Distribution-free consistent independence tests via Hallin’s multivariate rank

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Abstract

This paper investigates the problem of testing independence of two random vectors of general dimensions. For this, we give for the first time a distribution-free consistent test. Our approach combines distance covariance with a new multivariate rank statistic recently introduced by Hallin (2017). In technical terms, the proposed test is consistent and distribution-free in the family of multivariate distributions with nonvanishing (Lebesgue) probability densities. Exploiting the (degenerate) U-statistic structure of the distance covariance and the combinatorial nature of Hallin’s rank, we are able to derive the limiting null distribution of our test statistic. The resulting asymptotic approximation is accurate already for moderate sample sizes and makes the test implementable without requiring permutation. The limiting distribution is derived via a more general result that gives a new type of combinatorial non-central limit theorem for double- and multiple-indexed permutation statistics.

Keywords: Combinatorial non-central limit theorem, degenerate U-statistics, distance covariance, Hallin’s multivariate rank, independence test.

1 Introduction

Let \( X \) and \( Y \) be two real random vectors, with \( X \in \mathbb{R}^p \) and \( Y \in \mathbb{R}^q \). This paper treats the problem of testing the null hypothesis

\[
H_0 : X \text{ and } Y \text{ are independent},
\]

(1.1)

based on \( n \) independent copies \((X_1, Y_1), \ldots, (X_n, Y_n)\) of \((X, Y)\). Testing independence is a fundamental statistical problem that has received much attention in literature.

For the simplest instance, the bivariate case with \( p = q = 1 \), Höffding (1940), Hoeffding (1948), Blum et al. (1961), Yanagimoto (1970), Feuerverger (1993), Bergsma and Dassios (2014), among many others, have proposed tests that are consistent against all alternatives from slightly different but rather general classes of distributions. The tests are usually formulated using (univariate) ranks of the data, although recently more tests were proposed based on alternative summaries of the data,
including (i) binning approaches based on a partition of the sample space (Heller et al., 2013, 2016; Ma and Mao, 2019; Zhang, 2019), (ii) mutual information (Kraskov et al., 2004; Kinney and Atwal, 2014; Berrett and Samworth, 2019), and (iii) the maximal information coefficient (Reshef et al., 2011, 2016, 2018).

Testing independence of $X$ and $Y$ consistently when one or both of the dimensions $p$ and $q$ are larger than one is substantially more challenging, as noted in Feuerverger (1993, Section 7). Solutions have not been discovered until much more recently. Two tracks were pursued. First, Székely et al. (2007) generalized Feuerverger’s statistic to multivariate cases and proposed a new dependence measure termed “distance covariance”. It has been shown that under the existence of finite marginal first moments, the distance covariance is zero if and only if $H_0$ holds. For further extensions, Lyons (2013) generalized distance covariance/correlation to general metric spaces, and Jakobsen (2017) considered the corresponding test of independence in metric spaces.

The second track to characterize non-linear, non-monotone dependence is based on the maximal correlation introduced in Hirschfeld (1935) and Gebelein (1941), reformulated and examined by Rényi (1959a,b). Gretton et al. (2005c,a,b) extended this idea to examine multivariate cases, resulting in the Hilbert-Schmidt independence criterion (HSIC), which is a consistent kernel-based measure of dependence in multivariate cases. Interestingly, Gretton et al. (2008) connected HSIC with a Gaussian kernel to the characteristic function-based statistic raised in Feuerverger (1993), and Sejdinovic et al. (2013) pointed out the equivalence between distance covariance in general metric spaces and the kernel-based independence criterion.

A notable feature of both distance- and kernel-based statistics is that their null distributions depend on the distributions of $X$ and $Y$ even in the large-sample limit. This dependence arises already for $p = q = 1$ and is usually difficult to estimate. As a consequence, the tests are, unlike the rank tests of, e.g., Hoeffding (1948) and Blum et al. (1961), no longer distribution-free and permutation analysis has to be conducted to implement them. To remedy this problem, Székely et al. (2007) proposed a nonparametric test based on distance correlation by applying a universal upper tail probability bound for all quadratic forms of centered Gaussian random variables that have their mean equal to one (Székely and Bakirov, 2003). However, in practice this upper bound is usually too conservative for the approach to be a competitor to the computationally much more expensive permutation test (Székely and Rizzo, 2009; Gretton et al., 2008). This triggers the following question: For general $p, q > 1$, does there exist an asymptotically accurate consistent test of $H_0$ that is distribution-free and hence directly implementable?

Rank-based tests constitute a natural approach to answering the above question. Indeed, in contrast to Székely and Rizzo (2009), Rémillard (2009) claimed that the methods based on marginal ranks are effective and as powerful as original ones when the sample size is moderately large and this idea has been explored in depth in Lin (2017). However, Bakirov et al. (2006) notes that “[t]he method is also applicable for ranks, but this does not make [the] test distribution-free because ranks typically make tests distribution-free only in one dimension”, which is also recorded in, e.g., Theorem 2.3.2 in Lin (2017). Using the idea of projection from Escanciano (2006), Zhu et al. (2017) generalized Hoeffding’s $D$ to multivariate cases, and Kim et al. (2018) proposed the analogues of Blum–Kiefer–Rosenblatt’s $R$ and Bergsma–Dassios–Yanagimoto’s $\tau^*$. Weihs et al. (2018) proposed other multivariate extensions of Hoeffding’s $D$, Blum–Kiefer–Rosenblatt’s $R$, and Bergsma–Dassios–
Yanagimoto’s $\tau^*$, and did numerical studies comparing them to distance covariance applied to marginal ranks. Alternatively, Heller et al. (2013) developed a consistent multivariate test based on ranked distance covariance by transferring the original problem to testing independence of an aggregated $2 \times 2$ contingency table. However, all the aforementioned tests are not distribution-free when $p$ or $q$ is larger than 1, and due to the difficulty of accounting for the dependence within $X$ and $Y$, permutation analysis is required for their implementation. On the other hand, Heller et al. (2012) introduced distribution-free graph-based tests; however, it is unclear if their proposed tests are consistent.

This paper proposes a solution to the above question by combining Székely, Rizzo, and Bakirov’s distance covariance with a recently defined multivariate rank due to Hallin (2017), hereafter called Hallin’s (multivariate) rank. Due to the lack of a canonical ordering on $\mathbb{R}^d$ for $d > 1$, fundamental concepts related to distribution functions in dimension $d = 1$, such as ranks and quantiles, do not admit a simple extension for $d \geq 2$ that maintains properties such as distribution-freeness. To overcome this limitation, several types of multivariate ranks have been introduced; see Hallin (2017, Sec. 1.3) and, more recently, Ghosal and Sen (2019) for a literature review. None of them, however, is distribution-free except for pseudo-Mahalanobis ranks (Hallin and Paindaveine, 2002b,a), but these are restricted to the class of elliptically symmetric distributions (Fang et al., 1990). Recently, Chernozhukov et al. (2017) introduced the concept of Monge–Kantorovich ranks for all distributions with convex and compact supports, which is the first type of multivariate ranks that enjoys distribution-freeness for a rich class of distributions. Hallin (2017) generalized this definition further by refraining from moment assumptions and making the solution more explicit. As shall be seen soon, the explicit nature of the solution is important as it allows for more delicate manipulations and ultimately allows us to form a test statistic of $H_0$ whose limiting null distribution can be determined. The limiting distribution furnishes an accurate approximation to the statistic’s null distribution already for moderate sample sizes and allows us to avoid computationally more involved permutation analysis.

In detail, our proposed test is based on applying distance covariance to Hallin’s vector-valued ranks. We show that the test is consistent and distribution-free over the class of multivariate distributions with nonvanishing (Lebesgue) probability densities; see Section 2 for the precise definition of this class. The consistency is a consequence of a result of Figalli (2018). In light of the prior work of Székely et al. (2007), Hallin (2017), and Figalli (2018), our major new discovery is the form of the limiting null distribution of the test statistic, which is established with all parameters given explicitly. To this end, we study the weak convergence of U-statistics with a “degenerate” kernel and dependent (permutation) inputs, and derive a general combinatorial non-central limit theorem (non-CLT) for double- and multiple-indexed permutation statistics. This theorem is new and of independent interest beyond our particular application of asymptotic calibration of the size of the independence test under $H_0$.

As we were completing this manuscript, we became aware of an independent work by Deb and Sen (Deb and Sen, 2019) who also propose a rank-distance-covariance-based independence test. Their preprint was posted a few days before ours and presents, in particular, a result very similar to our Corollary 4.1. The derivations differ markedly, however. Deb and Sen’s proof uses techniques based on characteristic functions, whereas we develop a general combinatorial non-CLT theorem for
double- and multiple-indexed permutation statistics that can be applied to the considered statistic as well as possible modifications. There are further differences in the precise setup of multivariate ranks, and while we base ourselves directly on recent work by Hallin and by Figalli, Deb and Sen present weakened assumptions in the definition of the ranks.

The rest of the paper is organized as follows. Section 2 introduces Hallin’s multivariate rank, and Section 3 specifies the proposed test. Section 4 gives the theoretical analysis, including the combinatorial non-CLT and a study of the proposed test. Computational aspects are discussed in Section 5, and numerical studies of the finite-sample behavior of our test are presented in Section 6. All proofs are relegated to a supplement.

**Notation.** The sets of real and positive integer numbers are denoted \( \mathbb{R} \) and \( \mathbb{Z}_+ \), respectively. For \( n \in \mathbb{Z}_+ \), we define \( [n] = \{1, 2, \ldots, n\} \). We write \( \{x_1, \ldots, x_n\} \) and \( \{x_i\}_{i=1}^n \) for the multiset consisting of (possibly duplicate) elements \( x_1, \ldots, x_n \). We use \( [x_1, \ldots, x_n] \) and \( [x_i]_{i=1}^n \) to denote sequences. A permutation of a multiset \( S = \{x_1, \ldots, x_n\} \) is a sequence \( [x_{\sigma(i)}]_{i=1}^n \), where \( \sigma \) is a bijection from \( [n] \) to itself. The family of all distinct permutations of a multiset \( S \) is denoted \( \mathcal{P}(S) \). The Euclidean norm of \( v \in \mathbb{R}^d \) is written \( \|v\| \). We write \( I_d \) and \( J_d \) for the identity matrix and all-ones matrix in \( \mathbb{R}^{d \times d} \), respectively.

For a sequence of vectors \( v_1, \ldots, v_d \), we use \( (v_1, \ldots, v_d) \) as a shorthand of \( (v_1^T, \ldots, v_d^T)^T \). For a function \( f: \mathcal{X} \to \mathbb{R} \), we define \( \|f\|_\infty := \max_{x \in \mathcal{X}} |f(x)| \). The greatest integer less than or equal to \( x \in \mathbb{R} \) is denoted \( \lfloor x \rfloor \). The symbol \( 1(\cdot) \) stands for the indicator function. Throughout, \( c \) and \( C \) refer to positive absolute constants whose values may differ in different parts of the paper. For any two real sequences \( [a_n]_n \) and \( [b_n]_n \), we write \( a_n = O(b_n) \) if there exists \( C > 0 \) such that \( |a_n| \leq C|b_n| \) for all \( n \) large enough, and \( a_n = o(b_n) \) if for any \( c > 0 \), \( |a_n| \leq c|b_n| \) holds for all \( n \) large enough. The symbols \( S_d, \mathbb{S}_d, \mathbb{S}_{d-1} \) stand for the open unit ball, the closed unit ball, and the unit sphere in \( \mathbb{R}^d \), respectively. We use \( \xrightarrow{d} \) and \( \xrightarrow{a.s.} \) to denote convergence in distribution and almost sure convergence.

## 2 Hallin’s multivariate rank

In this section, we introduces necessary background on Hallin’s multivariate rank. As in Hallin (2017), we will be focused on the family of absolutely continuous distributions on \( \mathbb{R}^d \) that have a nonvanishing (Lebesgue) probability density (Definition 2.1 below). In what follows it is understood that the dimension \( d \) could be larger than 1 and that all considered probability measures are fixed, and not to be changed with the sample size \( n \) in particular.

**Definition 2.1.** Let \( P \) be an absolutely continuous probability measure on \( \mathbb{R}^d \) with (Lebesgue) density \( f \). Such \( P \) is said to be a nonvanishing probability measure/distribution if for all \( D > 0 \) there exist constants \( \Lambda_{D,f} \geq \lambda_{D,f} > 0 \) such that \( \lambda_{D,f} \leq f(x) \leq \Lambda_{D,f} \) for all \( \|x\| \leq D \). We write \( \mathcal{P}_d \) for the family of all nonvanishing probability measures/distributions on \( \mathbb{R}^d \).

The considered generalization of ranks to higher dimensions rests on the following concept of a center-outward distribution function, whose existence and uniqueness within the family \( \mathcal{P}_d \) is guaranteed by the Main Theorem in McCann (1995, p. 310).
Definition 2.2 (Definition 4.1 in Hallin, 2017). The center-outward distribution function $F_{\pm}$ of a probability measure $P \in \mathcal{P}_d$ is the unique function that (i) is the gradient of a convex function on $\mathbb{R}^d$, (ii) maps $\mathbb{R}^d$ to the open unit ball $S_d$, and (iii) pushes $P$ forward to $U_d$, where $U_d$ is the product of the uniform measure on $[0,1)$ (for the radius) and the uniform measure on the unit sphere $S_{d-1}$. To be explicit, property (iii) requires $U_d(B) = P(\mathbf{F}_\pm(B))$ for any Borel set $B \subseteq S_d$.

If $X \sim P \in \mathcal{P}_d$ and we further have $\mathbb{E}\|X\|^2 < \infty$, then the center-outward distribution function $F_{\pm}$ of $P$ coincides with the $L_2$-optimal transport from $P$ to $U_d$ (Villani, 2009, Theorem 9.4), i.e., it is the unique solution to the following optimization problem,

$$\inf_T \int_{\mathbb{R}^d} \|T(x) - x\|^2 dP \quad \text{subject to } T_*P = U_d,$$

where $T_*P$ denotes the push forward of $P$ under map $T$. In other words, the optimization is done over all Borel-measurable maps from $\mathbb{R}^d$ to $\mathbb{R}^d$ pushing $P$ forward to $U_d$. Assuming further that the Caffarelli’s regularity conditions including compactness of support (Chernozhukov et al., 2017, Lemma 2.1) hold, $F_{\pm}$ coincides with the Monge–Kantorovich vector rank transformation $R_P$ proposed in Definition 2.1 in Chernozhukov et al. (2017). Lastly, it can be easily checked that when $d = 1$, $F_{\pm}$ reduces to $2F - 1$, where $F$ is the usual cumulative distribution function.

In dimension $d = 1$, the distribution function $F$ determines the underlying probability distribution $P$. A natural question is then whether $F_{\pm}$ similarly preserves all information about a distribution $P \in \mathcal{P}_d$ when $d > 1$. That this is indeed the case turns out to be highly nontrivial, and was not resolved until very recently. The following proposition shows that $F_{\pm}$ is (nearly) a homeomorphism from $\mathbb{R}^d$ to $S_d$, indicating that all the information about the probability measure $P \in \mathcal{P}_d$ can be captured using $F_{\pm}$. This proposition will play a key role in our later justification of the consistency of our proposed test (Theorem 3.1).

Proposition 2.1 (Theorem 1.1 in Figalli, 2018; Propositions 4.1, 4.2 in Hallin, 2017). Let $P \in \mathcal{P}_d$, with center-outward distribution function $F_{\pm}$. Then,

(i) $F_{\pm}$ is a probability integral transformation of $\mathbb{R}^d$, that is, $X \sim P$ iff $F_{\pm}(X) \sim U_d$;

(ii) The set $F_{\pm}^{-1}(0)$ is compact and of Lebesgue measure zero. The restrictions of $F_{\pm}$ and $F_{\pm}^{-1}$ to $\mathbb{R}^d \setminus F_{\pm}^{-1}(0)$ and $S_d \setminus \{0\}$ are homeomorphisms between $\mathbb{R}^d \setminus F_{\pm}^{-1}(0)$ and $S_d \setminus \{0\}$. If $d = 1, 2,$

then the set $F_{\pm}^{-1}(0)$ is singleton, and $F_{\pm}$ and $F_{\pm}^{-1}$ are homeomorphisms between $\mathbb{R}^d$ and $S_d$.

We now move on to estimation of $F_{\pm}$ based on $n$ independent copies of $X \sim P \in \mathcal{P}_d$. The considered estimator mimics the empirical version of the Monge–Kantorovich problem (2.1), and the key step is to “discretize” the unit ball $S_d$ to $n$ grid points. In the following we sketch Hallin’s approach to the construction of such an estimator, with a focus on how to form the grid points when $d > 2$. To this end, let us first factorize $n$ into the following form, whose existence is clear:

$$n = n_R n_S + n_0, \quad n_S = \prod_{m=1}^{d-1} n_m, \quad n_R, n_1, n_2, \ldots, n_{d-1} \in \mathbb{Z}_+, \quad 0 \leq n_0 < \min\{n_R, n_S\},$$

with $n_R, n_1, n_2, \ldots, n_{d-1} \to \infty$ as $n \to \infty$. (2.2)

To construct deterministic points inside the unit ball, we consider spherical coordinates. Let $t = (t_1, \ldots, t_d)^\top \in \mathbb{R}^d$ be a vector in Cartesian coordinates. Its spherical coordinates $(r, \varphi_1, \ldots, \varphi_{d-1})^\top$
are defined implicitly as
\[ t_1 = r \cos(\varphi_1), \quad t_2 = r \sin(\varphi_1) \cos(\varphi_2), \]
\[ \vdots \]
\[ t_{d-1} = r \sin(\varphi_1) \cdots \sin(\varphi_{d-2}) \cos(\varphi_{d-1}), \]
\[ t_d = r \sin(\varphi_1) \cdots \sin(\varphi_{d-2}) \sin(\varphi_{d-1}), \]
(2.3)

where \( r \in [0, \infty), \varphi_1, \ldots, \varphi_{d-2} \in [0, \pi], \) and \( \varphi_{d-1} \in [0, 2\pi). \) Notice that the inverse transform is unique, while the transform is not unique in some special cases: if \( r = 0, \) then \( \varphi_1, \ldots, \varphi_{d-1} \) are arbitrary; if \( \varphi_m \in \{0, \pi\}, \) then \( \varphi_{m+1}, \ldots, \varphi_{d-1} \) are arbitrary. To avoid any ambiguity, we make the spherical coordinates unique by specifying that arbitrary coordinates are zero in these cases.

