On Azadkia–Chatterjee's conditional dependence coefficient

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In recent work, Azadkia and Chatterjee (*Ann. Statist.* **49** (2021) 3070–3102) laid out an ingenious approach to defining consistent measures of conditional dependence. Their fully nonparametric approach forms statistics based on ranks and nearest neighbor graphs. The appealing nonparametric consistency of the resulting conditional dependence measure and the associated empirical conditional dependence coefficient has quickly prompted follow-up work that seeks to study its statistical efficiency. In this paper, we take up the framework of conditional randomization tests (CRT) for conditional independence and conduct a power analysis that considers two types of local alternatives, namely, parametric quadratic mean differentiable alternatives and nonparametric Hölder smooth alternatives. Our local power analysis shows that conditional independence tests using the Azadkia–Chatterjee coefficient remain inefficient even when aided with the CRT framework, and serves as motivation to develop variants of the approach; cf. Lin and Han (*Biometrika* **110** (2023) 283–299). As a byproduct, we resolve a conjecture of Azadkia and Chatterjee by proving central limit theorems for the considered conditional dependence coefficients, with explicit formulas for the asymptotic variances.

Keywords: Conditional independence; graph-based test; rank-based test; nearest neighbor graphs; local power analysis

1. Introduction

Conditional (in)dependence is a fundamental statistical concept that plays a central role in statistical inference and theory (Dawid, 1979, 1980). Testing conditional independence is nowadays a routine task in graphical modeling (Maathuis et al., 2019), causal discovery (Peters, Janzing and Schölkopf, 2017), feature selection (Koller and Sahami, 1996), and many other statistical applications. Formally, the problem of interest is to test for three random vectors X, Y, Z the hypothesis

$$H_0: Y$$
 and Z are conditionally independent given X , (1)

based on a finite sample of size n from the joint distribution of (X,Y,Z). It is customary to denote the conditional independence by $Y \perp \!\!\! \perp Z \mid X$.

In contrast to the discrete/categorical case or favorable parametric settings such as multivariate normality, the general problem of testing (1) when *X* is continuous is a remarkably challenging task (Bergsma, 2004, Neykov, Balakrishnan and Wasserman, 2021, Shah and Peters, 2020). A number of attempts have been made to provide nonparametric solutions, and notable examples include Linton and Gozalo (1997) (on conditional cumulative distribution functions); Su and White (2007, 2008, 2014) (on conditional characteristic functions, conditional probability density functions, and smoothed empirical likelihood ratios, respectively); Huang (2010) (on maximal nonlinear conditional correlation); Fukumizu et al. (2008), Zhang et al. (2011), Doran et al. (2014), and Strobl, Zhang and Visweswaran (2019) (on kernel-based conditional dependence); Póczos and Schneider (2012) and Runge (2018) (on conditional mutual information); Székely and Rizzo (2014) and Wang et al. (2015) (on conditional distance

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correlation); Song (2009) and Cai, Li and Zhang (2022) (based on Rosenblatt transformation); Bergsma (2004, 2011) and Veraverbeke, Omelka and Gijbels (2011) (copula-based); Hoyer et al. (2009), Peters, Janzing and Schölkopf (2011), Shah and Peters (2020), and Petersen and Hansen (2021) (regression-based); Canonne et al. (2018) and Neykov, Balakrishnan and Wasserman (2021) (binning-based).

For the important special case where Y is a random scalar (and hence denoted in regular font by Y), Azadkia and Chatterjee (2021) introduced a novel and rather different conditional dependence measure whose estimate ingenuously combines ideas from rank statistics, nearest neighbor graphs and associated minimum spanning trees for data sets. The dependence measure and estimate were shown to possess the following four appealing properties:

- (1) the conditional dependence measure takes values in [0,1], is 0 if and only if $Y \perp \mathbb{Z} \mid X$, and is 1 if and only if Y is almost surely (a.s.) equal to a measurable function of \mathbb{Z} given X;
- (2) the estimate has a simple expression and can be computed in $O(n \log n)$ time;
- (3) the estimate is fully nonparametric and has no tuning parameter;
- (4) the estimate is consistent as long as Y is not a.s. equal to a measurable function of X.

The new approach has quickly caught attention. First follow-up work studies extensions to topological spaces and multidimensional *Y* and explores connections to general random graphs; see Deb, Ghosal and Sen (2020) and Huang, Deb and Sen (2022). Moreover, for the case of unconditional dependence, analyses were conducted to better understand the statistical power of the approach. These analyses treat the very closely related coefficient presented by Chatterjee (2021); see Cao and Bickel (2020), Shi, Drton and Han (2022a), and Auddy, Deb and Nandy (2023).

In this paper, we study the statistical efficiency of Azadkia—Chatterjee's conditional dependence coefficient in testing the hypothesis of conditional independence from (1). Azadkia and Chatterjee (2021) themselves did not pursue using their coefficient for inferential problems such as testing. To implement a test, we employ the conditional randomization test (CRT) framework developed in Candès et al. (2018); see Berrett et al. (2020) for a related proposal. The CRT framework assumes that the conditional distribution of Y given X is known, and thus the null distribution of any conditional dependence coefficient can be approximated by simulation.

Local power analyses for tests rely on a choice of local alternatives. In the context of this paper, an important subtlety lies in the fact that in order to be relevant for a CRT-based Azadkia–Chatterjee-type test, the conditional distribution of Y given X should be identical between the null and local alternatives. Two such families of local alternatives are considered in this manuscript:

- (a) the joint density of (X,Y,Z) in the alternative is assumed to be "smoothly" changing to the null in the sense of quadratic mean differentiability (Lehmann and Romano, 2005, Definition 12.2.1). This is akin to parametric settings, and such families of local alternatives have been explored in studies of rank- and graph-based tests in related statistical problems (Bhattacharya, 2019, Cao and Bickel, 2020, Shi et al., 2022). The critical detection boundary in such cases is known to be at root-n;
- (b) the conditional distribution of (Y, \mathbb{Z}) given X is assumed to be Hölder smoothly changing with regard to X. This is akin to nonparametric settings, and the case we will consider is an extension of the one that has been examined by Neykov, Balakrishnan and Wasserman (2021). There, as X,Y,\mathbb{Z} are all random scalars, the critical detection boundary is $n^{-2s/(4s+3)}$, where s denotes the Hölder smoothness exponent.

The local power analyses we report on in this manuscript provide, in both of the above scenarios, examples that show that the CRT-based Azadkia–Chatterjee-type test is unfortunately unable to achieve the critical detection boundary, i.e., the sum of type-I and type-II errors will not decrease to zero along the boundary. We emphasize here that the power of CRT-based Azadkia–Chatterjee-type test

cannot simply be boosted to achieve the detection boundary by using the additional information coming from the CRT framework, in view of the Hájek representation theorem; compare Equation (S4) in Shi, Drton and Han (2022b). Our theoretical analysis thus echoes the empirical observations made in Huang, Deb and Sen (2022) and calls for developing new variants of the tests that use an increasing number of nearest neighbors when constructing the nearest neighbor graphs; see Bhattacharya (2019, Proposition 1), Deb, Ghosal and Sen (2020, Remark 4.3), and in particular, a recent work by Lin and Han (2023) on boosting the power of Chatterjee's original proposal which however cannot be directly applied to multidimensional cases. These conclusions are also connected to related claims made by Stone (1977, Corollary 3), Biau and Devroye (2015), and Berrett, Samworth and Yuan (2019, Theorems 1 and 2) in other settings of nonparametric statistics.

Our local power analysis in Case (a) is built on the innovative new work of Deb, Ghosal and Sen (2020), who developed a general framework to study normalized graph-based dependence measures (combined with rank- and kernel-based ones) that invokes a Berry–Esseen theorem for dependency graphs (Chen and Shao, 2004). In order to complete our analysis of the local power, however, an additional ingredient is needed, namely, we have to prove the existence as well as calculate the asymptotic variance of the (unnormalized) Azadkia–Chatterjee conditional dependence coefficient. To obtain this crucial result we use asymptotic techniques devised for 1-nearest neighbor graphs in Henze (1987) and Devroye (1988). This part of our derivations shall occupy the main body of the proofs of our local power results. Our analysis covers as a special instance the case of full independence and, thus, resolves a conjecture of Azadkia and Chatterjee (2021) about a central limit theorem (CLT) for their statistic under full independence; see Section 3 ahead for details.

Our local power analysis in Case (b), on the other hand, is based on a brute-force calculation of the mean and variance of the Azadkia–Chatterjee conditional dependence coefficient along a special non-standard local alternative sequence that serves as the "worst case" in the minimax lower bound construction of Neykov, Balakrishnan and Wasserman (2021). This involves handling permutation statistics for which permutation randomness is not (though close to) uniform over all possible rearrangements, a notoriously difficult task. Interestingly, in a very recent preprint, Auddy, Deb and Nandy (2023) did related calculations in analyzing the local power of Chatterjee's rank correlation coefficient (Chatterjee, 2021) against a different family of non-standard local alternative sequences; see the proof of their Theorem 2.1. It appears, though, that the techniques used are substantially different from the ones present here, which of course also differs through the focus on conditional (in-)dependence.

The rest of the paper is organized as follows. Section 2 reviews the conditional dependence coefficient proposed by Azadkia and Chatterjee (2021), denoted ξ_n , as well as the conditional randomization test framework proposed by Candès et al. (2018). Section 3 presents the asymptotic normality of ξ_n under independence. Local power analyses of CRTs based on ξ_n , in the two cases of alternatives are presented in Section 4 and Section 5, respectively. A brief conclusion is provided in Section 6. The proof of Theorem 4.4 is given in Section 7, with auxiliary results and remaining proofs deferred to the supplement (Shi, Drton and Han, 2024).

Notation. For an integer $n \ge 1$, let $[\![n]\!] := \{1,2,\ldots,n\}$. A set consisting of distinct elements x_1,\ldots,x_n is written as either $\{x_1,\ldots,x_n\}$ or $\{x_i\}_{i=1}^n$. The corresponding sequence is denoted $[x_1,\ldots,x_n]$ or $[x_i]_{i=1}^n$. For a sequence of vectors v_1,\ldots,v_k , we use (v_1,\ldots,v_k) as a shorthand for $(v_1^\top,\ldots,v_k^\top)^\top$. For a vector $v \in \mathbb{R}^d$, ||v|| stands for the Euclidean norm. The symbols $[\cdot]$ and $[\cdot]$ denote the floor and ceiling functions, respectively. The notation $\mathbb{1}(\cdot)$ is used for the indicator function. For any real-valued random vectors U and V, the (induced) probability measure, cumulative distribution function, and the probability density function of U (if existing) are denoted as P_U , F_U , and q_U , respectively; the conditional probability density function of U given V (if existing) is written as $q_U|_V$. In the following, the terms "absolutely continuous" and "almost everywhere" (shorthanded as "a.e.") are with respect to Lebesgue measure.

2. Conditional dependence measures and tests

In the sequel, let $Y \in \mathbb{R}$ be a random scalar, and let $X \in \mathbb{R}^p$ and $Z \in \mathbb{R}^q$ be two random vectors, all defined on the same probability space. The goal is to test (1) based on observations $(X_1, Y_1, Z_1), \ldots, (X_n, Y_n, Z_n)$ that consist of n independent copies of the triple (X, Y, Z). Note that the joint distribution of (X, Y, Z) need not be continuous.

