

Limiting distributions of graph-based test statistics on sparse and dense graphs

YEJIONG ZHU^a and HAO CHEN^b

University of California, Davis, USA, ^ayjzhu@ucdavis.edu, ^bhxchen@ucdavis.edu

Two-sample tests utilizing a similarity graph on observations are useful for high-dimensional and non-Euclidean data due to their flexibility and good performance under a wide range of alternatives. Existing works mainly focused on sparse graphs, such as graphs with the number of edges in the order of the number of observations, and their asymptotic results imposed strong conditions on the graph that can easily be violated by commonly constructed graphs they suggested. Moreover, the graph-based tests have better performance with denser graphs under many settings. In this work, we establish the theoretical ground for graph-based tests with graphs ranging from those recommended in current literature to much denser ones.

Keywords: Dense graphs; graph-based methods; nonparametric two-sample tests; Stein's method

1. Introduction

Given two random samples, $X_1, \dots, X_m \stackrel{\text{iid}}{\sim} F_X, Y_1, \dots, Y_n \stackrel{\text{iid}}{\sim} F_Y$, we consider the hypothesis testing problem $H_0 : F_X = F_Y$ against $H_a : F_X \neq F_Y$. This two-sample testing problem is a fundamental problem in statistics and has been extensively studied for univariate and low-dimensional data. Nowadays, it is common that observations are in high dimensions (Feigenson et al., 2014, Network et al., 2012, Zhang et al., 2020), or non-Euclidean, such as networks (Beckmann et al., 2021, Biswal et al., 2010, Bullmore and Sporns, 2009). In many of these applications, one has little knowledge on F_X or F_Y , making parametric tests unapproachable.

Nonparametric methods play important roles in solving two-sample testing problems and have a long history. For univariate data, some common choices are the Kolmogorov–Smirnov test (Smirnov, 1939), the Wald–Wolfowitz runs test (Wald and Wolfowitz, 1940) and the Mann–Whitney rank-sum test (Mann and Whitney, 1947). Since the middle of the 20th century, researchers have tried to extend these methods to multivariate data (Bickel, 1968, Weiss, 1960). The first practical test that can be applied to data in an arbitrary dimension or non-Euclidean data was proposed by Friedman and Rafsky (1979), which is based on a similarity graph and is the start of graph-based tests. Over the years, graph-based tests evolved a lot and showed good power for a variety of alternatives and different kinds of data (Chen, Chen and Su, 2018, Chen and Friedman, 2017, Chen and Zhang, 2013, Chu and Chen, 2019, Henze and Penrose, 1999, Rosenbaum, 2005, Schilling, 1986, Zhang and Chen, 2022). In the following, we give a brief review of the graph-based tests and discuss their limitations.

1.1. A review of graph-based tests

Friedman and Rafsky (1979) proposed to pool all observations from both samples to construct the minimum spanning tree (MST), which is a tree connecting all observations such that the sum of edge lengths that are measured by the distance between two endpoints is minimized. They then count the number of edges that connect observations from different samples and reject H_0 when this count is significantly small. The rationale is that when two samples are from the same distribution, they are

well mixed and this count shall be relatively large, so a small count suggests separation of the two samples and rejection of H_0 . We refer this test to be the *original edge-count test* (OET). This test is not limited to the MST. [Friedman and Rafsky \(1979\)](#) also applied it to the K -MST¹. Later, [Schilling \(1986\)](#) and [Henze \(1988\)](#) applied it to the K -nearest neighbor graphs (K -NNG), and [Rosenbaum \(2005\)](#) applied it to the cross-match graph. [Zhang and Chen \(2022\)](#) extended the test to accommodate data with repeated observations.

Recently, [Chen and Friedman \(2017\)](#) noticed an issue of OET caused by the curse of dimensionality. They made use of a common pattern under moderate to high dimensions and proposed the *generalized edge-count test* (GET), which exhibits substantial power improvements over OET under a wide range of alternatives. Later, two more edge-count tests were proposed, the *weighted edge-count test* (WET) ([Chen, Chen and Su, 2018](#)) and the *max-type edge-count test* (MET) ([Chu and Chen, 2019](#)). WET addresses an issue of OET under unequal sample sizes, but it focuses on the locational alternatives. MET performs similarly to GET while it has some advantages under change-point settings.