The approximation problem is then settled in two steps. In the first step, and specified in the following lemma, we choose a set of points on the unit sphere such that the uniform distribution on this set will weakly converge to the uniform distribution over \( S_{d-1}. \)

**Lemma 2.1.** For each \( m \in [d-1], \) let \( u_{m,j} = (2j - 1)/(2n_m) \) for \( j \in [n_m], \) and define the function \( g_m : [0, \pi] \to \mathbb{R} \) as
\[ g_m(\theta) := \begin{cases} 
  \frac{1}{2^{m-1}} \sum_{k=0}^{(m-1)/2} (-1)^{(m-1)/2-k} \binom{m}{k} \frac{1 - \cos((m-2k)\theta)}{m-2k}, & \text{if } m \text{ is odd}, \\
  \frac{1}{2^m} \binom{m}{m/2} \theta + \frac{1}{2^{m-1}} \sum_{k=0}^{(m-2)/2} (-1)^{(m/2-k)} \binom{m}{k} \frac{\sin((m-2k)\theta)}{m-2k}, & \text{if } m \text{ is even.}
\end{cases} \]
(2.4)

Let
\[ \varphi_{m,j} = \begin{cases} 
  g_{d-1-m}^{-1} \left( \frac{\sqrt{n}}{2 \pi u_{d-1,j}} \right) u_{m,j}, & \text{for } m \in [d-2] \text{ and } j \in [n_m], \\
  2\pi u_{d-1,j}, & \text{for } m = d-1 \text{ and } j \in [n_{d-1}].
\end{cases} \]
(2.5)

Then the uniform distribution on the set \( \{ t_{j_1,\ldots,j_{d-1}}; j_1 \in [n_1], \ldots, j_{d-1} \in [n_{d-1}] \} \) of points with spherical coordinates \( (1, \varphi_{1,j_1}, \ldots, \varphi_{d-1,j_{d-1}})^T \) weakly converges to the uniform distribution over \( S_{d-1} \) as \( n_1, \ldots, n_{d-1} \to \infty. \)

In the second step, we expand the above approximation over the sphere to an approximating augmented grid for the ball.

**Definition 2.3.** Let \( r_j = j/(n_R + 1) \) for \( j \in [n_R], \) and define \( \varphi_{m,j} \) for \( m \in [d-1], j \in [n_m] \) as in (2.5). With notation \( n_S := (n_1, \ldots, n_{d-1})^T, \) the augmented grid \( \mathcal{G}_{n_0,n_R,n_S}^d \) is the multiset consisting of \( n_0 \) copies of the origin \( 0 \) whenever \( n_0 > 0 \) and the points \( t_{j_{R},j_1,\ldots,j_{d-1}} \) for \( j_R \in [n_R], j_1 \in [n_1], \ldots, j_{d-1} \in [n_{d-1}] \) that have spherical coordinates \( (r_j, \varphi_{1,j_1}, \ldots, \varphi_{d-1,j_{d-1}})^T. \)

The following proposition is an immediate corollary of Lemma 2.1 and shall later be used in justifying our proposed test.

**Proposition 2.2.** The uniform distribution on the augmented grid \( \mathcal{G}_{n_0,n_R,n_S}^d, \) which assigns mass \( n_0/n \) to the origin and mass \( 1/n \) to every other grid point, weakly converges to \( U_d. \)
We are now ready to introduce Hallin’s estimator, $F_{\pm}^{(n)}$, of $F_{\pm}$. It is defined via the optimal coupling between the observed data points and the augmented grid $G_{n_0,n_R,n_S}^d$.

**Definition 2.4** (Definition 4.2 in Hallin, 2017). Let $x_1, \ldots, x_n$ be data points in $\mathbb{R}^d$. Let $T$ be the collection of all bijective mappings between the multiset $\{x_i\}_{i=1}^n$ and the augmented grid $G_{n_0,n_R,n_S}^d$.

The empirical center-outward distribution function is defined as

$$F_{\pm}^{(n)} := \arg\min_{T \in T} \sum_{i=1}^n \|x_i - T(x_i)\|^2,$$

and $F_{\pm}^{(n)}(x_i)$ is called Hallin’s (multivariate) rank of $x_i$.

The following two propositions from Hallin (2017) give the Glivenko–Cantelli strong consistency and distribution-freeness of the empirical center-outward distribution function. Both shall play key roles for the asymptotic consistency and limiting null distribution of the test statistic that will be proposed in Section 3.

**Proposition 2.3** (Glivenko–Cantelli, Proposition 5.1 in Hallin, 2017, Theorem 3.1 in del Barrio et al., 2018). Let $X_1, \ldots, X_n$ be i.i.d. with distribution $P \in \mathcal{P}_d$, center-outward distribution function $F_{\pm}$, and empirical center-outward distribution function $F_{\pm}^{(n)}$. Then

$$\max_{1 \leq i \leq n} \left\| F_{\pm}^{(n)}(X_i) - F_{\pm}(X_i) \right\| \overset{a.s.}{\rightarrow} 0$$

(2.7) when $n \to \infty$ and (2.2) holds.

**Proposition 2.4** (Distribution-freeness, Proposition 6.1 in Hallin, 2017). Let $X_1, \ldots, X_n$ be i.i.d. with distribution $P \in \mathcal{P}_d$. Let $F_{\pm}^{(n)}$ be their empirical center-outward distribution function. Then for any decomposition $n_0, n_R, n_S$ of $n$, the random vector $[F_{\pm}^{(n)}(X_1), \ldots, F_{\pm}^{(n)}(X_n)]$ is uniformly distributed over $\mathcal{P}(G_{n_0,n_R,n_S}^d)$. The latter set is comprised of all permutations of the multiset $G_{n_0,n_R,n_S}^d$; recall the notation introduced at the end of Section 1.

## 3 A distribution-free test of independence

This section introduces the proposed distribution-free test of $H_0$ in (1.1) built on Hallin’s rank. The main new methodological idea is simple: We propose to plug the calculated Hallin’s multivariate ranks, instead of the original data, into the consistent test statistics presented in the introduction (Section 1). The distribution theory for the proposed test statistic, however, is non-trivial and requires new technical developments, which shall be detailed in Section 4.

To illustrate our idea, we will focus on one particular consistent test statistic in the sequel, namely, the distance covariance of Székely et al. (2007). Other choices including HSIC and more recent proposals like the ball covariance proposed in Pan et al. (2019) shall be discussed in Section 4 following the presentation of our general combinatorial non-CLT.

We begin with details on the distance covariance that are necessary to convey the main idea. We first introduce a representation of the associated measure of dependence.
Definition 3.1 (Distance covariance measure of dependence, Székely et al. (2007)). Let $X \in \mathbb{R}^p$ and $Y \in \mathbb{R}^q$ be two random vectors with $\mathbb{E}(\|X\| + \|Y\|) < \infty$, and let $(X', Y')$ be an independent copy of $(X, Y)$. The distance covariance of $(X, Y)$ is defined as
\[
d Cov^2(X, Y) := \mathbb{E}(d_X(x, X')d_Y(y, Y')),
\] which is finite and uses the kernel function
\[
d_X(x, x') := \|x - x'\| - \mathbb{E}\|x - X'\| - \mathbb{E}\|x - X'\| + \mathbb{E}\|x - X'\|,
\] and its analogue $d_Y(y, y')$.

The finiteness of $d Cov^2(X, Y)$ in (3.1) was proved by Lyons (2013, Proposition 2.3). It can be shown that under the same conditions as in Definition 3.1,
\[
d Cov^2(X, Y) = \frac{1}{4}\mathbb{E}(s(X_1, X_2, X_3, X_4)s(Y_1, Y_2, Y_3, Y_4)),
\] where $(X_1, Y_1), \ldots, (X_4, Y_4)$ are independent copies of $(X, Y)$ and
\[
s(t_1, t_2, t_3, t_4) := \|t_1 - t_2\| + \|t_3 - t_4\| - \|t_1 - t_3\| - \|t_2 - t_4\|;
\] see also Bergsma and Dassios (2014, Sec. 3.4). Accordingly, we have an unbiased estimator of the distance covariance between $X$ and $Y$ as follows.

Definition 3.2 (Sample distance covariance, Székely and Rizzo (2013)). Let $(X_1, Y_1), \ldots, (X_n, Y_n)$ be independent copies of $(X, Y)$ with $X \in \mathbb{R}^p$, $Y \in \mathbb{R}^q$, $\mathbb{E}(\|X\| + \|Y\|) < \infty$. The sample distance covariance is defined as
\[
d Cov^2_n([X_i]_{i=1}^n, [Y_i]_{i=1}^n) = \left(\frac{n}{4}\right)^{-1}\sum_{1 \leq i_1 < \cdots < i_4 \leq n} K((X_{i_1}, Y_{i_1}), \ldots, (X_{i_4}, Y_{i_4})),
\] where
\[
K((x_1, y_1), \ldots, (x_4, y_4)) := \frac{1}{4 \cdot 4!}\sum_{[i_1, \ldots, i_4] \in \mathcal{S}(\{4\})} s(x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4})s(y_{i_1}, y_{i_2}, y_{i_3}, y_{i_4}).
\]
This definition is equivalent to Definition 5.3 in Jakobsen (2017).

We are now ready to describe our distribution-free test of independence, which combines distance covariance with Hallin’s rank. In particular, we derive the limiting null distribution of our proposed statistics. To this end, let $(X_1, Y_1), \ldots, (X_n, Y_n)$ be a sample consisting of independent copies of $(X, Y)$, where $X \sim P$ for $P \in \mathcal{P}_p$ with center-outward distribution function $F_{1, \pm}$, and $Y \sim Q$ for $Q \in \mathcal{P}_q$ with center-outward distribution function $F_{2, \pm}$. We find it helpful to first consider the following “oracle” and infeasible test statistic:
\[
\tilde{M}_n := n \cdot d Cov^2_n([F_{1, \pm}(X_i)]_{i=1}^n, [F_{2, \pm}(Y_i)]_{i=1}^n).
\] The infeasibility stems from the use of the population center-outward distribution functions. Theorem 5.10 in Jakobsen (2017) then leads to the following proposition.

Proposition 3.1. Let $(U_1, V_1), \ldots, (U_n, V_n)$ be independent copies of $(U, V)$, where $U \sim U_p$ and
\( \mathbf{V} \sim \mathbf{U}_q \) are independent. As \( n \to \infty \),

\[
n \cdot \text{dCov}^2_n \left( [\mathbf{U}]_{i=1}^n, [\mathbf{V}]_{i=1}^n \right) \xrightarrow{d} \sum_{k=1}^{\infty} \lambda_k (\xi_k^2 - 1),
\]

where \( \lambda_k, k \in \mathbb{Z}_+ \), are the non-zero eigenvalues of the integral equation

\[
\mathbb{E}(d_\mathbf{U}(\mathbf{u}, \mathbf{U})d_\mathbf{V}(\mathbf{v}, \mathbf{V})\phi(\mathbf{U}, \mathbf{V})) = \lambda \phi(\mathbf{u}, \mathbf{v}),
\]

in which \( d_\mathbf{U}(\mathbf{u}, \mathbf{u}') \) and \( d_\mathbf{V}(\mathbf{v}, \mathbf{v}') \) are defined as in (3.2), and \( [\xi_k]_{k=1}^\infty \) is a sequence of independent standard Gaussian random variables.

An immediate corollary of Proposition 3.1 gives the asymptotic distribution of the infeasible test statistic \( \widetilde{M}_n \).

**Corollary 3.1.** Let \( (\mathbf{X}_1, \mathbf{Y}_1), \ldots, (\mathbf{X}_n, \mathbf{Y}_n) \) be independent copies of \((\mathbf{X}, \mathbf{Y})\), where \( \mathbf{X} \sim P \) with \( P \in \mathcal{P}_p \), \( \mathbf{Y} \sim Q \) with \( Q \in \mathcal{P}_q \), and \( \mathbf{X} \) and \( \mathbf{Y} \) are independent. Then it holds that

\[
\widetilde{M}_n \xrightarrow{d} \sum_{k=1}^{\infty} \lambda_k (\xi_k^2 - 1),
\]

as \( n \to \infty \), where \( [\lambda_k]_{k=1}^\infty \) and \( [\xi_k]_{k=1}^\infty \) are defined as in Proposition 3.1.

Therefore, we have an infeasible test using statistic \( \widetilde{M}_n \) for any pre-specified significance level \( \alpha \in (0, 1) \) as follows:

\[
\overline{T}_\alpha := I \left( \widetilde{M}_n > Q_{1-\alpha} \right), \quad Q_{1-\alpha} := \inf \left\{ x \in \mathbb{R} : \mathbb{P} \left( \sum_{k=1}^{\infty} \lambda_k (\xi_k^2 - 1) \leq x \right) \geq 1 - \alpha \right\}.
\]

It should be highlighted that the values of \( \lambda_k \)'s are distribution independent and only depend on the dimensions \( p \) and \( q \). The values may thus be calculated using numerical methods (for each pair of \( p \) and \( q \)). The details of the computation of \( Q_{1-\alpha} \) will be described in Section 5.2.

The infeasibility of the above test \( \overline{T}_\alpha \) results from the fact that in practice we do not know the values of \([F_{1,\pm}(\mathbf{X}_i)]_{i=1}^n\) and \([F_{2,\pm}(\mathbf{Y}_i)]_{i=1}^n\) based only on finite samples. However, it is reasonable to approximate \([F_{1,\pm}(\mathbf{X}_i)]_{i=1}^n\) and \([F_{2,\pm}(\mathbf{Y}_i)]_{i=1}^n\) by their empirical counterparts in view of Proposition 2.3. We hence make the following proposal for a feasible test statistic:

**Definition 3.3 (The proposed distribution-free test statistic).** Let \( (\mathbf{X}_1, \mathbf{Y}_1), \ldots, (\mathbf{X}_n, \mathbf{Y}_n) \) be independent copies of \((\mathbf{X}, \mathbf{Y})\), where \( \mathbf{X} \in \mathbb{R}^p \) and \( \mathbf{Y} \in \mathbb{R}^q \). Let \( \mathbf{F}_{1,\pm}^{(n)} \) and \( \mathbf{F}_{2,\pm}^{(n)} \) be the empirical center-outward distribution functions for \( \{\mathbf{X}_i\}_{i=1}^n \) and \( \{\mathbf{Y}_i\}_{i=1}^n \). We define the test statistic

\[
\widetilde{M}_n := n \cdot \text{dCov}^2_n \left( [\mathbf{F}_{1,\pm}^{(n)}(\mathbf{X}_i)]_{i=1}^n, [\mathbf{F}_{2,\pm}^{(n)}(\mathbf{Y}_i)]_{i=1}^n \right).
\]

Due to (i) the near-homeomorphism property of the center-outward distribution function shown in Proposition 2.1; (ii) the strong Glivenko-Cantelli consistency of Hallin’s ranks shown in Proposition 2.3; and (iii) the fact that the distance covariance measure of dependence is zero if and only if \( H_0 \) holds under finiteness of marginal first moments (Lyons, 2013, Theorem 3.11), it holds that \( \widetilde{M}_n \) is asymptotically consistent. This fact is summarized in the following theorem.
Theorem 3.1 (Asymptotic consistency). Let \((X_1, Y_1), \ldots, (X_n, Y_n)\) be independent copies of \((X, Y)\), where \(X \sim P\) for \(P \in P_p\) with center-outward distribution function \(F_{1,\pm}\), and \(Y \sim Q\) for \(Q \in P_q\) with center-outward distribution function \(F_{2,\pm}\). We then have
\[
\frac{\hat{M}_n}{n} \overset{a.s.}{\to} \text{dCov}^2\left(F_{1,\pm}(X), F_{2,\pm}(Y)\right)
\]
as \(n \to \infty\) and (2.2) holds. In addition, \(\text{dCov}^2\left(F_{1,\pm}(X), F_{2,\pm}(Y)\right) \geq 0\) with equality if and only if \(X\) and \(Y\) are independent.

By Proposition 2.4, the statistic \(\hat{M}_n\) is distribution-free under the independence hypothesis \(H_0\) in (1.1). Hence, an exact critical value for rejection of \(H_0\) can be approximated via Monte Carlo simulation. Numerically less demanding, one could instead adopt the critical value that comes from the asymptotic form of the infeasible test statistic \(\tilde{M}_n\) shown in Corollary 3.1, i.e., \(H_0\) is rejected if
\[
\hat{M}_n > Q_{1-\alpha},
\]
where \(Q_{1-\alpha}\) is defined as in (3.4). For any pre-specified significance level \(\alpha \in (0, 1)\), our proposed test is hence
\[
T_\alpha := \mathbb{1}\left(\hat{M}_n > Q_{1-\alpha}\right).
\]
In Section 4 we will show that this test is indeed able to accurately control the size as \(n \to \infty\). In fact, somewhat surprising to us, the limiting null distribution of \(\hat{M}_n\) is the same as that of \(\tilde{M}_n\).

4 Theoretical analysis

This section provides the theoretical justification for the test from (3.7). By Proposition 2.4, both \([F_{1,\pm}^{(n)}(X_i)]_{i=1}^n\) and \([F_{2,\pm}^{(n)}(Y_i)]_{i=1}^n\) are generated from uniform permutation measures. In view of Definition 3.3, it is hence clear that under \(H_0\) the test statistic \(\hat{M}_n\) is a summation over the product space of two uniform permutation measures, which belongs to the family of permutation statistics.

The study of permutation statistics can be traced back at least to Wald and Wolfowitz (1944), who proved an asymptotic normality result for single-indexed permutation statistics of the form \(\sum_{i=1}^n x_i^{(n)} y_i^{(n)}\). Here \(x^{(n)}\) and \(y^{(n)}\) are vectors that are possibly varying with \(n\), and \(\pi\) is uniformly distributed on \(\mathcal{P}([n])\). Later, Hoeffding (1951), Motoo (1957), and Hájek (1961), among many others, generalized Wald and Wolfowitz’s results in different ways, and Bolthausen (1984) gave a sharp Berry–Esseen bound for such permutation statistics using Stein’s method.

Double-indexed permutation statistics, of the form \(\sum_{i \neq j} A_{ij}^{(n)} B_{\pi_i, \pi_j}^{(n)}\) with \(A^{(n)}\) and \(B^{(n)}\) as matrices possibly varying with \(n\), are more difficult to tackle. They were first investigated by Daniels (1944), who gave sufficient conditions for asymptotic normality. Later, various weakened conditions were introduced in, e.g., Bloemena (1964, Chap. 4.1), Jogdeo (1968), Abe (1969), Cliff and Ord (1973, Chap. 2.4), Shapiro and Hubert (1979), Barbour and Eagleson (1986), Pham et al. (1989), and the Berry–Esseen bound was established in Zhao et al. (1997), Barbour and Chen (2005), and Reinert and Röllin (2009).

Despite this vast literature, there is a notable absence of results on permutation statistics which, as its degenerate U-statistics “cousins”, may weakly converge to a non-normal distribution. Our
analysis of $\hat{M}_n$, however, hinges on such a combinatorial non-CLT. In the following, we present two general theorems that fill the gap.

Before stating the two theorems, we introduce some notions needed. For each $i = 1, 2$, let $\mathbf{Z}_i$ be a random vector taking values in $\Omega_i$, a compact subset of $\mathbb{R}^{p_i}$. We consider triangular arrays 
\begin{equation*}
\{\mathbf{z}_{i,j}^{(n)}, n \in \mathbb{Z}_+, j \in \{1, \ldots, n\}\}, \text{ for } i = 1, 2,
\end{equation*}

such that the random variables with uniform distributions on the respective multisets 
\begin{equation*}
\{\mathbf{z}_{i,j}^{(n)}, j \in \{1, \ldots, n\}\}, \text{ denoted by } \mathbf{Z}_i^{(n)},
\end{equation*}

weakly converge to $\mathbf{Z}_i$ as $n \to \infty$. We further introduce an independent copy of $\mathbf{Z}_i$, denoted $\mathbf{Z}_i'$, and independent copies of the $\mathbf{Z}_i^{(n)}$, denoted $\mathbf{Z}_i^{(n)'}$. Finally, for $i = 1, 2$ and $n \in \mathbb{Z}_+$, let $g_i^{(n)}, g_i : \Omega_i \to \mathbb{R}$ be real-valued functions, the former of which may change with $n$.