2.1. Conditional dependence measures and coefficients

Azadkia and Chatterjee (2021) proposed the following measure of conditional dependence between Y and Z given X:

$$\xi = \xi(Y, \mathbf{Z} \mid \mathbf{X}) := \frac{\int \mathbb{E}\left[\operatorname{Var}\left\{P(Y \ge y \mid \mathbf{X}, \mathbf{Z}) \mid \mathbf{X}\right\}\right] dP_Y(y)}{\int \mathbb{E}\left[\operatorname{Var}\left\{\mathbb{1}\left(Y \ge y\right) \mid \mathbf{X}\right\}\right] dP_Y(y)}.$$
 (2)

The following proposition describes the appealing properties we pointed out in the introduction.

Proposition 2.1 ((Azadkia and Chatterjee, 2021, Theorem 2.1)). Suppose that Y is not a.s. equal to a measurable function of X. Then ξ is well-defined and belongs to the interval [0,1]. Moreover, ξ is a consistent measure of conditional dependence with tailored extremal properties in the sense that $\xi = 0$ if and only if Y and Z are conditionally independent given X, and $\xi = 1$ if and only if Y is a.s. equal to a measurable function of Z given X.

The dependence measure ξ clearly extends an earlier introduced measure of marginal dependence between Y and (a random scalar) Z, namely,

$$\xi^{\text{DSS}} = \xi^{\text{DSS}}(Y, Z) := \frac{\int \text{Var}\{P(Y \ge y \mid Z)\} dP_Y(y)}{\int \text{Var}\{\mathbb{1}(Y \ge y)\} dP_Y(y)},$$
(3)

which Dette, Siburg and Stoimenov (2013) introduced for continuous distributions and Chatterjee (2021) considered in general. The quantities ξ and ξ^{DSS} share similar properties: (i) the consistency in measuring dependence is natural as the numerator (a nonnegative scalar) is zero if and only if either Y is independent of Z (for ξ^{DSS}), or Y is independent of Z given X (for ξ); (ii) the self-normalization structure yields tailored extremal properties as the numerator is always upper bounded by the denominator; (iii) both the numerator and the denominator involve the indicator $\mathbb{1}(Y \ge y)$, which motivates estimation using the ranks of the Y_i 's and their regression on the Z_i 's or (X_i, Z_i) ' to account for the conditioning in each term.

Both Chatterjee (2021) and Azadkia and Chatterjee (2021) advocate a 1-nearest neighbor (1-NN) approach to performing the aforementioned regression; note that in one dimension 1-NN is obviously corresponding to working with ranks. In detail, let

$$R_i := \sum_{j=1}^n \mathbb{1}(Y_j \le Y_i) \tag{4}$$

be the rank of Y_i among Y_1, \ldots, Y_n , and define

$$N(i) := \left\{ j \neq i : X_j \text{ is the nearest neighbor of } X_i \right\},$$

$$M(i) := \left\{ j \neq i : (X_i, Z_i) \text{ is the nearest neighbor of } (X_i, Z_i) \right\},$$
(5)

to be the indices of the nearest neighbors of X_i and (X_i, Z_i) , respectively. Here, nearest neighbors are determined by Euclidean distance and possible ties in distance are broken at random. Azadkia and Chatterjee's conditional dependence coefficient is then defined as

$$\xi_n = \xi_n \left(\left[(X_i, Y_i, \mathbf{Z}_i) \right]_{i=1}^n \right) := \frac{\sum_{i=1}^n \left\{ \min(R_i, R_{M(i)}) - \min(R_i, R_{N(i)}) \right\}}{\sum_{i=1}^n \left\{ R_i - \min(R_i, R_{N(i)}) \right\}}.$$
 (6)

Although not at all immediate at first sight, Azadkia and Chatterjee (2021) showed that ξ_n is a strongly consistent estimator of ξ as long as the latter is well-defined. We summarize the fact in the following proposition.

Proposition 2.2 ((Azadkia and Chatterjee, 2021, Theorem 2.2)). As long as Y is not a.s. equal to a measurable function of X, it holds that ξ_n converges to ξ a.s. as $n \to \infty$.

Remark 2.3. The intuition behind the convergence is by no means transparent. We refer the readers of interest to Chatterjee (2021, Section 8) and the following heuristic argument:

$$\begin{split} \mathbf{E}\Big[n^{-1}\{R_1-\min(R_1,R_{N(1)})\}\Big] &\approx \mathbf{E}\Big[F_Y(Y_1)-\min\{F_Y(Y_1),F_Y(Y_{N(1)})\}\Big] \\ &= \mathbf{E}\Big[\int \Big\{\mathbb{1}(Y_1\geq t)-\mathbb{1}(Y_1\geq t)\mathbb{1}(Y_{N(1)}\geq t)\Big\}\mathrm{d}\mathbf{P}_Y(t)\Big] \\ &\approx \mathbf{E}\Big[\frac{1}{2}\int \Big\{\mathbb{1}(Y_1\geq t)-\mathbb{1}(Y_{N(1)}\geq t)\Big\}^2\mathrm{d}\mathbf{P}_Y(t)\Big], \end{split}$$

with

$$E\{\mathbb{1}(Y_1 \ge t) - \mathbb{1}(Y_{N(1)} \ge t)\}^2 \approx 2E[Var\{\mathbb{1}(Y_1 \ge t) \mid X_1\}].$$

Here the last step is intrinsically performed using an 1-NN regression.

2.2. Conditional randomization tests

Next we introduce the conditional randomization test (CRT) framework of Candès et al. (2018). This framework is designed for settings where the conditional distribution of Y given X is known or can be accurately inferred from a large out-of-sample data set. See also Berrett et al. (2020, Section 2.2) for an illustration of application scenarios of this framework. In the sequel, we use $Q = Q(\cdot | x)$ to denote the Markov kernel used in the algorithm implementing the test of conditional independence. Ideally, Q is (very close to) the conditional distribution of Y given X = x.

The CRT framework leverages that under H_0 the conditional distribution of Y given (X, Z) is the same as that of Y given X. This yields the following observation: if Q equals the conditional distribution of Y given X = x and $Y^{(1)}$ is drawn independently from $Q(\cdot | X)$, then the two triples (X, Y, Z) and $(X, Y^{(1)}, Z)$ are equal in distribution under H_0 . In contrast, any difference between the distributions of (X, Y, Z) and $(X, Y^{(1)}, Z)$ will manifest itself as evidence against H_0 .

Algorithm 1: Conditional randomization test (CRT)

Input: Data $\left[(X_i, Y_i, Z_i)\right]_{i=1}^n$, the chosen conditional distribution Q, test statistic ψ_n , number of simulations B, and significance level $\alpha \in (0, 1)$.

for $b = 1, \ldots, B$ do

Draw a sample $[Y_i^{(b)}]_{i=1}^n$ from the product distribution $\bigotimes_{i=1}^n Q(\cdot \mid X_i)$, independent of the observed $[(Y_i, \mathbf{Z}_i)]_{i=1}^n$ and conditionally on $[X_i]_{i=1}^n$.

end

Output: CRT p-value defined as

$$p_{\text{CRT}} = (1+B)^{-1} \left[1 + \sum_{b=1}^{B} \mathbb{1} \left\{ \psi_n \left(\left[(\boldsymbol{X}_i, Y_i^{(b)}, \boldsymbol{Z}_i) \right]_{i=1}^n \right) \ge \psi_n \left(\left[(\boldsymbol{X}_i, Y_i, \boldsymbol{Z}_i) \right]_{i=1}^n \right) \right\} \right].$$

The CRT is then

$$\mathsf{T}^{\mathrm{Q},\psi_n}_\alpha\left(\left[(\boldsymbol{X}_i,Y_i,\boldsymbol{Z}_i)\right]_{i=1}^n\right)=\mathbb{1}(p_{\mathrm{CRT}}\leq\alpha).$$

To make the idea practical, consider a real-valued test statistic ψ_n defined on the range of $\left[(X_i,Y_i,Z_i)\right]_{i=1}^n$. Let B be a chosen number of Monte Carlo simulations. Then in each round $b \in \llbracket B \rrbracket$, one independently draws a new copy $Y_i^{(b)}$ from $Q(\cdot | X_i)$ for $i \in \llbracket n \rrbracket$, and calculates $\psi_n(\left[(X_i,Y_i^{(b)},Z_i)\right]_{i=1}^n)$. The CRT then examines the difference between the distributions of (X,Y,Z) and $(X,Y^{(1)},Z)$ by comparing the observed test statistic $\psi_n(\left[(X_i,Y_i,Z_i)\right]_{i=1}^n)$ to the simulated values $\psi_n(\left[(X_i,Y_i^{(b)},Z_i)\right]_{i=1}^n)$. The procedure is detailed in Algorithm 1.

2.3. CRT using the Azadkia-Chatterjee coefficient

We will be concerned with the CRT that is obtained by taking the test statistic ψ_n in Algorithm 1 to be ξ_n , the Azadkia–Chatterjee conditional dependence coefficient. The resulting test for significance level α is denoted by $\mathsf{T}_{\alpha}^{Q,\xi_n}$; here Q is added to highlight the dependence of the implementation on the chosen conditional distribution Q.

Remark 2.4. Berrett et al. (2020, Section 2.2) argued that in many cases the unlabeled data, i.e., data on (X,Y) but without the Z component, are plentiful, but labeled data on (X,Y,Z) jointly are scarce. In such cases, it is natural to assume that one not only knows (or may very accurately estimate) the needed conditional distribution but also the joint distribution of (X,Y). When the distribution of (X,Y) is known, the only term to be estimated from data is the numerator in (2); the denominator in (2) only depends on the distribution of (X,Y).

However, we would like to emphasize that, in view of the Hájek representation theorem as given in Equation (S4) in Shi, Drton and Han (2022b), replacing each R_i by $nF_Y(Y_i)$ in ξ_n will not result in an (asymptotic) improvement of ξ_n . In detail, although it is tempting to define an "oracle version" of ξ_n that uses more information as

$$\widecheck{\xi}_n = \widecheck{\xi}_n \Big(\big[(\boldsymbol{X}_i, Y_i, \boldsymbol{Z}_i) \big]_{i=1}^n \Big) := \frac{n^{-1} \sum_{i=1}^n \big[\min\{F_Y(Y_i), F_Y(Y_{M(i)})\} - \min\{F_Y(Y_i), F_Y(Y_{N(i)})\} \big]}{\int \mathrm{E}[\mathrm{Var}\{\mathbb{1}(Y \geq y) \,|\, \boldsymbol{X}\}] \mathrm{dP}_Y(y)},$$

this change will not increase the CRT's power (asymptotically), at least in all settings considered in this paper.

Later, in Sections 4–5, we shall study in detail the test based on ξ_n . However, some preliminary results deserve to be documented first. In the following, let \mathcal{P}_Q be the family of all joint distributions for (X,Y,Z) such that Y is not a.s. equal to a measurable function of X and the conditional distribution of Y given X = x coincides with a given (non-trivial) Markov kernel Q.

Proposition 2.5 (Control of size and consistency). Fix a Markov kernel Q for Y given X.