In the following, we express the four graph-based test statistics with rigorous notations. The two samples X_1, \dots, X_m and Y_1, \dots, Y_n , are pooled together and indexed by $1, \dots, N$ ($N = m + n$). Let G be the set of all edges in the similarity graph, such as the K -MST. For an edge $e \in G$, let e^+, e^- be two endpoints of the edge e , i.e. $e = (e^+, e^-)$. Let g_i be the group label of i -th observation with

$$g_i = \begin{cases} 1 & \text{if observation } i \text{ is from sample X} \\ 2 & \text{if observation } i \text{ is from sample Y,} \end{cases}$$

and R_1, R_2 be the numbers of within-sample edges of sample X and sample Y, respectively, formally defined as

$$R_j = \sum_{e \in G} 1_{\{J_e=j\}}, \quad j = 1, 2,$$

where $1_{\{A\}}$ is the indicator function that takes value 1 if event A occurs and takes value 0 otherwise, and

$$J_e = \begin{cases} 0 & \text{if } g_{e^+} \neq g_{e^-} \\ 1 & \text{if } g_{e^+} = g_{e^-} = 1 \\ 2 & \text{if } g_{e^+} = g_{e^-} = 2. \end{cases}$$

Since no distributional assumption was made for F_X and F_Y , we use the permutation null distribution, which places probability $1/\binom{N}{m}$ on each selection of m observations among pooled observations as sample X. Let $E_P, \text{Var}_P, \text{Cov}_P$ be the expectation, variance and covariance under the permutation null distribution.

The four graph-based test statistics mentioned above can be expressed as follows:

1. OET: $Z_o^P = (R_1 + R_2 - E_P(R_1 + R_2)) / \sqrt{\text{Var}_P(R_1 + R_2)}$;
2. GET: $S = (R_1 - E_P(R_1) \quad R_2 - E_P(R_2)) \Sigma_R^{-1} \begin{pmatrix} R_1 - E_P(R_1) \\ R_2 - E_P(R_2) \end{pmatrix}$, where $\Sigma_R = \text{Var}_P(R_1, R_2)^T$;

¹A K -MST is the union of the 1st, \dots , K th MSTs, where the 1st MST is the MST and the k th ($k > 1$) MST is a tree connecting all observations that minimizes the sum of distance across edges subject to the constraint that this tree does not contain any edge in the 1st, \dots , $k - 1$ th MST(s).

3. WET: $Z_w^P = (R_w - E_P(R_w)) / \sqrt{\text{Var}_P(R_w)}$, where $R_w = R_1(n-1)/(N-2) + R_2(m-1)/(N-2)$;
4. MET: $\max\{Z_w^P, Z_{\text{diff}}^P\}$, where $Z_{\text{diff}}^P = (R_{\text{diff}} - E_P(R_{\text{diff}})) / \sqrt{\text{Var}_P(R_{\text{diff}})}$ with $R_{\text{diff}} = R_1 - R_2$.

The analytic formulas for the expectations and variances of $R_1 + R_2$, $(R_1, R_2)^T$, R_w , R_{diff} can be found in Chen, Chen and Su (2018), Chen and Friedman (2017), Chu and Chen (2019). It was also shown in Chu and Chen (2019) that the statistic S can be decomposed as

$$S = (Z_w^P)^2 + (Z_{\text{diff}}^P)^2 \tag{1}$$

and $\text{Cov}_P(Z_w^P, Z_{\text{diff}}^P) = 0$.

1.2. Limitations of existing theorems on graph-based test statistics

Since the computation of p -values by drawing random permutations is time-consuming, approximated p -values from the asymptotic null distributions of the graph-based test statistics are useful in practice. Some existing theorems provide sufficient conditions for the validity of the asymptotic distributions. Before stating these results, we first define some essential notations.

For each node $i \in \mathcal{N} \triangleq \{1, \dots, N\}$, let G_i be the set of edges with one endpoint node i , node_{G_i} be the set of nodes connected by G_i excluding node i , $G_{i,2}$ be the set of edges with at least one endpoint in node_{G_i} , and $\text{node}_{G_{i,2}}$ be the set of nodes connected by $G_{i,2}$ excluding node i . For each edge $e = (e^+, e^-) \in G$, define $A_e = G_{e^+} \cup G_{e^-}$, $B_e = G_{e^+,2} \cup G_{e^-,2}$ and C_e be the set of edges that share at least one common node with an edge in B_e . We use $|\cdot|$ to denote the cardinality of a set. Then $|G_i|$ is the degree of the node i . Figure 1 plots the quantities related to a node i and an edge e , respectively.