Our first theorem is then focused on double-indexed permutation-statistics of the form

\begin{equation}
\hat{D}^{(n)} = \left( \frac{n}{2} \right)^{-1} \sum_{1 \leq j_1 < j_2 \leq n} g_1^{(n)}(\mathbf{z}_{1,j_1}^{(n)}, \mathbf{z}_{1,j_2}^{(n)}) g_2^{(n)}(\mathbf{z}_{2,j_1}^{(n)}, \mathbf{z}_{2,j_2}^{(n)}),
\end{equation}

where $\pi$ is uniformly distributed on $\mathcal{P}(\{1, \ldots, n\})$.

**Theorem 4.1.** Assume that for each $i = 1, 2$, the functions $g_i^{(n)}$, $n \in \mathbb{Z}_+$, and $g_i$ satisfy the following conditions:

(i) each $g_i^{(n)}$ is symmetric, i.e., $g_i^{(n)}(z, z') = g_i^{(n)}(z', z)$ for all $z, z' \in \Omega_i$;

(ii) the family $g_i^{(n)}$, $n \in \mathbb{Z}_+$, is equicontinuous;

(iii) each $g_i^{(n)}$ is non-negative definite, i.e.,

\begin{equation*}
\sum_{j_1, j_2 = 1}^{\ell} c_{j_1} c_{j_2} g_i^{(n)}(z_{j_1}, z_{j_2}) \geq 0
\end{equation*}

for all $c_1, \ldots, c_\ell \in \mathbb{R}$, $z_1, \ldots, z_\ell \in \Omega_i$, $\ell \in \mathbb{Z}_+$;

(iv) each $g_i^{(n)}$ has $\mathbb{E}(g_i^{(n)}(z, \mathbf{Z}_i^{(n)})) = 0$;

(v) each $g_i^{(n)}$ has $\mathbb{E}(g_i^{(n)}(\mathbf{Z}_i^{(n)})) \in (0, +\infty)$;

(vi) as $n \to \infty$, the functions $g_i^{(n)}$ converge uniformly on $\Omega_i$ to $g_i$, with $\mathbb{E}(g_i(\mathbf{Z}_i, \mathbf{Z}_i')^2) \in (0, +\infty)$.

It then holds that

\begin{equation*}
n \hat{D}^{(n)} \xrightarrow{d} \sum_{k_1, k_2 = 1}^{\infty} \lambda_{1,k_1} \lambda_{2,k_2} (\xi_{k_1,k_2}^2 - 1)
\end{equation*}

as $n \to \infty$, where $\xi_{k_1,k_2}, k_1, k_2 \in \mathbb{Z}_+$, are i.i.d. standard Gaussian, and the $\lambda_{i,k} \geq 0$, $k \in \mathbb{Z}_+$, are eigenvalues of the Hilbert-Schmidt integral operator given by $g_i$. So, for each $i$ the $\lambda_{i,k}$ solve the integral equations

\begin{equation*}
\mathbb{E}(g_i(z_i, \mathbf{Z}_i)e_{i,k}(\mathbf{Z}_i)) = \lambda_{i,k} e_{i,k}(z_i)
\end{equation*}

for a system of orthonormal eigenfunctions $e_{i,k}$.

Theorem 4.1 provides the essential component of our analysis for $\hat{M}_n$. However, $\hat{M}_n$ is a permutation statistic that is not double- but quadruple-indexed. To cover this case, we have to extend
Theorem 4.1 to multiple-indexed permutation statistics, the study of which is much more sparse (see, for example, Raič (2015) for some recent progresses). Further notation is needed.

For all \( j \in \mathbb{Z}_+ \), let \( w_j = (z_{1,j}, z_{2,j}) \) be a vector with \( z_{i,j} \in \Omega_i \), for \( i = 1, 2 \). Let \( h : (\Omega_1 \times \Omega_2)^m \to \mathbb{R} \) be a symmetric kernel of order \( m \), i.e., \( h(w_1, \ldots, w_m) = h(w_{\sigma(1)}, \ldots, w_{\sigma(m)}) \) for all permutations \( \sigma \in \mathcal{P}(\lfloor m \rfloor) \) and \( w_1, \ldots, w_m \in \Omega_1 \times \Omega_2 \). For any integer \( \ell \in \lfloor m \rfloor \), and any measure \( \mathbb{P}_w \), we let

\[
h_{\ell}(w_1, \ldots, w_\ell; \mathbb{P}_w) := \mathbb{E}(h(w_1, \ldots, w_\ell, W_{\ell+1}, \ldots, W_m)),
\]

where \( W_1, \ldots, W_m \) are \( m \) independent random vectors with distribution \( \mathbb{P}_w \).

The next theorem treats a multiple-indexed permutation-statistic of order \( m \) defined as

\[
\hat{\Pi}^{(n)} = \left( \begin{array}{c} n \\ m \end{array} \right)^{-1} \sum_{1 \leq j_1 < \cdots < j_m \leq n} h\left( \left( z_{1,j_1}^{(n)}, z_{2,j_1}^{(n)} \right), \ldots, \left( z_{1,j_m}^{(n)}, z_{2,j_m}^{(n)} \right) \right),
\]

(4.2)

where \( \pi \) is uniformly distributed on \( \mathcal{P}(\lfloor n \rfloor) \), and the triangular arrays \( \{ z_{i,j}^{(n)}, n \in \mathbb{Z}_+, j \in \lfloor n \rfloor \}, i = 1, 2 \) are as introduced before the statement of Theorem 4.1.

**Theorem 4.2.** Let \( Z_i \) and \( Z_i^{(n)} \), \( i = 1, 2 \), be defined as for Theorem 4.1. Assume the kernel \( h \) has the following three properties:

(I) \( h \) is continuous with \( \| h \|_\infty < \infty \);

(II) \( h_1(w_1; \mathbb{P}_Z^{(n)} \times \mathbb{P}_Z^{(n)}) = 0 \);

(III) one has

\[
\binom{m}{2} h_2\left( w_1, w_2; \mathbb{P}_Z^{(n)} \times \mathbb{P}_Z^{(n)} \right) = g_1^{(n)}(z_{1,1}^{(n)}, z_{1,2}^{(n)})g_2^{(n)}(z_{2,1}^{(n)}, z_{2,2}^{(n)}),
\]

and

\[
\binom{m}{2} h_2\left( w_1, w_2; \mathbb{P}_Z^{(n)} \times \mathbb{P}_Z^{(n)} \right) = g_1(z_{1,1}^{(n)}, z_{1,2}^{(n)})g_2(z_{2,1}^{(n)}, z_{2,2}^{(n)}),
\]

where for each \( i = 1, 2 \), \( g_i^{(n)}, n \in \mathbb{Z}_+ \), and \( g_i \) satisfy Assumptions (i)–(vi) from Theorem 4.1.

We then have

\[
n\hat{\Pi}^{(n)} \overset{d}{\to} \sum_{k_1,k_2=1}^{\infty} \lambda_{1,k_1}\lambda_{2,k_2} (\xi_{k_1,k_2}^2 - 1)
\]

as \( n \to \infty \), where \( \lambda_{i,k} \) and \( \xi_{k_1,k_2} \) are defined as in Theorem 4.1.

With the aid of Theorem 4.2, we are now ready to present the limiting null distribution of \( \hat{M}_n \). In our context, \( p_1 = p, p_2 = q, m = 4 \), and \( h \) is the kernel \( K \) defined in (3.3). The multiset \( \{ z_{1,j}^{(n)}, j \in \lfloor n \rfloor \} \) and \( \{ z_{2,j}^{(n)}, j \in \lfloor n \rfloor \} \) are taken to be \( \{ u_j^{(n)}, j \in \lfloor n \rfloor \} := \mathcal{G}_0^{(n)} \) and \( \{ v_j^{(n)}, j \in \lfloor n \rfloor \} := \mathcal{G}_0^{(n)} \), respectively. Accordingly, \( Z_i^{(n)} \) follows the uniform distribution over \( \mathcal{G}_0^{(n)} \), denoted by \( U^{(n)} \), and \( Z_2^{(n)} \) has a uniform distribution over \( \mathcal{G}_0^{(n)} \), denoted by \( V^{(n)} \). The functions \( g_1^{(n)}, g_2^{(n)}, g_1, g_2 \) can be chosen as \( d_{U^{(n)}}, d_{V^{(n)}}, d_U, \) and \( d_V \), defined in the manner of (3.2), respectively.

We now verify properties (I)–(III). Write \( w = (u, v) \) and \( w' = (u', v') \). Notice that the kernel \( K \) is symmetric and continuous on \( \overline{\mathbb{R}}_p \times \overline{\mathbb{R}}_q \). We have

\[
K_1\left( w; \mathbb{P}_U^{(n)} \right) = 0, \quad 6K_2\left( w, w'; \mathbb{P}_U^{(n)} \right) = d_{U^{(n)}}(u, u')d_{V^{(n)}}(v, v'),
\]

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and \(6K_2 \left( \mathbf{w}, \mathbf{w}'; \mathbb{P}_U \times \mathbb{P}_V \right) = d_U(\mathbf{u}, \mathbf{u}')d_V(\mathbf{v}, \mathbf{v}')\), by Yao et al. (2018, Sec. 1.1). Moreover, the \(-d_U(\mathbf{u}, \mathbf{u}')\) are symmetric, non-negative definite (Lyons, 2013, p. 3291), and equicontinuous since
\[
|d_U(\mathbf{u}, \mathbf{u}') - d_U(\mathbf{u}'', \mathbf{u}'')| \leq 2\|\mathbf{u} - \mathbf{u}'\| + 2\|\mathbf{u}' - \mathbf{u}''\|. 
\]
One can verify that \(-d_U(\mathbf{u}, \mathbf{u}')\) converges uniformly to \(-d_U(\mathbf{u}, \mathbf{u}')\) by combining the pointwise convergence using the Portmanteau Lemma (van der Vaart, 1998, Lemma 2.2) and the equicontinuity of \(-d_U(\mathbf{u}, \mathbf{u}')\) (Rudin, 1976, Exercise 7.16). The similar results hold for \(-d_V(\mathbf{v}, \mathbf{v}')\) and \(-d_V(\mathbf{v}, \mathbf{v}')\). Lastly, under \(H_0\), \([F_{1,\pm}(X_i)]_{i=1}^n\) and \([F_{2,\pm}(Y_i)]_{i=1}^n\) are independent with margins uniformly distributed on \(\mathcal{P}(G_{R,0,n_R,n_S})\) and \(\mathcal{P}(G_{Q,0,n_R,n_S})\), respectively. Hence our statistic is distributed of the form (4.2).

In summary, Theorem 4.2 may be applied to the statistic \(\hat{M}_n\) and the following corollary summarizes the result from the above derivations.

**Corollary 4.1** (Limiting null distribution). Let \((X_1, Y_1), \ldots, (X_n, Y_n)\) be independent copies of \((X, Y)\), where \(X \sim P, P \in \mathcal{P}_p, Y \sim Q, Q \in \mathcal{P}_q\), and \(X\) and \(Y\) are independent. Then we have
\[
\hat{M}_n \xrightarrow{d} \sum_{k=1}^\infty \lambda_k(\xi_k^2 - 1),
\]
as \(n \to \infty\) and (2.2) holds, where \(|\lambda_k|_{k=1}^\infty\) and \(|\xi_k|_{k=1}^\infty\) are defined as in Proposition 3.1. Consequently,
\[
\mathbb{P}(T_\alpha = 1 \mid H_0) = \alpha + o(1).
\]

We remark that combining Corollary 4.1 and Theorem 3.1 shows the consistency of the proposed test against any fixed alternative. In addition, although our focus is on the combination of Hallin’s rank with the distance covariance statistic, the general form of our combinatorial non-CLTs (Theorems 4.1 and 4.2) also yields the limiting null distributions for test statistics based on plugging Hallin’s ranks into HSIC-type or ball-covariance statistics (Gretton et al., 2005c,a,b; Pan et al., 2019). We omit the details for these analogies.

### 5 Computational aspects

In this section, we describe the practical implementation of our test. To perform the proposed test, for any given \(n\), we fix a factorization such that
\[
n = n_R n_S + n_0, \quad n_S = \prod_{m=1}^{d-1} n_m, \quad n_R, n_1, n_2, \ldots, n_{d-1} \in \mathbb{Z}_+, \quad 0 \leq n_0 < \min\{n_R, n_S\},
\]
where \(n_R, n_1, \ldots, n_{d-1}\) are chosen to be as close to each other as possible.

First, we need to compute \([F_{1,\pm}(X_i)]_{i=1}^n\) and \([F_{2,\pm}(Y_i)]_{i=1}^n\) as defined in (2.6). This step is discussed in Section 5.1. After obtaining \([F_{1,\pm}(X_i)]_{i=1}^n\) and \([F_{2,\pm}(Y_i)]_{i=1}^n\), the test statistic \(\hat{M}_n\) in (3.5) can be computed using Equation (3.3) in Huo and Székely (2016) in \(O(n^2)\) time. Second, we have to calculate the critical value \(Q_{1-\alpha}\) defined in (3.4). This value can be estimated numerically, as detailed in Section 5.2.
5.1 Assignment problems

Problem (2.6) amounts to a linear sum assignment problem (LSAP), a fundamental problem in linear programming and combinatorial optimization. We define LSAP through graph theory. Consider a weighted (complete) bipartite graph \((S, T; E)\) with \(S := \{s_i\}_{i=1}^n\), \(T := \{t_j\}_{j=1}^n\), \(s_i, t_j \in \mathbb{R}^d\), where in Problem (2.6), \(S = \{X_i\}_{i=1}^n\) and \(T = G_{n_R}^d\). The edge between \(s_i\) and \(t_j\), denoted by \((s_i, t_j)\), has a nonnegative weight \(c_{ij} := \|s_i - t_j\|^2\), \(i, j \in [n]\). We want to find an optimal matching, i.e., a subset of edges such that each vertex is an endpoint of exactly one edge in this subset with a minimum sum of weights of its edges; see Figure 1 for an illustration of \(n = 3\), where edges in the optimal matching are marked in red.

![Figure 1: Bipartite graph formulation of a linear sum assignment problem (LSAP)](image)

Introducing the dummy variables \(x_{ij}\) defined as

\[
x_{ij} = \begin{cases} 1, & \text{if edge } (s_i, t_j) \text{ is in the optimal matching}, \\ 0, & \text{otherwise}, \end{cases}
\]

LSAP can be formulated as a linear program:

\[
\begin{align*}
\min_{x_{ij}} & \quad \sum_{i,j} c_{ij} x_{ij} \\
\text{subject to} & \quad \sum_{j=1}^n x_{ij} = 1, \text{ for } i \in [n]; \quad \sum_{i=1}^n x_{ij} = 1, \text{ for } j \in [n]; \quad x_{ij} \in \{0, 1\}, \quad \text{for } i, j \in [n].
\end{align*}
\]

Then an edge \((s_i, t_j)\) is in the optimal matching if and only if \(x_{ij} = 1\). The dual linear program is

\[
\begin{align*}
\max_{\alpha_i, \beta_j} & \quad \sum_i \alpha_i + \sum_j \beta_j \\
\text{subject to} & \quad \alpha_i + \beta_j \leq c_{ij}, \quad \text{for } i, j \in [n]; \quad \alpha_i, \beta_j \text{ unconstrained.}
\end{align*}
\]

The sufficient and necessary condition for an optimal solution is

\[
\begin{align*}
\alpha_i + \beta_j & \leq c_{ij}, \quad \text{for } i, j \in [n], \\
\alpha_i + \beta_j & = c_{ij}, \quad \text{for } x_{ij} = 1.
\end{align*}
\]

We introduce some terms to state the theorem below. A perfect matching is a subset of edges such
the squared distances if its total weight is no larger than 5
(Gabow and Tarjan (1989), Sharathkumar and Agarwal (2012), Agarwal and Sharathkumar (2014)). Assume that points $s_i, t_j \in \mathbb{R}^d, i, j \in [n]$, have bounded integer coordinates, and that the squared distances $\|s_i - t_j\|^2$, $i, j \in [n]$ are all bounded by some integer $N$. Then there exists an algorithm to find the optimal matching in $O(n^{5/2} \log(nN))$ time. Furthermore,

(i) if $d = 2$, there exists an exact algorithm for computing the optimal matching in $O(n^{3/2 + \delta} \log(N))$ time for any arbitrarily small constant $\delta > 0$;

(ii) if $d \geq 3$, there is an algorithm to compute a $(1 + \epsilon)$-approximate perfect matching in $O(\epsilon^{-1} n^{3/2} \tau(n, \epsilon) \log^4(n/\epsilon) \log(\max c_{ij}/\min c_{ij}))$ time, where $\tau(n, \epsilon)$ depending on $n, \epsilon$ is small.

In the following we will only describe the algorithm developed by Gabow and Tarjan (1989) under the basic settings, while ignoring the details of the faster exact algorithm for $d = 2$ by Sharathkumar and Agarwal (2012) and the approximate algorithm for $d \geq 3$ by Agarwal and Sharathkumar (2014). The Gabow–Tarjan algorithm described below is essentially the combination of Hungarian method (Kuhn, 1955, 1956; Munkres, 1957) and Hopcroft–Karp algorithm (Hopcroft and Karp, 1973).

We introduce more terms for convenience of description. A matching is a subset of edges whose vertices are disjoint. A matching $M$ is 1-feasible if the dual variables satisfy that

$$
\alpha_i + \beta_j \leq c_{ij} + 1, \\
\alpha_i + \beta_j = c_{ij},
$$

for $i, j \in [n]$, $(s_i, t_j) \in M$.

A 1-optimal matching is a 1-feasible perfect matching. An edge $(s_i, t_j)$ is called admissible with regard to a matching $M$ if $\alpha_i + \beta_j = c_{ij} + 1((s_i, t_j) \notin M)$. An admissible graph is the union of matching $M$ and the set of all admissible edges. A vertex is called exposed if it is not incident to any edge in the current matching. An alternating path is one that starts with an exposed vertex and alternatingly traverses edges in the matching and not. An alternating tree is a rooted tree whose paths are alternating paths from its root. A labelled vertex is one that belongs to any alternating tree. An augmenting path is an alternating path between two exposed vertices.

For every $s_i \in S$, $t_j \in T$, let $c_{ij}^* = (n + 1)c_{ij}$. It is equivalent to find the optimal matching for the weights $c_{ij}^*$ and that for the weights $c_{ij}$. Let $b_1b_2 \cdots b_{k(2)}$ stand for the binary representation of $c_{ij}^*$, where $k \leq \lceil \log_2((n + 1)N) \rceil + 1$. We initialize the weights $c_{ij}^{(0)}$ and the dual variables $\alpha_i^{(0)}, \beta_j^{(0)}$, $i, j \in [n]$ to zero and the matching $M$ to empty matching. The scaling algorithm proceeds in $k$ stages. At the $r$-th stage, we go through match routines to find a 1-optimal matching, where the weight $c_{ij}^{(r)}$ of edge $(s_i, t_j)$ has the binary representation $b_1b_2 \cdots b_{r(2)}$ (and thus is equal to $2c_{ij}^{(r-1)}$ or $2c_{ij}^{(r-1)} + 1$), starting from dual variables $\alpha_i^{(r)} := 2\alpha_i^{(r-1)}, \beta_j^{(r)} := 2\beta_j^{(r-1)}, i, j \in [n]$.

