.493	0.138	0.516	0.172	0.801	0.226	0.813
	10	5	0.050	0.231	0.495	0.254	0.519	0.236	0.724	0.256	0.736	0.356	0.927	0.398	0.938
	10	5	0.100	0.325	0.618	0.332	0.628	0.325	0.828	0.336	0.834	0.495	0.968	0.506	0.969
	10	30	0.010	0.032	0.286	0.028	0.267	0.032	0.543	0.030	0.513	0.044	0.848	0.041	0.838
	10	30	0.050	0.101	0.526	0.098	0.523	0.098	0.769	0.099	0.763	0.124	0.945	0.128	0.947
	10	30	0.100	0.158	0.669	0.162	0.666	0.160	0.858	0.160	0.858	0.203	0.978	0.205	0.977
	30	5	0.010	0.440	0.997	0.499	0.999	0.518	1	0.583	1	0.924	1	0.956	1
	30	5	0.050	0.651	1.000	0.679	1.000	0.741	1	0.768	1	0.987	1	0.988	1
	30	5	0.100	0.766	1.000	0.773	1	0.836	1	0.845	1	0.994	1	0.995	1
	30	30	0.010	0.084	1.000	0.082	1.000	0.085	1	0.082	1	0.194	1	0.192	1
	30	30	0.050	0.190	1	0.187	1	0.192	1	0.192	1	0.365	1	0.365	1
	30	30	0.100	0.275	1	0.272	1	0.280	1	0.276	1	0.476	1	0.478	1
	60	5	0.010	0.948	1	0.976	1	0.983	1	0.992	1	1	1	1	1
	60	5	0.050	0.994	1	0.996	1	0.998	1	0.999	1	1	1	1	1
	60	5	0.100	0.999	1	0.999	1	1.000	1	1.000	1	1	1	1	1
	60	30	0.010	0.185	1	0.173	1	0.194	1	0.183	1	0.587	1	0.587	1
	60	30	0.050	0.346	1	0.346	1	0.361	1	0.360	1	0.779	1	0.782	1
	60	30	0.100	0.462	1	0.459	1	0.475	1	0.473	1	0.861	1	0.864	1
10	5	0.010	0.167	0.232	0.237	0.296	0.192	0.347	0.263	0.410	0.279	0.595	0.391	0.652	
10	5	0.050	0.306	0.386	0.341	0.421	0.356	0.570	0.401	0.606	0.525	0.806	0.584	0.832	
10	5	0.100	0.401	0.489	0.409	0.500	0.479	0.699	0.487	0.709	0.674	0.892	0.689	0.901	
10	30	0.010	0.080	0.202	0.091	0.210	0.082	0.376	0.091	0.366	0.099	0.646	0.123	0.634	
10	30	0.050	0.178	0.369	0.191	0.378	0.179	0.605	0.192	0.610	0.229	0.834	0.252	0.837	
10	30	0.100	0.257	0.492	0.259	0.492	0.264	0.728	0.265	0.730	0.342	0.906	0.351	0.909	
30	5	0.010	0.623	0.847	0.781	0.950	0.895	0.999	0.957	1	0.995	1	0.999	1	
30	5	0.050	0.872	0.984	0.902	0.990	0.982	1	0.990	1	1.000	1	1	1	
30	5	0.100	0.940	0.996	0.945	0.995	0.994	1	0.994	1	1	1	1	1	
30	30	0.010	0.251	0.929	0.277	0.944	0.307	1	0.336	1	0.629	1	0.686	1	
30	30	0.050	0.419	0.982	0.434	0.985	0.499	1	0.517	1	0.830	1	0.849	1	
30	30	0.100	0.532	0.995	0.532	0.995	0.613	1	0.622	1	0.905	1	0.909	1	
60	5	0.010	0.999	1	1	1	1	1	1	1	1	1	1	1	
60	5	0.050	1	1	1	1	1	1	1	1	1	1	1	1	
60	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1	
60	30	0.010	0.643	1	0.684	1	0.790	1	0.833	1	0.996	1	0.999	1	
60	30	0.050	0.824	1	0.836	1	0.918	1	0.930	1	1.000	1	1.000	1	
60	30	0.100	0.894	1	0.896	1	0.955	1	0.958	1	1	1	1	1	
10	5	0.010	0.043	0.233	0.060	0.257	0.042	0.434	0.053	0.447	0.076	0.768	0.098	0.785	
10	5	0.050	0.121	0.466	0.141	0.490	0.119	0.680	0.137	0.698	0.191	0.924	0.214	0.927	
10	5	0.100	0.201	0.616	0.212	0.624	0.203	0.808	0.210	0.810	0.291	0.963	0.298	0.964	
10	30	0.010	0.017	0.260	0.013	0.242	0.017	0.482	0.012	0.445	0.021	0.830	0.017	0.811	
10	30	0.050	0.062	0.488	0.062	0.487	0.063	0.729	0.062	0.727	0.071	0.941	0.070	0.940	
10	30	0.100	0.120	0.632	0.116	0.630	0.118	0.837	0.115	0.836	0.131	0.972	0.130	0.975	
30	5	0.010	0.146	0.999	0.191	1	0.153	1	0.187	1	0.464	1	0.529	1	
30	5	0.050	0.346	1	0.375	1	0.347	1	0.380	1	0.723	1	0.747	1	
30	5	0.100	0.484	1	0.497	1	0.496	1	0.501	1	0.835	1	0.840	1	
30	30	0.010	0.024	1.000	0.022	1.000	0.026	1	0.022	1	0.038	1	0.037	1	
30	30	0.050	0.088	1	0.085	1	0.086	1	0.085	1	0.117	1	0.115	1	
30	30	0.100	0.149	1	0.147	1	0.148	1	0.144	1	0.195	1	0.193	1	
60	5	0.010	0.547	1	0.630	1	0.566	1	0.642	1	0.978	1	0.988	1	
60	5	0.050	0.802	1	0.835	1	0.808	1	0.836	1	0.997	1	0.998	1	
60	5	0.100	0.907	1	0.911	1	0.905	1	0.913	1	0.999	1	0.999	1	
60	30	0.010	0.038	1	0.030	1	0.038	1	0.029	1	0.089	1	0.080	1	
60	30	0.050	0.122	1	0.117	1	0.119	1	0.119	1	0.217	1	0.214	1	
60	30	0.100	0.198	1	0.196	1	0.199	1	0.197	1	0.326	1	0.325	1	

EXAMPLE 3.3. Generate *i.i.d.* samples from the following models for  $i = 1, \dots, n$ .

- (i) Let  $\circ$  denotes the Hadamard product,  $X_i = (x_{i1}, \dots, x_{ip})^T \stackrel{i.i.d.}{\sim} U(-1, 1)$ ,  
 $Y_i = X_i \circ X_i$ .
- (ii)  $X_i = (x_{i1}, \dots, x_{ip})^T \stackrel{i.i.d.}{\sim} U(0, 1)$ ,  $Y_i = 4X_i \circ X_i \circ X_i - 3.6X_i + 0.8$ .
- (iii)  $Z_i = (z_{i1}, \dots, z_{ip})^T \stackrel{i.i.d.}{\sim} U(0, 2\pi)$ ,  $X_i = \sin(Z_i)$ ,  $Y_i = \cos(Z_i)$ .

Notice that in the above two examples,  $\text{cov}^2(x_i, y_j) = 0$  but  $\text{dCov}^2(x_i, y_j) \neq 0$  for all  $(i, j)$ s, that is,  $(X, Y) \in H_{A_s}$ . From Table 2, we can observe that for Example 3.2, the “joint” tests suffer substantial power loss as dimension increases for fixed sample size. The power loss is less severe in case (ii) than the ones in cases (i) and (iii), due to the dependence between the components. On the other hand, the powers corresponding to the marginal test statistics consistently outperform their joint counterparts with very little to none power reduction as the dimension increases. Similar phenomenon can be observed for Example 3.3; see Table 3. In addition, for all the cases in both Example 3.2 and Example 3.3, the power loss corresponding to Laplacian kernel is consistently less than that for Gaussian kernel. In general, we observe that the tests based on distance covariance, Hilbert-Schmidt covariance with Gaussian kernel, and Hilbert-Schmidt covariance with Laplacian kernel, are all admissible, as none of them dominate the others in all situations. In the following example, we examine the afore-mentioned tests on a real data set.

**EXAMPLE 3.4.** *We consider the Earthquake data set, which is originally from the Northern California Earthquake Data Center and has classes of positive and negative major earthquake events. There are 368 negative and 93 positive cases and each data point is of length 512. This data set can be downloaded from UCR Time Series Classification Archive [Dau et al. (2018)]. Here we only consider the negative cases. Let  $Z_i = (z_{i,1}, z_{i,2}, \dots, z_{i,512})^T$  denote the record of a negative event, then set  $X_i = (z_{i,150-p+1}, \dots, z_{i,150})^T$  and  $Y_i = (z_{i,151}, \dots, z_{i,150+p})^T$ ,  $i = 1, \dots, 368$ . We apply all tests to test the independence between  $X_i$  and  $Y_i$ , which are expected to be dependent due to the serial nature of  $Z_i$ . For each  $p = 5, 30$  and  $n = 10, 30, 60$ , we randomly sample  $n$  rows from the full dataset  $(X_i, Y_i)_{i=1}^{368}$  without replacement and apply the afore-mentioned tests based on the subsample. Next, the above procedure is repeated 5000 times to calculate the power.*

The results are presented in Table 4. It can be seen that the powers of the marginal tests increase as the dimension grows, whereas the powers of all joint tests experience a decay as  $p$  grows and are nearly trivial when  $p = 30$ . This finding is consistent for all tests including hCov-based ones

TABLE 3  
Power comparison under  $H_{A_s}$  from Example 3.3

$n$	$p$	$\alpha$	dCov	mdCov	$T_{dCov}$	$T_{mdCov}$	Gaussian Kernel				Laplacian Kernel				
							hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	
(i)	10	5	0.010	0.044	0.196	0.055	0.218	0.042	0.348	0.052	0.367	0.074	0.672	0.098	0.685
	10	5	0.050	0.120	0.390	0.136	0.416	0.114	0.582	0.129	0.604	0.183	0.859	0.209	0.870
	10	5	0.100	0.201	0.542	0.209	0.546	0.191	0.722	0.197	0.731	0.292	0.927	0.304	0.931
	10	30	0.010	0.018	0.212	0.014	0.194	0.017	0.387	0.014	0.362	0.022	0.722	0.017	0.706
	10	30	0.050	0.066	0.434	0.064	0.428	0.066	0.627	0.064	0.625	0.075	0.892	0.077	0.891
	10	30	0.100	0.123	0.571	0.121	0.568	0.123	0.749	0.119	0.750	0.135	0.944	0.132	0.946
	30	5	0.010	0.158	0.988	0.197	0.996	0.136	1	0.163	1	0.486	1	0.555	1
	30	5	0.050	0.341	1.000	0.369	1	0.303	1	0.328	1	0.725	1	0.756	1
	30	5	0.100	0.483	1	0.488	1	0.433	1	0.444	1	0.838	1	0.846	1
	30	30	0.010	0.026	0.996	0.023	0.996	0.027	1.000	0.022	1.000	0.043	1	0.038	1
	30	30	0.050	0.089	1.000	0.084	0.999	0.088	1	0.083	1	0.123	1	0.125	1
	30	30	0.100	0.153	1.000	0.152	1.000	0.151	1	0.152	1	0.209	1	0.204	1
	60	5	0.010	0.559	1	0.637	1	0.461	1	0.539	1	0.989	1	0.996	1
	60	5	0.050	0.816	1	0.847	1	0.738	1	0.774	1	1.000	1	1	1
	60	5	0.100	0.916	1	0.925	1	0.861	1	0.870	1	1	1	1	1
	60	30	0.010	0.037	1	0.032	1	0.036	1	0.031	1	0.091	1	0.085	1
	60	30	0.050	0.125	1	0.119	1	0.122	1	0.115	1	0.231	1	0.228	1
	60	30	0.100	0.208	1	0.207	1	0.204	1	0.202	1	0.350	1	0.346	1
(ii)	10	5	0.010	0.044	0.217	0.059	0.242	0.040	0.393	0.055	0.413	0.077	0.713	0.106	0.732
	10	5	0.050	0.124	0.432	0.141	0.453	0.117	0.637	0.131	0.655	0.202	0.886	0.224	0.895
	10	5	0.100	0.210	0.577	0.213	0.583	0.196	0.771	0.204	0.775	0.304	0.942	0.318	0.942
	10	30	0.010	0.020	0.247	0.013	0.224	0.019	0.439	0.013	0.409	0.022	0.774	0.018	0.763
	10	30	0.050	0.064	0.474	0.064	0.474	0.063	0.677	0.063	0.676	0.075	0.913	0.076	0.913
	10	30	0.100	0.126	0.606	0.125	0.604	0.126	0.795	0.126	0.790	0.141	0.956	0.138	0.955
	30	5	0.010	0.178	0.995	0.221	0.999	0.148	1	0.186	1	0.544	1	0.608	1
	30	5	0.050	0.376	1	0.409	1	0.333	1	0.358	1	0.775	1	0.797	1
	30	5	0.100	0.518	1	0.526	1	0.468	1	0.478	1	0.871	1	0.880	1
	30	30	0.010	0.027	0.998	0.023	0.998	0.026	1.000	0.022	1	0.043	1	0.038	1
	30	30	0.050	0.088	1.000	0.087	1.000	0.088	1	0.086	1	0.128	1	0.128	1
	30	30	0.100	0.155	1.000	0.152	1.000	0.154	1	0.152	1	0.218	1	0.213	1
	60	5	0.010	0.632	1	0.709	1	0.526	1	0.609	1	0.995	1	0.999	1
	60	5	0.050	0.870	1	0.895	1	0.792	1	0.826	1	1	1	1	1
	60	5	0.100	0.946	1	0.952	1	0.904	1	0.911	1	1	1	1	1
	60	30	0.010	0.044	1	0.037	1	0.043	1	0.036	1	0.105	1	0.096	1
	60	30	0.050	0.126	1	0.125	1	0.123	1	0.121	1	0.251	1	0.244	1
	60	30	0.100	0.213	1	0.211	1	0.211	1	0.206	1	0.368	1	0.366	1
(iii)	10	5	0.010	0.019	0.024	0.023	0.028	0.017	0.033	0.022	0.040	0.023	0.090	0.029	0.095
	10	5	0.050	0.058	0.079	0.068	0.089	0.057	0.111	0.067	0.115	0.068	0.232	0.081	0.242
	10	5	0.100	0.113	0.148	0.117	0.151	0.114	0.194	0.118	0.196	0.124	0.351	0.129	0.355
	10	30	0.010	0.016	0.026	0.012	0.020	0.016	0.037	0.012	0.030	0.017	0.089	0.013	0.076
	10	30	0.050	0.059	0.086	0.057	0.083	0.060	0.112	0.058	0.105	0.061	0.233	0.060	0.225
	10	30	0.100	0.111	0.156	0.108	0.153	0.112	0.199	0.108	0.193	0.112	0.357	0.109	0.346
	30	5	0.010	0.019	0.051	0.021	0.068	0.017	0.141	0.021	0.170	0.026	0.673	0.032	0.724
	30	5	0.050	0.061	0.166	0.070	0.188	0.058	0.339	0.066	0.360	0.083	0.889	0.091	0.903
	30	5	0.100	0.117	0.283	0.117	0.288	0.117	0.488	0.116	0.497	0.153	0.953	0.153	0.955
	30	30	0.010	0.017	0.074	0.012	0.065	0.017	0.182	0.012	0.165	0.017	0.754	0.012	0.742
	30	30	0.050	0.061	0.202	0.058	0.198	0.061	0.378	0.059	0.373	0.063	0.913	0.061	0.913
	30	30	0.100	0.112	0.309	0.110	0.307	0.113	0.518	0.110	0.517	0.117	0.960	0.114	0.959
	60	5	0.010	0.019	0.174	0.024	0.219	0.017	0.580	0.022	0.666	0.034	1.000	0.041	1
	60	5	0.050	0.066	0.421	0.073	0.458	0.061	0.853	0.069	0.883	0.108	1	0.119	1
	60	5	0.100	0.123	0.600	0.128	0.612	0.119	0.941	0.122	0.949	0.179	1	0.183	1
	60	30	0.010	0.013	0.251	0.009	0.233	0.013	0.680	0.010	0.665	0.014	1.000	0.010	1
	60	30	0.050	0.053	0.485	0.051	0.484	0.052	0.869	0.050	0.871	0.056	1	0.055	1
	60	30	0.100	0.105	0.620	0.101	0.619	0.106	0.930	0.101	0.929	0.107	1	0.106	1

with Gaussian and Laplacian kernels. In addition, we also note that the marginal tests with Gaussian or Laplacian kernel have consistently higher power as compared to the Euclidean distance based tests.

TABLE 4  
*Power Comparison on Earthquake data*

$n$	$p$	$\alpha$	dCov	mdCov	$T_{dCov}$	$T_{mdCov}$	Gaussian Kernel				Laplacian Kernel			
							hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	hCov	mhCov	$T_{hCov}$	$T_{mhCov}$
10	5	0.010	0.021	0.054	0.041	0.079	0.021	0.851	0.038	0.883	0.035	0.937	0.060	0.952
10	5	0.050	0.070	0.144	0.085	0.160	0.065	0.927	0.080	0.937	0.091	0.975	0.112	0.979
10	5	0.100	0.120	0.235	0.126	0.230	0.114	0.956	0.117	0.959	0.155	0.985	0.160	0.985
10	30	0.010	0.012	0.218	0.013	0.226	0.012	1.000	0.012	1.000	0.013	1	0.016	1
10	30	0.050	0.046	0.412	0.047	0.421	0.046	1.000	0.046	1.000	0.050	1	0.054	1
10	30	0.100	0.095	0.537	0.093	0.541	0.096	1	0.095	1	0.094	1	0.091	1
30	5	0.010	0.034	0.155	0.055	0.196	0.026	1	0.042	1	0.078	1	0.124	1
30	5	0.050	0.106	0.333	0.128	0.356	0.082	1	0.096	1	0.188	1	0.210	1
30	5	0.100	0.177	0.460	0.183	0.461	0.139	1	0.146	1	0.278	1	0.273	1
30	30	0.010	0.009	0.936	0.009	0.941	0.009	1	0.009	1	0.011	1	0.012	1
30	30	0.050	0.040	0.977	0.041	0.976	0.043	1	0.043	1	0.040	1	0.041	1
30	30	0.100	0.081	0.988	0.080	0.988	0.086	1	0.085	1	0.085	1	0.082	1
60	5	0.010	0.060	0.473	0.086	0.549	0.034	1	0.050	1	0.171	1	0.245	1
60	5	0.050	0.147	0.722	0.171	0.749	0.096	1	0.107	1	0.341	1	0.370	1
60	5	0.100	0.240	0.835	0.244	0.838	0.162	1	0.167	1	0.457	1	0.458	1
60	30	0.010	0.006	1	0.006	1	0.006	1	0.006	1	0.008	1	0.008	1
60	30	0.050	0.030	1	0.031	1	0.032	1	0.031	1	0.033	1	0.034	1
60	30	0.100	0.066	1	0.065	1	0.068	1	0.070	1	0.067	1	0.066	1

**4. Conclusion.** In this article, we investigate the behavior of the distance covariance and Hilbert-Schmidt covariance in the high dimensional setting. We discover that the standard distance covariance and Hilbert-Schmidt covariance, which are well-known to capture nonlinear dependence in low/fixed dimensional context, can only capture linear componentwise cross-dependence (to the first order) in the high-dimensional environment. We believe that this is a new finding that may have significant implications to the design of tests for independence for high dimensional data. On one hand, we reveal the limitation of distance covariance and variants in the high dimensional context, and suggest to use marginally aggregated (sample) distance covariance as a way out, where the latter targets the low dimensional nonlinear dependence. On the other hand, we speculate whether it is possible to capture all kinds of dependence between high dimensional vectors  $X$  and  $Y$ , in a limited sample size framework. If the sample size is fixed, we would conjecture that an omnibus test does not exist; If the sample size can grow faster than the dimension, it seems possible but unclear to us how to develop an omnibus test in an asymptotic sense. We hope the results presented in this paper shed some light on the challenges in the high dimensional dependence testing and will motivate more work in this area.

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## SUPPLEMENTARY MATERIAL

### Supplement to: “Distance-based and RKHS-based Dependence Metrics in High Dimension”

( ). This supplement contains (1) some theoretical results derived under the high dimension and medium sample size setting, where the sample size is also allowed to grow as the dimension grows, albeit at a slower rate; (2) additional simulation examples, and comparisons with five nonparametric dependence tests that are not covered by our kernel class; (3) proof details for all theory presented in the paper.