We also define $\tilde{d}_i = |G_i| - 2|G|/N$ to be the centered degree of node i and $V_G = \sum_{i=1}^N \tilde{d}_i^2 = \sum_{i=1}^N |G_i|^2 - 4|G|^2/N$ that measures the variability of $|G_i|$'s. Besides, $a_n = o(b_n)$ or $a_n < b_n$ means that a_n is dominated by b_n asymptotically, i.e. $\lim_{n \rightarrow \infty} a_n/b_n = 0$, $a_n \lesssim b_n$ means that a_n is bounded above by b_n (up to a constant factor) asymptotically, and $a_n = O(b_n)$ or $a_n \asymp b_n$ means that a_n is

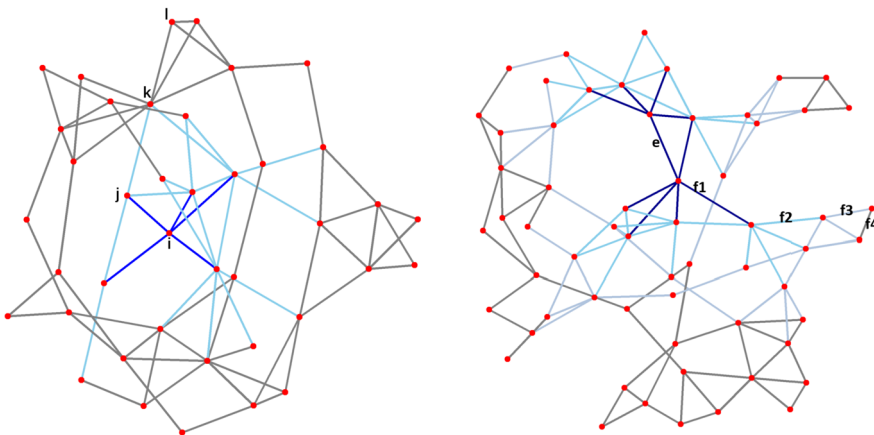


Figure 1. The left panel is an illustration of notations related to a node i : $G_i = \{\text{blue edges}\}$, $G_{i,2} = \{\text{sky blue edges}\} \cup \{\text{blue edges}\}$; $j \in \text{node}_{G_i}, k \in \text{node}_{G_{i,2}} \setminus \text{node}_{G_i}, l \notin \text{node}_{G_{i,2}}$, and the right panel is an illustration of notations related to an edge e : $A_e = \{\text{dark blue edges}\}, B_e \setminus A_e = \{\text{sky blue edges}\}, C_e \setminus B_e = \{\text{light steel blue edges}\}$; $f_1 \in A_e, f_2 \in B_e \setminus A_e, f_3 \in C_e \setminus B_e, f_4 \notin C_e$. Both graphs are plotted by the ‘ggnet2’ function in R.

Table 1. Major existing works on graph-based tests and their conditions on the graph for asymptotic distributions.

	Test Statistic	Graph conditions	max size of possible graphs
Friedman and Rafsky (1979)	Original	MST with $\sum_{i=1}^N G_i ^2 = O(N)$	$N - 1$
Schilling (1986)	Original	K -NNG, $K = O(1)$ for low-dimensional data	$O(N)$
Henze (1988)	Original	K -NNG, $K = O(1)$ with bounded maximal indegrees	$O(N)$
Rosenbaum (2005)	Original	cross-match graph	$N/2$ or $(N - 1)/2$
Chen and Zhang (2015)	Original	$ G = O(N^\alpha)$, $0 < \alpha < 1.125$ $\sum_{e \in G} A_e B_e = o(N^{1.5(\alpha \wedge 1)})$	$O(N^\alpha)$, $\alpha < 1.125$
Chen and Friedman (2017)	Generalized	$ G = O(N)$ $\sum_{i=1}^N G_i ^2 = O(N)$ $\sum_{e \in G} A_e B_e = o(N^{1.5})$	$O(N)$
Chen, Chen and Su (2018)	Weighted	$ G = O(N^\alpha)$, $1 \leq \alpha < 1.25$ $\sum_{e \in G} A_e B_e = o(N^{1.5\alpha})$ $\sum_{e \in G} A_e ^2 = o(N^{\alpha+0.5})$	$O(N^\alpha)$, $\alpha < 1.25$
Chu and Chen (2019)	Generalized Weighted Max-type	$ G = O(N^\alpha)$, $1 \leq \alpha < 1.25$ $\sum_{e \in G} A_e B_e = o(N^{1.5\alpha})$ $\sum_{e \in G} A_e ^2 = o(N^{\alpha+0.5})$ $V_G = O(\sum_{i=1}^N G_i ^2)$	$O(N^\alpha)$, $\alpha < 1.25$