The match routine computes a 1-optimal matching in several phases, each of which consists of augmenting the matching and doing a Hungarian search. Let $M$ be the current matching initialized to empty matching. We will omit the superscript index $(r)$ when there is no confusion.

**Step I.** We first obtain a maximal set $\mathcal{P}$ of vertex-disjoint augmenting paths in the admissible graph by performing a depth first search. The depth first search marks every vertex visited; initially
no vertex is marked. We grow an augmenting path $P$ starting from an exposed vertex $t_j \in T$ by searching all admissible edges and finding an edge $(t_j, s_i)$ where $s_i \in S$ is not marked. If such $s_i$ exists, we mark $s_i$, add edge $(t_j, s_i)$ to $P$, and then (1) if $s_i$ is also exposed, add the augmenting path $P$ to $\mathcal{P}$, and start finding the next augmenting path; (2) if $s_i$ is matched to $t_k$ ($k \neq j$ since $s_i$ has not been marked until this step), we mark $t_k$, add edge $(s_i, t_k)$ to $P$, and continue searching from $t_k$. If there is no $s_i$ unmarked, we delete the last two edges in path $P$ and (1) restart searching if $P$ is not empty; (2) initialize a new path otherwise. We repeat these steps until going through all exposed vertices in $T$. Then for each path $P \in \mathcal{P}$, we augment the matching $M$ by replacing edges in the even step with the ones in the odd steps, and decrease dual variables $\alpha_i$ by 1 for all $s_i \in A \cap P$ to maintain 1-feasibility. If the new matching is perfect, the routine halts, otherwise we do a Hungarian search as below.

**Step II.** For each exposed vertex $t_j \in T$, we grow an alternating tree rooted at $t_j$ such that each vertex in $S \cup T$ that in this tree is reachable from the root via an alternating path consisting only of admissible edges. For a vertex in $S$ (resp. $T$) in an alternating tree, the path from the root is augmenting (resp. not augmenting). Let $LS$ (resp. $LT$) denote the set of vertices in $S$ (resp. $T$) that are labelled. At the beginning of Hungarian search, $LT$ is defined as the set of the exposed vertices in $T$ and $LS = \emptyset$. Define

$$
\delta = \min_{s_i \in S-LS, t_j \in LT} \left\{ c_{ij} + 1((s_i, t_j) \notin M) - \alpha_i - \beta_j \right\}.
$$

Depending on whether $\delta = 0$ or $\delta > 0$, one of the following steps is taken:

Case 1. $\delta = 0$ (find an augmenting path or add to alternating trees). Let $(s_i, t_j)$ for $s_i \in S - LS$ and $t_j \in LT$ be an admissible edge, where the existence is guaranteed by $\delta = 0$. If $s_i$ is exposed, an augmenting path has been found and the Hungarian search ends. If $s_i$ is matched to $t_k$ for some $k \neq j$ (notice that $s_i$ cannot be matched to $t_j$ since $s_i$ is not labelled currently), we add the edges $(t_j, s_i)$ and $(s_i, t_k)$ to all the alternating trees that involve $t_j$, update $LS$ and $LT$ by adding vertices $s_i$ and $t_k$ respectively, and recompute $\delta$.

Case 2. $\delta > 0$ (update the dual solution). We decrease $\alpha_i$ by $\delta$ for each $s_i \in LS$, increase $\beta_j$ by $\delta$ for each $t_j \in LT$, and recompute $\delta$.

In summary, there are $O(\log(nN))$ stages. At each stage, one routine consists of $O(\sqrt{n})$ phases, and each phase runs in $O(n^2)$ time. The overall running time is $O(n^{5/2} \log(nN))$.

### 5.2 Eigenvalues and quadratic forms in normal variables

In Proposition 3.1, $\lambda_k$, $k \in \mathbb{Z}_+$, are non-zero eigenvalues (counted with multiplicity) of the integral equation

$$
\mathbb{E}(d_U(u, U')d_V(v, V')\phi(U', V')) = \lambda \phi(u, v).
$$

Under the independence hypothesis $H_0$, the eigenvalues $\lambda_k$, $k \in \mathbb{Z}_+$, are given by all the products $\lambda_1,j_1 \lambda_2,j_2$, $j_1,j_2 \in \mathbb{Z}_+$, where $\lambda_1,j$, $j \in \mathbb{Z}_+$, and $\lambda_2,j$, $j \in \mathbb{Z}_+$, are the non-zero eigenvalues of the integral equations

$$
\mathbb{E}(d_U(u, U')\phi_1(U')) = \lambda_1 \phi_1(u) \quad \text{and} \quad \mathbb{E}(d_V(v, V')\phi_2(V')) = \lambda_2 \phi_2(v),
$$

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The non-zero eigenvalues of integral equation
\[ \mathbb{E}(d_{U}(u, U') \phi(u)) = \lambda_{1} \phi(u) \]
where \( U' \sim U_{p} \) are given by
\[ -4/(\pi^{2} j^{2}), \quad \text{for all } j \in \mathbb{Z}_{+} \text{ when } p = 1. \]

We are not aware of any closed form formulas for the eigenvalues when \( p \geq 2 \). However, in practice, the non-zero eigenvalues \( \{\lambda_{1,j}\}_{j=1}^{\infty} \) can be numerically estimated by the non-zero eigenvalues of the matrix
\[
(I_{N_{1}} - J_{N_{1}}/N_{1})D^{(N_{1})}(I_{N_{1}} - J_{N_{1}}/N_{1})/N_{1},
\]
denoted by \( \lambda^{(N_{1})}_{1,j}, j \in [N^{*}_{1}] \), where \( N_{1} = M^{p}, N^{*}_{1} = N_{1} - 1, D^{(N_{1})} = [D_{jj'}^{(N_{1})}], D_{jj'}^{(N_{1})} = \|u_{j}^{(N_{1})} - u_{j'}^{(N_{1})}\| \) and \( u_{j}^{(N_{1})}, j \in [N_{1}] \), are points in the set \( G_{0, M, M, \ldots, M}^{p} \). Here \( \lambda^{(N_{1})}_{1,j}, j \in [N^{*}_{1}] \) are all negative (Lyons, 2013, p. 3291). For \( p = 1 \), we take \( \lambda^{(N_{1})}_{1,j} = -4/(\pi^{2} j^{2}) \). We can obtain eigenvalues \( \lambda^{(N_{2})}_{2,j}, j \in [N^{*}_{2}], \) where \( N_{2} = M^{q} \), similarly. Then we sort the positive products \( \lambda^{(N_{1})}_{1,j_1} \lambda^{(N_{2})}_{2,j_2}, j_1 \in [N^{*}_{1}], j_2 \in [N^{*}_{2}] \) into a descendingly ordered sequence \( [\lambda^{(M)}_{k}]_{k=1}^{\infty} \), and have the following theorem.

**Theorem 5.2.** Let \( [\lambda_{k}]_{k=1}^{\infty} \) and \( [\lambda^{(M)}_{k}]_{k=1}^{N^{*}_{1}N^{*}_{2}} \) be eigenvalues as defined in Proposition 3.1 and above, respectively. Let \( [\xi_{k}]_{k=1}^{\infty} \) be a sequence of independent standard Gaussian random variables. Then it holds for any pre-specified significance level \( \alpha \in (0, 1) \) that
\[ Q_{1-\alpha}^{(M)} \rightarrow Q_{1-\alpha} \]
as \( M \rightarrow \infty \), where \( Q_{1-\alpha}^{(M)} \) and \( Q_{1-\alpha} \) are the \( (1 - \alpha) \) quantiles of
\[
\sum_{k=1}^{N^{*}_{1}N^{*}_{2}} \lambda^{(M)}_{k} \xi_{k}^{2} - 1 \quad \text{and} \quad \sum_{k=1}^{\infty} \lambda_{k} \xi_{k}^{2} - 1,
\]
respectively.

Consequently, we can approximate the \( (1 - \alpha) \) quantile of quadratic form \( \sum_{k=1}^{\infty} \lambda_{k} \xi_{k}^{2} - 1 \) by estimating that of quadratic form \( \sum_{k=1}^{N^{*}_{1}N^{*}_{2}} \lambda^{(M)}_{k} \xi_{k}^{2} - 1 \) for a sufficiently large \( M \). The latter is done by solving the inverse of the cumulative distribution function of quadratic form \( \sum_{k=1}^{N^{*}_{1}N^{*}_{2}} \lambda^{(M)}_{k} \xi_{k}^{2} - 1 \), which can be numerically evaluated using Farebrother’s (1984) algorithm or Imhof’s (1961) method.

### 6 Numerical studies

We now turn to Monte Carlo simulation experiments on the finite-sample performance of the proposed test from Section 3. We compare the performances of our test using (i) theoretical and (ii) simulation-based rejection thresholds to the existing tests of independence via

(iii) distance covariance with marginal ranks (Lin, 2017);
(iv) distance covariance (Székely and Rizzo, 2013);

We evaluate the empirical sizes and powers of the six competing tests stated above for both Gaussian and non-Gaussian distributions. The values reported below are based on 1, 000 simulations at the nominal significance level of 0.05, with sample size \( n \in \{216, 432, 864, 1728\} \), dimensions
Table 1: Empirical sizes of the proposed test using theoretical (shown in bold font) and simulation-based (shown in parentheses) rejection threshold in Example 6.1.

| n   | p = q = 2  | p = q = 3  | p = q = 5  |
|-----|-----------|-----------|-----------|
| 216 | 0.040 (0.043) | 0.047 (0.047) | 0.040 (0.043) |
| 432 | 0.037 (0.047) | 0.047 (0.047) | 0.033 (0.043) |
| 864 | 0.045 (0.045) | 0.047 (0.053) | 0.047 (0.050) |
| 1728| 0.054 (0.054) | 0.049 (0.049) | 0.059 (0.059) |

$p = q \in \{2, 3, 5\}$, and correlation $\rho \in \{0, 0.005, 0.01, \ldots, 0.15\}$. In addition, we resample $n$ times in the permutation procedure used for tests (iii) and (iv). All data sets are generated as an i.i.d. sample from a distribution as specified below.

Example 6.1. The data $(X, Y)$ are generated from multivariate normal distribution with mean zero and covariance matrix $I_{p+q}$ but

(a) $\text{Cov}(X_1, X_2) = 0.5$, $\text{Cov}(X_1, Y_1) = \rho$;

(b) $\text{Cov}(X_1, Y_1) = \rho$;

Example 6.2. The data $(X, Y)$ are given by $X_i = Q_{t(1)}(\Phi(X_i^*))$, $i \in [p]$ and $Y_j = Q_{t(1)}(\Phi(Y_j^*))$, $j \in [q]$, where $Q_{t(1)}$ stands for the quantile function for Student’s $t$-distribution with 1 degree of freedom (Cauchy distribution), and $(X^*, Y^*)$ are generated as in Example 6.1.

In these two examples, the independence hypothesis holds when $\rho = 0$. We first report the empirical sizes of the proposed tests using theoretical and simulation-based rejection thresholds, which are presented in Table 1. It can be observed that the proposed test with either rejection threshold controls the size effectively.

The empirical powers for Examples 6.1–6.2 are summarized in Figures 2–3. For the proposed test, we present results only for the theoretical rejection threshold and the results for the simulation-based threshold are similar and hence omitted.

Several facts are noteworthy. First, the performance of the proposed test is no worse than the other two competing ones when the sample size is large and the dimension is two or three, where surprisingly the proposed test can even beat the other two when the within-group correlation is high, as in Example 6.1(a) and Example 6.2(a). It should also be highlighted that our method is computationally much faster than the competing ones, as shown in Figure 4. Second, for heavy-tailed distributions, the tests via distance covariance with Hallin’s and marginal ranks perform better than the original distance covariance test. Third, compared to setting (b) the proposed test performs better under setting (a), when there is higher within-group correlation. Lastly, compared to its competitors, the proposed test appears to be more sensitive to dimension. This is as expected.

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Figure 2: Empirical powers of the three competing tests in Example 6.1(a) (first three rows) and 6.1(b) (last three rows). The y-axis represents the power based on 1,000 replicates and the x-axis represents the level of a desired signal.
Figure 3: Empirical powers of the three competing tests in Example 6.2(a) (first three rows) and 6.2(b) (last three rows). The y-axis represents the power based on 1,000 replicates and the x-axis represents the level of a desired signal.
Figure 4: A comparison of computation time in Example 6.1 when $\rho = 0$ for the three tests. The y-axis represents the averaged computation elapsed time (in seconds) of 1,000 replicates of a single experiment and the x-axis represents the sample size. To compute the optimal matching, we used the algorithm in Gabow and Tarjan (1989).

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Further concepts concerning U-statistics are needed. For any symmetric kernel \( h \), any integer \( \ell \in \{ m \} \), and any probability measure \( \mathbb{P}_X \), we write
\[
h_\ell(x_1, \ldots, x_\ell; \mathbb{P}_X) = \mathbb{E}h(x_1, \ldots, x_\ell, X_{\ell+1}, \ldots, X_m),
\]
\[
\tilde{h}_\ell(x_1, \ldots, x_\ell; \mathbb{P}_X) = h_\ell(x_1, \ldots, x_\ell; \mathbb{P}_X) - \mathbb{E}h - \sum_{k=1}^{\ell-1} \sum_{1 \leq i_1 < \cdots < i_k \leq \ell} \tilde{h}_k(x_{i_1}, \ldots, x_{i_k}; \mathbb{P}_X),
\]
where \( X_1, \ldots, X_m \) are \( m \) independent random variables with law \( \mathbb{P}_X \) and \( \mathbb{E}h := \mathbb{E}h(X_1, \ldots, X_m) \). The kernel as well as the corresponding U-statistic are said to be \textit{completely degenerate} under \( \mathbb{P}_X \) if \( h_1(\cdot) \) has variance zero. We use the term \textit{completely degenerate} to indicate that the variances of \( h_1(\cdot), \ldots, h_{m-1}(\cdot) \) are all zero. We also have
\[
\binom{n}{m}^{-1} \sum_{1 \leq i_1 < i_2 < \cdots < i_m \leq n} h(X'_{i_1}, \ldots, X'_{i_m}) = \mathbb{E}h + \sum_{\ell=1}^{m} \binom{m}{\ell} \binom{n}{\ell}^{-1} \sum_{1 \leq i_1 < i_2 < \cdots < i_\ell \leq n} \tilde{h}_\ell(X'_{i_1}, \ldots, X'_{i_\ell}; \mathbb{P}_X),
\]
for any (possibly dependent) random variables \( X'_1, \ldots, X'_n \). This is the Hoeffding decomposition with respect to \( \mathbb{P}_X \).

**Notation.** Let \( (n)_r \) denote \( n!/(n-r)! \). The cardinality of a set \( S \) is written \( \text{card}(S) \). For a multiset \( M = \{ x_1, \ldots, x_n \} \) and \( r \in \{ n \} \), an \( r \)-permutation of \( M \) is a sequence \( [x_\sigma(i)]_{i=1}^r \), given \( \sigma \) is a bijection from \( [n] \) to itself. For \( r \in \{ n \} \), let \( I^n_r \) denote the family of all \( (n)_r \) possible \( r \)-permutations of set \( [n] \). For \( x \in \mathbb{R} \), let \( x_+ \) denote the positive part of \( x \), defined as \( \max\{ x, 0 \} \). Let \( x \circ y \) and \( x \cdot y \) denote the Hadamard product and dot product of two vectors \( x, y \in \mathbb{R}^d \). We use \( \xrightarrow{p} \) to denote convergence in probability.

**A.1 Proofs for Section 2 of the main paper**

**A.1.1 Proof of Lemma 2.1.** We proceed in three steps. First, we give an alternative form of the uniform distribution on the points \( \{ t_{j_1, \ldots, j_{d-1}}; j_1 \in \{ n_1 \}, \ldots, j_{d-1} \in \{ n_{d-1} \} \} \) with spherical coordinates \((1, \varphi_{1,j_1}, \ldots, \varphi_{d-1,j_{d-1}})^T\). Next, we find this uniform distribution’s limiting distribution as \( n_1, \ldots, n_{d-1} \to \infty \). Lastly, we prove that this limiting distribution is uniformly distributed over the unit sphere \( S_{d-1} \).

First, let \( Z_m^{(nm)} \) be the uniform distribution on the points \( \{ u_{m,j}; j \in \{ n_m \} \} \) for each \( m \in \{ d-1 \} \) such that \( Z_1^{(n_1)}, \ldots, Z_{d-1}^{(n_{d-1})} \) are mutually independent. Notice that the uniform distribution on the points \( \{ t_{j_1, \ldots, j_{d-1}}; j_1 \in \{ n_1 \}, \ldots, j_{d-1} \in \{ n_{d-1} \} \} \) with spherical coordinates \((1, \varphi_{1,j_1}, \ldots, \varphi_{d-1,j_{d-1}})^T\)
is identical to the distribution given by random spherical coordinates \((1, \Phi_1^{(n_1)}, \ldots, \Phi_{d-1}^{(n_{d-1})})^\top\), where
\[
\Phi_m^{(n_m)} = \begin{cases} 
  g_{d-1-m}^{-1} \left( \frac{\sqrt{\pi} \Gamma((m+1)/2)}{\Gamma(m/2+1)} Z_m^{(n_m)} \right), & \text{for } m \in [d-2], \\
  2\pi Z_d^{(n_{d-1})}, & \text{for } m = d-1.
\end{cases}
\tag{A.3}
\]

Second, we determine the limit of the distribution with random spherical coordinates \((A.3)\) as \(n_1, \ldots, n_{d-1} \to \infty\). Let \(Z_1, \ldots, Z_{d-1}\) be independent random variables that are uniformly distributed on \((0, 1)\). We have \(Z_m^{(n_m)} \to Z_m\) for \(m \in [d-1]\) as \(n_m \to \infty\) by the following argument:
\[
\mathbb{P}(Z_m^{(n_m)} \leq x) = \frac{[n_m x + 1/2]}{n_m} \to x = \mathbb{P}(Z_m \leq x), \quad \text{for } x \in (0, 1),
\tag{A.4}
\]
as \(n_m \to \infty\). Accordingly, the limiting distribution of \((A.3)\) is given by random spherical coordinates \((1, \Phi_1, \ldots, \Phi_{d-1})^\top\), where
\[
\Phi_m = \begin{cases} 
  g_{d-1-m}^{-1} \left( \frac{\sqrt{\pi} \Gamma((m+1)/2)}{\Gamma(m/2+1)} Z_m \right), & \text{for } m \in [d-2], \\
  2\pi Z_d, & \text{for } m = d-1,
\end{cases}
\tag{A.5}
\]
due to the continuous mapping theorem (van der Vaart, 1998, Theorem 2.3).