### References.

- AHN, J., MARRON, J., MULLER, K. M. and CHI, Y.-Y. (2007). The high-dimension, low-sample-size geometric representation holds under mild conditions. *Biometrika* **94** 760–766.
- AOSHIMA, M., SHEN, D., SHEN, H., YATA, K., ZHOU, Y.-H. and MARRON, J. (2018). A survey of high dimension low sample size asymptotics. *Australian & New Zealand Journal of Statistics* **60** 4–19.
- BEDO, J. (2008). Microarray design using the Hilbert–Schmidt independence criterion. In *IAPR International Conference on Pattern Recognition in Bioinformatics* 288–298. Springer.
- BERGSMA, W. and DASSIOS, A. (2014). A consistent test of independence based on a sign covariance related to Kendalls tau. *Bernoulli* **20** 1006–1028.
- BERRETT, T. B. and SAMWORTH, R. J. (2019). Nonparametric independence testing via mutual information. *Biometrika* **106** 547–566.
- BLUM, J. R., KIEFER, J. and ROSENBLATT, M. (1961). Distribution free tests of independence based on the sample distribution function. *The Annals of Mathematical Statistics* 485–498.
- BRADLEY, R. C. (2007). *Introduction to Strong Mixing Conditions, Volume 1*. Kendrick Press, Heber City, Utah.
- CHAKRABORTY, S. and ZHANG, X. (2018). Distance metrics for measuring joint dependence with application to causal inference. *Arxiv*: <https://arxiv.org/abs/1711.09179>.
- CHAKRABORTY, S. and ZHANG, X. (2019). A New Framework for Distance and Kernel-based Metrics in High Dimensions. <https://arxiv.org/abs/1909.13469>.
- CSÖRGŐ, S. (1985). Testing for independence by the empirical characteristic function. *Journal of Multivariate Analysis* **16** 290–299.
- DASGUPTA, A. (2008). *Asymptotic Theory of Statistics and Probability*. Springer Texts in Statistics. Springer New York.
- DAU, H. A., KEOGH, E., KAMGAR, K., YEH, C.-C. M., ZHU, Y., GHARGHABI, S., RATANAMAHATANA, C. A., YANPING, HU, B., BEGUM, N., BAGNALL, A., MUEEN, A. and BATISTA, G. (2018). The UCR Time Series Classification Archive. [https://www.cs.ucr.edu/~eamonn/time\\_series\\_data\\_2018/](https://www.cs.ucr.edu/~eamonn/time_series_data_2018/).
- DAVIDSON, J. (1994). *Stochastic Limit Theory*. Oxford University Press.
- DE WET, T. (1980). Cramér–von Mises tests for independence. *Journal of Multivariate Analysis* **10** 38–50.

- DEHEUVELS, P. (1981). An asymptotic decomposition for multivariate distribution-free tests of independence. *Journal of Multivariate Analysis* **11** 102–113.
- DOUKHAN, P. and NEUMANN, M. H. (2008). The notion of  $\psi$ -weak dependence and its applications to bootstrapping time series. *Probability Surveys* **5** 146–168.
- DUECK, J., EDELMANN, D., GNEITING, T. and RICHARDS, D. (2014). The affinely invariant distance correlation. *Bernoulli* **20** 2305–2330.
- EDELMANN, D., RICHARDS, D. and VOGEL, D. (2017). The Distance Standard Deviation. *arXiv preprint arXiv:1705.05777*.
- FAN, J. and LV, J. (2008). Sure independence screening for ultrahigh dimensional feature space. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **70** 849–911.
- GALLANT, A. R. and WHITE, H. (1988). *A Unified Theory of Estimation and Inference for Nonlinear Dynamic Models*. Basil Blackwell.
- GIESER, P. W. and RANDLES, R. H. (1997). A nonparametric test of independence between two vectors. *Journal of the American Statistical Association* **92** 561–567.
- GRETTON, A., FUKUMIZU, K., TEO, C. H., SONG, L., SCHÖLKOPF, B. and SMOLA, A. J. (2008). A kernel statistical test of independence. In *Advances in Neural Information Processing Systems* 585–592.
- GRETTON, A., BORGWARDT, K. M., RASCH, M. J., SCHÖLKOPF, B. and SMOLA, A. (2012). A kernel two-sample test. *Journal of Machine Learning Research* **13** 723–773.
- HALL, P. and HEYDE, C. C. (2014). *Martingale limit theory and its application*. Academic press.
- HALL, P., MARRON, J. S. and NEEMAN, A. (2005). Geometric representation of high dimension, low sample size data. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **67** 427–444.
- HAN, F., CHEN, S. and LIU, H. (2017). Distribution-free tests of independence in high dimensions. *Biometrika* **104** 813–828.
- HELLER, R., HELLER, Y. and GORFINE, M. (2012). A consistent multivariate test of association based on ranks of distances. *Biometrika* **100** 503–510.
- HETTMANSPERGER, T. P. and OJA, H. (1994). Affine invariant multivariate multisample sign tests. *Journal of the Royal Statistical Society. Series B (Methodological)* 235–249.
- HOEFFDING, W. (1948). A non-parametric test of independence. *The Annals of Mathematical Statistics* 546–557.
- HUA, W.-Y. and GHOSH, D. (2015). Equivalence of kernel machine regression and kernel distance covariance for multidimensional phenotype association studies. *Biometrics* **71** 812–820.
- JUNG, S. and MARRON, J. S. (2009). PCA consistency in high dimension, low sample size context. *The Annals of Statistics* **37** 4104–4130.
- KONG, J., KLEIN, B. E., KLEIN, R., LEE, K. E. and WAHBA, G. (2012). Using distance correlation and SS-ANOVA to assess associations of familial relationships, lifestyle factors, diseases, and mortality. *Proceedings of the National Academy of Sciences* **109** 20352–20357.
- KROUPI, E., YAZDANI, A., VESIN, J.-M. and EBRAHIMI, T. (2012). Multivariate spectral analysis for identifying the brain activations during olfactory perception. In *2012 Annual International Conference of the IEEE Engineering in Medicine and Biology Society* 6172–6175. IEEE.
- KROUPI, E., YAZDANI, A., VESIN, J.-M. and EBRAHIMI, T. (2014). EEG correlates of pleasant and unpleasant odor perception. *ACM Transactions on Multimedia Computing, Communications, and Applications (TOMM)* **11** 13.
- LAFORGIA, A. and NATALINI, P. (2012). On the asymptotic expansion of a ratio of gamma

- functions. *Journal of Mathematical Analysis and Applications* **389** 833–837.
- LEUNG, D. and DRTON, M. (2018). Testing independence in high dimensions with sums of rank correlations. *The Annals of Statistics* **46** 280–307.
- LI, R., ZHONG, W. and ZHU, L. (2012). Feature screening via distance correlation learning. *Journal of the American Statistical Association* **107** 1129–1139.
- LYONS, R. (2013). Distance covariance in metric spaces. *The Annals of Probability* **41** 3284–3305.
- MATTESON, D. S. and TSAY, R. S. (2017). Independent component analysis via distance covariance. *Journal of the American Statistical Association* **112** 623–637.
- MIKALSEN, K. Ø., SOGUERO-RUIZ, C., BIANCHI, F. M. and JENSSEN, R. (2019). Noisy multi-label semi-supervised dimensionality reduction. *Pattern Recognition* **90** 257–270.
- PAN, G., GAO, J. and YANG, Y. (2014). Testing Independence Among a Large Number of High-Dimensional Random Vectors. *Journal of the American Statistical Association* **109** 600–612.
- PARK, T., SHAO, X. and YAO, S. (2015). Partial martingale difference correlation. *Electronic Journal of Statistics* **9** 1492–1517.
- RAMDAS, A., REDDI, S. J., PÓCZOS, B., SINGH, A. and WASSERMAN, L. (2015). On the decreasing power of kernel and distance based nonparametric hypothesis tests in high dimensions. In *Twenty-Ninth AAAI Conference on Artificial Intelligence*.
- SEJDINOVIC, D., SRIPERUMBUDUR, B., GRETTON, A. and FUKUMIZU, K. (2013). Equivalence of distance-based and RKHS-based statistics in hypothesis testing. *The Annals of Statistics* **41** 2263–2291.
- SHAO, X. and ZHANG, J. (2014). Martingale difference correlation and its use in high-dimensional variable screening. *Journal of the American Statistical Association* **109** 1302–1318.
- SHEN, C., PRIEBE, C. E. and VOGELSTEIN, J. T. (2018). From distance correlation to multiscale graph correlation. *Journal of the American Statistical Association* **just-accepted** 1–39.
- SINHA, B. K. and WIEAND, H. (1977). Multivariate nonparametric tests for independence. *Journal of Multivariate Analysis* **7** 572–583.
- SZEKELY, G. J. and RIZZO, M. L. (2004). Testing for equal distributions in high dimension. *InterStat* **5** 1–6.
- SZÉKELY, G. J., RIZZO, M. L. and BAKIROV, N. K. (2007). Measuring and testing dependence by correlation of distances. *The Annals of Statistics* **35** 2769–2794.
- SZÉKELY, G. J. and RIZZO, M. L. (2009). Brownian distance covariance. *The Annals of Applied Statistics* **3** 1236–1265.
- SZÉKELY, G. J. and RIZZO, M. L. (2013). The distance correlation  $t$ -test of independence in high dimension. *Journal of Multivariate Analysis* **117** 193–213.
- SZÉKELY, G. J. and RIZZO, M. L. (2014). Partial distance correlation with methods for dissimilarities. *The Annals of Statistics* **42** 2382–2412.
- TASKINEN, S., KANKAINEN, A. and OJA, H. (2003). Sign test of independence between two random vectors. *Statistics & Probability Letters* **62** 9–21.
- TRICOMI, F. and ERDÉLYI, A. (1951). The asymptotic expansion of a ratio of gamma functions. *Pacific Journal of Mathematics* **1** 133–142.
- WALCK, C. (1996). Hand-book on statistical distributions for experimentalists Technical Report.
- WEI, S., LEE, C., WICHERS, L. and MARRON, J. S. (2016). Direction-Projection-Permutation for High-Dimensional Hypothesis Tests. *Journal of Computational and Graphical Statistics* **25** 549–569.
- WU, W. B. (2005). Nonlinear system theory: another look at dependence. *Proceedings of*



- the National Academy of Sciences USA* **102** 14150–14154.
- XU, J., LIU, J., YIN, J. and SUN, C. (2016). A multi-label feature extraction algorithm via maximizing feature variance and feature-label dependence simultaneously. *Knowledge-Based Systems* **98** 172–184.
- YANG, Y. (2017). Source-Space Analyses in MEG/EEG and Applications to Explore Spatio-temporal Neural Dynamics in Human Vision, PhD thesis.
- YANG, Y. and PAN, G. (2015). Independence test for high dimensional data based on regularized canonical correlation coefficients. *Annals of Statistics* **43** 467–500.
- YAO, S., ZHANG, X. and SHAO, X. (2018). Testing mutual independence in high dimension via distance covariance. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* **80** 455–480.
- YATA, K. and AOSHIMA, M. (2010). Effective PCA for high-dimension, low-sample-size data with singular value decomposition of cross data matrix. *Journal of multivariate analysis* **101** 2060–2077.
- ZHANG, Y. and ZHOU, Z.-H. (2010). Multilabel dimensionality reduction via dependence maximization. *ACM Transactions on Knowledge Discovery from Data (TKDD)* **4** 14.
- ZHANG, X., YAO, S., SHAO, X. et al. (2018). Conditional mean and quantile dependence testing in high dimension. *The Annals of Statistics* **46** 219–246.
- ZHOU, Z. (2012). Measuring nonlinear dependence in time-series, a distance correlation approach. *Journal of Time Series Analysis* **33** 438–457.
- ZHU, C. and SHAO, X. (2019). Interpoint distance based two sample tests in high dimension. <https://arxiv.org/pdf/1902.07279.pdf>.
- ZHU, L., XU, K., LI, R. and ZHONG, W. (2017). Projection correlation between two random vectors. *Biometrika* **104** 829–843.

**SUPPLEMENT TO “DISTANCE-BASED AND  
RKHS-BASED DEPENDENCE METRICS IN HIGH  
DIMENSION”**

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The supplement is organized as follows. In Section [A](#), we present some corresponding theory under the framework where both sample size and the dimension grow. Section [B](#) contains two additional examples and some numerical comparisons with five recent nonparametric tests. All the technical details are gathered in Section [C](#).

APPENDIX A: HIGH DIMENSION MEDIUM SAMPLE SIZE

Another type of asymptotics closely related to HDLSS is the high dimension medium sample size (HDMSS) setting [[Aoshima et al. \(2018\)](#)], where  $p \wedge q \rightarrow \infty$  and  $n \rightarrow \infty$  at a slower rate comparing to  $p, q$ . The HDMSS setting has been studied by [Fan and Lv \(2008\)](#) and [Yata and Aoshima \(2010\)](#), among others.

From the previous sections, we know that the distance/Hilbert-Schmidt covariance can only detect linear dependencies between pair-wise components when  $p \wedge q \rightarrow \infty$  and  $n$  is fixed. In this section, we show that this surprising phenomenon still holds under the high dimension medium sample size setting. Consequently, a unified approach is used to show that  $T_R$  converges in distribution to standard normal under the null hypothesis, but the technical details of handling the leading term and controlling the remainder are totally different from the fixed  $n$  case.

**A.1. Distance Covariance and Variants.** We first state the following assumption which can be seen as an extension of Assumption [D2](#).

ASSUMPTION D4. Denote  $E[L_X(X, X')^2] = \alpha_p^2, E[L_Y(Y, Y')^2] = \beta_q^2, E[L_X(X, X')^4] = \gamma_p^2$  and  $E[L_Y(Y, Y')^4] = \lambda_q^2$ , where  $\alpha_p, \beta_q, \gamma_p, \lambda_q$  are sequences of numbers such that as  $n \wedge p \wedge q \rightarrow \infty$

$$n\alpha_p = o(1), n\beta_q = o(1), \\ \tau_X^2(\alpha_p\gamma_p + \gamma_p^2) = o(1), \tau_Y^2(\beta_q\lambda_q + \lambda_q^2) = o(1), \tau(\alpha_p\lambda_q + \gamma_p\beta_q + \gamma_p\lambda_q) = o(1).$$

REMARK A.1.1. For the  $m$ -dependence structure, i.e.,  $x_i \perp x_j$  if  $|i-j| > m$  and  $y_{i'} \perp y_{j'}$  if  $|i'-j'| > m'$ , where  $\sup_i \mathbb{E}(x_i^8) < \infty$  and  $\sup_i \mathbb{E}(y_i^8) < \infty$ , we can show that  $\alpha_p = O(\sqrt{m/p})$ ,  $\beta_q = O(\sqrt{m'/q})$ ,  $\gamma_p = O(m/p)$  and  $\lambda_q = O(m'/q)$ . Thus, Assumption D4 holds under the  $m$ -dependence model if  $n$  and  $m, m'$  satisfies

$$\begin{aligned} n^2 m &= o(p), & n^2 m' &= o(q), \\ m^3 &= o(p), & m'^3 &= o(q), & m' m^2 &= o(p), & m m'^2 &= o(q). \end{aligned}$$

The following theorem shows that the decomposition property (7) for distance covariance still holds under high dimension medium sample size setting.

THEOREM A.1.1. Under Assumption D1, we can show that

(i)

$$(9) \quad \text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n.$$

Here  $\text{cov}_n^2$  is defined the same as in Theorem 2.1.1 and  $\mathcal{R}_n$  is the remainder term.

(ii) Further suppose Assumption D4 holds. Then we have

$$\begin{aligned} \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) &= O_p(\tau \alpha_p \beta_q), \\ \mathcal{R}_n &= O_p(\tau \alpha_p \lambda_q + \tau \gamma_p \beta_q + \tau \gamma_p \lambda_q) = o_p(1). \end{aligned}$$

Similarly, as shown in the following, hCov also has the decomposition property under HDMSS.

THEOREM A.1.2. Under Assumption D1, we have

(i)

$$(10) \quad \begin{aligned} &\tau \times \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) \\ &= f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_X}{\gamma_X} \frac{\tau_Y}{\gamma_Y} \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n, \end{aligned}$$

where  $\text{cov}_n^2$  is defined the same as in Theorem 2.1.1 and  $\mathcal{R}_n$  is the remainder term.

(ii) Further suppose Assumption [D4](#) holds. Then

$$\begin{aligned} f^{(1)}\left(\frac{\tau_X}{\gamma_X}\right) g^{(1)}\left(\frac{\tau_Y}{\gamma_Y}\right) \frac{\tau_X}{\gamma_X} \frac{\tau_Y}{\gamma_Y} &\asymp_p 1, \\ \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) &= O_p(\tau \alpha_p \beta_q), \\ \mathcal{R}_n &= O_p(\tau \alpha_p \lambda_q + \tau \gamma_p \beta_q + \tau \gamma_p \lambda_q) = o_p(1). \end{aligned}$$

From Equations [\(9\)](#) and [\(10\)](#), we can see that under the HDMSS setting, it is still true that distance/Hilbert-Schmidt covariance can only detect the linear dependence between the components of  $X$  and  $Y$ .

**A.2. Studentized Test Statistics.** Similar to Section [2.2](#), we provide a unified approach to analyze the studentized dCov, hCov, mdCov. Since now the sample size is growing, the element-wise argument used to prove the results in Section [2.2](#) will no longer work. Inspired by [Zhang et al. \(2018\)](#) and [Yao, Zhang and Shao \(2018\)](#), we derive the asymptotic distribution by constructing a martingale sequence and using martingale CLT.

**A.2.1. Unified Approach.** For notational convenience, we first define the following metrics,

$$U(X_s, X_t) := \frac{1}{\sqrt{p}} \sum_{i=1}^p k_{st}(i), \quad V(Y_s, Y_t) := \frac{1}{\sqrt{q}} \sum_{i=1}^q l_{st}(i),$$

where  $k_{st}(i)$  and  $l_{st}(i)$  are defined in Section [2.2.1](#). To show that the studentized test statistic converges to standard normal, we essentially use the martingale CLT [[Hall and Heyde \(2014\)](#)] and the following assumptions are used to guarantee the conditions in martingale CLT.

ASSUMPTION D5.

$$(11) \quad \frac{\mathbb{E}[U(X, X')^4]}{\sqrt{n}(\mathbb{E}[U(X, X')^2])^2} \rightarrow 0,$$

$$(12) \quad \frac{\mathbb{E}[U(X, X')U(X', X'')U(X'', X''')U(X''', X)]}{(\mathbb{E}[U(X, X')^2])^2} \rightarrow 0,$$

and similar assumptions hold for  $Y$ .

REMARK A.2.1. When  $k(x, y) = l(x, y) = |x - y|$ , Assumption [D5](#) has been studied in Propositions [2.1](#) and [2.2](#) of [Zhang et al. \(2018\)](#).

REMARK A.2.2. When  $k(x, y) = l(x, y) = |x - y|^2$ , Equations (11) and (12) can be simplified to

$$\frac{\sum_{i,j,r,w=1}^p \mathbb{E}^2 [(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j])(x_r - \mathbb{E}[x_r])(x_w - \mathbb{E}[x_w])] }{\sqrt{n} \text{Tr}^2(\Sigma_X^2)} \rightarrow 0,$$

$$\frac{\text{Tr}(\Sigma_X^4)}{\text{Tr}^2(\Sigma_X^2)} \rightarrow 0, \quad \text{where } \Sigma_X = \text{cov}(X, X).$$

Notice that  $\text{Tr}(\Sigma_X^2) = \sum_{i=1}^p \sum_{j=1}^p \text{cov}^2(x_i, x_j)$ . Consider the  $m$ -dependence model in Remark A.1.1. Assuming  $\sup_i \mathbb{E}(x_i^4) < \infty$ , we have  $\text{Tr}(\Sigma_X^4) = O(m^3 p)$  and

$$\sum_{i,j,r,w=1}^p \mathbb{E}^2 [(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j])(x_r - \mathbb{E}[x_r])(x_w - \mathbb{E}[x_w])] = O(m^2 p^2).$$

Consequently, it can be seen that the  $m$ -dependence model in Remark A.1.1 also satisfies Equations (11) and (12) by controlling the orders of  $n, m, m'$ .

Then, we can show that the normalized  $\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})$  converges to standard normal distribution under the high dimension medium sample size regime.

THEOREM A.2.1. Let  $n \wedge p \wedge q \rightarrow \infty$ . Under  $H_0$  and Assumption D5, we have

$$\sqrt{\binom{n}{2}} \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\mathcal{S}} \xrightarrow{d} N(0, 1), \quad \text{where } \mathcal{S}^2 = \mathbb{E}[U(X, X')^2] \mathbb{E}[V(Y, Y')^2].$$

Consequently, we have the following result.