*For the conditions in Chen, Chen and Su (2018) and Chu and Chen (2019), the size of the graph is bounded by the condition on $|A_e|^2$: $\sum_{e \in G} |A_e|^2 = o(N^{\alpha+0.5})$ requires that $\alpha < 1.25$.

bounded both above and below by b_n asymptotically. We use $a \wedge b$ for $\min\{a, b\}$. For two sets S_1 and S_2 , $S_1 \setminus S_2$ is used for the set that contains elements in S_1 but not in S_2 .

The major existing works that studied the asymptotic null distributions of the graph-based test statistics are listed in Table 1. In general, these works put requirements on the graph such as the maximum in-degree, $\sum |G_i|^2$, $\sum |A_e|^2$ and $\sum |A_e||B_e|$. The conditions in Friedman and Rafsky (1979) are limited to the MST, while K -MST with $K > 1$ has a better performance in general (Chen and Friedman, 2017). For those that are more relaxed on the graph and data, Henze (1988) requires a bounded maximal in-degree in K -NNG, Chen and Friedman (2017) requires $\sum |G_i|^2$ to be of the same order as N , and Chen, Chen and Su (2018) and Chu and Chen (2019) provide the current weakest conditions that require $\sum |A_e|^2 = o(|G|\sqrt{N})$ and $\sum |A_e||B_e| = o(|G|^{1.5})$. However, those conditions are often too strong to hold under even simple scenarios. For example, we generate two samples with equal sample size ($m = n = N/2$) from the 500-dimensional standard multivariate normal distribution, and construct the 5-MST and 5-NNG using the Euclidean distance. Figure 2 plots the maximum in-degree, $\sum_{i=1}^N |G_i|^2/N$, $\sum |A_e|^2/(|G|\sqrt{N})$ and $\sum |A_e||B_e|/|G|^{1.5}$ with different N 's. We see that the conditions on them are badly violated: the maximum in-degree goes up rather than bounded by a constant, $\sum_{i=1}^N |G_i|^2/N$ increases with N rather than bounded by a constant, and $\sum_{e \in G} |A_e|^2/(|G|\sqrt{N})$ and $\sum_{e \in G} |A_e||B_e|/|G|^{1.5}$ stay at a large value (in hundreds) as N increases rather than $o(1)$ as required by the conditions. If we