Lastly, we show that the distribution given by random spherical coordinates \((A.5)\) is uniformly distributed over the unit sphere \(S_{d-1}\). The area element of \(S_{d-1}\), denoted by \(dS_{d-1} V\), can be written in terms of spherical coordinates as
\[
dS_{d-1} V = \left( \prod_{m=1}^{d-2} \sin^{d-1-m}(\varphi_m) d\varphi_m \right) \cdot d\varphi_{d-1} = \left( \prod_{m=1}^{d-2} d(g_{d-1-m}(\varphi_m)) \right) \cdot d\varphi_{d-1},
\tag{A.6}
\]
where the first equality is by Blumenson (1960) and the last equality is using the trigonometric power-reduction formulas (Beyer, 1987, p. 388). Here \(g_m(\theta)\) is defined as (2.4). The transformation corresponding to \((A.5)\) is
\[
\varphi_m = \begin{cases} 
  g_{d-1-m}^{-1} \left( \frac{\sqrt{\pi} \Gamma((m+1)/2)}{\Gamma(m/2+1)} z_m \right), & \text{for } m \in [d-2], \\
  2\pi z_{d-1}, & \text{for } m = d-1,
\end{cases}
\tag{A.7}
\]
which is a bijection between \((0, 1)\) and \((0, \pi)\) for \(m \in [d-2]\) (Beyer, 1987, p. 381), and a bijection between \((0, 1)\) and \((0, 2\pi)\) for \(m = d-1\). In view of \((A.7)\), we have
\[
\frac{d(g_{d-1-m}(\varphi_m))}{dz_m} = \frac{\sqrt{\pi} \Gamma((m+1)/2)}{\Gamma(m/2+1)}, \quad \text{for } m \in [d-2], \quad \text{and} \quad \frac{d\varphi_{d-1}}{dz_{d-1}} = 2\pi.
\tag{A.8}
\]
Plugging \((A.8)\) into \((A.6)\) yields
\[
dS_{d-1} V = 2\pi \prod_{m=1}^{d-2} \frac{\sqrt{\pi} \Gamma((m+1)/2)}{\Gamma(m/2+1)} \cdot \prod_{m=1}^{d-1} d z_m.
\]
This together with the fact that, \((A.5)\) ranges over \((0, \pi)\) for \(m \in [d-2]\) and ranges over \((0, 2\pi)\) for \(m = d-1\), proves the distribution given by random spherical coordinates \((A.5)\) is uniformly distributed over \(S_{d-1}\). \(\square\)
A.1.2 Proof of Proposition 2.2

Proof of Proposition 2.2. We first prove the case $n_0 = 0$ and then generalize to $n_0 > 0$. For simpler presentation, let $\lambda_{n_0,n,R,n_S}$ denote the uniform measure (distribution) on the augmented grid $G^d_{n_0,n,R,n_S}$, let $\mu_{n,R}$ denote the uniform measure on the points $\{r_j, j \in [n_R]\}$, let $\nu_{n_S}$ denote the uniform measure on the points $\{t_{j_1,\ldots,j_{d-1}}; j_i \in [n],\ldots,j_{d-1} \in [n_{d-1}]\}$ with spherical coordinates $(1, \varphi_{1,j_1}, \ldots, \varphi_{d-1,j_{d-1}})^T$, let $\mu$ denote the uniform measure on $[0,1)$, and let $\nu$ denote the uniform measure over the unit sphere $S_{d-1}$.

If $n_0 = 0$, then $\lambda_{n_0,n,R,n_S}$ is the product measure of $\mu_{n,R}$ (for the radius) and $\nu_{n_S}$ (for the unit sphere). We have proven in Lemma 2.1 that $\nu_{n_S}$ weakly converges to $\nu$ as $n_1,\ldots,n_{d-1} \to \infty$. We also have that $\mu_{n,R}$ weakly converges to $\mu$ as $n_R \to \infty$ via a similar argument as (A.4). Combining these facts, and applying Theorem 2.8 in Billingsley (1999) to the separable space $S_d$, we deduce that $\lambda_{n_0,n,R,n_S}$, the product measure of $\mu_{n,R}$ and $\nu_{n_S}$, weakly converges to $\mu \times \nu = \mathcal{U}_d$ as $n_R,n_1,\ldots,n_{d-1} \to \infty$.

If $n_0 > 0$, we compare the uniform measure on the augmented grid $G^d_{0,n,R,n_S}$ (denoted by $\lambda_{0,n,R,n_S}$) and that on $G^d_{n_0,n,R,n_S}$. For any $\mathcal{U}_d$-continuity Borel set $D \subseteq S_d$, we have

$$\lambda_{0,n,R,n_S}(D) = \frac{\text{card}(D \cap G^d_{0,n,R,n_S})}{n-n_0} \quad \text{and} \quad \lambda_{n_0,n,R,n_S}(D) = \frac{\text{card}(D \cap G^d_{n_0,n,R,n_S}) + n_0 \mathbb{1}(\mathbf{0} \in D)}{n}.$$ 

Therefore,

$$|\lambda_{0,n,R,n_S}(D) - \lambda_{n_0,n,R,n_S}(D)| \leq \left( \frac{1}{n-n_0} - \frac{1}{n} \right) \text{card}(D \cap G^d_{0,n,R,n_S}) + \frac{n_0}{n} \leq \left( \frac{1}{n-n_0} - \frac{1}{n} \right) (n-n_0) + \frac{n_0}{n} = \frac{2n_0}{n} \to 0,$$

where the last step follows by noticing

$$\frac{n_0}{n} < \min\{n_R,n_S\} \leq \frac{n_S}{n_Rn_S + n_0} \leq \frac{1}{n_R} \to 0$$

as $n_R \to \infty$. We have proven in the case $n_0 = 0$ that $\lambda_{0,n,R,n_S}$ weakly converges to $\mathcal{U}_d$ and then $\lambda_{0,n,R,n_S}(D) \to \mathcal{U}_d(D)$. This, together with (A.9), proves that $\lambda_{n_0,n,R,n_S}(D) \to \mathcal{U}_d(D)$ for any $\mathcal{U}_d$-continuity Borel set $D \subseteq S_d$, and equivalently, $\lambda_{n_0,n,R,n_S}$ weakly converges to $\mathcal{U}_d$ as $n_R,n_1,\ldots,n_{d-1} \to \infty$. \hfill \square

A.2 Proofs for Section 3 of the main paper

A.2.1 Proof of Theorem 3.1

Proof of Theorem 3.1. We begin by proving the first claim (3.6). Let $\mathbf{U}_i$, $\mathbf{V}_i$, $\mathbf{U}_i^{(n)}$, $\mathbf{V}_i^{(n)}$ denote $\mathbf{F}_{1,\pm}(\mathbf{X}_i)$, $\mathbf{F}_{2,\pm}(\mathbf{Y}_i)$, $\mathbf{F}_{1,\pm}^{(n)}(\mathbf{X}_i)$, $\mathbf{F}_{2,\pm}^{(n)}(\mathbf{Y}_i)$, respectively. Write $\mathbf{W}_i := (\mathbf{U}_i, \mathbf{V}_i)$, $\mathbf{W}_i^{(n)} := (\mathbf{U}_i^{(n)}, \mathbf{V}_i^{(n)})$, and $\mathbf{w}_i := (u_i, v_i)$. The main idea here is to bound

$$\left| \text{dCov}^2_n([U_i^{(n)}]_{i=1}^n, [V_i^{(n)}]_{i=1}^n) - \text{dCov}^2_n([U_i]_{i=1}^n, [V_i]_{i=1}^n) \right|.$$ 

Recall that

$$\text{dCov}^2_n([U_i^{(n)}]_{i=1}^n, [V_i^{(n)}]_{i=1}^n) = (\binom{n}{4})^{-1} \sum_{1 \leq i_1 < \cdots < i_4 \leq n} K(W_{i_1}^{(n)}, W_{i_2}^{(n)}, W_{i_3}^{(n)}, W_{i_4}^{(n)}),$$
\[
d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) = \frac{n}{4} - \sum_{1 \leq i_1 < \cdots < i_4 \leq n} K(W_{i_1}, W_{i_2}, W_{i_3}, W_{i_4}),
\]

where
\[
K(w_1, \ldots, w_4) := \frac{1}{4 \cdot 4!} \sum_{[i_1, \ldots, i_4] \in \mathcal{P}([4])} s(u_{i_1}, u_{i_2}, u_{i_3}, u_{i_4}) s(v_{i_1}, v_{i_2}, v_{i_3}, v_{i_4}),
\]

and \(s(t_1, t_2, t_3, t_4) := ||t_1 - t_2|| + ||t_3 - t_4|| - ||t_1 - t_3|| - ||t_2 - t_4||\). Using the inequality
\[
\left\| U_{i_1}^{(n)} - U_{i_2}^{(n)} \right\| \cdot \left\| V_{i_3}^{(n)} - V_{i_4}^{(n)} \right\| - \left\| U_{i_1} - U_{i_2} \right\| \cdot \left\| V_{i_3} - V_{i_4} \right\|
\leq \left( \left\| U_{i_1}^{(n)} - U_{i_1} \right\| + \left\| U_{i_2}^{(n)} - U_{i_2} \right\| \right) \cdot 2 + \left( \left\| V_{i_3}^{(n)} - V_{i_3} \right\| + \left\| V_{i_4}^{(n)} - V_{i_4} \right\| \right) \cdot 2
\leq 4 \sup_{1 \leq i \leq n} \left\| U_{i}^{(n)} - U_{i} \right\| + 4 \sup_{1 \leq i \leq n} \left\| V_{i}^{(n)} - V_{i} \right\|[16 (\sup_{1 \leq i \leq n} \left\| U_{i}^{(n)} - U_{i} \right\| + \sup_{1 \leq i \leq n} \left\| V_{i}^{(n)} - V_{i} \right\|).
\]

This implies
\[
\left| d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) - d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) \right| \leq 16 \left( \sup_{1 \leq i \leq n} \left\| U_{i}^{(n)} - U_{i} \right\| + \sup_{1 \leq i \leq n} \left\| V_{i}^{(n)} - V_{i} \right\|.
\]

Applying Proposition 2.3 (Glivenko–Cantelli) to (A.12) yields that
\[
\left| d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) - d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) \right| \overset{a.s.}{\rightarrow} 0.\] (A.13)

This together with
\[
d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) \overset{a.s.}{\rightarrow} d\text{Cov}^2\left(F_{1,\pm}(X), F_{2,\pm}(Y)\right),
\]
the strong consistency of \(d\text{Cov}_n^2([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n})\) (Jakobsen, 2017, Theorem 5.5), yields
\[
\tilde{M}_n / n = d\text{Cov}_n^2\left([U_i]_{i=1}^{n}, [V_i]_{i=1}^{n}\right) \overset{a.s.}{\rightarrow} d\text{Cov}^2\left(F_{1,\pm}(X), F_{2,\pm}(Y)\right).
\]

Next we prove the second claim. It has been proved by Székely et al. (2007, Theorem 3(i)) that \(d\text{Cov}^2(F_{1,\pm}(X), F_{2,\pm}(Y)) \geq 0\) and equality holds if and only if \(F_{1,\pm}(X)\) and \(F_{2,\pm}(Y)\) are independent. It remains to show that (a) the independence of \(F_{1,\pm}(X)\) and \(F_{2,\pm}(Y)\) is equivalent to (b) the independence of \(X\) and \(Y\). It is obvious that (b) implies (a). Then we prove (a) implies (b). For any Borel sets \(B_1 \in \mathbb{R}^p\) and \(B_2 \in \mathbb{R}^q\), using Proposition 2.1(ii) and Definition 2.1, we deduce
\[
P(X \in B_1, Y \in B_2) = P(X \in B_1, Y \in B_2) - P(X \in F_{1,\pm}^{-1}(0)) = P(Y \in F_{2,\pm}^{-1}(0))
\leq P(X \in B_1 \setminus F_{1,\pm}^{-1}(0), Y \in B_2 \setminus F_{2,\pm}^{-1}(0)) \leq P(X \in B_1, Y \in B_2),
\]
and thus
\[
P(X \in B_1, Y \in B_2) = P(X \in B_1 \setminus F_{1,\pm}^{-1}(0), Y \in B_2 \setminus F_{2,\pm}^{-1}(0)).\] (A.14)
We can similarly obtain
\[
\mathbb{P}(X \in B_1) = \mathbb{P}(X \in B_1 \setminus F_{1,\pm}^{-1}(0)) \quad \text{and} \quad \mathbb{P}(Y \in B_2) = \mathbb{P}(Y \in B_2 \setminus F_{2,\pm}^{-1}(0)).
\] (A.15)

It follows that
\[
\begin{align*}
\mathbb{P}(X \in B_1, Y \in B_2) &= \frac{\mathbb{P}(X \in B_1 \setminus F_{1,\pm}^{-1}(0), Y \in B_2 \setminus F_{2,\pm}^{-1}(0))}{\mathbb{P}(X \in B_1 \setminus F_{1,\pm}^{-1}(0)) \cdot \mathbb{P}(Y \in B_2 \setminus F_{2,\pm}^{-1}(0))} \\
&\overset{\text{Prop. 2.1(ii)}}{=} \mathbb{P}\{F_{1,\pm}(X) \in F_{1,\pm}(B_1 \setminus F_{1,\pm}^{-1}(0)), F_{2,\pm}(Y) \in F_{2,\pm}(B_2 \setminus F_{2,\pm}^{-1}(0))\} \\
&\overset{\text{Prop. 2.1(ii)}}{=} \mathbb{P}(X \in B_1 \setminus F_{1,\pm}^{-1}(0)) \cdot \mathbb{P}(Y \in B_2 \setminus F_{2,\pm}^{-1}(0)) \overset{\text{(A.15)}}{=} \mathbb{P}(X \in B_1) \cdot \mathbb{P}(Y \in B_2).
\end{align*}
\]

This completes the proof. \(\square\)

A.3 Proofs for Section 4 of the main paper

A.3.1 Proof of Theorem 4.1

We first state the following properties of \(g_i, \ i = 1, 2:\)

**Lemma A.1.** For the limiting functions \(g_i,\ i = 1, 2,\) we have

(i') \(g_i\) is symmetric, i.e., \(g_i(z, z') = g_i(z', z)\) for all \(z, z' \in \Omega_i;\)

(ii') \(g_i\) is continuous;

(iii') \(g_i\) is non-negative definite;

(iv') \(E(g_i(z, Z_i)) = 0;\)

(v') \(E(g_i(Z_i, Z'_i)) \in (0, +\infty).\)

**Proof of Lemma A.1.** Given Assumption (vi), Properties (i') and (iii') readily follow from Assumptions (i) and (iii), respectively. Property (ii') follows from Assumptions (ii) and (vi) by Theorem 7.12 in Rudin (1976). Property (iv') holds by noticing \(E(g_i(z, Z_i^{(n)})) \rightarrow E(g_i(z, Z_i))\) by Property (ii') and the portmanteau lemma (van der Vaart, 1998, Lemma 2.2), and
\[
|E g_i(z_i, Z_i^{(n)})| = |E g_i^{(n)}(z_i, Z_i^{(n)}) - E g_i(z_i, Z_i^{(n)})| \leq E |g_i^{(n)}(z_i, Z_i^{(n)}) - g_i(z_i, Z_i^{(n)})| \leq \|g_i^{(n)} - g_i\|_\infty \rightarrow 0,
\]
where the first step is by Assumption (iv), and the last step is due to Assumption (vi). For Property (v'), \(E(g_i(Z_i, Z_i')) \geq 0\) has been assumed in Property (vi), and \(E(g_i(Z_i, Z_i')) < \infty\) since \(\Omega_i\) is compact and Property (ii'). \(\square\)

**Proof of Theorem 4.1.** The proof is divided into two steps. The first step consists of defining a “truncated” version \(\hat{D}_K^{(n)}\) of \(\hat{D}^{(n)}\) and finding the limiting distribution of \(\hat{D}_K^{(n)}\). The second step is to bound the difference between \(\hat{D}_K^{(n)}\) and \(\hat{D}^{(n)}\) and then show the limiting distribution of \(\hat{D}^{(n)}\). To this end, we do some preliminary work. Using Hilbert–Schmidt theorem (Simon, 2015a, Theorem 3.2.1, Example 3.1.15), \(g_i^{(n)}\) admits the following eigenfunction expansion by Assumptions (i) and (v),
\[
g_i^{(n)}(z, z') = \sum_{k=1}^{\infty} \lambda_{i,k}^{(n)}(z) \exp_{i,k}(z'),
\]
where $\lambda_{i,k}^{(n)}, k \in \mathbb{Z}_+$ are all the non-zero eigenvalues of the integral equation
\[
Eg_i(z, Z_i^{(n)})e_{i,k}^{(n)}(Z_i^{(n)}) = \lambda_{i,k}^{(n)}e_{i,k}^{(n)}(z)
\]
with $\lambda_{i,1}^{(n)} \geq \lambda_{i,2}^{(n)} \geq \lambda_{i,3}^{(n)} \geq \cdots > 0$ by Assumption (iii), and orthonormal eigenfunctions $e_{i,k}^{(n)}(z), k \in \mathbb{Z}_+$ are such that
\[
Ee_{i,k}^{(n)}(Z_i^{(n)})e_{i,k'}^{(n)}(Z_i^{(n)}) = \mathbb{I}(k = k').
\]
(A.16)
Since the constant function $1$ is an eigenfunction associated with eigenvalue $0$ by Assumption (iv), using the orthogonality between $e_{i,k}^{(n)}$ and the constant function $1$ (Simon, 2015a, Theorem 3.2.1) yields
\[
Ee_{i,k}^{(n)}(Z_i^{(n)}) = 0.
\]
(A.17)
We also define $\lambda_{i,k}, k \in \mathbb{Z}_+$ as all the non-zero eigenvalues of the integral equation $Eg_i(z, Z_i)e_{i,k}(Z_i) = \lambda_{i,k}e_{i,k}(z)$ with $\lambda_{i,1} \geq \lambda_{i,2} \geq \lambda_{i,3} \geq \cdots > 0$ by Property (iii'), and orthonormal eigenfunctions $e_{i,k}(z), k \in \mathbb{Z}_+$ are such that $Ee_{i,k}(Z_i)e_{i,k'}(Z_i) = \mathbb{I}(k = k')$. Denote $k := [k_1, k_2], \gamma_{k}^{(n)} := \lambda_{1,k_1,1,k_2}^{(n)}$, and $\Phi_{k}^{(n)}(j_1, j_2) := e_{1,k_1}^{(n)}(z_{1,j_1})e_{2,k_2}^{(n)}(z_{2,j_2})$.