(i) The test T_{α}^{Q,ξ_n} is valid in the sense that for any $P_{(X,Y,Z)} \in \mathcal{P}_Q$ satisfying H_0 , denoting $P_{H_0} := P_{(X,Y,Z)}^{\otimes n}$ as the corresponding product measure, it holds for any $n \ge 1$ that

$$P_{H_0}(\mathsf{T}^{\mathsf{Q},\xi_n}_{\alpha}=1) \leq \alpha;$$

notice that no assumption concerning the number of simulations B is required at all.

(ii) In addition, $\mathsf{T}_{\alpha}^{\mathsf{Q},\xi_n}$ is consistent in the sense that for any $\mathsf{P}_{(X,Y,\mathbf{Z})} \in \mathcal{P}_{\mathsf{Q}}$ violating H_0 , denoting P_{H_1} as the corresponding product measure, we have

$$\lim_{n\to\infty} P_{H_1}(\mathsf{T}_{\alpha}^{\mathbb{Q},\xi_n}=1)=1$$

as long as the number of simulations B tends to infinity as $n \to \infty$.

Remark 2.6. Of note, Petersen and Hansen (2021, Corollary 23) and Lundborg, Shah and Peters (2022, Theorem 4), among many others, proved uniform consistency of their conditional independence tests against particular subsets of alternative hypotheses. Their results are established via some careful non-asymptotic analysis of the test statistic along such local alternatives. It will be a statistically and also technically very interesting question to examine whether T_{α}^{Q,ξ_n} also enjoys similar properties. This is still an open problem.

3. Asymptotic normality under independence

In this section we consider the asymptotic behavior of ξ_n under independence of Y and (X, Z), which constitutes a special subfamily of the conditional independence hypothesis H_0 that our subsequent theoretic analysis shall be built on. In this (unconditional) independence scenario we then consider the coefficient ξ_n from Section 2 as well as a variant introduced in Azadkia and Chatterjee (2021).

In detail, Azadkia and Chatterjee (2021) also examined the case when p = 0, i.e., X has no component. In this case, the conditional dependence measure ξ from (2) reduces to the unconditional dependence measure defined analogous to ξ^{DSS} from (3); here the dimension of Z is not necessarily one. They then introduced the following coefficient $\xi_n^\#$, which extends the original proposal of Chatterjee (2021, Eqn. (1)) to higher dimension $q \ge 1$:

$$\xi_n^{\#} := \frac{\sum_{i=1}^n \{ n \min(R_i, R_{M(i)}) - L_i^2 \}}{\sum_{i=1}^n L_i (n - L_i)}.$$
 (7)

Here R_i and M(i) are defined in (4) and (5), respectively, with the understanding that X's part in (5) is removed since it is of no component, and $L_i := \sum_{j=1}^n \mathbb{1}(Y_j \ge Y_i)$.

Azadkia and Chatterjee (2021) conjectured that under independence between Y and Z, $\sqrt{n}\xi_n^{\#}$ obeys a CLT. Building on results of Deb, Ghosal and Sen (2020), we are able to derive the following theorem that, in particular, gives an affirmative answer to this conjecture under (absolute) continuity.

Theorem 3.1 (Asymptotic normality).

(i) Assume that $Y \in \mathbb{R}$ is continuous and independent of $(X, \mathbb{Z}) \in \mathbb{R}^{p+q}$. In addition, assume (X, \mathbb{Z}) is absolutely continuous admitting a density continuous over its support. We then have as, $n \to \infty$,

$$\sqrt{n}\xi_n \stackrel{\mathrm{d}}{\longrightarrow} N\Big(0, \frac{4}{5} + \frac{2}{5}\Big\{\mathfrak{q}_{p+q} + \mathfrak{q}_p\Big\} + \frac{4}{5}\Big\{\mathfrak{o}_{p+q} + \mathfrak{o}_p\Big\}\Big),$$

where for any integer $d \ge 1$, q_d and o_d are positive constants depending only on d. Their values are

$$q_d := \left\{ 2 - I_{3/4} \left(\frac{d+1}{2}, \frac{1}{2} \right) \right\}^{-1}, \quad I_x(a,b) := \frac{\int_0^x t^{a-1} (1-t)^{b-1} dt}{\int_0^1 t^{a-1} (1-t)^{b-1} dt}, \tag{8}$$

$$\mathfrak{o}_d := \int_{\Gamma_{d-2}} \exp\left[-\lambda \left\{ B(w_1, ||w_1||) \cup B(w_2, ||w_2||) \right\} \right] d(w_1, w_2), \tag{9}$$

$$\Gamma_{d;2} := \left\{ (w_1, w_2) \in (\mathbb{R}^d)^2 : \max(\|w_1\|, \|w_2\|) < \|w_1 - w_2\| \right\},\,$$

where $B(\mathbf{w}_1, r)$ is the ball of radius r centered at \mathbf{w}_1 , and $\lambda(\cdot)$ is the Lebesgue measure.

(ii) Assume $Y \in \mathbb{R}$ is continuous and independent of $\mathbf{Z} \in \mathbb{R}^q$. In addition, assume \mathbf{Z} is absolutely continuous. We then have, as $n \to \infty$,

$$\sqrt{n}\xi_n^{\#} \stackrel{\mathsf{d}}{\longrightarrow} N\left(0, \frac{2}{5} + \frac{2}{5}\mathfrak{q}_q + \frac{4}{5}\mathfrak{o}_q\right).$$

Remark 3.2. The asymptotic variance of $\sqrt{n}\xi_n$ (or $\sqrt{n}\xi_n^{\#}$) under independence between Y and (X,Z) (or Z) is seen to be distribution-free, i.e., its value will not change with the particular distribution of $P_{(X,Y,Z)}$ as long as the (absolute) continuity conditions in Theorem 3.1 hold. This (asymptotic) distribution-freeness is in line with similar observations made earlier for related problems such as two-sample goodness-of-fit tests, where Friedman and Rafsky (1979) extended Wald and Wolfowitz (1940)'s rank-based run test to multivariate spaces via minimum spanning trees; see, also, Henze (1988), Liu and Singh (1993), Henze and Penrose (1999), and Bhattacharya (2019) for other notable results along that track, and Devroye et al. (2018), Gamboa et al. (2022), Lin and Han (2022, 2023) for more related work.

Remark 3.3. It may be interesting to note that the asymptotic variance of $\sqrt{n}\xi_n^{\#}$ is strictly larger than 2/5, the asymptotic variance of the rank correlation from Equation (1) in Chatterjee (2021). However, this observation should not be interpreted as an advantage of Chatterjee's rank correlation over $\sqrt{n}\xi_n^{\#}$ in terms of statistical efficiency. As a matter of fact, both are powerless when used for testing independence; cf. Shi, Drton and Han (2022a, Theorem 1) and Theorem 4.4 ahead.

Remark 3.4. In order to derive the above CLTs for ξ_n and $\xi_n^{\#}$, we adopt techniques devised in Deb, Ghosal and Sen (2020). We highlight here some of these technical ingredients of our proof. Deb, Ghosal and Sen (2020) were focused on establishing general asymptotic results for graph-based statistics with an additional self-normalization step. In the present context of our Theorem 3.1, following Deb, Ghosal and Sen (2020, Theorem 4.1), it is readily shown that

$$\sqrt{n}\xi_n / \left\{ \hat{\operatorname{Var}}(\xi_n) \right\}^{1/2} \stackrel{\mathsf{d}}{\longrightarrow} N(0,1),$$

for some data-based normalization statistic $\hat{\text{Var}}(\xi_n)$. Our main focus, accordingly, can be understood as proving the existence as well as deriving the value of the limit of $\hat{\text{Var}}(\xi_n)$ as $n \to \infty$. This problem was not touched upon in Deb, Ghosal and Sen (2020) for a good reason, but is crucial for our analysis of the power ahead. To fill the gap, our proof draws on the remarkable techniques developed in Henze (1987) and Devroye (1988), which will be detailed blow.

The asymptotic variances of ξ_n and $\xi_n^{\#}$ may look mysterious but they are in fact connected to the behavior of nearest neighbor graphs. We present here a series of results that illustrate this connection. The first is a well-known result by Bickel and Breiman (1983, Corollary S1) on maximum degrees in 1-NN graphs.

Lemma 3.5 (Maximum degree in nearest neighbor graphs). Let $w_1, ..., w_n$ be any collection of n distinct points in \mathbb{R}^d . Then there exists a constant \mathfrak{C}_d depending only on the dimension d such that w_1 is the nearest neighbor of at most \mathfrak{C}_d points from $\{w_2, ..., w_n\}$.

The notation \mathfrak{C}_d , representing a constant upper bound of the maximum degree, will be used throughout the manuscript. For convenience, we take \mathfrak{C}_d as the smallest constant for which the property in Lemma 3.5 holds.

In the following, consider a sample $[W_i]_{i=1}^n$ comprised of n independent copies of a random vector $W \in \mathbb{R}^d$. Let \mathcal{G}_n be the associated directed nearest neighbor graph (NNG), i.e., \mathcal{G}_n has vertex set [n] and contains a directed edge from i to j whenever W_j is a nearest neighbor of W_i . We write $\mathcal{E}(\mathcal{G}_n)$ for the edge set of \mathcal{G}_n .

The parameter q_d in Theorem 3.1 comes from the following crucial result of Devroye (1988, Theorem 2).

Lemma 3.6 (Expected number of nearest-neighbor pairs). As long as W is absolutely continuous, we have

$$\mathrm{E}\left(\frac{1}{n}\#\left\{(i,j)\;distinct:\,i\to j,j\to i\in\mathcal{E}(\mathcal{G}_n)\right\}\right)\;\longrightarrow\;\frac{V_d}{U_d}=\mathfrak{q}_d,$$

where V_d is the volume of the unit ball in \mathbb{R}^d , and U_d is the volume of the union of two unit balls in \mathbb{R}^d whose centers are a unit distance apart. The explicit value of \mathfrak{q}_d shown in (8) is given by Li (2011, Equation (3)).

The parameter \mathfrak{o}_d in Theorem 3.1, on the other hand, comes from the following new lemma, which is developed in this manuscript. The lemma builds on an earlier result of Henze (1987).

Lemma 3.7. As long as **W** is absolutely continuous, we have

$$E\left(\frac{1}{n}\#\left\{(i,j,k) \ distinct: i \to k, j \to k \in \mathcal{E}(\mathcal{G}_n)\right\}\right) \longrightarrow \mathfrak{o}_d,$$

where $\mathfrak{d}_d = \mathfrak{d}_{d:2}$ is a special case of $\mathfrak{d}_{d:r}$, a quantity defined in Lemma 3.8 below.

The next lemma is due to Henze (1987, Theorem 1.4, Corollaries 1.5 and 1.6).