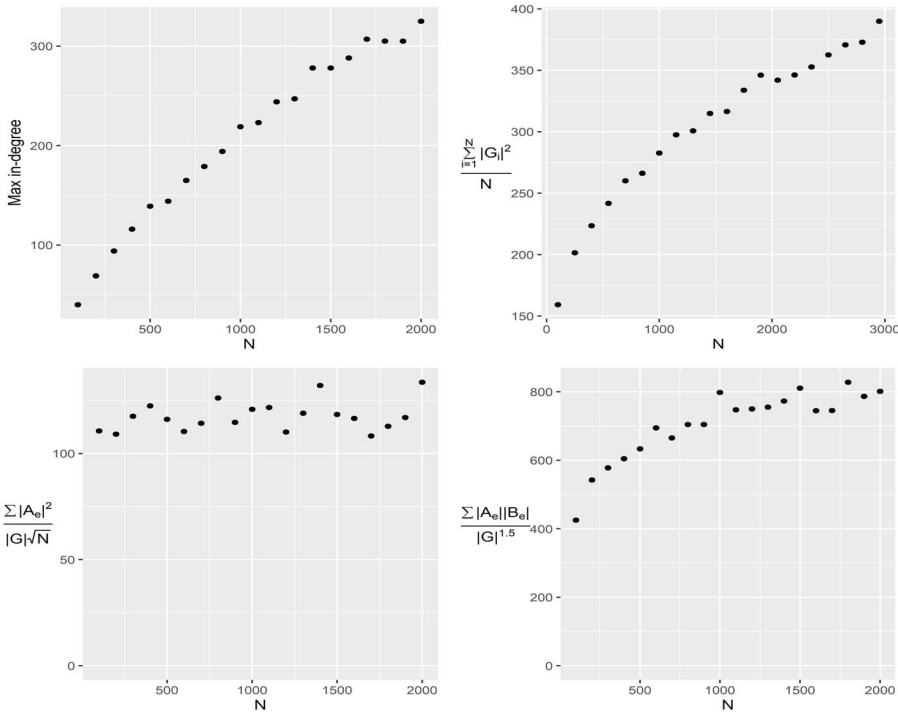


Figure 2. Key quantities with respect to N . Top-left: the maximum in-degree in the 5-NNG; top-right: the ratio of $\sum_{i=1}^N |G_i|^2$ to N in the 5-MST; bottom-left: the ratio of $\sum |A_e|^2$ to $|G|\sqrt{N}$ in the 5-MST; bottom-right: the ratio of $\sum |A_e||B_e|$ to $|G|^{1.5}$ in the 5-MST.

make the graph denser, such as 10-MST, these conditions are even more badly violated. However, in many settings, the graph-based tests work better under denser graphs (see Section 1.3).

1.3. The merits of denser graphs in improving power for graph-based tests

Friedman and Rafsky (1979) found that the original edge-count test in general had a higher power under the 3-MST than that under the 1-MST. Similarly, Chen and Friedman (2017) found that the generalized edge-count test in general had a higher power under the 5-MST than that under the 1-MST. We here check the performance of these tests under even denser graphs. In particular, for $m = n = 100$, we consider the generalized edge-count tests on the 5-MST (GET₅) and on the 50-MST (GET₅₀), the original edge-count tests on the 5-MST (OET₅) and on the 50-MST (OET₅₀). All K -MSTs here are constructed under the Euclidean distance. We also include two other tests as baselines: the kernel two-sample test in Gretton et al. (2012) with the p -value approximated by 10,000 bootstrap samples (Kernel) and the Adaptable Regularized Hotelling’s T^2 test (Li et al., 2020) (ARHT).

We consider different distributions in the comparison. Explicitly,

$$X_i = \Sigma^{\frac{1}{2}} U_i, \quad i = 1, \dots, 100, \quad Y_j = (1 + ad^{-\frac{1}{3}}) \Sigma^{\frac{1}{2}} V_j - bd^{-\frac{1}{3}} \mathbf{1}_d, \quad j = 1, \dots, 100,$$