**Step I.** We write by Theorem 4.11.8 in Simon (2015b),
\[
\hat{D}^{(n)} = \frac{1}{n(n-1)} \sum_{j_1 \neq j_2} \sum_{k_1, k_2 = 1}^{\infty} \gamma_{k}^{(n)} \Phi_{k}^{(n)}(j_1, \pi_{j_1})\Phi_{k}^{(n)}(j_2, \pi_{j_2}).
\]
For each integer $K$, we define the “truncated” permutation statistic
\[
\hat{D}_{K}^{(n)} := \frac{1}{n(n-1)} \sum_{j_1 \neq j_2} \sum_{k_1, k_2 = 1}^{K} \gamma_{k}^{(n)} \Phi_{k}^{(n)}(j_1, \pi_{j_1})\Phi_{k}^{(n)}(j_2, \pi_{j_2}),
\]
and derive the limiting distribution of $n\hat{D}_{K}^{(n)}$ as $n \to \infty$. Notice that $n\hat{D}_{K}^{(n)}$ can be written as
\[
n\hat{D}_{K}^{(n)} = \frac{n}{n-1} \left\{ \sum_{k_1, k_2 = 1}^{K} \gamma_{k}^{(n)} \left( \sum_{j=1}^{n} \frac{\Phi_{k_1,k_2}^{(n)}(j, \pi_{j})}{\sqrt{n}} \right)^2 - \sum_{k_1, k_2 = 1}^{K} \gamma_{k}^{(n)} \left( \frac{\sum_{j=1}^{n} \Phi_{k_1,k_2}^{(n)}(j, \pi_{j})}{n} \right)^2 \right\}.
\]
(A.18)
We separately study the two terms on the right-hand side of (A.18), starting from the first term. We first establish that, for any fixed $K \in \mathbb{Z}_+$, the random vector
\[
\Xi_{K}^{(n)} := \left( \frac{\sum_{j=1}^{n} \Phi_{[1,1]}^{(n)}(j, \pi_{j})}{\sqrt{n}}, \ldots, \frac{\sum_{j=1}^{n} \Phi_{[1,K]}^{(n)}(j, \pi_{j})}{\sqrt{n}}, \ldots, \frac{\sum_{j=1}^{n} \Phi_{[K,1]}^{(n)}(j, \pi_{j})}{\sqrt{n}}, \ldots, \frac{\sum_{j=1}^{n} \Phi_{[K,K]}^{(n)}(j, \pi_{j})}{\sqrt{n}} \right) \top
\]
has a mean of $0$ and a variance-covariance matrix of $\frac{n}{n-1}I_{K^2}$. We have for $k = [k_1, k_2] \in \mathbb{K} \times \mathbb{K},$
\[
E \sum_{j=1}^{n} \Phi_{k}^{(n)}(j, \pi_{j}) = \frac{1}{n} \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} \Phi_{k_1,k_2}^{(n)}(j_1, j_2)
\]
\[
= \frac{1}{n} \sum_{j_1=1}^{n} e_{1,k_1}^{(n)}(z_{1,j_1}) \sum_{j_2=1}^{n} e_{2,k_2}^{(n)}(z_{2,j_2}) = nE[e_{1,k_1}^{(n)}(Z_1^{(n)})]E[e_{2,k_2}^{(n)}(Z_2^{(n)})] = 0,
\]
(A.19)
where the last step is by (A.17). For \( k = [k_1, k_2] \) and \( k' = [k'_1, k'_2] \), it holds that

\[
\mathbb{E} \left[ \sum_{j_1=1}^{n} \Phi^{(n)}_{k} (j_1, \pi_{j_1}) \sum_{j_3=1}^{n} \Phi^{(n)}_{k'} (j_3, \pi_{j_3}) \right]
\]

\[
= \mathbb{E} \left[ \sum_{j_1=1}^{n} \Phi^{(n)}_{k} (j_1, \pi_{j_1}) \Phi^{(n)}_{k'} (j_1, \pi_{j_1}) + \sum_{j_1 \neq j_3} \Phi^{(n)}_{k} (j_1, \pi_{j_1}) \Phi^{(n)}_{k'} (j_3, \pi_{j_3}) \right]
\]

\[
= \frac{1}{n} \sum_{j_1,j_2} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_1, j_2)
\]

\[
+ \frac{1}{n(n-1)} \left( \sum_{j_1,j_2,j_3,j_4=1}^{n} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_3, j_4) - \sum_{j_1,j_2,j_4=1}^{n} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_4, j_1) \right)
\]

and thus

\[
\text{Cov} \left( \sum_{j_1=1}^{n} \Phi^{(n)}_{k} (j_1, \pi_{j_1}), \sum_{j_3=1}^{n} \Phi^{(n)}_{k'} (j_3, \pi_{j_3}) \right)
\]

\[
= \mathbb{E} \left[ \sum_{j_1=1}^{n} \Phi^{(n)}_{k} (j_1, \pi_{j_1}) \sum_{j_3=1}^{n} \Phi^{(n)}_{k'} (j_3, \pi_{j_3}) \right] - \left( \mathbb{E} \sum_{j_1=1}^{n} \Phi^{(n)}_{k} (j_1, \pi_{j_1}) \right) \left( \mathbb{E} \sum_{j_3=1}^{n} \Phi^{(n)}_{k'} (j_3, \pi_{j_3}) \right)
\]

\[
= \frac{n^2}{n-1} \left( \frac{1}{n^2} \sum_{j_1,j_2=1}^{n} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_1, j_2) - \frac{1}{n^3} \sum_{j_1,j_2,j_3=1}^{n} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_3, j_2) \right)
\]

\[
- \frac{1}{n^3} \sum_{j_1,j_2,j_4=1}^{n} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_3, j_4) + \frac{1}{n^4} \sum_{j_1,j_2,j_3,j_4=1}^{n} \Phi^{(n)}_{k} (j_1, j_2) \Phi^{(n)}_{k'} (j_3, j_4)
\]

\[
= \frac{n^2}{n-1} \left\{ \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_1}) \left( \frac{1}{n} \sum_{j_2=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) e^{(n)}_{2,k'_2} (z^{(n)}_{2,j_2}) \right) \right. \\
- \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) \left( \frac{1}{n} \sum_{j_3=1}^{n} e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_3}) \right) \left( \frac{1}{n} \sum_{j_2=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) e^{(n)}_{2,k'_2} (z^{(n)}_{2,j_2}) \right) \left( \frac{1}{n} \sum_{j_4=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_4}) \right) \right. \\
- \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) \left( \frac{1}{n} \sum_{j_4=1}^{n} e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_4}) \right) \left( \frac{1}{n} \sum_{j_2=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) \right) \left( \frac{1}{n} \sum_{j_3=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_3}) \right) \right. \\
- \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) \left( \frac{1}{n} \sum_{j_3=1}^{n} e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_3}) \right) \left( \frac{1}{n} \sum_{j_4=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_4}) \right) \left( \frac{1}{n} \sum_{j_2=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) \right) \right. \\
\left. + \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) \left( \frac{1}{n} \sum_{j_3=1}^{n} e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_3}) \right) \left( \frac{1}{n} \sum_{j_2=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) \right) \left( \frac{1}{n} \sum_{j_4=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_4}) \right) \right\}
\]

\[
= \frac{n^2}{n-1} \left\{ \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_1}) - \left( \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{1,k_1} (z^{(n)}_{1,j_1}) \left( \frac{1}{n} \sum_{j_3=1}^{n} e^{(n)}_{1,k'_1} (z^{(n)}_{1,j_3}) \right) \right) \right. \\
\left. + \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) e^{(n)}_{2,k'_2} (z^{(n)}_{2,j_2}) - \left( \frac{1}{n} \sum_{j_1=1}^{n} e^{(n)}_{2,k_2} (z^{(n)}_{2,j_2}) \left( \frac{1}{n} \sum_{j_4=1}^{n} e^{(n)}_{2,k'_2} (z^{(n)}_{2,j_4}) \right) \right) \right\}
\]

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\[ = \frac{n^2}{n-1} \text{Cov} \left( e_{1,k_1}^{(n)} (Z_1^{(n)}), e_{1,k_1'}^{(n)} (Z_1^{(n)}) \right) \text{Cov} \left( e_{2,k_2}^{(n)} (Z_2^{(n)}), e_{2,k_2'}^{(n)} (Z_2^{(n)}) \right) = \frac{n^2}{n-1} \mathbf{I} (k = k'), \quad \text{(A.21)} \]

where the last step is by (A.16) and (A.17). Combining (A.19) and (A.21) confirms the claim that the mean and the variance-covariance matrix of \( \sqrt{(n-1)/n} \mathbf{E}_{K^2}^{(n)} \) are \( \mathbf{0} \) and \( \mathbf{I}_{K^2} \), respectively.

This claim about \( \sqrt{(n-1)/n} \mathbf{E}_{K^2}^{(n)} \) allows us to use the multivariate Berry–Esséen theorem for permutation statistics (Bolthausen and Götze, 1993, Theorem 1). Specifically, we present the version revised by Raič (2015, p. 3) here. Define \( \mathbf{E}_{K^2} \) as a standard \( K^2 \)-dimensional Gaussian random vector with independent univariate standard Gaussian entries

\[ \mathbf{E}_{K^2} = (\xi_{[1,1]}, \ldots, \xi_{[1,K]}, \ldots, \xi_{[K,1]}, \ldots, \xi_{[K,K]})^\top, \]

and \( \mathcal{H} \) as the family of all measurable convex sets in \( \mathbb{R}^{K^2} \). We obtain for all \( H \in \mathcal{H} \), there exists a universal constant \( c_1 \) such that

\[
\left| \mathbb{P} \left( \frac{n-1}{n} \mathbf{E}_{K^2}^{(n)} \in H \right) - \mathbb{P} (\mathbf{E}_{K^2} \in H) \right| \leq c_1 (K^2)^{1/4} \frac{1}{n} \sum_{j_1, j_2 = 1}^{n} \left( \sum_{k_1, k_2 = 1}^{K} \left\{ \sqrt{\frac{n-1}{n^2}} \Phi_k^{(n)} (j_1, j_2) \right\}^2 \right)^{3/2} \leq c_1 K^{1/2} \frac{1}{n^{5/2}} \sum_{j_1, j_2 = 1}^{n} \left( \sum_{k_1, k_2 = 1}^{K} \left\{ e_{1,k_1}^{(n)} (Z_{1,j_1}) \right\}^2 e_{2,k_2}^{(n)} (Z_{2,j_2}) \right)^{3/2} = O(n^{-1/2}), \quad \text{(A.22)}
\]

where the last step is due to the facts that \( K \) is fixed and that \( \sup_n \| e_i^{(n)} \|_\infty < \infty \) for each \( i = 1, 2 \) and any fixed \( k \), as we will show in Lemma A.2(b). Notice for any \( a_1, \ldots, a_{K^2} \in \mathbb{R} \), the set \( (-\infty, a_1] \times \cdots \times (-\infty, a_{K^2}] \) is a convex subset of \( \mathbb{R}^{K^2} \). It follows that \( \sqrt{(n-1)/n} \mathbf{E}_{K^2}^{(n)} \overset{d}{\to} \mathbf{E}_{K^2} \), and moreover, \( \mathbf{E}_{K^2}^{(n)} \overset{d}{\to} \mathbf{E}_{K^2} \) by Slutsky’s theorem (van der Vaart, 1998, Theorem 2.8). On the other hand, since

\[ \gamma_k^{(n)} = \lambda_{1,k_1}^{(n)} \lambda_{2,k_2}^{(n)} \rightarrow \lambda_{1,k_1} \lambda_{2,k_2} = \gamma_k \quad \text{(A.23)} \]

by Lemma A.2(a), we have \( \mathbf{I}_{K^2}^{(n)} \rightarrow \mathbf{I}_{K^2} \) where

\[ \mathbf{I}_{K^2} := (\gamma_{[1,1]}, \ldots, \gamma_{[1,K]}, \ldots, \gamma_{[K,1]}, \ldots, \gamma_{[K,K]})^\top, \]

and \( \mathbf{I}_{K^2} := (\gamma_{[1,1]}, \ldots, \gamma_{[1,K]}, \ldots, \gamma_{[K,1]}, \ldots, \gamma_{[K,K]})^\top \).

We find using generalized Slutsky’s theorem (as a consequence of Theorem 2.7 in van der Vaart, 1998, p.10–11) that

\[ \sum_{k_1, k_2 = 1}^{K} \gamma_k^{(n)} \left( \sum_{j=1}^{\sqrt{n}} \frac{\Phi_k^{(n)} (j, \pi_j)}{\sqrt{n}} \right)^2 = (\mathbf{I}_{K^2} \circ \mathbf{E}_{K^2}^{(n)}) \cdot \mathbf{E}_{K^2} \overset{d}{\to} (\mathbf{I}_{K^2} \circ \mathbf{E}_{K^2}) \cdot \mathbf{E}_{K^2} = \sum_{k_1, k_2 = 1}^{K} \gamma_k \xi_k^2, \quad \text{(A.24)} \]

recognizing the function \( f(x, y) = (x \circ y) \cdot y \) for \( x, y \in \mathbb{R}^{K^2} \) as continuous. This completes the analysis of the first term in (A.18).

We turn to the second term in (A.18). Denoting \( n^{-1} \sum_{j=1}^{n} \left( \Phi_k^{(n)} (j, \pi_j) \right)^2 \) by \( T_k^{(n)} \), we have by
where the last step in (A.26) is by Lemma A.2(b) as well. Therefore, we have

\[ \mathbb{E} \left[ \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \right] = \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} \mathbb{E}[T_k^{(n)}] = \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)}, \]  

(A.27)

and

\[ \text{Var} \left( \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \right) \leq \left( \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} \text{Var}(T_k^{(n)}) \right)^{1/2} = O(n^{-1}), \]  

(A.28)

where the first step in (A.28) is by Minkowski’s inequality (Billingsley, 1995, p. 242) and the last step is by (A.23) and (A.26). It follows by DeGroot and Schervish (2012, Exercise. 4.3.5) that

\[ \mathbb{E} \left[ \left( \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \right)^2 - \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} \right] = \left( \mathbb{E} \left[ \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \right] - \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} \right)^2 + \text{Var} \left( \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \right) \]

\[ = \sum_{k_1, k_2=1}^{K} \left( \gamma_k^{(n)} - \gamma_k^{(n)} \right)^2 + \text{Var} \left( \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \right) = o(1). \]  

(A.29)

Here the second last step is by (A.27), and the last step is by (A.23) and (A.28). Hence for the second term in (A.18), we have

\[ \sum_{k_1, k_2=1}^{K} \gamma_k^{(n)} T_k^{(n)} \xrightarrow{p} \sum_{k_1, k_2=1}^{K} \gamma_k. \]  

(A.30)

Putting two pieces (A.24) and (A.30) together, and using Slutsky’s theorem once again, we have

\[ n \hat{D}^{(n)} \xrightarrow{d} \sum_{k_1, k_2=1}^{K} \gamma_k (\xi_k^2 - 1). \]  

(A.31)

This achieves the goal of Step I.

**Step II.** We will prove \( n \hat{D}^{(n)} \xrightarrow{d} \sum_k \gamma_k (\xi_k^2 - 1) \) starting from (A.31). Following arguments of Serfling (1980, Chap. 5.5.2), we first control \( \mathbb{E}[|n \hat{D}^{(n)} - n \hat{D}_K^{(n)}|^2] \). Letting

\[ S_k^{(n)} := \sum_{j_1 \neq j_2} \Phi_k^{(n)}(j_1, \pi_{j_1}) \Phi_k^{(n)}(j_2, \pi_{j_2}) = \sum_{j_1 \neq j_2} \epsilon_{1,k_1}^{(n)}(z_{1,j_1}) \epsilon_{1,k_2}^{(n)}(z_{1,j_1}) \epsilon_{2,k_2}^{(n)}(z_{2,j_2}) \epsilon_{2,k_2}^{(n)}(z_{2,j_2}), \]

we have

\[ n \hat{D}^{(n)} - n \hat{D}_K^{(n)} = \frac{1}{n-1} \sum_{k \in [K]} \gamma_k^{(n)} S_k^{(n)}. \]  

(A.32)

Equations (2.2)–(2.3) in Barbour and Eagleson (1986) give

\[ \mathbb{E}[S_k^{(n)}] = n(n-1) \mu_{1,k_1}^{(n)} \mu_{2,k_2}^{(n)} = n(n-1) \left( -\frac{1}{n-1} \right) \left( -\frac{1}{n-1} \right) = \frac{n}{n-1}, \]  

(A.33)
Combining (A.33) and (A.35), we deduce for
\[ \frac{4n^2(n-2)^2}{(n-1)^2} \left( \sum_{j=1}^{n} \{ \xi_{j;1}^{(n)}/(n-2) \}^2 \right) \left( \sum_{j=1}^{n} \{ \xi_{j;2}^{(n)}/(n-2) \}^2 \right) \\
+ \frac{2n(n-1)^2}{n-3} \left( \sum_{j_1 \neq j_2} \{ \eta_{j,1}^{(n)} \}^2 \right) \left( \sum_{j_1 \neq j_2} \{ \eta_{j,2}^{(n)} \}^2 \right), \]  
where for \( i = 1, 2, \)
\[ \mu_{i,k}^{(n)} := \frac{1}{n(n-1)} \sum_{j_1 \neq j_2} e_{i,k}^{(n)} (z_{i;j_1}) e_{i,k}^{(n)} (z_{i;j_2}) = -\frac{1}{n(n-1)} \sum_{j=1}^{n} \{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 = -\frac{1}{n-1}, \]
\[ \zeta_{i,j_1}$j_2}^{(n)} := \sum_{j_2:j_2 \neq j_1} \{ e_{i,k}^{(n)} (z_{i;j_1}) e_{i,k}^{(n)} (z_{i;j_2}) - \mu_{i,k}^{(n)} \} = -\{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 + 1, \]
and \[ \eta_{i,j_1,j_2}^{(n)} := e_{i,k}^{(n)} (z_{i;j_1}) e_{i,k}^{(n)} (z_{i;j_2}) - \zeta_{i,j_1\#j_2}^{(n)} - \zeta_{i,j_1\#j_2}^{(n)} - \zeta_{i,k}^{(n)} \]
\[ = e_{i,k}^{(n)} (z_{i;j_1}) e_{i,k}^{(n)} (z_{i;j_2}) + \frac{\{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 - 1}{n-2} + \frac{\{ e_{i,k}^{(n)} (z_{i;j_2}) \}^2 - 1}{n-2} + \frac{1}{n-1}. \]
To further bound (A.34), using the inequalities for \( i = 1, 2 \) as below:
\[ \sum_{j=1}^{n} \{ \zeta_{i,j_1}^{(n)} \}^2 = \sum_{j=1}^{n} (1 - \zeta_{i,j_1}^{(n)})^2 - n = \sum_{j=1}^{n} \left( n - \sum_{j_2 \neq j_1} \{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 \right) \left( \{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 \right) - n \]
\[ \leq n \sum_{j=1}^{n} \{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 - n = n(n-1), \]
and
\[ \sum_{j_1 \neq j_2} \{ \eta_{i,j_1,j_2}^{(n)} \}^2 = n(n-1) - \frac{n}{n-1} - \frac{n}{n-2} \sum_{j=1}^{n} \left( \{ e_{i,k}^{(n)} (z_{i;j_1}) \}^2 - 1 \right)^2 \leq n(n-1) - \frac{n}{n-1}, \]
we deduce for all \( k \in \mathbb{Z}_+ \times \mathbb{Z}_+, \)
\[ \text{Var}(S_k^{(n)}) \leq \frac{4n^2(n-1)^2}{(n-2)^2} + \frac{2n(n-1)^2}{n-3}. \]
Combining (A.33) and (A.35), we deduce for \( n \geq 14, \)
\[ \mathbb{E}[n \hat{D}^{(n)} - n \hat{D}_K^{(n)}]^2 = \frac{1}{(n-1)^2} \left[ \mathbb{E} \sum_{k \in K} \gamma_k^{(n)} S_k^{(n)} \right]^2 + \text{Var} \left( \sum_{k \in K} \gamma_k^{(n)} S_k^{(n)} \right) \\
\leq \frac{1}{(n-1)^2} \left[ \left( \sum_{k \in K} \gamma_k^{(n)} \mathbb{E} S_k^{(n)} \right)^2 + \left( \sum_{k \in K} \gamma_k^{(n)} \sqrt{\text{Var}(S_k^{(n)})} \right)^2 \right] \\
\leq \frac{1}{(n-1)^2} \left[ \left( \frac{n}{n-1} \right)^2 + 4 \frac{n^2(n-1)}{(n-2)^2} + \frac{2n^2(n-1)^2}{(n-3)} \right] \left( \sum_{k \in K} \gamma_k^{(n)} \right)^2 \leq 3 \left( \sum_{k \in K} \gamma_k^{(n)} \right)^2 \\
\leq 9 \left( \sum_{k \in K} \gamma_k \right)^2 \leq 9 \left( \sum_{k \in K} \gamma_k \right)^2 \leq 9 \left( \sum_{k \in K} \gamma_k \right)^2 \leq 9 \left( \sum_{k \in K} \gamma_k \right)^2 \leq 9 \left( \sum_{k \in K} \gamma_k \right)^2. \]  
We next verify that \( \mathbb{E}[n \hat{D}^{(n)} - n \hat{D}_K^{(n)}]^2 \) can be arbitrarily small for all \( K \) large enough and all \( n \geq N(K) \) with \( N(K) \) possibly depending on \( K \). Fix any arbitrarily small \( \epsilon > 0 \). We have the first
term in (A.36) is smaller than \( \epsilon / 3 \) as long as \( K \) is large enough, since
\[
\sum_{k \in \mathbb{Z}^+} \gamma_k = \mathbb{E} g_1(Z_1, Z_1) \cdot \mathbb{E} g_2(Z_2, Z_2) < \infty
\]
by Properties (i)–(iii) and Mercer’s theorem (Simon, 2015a, Theorem 3.11.9(b)). In view of (A.23),
the second term in (A.36) will be smaller than \( \epsilon / 3 \) for each fixed \( K \) and all \( n \geq N(K) \), where \( N(K) \)
may depend on \( K \). For the third term, combining the facts that \( \mathbb{E} g_i(Z_i^{(n)}, Z_i^{(n)}) \rightarrow \mathbb{E} g_i(Z_i, Z_i) \) by
the portmanteau lemma (van der Vaart, 1998, Lemma 2.2), and that
\[
\mathbb{E} |g_i^{(n)}(Z_i^{(n)}, Z_i^{(n)}) - g_i(Z_i^{(n)}, Z_i^{(n)})| \leq \|g_i^{(n)} - g_i\|_\infty \rightarrow 0,
\]
by Assumption (vi), we deduce for \( i = 1, 2 \), \( \mathbb{E} g_i^{(n)}(Z_i^{(n)}, Z_i^{(n)}) \rightarrow \mathbb{E} g_i(Z_i, Z_i) \) as \( n \rightarrow \infty \). Recalling
Assumptions (i)–(iii) and Properties (i')–(iii'), it holds by Mercer’s theorem once again (Simon,
2015a, Theorem 3.11.9(b)) that
\[
\left( \sum_{k \in \mathbb{Z}^+} \gamma_k^{(n)} - \sum_{k \in \mathbb{Z}^+} \gamma_k \right)^2 = \left( \mathbb{E} g_1(Z_1^{(n)}, Z_1^{(n)}) \cdot \mathbb{E} g_2(Z_2^{(n)}, Z_2^{(n)}) - \mathbb{E} g_1(Z_1, Z_1) \cdot \mathbb{E} g_2(Z_2, Z_2) \right)^2,
\]
which is smaller than \( \epsilon / 3 \) so long as \( n \) is large enough. Adding these three terms together concludes
the result.