Lemma 3.8 (Expected number of vertices of specified degree). Let d_j^- be the in-degree of vertex W_j in \mathcal{G}_n , i.e., $d_j^- := \#\{i : i \to j \in \mathcal{E}(\mathcal{G}_n)\}$. If W is absolutely continuous with a density continuous a.e., then for any integer $k \in [0, \mathbb{C}_d]$, we have

$$\mathrm{E}\Big(\frac{1}{n}\#\{j:d_j^-=k\}\Big)\longrightarrow \mathfrak{p}_{d;k} \quad and \quad \mathrm{Var}(d_1^-)\longrightarrow \mathfrak{d}_{d;2},$$

where

$$\mathfrak{p}_{d;k} = \frac{1}{k!} \sum_{u=0}^{\mathfrak{C}_d - k} \frac{1}{u!} (-1)^u \mathfrak{d}_{d;k+u}, \quad 0 \le k \le \mathfrak{C}_d,$$

and

$$b_{d;0} = b_{d;1} = 1, \quad b_{d;r} = \int_{\Gamma_{d;r}} \exp\left[-\lambda \left\{ \bigcup_{i=1}^{r} B(w_i, ||w_i||) \right\} \right] d(w_1, \dots, w_r),$$

$$\Gamma_{d;r} = \left\{ (w_1, \dots, w_r) \in (\mathbb{R}^d)^r : ||w_i|| < \min_{1 \le i \le r; i \ne i} ||w_i - w_j||, 1 \le i \le r \right\}, \quad 2 \le r \le \mathfrak{C}_d.$$

Notice that $\mathfrak{p}_{d:k} \in [0,1]$ *is a constant only depending on d and k.*

Remark 3.9. We note that in Theorem 3.1(i), a slightly stronger condition (continuity over its support) is required for the density function in order to establish CLTs. This additional requirement is made for handling the "cross terms" of 1-NN graphs built on $[(X_i, Z_i)]_{i=1}^n$ and $[X_i]_{i=1}^n$ separately (cf. Lemma 7.4 ahead as an analogue of Lemmas 3.6–3.8 for the cross terms). Such cross terms are not present in Devroye (1988) and Henze (1987). Roughly speaking, we will prove that the two 1-NN graphs built on $[(X_i, Z_i)]_{i=1}^n$ and $[X_i]_{i=1}^n$ are nearly independent from each other. The proof of Lemma 7.4 adopts Devroye's and Henze's ideas but involves further analysis.

4. Power analysis: Parametric case

This section investigates the local power of the proposed tests for quadratic mean differentiable classes of alternatives (Lehmann and Romano, 2005, Definition 12.2.1), for which we show that the CRT based on Azadkia and Chatterjee ξ_n possesses only trivial power in $n^{-1/2}$ neighborhoods.

We begin with a set of local alternatives

$$\left\{ q_{\Delta}(\boldsymbol{x}, y, \boldsymbol{z}) : |\Delta| < \Delta^* \right\}, \quad \Delta^* > 0, \tag{10}$$

where for each $|\Delta| < \Delta^*$, $q_{\Delta}(x, y, z)$ is a joint density with respect to the Lebesgue measure. We then make assumptions on the set in (10). In the following, $E_0(\cdot)$ is understood to be the expectation operator with regard to the density function $q_0(x, y, z)$ obtained for $\Delta = 0$.

Assumption 4.1. It is assumed that

- (i) $q_0(x, y, z)$ is such that Y and Z are conditionally independent given X;
- (ii) for all $|\Delta| < \Delta^*$,

$$\int q_{\Delta}(\mathbf{x}, \mathbf{y}, \mathbf{z}) d\mathbf{z} = q_{\mathbf{X}, \mathbf{Y}}(\mathbf{x}, \mathbf{y}),$$

where $q_{X,Y}(\cdot,\cdot)$, the density of $P_{(X,Y)}$, is fixed and equal to the product of densities of P_X and P_Y , and invariant with regard to Δ ;

(iii) the score function

$$\dot{\ell}_{\Delta}(x, y, z) := \frac{\partial}{\partial \Delta} \log q_{\Delta}(x, y, z)$$

exists at $\Delta = 0$, and the family $\{q_{\Delta}(x, y, z)\}_{|\Delta| < \Delta^*}$ is quadratic mean differentiable (QMD) at $\Delta = 0$ with score function $\dot{\ell}_0$, that is,

$$\int \left(\sqrt{q_{\Delta}(\boldsymbol{x},y,z)} - \sqrt{q_{0}(\boldsymbol{x},y,z)} - \frac{1}{2}\Delta\dot{\ell}_{0}(\boldsymbol{x},y,z)\sqrt{q_{0}(\boldsymbol{x},y,z)}\right)^{2}\mathrm{d}(\boldsymbol{x},y,z) = o(\Delta^{2})$$

as $\Delta \rightarrow 0$:

- (iv) $E_0\{\dot{\ell}_0(X,Y,\mathbf{Z})^2\} > 0$ (Assumption (iii) implies $E_0\{\dot{\ell}_0(X,Y,\mathbf{Z})^2\} < \infty$ and $E_0\{\dot{\ell}_0(X,Y,\mathbf{Z})\} = 0$);
- (v) $E_0\{\dot{\ell}_0(X,Y,Z) \mid X,Z\} = 0$ almost surely;
- (vi) $E_0\{|\dot{\ell}_0(X,Y,Z)|^{4+\epsilon}\}<\infty$ for some fixed constant $\epsilon>0$;
- (vii) $\dot{\ell}_0(x, y, z)$ cannot be written as $h_1(y) + h_2(x, z)$.

Example 4.2 (Rotation alternatives). Suppose that $X^* \in \mathbb{R}^p$, $Y^* \in \mathbb{R}$, and $Z^* \in \mathbb{R}^q$ are centered and jointly normally distributed random variables such that Y^* is independent of (X^*, Z^*) . Then Assumption 4.1 holds for rotation alternatives given as

$$(X,Y,Z) = (X^*,Y^*,Z^* + \Delta(AX^* + BY^*)),$$

where $\mathbf{A} \in \mathbb{R}^{q \times p}$, $\mathbf{B} \in \mathbb{R}^{q \times 1}$ are deterministic matrices, and \mathbf{B} is nonzero.

Example 4.3 (Farlie alternatives). Suppose that $X^* \in \mathbb{R}^p$, $Y^* \in \mathbb{R}$, and $Z^* \in \mathbb{R}^q$ are absolutely continuous random variables such that Y^* is independent of (X^*, Z^*) . Then Assumption 4.1 holds for the (generalized) Farlie alternatives (see Kössler and Rödel (2007, Sec. 1.1.5) for the one-dimensional case) that are defined as

$$q_{\Delta}(\mathbf{x}, y, \mathbf{z}) := q_{\mathbf{Y}^*}(y) q_{(\mathbf{X}^*, \mathbf{Z}^*)}(\mathbf{x}, \mathbf{z}) \left[1 + \Delta \{1 - 2F_{\mathbf{Y}^*}(y)\} \{1 - 2F_{(\mathbf{X}^*, \mathbf{Z}^*)}(\mathbf{x}, \mathbf{z})\} \right].$$

For a local power analysis for an alternative set under the listed assumptions, we examine the asymptotic power along a respective sequence of alternatives obtained as

$$H_{1,n}(\Delta_0): \Delta = \Delta_n$$
, where $\Delta_n := n^{-1/2} \Delta_0$ (11)

with some constant $\Delta_0 \neq 0$. In this local model, testing the null hypothesis of independence reduces to testing

$$H_0: \Delta_0 = 0$$
 versus $H_1: \Delta_0 \neq 0$.

We obtain the following theorem on the local power of the discussed tests. The result demonstrates the trivial power claimed for ξ_n in the beginning of this section.

Theorem 4.4 (Power analysis for ξ_n). Suppose that the considered set of local alternatives in (10) satisfies Assumption 4.1 and constitutes a subset of \mathcal{P}_Q . Then for any sequence of alternatives given in (11), for any fixed constant $\Delta_0 > 0$,

(i) assuming the number of simulations B for the CRT tends to infinity as $n \to \infty$, it holds that

$$\lim_{n\to\infty} P_{H_{1,n}(\Delta_0)}(\mathsf{T}_{\alpha}^{\mathsf{Q},\xi_n}=1) \leq \alpha;$$

(ii) in contrast, there exists a test T_{α}^{opt} such that for any $\alpha, \beta \in (0,1)$, as long as Δ_0 is sufficiently large, it holds that

$$\lim_{n\to\infty} P_{H_0}(\mathsf{T}_{\alpha}^{\mathrm{opt}}=1) \leq \alpha \quad and \quad \lim_{n\to\infty} P_{H_{1,n}(\Delta_0)}(\mathsf{T}_{\alpha}^{\mathrm{opt}}=1) \geq 1-\beta,$$

while for small Δ_0 the total variation distance vanishes as

$$\lim_{\Delta_0 \to 0} \lim_{n \to \infty} \text{TV}(H_{1,n}(\Delta_0), H_0) = 0,$$

and hence

$$\lim_{\Delta_0 \to 0} \lim_{n \to \infty} \inf_{\overline{\mathsf{T}}_\alpha \in \mathcal{T}_\alpha} \mathsf{P}_{H_{1,n}(\Delta_0)}(\overline{\mathsf{T}}_\alpha = 0) \geq 1 - \alpha.$$

Here the infimum is taken over all size- α tests.

Remark 4.5. We give a rigorous proof of Theorem 4.4(i) in Section 7.1. The main idea is to first derive the joint limiting null distribution of $\sqrt{n}\xi_n$ and the log likelihood ratio between two hypotheses, and then to use Le Cam's third lemma. In addition to Theorem 3.1(i), combining results from Azadkia and Chatterjee (2021), we are able to prove joint asymptotic normality with deterministic variance of $\sqrt{n}\xi_n$ and the log likelihood ratio; in particular, zero asymptotic covariance between $\sqrt{n}\xi_n$ and the log likelihood ratio is the technical reason why the CRT-based Azadkia–Chatterjee-type test is inefficient in the quadratic mean differentiable class.

Remark 4.6. The phenomenon that a (1-NN) graph-based test has zero asymptotic efficiency has been encountered also in other situations. For example, the lack of power of the Wald–Wolfowitz runs test is a classic result in the literature (Hájek, Šidák and Sen, 1999, p. 102). A systematic analysis of this phenomenon in the two-sample test context was done recently in Bhattacharya (2019) and similar analyses for Chatterjee's 1-NN tests of unconditional independence were performed in Cao and Bickel (2020), Shi, Drton and Han (2022a), and Auddy, Deb and Nandy (2023).

5. Power analysis: Nonparametric case

In this section, we conduct local power analyses of the proposed tests within the Hölder smooth class inspired by the work of Neykov, Balakrishnan and Wasserman (2021). In this class, the conditional distribution of (Y, \mathbb{Z}) is allowed to change more dramatically (beyond the limit of QMD classes established in Section 4) as X changes. In the sequel, following the settings treated in Neykov, Balakrishnan and Wasserman (2021), we consider $X \in [0,1]^p$, $Y \in [0,1]$, and $Z \in [0,1]$ to be continuous random vector/variables.

5.1. Rate of convergence

Let $\mathcal{E}_{[0,1]^{p+2}}$ be the set of all absolutely continuous distributions $(X,Y,Z) \in [0,1]^{p+2}$ such that the randomness of the triplet can be understood as first sampling X from a density q_X with support $[0,1]^p$,

and then sampling Y and Z from a conditional distribution $q_{(Y,Z)|X}$ of support $[0,1] \times [0,1]$ for (almost) all X. Let $\mathcal{P}_0 \subseteq \mathcal{E}_{[0,1]^{p+2}}$ be the subset for which $Y \perp \!\!\! \perp Z \mid X$, and let $\mathcal{P}_1 = \mathcal{E}_{[0,1]^{p+2}} \backslash \mathcal{P}_0$.

Next we separately define the two Hölder classes of density functions, belonging to \mathcal{P}_0 (the null class) and \mathcal{P}_1 . Our main interest is on exponents s that are close to 0, representing those conditional distributions of (Y, Z) that change possibly very roughly with the values of X.