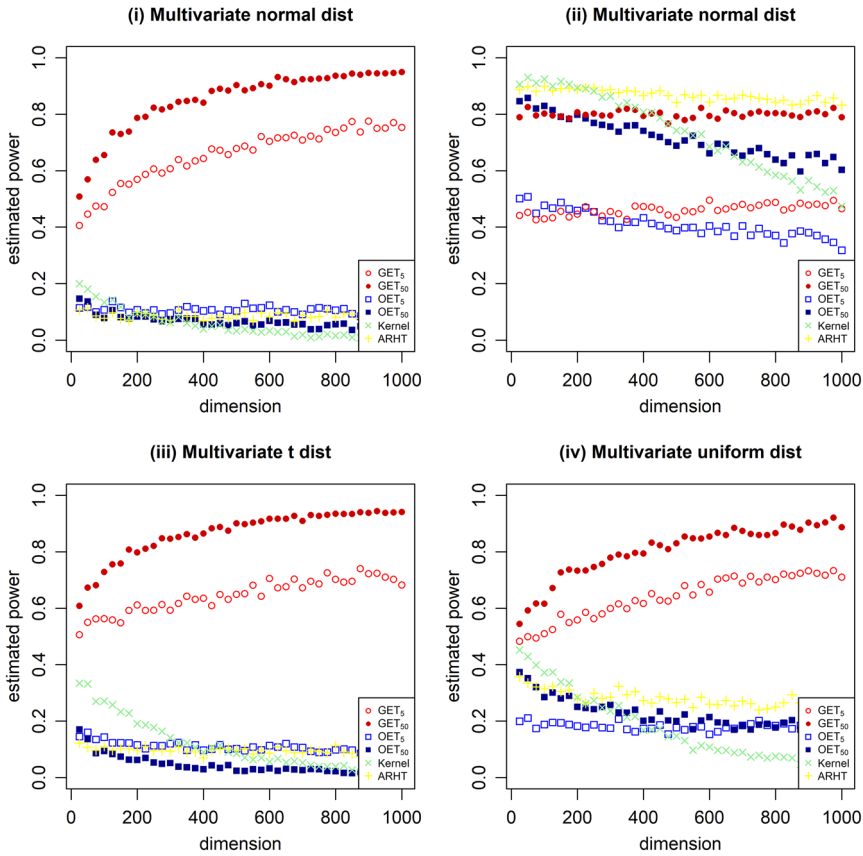


Figure 3. Estimated power of the generalized edge-count tests on the 5-MST (GET₅) and on the 50-MST (GET₅₀), the original edge-count tests on the 5-MST (OET₅) and on the 50-MST (OET₅₀), the kernel test (Kernel), and the Adaptable Regularized Hotelling’s T² test (ARHT) under different simulation settings (i) - (iv).

with $\Sigma = (0.5^{|i-j|})_{1 \leq i, j \leq d}$, where d is the dimension of the data, $\mathbf{1}_d$ is a d -length vector of all ones. Let $\mathbf{0}_d$ be a d -length vector of all zeros and I_d be a d -dimensional identity matrix. We consider four different settings:

- (i) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} N(\mathbf{0}_d, I_d), a = b = 0.17,$
- (ii) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} N(\mathbf{0}_d, I_d), a = 0.1, b = 0.6,$
- (iii) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} t_5(\mathbf{0}_d, I_d), a = b = 0.25,$
- (iv) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} \text{Uniform}[-0.5, 0.5]^d, a = 0.12, b = 0.1.$

Here, a and b are chosen so that the tests have moderate power in low dimensions. The dimension d ranges from 25 to 1000 with an increment of 25. The power of tests are estimated through 1,000 simulation runs (Figure 3). We see that GET₅₀ works well in these settings, either having the best power or on par with the test of the best power. GET₅ in general has a lower power than GET₅₀. For OET, it is only powerful under setting (ii). The worse performance of OET compared to GET is expected as OET covers less alternatives than GET for high-dimensional data (Chen and Friedman, 2017). Under setting (ii) where OET is powerful, OET₅₀ has a higher power than OET₅.

1.4. Our contribution

From Section 1.3, we see that the use of denser graphs has a promising effect in improving power for graph-based tests. So far, the best theoretical results on dense graphs are in [Chen, Chen and Su \(2018\)](#) and [Chu and Chen \(2019\)](#), which allow the maximum size of possible graphs to be of order N^α , $1 \leq \alpha < 1.25$. But in the numerical studies in Section 1.3 where $N = 200$, the number of edges in the 50-MST is 9950 ($\approx N^{1.74}$). Existing conditions cannot work for such dense graphs. In addition, even for sparse graphs, current existing conditions usually do not hold (see Section 1.2). Therefore, it is important to figure out whether the conditions on graphs can be weakened and to what extent. Throughout the paper, we consider simple undirected graphs that contain no duplicate edges and no loops.

[Friedman and Rafsky \(1979\)](#) applied the moment-based method in [Daniels \(1944\)](#) to derive sufficient conditions for the asymptotic normality of Z_o^P , and [Chen, Chen and Su \(2018\)](#), [Chen and Friedman \(2017\)](#), [Chu and Chen \(2019\)](#) made use of the bootstrap null distribution and the second neighbor dependent Stein's method to show the asymptotic normality of $(R_1, R_2)^T$ and Z_w^P under the permutation null distribution. In this paper, we seek improvements in both directions, especially the latter one. In particular, we propose to use a "locSCB" (local Stein's method on Conditioning Bootstrap) approach that use Stein's method to carefully deal with all the first neighbor dependency under the bootstrap null distribution and link the permutation null distribution and bootstrap null distribution through conditioning. By doing this, we are able to weaken the conditions on the graphs to a tremendous amount. Under new conditions, the maximum size of possible graphs can be as large as $M^{1-\epsilon}$ with an arbitrarily small ϵ , where $M = \binom{N}{2}$ is the size of the complete graph. In addition, we also quantify the upper bound of Stein's inequality.