PROPOSITION A.2.1. Let  $n \wedge p \wedge q \rightarrow \infty$ . Under  $H_0$  and Assumption D5, we have

$$T_u \xrightarrow{d} N(0, 1).$$

A.2.2. *Studentized Tests.* The following result shows that as  $n \wedge p \wedge q \rightarrow \infty$ , scaled dCov, hCov and mdCov are all equal to uCov up to an asymptotically constant factor.

PROPOSITION A.2.2. Under Assumption D1,

(i) When  $k(x, y) = l(x, y) = |x - y|^2$ ,

$$\begin{aligned} \text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) &= \frac{1}{4} \frac{\sqrt{pq}}{\tau} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) + \mathcal{R}'_n, \\ \tau \times \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) &= \frac{\sqrt{pq}}{4\gamma_{\mathbf{X}}\gamma_{\mathbf{Y}}} f^{(1)}\left(\frac{\tau_{\mathbf{X}}}{\gamma_{\mathbf{X}}}\right) g^{(1)}\left(\frac{\tau_{\mathbf{Y}}}{\gamma_{\mathbf{Y}}}\right) \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) + \mathcal{R}''_n, \end{aligned}$$

where  $\mathcal{R}'_n, \mathcal{R}''_n$  are the remainder terms. Further suppose Assumption [D4](#) holds. Then

$$\begin{aligned} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &= O_p(\tau\alpha_p\beta_q), \\ \mathcal{R}'_n &= O_p(\tau\alpha_p\lambda_q + \tau\gamma_p\beta_q + \tau\gamma_p\lambda_q) = o_p(1), \\ \mathcal{R}''_n &= O_p(\tau\alpha_p\lambda_q + \tau\gamma_p\beta_q + \tau\gamma_p\lambda_q) = o_p(1). \end{aligned}$$

(ii) When  $k(x, y) = l(x, y) = |x - y|$ ,

$$\text{mdCov}_n^2(\mathbf{X}, \mathbf{Y}) = \sqrt{pq} \sqrt{\binom{n}{2}} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}).$$

Finally, by adopting a unified approach, we have the following Corollary.

**COROLLARY A.2.1.** *Let  $n \wedge p \wedge q \rightarrow \infty$ . Under  $H_0$  and Assumption [D5](#), we have*

(i)

$$T_{\text{mdCov}} \xrightarrow{d} N(0, 1).$$

(ii) Further suppose Assumption [D4](#) and

$$(13) \quad \frac{n}{\sqrt{\frac{1}{p}\text{Tr}(\boldsymbol{\Sigma}_{\mathbf{X}}^2)\frac{1}{q}\text{Tr}(\boldsymbol{\Sigma}_{\mathbf{Y}}^2)}} \tau(\alpha_p\lambda_q + \gamma_p\beta_q + \gamma_p\lambda_q) = o(1).$$

Then, for each  $R \in \{\text{dCov}, \text{hCov}\}$ , we have

$$T_R \xrightarrow{d} N(0, 1).$$

**REMARK A.2.3.** *The  $m$ -dependence model in Remark [A.1.1](#) can also satisfy Equation (13) by controlling the orders of  $n, m, m'$  based on the magnitude of  $\text{Tr}(\boldsymbol{\Sigma}_{\mathbf{X}}^2)/p$  and  $\text{Tr}(\boldsymbol{\Sigma}_{\mathbf{Y}}^2)/q$ .*

APPENDIX B: ADDITIONAL SIMULATION EXAMPLES AND  
COMPARISONS

The asymptotic validity of our  $t$ -tests depend on the weak dependence assumption among the components of  $X$  and  $Y$ . In the following, we conduct some sensitivity analysis and examine a few cases where the weak dependence assumption is violated.

EXAMPLE B.1. *Generate i.i.d. samples from the following models for  $i = 1, \dots, n$ .*

- (i) *Let ARFIMA( $\phi, d, 0$ ) denotes the autoregressive fractionally integrated moving average (ARFIMA) model with autoregressive order 1 parameter  $\phi$ , moving average parameter 0 and fractional differencing parameter  $d$ ,  $X_i = (x_{i1}, \dots, x_{ip})^T \sim \text{ARFIMA}(0.5, d, 0)$  and  $Y_i = (y_{i1}, \dots, y_{ip})^T \sim \text{ARFIMA}(0.5, d, 0)$ .*
- (ii) *We consider the compound symmetric covariance structure, i.e., let*

$$\Sigma_d = (0.5 + 0.5\mathbb{I}_{\{i=j\}})_{i,j=1}^d \quad \text{and} \quad \Sigma = \begin{pmatrix} \mathbf{I}_{\lfloor p/d \rfloor} \otimes \Sigma_d & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{p - \lfloor p/d \rfloor \times d} \end{pmatrix},$$

where  $\otimes$  is the Kronecker product. Then,  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \Sigma)$  and  $Y_i = (y_{i1}, \dots, y_{ip})^T \sim N(\mathbf{0}, \Sigma)$ .

- (iii) *Let  $X_i = (x_{i1}, \dots, x_{ip})^T \sim N(\mathbf{0}, \Sigma)$  and  $Y_i = (y_{i1}, \dots, y_{ip})^T \sim N(\mathbf{0}, \Sigma)$ , where*

$$\Sigma_d = (0.5 + 0.5\mathbb{I}_{\{i=j\}})_{i,j=1}^d \quad \text{and} \quad \Sigma = \begin{pmatrix} \Sigma_d & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{p-d} \end{pmatrix}.$$

In Example B.1 (i), as  $d$  increases from 0 to 0.45, the dependence among components become stronger. The weak dependence assumptions, i.e. Assumptions D2 and D3, are not expected to hold, thus the limiting null distribution of our test statistics may not be  $t$ -distribution. The results in Table 5 show there is a mild size distortion and the approximation by  $t$ -distribution might still work in this case. For Example B.1 (ii) and (iii), the larger  $d$  is, the more dependence there are in the components. For relatively large  $d$ , i.e.,  $d = 30$  in Example B.1 (ii) & (iii), some of the  $t$ -tests have size over 0.07, showing the impact of strong componentwise dependence. In general, the magnitude of distortion is moderate under all examples in B.1.

Notice that under the high dimensional case, the ‘‘joint’’ tests can be seen as the aggregation of component-wise sample squared covariances. On the other hand, the ‘‘marginal’’ tests are the accumulation of component-wise sample distance/Hilbert-Schmidt covariances. When  $(X, Y)$  are generated

TABLE 5  
*Size comparison from Example B.1*

$d$	$n$	dCov	mdCov	$T_{dCov}$	$T_{mdCov}$	Gaussian Kernel				Laplacian Kernel				
						hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	
	0	10	0.057	0.059	0.059	0.058	0.058	0.053	0.059	0.051	0.056	0.055	0.058	0.051
	0.050	10	0.057	0.058	0.058	0.059	0.056	0.053	0.059	0.054	0.055	0.054	0.057	0.051
	0.100	10	0.055	0.058	0.058	0.060	0.056	0.053	0.058	0.055	0.055	0.052	0.057	0.049
	0.150	10	0.056	0.057	0.058	0.059	0.055	0.054	0.057	0.051	0.053	0.051	0.056	0.050
	0.200	10	0.054	0.055	0.058	0.062	0.055	0.052	0.057	0.055	0.053	0.052	0.057	0.054
	0.250	10	0.053	0.055	0.059	0.059	0.053	0.052	0.057	0.054	0.054	0.053	0.059	0.058
	0.350	10	0.054	0.055	0.063	0.061	0.053	0.056	0.063	0.057	0.053	0.058	0.062	0.061
	0.450	10	0.058	0.054	0.066	0.060	0.056	0.053	0.066	0.059	0.056	0.052	0.061	0.058
(i)	0	30	0.055	0.052	0.058	0.052	0.055	0.053	0.059	0.054	0.058	0.049	0.061	0.049
	0.050	30	0.054	0.051	0.059	0.051	0.054	0.052	0.058	0.052	0.058	0.052	0.059	0.049
	0.100	30	0.053	0.049	0.060	0.052	0.055	0.052	0.059	0.051	0.056	0.049	0.059	0.047
	0.150	30	0.055	0.049	0.059	0.055	0.055	0.050	0.059	0.054	0.055	0.048	0.059	0.049
	0.200	30	0.055	0.050	0.058	0.057	0.055	0.048	0.058	0.054	0.054	0.051	0.058	0.048
	0.250	30	0.054	0.051	0.060	0.059	0.053	0.052	0.058	0.054	0.054	0.056	0.059	0.057
	0.350	30	0.052	0.052	0.057	0.058	0.053	0.051	0.059	0.056	0.054	0.057	0.062	0.058
	0.450	30	0.053	0.052	0.062	0.061	0.052	0.055	0.061	0.059	0.054	0.057	0.060	0.059
	2	10	0.056	0.056	0.054	0.056	0.055	0.058	0.053	0.056	0.057	0.056	0.053	0.051
	3	10	0.055	0.056	0.056	0.054	0.055	0.052	0.057	0.051	0.056	0.055	0.056	0.054
	5	10	0.060	0.058	0.063	0.059	0.060	0.052	0.064	0.052	0.059	0.054	0.062	0.051
	6	10	0.058	0.052	0.062	0.057	0.055	0.059	0.061	0.059	0.056	0.059	0.062	0.058
	10	10	0.055	0.055	0.064	0.064	0.057	0.059	0.065	0.061	0.058	0.060	0.064	0.060
	15	10	0.054	0.051	0.065	0.062	0.054	0.050	0.065	0.059	0.055	0.050	0.065	0.057
	30	10	0.056	0.053	0.075	0.072	0.056	0.054	0.074	0.069	0.053	0.055	0.073	0.068
(ii)	2	30	0.056	0.054	0.055	0.054	0.056	0.059	0.055	0.057	0.056	0.057	0.055	0.055
	3	30	0.056	0.057	0.057	0.058	0.056	0.053	0.057	0.053	0.056	0.055	0.059	0.052
	5	30	0.055	0.056	0.059	0.055	0.057	0.054	0.059	0.055	0.059	0.050	0.061	0.050
	6	30	0.051	0.053	0.056	0.054	0.052	0.051	0.055	0.051	0.053	0.051	0.056	0.051
	10	30	0.057	0.052	0.066	0.060	0.057	0.051	0.065	0.060	0.056	0.053	0.064	0.054
	15	30	0.050	0.051	0.064	0.064	0.050	0.051	0.063	0.059	0.054	0.050	0.064	0.059
	30	30	0.053	0.054	0.067	0.069	0.054	0.053	0.068	0.065	0.052	0.052	0.065	0.062
	2	10	0.057	0.056	0.056	0.055	0.057	0.058	0.055	0.056	0.055	0.055	0.055	0.051
	6	10	0.058	0.055	0.057	0.054	0.057	0.054	0.057	0.052	0.057	0.052	0.058	0.049
	10	10	0.057	0.060	0.062	0.061	0.057	0.058	0.062	0.059	0.057	0.057	0.061	0.059
	14	10	0.060	0.056	0.063	0.061	0.060	0.058	0.062	0.061	0.056	0.059	0.062	0.056
	18	10	0.055	0.053	0.067	0.064	0.056	0.053	0.067	0.060	0.059	0.052	0.068	0.057
	24	10	0.051	0.052	0.067	0.065	0.051	0.053	0.065	0.063	0.054	0.053	0.068	0.062
	30	10	0.056	0.053	0.075	0.072	0.056	0.054	0.074	0.069	0.053	0.055	0.073	0.068
(iii)	2	30	0.049	0.054	0.048	0.052	0.050	0.056	0.048	0.053	0.050	0.056	0.049	0.053
	6	30	0.049	0.050	0.048	0.050	0.048	0.055	0.047	0.055	0.048	0.057	0.049	0.055
	10	30	0.050	0.053	0.052	0.057	0.049	0.052	0.051	0.054	0.047	0.053	0.050	0.051
	14	30	0.052	0.054	0.058	0.059	0.049	0.050	0.056	0.059	0.049	0.053	0.056	0.054
	18	30	0.053	0.055	0.062	0.061	0.054	0.053	0.062	0.058	0.054	0.051	0.059	0.054
	24	30	0.044	0.046	0.055	0.060	0.046	0.048	0.055	0.060	0.046	0.047	0.056	0.055
	30	30	0.053	0.054	0.067	0.069	0.054	0.053	0.068	0.065	0.052	0.052	0.065	0.062



from the model in Proposition 2.2.5, it is expected that there is power loss for mdCov and mhCov based permutation test comparing to dCov and hCov based permutation tests and similar phenomenon is expected for mdCov and mhCov based  $t$ -tests comparing to dCov and hCov based  $t$ -tests. The following example demonstrates this phenomenon.

EXAMPLE B.2. *Generate i.i.d. samples from the following models for  $i = 1, \dots, n$ .*

(i) *Let  $\rho = 0.5$ ,*

$$\begin{aligned} Z_i &= (z_{i1}, \dots, z_{ip}) \sim N(\mathbf{0}, \mathbf{I}_p), \\ X_i &= (x_{i1}, \dots, x_{ip}) \sim N(\mathbf{0}, \mathbf{I}_p), \\ Y_i &= \frac{\rho X_i + (1-\rho)Z_i}{\sqrt{\rho^2 + (1-\rho)^2}}. \end{aligned}$$

(ii) *Let  $\rho = 0.7$  and  $(X_i, Y_i, Z_i)$  be defined in the same way as in (i).*

(iii) *Let  $\rho = 0.5$  and  $\otimes$  denote the Kronecker product. Define*

$$\begin{aligned} Z_i &= (z_{i1}, \dots, z_{ip}) \sim N(\mathbf{0}, \mathbf{I}_p), \\ X_i &= (x_{i1}, \dots, x_{ip}) \sim N(\mathbf{0}, \mathbf{I}_p), \\ Y_i &= \frac{\rho \Sigma X_i + (1-\rho)Z_i}{\sqrt{\rho^2 + (1-\rho)^2}}, \end{aligned}$$

where  $\Sigma = \mathbf{I} \otimes \mathbf{A}$  and  $\mathbf{A}$  is an orthogonal matrix defined as

$$\mathbf{A} = \begin{pmatrix} 0 & \sqrt{\frac{1}{4}} & \sqrt{\frac{1}{5}} & -\sqrt{\frac{1}{4}} & -\sqrt{\frac{3}{10}} \\ \sqrt{\frac{1}{6}} & \sqrt{\frac{1}{4}} & \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{4}} & \sqrt{\frac{2}{15}} \\ -\sqrt{\frac{2}{3}} & 0 & \sqrt{\frac{1}{5}} & 0 & \sqrt{\frac{2}{15}} \\ \sqrt{\frac{1}{6}} & -\sqrt{\frac{1}{4}} & \sqrt{\frac{1}{5}} & -\sqrt{\frac{1}{4}} & \sqrt{\frac{2}{15}} \\ 0 & -\sqrt{\frac{1}{4}} & \sqrt{\frac{1}{5}} & \sqrt{\frac{1}{4}} & -\sqrt{\frac{3}{10}} \end{pmatrix}.$$

From Table 6, we can see that there is indeed a power loss for the “marginal” tests compared to the “joint” tests, but the loss of power appears fairly moderate, which is consistent with our theory. For Example B.2, it can also be observed that the power decrease for the Hilbert-Schmidt covariance based tests is a bit more than the power decrease of distance covariance based tests. Moreover, the power drop is slightly smaller for Gaussian kernel comparing with Laplacian kernel.

We also compare the marginal distance/Hilbert-Schmidt covariance based statistics with five recently proposed nonparametric tests, namely Heller-Heller-Gorfine test (HHG) [Heller, Heller and Gorfine (2012)], Projection

TABLE 6  
*Power comparison from Example B.2*

$n$	$p$	$\alpha$	dCov	mdCov	$T_{dCov}$	$T_{mdCov}$	Gaussian Kernel				Laplacian Kernel			
							hCov	mhCov	$T_{hCov}$	$T_{mhCov}$	hCov	mhCov	$T_{hCov}$	$T_{mhCov}$
10	5	0.010	0.635	0.560	0.691	0.597	0.629	0.371	0.685	0.392	0.516	0.237	0.585	0.246
10	5	0.050	0.833	0.774	0.855	0.792	0.825	0.598	0.849	0.610	0.741	0.450	0.772	0.458
10	5	0.100	0.910	0.861	0.914	0.867	0.906	0.717	0.912	0.721	0.839	0.581	0.851	0.586
10	30	0.010	0.795	0.654	0.788	0.634	0.796	0.410	0.787	0.379	0.769	0.247	0.762	0.219
10	30	0.050	0.936	0.849	0.937	0.851	0.935	0.648	0.937	0.644	0.921	0.468	0.924	0.460
10	30	0.100	0.970	0.914	0.970	0.916	0.970	0.767	0.970	0.768	0.963	0.604	0.964	0.603
30	5	0.010	1	1	1	1	1	0.999	1	0.998	1	0.980	1	0.982
30	5	0.050	1	1	1	1	1	1.000	1	1.000	1	0.996	1	0.996
30	5	0.100	1	1	1	1	1	1.000	1	1.000	1	0.998	1	0.998
30	30	0.010	1	1	1	1	1	1	1	1	1	0.996	1	0.996
30	30	0.050	1	1	1	1	1	1	1	1	1	0.999	1	0.999
30	30	0.100	1	1	1	1	1	1	1	1	1	1.000	1	1.000
60	5	0.010	1	1	1	1	1	1	1	1	1	1	1	1
60	5	0.050	1	1	1	1	1	1	1	1	1	1	1	1
60	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.010	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.050	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.100	1	1	1	1	1	1	1	1	1	1	1	1
10	5	0.010	1.000	0.999	1.000	0.999	1.000	0.986	1.000	0.989	0.997	0.935	0.999	0.942
10	5	0.050	1.000	1.000	1.000	1.000	1.000	0.997	1.000	0.997	0.999	0.983	1.000	0.983
10	5	0.100	1.000	1.000	1.000	1.000	1.000	0.999	1.000	0.999	1.000	0.992	1.000	0.993
10	30	0.010	1	1	1	1.000	1	0.998	1	0.998	1	0.973	1	0.970
10	30	0.050	1	1	1	1	1	1.000	1	1.000	1	0.995	1	0.995
10	30	0.100	1	1	1	1	1	1.000	1	1.000	1	0.997	1	0.997
30	5	0.010	1	1	1	1	1	1	1	1	1	1	1	1
30	5	0.050	1	1	1	1	1	1	1	1	1	1	1	1
30	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1
30	30	0.010	1	1	1	1	1	1	1	1	1	1	1	1
30	30	0.050	1	1	1	1	1	1	1	1	1	1	1	1
30	30	0.100	1	1	1	1	1	1	1	1	1	1	1	1
60	5	0.010	1	1	1	1	1	1	1	1	1	1	1	1
60	5	0.050	1	1	1	1	1	1	1	1	1	1	1	1
60	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.010	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.050	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.100	1	1	1	1	1	1	1	1	1	1	1	1
10	5	0.010	0.635	0.497	0.685	0.537	0.633	0.238	0.681	0.260	0.525	0.138	0.584	0.135
10	5	0.050	0.831	0.728	0.848	0.748	0.824	0.460	0.844	0.477	0.740	0.311	0.768	0.323
10	5	0.100	0.903	0.830	0.911	0.835	0.899	0.597	0.905	0.604	0.835	0.440	0.844	0.446
10	30	0.010	0.790	0.583	0.784	0.555	0.789	0.273	0.785	0.247	0.763	0.147	0.761	0.122
10	30	0.050	0.928	0.800	0.930	0.797	0.928	0.490	0.930	0.486	0.915	0.331	0.919	0.324
10	30	0.100	0.966	0.888	0.964	0.889	0.965	0.628	0.964	0.626	0.960	0.460	0.957	0.453
30	5	0.010	1	1.000	1	1	1	0.985	1	0.989	1.000	0.890	1.000	0.898
30	5	0.050	1	1	1	1	1	0.996	1	0.997	1	0.971	1	0.971
30	5	0.100	1	1	1	1	1	0.999	1	0.999	1	0.984	1	0.984
30	30	0.010	1	1	1	1	1	0.998	1	0.999	1	0.950	1	0.948
30	30	0.050	1	1	1	1	1	1.000	1	1.000	1	0.990	1	0.990
30	30	0.100	1	1	1	1	1	1.000	1	1.000	1	0.997	1	0.997
60	5	0.010	1	1	1	1	1	1	1	1	1	1.000	1	1
60	5	0.050	1	1	1	1	1	1	1	1	1	1	1	1
60	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.010	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.050	1	1	1	1	1	1	1	1	1	1	1	1
60	30	0.100	1	1	1	1	1	1	1	1	1	1	1	1

Correlation (PCOR) [Zhu et al. (2017)], Multiscale Graph Correlation (MGC) [Shen, Priebe and Vogelstein (2018)], Kendall's tau ( $R_\tau$ ) [Han, Chen and Liu (2017)] and Spearman's rho ( $R_\rho$ ) [Han, Chen and Liu (2017)]. We want to remark that Han, Chen and Liu (2017) aim to test the mutual independence among the components of  $X$  based on a random sample  $\{X_i\}_{i=1}^n$ , whereas we test the independence of  $X$  and  $Y$  based on paired high dimensional samples  $\{(X_i, Y_i)\}_{i=1}^n$ . Thus, the asymptotic theory in Han, Chen and Liu (2017) is not directly applicable to our setting. To circumvent the difficulty, we shall apply a simple permutation procedure to the following test statistics  $R_\tau$  and  $R_\rho$ , where

$$R_\rho = \max_{j=1}^p \max_{k=1}^q \rho_{j,k}^2 \quad \text{and} \quad R_\tau = \max_{j=1}^p \max_{k=1}^q \tau_{j,k}^2,$$

where  $\rho_{j,k}$  is the Spearman's  $\rho$  and  $\tau_{j,k}$  is the Kendall's tau between component samples  $\mathcal{X}_j$  and  $\mathcal{Y}_k$  respectively. Let  $Q_{ni}^j$  and  $Q_{ni}^k$  be the ranks of  $x_{i,j}$  and  $x_{i,k}$  among  $\{x_{1,j}, \dots, x_{n,j}\}$  and  $\{x_{1,k}, \dots, x_{n,k}\}$  respectively,  $\rho_{j,k}$  and  $\tau_{j,k}$  are formally defined as

$$\rho_{j,k} = \frac{\sum_{i=1}^n (Q_{ni}^j - \bar{Q}_n^j)(Q_{ni}^k - \bar{Q}_n^k)}{\{\sum_{i=1}^n (Q_{ni}^j - \bar{Q}_n^j)^2 \sum_{i=1}^n (Q_{ni}^k - \bar{Q}_n^k)^2\}^{1/2}},$$

$$\tau_{j,k} = \frac{2}{n(n-1)} \sum_{1 \leq i < i' \leq n} \text{sign}(x_{i',j} - x_{i,j}) \text{sign}(y_{i',k} - y_{i,k}).$$

From Table 7, the sizes for all three tests appear very accurate due to the use of permutation-based critical values except for the two rank-correlation based tests at small sample size  $n = 10$ . Comparing Table 6 to Table 8, we can see that the performance of dCov/hCov based tests (except for Laplacian kernel) are comparable to PCOR and MGC, which outperform all other tests (HHG,  $R_\tau$ ,  $R_\rho$ ). The power of  $R_\tau$  and  $R_\rho$  are almost trivial in the case of Example B.2 (iii).