Definition 5.1 (Null Hölder class). Let $\mathcal{P}_0(L,s) \subseteq \mathcal{P}_0$ with L > 1 and $s \in (0,1]$ be the collection of joint distributions of (X,Y,Z) such that, for all $x,x' \in [0,1]^p$, $y,y',z,z' \in [0,1]$, we have

$$\left| q_{Y|X}(y|x) - q_{Y|X}(y|x') \right| \le L \|x - x'\|^{s}$$
and
$$\left| q_{Z|X}(z|x) - q_{Z|X}(z|x') \right| \le L \|x - x'\|^{s}.$$

Definition 5.2 (Alternative Hölder class). Let $\mathcal{P}_1(L,s) \subseteq \mathcal{P}_1$ with L > 1 and $s \in (0,1]$ be the collection of joint distributions of (X,Y,Z) such that, for all $x,x' \in [0,1]^p$, $y,y',z,z' \in [0,1]$, we have

$$\left| q_{(Y,Z)|X}(y,z|x) - q_{(Y,Z)|X}(y,z|x') \right| \le L \|x - x'\|^{s},$$

$$\left| q_{(Y,Z)|X}(y,z|x) - q_{(Y,Z)|X}(y',z'|x) \right| \le L \left(|y - y'|^{s} + |z - z'|^{s} \right),$$
and $L^{-1} \le q_{Y,Z|X}(y,z|x) \le L.$

To obtain the rate of convergence for ξ_n under $\mathcal{P}_0(L,s)$ as well as $\mathcal{P}_1(L,s)$, we establish the following two results. The first is a proposition that extends Theorem 4.1 in Azadkia and Chatterjee (2021), which focused on the Lipschitz class with s = 1. The second result is a lemma that shows that the distributions in $\mathcal{P}_0(L,s)$ and $\mathcal{P}_1(L,s)$ satisfy the conditions in the proposition.

Proposition 5.3. Restricted to this proposition, $Z \in \mathbb{R}^q$ is allowed to be multidimensional. Suppose then that Y is not a.s. equal to a measurable function of X and that

(i) there are universal constants $C_1 > 0$ and $s \in (0,1]$ such that for any $t \in \mathbb{R}$, $x, x' \in \mathbb{R}^p$, and $z, z' \in \mathbb{R}^q$,

$$\left| P(Y \ge t \mid X = x, Z = z) - P(Y \ge t \mid X = x', Z = z') \right| \le C_1 \left(\|x - x'\|^s + \|z - z'\|^s \right),$$
and
$$\left| P(Y \ge t \mid X = x) - P(Y \ge t \mid X = x') \right| \le C_1 \left(\|x - x'\|^s \right);$$

(ii) there exists a universal constant $C_2 > 0$ such that $P(||X|| \ge C_2) = 0$ and $P(||Z|| \ge C_2) = 0$.

Then, as $n \to \infty$,

$$\xi_n - \xi = O_{\mathbf{P}} \left(\frac{(\log n)^{p+q+1}}{n^{s/(p+q)}} \right).$$

Lemma 5.4.

(i) If $P_{(X,Y,Z)} \in \mathcal{P}_0(L,s)$ for a fixed L > 1 and $s \in (0,1]$, then for all $x, x' \in [0,1]^p$, $y, y', z, z' \in [0,1]$, we have

$$\left| q_{Y|(X,Z)}(y|x,z) - q_{Y|(X,Z)}(y|x',z') \right| \le L \|x - x'\|^{s}.$$

(ii) If $P_{(X,Y,Z)} \in \mathcal{P}_1(L,s)$ for a fixed L > 1 and $s \in (0,1]$, then for all $x, x' \in [0,1]^p$, $y, y', z, z' \in [0,1]$, we have

$$\left| q_{Y|(X,Z)}(y \mid x, z) - q_{Y|(X,Z)}(y \mid x', z') \right| \le L' \left(\|x - x'\|^s + |z - z'|^s \right)$$

for some $L' \leq 2L^4$.

Combining Lemma 5.4 with Proposition 5.3 gives the following corollary.

Corollary 5.5. Suppose $P_{(X,Y,Z)} \in \mathcal{P}_0(L,s)$, or $P_{(X,Y,Z)} \in \mathcal{P}_1(L,s)$ with Y not a.s. equal to a measurable function of X. Then as $n \to \infty$,

$$\xi_n - \xi = O_{\mathbf{P}} \left(\frac{(\log n)^{p+q+1}}{n^{s/(p+q)}} \right).$$

Remark 5.6. Huang, Deb and Sen (2022) proposed a measure of conditional dependence and a coefficient estimating the measure in general spaces by generalizing Azadkia and Chatterjee (2021)'s idea. In particular, they also explored the rate of convergence of such a coefficient in their Theorem 3.3, and mentioned that the rate of convergence may be arbitrarily slow without a smoothness assumption on the conditional distribution (Huang, Deb and Sen, 2022, Remark 8). While their Assumptions 4–8 are made for general spaces and the analysis techniques are not substantially different, ours are specifically designed to facilitate the local power analysis to be presented in the next section. We thus decide to still document these results for easy reference.

5.2. Power analysis

Fix L > 1 and $s \in (0,1]$. We consider now the problem of testing

$$H_0: P_{(X|Y|Z)} = P_0 \in \mathcal{P}_0(L,s)$$

against a sequence of local alternatives,

$$H_{1,n}: P_{(X,Y,Z)} = P_{1,n} \in \mathcal{P}_1(L,s).$$

Corollary 5.7. Assume both P_0 and $\{P_{1,n}, n = 1, 2, ...\}$ belong to \mathcal{P}_Q , and $\xi(P_{1,n})$, the conditional dependence measure ξ under the local alternative $P_{1,n}$, satisfies that

$$\xi(P_{1,n}) \gtrsim n^{-s/(p+1)+\delta}$$

for some (arbitrarily small) constant $\delta > 0$. Further assume that the number of simulations B tends to infinity as $n \to \infty$. Then

$$\lim_{n\to\infty} P_{H_{1,n}}(\mathsf{T}_{\alpha}^{\mathbb{Q},\xi_n}=1)=1.$$

We observe that unfortunately, even as the Hölder exponent s is small, the threshold $n^{-s/(p+1)}$ is (from a worst case perspective) not the critical boundary in the studied nonparametric class. The following theorem shall confirm it rigorously. To this end, we consider a simplified setting when p=1, so $X,Y,Z\in\mathbb{R}$. Define the class

$$\mathcal{P}_1(\epsilon; L, s) := \left\{ q \in \mathcal{P}_1(L, s) : \inf_{q^0 \in \mathcal{P}_0} \| q - q^0 \|_1 \ge \epsilon \right\},\,$$

where $||q - q^0||_1 := \int |q(x, y, z) - q^0(x, y, z)| d(x, y, z)$. Consider testing

$$H_0: P_{(X,Y,Z)} = P_0 \in \mathcal{P}_0(L,s)$$

against the following particular sequence of local alternatives:

$$H_{1,n}(\Delta_0): P_{(X,Y,Z)} = P_{1,n}(\Delta_0) \in \mathcal{P}_1(\Delta_0 n^{-2s/(4s+3)}; L, s)$$
.

Theorem 5.8. For any $s \in (0,1]$, there exist

$$P_0 \in \mathcal{P}_0(L, s)$$
 and $P_{1,n}(\Delta_0) \in \mathcal{P}_1(\Delta_0 n^{-2s/(4s+3)}; L, s)$

such that $P_{(X,Y)} \in \mathcal{P}_Q$ does not vary under both the null and local alternatives, and

(i) assuming the number of simulations B tends to infinity as $n \to \infty$, for any $\Delta_0 > 0$ and $\alpha < 0.1$, it holds that

$$\limsup_{n\to\infty} \mathrm{P}_{H_{1,n}(\Delta_0)}(\mathsf{T}_\alpha^{\mathrm{Q},\xi_n}=1) \leq \beta_\alpha,$$

where β_{α} < 1 is a constant only depending on α ;

(ii) if further $s \in [1/4, 1]$, then there exists a test T_{α}^{bin} such that, for any $\alpha, \beta \in (0, 1)$, as long as Δ_0 is sufficiently large,

$$P_{H_0}(\mathsf{T}^{\mathsf{bin}}_{\alpha} = 1) \leq \alpha \quad and \quad \lim_{n \to \infty} P_{H_{1,n}(\Delta_0)}(\mathsf{T}^{\mathsf{bin}}_{\alpha} = 1) \geq 1 - \beta;$$

in contrast, as Δ_0 becomes small,

$$\lim_{\Delta_0 \to 0} \lim_{n \to \infty} TV(H_{1,n}(\Delta_0), H_0) = 0.$$

Remark 5.9. Our proof of Theorem 5.8(i) is different from the approach we used to prove Theorem 4.4(i). It depends on the fact that $\sqrt{n}\xi_n$ has the same asymptotic mean and variance under a null hypothesis and a special non-standard local alternative sequence constructed in Neykov, Balakrishnan and Wasserman (2021). We show this in a direct calculation.

6. Conclusion

In this manuscript, we explore the use of Azadkia–Chatterjee's conditional dependence coefficient in inferential tasks. Specifically, we adopt the framework of conditional randomization tests in order to study the power of Azadkia–Chatterjee-type tests of conditional independence. Our analyses take up two types of local alternatives: First, a rather general quadratic mean differentiable class and second, a rougher Hölder class. In these settings, we prove that the CRT-based Azadkia–Chatterjee test is unfortunately statistically inefficient.

The current analyses are focused on the situation when X and Y are independent, which makes the required analysis of permutation statistics mathematically tractable. Indeed, while it would be natural and interesting to also study cases where X and Y are dependent, entirely new technical tools would need to be developed to attack this problem. This said, we conjecture that the inefficiency of Azadkia–Chatterjee-type test persists for more general local alternatives, with X and Y are dependent.

Finally, the inefficiency we demonstrate motivates further efforts to develop variants of the considered approach. One possible avenue would be to develop tests that use modified versions of Azadkia–Chatterjee's conditional dependence coefficient, in which one uses k-nearest neighbor graphs with k

allowed to tend to infinity as the sample size n increases; in the unconditional setting recent progress in this direction was made by Lin and Han (2023). Another interesting topic for future research would be a generalization of the coefficient to the setting where all of X, Y, Z are multivariate.

7. Proof of Theorem 4.4

7.1. Proof of Theorem 4.4(i)

Proof of Theorem 4.4(i). The proof is divided into three steps. The first step reviews Le Cam's third lemma and introduces graph theoretic notions. The second step derives the distribution of ξ_n under the local alternative. The third step computes the local power.