We are now ready to prove \( n \hat{D}^{(n)} \overset{d}{\rightarrow} \sum_k \gamma_k (\xi_k^2 - 1) \) using Lévy’s continuity theorem (Billingsley,
1995, Theorem 26.3). We have
\[
\begin{align*}
|\mathbb{E} \left[ \exp \left( itn \hat{D}^{(n)} \right) \right] - \mathbb{E} \left[ \exp \left( it \sum_k \gamma_k (\xi_k^2 - 1) \right) \right]| & \\
\leq |\mathbb{E} \left[ \exp \left( itn \hat{D}^{(n)} \right) \right] - \mathbb{E} \left[ \exp \left( it \sum_k \gamma_k (\xi_k^2 - 1) \right) \right]| + |\mathbb{E} \left[ \exp \left( itn \hat{D}^{(n)} \right) \right] - \mathbb{E} \left[ \exp \left( it \sum_k \gamma_k (\xi_k^2 - 1) \right) \right]| \\
& \\
& + |t| \left( \mathbb{E} \left[ |n \hat{D}^{(n)} - n \hat{D}^{(n)}_K|^2 \right] \right)^{1/2} + |t| \left( \mathbb{E} \left[ \exp \left( itn \hat{D}^{(n)}_K \right) \right] - \mathbb{E} \left[ \exp \left( it \sum_k \gamma_k (\xi_k^2 - 1) \right) \right] \right) \\
& \\
& + |t| \left( \sum_{k \in [K] \times [K]} \gamma_k^2 \right)^{1/2} =: I_{n,K} + II_{n,K} + III_{K}.
\end{align*}
\]
Here in the last inequality, the first term is because of \( |\mathbb{E}[e^{itX}] - \mathbb{E}[e^{itY}]| \leq |t||\mathbb{E}[X - Y]^2|^{1/2} \),
and the last term is due to Equation (4.3.10) in Koroljuk and Borovskich (1994). Fix \( t \) and let
arbitrarily small \( \epsilon > 0 \) be given. We have proven that there exists \( K_1 \) such that for all \( K \geq K_1 \)
and all \( n \geq N(K) \), where \( N(K) \) may depend on \( K \), such that \( I_{n,K} < \epsilon / 3 \). We can find \( K_2 \)
such that \( III_K < \epsilon / 3 \) for all \( K \geq K_2 \) because \( \sum_k \gamma_k^2 = \mathbb{E} \left[ \{g_1(Z_1, Z_1)^2 | \{g_2(Z_2, Z_2)^2} \right] < \infty \) by
Property (v'). Taking \( K_0 = \max(K_1, K_2) \), we can choose \( N_0 \geq N(K_0) \) so that \( II_{n,K_0} < \epsilon / 3 \) for all
\( n \geq N_0 \) since (A.31) holds for \( K_0 \). Then for all \( n \geq N_0 \),
\[
\left| \mathbb{E} \left[ \exp \left( itn \hat{D}^{(n)} \right) \right] - \mathbb{E} \left[ \exp \left( it \sum_k \gamma_k (\xi_k^2 - 1) \right) \right] \right| \leq I_{n,K_0} + II_{n,K_0} + III_{K_0} \leq \epsilon
\]
proving the theorem.
Lemma A.2. For each $i = 1, 2$ and any fixed $k \in \mathbb{Z}_+$, we have (a) $\lambda_{i,k}^{(n)} \to \lambda_{i,k}$ as $n \to \infty$; (b) $\sup_n \|e_{i,k}^{(n)}\|_\infty < \infty$.

Proof of Lemma A.2. We employ results in Atkinson (1967). Consider the Banach space $C(\Omega_i)$ of all continuous functions $f$ on $\Omega_i$ equipped with the sup norm $\|f\|_\infty := \sup_z |f(z)|$. Define operators $A$ and $A_n$ on $C(\Omega_i)$ for each $i = 1, 2$ as

$$ (Af)(z) := E g_i(z, Z_i) f(Z_i) \quad \text{and} \quad (A_n f)(z) := E g_i^{(n)}(z, Z_i^{(n)}) f(Z_i^{(n)}). \quad (A.38) $$

We first verify the three assumptions stated in Atkinson (1967, Sect. 1):

1. $A$ and $A_n$, $n \in \mathbb{Z}_+$ are linear operators on Banach space $C(\Omega_i)$ into itself;
2. $\|A_n f - A f\|_\infty \to 0$ for each $f \in C(\Omega_i)$;
3. $\{A_n, n \in \mathbb{Z}_+\}$ is collectively compact, i.e., the set

$$ \mathcal{B} := \left\{ A_n f : n \in \mathbb{Z}_+ \text{ and } \|f\|_\infty \leq 1, \text{ for } f \in C(\Omega_i) \right\} $$

has compact closure.

Notice Assumptions (2) and (3) together imply operator $A$ is compact (Anselone, 1971, Chap. 1.4). Assumption (1) is obvious by Property (ii') and Assumption (iii). We now verify Assumption (2). For each fixed $f \in C(\Omega_i)$ and any fixed $z$, $g_i(z, \cdot) f(\cdot)$ is a bounded and continuous function, and it follows from the portmanteau lemma (van der Vaart, 1998, Lemma 2.2) that $E g_i(z, Z_i^{(n)}) f(Z_i^{(n)}) \to (Af)(z)$ as $n \to \infty$. Since $f$ is continuous, we have $\|f\|_\infty < \infty$. We also have

$$ \| (A_n f)(z) - E g_i(z, Z_i^{(n)}) f(Z_i^{(n)}) \| \leq g_i^{(n)}(z) - g_i(z) \cdot \|f\|_\infty \to 0, \quad (A.39) $$

where the last step is by Assumption (vi); hence $(A_n f)(z) \to (Af)(z)$. Further than that, Assumption (2) holds by Theorem 7.9 and Exercise 7.16 in Rudin (1976) and noticing that the family of functions $\{A_n f : n \in \mathbb{Z}_+\}$ is equicontinuous for each fixed $f \in C(\Omega_i)$ via the following argument. Given an arbitrarily small $\epsilon > 0$, there exists $\delta > 0$ such that $\|z - z'\| < \delta$ implies by Assumption (ii) that $|g_i^{(n)}(z, z'') - g_i^{(n)}(z', z'')| < \epsilon/\|f\|_\infty$ for all $z'' \in \Omega_i$, where $\|f\|_\infty < \infty$, and thus implies

$$ |(A_n f)(z) - (A_n f)(z')| \leq E |g_i^{(n)}(z, Z_i^{(n)}) - g_i^{(n)}(z', Z_i^{(n)})| \cdot \|f\|_\infty < \epsilon. \quad (A.40) $$

For Assumption (3), the set $\mathcal{B}$ is bounded and equicontinuous by (A.40), and thus has compact closure by the Arzelà–Ascoli theorem (Simon, 2015a, Theorem 1.5.3).

To prove (a), using Theorems 2 and 3 in Atkinson (1967), we have for any fixed $k$, $\lambda_{i,k}^{(n)} \to \lambda_{i,k}$ as $n \to \infty$.

The proof of (b) is separated into two parts. In the first part, we show that for each $i = 1, 2$ and any fixed $k$, $e_{i,k}^{(n)}$ are uniformly upper bounded for all sufficiently large $n$. Applying Theorems 4 in Atkinson (1967) yields that, for any arbitrarily small $\epsilon > 0$, there exists a sufficiently large $N$ such that for each $n \geq N$, there exists an (not necessarily unique) eigenfunction $\tilde{e}_{i,k}$ satisfies that $E g_i(z, Z_i) \tilde{e}_{i,k}(Z_i) = \lambda_{i,k} \tilde{e}_{i,k}(z)$, $E[\tilde{e}_{i,k}(Z_i)]^2 = 1$, and

$$ \left\| \frac{e_{i,k}^{(n)}}{\|e_{i,k}^{(n)}\|_\infty} - \frac{\tilde{e}_{i,k}}{\|\tilde{e}_{i,k}\|_\infty} \right\|_\infty < \epsilon. $$
Invoking Properties (i)'–(iii'), Theorem 3.1.1 in König (1986) guarantees that there exists an absolute constant $C_1$ such that $\|\tilde{e}_{i,k}\|_\infty < C_1$ for all $k \in \mathbb{Z}_+$, and hence
\[
\frac{|e_{i,k}^{(n)}|}{\|e_{i,k}^{(n)}\|_\infty} \geq \left( \frac{|e_{i,k}|}{|e_{i,k}\|_\infty} - \epsilon \right) + \left( \frac{|\tilde{e}_{i,k}|}{C_1} - \epsilon \right).
\]
This together with $\sum_{j=1}^n \{e_{i,k}^{(n)}(z_{i,j}^{(n)})\}^2/n = 1$ implies that
\[
\|e_{i,k}^{(n)}\|_\infty^2 \leq \left[ \frac{1}{n} \sum_{j=1}^n \left( \frac{|\tilde{e}_{i,k}(z_{i,j}^{(n)})|}{C_1} - \epsilon \right)^2 \right]^{-1}. \tag{A.41}
\]
In order to prove $e_{i,k}^{(n)}$ are uniformly upper bounded for any fixed $k \in \mathbb{Z}_+$ and all $n$ large enough, it suffices to control the right-hand side of (A.41). Consider an orthonormal basis associated with eigenvalue $\lambda_{i,k}$: $\{e_{i,k_1}, \ldots, e_{i,k_{1'}}\}$, where $\ell$ is finite since
\[
\ell \lambda_{i,k} \leq \sum_{k'=1}^\infty \lambda_{i,k'} = \mathbb{E}g_i(Z_i, Z_i) < \infty,
\]
by Properties (i)'–(iii') and Mercer’s theorem (Simon, 2015a, Theorem 3.11.9(b)). Then $\tilde{e}_{i,k}$ can be represented by
\[
\tilde{e}_{i,k} = \sum_{v=1}^\ell \alpha_v e_{i,k_v}, \quad \text{where} \quad \sum_{v=1}^\ell \alpha_v^2 = 1. \tag{A.42}
\]
First, notice that there exists $N_1 \geq N$ such that for all $n \geq N_1$,
\[
\left| \frac{1}{n} \sum_{j=1}^n e_{i,k_v}(z_{i,j}^{(n)})e_{i,k'_{v'}}(z_{i,j}^{(n)}) - \mathbb{I}(v = v') \right| < \epsilon, \quad \text{for all} \ v, v' \in [\ell], \tag{A.43}
\]
using the continuity of eigenfunctions $e_{i,k_v}$ by Property (ii') and Corollary 2 in Cucker and Smale (2002, p. 34), and the portmanteau lemma (van der Vaart, 1998, Lemma 2.2). Then combining (A.42) and (A.43), we have for $n \geq N_1$,
\[
\frac{1}{n} \sum_{j=1}^n \left( \frac{|\tilde{e}_{i,k}(z_{i,j}^{(n)})|}{C_1} - \epsilon \right)^2 \geq \frac{1}{C_1^2} \cdot \frac{1}{n} \sum_{j=1}^n \{\tilde{e}_{i,k}(z_{i,j}^{(n)})\}^2 - \frac{2\epsilon}{C_1} \cdot \frac{1}{n} \sum_{j=1}^n |\tilde{e}_{i,k}(z_{i,j}^{(n)})|
\]
\[
= \frac{1}{C_1^2} \cdot \frac{\ell}{n} \sum_{v=1}^\ell \alpha_v^2 \sum_{j=1}^n |e_{i,k_v}(z_{i,j}^{(n)})|^2 + \frac{2}{C_1^2} \sum_{v < v'} \frac{\alpha_v \alpha_{v'}}{n} \sum_{j=1}^n e_{i,k_v}(z_{i,j}^{(n)})e_{i,k'_{v'}}(z_{i,j}^{(n)}) - \frac{2\epsilon}{C_1} \cdot \frac{1}{n} \sum_{j=1}^n |\tilde{e}_{i,k}(z_{i,j}^{(n)})|
\]
\[
\geq \frac{1}{C_1^2} \cdot \frac{\ell}{n} \sum_{v=1}^\ell \alpha_v^2 (1 - \epsilon) - \frac{2}{C_1^2} \cdot \sum_{v < v'} |\alpha_v \alpha_{v'}| \epsilon - 2\epsilon = \frac{1}{C_1^2} - \frac{\epsilon}{C_1^2} \left( \sum_{v=1}^\ell |\alpha_v| \right)^2 - 2\epsilon \geq \frac{1 - \epsilon \ell}{C_1^2} - 2\epsilon. \tag{A.44}
\]
This completes the first part by taking sufficiently small $\epsilon$.

We then show the remaining part; we have $\sup_{n < N_1} \|e_{i,k}^{(n)}\|_\infty < \infty$ as proven below. Using Assumption (ii'), and once again, Corollary 2 in Cucker and Smale (2002, p. 34), we have eigenfunctions $e_{i,k}^{(n)}$, $n < N_1$ are continuous, and the result hence follows from the facts that $\Omega_i$ is compact and that $N_1$ is finite. The proof is thus completed.
A.3.2 Proof of Theorem 4.2

Proof of Theorem 4.2. We consider the Hoeffding decomposition with respect to product measure \( \mathbb{P}_{Z_1(n)} \times \mathbb{P}_{Z_2(n)} \):

\[
\widehat{\Pi}^{(n)} = \sum_{\ell=2}^{m} \binom{m}{\ell} \binom{n}{\ell}^{-1} \sum_{1 \leq i_1 < \cdots < i_\ell \leq n} \widehat{h}_\ell( (z_{1:i_1}^{(n)}, z_{2:i_1}^{(n)}), \ldots, (z_{1:i_\ell}^{(n)}, z_{2:i_\ell}^{(n)}); \mathbb{P}_{Z_1(n)} \times \mathbb{P}_{Z_2(n)} ).
\]

We have proven in Theorem 4.1 that

\[
\left( \binom{m}{2} \right)^{-1} n \mathcal{D}_2^{(n)} \overset{d}{\longrightarrow} \sum_{k_1, k_2 = 1}^{\infty} \lambda_1, k_1 \lambda_2, k_2 (\xi_{k_1, k_2}^2 - 1)
\]

as \( n \to \infty \). In order to prove that \( n \widehat{\Pi}^{(n)} \) and \( n \mathcal{D}_2^{(n)} \) have the same limiting distribution, we only need to show that \( n \mathcal{D}_2^{(n)} \overset{p}{\to} 0 \) for \( \ell = 3, \ldots, m \) by Slutsky’s theorem (van der Vaart, 1998, Theorem 2.8). It suffices to establish that \( \mathbb{E}(n \mathcal{D}_2^{(n)})^2 = O(n^{-1}) \) for \( \ell = 3, \ldots, m \).