A comparison of Table 9 with Table 2 (Table 10 with Table 3) shows that the mdCov/mhCov based statistics have superior power compared with HHG, PCOR, MGC,  $R_\rho$  and  $R_\tau$  for Example 3.2 (iii) and Example 3.3 (i) & (ii). In addition, HHG, PCOR and MGC all experience a power drop as the dimension grows. For Example 3.2 (i) & (ii), MGC and PCOR have a noticeable power drop for higher dimensional case, while HHG performs comparably with marginal distance/Hilbert-Schmidt covariance based statistics. Next, for Example 3.3 (iii), mhCov based statistics have better power than HHG, PCOR and MGC, while the performance of mdCov based statistics and HHG are similar. In addition, for Example 3.2 (i) & (ii) and Example 3.3 (iii),  $R_\rho$  and  $R_\tau$  experience low power.

Finally, the experimental results of these five tests on the Earthquake data are shown in Table 11, from which we can observe that HHG, PCOR and MGC all suffer substantial power drop as the dimension increases, while the tests  $R_\rho$  and  $R_\tau$  exhibit higher power with increasing dimension. Overall, HHG, PCOR and MGC exhibit similar phenomenon as what we observed for distance/Hilbert-Schmidt covariance applied to the whole components jointly and their ability of detecting nonlinear dependence gets compromised as the dimension grows with a fixed sample size. As for  $R_\rho$  and  $R_\tau$ , although they do not seem to suffer from high dimensionality, these two tests have little power for detecting some none-monotone dependence due to their rank-based nature. The class of kernels we consider, however, does not include any of these five tests, so a rigorous theoretical justification for these five tests would be interesting and merits future investigation.

TABLE 7  
Size comparison from Example 3.1

$n$	$p$	$\alpha$	(i)					(ii)					(iii)				
			HHG	PCOR	MGC	$R_\rho$	$R_\tau$	HHG	PCOR	MGC	$R_\rho$	$R_\tau$	HHG	PCOR	MGC	$R_\rho$	$R_\tau$
10	5	0.010	0.008	0.012	0.008	0.014	0.011	0.008	0.010	0.009	0.012	0.010	0.008	0.009	0.008	0.014	0.011
10	5	0.050	0.048	0.052	0.054	0.051	0.039	0.052	0.048	0.053	0.045	0.04	0.044	0.050	0.051	0.049	0.041
10	5	0.100	0.095	0.104	0.099	0.092	0.074	0.104	0.100	0.097	0.089	0.072	0.095	0.106	0.099	0.096	0.079
10	30	0.010	0.011	0.011	0.010	0.007	0.005	0.009	0.011	0.010	0.006	0.005	0.010	0.008	0.007	0.009	0.007
10	30	0.050	0.047	0.049	0.053	0.036	0.030	0.045	0.056	0.058	0.039	0.033	0.050	0.046	0.049	0.037	0.034
10	30	0.100	0.098	0.099	0.096	0.075	0.047	0.096	0.109	0.105	0.079	0.051	0.100	0.102	0.094	0.078	0.053
30	5	0.010	0.007	0.010	0.010	0.013	0.012	0.008	0.005	0.008	0.015	0.016	0.008	0.009	0.009	0.016	0.013
30	5	0.050	0.044	0.048	0.055	0.054	0.048	0.048	0.041	0.048	0.055	0.052	0.044	0.045	0.051	0.055	0.052
30	5	0.100	0.098	0.104	0.099	0.105	0.102	0.095	0.099	0.090	0.102	0.097	0.095	0.100	0.095	0.105	0.107
30	30	0.010	0.009	0.008	0.007	0.013	0.010	0.008	0.011	0.011	0.016	0.016	0.011	0.010	0.011	0.016	0.013
30	30	0.050	0.047	0.048	0.054	0.050	0.050	0.042	0.057	0.061	0.056	0.053	0.049	0.051	0.058	0.053	0.051
30	30	0.100	0.096	0.099	0.091	0.097	0.097	0.095	0.110	0.104	0.101	0.101	0.095	0.103	0.099	0.104	0.098
60	5	0.010	0.008	0.011	0.010	0.016	0.016	0.011	0.009	0.009	0.017	0.016	0.011	0.008	0.009	0.016	0.015
60	5	0.050	0.050	0.047	0.051	0.056	0.056	0.054	0.048	0.052	0.056	0.056	0.046	0.047	0.051	0.054	0.055
60	5	0.100	0.101	0.105	0.100	0.107	0.102	0.112	0.101	0.098	0.103	0.101	0.095	0.098	0.093	0.101	0.102
60	30	0.010	0.011	0.013	0.007	0.016	0.016	0.009	0.008	0.012	0.014	0.015	0.008	0.012	0.010	0.014	0.014
60	30	0.050	0.048	0.055	0.057	0.054	0.056	0.047	0.049	0.056	0.055	0.052	0.047	0.054	0.056	0.057	0.055
60	30	0.100	0.092	0.112	0.104	0.106	0.105	0.100	0.108	0.106	0.105	0.102	0.096	0.101	0.097	0.107	0.11

TABLE 8  
Power comparison from Example B.2

$n$	$p$	$\alpha$	(i)					(ii)					(iii)				
			HHG	PCOR	MGC	$R_\rho$	$R_\tau$	HHG	PCOR	MGC	$R_\rho$	$R_\tau$	HHG	PCOR	MGC	$R_\rho$	$R_\tau$
10	5	0.010	0.350	0.614	0.266	0.311	0.27	0.994	1.000	0.711	0.945	0.928	0.358	0.613	0.277	0.062	0.049
10	5	0.050	0.580	0.844	0.847	0.622	0.572	0.999	1.000	0.987	0.998	0.995	0.573	0.840	0.842	0.199	0.161
10	5	0.100	0.681	0.917	0.929	0.787	0.742	1.000	1	0.998	1	1	0.674	0.916	0.922	0.334	0.288
10	30	0.010	0.395	0.749	0.341	0.114	0.098	0.998	1	0.674	0.850	0.808	0.367	0.751	0.348	0.017	0.013
10	30	0.050	0.622	0.934	0.917	0.336	0.302	0.999	1	0.968	0.994	0.984	0.615	0.925	0.916	0.068	0.060
10	30	0.100	0.724	0.973	0.974	0.516	0.406	1	1	0.991	0.999	0.998	0.717	0.967	0.967	0.138	0.094
30	5	0.010	0.999	1	0.992	1	1	1	1	1	1	1	0.998	1	0.994	0.438	0.429
30	5	0.050	1	1	1	1	1	1	1	1	1	1	1.000	1	1	0.771	0.756
30	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1	1	0.902	0.893
30	30	0.010	1	1	0.966	1	1	1	1	0.997	1	1	1	1	0.967	0.268	0.257
30	30	0.050	1	1	1	1	1	1	1	1.000	1	1	1	1	1	0.563	0.553
30	30	0.100	1	1	1	1	1	1	1	1	1	1	1	1	1	0.748	0.734
60	5	0.010	1	1	1	1	1	1	1	1	1	1	1	1	1	0.927	0.924
60	5	0.050	1	1	1	1	1	1	1	1	1	1	1	1	1	0.995	0.996
60	5	0.100	1	1	1	1	1	1	1	1	1	1	1	1	1	0.999	1
60	30	0.010	1	1	1	1	1	1	1	1	1	1	1	1	1	0.893	0.899
60	30	0.050	1	1	1	1	1	1	1	1	1	1	1	1	1	0.994	0.992
60	30	0.100	1	1	1	1	1	1	1	1	1	1	1	1	1	0.999	0.999

TABLE 9  
Power comparison from Example 3.2

n	p	α	(i)						(ii)						(iii)					
			HHG	PCOR	MGC	R <sub>ρ</sub>	R <sub>τ</sub>	HHG	PCOR	MGC	R <sub>ρ</sub>	R <sub>τ</sub>	HHG	PCOR	MGC	R <sub>ρ</sub>	R <sub>τ</sub>			
10	5	0.010	0.403	0.075	0.200	0.076	0.092	0.591	0.107	0.256	0.068	0.080	0.032	0.027	0.052	0.076	0.092			
10	5	0.050	0.643	0.187	0.430	0.132	0.169	0.814	0.240	0.525	0.128	0.153	0.113	0.108	0.141	0.132	0.169			
10	5	0.100	0.742	0.280	0.516	0.200	0.238	0.879	0.346	0.606	0.190	0.211	0.191	0.188	0.208	0.200	0.238			
10	30	0.010	0.185	0.021	0.072	0.124	0.135	0.377	0.044	0.140	0.112	0.117	0.011	0.009	0.013	0.124	0.135			
10	30	0.050	0.423	0.082	0.265	0.218	0.236	0.627	0.139	0.391	0.186	0.196	0.052	0.055	0.067	0.218	0.236			
10	30	0.100	0.534	0.146	0.354	0.275	0.292	0.730	0.216	0.491	0.235	0.239	0.106	0.115	0.118	0.275	0.292			
30	5	0.010	1	0.266	0.961	0.056	0.133	1	0.433	0.992	0.047	0.107	0.282	0.080	0.613	0.056	0.133			
30	5	0.050	1	0.510	0.999	0.127	0.230	1	0.774	1	0.110	0.185	0.587	0.266	0.791	0.127	0.230			
30	5	0.100	1	0.643	0.999	0.196	0.308	1	0.901	1	0.170	0.249	0.720	0.419	0.806	0.196	0.308			
30	30	0.010	0.984	0.048	0.323	0.055	0.190	0.999	0.129	0.658	0.053	0.157	0.010	0.013	0.051	0.055	0.190			
30	30	0.050	0.997	0.135	0.767	0.135	0.332	1	0.278	0.974	0.122	0.259	0.069	0.072	0.134	0.135	0.332			
30	30	0.100	0.999	0.222	0.792	0.207	0.425	1	0.392	0.979	0.192	0.340	0.130	0.133	0.186	0.207	0.425			
60	5	0.010	1	0.781	1	0.056	0.140	1	0.993	1	0.043	0.106	0.862	0.338	0.999	0.056	0.140			
60	5	0.050	1	0.955	1	0.123	0.248	1	1	1	0.104	0.196	0.985	0.676	1	0.123	0.248			
60	5	0.100	1	0.988	1	0.198	0.330	1	1	1	0.161	0.258	0.995	0.828	1	0.198	0.330			
60	30	0.010	1	0.081	0.826	0.043	0.203	1	0.316	0.991	0.043	0.161	0.018	0.019	0.171	0.043	0.203			
60	30	0.050	1	0.212	0.999	0.109	0.333	1	0.562	1	0.114	0.263	0.095	0.093	0.409	0.109	0.333			
60	30	0.100	1	0.324	1.000	0.176	0.427	1	0.689	1	0.178	0.350	0.188	0.165	0.434	0.176	0.427			

TABLE 10  
Power comparison from Example 3.3

n	p	α	(i)						(ii)						(iii)					
			HHG	PCOR	MGC	R <sub>ρ</sub>	R <sub>τ</sub>	HHG	PCOR	MGC	R <sub>ρ</sub>	R <sub>τ</sub>	HHG	PCOR	MGC	R <sub>ρ</sub>	R <sub>τ</sub>			
10	5	0.010	0.077	0.028	0.067	0.076	0.093	0.080	0.030	0.073	0.047	0.053	0.010	0.010	0.015	0.011	0.008			
10	5	0.050	0.199	0.107	0.163	0.142	0.181	0.202	0.109	0.168	0.096	0.11	0.054	0.048	0.056	0.038	0.034			
10	5	0.100	0.292	0.194	0.236	0.210	0.250	0.294	0.196	0.238	0.154	0.171	0.117	0.107	0.096	0.078	0.064			
10	30	0.010	0.020	0.013	0.022	0.134	0.151	0.021	0.011	0.023	0.065	0.071	0.012	0.011	0.011	0.012	0.010			
10	30	0.050	0.080	0.059	0.085	0.222	0.241	0.079	0.056	0.089	0.129	0.132	0.062	0.055	0.052	0.041	0.037			
10	30	0.100	0.143	0.118	0.142	0.271	0.293	0.138	0.123	0.146	0.178	0.173	0.125	0.111	0.093	0.079	0.056			
30	5	0.010	0.728	0.101	0.737	0.055	0.128	0.737	0.112	0.768	0.027	0.052	0.034	0.008	0.034	0.009	0.011			
30	5	0.050	0.893	0.270	0.825	0.125	0.234	0.891	0.301	0.854	0.078	0.114	0.172	0.053	0.070	0.04	0.037			
30	5	0.100	0.935	0.413	0.838	0.193	0.314	0.938	0.445	0.862	0.135	0.180	0.305	0.107	0.109	0.078	0.074			
30	30	0.010	0.198	0.016	0.083	0.054	0.191	0.186	0.016	0.093	0.024	0.066	0.093	0.011	0.011	0.015	0.015			
30	30	0.050	0.371	0.072	0.165	0.122	0.323	0.364	0.074	0.179	0.076	0.139	0.232	0.053	0.052	0.052	0.052			
30	30	0.100	0.482	0.141	0.216	0.188	0.411	0.478	0.140	0.226	0.135	0.202	0.337	0.112	0.094	0.104	0.096			
60	5	0.010	0.999	0.349	1	0.049	0.143	0.999	0.401	1	0.024	0.041	0.263	0.010	0.073	0.013	0.011			
60	5	0.050	1	0.680	1	0.124	0.25	1.000	0.734	1	0.075	0.102	0.633	0.053	0.109	0.041	0.045			
60	5	0.100	1	0.836	1	0.198	0.332	1	0.871	1	0.13	0.155	0.793	0.117	0.146	0.079	0.078			
60	30	0.010	0.758	0.019	0.338	0.049	0.217	0.730	0.022	0.366	0.024	0.045	0.487	0.009	0.012	0.015	0.014			
60	30	0.050	0.882	0.095	0.471	0.116	0.354	0.873	0.098	0.511	0.074	0.108	0.706	0.047	0.046	0.052	0.050			
60	30	0.100	0.925	0.173	0.494	0.19	0.442	0.915	0.179	0.530	0.123	0.173	0.801	0.105	0.088	0.099	0.097			

APPENDIX C: TECHNICAL DETAILS

C.1. Proof of Proposition 2.1.1.

PROOF. Denote  $f^{(2)}(t) = -\frac{1}{4}(1+t)^{-\frac{3}{2}}$ . The remainder term can be written as

$$R_X(X_s, X_t) = \int_0^1 \int_0^1 v f^{(2)}(uvL_X(X_s, X_t)) dudv \times (L_X(X_s, X_t))^2.$$

Set  $\varphi(x) = \int_0^1 \int_0^1 v f^{(2)}(uvx) dudv$ . Then  $\varphi(x)$  is continuous at 0. Next, by the continuous mapping theorem, we have

$$\int_0^1 \int_0^1 v f^{(2)}(uvL_X(X_s, X_t)) dudv \xrightarrow{P} \int_0^1 \int_0^1 v f^{(2)}(0) dudv.$$

TABLE 11  
Power Comparison on Earthquake data

$n$	$p$	$\alpha$	HHG	PCOR	MGC	$R_p$	$R_r$
10	5	0.010	0.067	0.085	0.032	0.791	0.874
10	5	0.050	0.169	0.179	0.102	0.873	0.958
10	5	0.100	0.236	0.256	0.156	0.914	0.983
10	30	0.010	0.008	0.009	0.007	1	1
10	30	0.050	0.050	0.043	0.050	1	1
10	30	0.100	0.097	0.094	0.090	1	1
30	5	0.010	0.333	0.413	0.136	0.922	1.000
30	5	0.050	0.548	0.570	0.313	0.983	1
30	5	0.100	0.638	0.657	0.350	0.994	1
30	30	0.010	0.009	0.007	0.015	1	1
30	30	0.050	0.048	0.038	0.050	1	1
30	30	0.100	0.100	0.088	0.088	1	1
60	5	0.010	0.725	0.812	0.427	0.997	1
60	5	0.050	0.906	0.903	0.750	1	1
60	5	0.100	0.945	0.936	0.779	1	1
60	30	0.010	0.005	0.003	0.017	1	1
60	30	0.050	0.037	0.027	0.056	1	1
60	30	0.100	0.077	0.069	0.085	1	1

So,  $R_X(X_s, X_t) \asymp_p (L_X(X_s, X_t))^2$ . Similar arguments hold for  $R_Y(Y_s, Y_t)$ .  $\square$

### C.2. Proof of Remark 2.1.1.

PROOF. Denote  $\mathbf{C} = (c_{ij}) = \mathbf{A}^T \mathbf{A} \in \mathbb{R}^{s_1 \times s_1}$ . We obtain that

$$\begin{aligned}
\text{var}[L(X, X')] &= \frac{\text{var}[(U - U')^T \mathbf{A}^T \mathbf{A} (U - U')]}{4\text{tr}^2(\mathbf{A}\mathbf{A}^T)} \\
&= \frac{\text{var}\left[\sum_{i=1}^{s_1} \sum_{j=1}^{s_1} c_{ij} (u_i - u'_i)(u_j - u'_j)\right]}{4\text{tr}^2(\mathbf{A}\mathbf{A}^T)} \\
&\leq \frac{\sum_{i=1}^{s_1} \sum_{j=1}^{s_1} c_{ij}^2 \text{var}[(u_i - u'_i)(u_j - u'_j)]}{\text{tr}^2(\mathbf{A}\mathbf{A}^T)} \\
&\leq \frac{C \sum_{i=1}^{s_1} \sum_{j=1}^{s_1} c_{ij}^2}{\text{tr}^2(\mathbf{A}\mathbf{A}^T)} \\
&= \frac{C \text{tr}(\mathbf{A}^T \mathbf{A} \mathbf{A}^T \mathbf{A})}{\text{tr}^2(\mathbf{A}\mathbf{A}^T)} = O(p^{-1})
\end{aligned}$$

for some constant  $C > 0$ , where we have used the fact that the fourth moment of  $u_i$  is uniformly bounded. It follows that  $a_p = 1/\sqrt{p}$ .  $\square$

### C.3. Proof of Theorem 2.1.1.

PROOF. (i) Recall that  $\text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = (\tilde{\mathbf{A}} \cdot \tilde{\mathbf{B}})$ . For any matrix  $\mathbf{A}$ , the matrix  $\mathbf{A}_{-D}$  is just  $\mathbf{A}$  with its diagonal elements setting to be 0. Using the

expansion for  $a_{st}$  in Proposition 2.1.1, we have

$$\frac{1}{\tau_X} \tilde{\mathbf{A}} = (\widetilde{\mathbf{1}_{n \times n}})_{-D} + \frac{1}{2} \tilde{\mathbf{L}}_X + \tilde{\mathbf{R}}_X = \frac{1}{2} \tilde{\mathbf{L}}_X + \tilde{\mathbf{R}}_X,$$

where  $\mathbf{L}_X = ((L_X(X_s, X_t))_{s,t=1}^n)_{-D}$  and  $\mathbf{R}_X = ((R_X(X_s, X_t))_{s,t=1}^n)_{-D}$ . Similarly,  $\frac{1}{\tau_Y} \tilde{\mathbf{B}} = \frac{1}{2} \tilde{\mathbf{L}}_Y + \tilde{\mathbf{R}}_Y$ . Then, we have

$$\begin{aligned} \frac{\text{dCov}_n^2(\mathbf{X}, \mathbf{Y})}{\tau} &= \left( \left( \frac{1}{2} \tilde{\mathbf{L}}_X + \tilde{\mathbf{R}}_X \right) \cdot \left( \frac{1}{2} \tilde{\mathbf{L}}_Y + \tilde{\mathbf{R}}_Y \right) \right) \\ &= \frac{1}{4} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y) + \frac{1}{2} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) + \frac{1}{2} (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) + (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y). \end{aligned}$$

Let  $R_n = \frac{1}{2} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) + \frac{1}{2} (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) + (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y)$ . We show that  $\frac{1}{4} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y)$  can be written as sum of sample component-wise cross-covariances up to a constant factor in the following Lemma.