Step I-1. To derive the local alternative distribution of ξ_n , we will use Le Cam's third lemma (van der Vaart, 1998, Theorem 7.2 and Example 6.7). The lemma states that if under the null hypothesis,

$$\left(\sqrt{n}\xi_{n}, \frac{1}{\sqrt{n}}\sum_{i=1}^{n}\dot{\ell}_{0}(\boldsymbol{X}_{i}, Y_{i}, \boldsymbol{Z}_{i})\right) \stackrel{\mathsf{d}}{\longrightarrow} N\left(\begin{pmatrix} 0\\0 \end{pmatrix}, \begin{pmatrix} \sigma^{2} & \tau\\ \tau & I_{0} \end{pmatrix}\right) \tag{12}$$

where σ^2 , τ are fixed constants and $I_0 := \mathbb{E}\{\dot{\ell}_0(X,Y,Z)^2\}$ equals the Fisher information for Δ at 0, then under the local alternative hypothesis, we have

$$\sqrt{n}\xi_n \stackrel{\mathsf{d}}{\longrightarrow} N(\Delta_0 \tau, \sigma^2).$$

In order to employ the Cramér–Wold device to prove (12) for some σ^2 and τ , we need to show that under the null, for any real numbers a and b,

$$a\sqrt{n}\xi_n + bn^{-1/2} \sum_{i=1}^n \dot{\ell}_0(X_i, Y_i, \mathbf{Z}_i) \xrightarrow{d} N(0, a^2\sigma^2 + 2ab\tau + b^2I_0).$$
 (13)

To this end, first notice that Azadkia and Chatterjee (2021, Theorem 9.1) show

$$\frac{1}{n^2} \sum_{i=1}^n \{ R_i - \min(R_i, R_{N(i)}) \} \xrightarrow{\text{a.s.}} \int \mathbb{E}[\operatorname{Var}\{\mathbb{1}(Y \ge t) \mid X\}] dP_Y(t).$$

Therefore, by Slutsky's theorem, it suffices to establish (12) for $\sqrt{n}\hat{\xi}_n$ instead of $\sqrt{n}\xi_n$, where

$$\widehat{\xi}_n := \frac{n^{-2} \sum_{i=1}^n \{ \min(R_i, R_{M(i)}) - \min(R_i, R_{N(i)}) \}}{\int \mathbb{E}[\text{Var}\{\mathbb{1}(Y \ge t) \mid X\}] dP_Y(t)}.$$
(14)

Moreover, consider the "oracle" version of $\widehat{\xi}_n$ defined as

$$\widetilde{\xi}_n := \frac{n^{-1} \sum_{i=1}^n [\min\{F_Y(Y_i), F_Y(Y_{M(i)})\} - \min\{F_Y(Y_i), F_Y(Y_{N(i)})\}]}{\int \mathbb{E}[\operatorname{Var}\{\mathbb{1}(Y \ge t) \mid X\}] dP_Y(t)}.$$
(15)

We have the following lemma for $\hat{\xi}_n$ and $\check{\xi}_n$. This result and lemmas given later in this section are derived in the supplement.

Lemma 7.1. Under the null hypothesis, $\sqrt{n}\widehat{\xi}_n - \sqrt{n}\widecheck{\xi}_n = o_P(1)$.

Thus we only need to show

$$a\sqrt{n}\widetilde{\xi}_n + bn^{-1/2} \sum_{i=1}^n \dot{\ell}_0(\boldsymbol{X}_i, Y_i, \boldsymbol{Z}_i) \xrightarrow{\mathsf{d}} N\left(0, a^2\sigma^2 + 2ab\tau + b^2I_0\right). \tag{16}$$

The idea of proving (16) is to first show a conditional central limit result,

$$a\sqrt{n}\tilde{\xi}_n + bn^{-1/2} \sum_{i=1}^n \dot{\ell}_0(X_i, Y_i, \mathbf{Z}_i) \Big| \mathcal{F}_n \xrightarrow{\mathsf{d}} N\Big(0, a^2\sigma^2 + 2ab\tau + b^2I_0\Big)$$
for almost every sequence $[(X_n, \mathbf{Z}_n)]_{n \ge 1}$, (17)

where \mathcal{F}_n denotes the σ -field generated by $(X_1, Z_1), \dots, (X_n, Z_n)$, i.e., for almost every ω of the probability space supporting the (X_i, Z_i) 's,

$$a\sqrt{n}\widetilde{\xi}_n\Big(\big[\big(X_i(\omega),Y_i,\boldsymbol{Z}_i(\omega)\big)\big]_{i=1}^n\Big) + bn^{-1/2}\sum_{i=1}^n \dot{\ell}_0\big(X_i(\omega),Y_i,\boldsymbol{Z}_i(\omega)\big) \stackrel{\mathsf{d}}{\longrightarrow} N(0,a^2\sigma^2 + 2ab\tau + b^2I_0)$$

(Ledoux and Talagrand, 1991, Theorem 10.14), and then deduce the desired unconditional central limit result (16), and thus (13).

Step I-2. To show (17), we introduce the language of graph theory. We write

$$\begin{split} S_{n} &= a\sqrt{n} \xi_{n} + bn^{-1/2} \sum_{i=1}^{n} \dot{\ell}_{0}(\boldsymbol{X}_{i}, Y_{i}, \boldsymbol{Z}_{i}) \\ &= a\gamma^{-1} n^{-1/2} \sum_{i=1}^{n} \min\{F_{Y}(Y_{i}), F_{Y}(Y_{M(i)})\} - a\gamma^{-1} n^{-1/2} \sum_{i=1}^{n} \min\{F_{Y}(Y_{i}), F_{Y}(Y_{N(i)})\} \\ &+ bn^{-1/2} \sum_{i=1}^{n} \dot{\ell}_{0}(\boldsymbol{X}_{i}, Y_{i}, \boldsymbol{Z}_{i}) \\ &= a\gamma^{-1} n^{-1/2} \sum_{i=1}^{n} \sum_{j: i \to j \in \mathcal{E}(\mathcal{G}_{n})} K_{\wedge}(Y_{i}, Y_{j}) - a\gamma^{-1} n^{-1/2} \sum_{i=1}^{n} \sum_{k: i \to k \in \mathcal{E}(\mathcal{G}_{n}^{X})} K_{\wedge}(Y_{i}, Y_{k}) \\ &+ bn^{-1/2} \sum_{i=1}^{n} \dot{\ell}_{0}(\boldsymbol{X}_{i}, Y_{i}, \boldsymbol{Z}_{i}), \end{split}$$

where for all Y independent of X,

$$\gamma := \int \mathrm{E}[\mathrm{Var}\{\mathbb{1}(Y \geq t) \mid X\}] \mathrm{dP}_Y(t) = \int \mathrm{E}[\mathrm{Var}\{\mathbb{1}(Y \geq t)\}] \mathrm{dP}_Y(t) = \frac{1}{6},$$

 \mathcal{G}_n is the directed nearest neighbor graph (NNG) of the vertices $[(X_i, \mathbf{Z}_i)]_{i=1}^n$, \mathcal{G}_n^X is the directed nearest neighbor graph (NNG) of the vertices $[X_i]_{i=1}^n$, and $K_{\wedge}(y_1, y_2) := \min\{F_Y(y_1), F_Y(y_2)\}$. Next we define

$$V_{i;1} := n^{-1/2} \left\{ 6a \sum_{j: i \to j \in \mathcal{E}(\mathcal{G}_n)} K_{\wedge}(Y_i, Y_j) - 6a \sum_{k: i \to k \in \mathcal{E}(\mathcal{G}_n^X)} K_{\wedge}(Y_i, Y_k) \right\},$$

$$V_{i:2} := n^{-1/2} b \dot{\ell}_0(X_i, Y_i, \mathbf{Z}_i), \quad \text{and} \quad V_i := V_{i:1} + V_{i:2},$$
 (18)

such that S_n can be written as $\sum_{i=1}^n V_i$. Observe that, since $[Y_i]_{i=1}^n$ is independent of $[(X_i, Z_i)]_{i=1}^n$ under the null,

$$E(V_{i;1} \mid \mathcal{F}_n) = n^{-1/2} \left[6a \operatorname{E} \left\{ K_{\wedge}(Y_i, Y_{M(i)}) \mid \mathcal{F}_n \right\} - 6a \operatorname{E} \left\{ K_{\wedge}(Y_i, Y_{N(i)}) \mid \mathcal{F}_n \right\} \right]$$

$$= n^{-1/2} \left\{ 6a(1/3) - 6a(1/3) \right\} = 0,$$

$$E(V_{i;2} \mid \mathcal{F}_n) = \operatorname{E} \left\{ \dot{\ell}_0(X_i, Y_i, \mathbf{Z}_i) \mid \mathcal{F}_n \right\} = 0, \quad \text{by Assumption 4.1(v)},$$
and
$$E(V_i \mid \mathcal{F}_n) = a \operatorname{E}(V_{i;1} \mid \mathcal{F}_n) + b \operatorname{E}(V_{i;2} \mid \mathcal{F}_n) = 0.$$

To establish a conditional central limit theorem for S_n , we make use of the following lemma.

Lemma 7.2. It holds that

$$\sup_{z \in \mathbb{R}} \left| \Pr\left(\frac{S_n}{\sqrt{\operatorname{Var}(S_n \mid \mathcal{F}_n)}} \le z \mid \mathcal{F}_n \right) - \Phi(z) \right| \le 75 C_{p+q}^{5(1+\epsilon)} \frac{\operatorname{E}(\sum_{i=1}^n |V_i|^{2+\epsilon} \mid \mathcal{F}_n)}{\{\operatorname{Var}(S_n \mid \mathcal{F}_n)\}^{(2+\epsilon)/2}} \quad a.s., \tag{19}$$

where C_{p+q} is a constant depending only on p+q.

To control the right-hand side of (19), we get by the " c_r -inequality" that

$$\mathbb{E}\left(\sum_{i=1}^{n}|V_{i}|^{2+\epsilon}\left|\mathcal{F}_{n}\right.\right)\leq2^{1+\epsilon}\left\{\mathbb{E}\left(\sum_{i=1}^{n}|V_{i;1}|^{2+\epsilon}\left|\mathcal{F}_{n}\right.\right)+\mathbb{E}\left(\sum_{i=1}^{n}|V_{i;2}|^{2+\epsilon}\left|\mathcal{F}_{n}\right.\right)\right\}.$$

Here

$$n^{\epsilon/2} \mathrm{E}\Big(\sum_{i=1}^{n} |V_{i;1}|^{2+\epsilon} \, \Big| \, \mathcal{F}_n\Big) \leq |6a|^{2+\epsilon} \quad \text{and} \quad n^{\epsilon/2} \mathrm{E}\Big(\sum_{i=1}^{n} |V_{i;2}|^{2+\epsilon} \, \Big| \, \mathcal{F}_n\Big) \xrightarrow{\text{a.s.}} \mathrm{E}\Big\{ |b\dot{\ell}_0(X,Y,\mathbf{Z})|^{2+\epsilon} \Big\},$$

where the former follows from $|V_{i;1}| \le |6a|n^{-1/2}$ and the latter from the strong law of large numbers and Assumption 4.1(vi).

Step II. In order to show (17), in view of (19), it suffices to show

$$Var(S_n \mid \mathcal{F}_n) \xrightarrow{\text{a.s.}} a^2 \sigma^2 + 2ab\tau + b^2 I_0.$$
 (20)

for some fixed $\sigma^2 > 0$ and τ , and recall $I_0 := \mathbb{E}\{\dot{\ell}_0(X,Y,\mathbf{Z})^2\}$. We proceed in two sub-steps. We will first compute $\operatorname{Var}(S_n \mid \mathcal{F}_n)$, then claim $\operatorname{Var}(S_n \mid \mathcal{F}_n) - \operatorname{Var}(S_n) \xrightarrow{\text{a.s.}} 0$ and determine the limit value of $\operatorname{Var}(S_n)$ accordingly.