We start from the scenario \( \ell = 3 \). The proof consists of two steps: (i) showing that \( \mathbb{E}[n \mathcal{D}_3^{(n)}] = O(n^{-1}) \), and (ii) proving that \( \text{Var}(n \mathcal{D}_3^{(n)}) = O(n^{-1}) \). We have by symmetry,

\[
\mathcal{D}_3^{(n)} = \binom{m}{3} (n)^{-1} \sum_{[i_1, i_2, i_3] \in T_3^n} \bar{h}_3( (z_{1:i_1}^{(n)}, z_{2:i_1}^{(n)}), (z_{1:i_2}^{(n)}, z_{2:i_2}^{(n)}), (z_{1:i_3}^{(n)}, z_{2:i_3}^{(n)}); \mathbb{P}_{Z_1(n)} \times \mathbb{P}_{Z_2(n)} ).
\]

One readily verifies \( \| \bar{h}_3 \|_{\infty} \leq 2^3 \| h \|_{\infty} \). Let \( \Delta_3^{(n)}(i_1, j_1; i_2, j_2; i_3, j_3) \) denote

\[
\bar{h}_3( (z_{1:i_1}^{(n)}, z_{2:i_1}^{(n)}), (z_{1:i_2}^{(n)}, z_{2:i_2}^{(n)}), (z_{1:i_3}^{(n)}, z_{2:i_3}^{(n)}); \mathbb{P}_{Z_1(n)} \times \mathbb{P}_{Z_2(n)} ).
\]

Moreover, we define averages of \( \Delta_3^{(n)}(i_1, j_1; i_2, j_2; i_3, j_3) \), in which replacing an index at any position by a “•” sign denotes average over all indices at this position:

\[
\Delta_3^{(n)}(\bullet, j_1; i_2, j_2; i_3, j_3) := \frac{1}{n} \sum_{i_1 = 1}^{n} \Delta_3^{(n)}(i_1, j_1; i_2, j_2; i_3, j_3),
\]

\[
\Delta_3^{(n)}(\bullet, \bullet; i_2, j_2; i_3, j_3) := \frac{1}{n^2} \sum_{i_1 = 1}^{n} \sum_{j_1 = 1}^{n} \Delta_3^{(n)}(i_1, j_1; i_2, j_2; i_3, j_3),
\]

\[
\cdots \Delta_3^{(n)}(\bullet; \bullet; \bullet; \bullet; \bullet; \bullet) := \frac{1}{n^6} \sum_{i_1 = 1}^{n} \sum_{i_2 = 1}^{n} \sum_{i_3 = 1}^{n} \Delta_3^{(n)}(i_1, j_1; i_2, j_2; i_3, j_3).
\]

and others are defined similarly. We obtain using the definition (A.46) that

\[
\Delta_3^{(n)}(\bullet, \bullet; i_2, j_2; i_3, j_3) = \Delta_3^{(n)}(i_1, j_1; \bullet, \bullet; i_3, j_3) = \Delta_3^{(n)}(i_1, j_1; i_2, j_2; \bullet, \bullet) = 0,
\]

\[
\Delta_3^{(n)}(\bullet, \bullet; \bullet; i_3, j_3) = \Delta_3^{(n)}(\bullet, \bullet; i_2, j_2; \bullet; \bullet) = \Delta_3^{(n)}(i_1, j_1; \bullet; \bullet; \bullet; \bullet; \bullet) = 0.
\]
Step I. We show that $\mathbb{E}[n\tilde{D}^{(n)}_3] = O(n^{-1})$. Applying (A.48), direct calculation yields

\[
\mathbb{E} \sum_{[i_1,i_2,i_3] \in I^*_3} \Delta^{(n)}_3(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}) = \frac{1}{(n)_3} \sum_{[i_1,i_2,i_3] \in I^*_3} \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_3, j_3)
\]

\[
= \frac{1}{(n)_3} \sum_{[i_1,i_2] \in I^*_2, [j_1,j_2] \in I^*_2} \left\{ -n\Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_1, \bullet) - n\Delta^{(n)}_3(i_1, j_1; i_2, j_2; \bullet, j_1) - \right.
\]

\[
- n\Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_1, \bullet) - n\Delta^{(n)}_3(i_1, j_1; i_2, j_2; \bullet, j_2) + \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_1, j_1) + \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_1, j_2)
\]

\[
+ \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_2, i_1) + \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_2, j_2)
\]

\[
= \frac{1}{(n-1)_2} \sum_{i_1 \in [n], j_1 \in [n]} \left\{ n\Delta^{(n)}_3(i_1, j_1; i_1, \bullet; i_1, \bullet) + n\Delta^{(n)}_3(i_1, j_1; \bullet; i_1, \bullet) - \Delta^{(n)}_3(i_1, j_1; i_1, j_1; i_1, \bullet) \right\}
\]

\[
+ \frac{1}{(n-1)_2} \sum_{i_2 \in [n], j_2 \in [n]} \left\{ n\Delta^{(n)}_3(i_2, j_2; i_2, j_2; i_2, j_2) + n\Delta^{(n)}_3(i_2, j_2; i_2, j_2; i_2, j_2) - \Delta^{(n)}_3(i_2, j_2; i_2, j_2; i_2, j_2) \right\}
\]

\[
+ \frac{1}{(n)_3} \sum_{[i_1,i_2] \in I^*_2, [j_1,j_2] \in I^*_2} \left\{ \left( \Delta^{(n)}_3(i_1, j_1; i_1, j_2; i_1, j_2) + \Delta^{(n)}_3(i_1, j_1; i_1, j_2; i_1, j_2) \right) + \right.
\]

\[
\left. + \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_2, j_2) + \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_2, j_2) \right\} = O(n), \quad (A.49)
\]

where the implicit constant depends only on $\|h\|_\infty$. This completes Step I in view of (A.45).

Step II. We prove that $\text{Var}(n\tilde{D}^{(n)}_3) = O(n^{-1})$. Notice that

\[
\sum_{[i_1,i_2,i_3] \in I^*_3} \Delta^{(n)}_3(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}) = A_3 - A_2 - A_1,
\]

where

\[
A_3 := \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \sum_{i_3=1}^{n} \Delta^{(n)}_3(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}),
\]

\[
A_2 := \sum_{[i_1,i_2] \in I^*_2} \left\{ \Delta^{(n)}_3(i_1, \pi_{i_1}; i_1, \pi_{i_1}; i_2, \pi_{i_2}) + \Delta^{(n)}_3(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_1, \pi_{i_1}) + \Delta^{(n)}_3(i_2, \pi_{i_2}; i_1, \pi_{i_1}; i_1, \pi_{i_1}) \right\},
\]

\[
A_1 := \sum_{i_1=1}^{n} \Delta^{(n)}_3(i_1, \pi_{i_1}; i_1, \pi_{i_1}; i_1, \pi_{i_1}).
\]

We set

\[
\bar{\Delta}^{(n)}_3(i_1, j_1; i_2, j_2; i_3, j_3)
\]

\[
:= \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_3, j_3) - \Delta^{(n)}_3(\bullet, j_1; i_2, j_2; i_3, j_3) - \cdots - \Delta^{(n)}_3(i_1, j_1; i_2, j_2; i_3; \bullet)
\]

\[
+ \Delta^{(n)}_3(\bullet; i_2, j_2; i_3, j_3) + \Delta^{(n)}_3(\bullet; j_1; \bullet, j_2; i_3, j_3) + \cdots + \Delta^{(n)}_3(i_1, j_1; i_2, j_2; \bullet, \bullet)
\]

\[
- \cdots + \Delta^{(n)}_3(\bullet; \bullet; \bullet; \bullet; \bullet; \bullet). \quad (A.50)
\]

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Combining (A.48) and (A.50), we deduce

\[ A_3 = \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \sum_{i_3=1}^{n} \Delta_3^{(n)}(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}). \]

Here, \( A_3 \) can be decomposed as \( A_3 = \tilde{A}_3 + \tilde{A}_2 + \tilde{A}_1 \), where

\[ \tilde{A}_3 := \sum_{[i_1,i_2,i_3] \in I_n^3} \Delta_3^{(n)}(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}), \]

\[ \tilde{A}_2 := \sum_{[i_1,i_2] \in I_n^2} \left\{ \Delta_3^{(n)}(i_1, \pi_{i_1}; i_2, \pi_{i_2}) + \Delta_3^{(n)}(i_1, \pi_{i_1}; i_2, \pi_{i_2}) + \Delta_3^{(n)}(i_2, \pi_{i_2}; i_1, \pi_{i_1}) \right\}, \]

\[ \tilde{A}_1 := \sum_{i_1=1}^{n} \tilde{\Delta}_3^{(n)}(i_1, \pi_{i_1}; i_1, \pi_{i_1}; i_1, \pi_{i_1}). \]

Hence

\[ \sum_{[i_1,i_2,i_3] \in I_n^3} \Delta_3^{(n)}(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}) = \tilde{A}_3 + (\tilde{A}_2 - A_2) + (\tilde{A}_1 - A_1). \]

Using \( \tilde{\Delta}_3^{(n)}(\bullet, j_1; i_2, j_2; i_3, j_3) = \cdots = \tilde{\Delta}_3^{(n)}(\bullet, \bullet, \bullet, \bullet, \bullet, \bullet) = 0 \), straightforward calculation confirms that \( \text{Var}(A_3) = O(n^3) \). First, for \( i_1, i_2, i_3, i'_1, i'_2, i'_3 \) distinct, we have

\[
\mathbb{E}[\Delta_3^{(n)}(i_1, \pi_{i_1}; i_2, \pi_{i_2}; i_3, \pi_{i_3}) \Delta_3^{(n)}(i'_1, \pi_{i'_1}; i'_2, \pi_{i'_2}; i'_3, \pi_{i'_3})] = \frac{1}{(n)^6} \sum_{[j_1,j_2,j_3,j'_1,j'_2,j'_3] \in I_n^6} \Delta_3^{(n)}(i_1,i_2,j_1,j_2,j_3,j_3) \Delta_3^{(n)}(i'_1,i'_2,j'_1,j'_2,j'_3,j'_3)
\]

where

\[
- \frac{1}{(n)^6} \sum_{[j_1,j_2,j_3,j'_1,j'_2,j'_3] \in I_n^6} \Delta_3^{(n)}(i_1,j_1,j_2,j_3,j_3) \Delta_3^{(n)}(i'_1,j'_1,j'_2,j'_3,j'_3) = \frac{1}{(n)^6} \sum_{[j_1,j_2,j_3,j'_1,j'_2,j'_3] \in I_n^6} \tilde{\Delta}_3^{(n)}(i_1,j_1,j_2,j_3,j_3) \tilde{\Delta}_3^{(n)}(i'_1,j'_1,j'_2,j'_3,j'_3), \quad (A.51)
\]

and other summands can be rewritten similarly. Moreover, we have in (A.51)

\[
\frac{1}{(n)^6} \sum_{[j_1,j_2,j_3,j'_1,j'_2,j'_3] \in I_n^6} \Delta_3^{(n)}(i_1,j_1,j_2,j_3,j_3) \Delta_3^{(n)}(i'_1,j'_1,j'_2,j'_3,j'_3) = - \frac{1}{(n)^6} \sum_{[j_1,j_2,j_3,j'_1,j'_2,j'_3] \in I_n^6} \tilde{\Delta}_3^{(n)}(i_1,j_1,j_2,j_3,j_3) \tilde{\Delta}_3^{(n)}(i'_1,j'_1,j'_2,j'_3,j'_3),
\]

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\[
\frac{1}{(n)_6} \sum_{[j_1,j_2,j_3] \in I^6_1} \bar{\Delta}_3^{(n)}(i_1,j_1; i_2,j_2; i_3,j_3) \bar{\Delta}_3^{(n)}(i_1',j_1'; i_2',j_2'; i_3',j_3') \\
= - \frac{1}{(n)_6} \sum_{[j_1,j_2,j_3] \in I^6_1} \sum_{j_3 \in \{j_1,j_2,j_3\}} \bar{\Delta}_3^{(n)}(i_1,j_1; i_2,j_2; i_3,j_3) \bar{\Delta}_3^{(n)}(i_1',j_1'; i_2',j_1; i_3',j_1'),
\]
and all the rest; in (A.52)
\[
\frac{1}{(n)_6} \sum_{[j_1,j_2,j_3,j_4] \in I^6_1} \bar{\Delta}_3^{(n)}(i_1,j_1; i_2,j_2; i_3,j_3) \bar{\Delta}_3^{(n)}(i_1',j_1'; i_2',j_1; i_3',j_1') \\
= - \frac{1}{(n)_6} \sum_{[j_1,j_2,j_3,j_4] \in I^6_1} \sum_{j_3 \in \{j_1,j_2,j_3,j_4\}} \bar{\Delta}_3^{(n)}(i_1,j_1; i_2,j_2; i_3,j_3) \bar{\Delta}_3^{(n)}(i_1',j_1'; i_2',j_1; i_3',j_1'),
\]
and all the rest. It follows that
\[
\sum_{[i_1,i_2,i_3,i_1',i_2',i_3'] \in I^6_1} \mathbb{E} \left[ \bar{\Delta}_3^{(n)}(i_1,\pi_{i_1}; i_2,\pi_{i_2}; i_3,\pi_{i_3}) \bar{\Delta}_3^{(n)}(i_1',\pi_{i_1'}; i_2',\pi_{i_2'}; i_3',\pi_{i_3'}) \right] = O(n^3).
\]
Similar calculations for the cases when the pairs \([i_1,i_2,i_3]\) and \([i_1',i_2',i_3']\) have one, two, or three indices in common, give a total contribution of at most \(O(n^3)\). Adding these together shows that \(\text{Var}(\bar{A}_3) = O(n^3)\). This together with \(\text{Var}(\bar{A}_2 - A_2) = O(n^3)\) (similar to Zhao et al., 1997, p. 2212; Barbour and Chen, 2005, Lemma 3.1) and \(\text{Var}(A_1 - A_1) = O(n)\) (Hoeffding, 1951, Theorem 2) concludes that \(\text{Var}(n \bar{D}_3^{(n)}) = O(n^{-1})\).

These two steps together prove \(\mathbb{E}[(n \bar{D}_3^{(n)})^2] = O(n^{-1})\). The proofs for \(\mathbb{E}[(n \bar{D}_\ell^{(n)})^2] = O(n^{-1})\), \(\ell = 4, \ldots, m\), are very similar and hence omitted. \(\square\)

### A.3.3 Proof of Corollary 4.1

**Proof of Corollary 4.1.** Recall the notations introduced right before Corollary 4.1. We verify the conditions in Theorem 4.2 as follows. Proposition 2.2 shows that \(U^{(n)}\) and \(V^{(n)}\) converge in distribution to \(U\) and \(V\), respectively. We also have (I) the kernel \(K\) is symmetric and continuous on \(\mathbb{R}^p \times \mathbb{R}^q\), and thus \(\|K\|_\infty < \infty\); (II) \(K_1(w; \mathbb{P}_{U^{(n)}} \times \mathbb{P}_{V^{(n)}}) = 0\); (III)
\[
6K_2\left( w, w'; \mathbb{P}_{U^{(n)}} \times \mathbb{P}_{V^{(n)}} \right) = d_{U^{(n)}}(u, u') d_{V^{(n)}}(v, v'),
\]
and
\[
6K_2\left( w, w'; \mathbb{P}_U \times \mathbb{P}_V \right) = d_U(u, u') d_V(v, v'),
\]
y by Yao et al. (2018, Sec. 1.1). Recall that
\[
d_{U^{(n)}}(u, u') := \|u - u'\| - \mathbb{E}\|u - U^{(n)}\| - \mathbb{E}\|U^{(n)} - u'\| + \mathbb{E}\|U^{(n)} - U^{(n)}\|,
\]
and
\[
d_U(u, u') := \|u - u'\| - \mathbb{E}\|u - U\| - \mathbb{E}\|U - u'\| + \mathbb{E}\|U - U\|,
\]
where \(U^{(n)}\) and \(U\) are independent copies of \(U^{(n)}\) and \(U\), respectively.
Next we verify Assumptions (i)–(vi) for $-d_{U(n)}(u, u')$ and $-d_U(u, u')$. It can be easily seen that $-d_{U(n)}(u, u')$ are symmetric (Assumption (i)), degenerate $E[d_{U(n)}(u, U(n))] = 0$ (Assumption (iv)), and $E[d_{U(n)}(U(n), U'_n)] \in (0, +\infty)$ (Assumption (v)) by Székely et al. (2007, Theorem 4(i)). Lyons (2013, p. 3291) has proved that functions $-d_{U(n)}(u, u')$ are non-negative definite (Assumption (iii)). These functions are equicontinuous (Assumption (ii)) since

$$|d_{U(n)}(u, u') - d_{U(n)}(u, u'')| = \left| \|u - u'\| - \|u - u''\| - E[(U'(n) - u') - (U(n) - u'')] \right|$$

$$\leq 2\|u' - u''\|,$$

and moreover, $|d_{U(n)}(u, u') - d_{U(n)}(u'', u'')| \leq 2\|u - u''\| + 2\|u' - u''\|$. It remains to prove that $-d_{U(n)}(u, u')$ converges uniformly to $-d_U(u, u')$ (Assumption (vi)). Using the portmanteau Lemma (van der Vaart, 1998, Lemma 2.2) and Proposition 2.2, we have for all $u, u' \in \mathbb{S}_p$,

$$E\|u - U_s(n)\| \to E\|u - U_s\|, \ E\|U'(n) - u'\| \to E\|U - u'\|, \text{ and } E\|U(n) - U'_n\| \to E\|U - U_s\|,$$

and thus $-d_{U(n)}(u, u')$ converges pointwise to $-d_U(u, u')$. Then the uniform convergence follows from the equicontinuity of $-d_{U(n)}(u, u')$ (Rudin, 1976, Exercise 7.16). Assumptions (i)–(vi) can be similarly verified for $-d_{V(n)}(v, v')$ and $-d_V(v, v')$ as well.

Lastly, using Proposition 2.4, $[F_{1,+(n)}(X_i)]_{i=1}^n$ and $[F_{2,+(n)}(Y_i)]_{i=1}^n$ are uniformly distributed on $\mathcal{P}(G_{\alpha,nR,ns})$ and $\mathcal{P}(G'_{\alpha,nR,ns})$, respectively. In addition, under $H_0$, $[F_{1,+(n)}(X_i)]_{i=1}^n$ and $[F_{2,+(n)}(Y_i)]_{i=1}^n$ are independent. Hence our statistic is distributed as

$$\widehat{M}_n = n \cdot \left(\begin{array}{c} n \\ 4 \end{array}\right)^{-1} \sum_{1 \leq j_1 < \cdots < j_4 \leq n} K\left(\left(u_{\pi'}^{(n)}(j_1), v_{\pi''}^{(n)}(j_1), \ldots, u_{\pi'}^{(n)}(j_4), v_{\pi''}^{(n)}(j_4)\right)\right),$$

where $\pi'$ and $\pi''$ are uniformly distributed on $\mathcal{P}([n])$ and independent, and thus the same as the form (4.2) by defining permutation $\pi$ for which $\pi_i = j$ subject to $\pi'_k = i$ and $\pi''_k = j$ for some $k$. \qed

### A.4 Proofs for Section 5 of the main paper

#### A.4.1 Proof of Theorem 5.2

**Proof of Theorem 5.2.** In order to prove $Q_{1-\alpha}^{(M)} \rightarrow Q_{1-\alpha}$ as $M \rightarrow \infty$, it suffices to show that

$$\sum_{k=1}^{N1N2} \lambda_k^{(M)}(\xi_k^2 - 1) \overset{d}{\rightarrow} \sum_{k=1}^{\infty} \lambda_k(\xi_k^2 - 1).$$

We only need to show the convergence of moment-generating functions:

$$E\left[ \exp\left( t \sum_{k=1}^{N1N2} \lambda_k^{(M)}(\xi_k^2 - 1) \right) \right] \to E\left[ \exp\left( t \sum_{k=1}^{\infty} \lambda_k(\xi_k^2 - 1) \right) \right] \quad \text{(A.54)}$$

as $M \to \infty$, for all $t \in [-r, r]$, some $r > 0$, by arguments in Billingsley (1995, p. 390). Notice that (A.54) is equivalent to

$$\prod_{k=1}^{N1N2} \left( \frac{1 - 2t\lambda_k^{(M)}}{\exp(\lambda_k^{(M)})} \right)^{-1/2} \rightarrow \prod_{k=1}^{\infty} \left( \frac{1 - 2t\lambda_k}{\exp(\lambda_k)} \right)^{-1/2} \quad \text{(A.55)}$$
Since we have, by Item (vi) in Lyons (2018), $\lambda_k > 0$ and
\[
\sum_{k=1}^{\infty} \lambda_k = \mathbb{E}\|U - U_*\| \cdot \mathbb{E}\|V - V_*\| < \infty,
\]
where $U \sim U_p$, $V \sim U_q$, and $U_*$ and $V_*$ are independent copies of $U$ and $V$, respectively, the right-hand side of (A.55) converges to a nonzero real number (Rudin, 1987, Theorem 15.5) for every $t \in [-r, r]$ where $r$ is some fixed small positive number. This together with the fact that, $\lambda_k^{(M)} \to \lambda_k$ for each fixed $k$ as $M \to \infty$ by (A.23), concludes (A.55). \qed