LEMMA 1.

$$\frac{1}{4} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y) = \frac{1}{\tau^2} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(x_i, y_j).$$

PROOF. By Lemma A.1. of Park, Shao and Yao (2015), since all diagonal entries of distance matrices  $\mathbf{A}$  and  $\mathbf{B}$  are equal to 0, we have  $(\tilde{\mathbf{A}} \cdot \tilde{\mathbf{B}}) = (\mathbf{A} \cdot \tilde{\tilde{\mathbf{B}}})$ . Then, it can be directly verified that for any  $1 \leq s, t \leq n$ ,  $\sum_{u=1}^n \tilde{b}_{ut} = \sum_{v=1}^n \tilde{b}_{sv} = 0$  and it further implies that  $\tilde{\tilde{\mathbf{B}}} = \tilde{\mathbf{B}}$ . Direct calculation shows that

$$\begin{aligned} (14) \quad (\tilde{\mathbf{A}} \cdot \tilde{\mathbf{B}}) &= (\mathbf{A} \cdot \tilde{\mathbf{B}}) = \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} a_{st} b_{st} \\ &\quad + \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in \mathbf{i}_4^n} a_{st} b_{uv} - \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in \mathbf{i}_3^n} a_{st} b_{su}, \end{aligned}$$

where  $\mathbf{i}_m^n$  denotes the set of all  $m$ -tuples drawn without replacement from  $\{1, 2, \dots, n\}$ . Equation (14) can be used as equivalent definition of the sample distance covariance. Notice that

$$\tilde{\mathbf{L}}_X = \tilde{\mathbf{D}}_X - (\widetilde{\mathbf{1}_{n \times n}})_{-D} = \tilde{\mathbf{D}}_X,$$

where  $\mathbf{D}_X = \frac{1}{\tau_X^2} ((|X_s - X_t|^2)_{s,t=1}^n)_{-D}$ . Similarly,  $\tilde{\mathbf{L}}_Y = \tilde{\mathbf{D}}_Y$ . Next, it can be verified directly that for any vector  $\mathbf{a} \in \mathbf{R}^n$ ,

$$(\widetilde{\mathbf{a} \mathbf{1}_n^T})_{-D} + (\widetilde{\mathbf{1}_n \mathbf{a}})_{-D} = 0.$$

Using this fact, we then can further decompose  $\tilde{\mathbf{D}}_X$  as follows,

$$\tilde{\mathbf{D}}_X = \tilde{\mathbf{D}}_{X,1} + \tilde{\mathbf{D}}_{X,2} + \tilde{\mathbf{D}}_{X,3} = \tilde{\mathbf{D}}_{X,2},$$

where  $\mathbf{D}_{X,1} = \frac{1}{\tau_X^2}((X_s^T X_s)_{s,t=1}^n)_{-D}$ ,  $\mathbf{D}_{X,2} = -2\frac{1}{\tau_X^2}((X_s^T X_t)_{s,t=1}^n)_{-D}$  and  $\mathbf{D}_{X,3} = \frac{1}{\tau_X^2}((X_t^T X_t)_{s,t=1}^n)_{-D}$ . Similarly,  $\tilde{\mathbf{D}}_Y = \tilde{\mathbf{D}}_{Y,2}$ . Next, using Equation (14), we have

$$\begin{aligned} & \tau^2 \times (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y) \\ &= \tau^2 \times (\tilde{\mathbf{D}}_{X,2} \cdot \tilde{\mathbf{D}}_{Y,2}) \\ &= 4 \left\{ \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in i_2^n} X_s^T X_t Y_s^T Y_t + \right. \\ & \quad \left. \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in i_4^n} X_s^T X_t Y_u^T Y_v - \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in i_3^n} X_s^T X_t Y_s^T Y_u \right\} \\ &= 4 \sum_{i=1}^p \sum_{j=1}^q \left\{ \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in i_2^n} x_{si} x_{ti} y_{sj} y_{tj} + \right. \\ & \quad \left. \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in i_4^n} x_{si} x_{ti} y_{uj} y_{vj} - \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in i_3^n} x_{si} x_{ti} y_{sj} y_{uj} \right\} \\ &= 4 \sum_{i=1}^p \sum_{j=1}^q \left\{ \frac{1}{\binom{n}{4}} \sum_{k < l < s < t} \frac{1}{4!} \sum_{*}^{(k,l,s,t)} \frac{(x_{ki} - x_{li})(y_{kj} - y_{lj})(x_{si} - x_{ti})(y_{sj} - y_{tj})}{4} \right\} \\ &= 4 \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j). \end{aligned}$$

□

Therefore, by Lemma 1, we have the following decomposition,

$$\text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n,$$

where  $\mathcal{R}_n = \tau R_n$ .

(ii) Note  $L_X(X_s, X_t) = O_p(a_p) = o_p(1)$  and  $L_Y(Y_s, Y_t) = O_p(b_q) = o_p(1)$  for  $s \neq t \in \{1, \dots, n\}$ . We can then apply Proposition 2.1.1, obtain that  $R_X(X_s, X_t) = O_p(L_X(X_s, X_t)^2)$  and  $R_Y(Y_s, Y_t) = O_p(L_Y(Y_s, Y_t)^2)$ . For the



leading term  $\tau(\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y)$ , it can be easily seen from Equation (14) that  $(\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y) = O_p(a_p b_q)$ . Similarly, for the remainder terms,  $(\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) = O_p(a_p b_q^2)$ ,  $(\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) = O_p(a_p^2 b_q)$  and  $(\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y) = O_p(a_p^2 b_q^2)$ . Thus, we have  $R_n = O_p(a_p^2 b_q + a_p b_q^2)$  and  $\mathcal{R}_n = \tau R_n = O_p(\tau a_p^2 b_q + \tau a_p b_q^2) = o_p(1)$ . Therefore the remainder terms are negligible comparing to the leading term.  $\square$

#### C.4. Proof of Theorem 2.1.2.

PROOF. (i) We first show that  $\gamma_{\mathbf{X}}$  is asymptotically equal to  $\tau_X$  (similar result applies to  $\gamma_{\mathbf{Y}}$  and  $\tau_Y$ ). Recall that for all  $s \neq t$ ,

$$L_X(X_s, X_t) = \frac{|X_s - X_t|^2 - \tau_X^2}{\tau_X^2}.$$

Since  $L_X(X_s, X_t) = O_p(a_p) = o_p(1)$ , we have  $\frac{|X_s - X_t|^2}{\tau_X^2} \xrightarrow{p} 1$ . Then

$$\frac{\text{median}\{|X_s - X_t|^2\}}{\tau_X^2} \xrightarrow{p} 1$$

and thus

$$\frac{\tau_X}{\gamma_{\mathbf{X}}} = \sqrt{\frac{\tau_X^2}{\text{median}\{|X_i - X_j|^2\}}} \xrightarrow{p} 1.$$

Similar arguments can also be used to show that  $\frac{\tau_Y}{\gamma_{\mathbf{Y}}} \xrightarrow{p} 1$ . Next, under Proposition 2.1.1, we can deduce that

$$\begin{aligned} & f\left(\frac{|X_s - X_t|}{\gamma_{\mathbf{X}}}\right) \\ &= f\left(\frac{|X_s - X_t|}{\tau_X} \frac{\tau_X}{\gamma_{\mathbf{X}}}\right) \\ &= f\left(\left\{1 + \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t)\right\} \frac{\tau_X}{\gamma_{\mathbf{X}}}\right) \\ &= f\left(\frac{\tau_X}{\gamma_{\mathbf{X}}}\right) + f^{(1)}\left(\frac{\tau_X}{\gamma_{\mathbf{X}}}\right) \left\{\frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t)\right\} \frac{\tau_X}{\gamma_{\mathbf{X}}} + R_f(X_s, X_t), \end{aligned}$$

where  $R_f(X_s, X_t)$  is the remainder term. Similarly,

$$\begin{aligned} g\left(\frac{|Y_s - Y_t|}{\gamma_{\mathbf{Y}}}\right) &= g\left(\frac{\tau_Y}{\gamma_{\mathbf{Y}}}\right) + \\ & g^{(1)}\left(\frac{\tau_Y}{\gamma_{\mathbf{Y}}}\right) \left\{\frac{L_Y(Y_s, Y_t)}{2} + R_Y(Y_s, Y_t)\right\} \frac{\tau_Y}{\gamma_{\mathbf{Y}}} + R_g(Y_s, Y_t). \end{aligned}$$

Similar to the proof of Theorem 2.1.1,

$$\begin{aligned} \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) &= (\tilde{\mathbf{R}} \cdot \tilde{\mathbf{H}}) \\ &= \frac{1}{4} f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_X}{\gamma_X} \frac{\tau_Y}{\gamma_Y} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y) + \frac{1}{2} f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) \frac{\tau_X}{\gamma_X} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) \\ &\quad + \frac{1}{2} g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_Y}{\gamma_Y} (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) + (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y), \end{aligned}$$

where  $\mathbf{L}_X = ((L_X(X_s, X_t))_{s,t=1}^n)_{-D}$ ,  $\mathbf{L}_Y = ((L_Y(Y_s, Y_t))_{s,t=1}^n)_{-D}$  and

$$\begin{aligned} \mathbf{R}_X &= \left( \left( f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) \frac{\tau_X}{\gamma_X} R_X(X_s, X_t) + R_f(X_s, X_t) \right)_{s,t=1}^n \right)_{-D}, \\ \mathbf{R}_Y &= \left( \left( g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_Y}{\gamma_Y} R_Y(Y_s, Y_t) + R_g(Y_s, Y_t) \right)_{s,t=1}^n \right)_{-D}. \end{aligned}$$

Denote  $R_n = \frac{1}{2} f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) \frac{\tau_X}{\gamma_X} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) + \frac{1}{2} g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_Y}{\gamma_Y} (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) + (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y)$  and  $\mathcal{R}_n = \tau R_n$ . By Lemma 1, we have

$$\begin{aligned} \tau \times \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) &= \\ &= f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_X}{\gamma_X} \frac{\tau_Y}{\gamma_Y} \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n. \end{aligned}$$

(ii) We present the following lemma which would be useful in subsequent arguments.

LEMMA 2. *Suppose  $f^{(2)}$  and  $g^{(2)}$  are continuous on some open interval containing 1. Then under the assumptions of Theorem 2.1.2,*

$$R_f(X_s, X_t) = O_p(L_X(X_s, X_t)^2), \quad R_g(Y_s, Y_t) = O_p(L_Y(Y_s, Y_t)^2).$$

PROOF. The remainder term can be written as

$$\begin{aligned} (15) \quad R_f(X_s, X_t) &= \\ &= \int_0^1 \int_0^1 v f^{(2)} \left( \frac{\tau_X}{\gamma_X} + uv \left\{ \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t) \right\} \frac{\tau_X}{\gamma_X} \right) dudv \\ &\quad \times \left( \frac{\tau_X}{\gamma_X} \right)^2 \left( \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t) \right)^2. \end{aligned}$$

Set  $\varphi(x, y) = \int_0^1 \int_0^1 v f^{(2)}(x + uv y) dudv$ . Then  $\varphi(x, y)$  is continuous at  $(1, 0)$ . By the continuous mapping theorem, we have

$$\begin{aligned} \int_0^1 \int_0^1 v f^{(2)} \left( \frac{\tau_X}{\gamma_{\mathbf{X}}} + uv \left\{ \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t) \right\} \frac{\tau_X}{\gamma_{\mathbf{X}}} \right) dudv \\ \xrightarrow{p} \int_0^1 \int_0^1 v f^{(2)}(1) dudv. \end{aligned}$$

So  $R_f(X_s, X_t) = O_p(1) \left( \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t) \right)^2 = O_p(L_X(X_s, X_t)^2)$ . Similar argument holds for  $R_g(Y_s, Y_t)$ .  $\square$

Both the Gaussian and Laplacian kernel have continuous second order derivatives. From Lemma 2, we know

$$\begin{aligned} f^{(1)} \left( \frac{\tau_X}{\gamma_{\mathbf{X}}} \right) \frac{\tau_X}{\gamma_{\mathbf{X}}} R_X(X_s, X_t) + R_f(X_s, X_t) &= O_p(L_X(X_s, X_t)^2), \\ g^{(1)} \left( \frac{\tau_Y}{\gamma_{\mathbf{Y}}} \right) \frac{\tau_Y}{\gamma_{\mathbf{Y}}} R_Y(Y_s, Y_t) + R_g(Y_s, Y_t) &= O_p(L_Y(Y_s, Y_t)^2). \end{aligned}$$

Thus, similar arguments in Theorem 2.1.1 can be used to show that  $\mathcal{R}_n = O_p(\tau a_p^2 b_q + \tau a_p b_q^2) = o_p(1)$ .  $\square$

### C.5. Proof of Proposition 2.2.1.

PROOF. Clearly,  $E[k_{st}(i)l_{uv}(j)] = 0$  when  $\{s, t\} \cap \{u, v\} = \emptyset$ . For any  $1 \leq i, i' \leq p, 1 \leq j, j' \leq q$ ,

$$\begin{aligned} &E[k_{st}(i)l_{su}(j)] \\ &= E[E[k_{st}(i)l_{su}(j)|x_{si}, y_{sj}]] \\ &= E[E[k_{st}(i)|x_{si}, y_{sj}]E[l_{su}(j)|x_{si}, y_{sj}]]. \end{aligned}$$

Notice that

$$\begin{aligned} &E[k_{st}(i)|x_{si}, y_{sj}] \\ &= E\{k(x_{si}, x_{ti}) - E[k(x_{si}, x_{ti})|x_{si}] - E[k(x_{si}, x_{ti})|x_{ti}] + E[k(x_{si}, x_{ti})|x_{si}, y_{sj}]\} \\ &= E[k(x_{si}, x_{ti})|x_{si}, y_{sj}] - E[k(x_{si}, x_{ti})|x_{si}] - E[k(x_{si}, x_{ti})] + E[k(x_{si}, x_{ti})] \\ &= 0. \end{aligned}$$

Thus  $E[k_{st}(i)l_{su}(j)] = 0$ . Similarly,  $E[k_{st}(i)k_{su}(i')] = E[l_{st}(j)l_{su}(j')] = 0$ .  $\square$

### C.6. Proof of Theorem 2.2.1 .

PROOF. Let  $\tilde{\mathbf{K}} = ((\tilde{k}_{st})_{s,t=1}^n)_{-D}$  and  $\tilde{\mathbf{L}} = ((\tilde{l}_{st})_{s,t=1}^n)_{-D}$ . Notice that

$$\begin{aligned} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &= (pq)^{-1/2} \sum_{i=1}^p \sum_{j=1}^q \frac{1}{n(n-3)} \sum_{s \neq t} \tilde{k}_{st}(i) \tilde{l}_{st}(j) \\ &= \frac{1}{n(n-3)} \sum_{s \neq t} \left( p^{-1/2} \sum_{i=1}^p \tilde{k}_{st}(i) \right) \left( q^{-1/2} \sum_{j=1}^q \tilde{l}_{st}(j) \right). \end{aligned}$$

Under Assumption D3, we have

$$\begin{aligned} & p^{-1/2} \sum_{i=1}^p \tilde{k}_{st}(i) \\ &= p^{-1/2} \sum_{i=1}^p k_{st}(i) - \frac{1}{n-2} \sum_{u \neq t} p^{-1/2} \sum_{i=1}^p k_{ut}(i) \\ & \quad - \frac{1}{n-2} \sum_{v \neq s} p^{-1/2} \sum_{i=1}^p k_{sv}(i) + \frac{1}{(n-1)(n-2)} \sum_{u \neq v} p^{-1/2} \sum_{i=1}^p k_{uv}(i) \\ & \xrightarrow{d} c_{st} - \frac{1}{n-2} \sum_{u \neq t} c_{ut} - \frac{1}{n-2} \sum_{v \neq s} c_{vs} + \frac{1}{(n-1)(n-2)} \sum_{u \neq v} c_{uv}. \end{aligned}$$

Then we get

$$\begin{aligned} & n(n-3) \times \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) \xrightarrow{d} \\ & \sum_{s \neq t} \left( c_{st} - \frac{1}{n-2} \sum_{u \neq t} c_{ut} - \frac{1}{n-2} \sum_{v \neq s} c_{sv} + \frac{1}{(n-1)(n-2)} \sum_{u \neq v} c_{uv} \right) \\ & \times \left( d_{st} - \frac{1}{n-2} \sum_{u \neq t} d_{ut} - \frac{1}{n-2} \sum_{v \neq s} d_{sv} + \frac{1}{(n-1)(n-2)} \sum_{u \neq v} d_{uv} \right). \end{aligned}$$

Set

$$\begin{aligned} \mathbf{c} &= (c_{12}, c_{13}, \dots, c_{1n}, c_{23}, \dots, c_{2n}, c_{34}, \dots, c_{n(n-1)})^T, \\ \mathbf{d} &= (d_{12}, d_{13}, \dots, d_{1n}, d_{23}, \dots, d_{2n}, d_{34}, \dots, d_{n(n-1)})^T. \end{aligned}$$

Under Assumption D3 and by Proposition 2.2.1, we know that

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} \sim N \left( \mathbf{0}, \begin{pmatrix} \sigma_x^2 \mathbf{I}_{n(n-1)/2} & \sigma_{xy}^2 \mathbf{I}_{n(n-1)/2} \\ \sigma_{xy}^2 \mathbf{I}_{n(n-1)/2} & \sigma_y^2 \mathbf{I}_{n(n-1)/2} \end{pmatrix} \right).$$

Define  $\mathbf{C} = (c_{st})_{s,t=1}^n$  such that  $c_{st} = c_{ts}$  and  $\tilde{\mathbf{C}} = (\tilde{c}_{st})_{s,t=1}^n$ . Here we assume that  $c_{ss} = 0$ . Following [Park, Shao and Yao \(2015\)](#), for any matrix  $\mathbf{A}$ , define  $\dot{\mathbf{A}}$  as

$$\dot{\mathbf{A}} = \mathbf{A} - \frac{1}{n-2} \mathbf{A} \mathbf{J} - \frac{1}{n-2} \mathbf{J} \mathbf{A} + \frac{1}{(n-1)(n-2)} \mathbf{J} \mathbf{A} \mathbf{J},$$

where  $\mathbf{J} = \mathbf{1}_{n \times n}$  is the  $n \times n$  matrix of ones. Let  $\text{vec}(\mathbf{A})$  is the usual vectorization of matrix  $\mathbf{A}$ , then it is straightforward to see that

$$\text{vec}(\dot{\mathbf{A}}) = \mathbf{S} \text{vec}(\mathbf{A}),$$

where

$$\mathbf{S} = \mathbf{I}_n \otimes \mathbf{I}_n - \frac{1}{n-2} \mathbf{J} \otimes \mathbf{I}_n - \frac{1}{n-2} \mathbf{I}_n \otimes \mathbf{J} + \frac{1}{(n-1)(n-2)} \mathbf{J} \otimes \mathbf{J}.$$

Also notice that  $\tilde{\mathbf{A}}$  is just  $\dot{\mathbf{A}}$  with diagonal replaced by 0. Putting things together, we have

$$\text{vec}(\tilde{\mathbf{C}}) = \mathbf{F} \mathbf{S} \text{vec}(\mathbf{C}) = \mathbf{F} \mathbf{S} \mathbf{F} \text{vec}(\mathbf{C}),$$

where  $\mathbf{F}$  is the matrix of the linear operator that sets the diagonal of a matrix to be 0, i.e.,  $\text{vec}(\mathbf{B}_{-D}) = \mathbf{F} \text{vec}(\mathbf{B})$ ,  $\mathbf{B}_{-D}$  is  $\mathbf{B}$  with its diagonal set to be 0.