Step II-1. Set

$$\begin{split} \gamma_{1;a} &:= \mathbb{E}\Big[\Big\{6aK_{\wedge}(Y,Y') - 2a\Big\}^2\Big], \qquad \gamma_{2;a} := \mathbb{E}\Big[\Big\{6aK_{\wedge}(Y,Y') - 2a\Big\}\Big\{6aK_{\wedge}(Y,Y'') - 2a\Big\}\Big], \\ \gamma_{4;a,b}^*(\mathbf{x},\mathbf{z}) &:= \mathbb{E}\Big[\Big\{6aK_{\wedge}(Y,Y') - 2a\Big\}\Big\{b\dot{\ell}_0(\mathbf{x},Y,\mathbf{z})\Big\}\Big], \qquad \gamma_{4;a,b} := \mathbb{E}\Big\{\gamma_{4;a,b}^*(\mathbf{X},\mathbf{Z})\Big\}, \\ \gamma_{5;b}^*(\mathbf{x},\mathbf{z}) &:= \mathbb{E}\Big[\Big\{b\dot{\ell}_0(\mathbf{x},Y,\mathbf{z})\Big\}^2\Big], \qquad \gamma_{5;b} := \mathbb{E}\Big\{\gamma_{5;b}^*(\mathbf{X},\mathbf{Z})\Big\}, \end{aligned}$$

where Y' and Y'' are independent copies of Y. We obtain

$$\operatorname{Var}(S_n \mid \mathcal{F}_n) = \operatorname{E}(S_n^2 \mid \mathcal{F}_n) = \sum_{i=1}^n \operatorname{E}(V_i^2 \mid \mathcal{F}_n) + \sum_{i \neq j} \operatorname{E}(V_i V_j \mid \mathcal{F}_n),$$

where

$$\sum_{i=1}^{n} \mathbb{E}(V_{i}^{2} \mid \mathcal{F}_{n}) = n^{-1} \sum_{i=1}^{n} \left\{ 2\gamma_{1;a} - 2 \sum_{j:i \to j \in \mathcal{E}(\mathcal{G}_{n}) \cap \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{1;a} - 2 \sum_{(j,k):i \to j \in \mathcal{E}(\mathcal{G}_{n}), i \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}), j \neq k} \gamma_{2;a} + \gamma_{5;a,b}^{*}(X_{i}, Z_{i}) \right\},$$

$$(22)$$

and

$$\sum_{i \neq j} E(V_{i}V_{j} | \mathcal{F}_{n})$$

$$= n^{-1} \left\{ \sum_{\substack{(i,j) \text{ distinct} \\ i \to j, j \to i \in \mathcal{E}(\mathcal{G}_{n}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}) \\ \text{ or } i \to k, j \to$$

Step II-2. We employ the following result.

Lemma 7.3.

$$\operatorname{Var}(S_n \mid \mathcal{F}_n) - \operatorname{Var}(S_n) \xrightarrow{\mathsf{a.s.}} 0.$$
 (24)

Then it remains to prove

$$Var(S_n) \to a^2 \sigma^2 + 2ab\tau + b^2 I_0 \tag{25}$$

for some fixed $\sigma^2 > 0$ and τ ; notice (24) and (25) will imply (20). To this end, in addition to Lemmas 3.6 and 3.8, we also need the following lemma, which is a "covariance" version of Lemmas 3.6 and 3.8.

Lemma 7.4. Let $[W_i]_{i=1}^n = [(X_i, Z_i)]_{i=1}^n$ be a sample comprised of n independent copies of W = (X, Z), with $X \in \mathbb{R}^p$ and $Z \in \mathbb{R}^q$. Let \mathcal{G}_n be the directed nearest neighbor graph (NNG) of the vertices $[W_i]_{i=1}^n$, and let \mathcal{G}_n^X be the directed nearest neighbor graph (NNG) of the vertices $[X_i]_{i=1}^n$. If random vector W

is absolutely continuous with a Lebesgue density f that is continuous, then

$$E\left(n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n) \cap \mathcal{E}(\mathcal{G}_n^X)}} 1\right) \to 0,$$
(26)

$$E\left(n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), j \to i \in \mathcal{E}(\mathcal{G}_n^X)}} 1\right) \to 0,$$
(27)

and
$$E\left(n^{-1}\sum_{\substack{(i,j,k) \text{ distinct} \\ i\to k\in\mathcal{E}(\mathcal{G}_n), j\to k\in\mathcal{E}(\mathcal{G}_n^X)}} 1\right)\to 1.$$
 (28)

Adding (22) and (23) together, we obtain

$$\operatorname{Var}(S_{n}) = \operatorname{E}\left(2n^{-1}\sum_{i=1}^{n}\gamma_{1;a}\right) - \operatorname{E}\left(2\sum_{(i,j) \text{ distinct} \atop i \to j \in \mathcal{E}(\mathcal{G}_{n}) \cap \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{1;a}\right)$$

$$- \operatorname{E}\left(2n^{-1}\sum_{(i,j) \text{ distinct} \atop i \to j \in \mathcal{E}(\mathcal{G}_{n}), i \to k \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{2;a}\right) + \operatorname{E}\left\{n^{-1}\sum_{i=1}^{n}\gamma_{5;a,b}^{*}(X_{i}, Z_{i})\right\}$$

$$+ \operatorname{E}\left(n^{-1}\sum_{(i,j) \text{ distinct} \atop i \to j, j \to i \in \mathcal{E}(\mathcal{G}_{n})} \gamma_{1;a}\right) + \operatorname{E}\left(n^{-1}\sum_{(i,j,k) \text{ distinct} \atop i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n})} \gamma_{2;a}\right)$$

$$+ \operatorname{E}\left(n^{-1}\sum_{(i,j) \text{ distinct} \atop i \to j, j \to i \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{1;a}\right) + \operatorname{E}\left(n^{-1}\sum_{(i,j,k) \text{ distinct} \atop i \to k, j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{2;a}\right)$$

$$- \operatorname{E}\left(2n^{-1}\sum_{(i,j) \text{ distinct} \atop i \to j \in \mathcal{E}(\mathcal{G}_{n}^{X}), j \to i \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{1;a}\right) - \operatorname{E}\left(2n^{-1}\sum_{(i,j,k) \text{ distinct} \atop i \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}), j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{2;a}\right)$$

$$+ \operatorname{E}\left\{2n^{-1}\sum_{(i,j) \text{ distinct} \atop i \to i \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{4;a,b}(X_{i}, Z_{i})\right\} - \operatorname{E}\left\{2n^{-1}\sum_{(i,j) \text{ distinct} \atop i \to k \in \mathcal{E}(\mathcal{G}_{n}^{X}), j \to k \in \mathcal{E}(\mathcal{G}_{n}^{X})} \gamma_{4;a,b}(X_{i}, Z_{i})\right\}. \tag{29}$$

The first term is $2\gamma_{1;a}$. The second term tends to 0 by Equation (26) in Lemma 7.4. For the third term, we have

$$\begin{split} \mathbf{E}\Big(2n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), i \to k \in \mathcal{E}(\mathcal{G}_n^X)}} \gamma_{2;a}\Big) &= 2\gamma_{2;a} \mathbf{E}\Big(n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), i \to j \notin \mathcal{E}(\mathcal{G}_n^X)}} 1\Big) \end{split}$$

$$= 2\gamma_{2;a} \mathbb{E}\left(1 - n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), i \to j \in \mathcal{E}(\mathcal{G}_n^X)}} 1\right) \to 2\gamma_{2;a},$$

where the last step is by Equation (26). The fourth term is $\gamma_{5;a}$. The fifth term tends to $\gamma_{1;a}\mathfrak{q}_{p+q}$ by Lemma 3.6. The sixth term can be rewritten as

$$\begin{split} &\gamma_{2;a} \mathbf{E} \Big(n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to k,j \to k \in \mathcal{E}(\mathcal{G}_n)}} 1 + n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to j,j \to k \in \mathcal{E}(\mathcal{G}_n)}} 1 + n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to k,j \to i \in \mathcal{E}(\mathcal{G}_n)}} 1 \Big) \\ &= \gamma_{2;a} \mathbf{E} \Big(n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to k,j \to k \in \mathcal{E}(\mathcal{G}_n)}} 1 + n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n),j \to i \notin \mathcal{E}(\mathcal{G}_n)}} 1 + n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n),j \to i \notin \mathcal{E}(\mathcal{G}_n)}} 1 \Big) \\ &= \gamma_{2;a} \mathbf{E} \Big\{ n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to k,j \to k \in \mathcal{E}(\mathcal{G}_n)}} 1 + \Big(1 - n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j,j \to i \in \mathcal{E}(\mathcal{G}_n)}} 1 \Big) + \Big(1 - n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j,j \to i \in \mathcal{E}(\mathcal{G}_n)}} 1 \Big) \Big\} \\ &\to \gamma_{2;a} \Big(\mathfrak{o}_{p+q} + 2 - 2\mathfrak{o}_{p+q} \Big), \end{split}$$

where the last step is by Lemmas 3.7 and 3.6. Similarly, the seventh and eighth terms tend to $\gamma_{1;a}q_p$ and $\gamma_{2;a}(\mathfrak{o}_p+2-2\mathfrak{q}_p)$, respectively. The ninth term tends to 0 by Equation (27) in Lemma 7.4. The tenth term is equal to

$$\begin{aligned} & 2\gamma_{2;a} \mathbf{E} \Big(n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to k \in \mathcal{E}(\mathcal{G}_n), j \to k \in \mathcal{E}(\mathcal{G}_n^X)}} 1 + n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), j \to k \in \mathcal{E}(\mathcal{G}_n^X)}} 1 + n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to k \in \mathcal{E}(\mathcal{G}_n), j \to i \in \mathcal{E}(\mathcal{G}_n^X)}} 1 \\ & = 2\gamma_{2;a} \mathbf{E} \Big(n^{-1} \sum_{\substack{(i,j,k) \text{ distinct} \\ i \to k \in \mathcal{E}(\mathcal{G}_n), j \to k \in \mathcal{E}(\mathcal{G}_n^X)}} 1 + n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), j \to i \in \mathcal{E}(\mathcal{G}_n^X)}} 1 + n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), j \to k \in \mathcal{E}(\mathcal{G}_n^X)}} 1 \Big) \\ & = 2\gamma_{2;a} \mathbf{E} \Big\{ n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to k \in \mathcal{E}(\mathcal{G}_n), j \to k \in \mathcal{E}(\mathcal{G}_n^X)}} 1 \\ & + \Big(1 - n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), j \to i \in \mathcal{E}(\mathcal{G}_n^X)}} 1 \Big) + \Big(1 - n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ i \to j \in \mathcal{E}(\mathcal{G}_n), j \to i \in \mathcal{E}(\mathcal{G}_n^X)}} 1 \Big) \Big\} \\ & \to 2\gamma_{2;a} \Big\{ 1 + (1 - 0) + (1 - 0) \Big\} = 6\gamma_{2;a}, \end{aligned}$$

where the second last step is by Lemma 7.4. For the last two terms in Equation (29), we obtain

$$\begin{split} \mathbf{E} \Big\{ n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ j \to i \in \mathcal{E}(\mathcal{G}_n)}} \gamma_{4;a,b}^*(X_i, \mathbf{Z}_i) \Big\} &= \mathbf{E} \Big\{ n^{-1} \sum_{i=1}^n \gamma_{4;a,b}^*(X_{M(i)}, \mathbf{Z}_{M(i)}) \Big\} \\ &= \mathbf{E} \Big\{ \gamma_{4;a,b}^*(X_{M(1)}, \mathbf{Z}_{M(1)}) \Big\} &= \mathbf{E} \Big[\mathbf{E} \Big\{ \gamma_{4;a,b}^*(X_{M(1)}, \mathbf{Z}_{M(1)}) \, \Big| \, M(1) \Big\} \, \Big] &= \gamma_{4;a,b}, \end{split}$$

and similarly

$$\mathbb{E}\left\{n^{-1} \sum_{\substack{(i,j) \text{ distinct} \\ j \to i \in \mathcal{E}(\mathcal{G}_n^X)}} \gamma_{4;a,b}^*(\boldsymbol{X}_i, \boldsymbol{Z}_i)\right\} = \gamma_{4;a,b}.$$

Thus the last two terms are canceled out. Plugging all terms back into (29) yields

$$\operatorname{Var}(S_n) \to \gamma_{1;a} \left\{ 2 + \left(\mathfrak{q}_{p+q} + \mathfrak{q}_p \right) \right\} + \gamma_{2;a} \left\{ -4 - 2\left(\mathfrak{q}_{p+q} + \mathfrak{q}_p \right) + \left(\mathfrak{o}_{p+q} + \mathfrak{o}_p \right) \right\} + \gamma_{5;b}.$$

In addition,

$$\gamma_{1;a} = 2a^2$$
, $\gamma_{2;a} = 4a^2/5$, $\gamma_{5;b} = b^2 I_0$.