Next, to simplify the following proof, we will use a different vectorization operator, which will align the upper triangular elements first, then the lower triangular elements and lastly the diagonal elements, i.e., define

$$\begin{aligned} \widetilde{\text{vec}}(\mathbf{C}) &= (\mathbf{c}_u^T, \mathbf{c}_l^T, \mathbf{c}_d^T)^T, \\ \mathbf{c}_u^T &= (c_{12}, c_{13}, \dots, c_{1n}, c_{23}, \dots, c_{2n}, c_{34}, \dots, c_{(n-1)n}), \\ \mathbf{c}_l^T &= (c_{21}, c_{31}, \dots, c_{n1}, c_{32}, \dots, c_{n2}, c_{43}, \dots, c_{n(n-1)}), \\ \mathbf{c}_d^T &= (c_{11}, c_{22}, \dots, c_{nn}). \end{aligned}$$

Notice that there is a permutation matrix  $\mathbf{P}_1$  such that  $\widetilde{\text{vec}}(\mathbf{C}) = \mathbf{P}_1 \text{vec}(\mathbf{C})$ . Then

$$\widetilde{\text{vec}}(\tilde{\mathbf{C}}) = \mathbf{P}_1 \mathbf{F} \mathbf{S} \mathbf{F} \mathbf{P}_1^T \widetilde{\text{vec}}(\mathbf{C}).$$

Observe that for any symmetric matrix  $\mathbf{C}$  with 0 diagonal, both the column sum and row sum of  $\tilde{\mathbf{C}}$  are 0. We can verify that  $\tilde{\tilde{\mathbf{C}}} = \tilde{\mathbf{C}}$ . Set  $\mathbf{U} = \mathbf{P}_1 \mathbf{F} \mathbf{S} \mathbf{F} \mathbf{P}_1^T$ . It follows that  $\mathbf{U}^2 \widetilde{\text{vec}}(\mathbf{C}) = \mathbf{U} \widetilde{\text{vec}}(\mathbf{C})$  and thus

$$(16) \quad (\mathbf{U}^2 - \mathbf{U}) \widetilde{\text{vec}}(\mathbf{C}) = 0.$$

We partition  $\mathbf{U}$  into three blocks corresponding to the upper triangular, lower triangular and diagonal elements respective, i.e., we write

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_1 & \mathbf{U}_2 & \mathbf{0} \\ \mathbf{U}_2 & \mathbf{U}_1 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix},$$

where we have used the symmetry for  $\mathbf{U}$ . Equation (16) is then equivalent to  $(\mathbf{U}_1^2 + \mathbf{U}_2^2 - \mathbf{U}_1)\mathbf{c}_u + (\mathbf{U}_1\mathbf{U}_2 + \mathbf{U}_2\mathbf{U}_1 - \mathbf{U}_2)\mathbf{c}_l = 0$ . Using the facts that  $\mathbf{c}_u$  is arbitrary and  $\mathbf{c}_u = \mathbf{c}_l$ , we can conclude that

$$\mathbf{U}_1^2 + \mathbf{U}_2^2 + \mathbf{U}_1\mathbf{U}_2 + \mathbf{U}_2\mathbf{U}_1 = \mathbf{U}_1 + \mathbf{U}_2.$$

Next, let  $\mathbf{C}^u$  ( $\mathbf{C}^l$ ) be the matrix by setting the lower (upper) triangular and diagonal elements in  $\mathbf{C}$  to be zero. Denote

$$\mathbf{P}_2 = \begin{pmatrix} \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{pmatrix}, \quad \mathbf{D} = \begin{pmatrix} \mathbf{I} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}.$$

Then, we see that  $\widetilde{\text{vec}}(\mathbf{C}^l) = \mathbf{P}_2\widetilde{\text{vec}}(\mathbf{C}^u)$  and

$$\mathbf{U}\widetilde{\text{vec}}(\mathbf{C}) = \mathbf{U}\widetilde{\text{vec}}(\mathbf{C}^u) + \mathbf{U}\mathbf{P}_2\widetilde{\text{vec}}(\mathbf{C}^u) = \mathbf{U}(\mathbf{I} + \mathbf{P}_2)\widetilde{\text{vec}}(\mathbf{C}^u) = \mathbf{U}(\mathbf{I} + \mathbf{P}_2)\mathbf{D}\mathbf{c}.$$

We note that

$$\mathbf{W} := \mathbf{D}^T(\mathbf{I} + \mathbf{P}_2)\mathbf{U}\mathbf{U}(\mathbf{I} + \mathbf{P}_2)\mathbf{D} = \mathbf{D}^T(\mathbf{U} + \mathbf{U}\mathbf{P}_2 + \mathbf{P}_2\mathbf{U} + \mathbf{P}_2\mathbf{U}\mathbf{P}_2)\mathbf{D}.$$

Then we have  $\mathbf{W} = 2(\mathbf{U}_1 + \mathbf{U}_2)$ . Also notice that

$$\mathbf{W}^2 = 4(\mathbf{U}_1 + \mathbf{U}_2)^2 = 4(\mathbf{U}_1^2 + \mathbf{U}_2^2 + \mathbf{U}_1\mathbf{U}_2 + \mathbf{U}_2\mathbf{U}_1) = 4(\mathbf{U}_1 + \mathbf{U}_2) = 2\mathbf{W},$$

which indicates that  $\mathbf{W}$  has eigenvalues which are either equal to two or zero. It remains to show that the rank of  $\mathbf{W}$  is  $n(n-3)/2$  or equivalently, the trace of  $\mathbf{W}/2 = \mathbf{U}_1 + \mathbf{U}_2$  is  $n(n-3)/2$ . Note that

$$\text{Tr}(\mathbf{W}/2) = \text{Tr}(\mathbf{U}_1 + \mathbf{U}_2) = \sum_{i=1}^{n(n-1)/2} \frac{\mathbf{r}_i^T \mathbf{U} \mathbf{r}_i}{2} = \frac{n(n-1)}{4} \widetilde{\text{vec}}(\widetilde{\mathbf{E}}_1)^T \widetilde{\text{vec}}(\widetilde{\mathbf{E}}_1),$$

where  $\mathbf{r}_i = (\mathbf{e}_i^T, \mathbf{e}_i^T, \mathbf{0}^T)^T$  and  $\mathbf{e}_i$  is a  $n(n-1)/2$ -dimensional vector with 1 on the  $i$ th position and zero otherwise;  $\widetilde{\mathbf{E}}_i$  denotes the  $\mathcal{U}$ -centering version of the matrix  $\mathbf{E}_i$  such that  $\widetilde{\text{vec}}(\widetilde{\mathbf{E}}_i) = \mathbf{r}_i$ . Direct calculation shows that

$$\begin{aligned} \text{vec}(\widetilde{\mathbf{E}}_1)^T \text{vec}(\widetilde{\mathbf{E}}_1) &= \frac{2(n-3)^2}{(n-1)^2} + 4(n-2) \frac{(n-3)^2}{(n-1)^2(n-2)^2} \\ &\quad + (n-2)(n-3) \frac{4}{(n-1)^2(n-2)^2} = \frac{2(n-3)}{n-1}, \end{aligned}$$

which implies that  $4^{-1}n(n-1)\widetilde{\text{vec}}(\widetilde{\mathbf{E}}_1)^T\widetilde{\text{vec}}(\widetilde{\mathbf{E}}_1) = n(n-3)/2$ . Using the above results and setting  $\mathbf{M} = \mathbf{W}/2$ , we have

$$\begin{aligned}\text{vec}(\widetilde{\mathbf{C}})^T\text{vec}(\widetilde{\mathbf{C}}) &= \widetilde{\text{vec}}(\widetilde{\mathbf{C}})^T\widetilde{\text{vec}}(\widetilde{\mathbf{C}}) = \widetilde{\text{vec}}(\mathbf{C})^T\mathbf{U}^2\widetilde{\text{vec}}(\mathbf{C}) \\ &= 2\mathbf{c}^T\mathbf{M}\mathbf{c} \sim 2\sigma_x^2\chi_{n(n-3)/2}^2.\end{aligned}$$

Thus,

$$\text{uCov}_n^2(\mathbf{X}, \mathbf{X}) \xrightarrow{d} \frac{2}{n(n-3)}\mathbf{c}^T\mathbf{M}\mathbf{c} \stackrel{d}{=} \frac{2}{n(n-3)}\sigma_x^2\chi_{n(n-3)/2}^2.$$

Similarly,

$$\begin{aligned}\text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &\xrightarrow{d} \frac{2}{n(n-3)}\mathbf{c}^T\mathbf{M}\mathbf{d}, \\ \text{uCov}_n^2(\mathbf{Y}, \mathbf{Y}) &\xrightarrow{d} \frac{2}{n(n-3)}\mathbf{d}^T\mathbf{M}\mathbf{d} \stackrel{d}{=} \frac{2}{n(n-3)}\sigma_y^2\chi_{n(n-3)/2}^2.\end{aligned}$$

□

### C.7. Proof of Proposition 2.2.2.

PROOF. Since

$$\begin{pmatrix} \mathbf{c} \\ \mathbf{d} \end{pmatrix} \stackrel{d}{=} N\left(\mathbf{0}, \begin{pmatrix} \sigma_x^2\mathbf{I}_{n(n-1)/2} & \sigma_{xy}\mathbf{I}_{n(n-1)/2} \\ \sigma_{xy}\mathbf{I}_{n(n-1)/2} & \sigma_y^2\mathbf{I}_{n(n-1)/2} \end{pmatrix}\right),$$

we have

$$\mathbf{c}|\mathbf{d} \stackrel{d}{=} N(\mu\mathbf{d}, \sigma^2\mathbf{I}_{n(n-1)/2}),$$

where  $\mu = \sigma_{xy}^2/\sigma_y^2$ ,  $\sigma^2 = (\sigma_x^2\sigma_y^2 - \sigma_{xy}^4)/\sigma_y^2$ . Set

$$\mathbf{z} = \frac{\mathbf{M}\mathbf{d}}{\sqrt{(\mathbf{d}^T\mathbf{M}\mathbf{d})}}.$$

It can be easily seen that conditional on  $\mathbf{d}$ ,

$$\mathbf{c}^T\mathbf{z}/\sigma \sim N(\mu\mathbf{z}^T\mathbf{d}/\sigma, 1),$$

which implies that  $(\mathbf{c}^T\mathbf{z})^2/\sigma^2 | \mathbf{d} \sim \chi_1^2(W^2)$ , where  $\chi_1^2(W^2)$  is the non-central chi-squared distribution and  $W^2 = \frac{\mu^2}{\sigma^2}\mathbf{d}^T\mathbf{M}\mathbf{d}$  is the non-centrality parameter. Note that conditioned on  $\mathbf{d}$ ,

$$\mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{c}/\sigma \sim N(\mathbf{0}, \mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{M}),$$

where we have used the fact that  $\mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{d} = 0$ . As  $\mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{M} = \mathbf{M} - \frac{\mathbf{M}\mathbf{d}\mathbf{d}^T\mathbf{M}}{\mathbf{d}^T\mathbf{M}\mathbf{d}}$  is a projection matrix with rank  $v - 1$ , it is easy to see that conditioned on  $\mathbf{d}$ ,

$$\mathbf{c}^T(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{c}/\sigma^2 \sim \chi_{v-1}^2.$$

Next, conditioned on  $\mathbf{d}$ , as  $\mathbf{z}^T\mathbf{c}$  and  $(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{c}$  are independent, we have  $(\mathbf{c}^T\mathbf{z})^2/\sigma^2$  and  $\mathbf{c}^T(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{c}$  are independent. Then,

$$\begin{aligned} P_{H_A}(T_u < t) &\rightarrow P\left(\sqrt{v-1}\frac{\frac{\mathbf{c}^T\mathbf{z}}{\sqrt{(\mathbf{c}^T\mathbf{M}\mathbf{c})}}}{\sqrt{1 - \left(\frac{\mathbf{c}^T\mathbf{z}}{\sqrt{(\mathbf{c}^T\mathbf{M}\mathbf{c})}}\right)^2}} < t\right) \\ &= \mathbb{E}\left[P\left(\sqrt{v-1}\frac{\frac{\mathbf{c}^T\mathbf{z}}{\sqrt{(\mathbf{c}^T\mathbf{M}\mathbf{c})}}}{\sqrt{1 - \left(\frac{\mathbf{c}^T\mathbf{z}}{\sqrt{(\mathbf{c}^T\mathbf{M}\mathbf{c})}}\right)^2}} < t \mid \mathbf{d}\right)\right] \\ &= \mathbb{E}\left[P\left(\sqrt{v-1}\frac{\mathbf{c}^T\mathbf{z}}{\sqrt{\mathbf{c}^T\mathbf{M}\mathbf{c} - (\mathbf{c}^T\mathbf{z})^2}} < t \mid \mathbf{d}\right)\right] \\ &= \mathbb{E}\left[P\left(\frac{\mathbf{c}^T\mathbf{z}}{\sqrt{\frac{1}{v-1}\mathbf{c}^T(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{M}(\mathbf{I} - \mathbf{z}\mathbf{z}^T)\mathbf{c}}} < t \mid \mathbf{d}\right)\right] \\ &= \mathbb{E}[P(t_{v-1,W} < t)] \end{aligned}$$

where  $t_{v-1,W}$  is a noncentral  $t$ -distribution with  $v - 1$  degrees of freedom and noncentrality parameter  $W = \frac{\mu}{\sigma}\sqrt{\mathbf{d}^T\mathbf{M}\mathbf{d}} \stackrel{d}{=} c\chi_v$  for  $c = \frac{\sigma_{xy}^2}{\sqrt{\sigma_x^2\sigma_y^2 - \sigma_{xy}^4}}$ . By setting  $c = 0$ , we get  $P_{H_0}(T_u < t) \rightarrow P(t_{v-1} < t)$ .  $\square$

### C.8. Proof of Proposition 2.2.3.

PROOF. Notice that

$$\phi = \frac{\phi_0}{\sqrt{v}} \Rightarrow c = \frac{\phi_0}{\sqrt{v - \phi_0^2}} = \frac{\phi_0}{\sqrt{v}} \left(1 + O\left(\frac{1}{v}\right)\right).$$



Next, by the definition of non-central  $t$ -distribution,

$$\begin{aligned}
P(t_{v-1,u} < t) &= P\left(\frac{Z + u}{\sqrt{\chi_{v-1}^2/(v-1)}} < t\right) \\
&= P\left(Z < t\sqrt{\chi_{v-1}^2/(v-1)} - u\right) \\
&= \mathbb{E}\left[P\left(Z < t\sqrt{\chi_{v-1}^2/(v-1)} - u \mid \chi_{v-1}^2\right)\right] \\
&= \mathbb{E}\left[\Phi\left(t\sqrt{\frac{\chi_{v-1}^2}{v-1}} - u\right)\right],
\end{aligned}$$

where  $\Phi$  is the cdf of standard normal. For notational convenience, set

$$g(u) = \mathbb{E}\left[\Phi\left(t\sqrt{\frac{\chi_{v-1}^2}{v-1}} - u\right)\right].$$

Notice that  $P(t_{v-1,W} < t) = g(W)$ . By the following asymptotic series [see [Laforgia and Natalini \(2012\)](#); [Tricomi and Erdélyi \(1951\)](#)],

$$\begin{aligned}
\frac{\Gamma(J+1/2)}{\Gamma(J)} &= \sqrt{J}\left(1 - \frac{1}{8J} + \frac{1}{128J^2} + \frac{5}{1024J^3} - \frac{21}{32768J^4} + \dots\right) \\
&= \sqrt{J}\left(1 + O\left(\frac{1}{J}\right)\right),
\end{aligned}$$

we can get,

$$\begin{aligned}
&\mathbb{E}[(W - \phi_0)] \\
&= \frac{\phi_0}{\sqrt{v}}\left(1 + O\left(\frac{1}{v}\right)\right)\sqrt{2}\frac{\Gamma((v+1)/2)}{\Gamma(v/2)} - \phi_0 \\
&= \phi_0\left(1 + O\left(\frac{1}{v}\right)\right) - \phi_0 \\
&= O\left(\frac{1}{v}\right),
\end{aligned}$$

as well as

$$\begin{aligned}
& \mathbf{E} [(W - \phi_0)^2] \\
&= \phi_0^2 \mathbf{E} \left[ \left( \frac{\chi_v}{\sqrt{v}} \left( 1 + O\left(\frac{1}{v}\right) \right) - 1 \right)^2 \right] \\
&= \phi_0^2 \mathbf{E} \left[ \frac{\chi_v^2}{v} \left( 1 + O\left(\frac{1}{v}\right) \right) - 2 \frac{\chi_v}{\sqrt{v}} \left( 1 + O\left(\frac{1}{v}\right) \right) + 1 \right] \\
&= \phi_0^2 \left\{ \left( 1 + O\left(\frac{1}{v}\right) \right) - 2 \left( 1 + O\left(\frac{1}{v}\right) \right) + 1 \right\} \\
&= O\left(\frac{1}{v}\right),
\end{aligned}$$

and

$$\begin{aligned}
& \mathbf{E} [W(W - \phi_0)^2] \\
&= \phi_0^3 \mathbf{E} \left[ \frac{\chi_v}{\sqrt{v}} \left( 1 + O\left(\frac{1}{v}\right) \right) \left( \frac{\chi_v}{\sqrt{v}} \left( 1 + O\left(\frac{1}{v}\right) \right) - 1 \right)^2 \right] \\
&= \phi_0^3 \mathbf{E} \left[ \frac{\chi_v^3}{v^{3/2}} - 2 \frac{\chi_v^2}{v} + \frac{\chi_v}{\sqrt{v}} \right] \left( 1 + O\left(\frac{1}{v}\right) \right) \\
&= \phi_0^3 \left\{ \frac{(v+1)}{v^{3/2}} \sqrt{v} \left( 1 + O\left(\frac{1}{v}\right) \right) - 2 + 1 + O\left(\frac{1}{v}\right) \right\} \left( 1 + O\left(\frac{1}{v}\right) \right) \\
&= O\left(\frac{1}{v}\right).
\end{aligned}$$

We note that

$$\begin{aligned}
\frac{\partial}{\partial u} \Phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) &= -\phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \\
\frac{\partial^2}{\partial u^2} \Phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) &= - \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right).
\end{aligned}$$

Thus,

$$\begin{aligned}
|g^{(2)}(u)| &= \left| \frac{\partial^2}{\partial u^2} \mathbb{E} \left[ \Phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \right] \right| \\
&= \left| \mathbb{E} \left[ \frac{\partial^2}{\partial u^2} \Phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \right] \right| \\
&= \left| \mathbb{E} \left[ - \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \right] \right| \\
&\leq \mathbb{E} \left[ \left| - \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \right| \phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \right] \\
&\leq \mathbb{E} \left[ \left( |t| \sqrt{\frac{\chi_{v-1}^2}{v-1}} + |u| \right) \phi \left( t \sqrt{\frac{\chi_{v-1}^2}{v-1}} - u \right) \right] \\
&< \mathbb{E} \left[ \left( |t| \sqrt{\frac{\chi_{v-1}^2}{v-1}} + |u| \right) \right] \\
&\leq \left( |t| \mathbb{E} \sqrt{\frac{\chi_{v-1}^2}{v-1}} + |u| \right) \\
&\leq \sqrt{2}|t| + |u|.
\end{aligned}$$

Next, we can bound the following integral,

$$\begin{aligned}
&\left| \int_0^1 \int_0^1 ag^{(2)}(\phi_0 + ab(W - \phi_0)) dbda \right| \\
&\leq \int_0^1 \int_0^1 |ag^{(2)}(\phi_0 + ab(W - \phi_0))| dbda \\
&\leq \int_0^1 \int_0^1 \sqrt{2}|t| + |\phi_0 + ab(W - \phi_0)| dbda \\
&\leq \int_0^1 \int_0^1 \sqrt{2}|t| + \phi_0 + |W| dbda \\
&= \sqrt{2}|t| + \phi_0 + W.
\end{aligned}$$

To calculate  $\mathbb{E}[P(t_{v-1,W} < t)] = \mathbb{E}[g(W)]$ , taking the Taylor expansion of

$g(W)$  around  $\phi_0$ , the asymptotic mean of  $W$ , we get

$$\begin{aligned}
&= \mathbb{E}[g(W)] \\
&= g(\phi_0) + g^{(1)}(\phi_0)\mathbb{E}[(W - \phi_0)] \\
&\quad + \mathbb{E}\left[\int_0^1 \int_0^1 ag^{(2)}(\phi_0 + ab(W - \phi_0))dbda (W - \phi_0)^2\right] \\
&= P(t_{v-1, \phi_0} < t) + O\left(\frac{1}{v}\right) \\
&\quad + \mathbb{E}\left[\int_0^1 \int_0^1 ag^{(2)}(\phi_0 + ab(W - \phi_0))dbda (W - \phi_0)^2\right].
\end{aligned}$$

Notice that,

$$\begin{aligned}
&\left| \mathbb{E}\left[\int_0^1 \int_0^1 ag^{(2)}(\phi_0 + ab(W - \phi_0))dbda (W - \phi_0)^2\right] \right| \\
&\leq \mathbb{E}\left[\left|\int_0^1 \int_0^1 ag^{(2)}(\phi_0 + ab(W - \phi_0))dbda (W - \phi_0)^2\right|\right] \\
&\leq \mathbb{E}\left[(\sqrt{2}|t| + \phi_0 + W)(W - \phi_0)^2\right] \\
&\leq (\sqrt{2}|t| + \phi_0)\mathbb{E}\left[(W - \phi_0)^2\right] + \mathbb{E}\left[W(W - \phi_0)^2\right] \\
&= O\left(\frac{1}{v}\right).
\end{aligned}$$

In conclusion, we have  $\mathbb{E}[P(t_{v-1, W} < t)] = P(t_{v-1, \phi_0} < t) + O\left(\frac{1}{v}\right)$ . Since  $t_{v-1}^{(\alpha)} \rightarrow Z^{(\alpha)}$  as  $n \rightarrow \infty$ , where  $Z^{(\alpha)}$  is the  $(1 - \alpha)$ th percentile of standard normal,  $t_{v-1}^{(\alpha)}$  is bounded. Then, all the above analysis still holds if we replace  $t$  with  $t_{v-1}^\alpha$ .  $\square$

Let  $B(\cdot, \cdot)$  denote the beta function and  $I_y(\cdot, \cdot)$  denote the regularized incomplete beta function. In the following, we express  $\mathbb{E}[P(t_{v-1, W} \leq t)]$  as a sum of infinite series.

LEMMA 3.  $\mathbb{E}[P(t_{v-1, W} \leq t)]$  can be calculated exactly as

$$\begin{aligned}
\mathbb{E}[P(t_{v-1, W} < t)] &= \left(\frac{1}{c^2 + 1}\right)^{v/2} \left\{ P(t_{v-1} \leq t) + \right. \\
&\quad \left. \sum_{j=1}^{\infty} \left(\frac{c^2}{c^2 + 1}\right)^{j/2} \frac{1}{jB(j/2, v/2)} \left( (-1)^j + I_{\frac{t^2}{t^2 + v - 1}}\left(\frac{j+1}{2}, \frac{v-1}{2}\right) \right) \right\}.
\end{aligned}$$

PROOF. Notice that from [Walck \(1996\)](#), the CDF of non-central  $t$ -distribution for  $t \geq 0$  can be written as

$$P(t_{v-1,W} < t) = \frac{1}{2\sqrt{\pi}} \times \sum_{j=0}^{\infty} \frac{2^{\frac{j}{2}}}{j!} W^j \exp\left\{-\frac{W^2}{2}\right\} \Gamma\left(\frac{j+1}{2}\right) \left((-1)^j + I_z\left(\frac{j+1}{2}, \frac{v-1}{2}\right)\right),$$

where

$$z = \frac{t^2}{t^2 + v - 1}, \quad v = \frac{n(n-3)}{2},$$

$I_y(\cdot, \cdot)$  is the regularized incomplete beta function,

$$W = \frac{\mu}{\sigma} \sqrt{\mathbf{d}^T \mathbf{M} \mathbf{d}} \stackrel{d}{=} c\chi_v, \quad c = \frac{\sigma_{xy}^2}{\sqrt{\sigma_x^2 \sigma_y^2 - \sigma_{xy}^4}}.$$

Next, we calculate the expectation by constructing a generalized gamma distribution,

$$\begin{aligned} & \mathbb{E}\left[W^j \exp\left\{-\frac{W^2}{2}\right\}\right] \\ &= \int_0^{\infty} w^j \exp\left\{-\frac{w^2}{2}\right\} \frac{1}{c} \frac{1}{2^{v/2-1} \Gamma(v/2)} \left(\frac{w}{c}\right)^{v-1} \exp\left\{-\frac{w^2}{2c^2}\right\} dw \\ &= \frac{1}{c^v} \frac{1}{2^{v/2-1} \Gamma(v/2)} \int_0^{\infty} \exp\left\{-\left(\frac{w}{\sqrt{2c^2/(c^2+1)}}\right)^2\right\} w^{j+v-1} dw \\ &= \frac{1}{c^v} \frac{1}{2^{v/2-1} \Gamma(v/2)} \frac{\Gamma(j/2 + v/2) (\sqrt{2c^2/(c^2+1)})^{j+v}}{2} \\ &= \frac{(\sqrt{2c^2/(c^2+1)})^{j+v}}{c^v} \frac{1}{2^{v/2}} \frac{\Gamma(j/2 + v/2)}{\Gamma(v/2)}. \end{aligned}$$

Then,

$$\begin{aligned} \mathbb{E}[P(t_{v-1,W} < t)] &= \frac{1}{2\sqrt{\pi}} \left(\sqrt{\frac{1}{c^2+1}}\right)^v \times \\ & \sum_{j=0}^{\infty} \left(\frac{4c^2}{c^2+1}\right)^{\frac{j}{2}} \frac{\Gamma((j+1)/2) \Gamma(j/2 + v/2)}{j! \Gamma(v/2)} \left((-1)^j + I_z\left(\frac{j+1}{2}, \frac{v-1}{2}\right)\right). \end{aligned}$$

According to the gamma duplicate formula,

$$\Gamma\left(\frac{j+1}{2}\right) = \frac{\sqrt{\pi}}{2^j} \frac{\Gamma(j+1)}{\Gamma(j/2+1)},$$

which further implies that

$$\begin{aligned} \frac{\Gamma((j+1)/2)\Gamma(j/2+v/2)}{j!\Gamma(v/2)} &= \frac{\sqrt{\pi}}{2^j} \frac{\Gamma(j+1)}{\Gamma(j/2+1)} \frac{\Gamma(j/2+v/2)}{j!\Gamma(v/2)} \\ &= \begin{cases} \sqrt{\pi}, & j=0 \\ \frac{\sqrt{\pi}}{2^{j-1}} \frac{1}{j\Gamma(j/2)} \frac{\Gamma(j/2+v/2)}{\Gamma(v/2)}, & j \geq 1 \end{cases} \\ &= \begin{cases} \sqrt{\pi}, & j=0 \\ \frac{\sqrt{\pi}}{j2^{j-1}} \frac{1}{B(j/2, v/2)}, & j \geq 1 \end{cases} \end{aligned}$$

where  $B(\cdot, \cdot)$  is the beta function. Then, the expectation can be further simplified as

$$\begin{aligned} \mathbb{E}[P(t_{v-1, W} < t)] &= \frac{1}{2} \left(\frac{1}{c^2+1}\right)^{v/2} \left(1 + I_z\left(\frac{1}{2}, \frac{v-1}{2}\right)\right) + \\ &\left(\frac{1}{c^2+1}\right)^{v/2} \sum_{j=1}^{\infty} \left(\frac{c^2}{c^2+1}\right)^{j/2} \frac{1}{jB(j/2, v/2)} \left((-1)^j + I_z\left(\frac{j+1}{2}, \frac{v-1}{2}\right)\right). \end{aligned}$$

Notice that

$$\frac{1}{2} \left(1 + I_z\left(\frac{1}{2}, \frac{v-1}{2}\right)\right) = P(t_{v-1} \leq t).$$

Thus,

$$\begin{aligned} \mathbb{E}[P(t_{v-1, W} < t)] &= \left(\frac{1}{c^2+1}\right)^{v/2} \left\{ P(t_{v-1} \leq t) + \right. \\ &\left. \sum_{j=1}^{\infty} \left(\frac{c^2}{c^2+1}\right)^{j/2} \frac{1}{jB(j/2, v/2)} \left((-1)^j + I_z\left(\frac{j+1}{2}, \frac{v-1}{2}\right)\right) \right\}. \end{aligned}$$

□

### C.9. Proof of Proposition 2.2.5.

PROOF. Since we have

$$\begin{pmatrix} X \\ Y \end{pmatrix} \sim N\left(\mathbf{0}, \begin{pmatrix} \mathbf{I}_p & \boldsymbol{\Sigma}_{XY} \\ \boldsymbol{\Sigma}_{XY}^T & \mathbf{I}_q \end{pmatrix}\right),$$

from Theorem 7 in Székely, Rizzo and Bakirov (2007), by setting  $c = \frac{1}{4(\pi/3 - \sqrt{3} + 1)}$ , we obtain

$$c \leq \frac{\text{dCor}^2(x_i, y_j)}{\text{cor}^2(x_i, y_j)} \leq 1,$$

$\text{cov}^2(x_i, y_j) = \text{cor}^2(x_i, y_j)$  and  $\text{dCor}^2(x_i, y_j) = \text{dCov}^2(x_i, y_j)\pi/c$ . Combine these results, we have

$$c \leq \frac{\text{dCov}^2(x_i, y_j)\pi/c}{\text{cov}^2(x_i, y_j)} \leq 1.$$

Notice also that  $\text{dCov}^2(x_i, x_i) = \text{dCov}^2(y_j, y_j) = c/\pi$  and  $\text{cov}^2(x_i, x_i) = \text{cov}^2(y_j, y_j) = 1$ . We finally get  $0.89^2\phi_2 \leq \phi_1 \leq \phi_2$ .  $\square$

### C.10. Proof of Proposition 2.2.4.

PROOF. (i) When  $k(x, y) = l(x, y) = |x - y|^2$ ,

$$\begin{aligned} k_{st}(i) &= -2(x_{si} - \mathbb{E}(x_{si}))(x_{ti} - \mathbb{E}(x_{ti})), \\ l_{st}(j) &= -2(y_{sj} - \mathbb{E}(y_{sj}))(y_{tj} - \mathbb{E}(y_{tj})). \end{aligned}$$

Thus, letting  $\mathbf{D}_X(i) = ((x_{si}x_{ti})_{s,t=1}^n)_{-D}$  and  $\mathbf{D}_Y(j) = ((y_{sj}y_{tj})_{s,t=1}^n)_{-D}$ , we have

$$\begin{aligned} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &= \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q (\tilde{\mathbf{K}}(i) \cdot \tilde{\mathbf{L}}(j)) \\ &= \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q 4(\tilde{\mathbf{D}}_X(i) \cdot \tilde{\mathbf{D}}_Y(j)) \\ &= 4 \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q \left\{ \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in i_2^n} x_{si}x_{ti}y_{sj}y_{tj} + \right. \\ &\quad \left. \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in i_4^n} x_{si}x_{ti}y_{uj}y_{vj} - \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in i_3^n} x_{si}x_{ti}y_{sj}y_{uj} \right\} \\ &= 4 \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j). \end{aligned}$$

Thus,

$$\text{dCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}'_n = \frac{1}{4} \frac{\sqrt{pq}}{\tau} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) + \mathcal{R}'_n$$

and

$$\begin{aligned}
& \tau \times \text{hCov}_n^2(\mathbf{X}, \mathbf{Y}) \\
&= f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_X}{\gamma_X} \frac{\tau_Y}{\gamma_Y} \frac{1}{\tau} \sum_{i=1}^p \sum_{j=1}^q \text{cov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) + \mathcal{R}_n'' \\
&= f^{(1)} \left( \frac{\tau_X}{\gamma_X} \right) g^{(1)} \left( \frac{\tau_Y}{\gamma_Y} \right) \frac{\tau_X}{\gamma_X} \frac{\tau_Y}{\gamma_Y} \frac{1}{4} \frac{\sqrt{pq}}{\tau} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) + \mathcal{R}_n''.
\end{aligned}$$

(ii) When  $k(x, y) = l(x, y) = |x - y|$ , we have

$$\tilde{\mathbf{K}}(i) = \tilde{\mathbf{K}}_1(i) - \tilde{\mathbf{K}}_2(i) - \tilde{\mathbf{K}}_3(i) + \tilde{\mathbf{K}}_4(i) = \tilde{\mathbf{K}}_1(i),$$

where

$$\begin{aligned}
\mathbf{K}_1(i) &= ((k(x_{si}, x_{ti}))_{s,t=1}^n)_{-D}, \mathbf{K}_2(i) = ((E[k(x_{si}, x_{ti})|x_{si}])_{s,t=1}^n)_{-D}, \\
\mathbf{K}_3(i) &= ((E[k(x_{si}, x_{ti})|x_{ti}])_{s,t=1}^n)_{-D}, (\mathbf{K}_4(i) = (E[k(x_{si}, x_{ti})])_{s,t=1}^n)_{-D}.
\end{aligned}$$

Similarly,  $\tilde{\mathbf{L}}(j) = \tilde{\mathbf{L}}_1(j)$  with  $\mathbf{L}_1(j) = (l(y_{sj}, l_{tj}))_{s,t=1}^n$ . Then, we have

$$\begin{aligned}
\text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &= \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q (\tilde{\mathbf{K}}_1(i) \cdot \tilde{\mathbf{L}}_1(j)) \\
&= \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q \text{dCov}_n^2(\mathcal{X}_i, \mathcal{Y}_j) \\
&= \frac{1}{\sqrt{pq}} \frac{1}{\sqrt{\binom{n}{2}}} \text{mdCov}_n^2(\mathbf{X}, \mathbf{Y}).
\end{aligned}$$

□

### C.11. Proof of Corollary 2.2.1.

PROOF. For any fixed  $t$  and each  $R \in \{\text{dCov}, \text{hCov}, \text{mdCov}\}$ , Proposition 2.2.4 and Theorem 2.2.1 imply that

$$T_R \xrightarrow{d} \sqrt{v-1} \frac{\Upsilon}{\sqrt{1-(\Upsilon)^2}}, \text{ where } \Upsilon = \frac{\mathbf{c}^T \mathbf{M} \mathbf{d}}{\sqrt{(\mathbf{c}^T \mathbf{M} \mathbf{c})(\mathbf{d}^T \mathbf{M} \mathbf{d})}}.$$

Then the results follow similarly from the proof of Proposition 2.2.2. □



**C.12. Proof of Remark A.1.1.**

PROOF. For notational convenience, set  $z_i = (x_i - x'_i)^2 - \mathbb{E}[(x_i - x'_i)^2]$ . Since  $\sup_i \mathbb{E}(x_i^8) < \infty$ , we get  $\sup_i \mathbb{E}(z_i^4) < \infty$ . Then, we have

$$\begin{aligned} \alpha_p^2 &\asymp \frac{\mathbb{E} \left[ \left( \sum_{i=1}^p z_i \right)^2 \right]}{p^2} \\ &= \frac{\mathbb{E} \left[ \sum_{s=1}^p \sum_{t \in [s-m, s+m]} z_s z_t \right]}{p^2} \\ &\leq \frac{(2m+1)p}{p^2} \sup_i \mathbb{E}(z_i^2) \\ &= O\left(\frac{m}{p}\right) \end{aligned}$$

and

$$\begin{aligned} \gamma_p^2 &\asymp \frac{\mathbb{E} \left[ \left( \sum_{i=1}^p z_i \right)^4 \right]}{p^4} \\ &\asymp \frac{m^3 p + m^2 p^2}{p^4} \sup_i \mathbb{E}(z_i^4) \\ &= O\left(\frac{m^2}{p^2}\right). \end{aligned}$$

Similarly, we can show that

$$\beta_q^2 = O\left(\frac{m'}{q}\right) \text{ and } \lambda_q^2 = O\left(\frac{m'^2}{q^2}\right).$$

Next, it follows that

$$\tau \alpha_p \lambda_q = O\left(\frac{m' \sqrt{m}}{\sqrt{q}}\right) = o(1).$$

The other results can be proved in a similar fashion.  $\square$

**C.13. Proof of Theorem A.1.1.**

PROOF. (i)&(ii) Following the proof of Theorem 2.1.1, we only need to check that  $\mathcal{R}_n = o_p(1)$  still holds as  $n \wedge p \wedge q \rightarrow \infty$ . Recall that the leading term is  $\tau \times (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y)$  and the remainder term is given as

$$\mathcal{R}_n = \frac{1}{2} \tau (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) + \frac{1}{2} \tau (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) + \tau (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y).$$

Then, using Equation (14), we have

$$\begin{aligned} (\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) &= \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_X(X_s, X_t) R_Y(Y_s, Y_t) \\ &\quad + \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in \mathbf{i}_4^n} L_X(X_s, X_t) R_Y(Y_u, Y_v) \\ &\quad - \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in \mathbf{i}_3^n} L_X(X_s, X_t) R_Y(Y_s, Y_u), \end{aligned}$$

and

$$\begin{aligned} (\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y) &= \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) \\ &\quad + \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in \mathbf{i}_4^n} R_X(X_s, X_t) R_Y(Y_u, Y_v) \\ &\quad - \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in \mathbf{i}_3^n} R_X(X_s, X_t) R_Y(Y_s, Y_u). \end{aligned}$$

To show that  $\mathcal{R}_n$  is asymptotically negligible, we consider the events  $B_{\mathbf{X}}, B_{\mathbf{Y}}$  and their complements  $B_{\mathbf{X}}^c, B_{\mathbf{Y}}^c$ , where

$$B_{\mathbf{Y}} = \left\{ \min_{1 \leq s < t \leq n} \frac{|Y_s - Y_t|^2}{\tau_X^2} \leq \frac{1}{2} \text{ or } \max_{1 \leq s < t \leq n} \frac{|Y_s - Y_t|^2}{\tau_X^2} \geq \frac{3}{2} \right\}.$$

Then, under Assumption D4, as  $n \wedge p \wedge q \rightarrow \infty$

$$\begin{aligned} P(B_{\mathbf{Y}}) &= P\left( \min_{1 \leq s < t \leq n} L_Y(Y_s, Y_t) \leq -\frac{1}{2} \text{ or } \max_{1 \leq s < t \leq n} L_Y(Y_s, Y_t) \geq \frac{1}{2} \right) \\ &= P\left( \bigcup_{1 \leq s < t \leq n} \left\{ L_Y(Y_s, Y_t) \leq -\frac{1}{2} \text{ or } L_Y(Y_s, Y_t) \geq \frac{1}{2} \right\} \right) \\ &\leq \sum_{1 \leq s < t \leq n} P\left( |L_Y(Y_s, Y_t)| \geq \frac{1}{2} \right) \\ &< n^2 P\left( |L_Y(Y_1, Y_2)| \geq \frac{1}{2} \right) \\ &\leq 4n^2 \mathbf{E}[L_Y(Y_1, Y_2)^2] \\ &= o(1). \end{aligned}$$

Also notice that  $P(B_{\mathbf{Y}}B_{\mathbf{X}}^c) \leq P(B_{\mathbf{Y}}) = o(1)$ . Similarly, we have  $P(B_{\mathbf{X}}) = o(1)$ ,  $P(B_{\mathbf{X}}B_{\mathbf{Y}}^c) = o(1)$  and  $P(B_{\mathbf{Y}}B_{\mathbf{X}}) = o(1)$ . By the proof of Proposition 2.1.1, the remainder term can be written as

$$R_X(X_s, X_t) = \int_0^1 \int_0^1 v f^{(2)}(uv L_X(X_s, X_t)) dudv \times (L_X(X_s, X_t))^2,$$

where  $f^{(2)}(t) = -\frac{1}{4}(1+t)^{-\frac{3}{2}}$  and similar formula holds for  $Y$ . Conditioned on the event  $B_{\mathbf{X}}^c B_{\mathbf{Y}}^c$ , we can easily show that

$$(17) \quad |R_X(X_s, X_t)| \leq \frac{\sqrt{2}}{4} (L_X(X_s, X_t))^2, |R_Y(Y_s, Y_t)| \leq \frac{\sqrt{2}}{4} (L_Y(Y_s, Y_t))^2.$$

Notice that

$$\begin{aligned} & \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) \\ &= \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) \mathbb{I}_{\{B_{\mathbf{X}}^c B_{\mathbf{Y}}^c\}} \\ & \quad + \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) \mathbb{I}_{\{B_{\mathbf{X}} B_{\mathbf{Y}}^c\}} \\ & \quad + \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) \mathbb{I}_{\{B_{\mathbf{X}}^c B_{\mathbf{Y}}\}} \\ & \quad + \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) \mathbb{I}_{\{B_{\mathbf{X}} B_{\mathbf{Y}}\}} \\ &= i + ii + iii + iv. \end{aligned}$$