Therefore,

$$\operatorname{Var}(S_n) \to a^2 \left\{ \frac{4}{5} + \frac{2}{5} \left(\mathfrak{q}_{p+q} + \mathfrak{q}_p \right) + \frac{4}{5} \left(\mathfrak{o}_{p+q} + \mathfrak{o}_p \right) \right\} + b^2 I_0.$$

This completes the proof of (17) and thus (13) and (12) with

$$\sigma^2 := \frac{4}{5} + \frac{2}{5} \left(\mathfrak{q}_{p+q} + \mathfrak{q}_p \right) + \frac{4}{5} \left(\mathfrak{o}_{p+q} + \mathfrak{o}_p \right) \quad \text{and} \quad \tau := 0.$$

Finally, by Le Cam's third lemma, under $\{P_{n,\Delta_n}\}_{n\geq 1}$,

$$\sqrt{n}\xi_n\Big(\big[(\boldsymbol{X}_i,Y_i,\boldsymbol{Z}_i)\big]_{i=1}^n\Big) \stackrel{\mathsf{d}}{\longrightarrow} N(0,\sigma^2).$$

Moreover, we also have

$$\sqrt{n}\xi_n\Big(\big[(\boldsymbol{X}_i,Y_i^{(b)},\boldsymbol{Z}_i)\big]_{i=1}^n\Big) \stackrel{\mathsf{d}}{\longrightarrow} N(0,\sigma^2).$$

Step III. Since B tends to infinity as $n \to \infty$, without loss of generality, we assume $B > \alpha^{-1} - 1$. With the shorthand notation

$$\xi_n^{(b)} \equiv \xi_n \Big(\big[(\boldsymbol{X}_i, Y_i^{(b)}, \boldsymbol{Z}_i) \big]_{i=1}^n \Big) \quad \text{and} \quad \xi_n^{\circ} \equiv \xi_n \Big(\big[(\boldsymbol{X}_i, Y_i, \boldsymbol{Z}_i) \big]_{i=1}^n \Big),$$

the test

$$\mathsf{T}_{\alpha}^{Q,\xi_{n}} := \mathbb{1}\Big(\frac{1 + \sum_{b=1}^{B} \mathbb{1}(\xi_{n}^{(b)} \ge \xi_{n}^{\circ})}{1 + B} \le \alpha\Big)$$

can be restated as

$$\mathsf{T}_{\alpha}^{\mathrm{Q},\xi_n} = \mathbb{1}\Big(\sqrt{n}\xi_n^{\circ} > \sqrt{n}\xi_n^{[1+B-\lfloor\alpha(1+B)\rfloor]}\Big),\tag{30}$$

where $\xi_n^{[1]}, \xi_n^{[2]}, \dots, \xi_n^{[B]}$ is a rearrangement of $\xi_n^{(1)}, \xi_n^{(2)}, \dots, \xi_n^{(B)}$ such that

$$\xi_n^{[1]} \le \xi_n^{[2]} \le \dots \le \xi_n^{[B]}$$
.

Write $\Phi_{\sigma}(\cdot)$ and $\Phi_{\sigma}^{-1}(\cdot)$ for the cumulative distribution function and quantile function of the normal distribution with mean zero and variance σ^2 . We wish to prove

$$\sqrt{n}\xi_n^{[1+B-\lfloor\alpha(1+B)\rfloor]} \xrightarrow{p} \Phi_{\sigma}^{-1}(1-\alpha). \tag{31}$$

Using Theorem 3.1 in Hoeffding (1952), it suffices to prove

$$B^{-1} \sum_{b=1}^{B} \mathbb{1}(\sqrt{n}\xi_n^{(b)} \le y) \xrightarrow{p} \Phi_{\sigma}(y),$$

which is immediate from

$$B^{-1} \sum_{b=1}^{B} \mathbb{1}(\sqrt{n}\xi_n^{(b)} \le y) \left| \mathcal{F}_n \xrightarrow{p} \Phi_{\sigma}(y) \right| \text{ for almost every sequence } [(X_n, Z_n)]_{n \ge 1}.$$

We obtain that

$$\begin{split} \lim_{n \to \infty} \mathbf{P}_{H_{1,n}(\Delta_0),\mathbf{Q}} \Big(\mathsf{T}_{\alpha}^{\mathbf{Q},\xi_n} &= 1 \Big) = \lim_{n \to \infty} \mathbf{P}_{H_{1,n}(\Delta_0),\mathbf{Q}} \Big(\sqrt{n} \xi_n^\circ > \sqrt{n} \xi_n^{[1+B-\lfloor \alpha(1+B)\rfloor]} \Big) \\ &= \lim_{n \to \infty} \mathbf{P}_{H_{1,n}(\Delta_0),\mathbf{Q}} \Big(\sqrt{n} \xi_n^\circ > \Phi_\sigma^{-1}(1-\alpha) \Big) = \alpha. \end{split}$$

This completes the proof.

7.2. Proof of Theorem 4.4(ii)

Proof of Theorem 4.4(ii). Given that Y is independent of X, the conditional independence between Y and Z given X is equivalent to the (unconditional) independence between Y and W = (X, Z).

To test the independence between $Y \in \mathbb{R}^1$ and $W \in \mathbb{R}^{p+q}$, we will adopt the test proposed in Shi, Drton and Han (2022c, Equation (13)); see Deb and Sen (2023) for a similar result. We will briefly illustrate the idea.

Let $(Y_1, W_1), \ldots, (Y_n, W_n)$ be independent copies of (Y, W). Let $\mathbf{F}_{Y,\pm}^{(n)}$ and $\mathbf{F}_{W,\pm}^{(n)}$ be the empirical center-outward distribution functions as defined in Hallin et al. (2021, Definition 2.3) for $\{Y_i\}_{i=1}^n$ and $\{W_i\}_{i=1}^n$, respectively. We define the test statistic

$$\widehat{M}_n := n \cdot d\text{Cov}_n^2 \Big([\mathbf{F}_{X,\pm}^{(n)}(X_i)]_{i=1}^n, [\mathbf{F}_{Y,\pm}^{(n)}(Y_i)]_{i=1}^n \Big),$$

where the (sampled) distance covariance $dCov_n^2(\cdot, \cdot)$ is given in Székely and Rizzo (2013, Definition 1), and then form the test

$$\mathsf{T}_{\alpha}^{\mathrm{opt}} := \mathbb{1}\Big(\widehat{M}_n > q_{1-\alpha}\Big), \quad q_{1-\alpha} := \inf\Big\{x \in \mathbb{R} : \mathsf{P}\Big(\sum_{k=1}^{\infty} \lambda_k (\xi_k^2 - 1) \le x\Big) \ge 1 - \alpha\Big\}.$$

Here, λ_k , $k \in \mathbb{Z}_+$, are the non-zero eigenvalues of the integral equation given by Shi, Drton and Han (2022c, Equation (12)) and depend only on p+q, and $[\xi_k]_{k=1}^{\infty}$ is a sequence of independent standard Gaussian random variables. Further details can be found in Shi, Drton and Han (2022c).

By Theorem 3.1 in Shi, Drton and Han (2022c),

$$\lim_{n \to \infty} P_{H_0}(\mathsf{T}_{\alpha}^{\text{opt}} = 1) \le \alpha,$$

and by Theorem 5.3 in Shi et al. (2022), for sufficiently large Δ_0 ,

$$\lim_{n\to\infty} P_{H_{1,n}(\Delta_0)}(\mathsf{T}^{\mathrm{opt}}_{\alpha}=1)\geq 1-\beta.$$

Finally, we prove that

$$\lim_{\Delta_0 \to 0} \lim_{n \to \infty} \text{TV}(H_0, H_{1,n}(\Delta_0)) = 0.$$

Equation (2.20) in Tsybakov (2009) states that total variation and Hellinger distances satisfy

$$TV(H_{1,n}(\Delta_0), H_0) \le HL(H_{1,n}(\Delta_0), H_0).$$

It is also known (Tsybakov, 2009, p. 83) that

$$1 - \frac{\mathrm{HL}^{2}(H_{1,n}(\Delta_{0}), H_{0})}{2} = \left(1 - \frac{\mathrm{HL}^{2}(P_{1,n}(\Delta_{0}), P_{0})}{2}\right)^{n}.$$

Lehmann and Romano (2005, Example 13.1.1) show that, under Assumption 4.1,

$$n \times \operatorname{HL}^{2}(P_{1,n}(\Delta_{0}), P_{0})) \to \frac{\Delta_{0}^{2} I_{X}(0)}{4};$$

notice that here the definition of $HL^2(Q,P)$ differs from that in Lehmann and Romano (2005, Definition 13.1.3) by a factor of 2. Therefore,

$$\frac{\mathrm{HL}^{2}(H_{1,n}(\Delta_{0}),H_{0})}{2}\longrightarrow 1-\exp\Big\{-\frac{\Delta_{0}^{2}I_{X}(0)}{8}\Big\}.$$

where the right-hand side tends to 0 as $\Delta_0 \rightarrow 0$. The last assertion is a direct corollary of the fact that the sum of probabilities of Type I error and Type II error has the following lower bound:

$$\inf_{\mathsf{T}} \left\{ P_{H_0}(\mathsf{T} = 1) + \mathrm{P}_{H_{1,n}(\Delta_0)}(\mathsf{T} = 0) \right\} = 1 - \mathrm{TV}(H_{1,n}(\Delta_0), H_0)$$

(Lehmann and Romano, 2005, Theorem 13.1.1). This completes the proof.

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Supplementary Material

Supplement to "On Azadkia–Chatterjee's conditional dependence coefficient" (DOI: 10.3150/22-BEJ1529SUPP; .pdf). The supplement consists of auxiliary results and proofs.

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