For any  $\epsilon > 0$ ,  $P(|\tau \times ii| > \epsilon) \leq P(B_{\mathbf{X}} B_{\mathbf{Y}}^c) = o(1)$ , which implies that  $\tau \times ii = o_p(1)$ . Similarly,  $\tau \times iii = o_p(1)$  and  $\tau \times iv = o_p(1)$ . For term  $i$ , by Equation (17), we have

$$\begin{aligned} |i| &\leq \left\{ \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} |R_X(X_s, X_t) R_Y(Y_s, Y_t)| \right\} B_{\mathbf{X}}^c B_{\mathbf{Y}}^c \\ &\leq \frac{1}{8} \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_X(X_s, X_t)^2 L_Y(Y_s, Y_t)^2 \\ &\leq \frac{1}{8} \left\{ \left( \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_X(X_s, X_t)^4 \right) \left( \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_Y(Y_s, Y_t)^4 \right) \right\}^{\frac{1}{2}}. \end{aligned}$$

Next, by the Markov's inequality

$$\begin{aligned} P\left(\frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_X(X_s, X_t)^4 > \epsilon\right) &\leq \frac{\mathbb{E}\left[\frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_X(X_s, X_t)^4\right]}{\epsilon} \\ &= \frac{1}{\epsilon} \mathbb{E}[L_X(X_1, X_2)^4] \\ &= \frac{1}{\epsilon} \gamma_p^2. \end{aligned}$$

Thus, we have  $\frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_X(X_s, X_t)^4 = O_p(\gamma_p^2)$  and similar proof shows that  $\frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} L_Y(Y_s, Y_t)^4 = O_p(\lambda_q^2)$ . So, we have  $\tau i = O_p(\tau \gamma_p \lambda_q)$  and

$$\tau \frac{1}{\binom{n}{2}} \frac{1}{2!} \sum_{(s,t) \in \mathbf{i}_2^n} R_X(X_s, X_t) R_Y(Y_s, Y_t) = O_p(\tau \gamma_p \lambda_q).$$

Similarly, it can be shown that

$$\begin{aligned} \tau \frac{1}{\binom{n}{4}} \frac{1}{4!} \sum_{(s,t,u,v) \in \mathbf{i}_4^n} R_X(X_s, X_t) R_Y(Y_u, Y_v) &= O_p(\tau \gamma_p \lambda_q), \\ \tau \frac{2}{\binom{n}{3}} \frac{1}{3!} \sum_{(s,t,u) \in \mathbf{i}_3^n} R_X(X_s, X_t) R_Y(Y_s, Y_u) &= O_p(\tau \gamma_p \lambda_q). \end{aligned}$$

In conclusion, we have  $\tau(\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{R}}_Y) = O_p(\tau \gamma_p \lambda_q)$ . Similarly, it can be shown that  $\tau(\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{L}}_Y) = O_p(\tau \alpha_p \beta_q)$ ,  $\tau(\tilde{\mathbf{L}}_X \cdot \tilde{\mathbf{R}}_Y) = O_p(\tau \alpha_p \lambda_q)$  and  $\tau(\tilde{\mathbf{R}}_X \cdot \tilde{\mathbf{L}}_Y) = O_p(\tau \gamma_p \beta_q)$ .  $\square$

#### C.14. Proof of Theorem A.1.2.

PROOF. (i)&(ii) Continuing with the proof of Theorem 2.1.2, we need to show that  $\mathcal{R}_n = o_p(1)$  and  $\gamma_{\mathbf{X}}$  is asymptotically equal to  $\tau_X$  as  $n \wedge p \wedge q \rightarrow \infty$  (similar result applies to  $\gamma_{\mathbf{Y}}$  and  $\tau_Y$ ). Recall that for all  $s \neq t$ ,

$$L_X(X_s, X_t) = \frac{|X_s - X_t|^2 - \tau_X^2}{\tau_X^2}.$$

Since for any  $\epsilon > 0$ , under Assumption D4,

$$\begin{aligned}
& P\left(\left|\frac{\text{median}\{|X_s - X_t|^2\}}{\tau_X^2} - 1\right| > \epsilon\right) \\
& \leq P\left(\min_{1 \leq s < t \leq n} L_X(X_s, X_t) \leq -\epsilon \text{ or } \max_{1 \leq s < t \leq n} L_X(X_s, X_t) \geq \epsilon\right) \\
& = P\left(\bigcup_{1 \leq s < t \leq n} \{L_X(X_s, X_t) \leq -\epsilon \text{ or } L_X(X_s, X_t) \geq \epsilon\}\right) \\
& \leq \sum_{1 \leq s < t \leq n} P(|L_X(X_s, X_t)| \geq \epsilon) \\
& < n^2 P(|L_X(X_1, X_2)| \geq \epsilon) \\
& \leq \frac{1}{\epsilon^2} n^2 \mathbb{E}[L_X(X_1, X_2)^2] \\
& = o(1).
\end{aligned}$$

Thus, we have  $\frac{\text{median}\{|X_s - X_t|^2\}}{\tau_X^2} \xrightarrow{p} 1$  and  $\frac{\tau_X}{\gamma_{\mathbf{X}}} = \sqrt{\frac{\tau_X^2}{\text{median}\{|X_i - X_j|^2\}}} \xrightarrow{p} 1$ .

Similar arguments can also be used to show that  $\frac{\tau_Y}{\gamma_{\mathbf{Y}}} \xrightarrow{p} 1$ .

Notice that conditioned on  $B_{\mathbf{X}}^c B_{\mathbf{Y}}^c$ , for all  $1 \leq s < t \leq n$ , we have

$$(18) \quad |L_X(X_s, X_t)| < 1/2 \text{ and } \frac{1}{2} < \frac{|X_s - X_t|^2}{\tau_X^2} < \frac{3}{2}.$$

Next, Inequalities (17) and (18) together imply that

$$\left| \frac{\tau_X}{\gamma_{\mathbf{X}}} + uv \left\{ \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t) \right\} \frac{\tau_X}{\gamma_{\mathbf{X}}} \right| \leq c,$$

where  $c$  is some constant. Since we choose kernels  $k$  and  $l$  to be the Gaussian or Laplacian kernel, it can be shown that

$$\left| \int_0^1 \int_0^1 v f^{(2)} \left( \frac{\tau_X}{\gamma_{\mathbf{X}}} + uv \left\{ \frac{L_X(X_s, X_t)}{2} + R_X(X_s, X_t) \right\} \frac{\tau_X}{\gamma_{\mathbf{X}}} \right) dudv \right| \leq c',$$

where  $c'$  is some constant. Then, we can easily see from Equation (15) that  $|R_f(X_s, X_t)| \leq c' L_X(X_s, X_t)^2$ . Similar result holds for  $Y$ . Finally, Theorem A.1.2 can be shown using similar arguments as in the proof of Theorem A.1.1.  $\square$

**C.15. Proof of Remark A.2.2.**

PROOF. When  $k(x, y) = l(x, y) = |x - y|^2$ ,

$$\begin{aligned} k_{st}(i) &= -2(x_{si} - \mathbb{E}(x_{si}))(x_{ti} - \mathbb{E}(x_{ti})), \\ l_{st}(j) &= -2(y_{sj} - \mathbb{E}(y_{sj}))(y_{tj} - \mathbb{E}(y_{tj})). \end{aligned}$$

Thus, we have

$$\begin{aligned} & \mathbb{E}[U(X_s, X_t)^2] \\ &= \mathbb{E} \left[ \frac{1}{p} \sum_{i=1}^p \sum_{j=1}^p k_{st}(i) k_{st}(j) \right] \\ &= \frac{4}{p} \sum_{i=1}^p \sum_{j=1}^p \mathbb{E} [(x_{si} - \mathbb{E}[x_{si}])(x_{ti} - \mathbb{E}[x_{ti}])(x_{sj} - \mathbb{E}[x_{sj}])(x_{tj} - \mathbb{E}[x_{tj}])] \\ &= \frac{4}{p} \sum_{i=1}^p \sum_{j=1}^p \text{cov}^2(x_i, x_j) \\ &= \frac{4}{p} \text{Tr}(\Sigma_X^2), \end{aligned}$$

and

$$\begin{aligned} & \mathbb{E}[U(X_s, X_t)^4] \\ &= \mathbb{E} \left[ \frac{1}{p^2} \sum_{i,j,r,w=1}^p k_{st}(i) k_{st}(j) k_{st}(r) k_{st}(w) \right] \\ &= \frac{16}{p^2} \sum_{i,j,r,w=1}^p \mathbb{E} \left[ (x_{si} - \mathbb{E}[x_{si}])(x_{ti} - \mathbb{E}[x_{ti}])(x_{sj} - \mathbb{E}[x_{sj}])(x_{tj} - \mathbb{E}[x_{tj}]) \right. \\ & \quad \left. (x_{sr} - \mathbb{E}[x_{sr}])(x_{tr} - \mathbb{E}[x_{tr}])(x_{sw} - \mathbb{E}[x_{sw}])(x_{tw} - \mathbb{E}[x_{tw}]) \right] \\ &= \frac{16}{p^2} \sum_{i,j,r,w=1}^p \mathbb{E}^2 [(x_i - \mathbb{E}[x_i])(x_j - \mathbb{E}[x_j])(x_r - \mathbb{E}[x_r])(x_w - \mathbb{E}[x_w])] \\ &\asymp \frac{m^3 p + m^2 p^2}{p^2} \sup_i \mathbb{E}^2(x_i^4) \\ &= O(m^2). \end{aligned}$$

Also,

$$\begin{aligned}
& \mathbb{E}[U(X_s, X_t)U(X_t, X_u)U(X_u, X_v)U(X_v, X_s)] \\
&= \mathbb{E} \left[ \frac{1}{p^2} \sum_{i,j,r,w=1}^p k_{st}(i)k_{tu}(j)k_{uv}(r)k_{vs}(w) \right] \\
&= \frac{16}{p^2} \sum_{i,j,r,w=1}^p \mathbb{E} \left[ (x_{si} - \mathbb{E}[x_{si}])(x_{ti} - \mathbb{E}[x_{ti}])(x_{tj} - \mathbb{E}[x_{tj}])(x_{uj} - \mathbb{E}[x_{uj}]) \right. \\
&\quad \left. (x_{ur} - \mathbb{E}[x_{ur}])(x_{vr} - \mathbb{E}[x_{vr}])(x_{vw} - \mathbb{E}[x_{vw}])(x_{sw} - \mathbb{E}[x_{sw}]) \right] \\
&= \frac{16}{p^2} \sum_{i,j,r,w=1}^p \text{cov}(x_i, x_j)\text{cov}(x_j, x_r)\text{cov}(x_r, x_w)\text{cov}(x_w, x_i) \\
&= \frac{16}{p^2} \text{Tr}(\Sigma_X^4) \\
&\asymp \frac{m^3 p}{p^2} \sup_i \mathbb{E}^4(x_i^2) \\
&= O\left(\frac{m^3}{p}\right).
\end{aligned}$$

□

### C.16. Proof of Theorem A.2.1.

PROOF. Firstly, the following lemma would be useful.

LEMMA 4. *Under null, we have*

$$\frac{1}{\mathcal{S}} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) = \frac{1}{\binom{n}{2}\mathcal{S}} \sum_{1 \leq s < t \leq n} H(Z_s, Z_t) + \mathcal{R}_n,$$

where  $\sqrt{\binom{n}{2}}\mathcal{R}_{n,p,q} = o_p(1)$  as  $n \wedge p \wedge q \rightarrow \infty$ ,  $Z_s = (X_s, Y_s)$  and  $H(\cdot, \cdot)$  is defined as

$$H(Z_s, Z_t) := U(X_s, X_t)V(Y_s, Y_t).$$

PROOF. Firstly, sample uCov can be written as

$$\begin{aligned} \text{uCov}_n^2(\mathbf{X}, \mathbf{Y}) &= \frac{1}{\sqrt{pq}} \sum_{i=1}^p \sum_{j=1}^q (\tilde{\mathbf{K}}(i) \cdot \tilde{\mathbf{L}}(j)) \\ &= \left( \frac{1}{\sqrt{p}} \sum_{i=1}^p \tilde{\mathbf{K}}(i) \cdot \frac{1}{\sqrt{q}} \sum_{j=1}^q \tilde{\mathbf{L}}(j) \right) \\ &= (\tilde{\mathbf{K}} \cdot \tilde{\mathbf{L}}), \end{aligned}$$

where  $\bar{\mathbf{K}} = (\bar{k}_{st})_{s,t=1}^n$ ,  $\bar{\mathbf{L}} = (\bar{l}_{st})_{s,t=1}^n$ ,  $\bar{k}_{st} = \frac{1}{\sqrt{p}} \sum_{i=1}^p k(x_{si}, x_{ti})$  and  $\bar{l}_{st} = \frac{1}{\sqrt{q}} \sum_{i=1}^q l(y_{si}, y_{ti})$ . Thus,  $\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})$  is just  $\text{dCov}_n^2(\mathbf{X}, \mathbf{Y})$  with kernel  $\bar{K}$  defines as  $\bar{K}(X_s, X_t) = \bar{k}_{st}$  and  $\bar{L}(Y_s, Y_t) = \bar{l}_{st}$ . Notice that

$$\begin{aligned} \bar{K}(X_s, X_t) - \mathbb{E}[\bar{K}(X_s, X_t)|X_s] - \mathbb{E}[\bar{K}(X_s, X_t)|X_t] + \mathbb{E}[\bar{K}(X_s, X_t)] &= \frac{1}{\sqrt{p}} \sum_{i=1}^p k_{st}(i), \\ \bar{L}(Y_s, Y_t) - \mathbb{E}[\bar{L}(Y_s, Y_t)|Y_s] - \mathbb{E}[\bar{L}(Y_s, Y_t)|Y_t] + \mathbb{E}[\bar{L}(Y_s, Y_t)] &= \frac{1}{\sqrt{q}} \sum_{i=1}^q l_{st}(i), \end{aligned}$$

where  $k_{st}(i)$  and  $l_{st}(i)$  are the double centered kernel distance defined in Section 2.2.1. By Proposition 2.1 of [Yao, Zhang and Shao \(2018\)](#), we have

$$\begin{aligned} \frac{1}{\mathcal{S}} (\tilde{\mathbf{K}} \cdot \tilde{\mathbf{L}}) &= \frac{1}{\binom{n}{2} \mathcal{S}} \sum_{1 \leq s < t \leq n} U(X_{s,n}, X_{t,n}) V(Y_{s,n}, Y_{t,n}) + \mathcal{R}_{n,p,q} \\ &= \frac{1}{\binom{n}{2} \mathcal{S}} \sum_{1 \leq s < t \leq n} \frac{1}{\sqrt{p}} \sum_{i=1}^p k_{st}(i) \frac{1}{\sqrt{q}} \sum_{i=1}^q l_{st}(i) + \mathcal{R}_{n,p,q}, \end{aligned}$$

where  $\sqrt{\binom{n}{2}} \mathcal{R}_{n,p,q} = o_p(1)$  as  $n \wedge p \wedge q \rightarrow \infty$ . □

By Lemma 4, we have

$$\sqrt{\binom{n}{2}} \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\mathcal{S}} = \frac{1}{\sqrt{\binom{n}{2}} \mathcal{S}} \sum_{1 \leq s < t \leq n} H(Z_s, Z_t) + \sqrt{\binom{n}{2}} \mathcal{R}_{n,p,q},$$

where  $\sqrt{\binom{n}{2}} \mathcal{R}_{n,p,q} = o_p(1)$ . By similar proof of Theorem 2.1 in [Zhang et al. \(2018\)](#), under  $H_0$ , we have

$$\frac{1}{\sqrt{\binom{n}{2}} \mathcal{S}} \sum_{1 \leq s < t \leq n} H(Z_s, Z_t) \xrightarrow{d} N(0, 1).$$

□



**C.17. Proof of Proposition A.2.1.**

PROOF. Notice that by the proof of Theorem 2.2 in Zhang et al. (2018), under null

$$(19) \quad \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{X})}{\mathbb{E}[U(X, X')^2]} \xrightarrow{p} 1, \quad \frac{\text{uCov}_n^2(\mathbf{Y}, \mathbf{Y})}{\mathbb{E}[V(Y, Y')^2]} \xrightarrow{p} 1.$$

So, by Theorem A.2.1

$$\sqrt{\binom{n}{2}} \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{\text{uCov}_n^2(\mathbf{X}, \mathbf{X})\text{uCov}_n^2(\mathbf{Y}, \mathbf{Y})}} \xrightarrow{d} N(0, 1),$$

and also

$$\frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{\text{uCov}_n^2(\mathbf{X}, \mathbf{X})\text{uCov}_n^2(\mathbf{Y}, \mathbf{Y})}} \xrightarrow{p} 0.$$

As a consequence, we have  $T_u \xrightarrow{d} N(0, 1)$ .  $\square$

**C.18. Proof of Proposition A.2.2.**

PROOF. Based on Theorem A.1.1 and A.1.2, the results follow similarly from the proof of Proposition 2.2.4.  $\square$

**C.19. Proof of Corollary A.2.1.**

PROOF. (i) If  $R = \text{mdCov}$ , the result follows from Proposition A.2.1 and the following observation

$$\sqrt{\binom{n}{2}} \frac{R_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{R_n^2(\mathbf{X}, \mathbf{X})R_n^2(\mathbf{Y}, \mathbf{Y})}} = \sqrt{\binom{n}{2}} \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{\text{uCov}_n^2(\mathbf{X}, \mathbf{X})\text{uCov}_n^2(\mathbf{Y}, \mathbf{Y})}}.$$

(ii) Recall that when  $k(x, y) = l(x, y) = |x - y|^2$ ,  $\mathbb{E}[U(X_s, X_t)^2] = \frac{4}{p} \text{Tr}(\boldsymbol{\Sigma}_X^2)$  and  $\mathbb{E}[V(Y_s, Y_t)^2] = \frac{4}{q} \text{Tr}(\boldsymbol{\Sigma}_Y^2)$ . If  $R = \text{hCov}$ , by Proposition A.2.2, we have

$$\sqrt{\binom{n}{2}} \tau \times \frac{R_n^2(\mathbf{X}, \mathbf{Y})}{\mathcal{S}} = A_p B_q \sqrt{\binom{n}{2}} \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\mathcal{S}} + \sqrt{\binom{n}{2}} \frac{\mathcal{R}_n''}{\mathcal{S}},$$

where  $A_p = \frac{\sqrt{p}}{2\tau_X} f^{(1)}\left(\frac{\tau_X}{\gamma_X}\right) \frac{\tau_X}{\gamma_X}$  and  $B_q = \frac{\sqrt{q}}{2\tau_Y} g^{(1)}\left(\frac{\tau_Y}{\gamma_Y}\right) \frac{\tau_Y}{\gamma_Y}$ . By Theorem A.2.1,

$$A_p B_q \sqrt{\binom{n}{2}} \frac{\text{uCov}_n^2(\mathbf{X}, \mathbf{Y})}{\mathcal{S}} \xrightarrow{d} cN(0, 1),$$

where  $c$  is some constant. Also notice that

$$\left| \sqrt{\binom{n}{2}} \frac{\mathcal{R}_n''}{\mathcal{S}} \right| \leq \left| \frac{n\mathcal{R}_n''}{4\sqrt{\frac{1}{p}\text{Tr}(\boldsymbol{\Sigma}_X^2)\frac{1}{q}\text{Tr}(\boldsymbol{\Sigma}_Y^2)}} \right| = o_p(1).$$

Thus, we have

$$\sqrt{\binom{n}{2}} \tau \times \frac{R_n^2(\mathbf{X}, \mathbf{Y})}{\mathcal{S}} \xrightarrow{d} cN(0, 1).$$

Next, under Assumption D4, by Equation (19) and Proposition A.2.2

$$\begin{aligned} & \tau \times \frac{\sqrt{R_n^2(\mathbf{X}, \mathbf{X})R_n^2(\mathbf{Y}, \mathbf{Y})}}{\mathcal{S}} \\ &= \sqrt{\left( \frac{A_p^2 \text{uCov}_n^2(\mathbf{X}, \mathbf{X}) + \mathcal{R}'''}{\mathbb{E}[U(X, X')^2]} \right) \left( \frac{B_q^2 \text{uCov}_n^2(\mathbf{Y}, \mathbf{Y}) + \mathcal{R}''''}{\mathbb{E}[U(Y, Y')^2]} \right)} \\ & \xrightarrow{p} c. \end{aligned}$$

Notice that Under Assumptions D1 and D4, Proposition A.2.2 also holds similarly when  $\mathbf{X} = \mathbf{Y}$  or  $\mathbf{Y} = \mathbf{X}$ . So  $\mathcal{R}'''$  and  $\mathcal{R}''''$  are both negligible. Thus, we have

$$\sqrt{\binom{n}{2}} \frac{R_n^2(\mathbf{X}, \mathbf{Y})}{\sqrt{R_n^2(\mathbf{X}, \mathbf{X})R_n^2(\mathbf{Y}, \mathbf{Y})}} \xrightarrow{d} N(0, 1)$$

and consequently  $T_R \xrightarrow{d} N(0, 1)$ . Similarly, it can be proved for  $R = \text{dCov}$ .  $\square$