The "locSCB" approach is not limited to show the asymptotic properties of these four graph-based test statistics listed in Section 1.1. It can be applied to some other nonparametric two-sample test statistics and K -sample test statistics under the permutation null distribution, and to the change-point analysis settings. The main theorems are provided in Section 2. We discuss the new conditions in Section 3 from various aspects. Section 4 provides detailed proof for the theorem on GET. The detailed proofs for other edge-count tests are deferred to the Supplementary Material ([Zhu and Chen, 2024](#)).

2. Asymptotic distribution under denser graphs

We first state the main results for the four statistics. The discussion of new conditions are deferred to Section 3. The proofs are provided in Section 4 and the Supplementary Material ([Zhu and Chen, 2024](#)).

We use $\xrightarrow{\mathcal{D}}$ to denote convergence in distribution, and use 'the usual limit regime' to refer $N \rightarrow \infty$ and $\lim_{N \rightarrow \infty} m/N = r \in (0, 1)$. We define N_{sq} as the number of squares in the graph, $N_{i,j}$ as the number of nodes connecting to nodes i and j simultaneously, and recall that $\tilde{d}_i = |G_i| - 2|G|/N$ (defined in Section 1.2). The conditions needed for the asymptotic results of the four statistics are listed below.

- C.1 $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$, $N_{sq} = o(|G|^2)$;
- C.2 $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$, $\sum_{i=1}^N \tilde{d}_i^3 = o(V_G \sqrt{|G|})$, $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k = o(|G|V_G)$;
- C.3 $\max(\tilde{d}_i^2) = o(V_G)$;
- C.4 $\sum_{i=1}^N |G_i|^2 = o(T^{1.5})$, $\sum_{i=1}^N |\tilde{d}_i|^3 = o(T^{1.5})$, $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k = o(T^2)$, with $T = |G| + V_G$.

2.1. Generalized edge-count test

Theorem 1. *Under Condition C.1 and C.2, in the usual limit regime, $S \xrightarrow{\mathcal{D}} \chi_2^2$ under the permutation null distribution.*

A detailed comparison of the conditions in Theorem 1 to the best existing conditions is provided in Section 3.1. We will see that Theorem 1 provides much weaker conditions.

The conditions in Theorem 1 are not easily understandable for a graph. In the following, we provide a set of conditions that only involve up to the second moment of the degree distribution, and are easier to understand. Let Q_G be a random variable generated from the degree distribution of a graph G built on N nodes. Then it is not hard to see that $E(Q_G) = 2|G|/N$ and $\text{Var}(Q_G) = V_G/N$.

Corollary 2. *Suppose $|G| = O(KN)$ with $1 \lesssim K < N$, if $\max(1, K^2/N) \lesssim \text{Var}(Q_G) < K^{1.5}\sqrt{N}$, and the concentration inequality*

$$P(|Q_G - E(Q_G)| \geq t) \leq 2\exp\left(-\frac{ct^2}{Na}\right), \quad t > 0, \tag{2}$$

holds for all large N with some constants $c > 0$ and $0 < a < 1$, then, in the usual limit regime, $S \xrightarrow{\mathcal{D}} \chi_2^2$ under the permutation null distribution.

Remark 3. Corollary 2 is derived from Theorem 1 at the cost of sacrificing some of its generality. The conditions in Corollary 2 could be further weakened when more information on the degree distribution is available. For the K -MST constructed on multivariate data, the maximum degree of the MST has been studied for fixed dimensions (Robins and Salowe, 1994), which is of $O(1)$. Hence, under fixed dimensions, the maximum degree of the K -MST has the order at most of K , which is sufficient for the conditions in Corollary 2 to hold when $K = O(N^\beta)$, $\beta < 0.5$. Similarly, under fixed dimensions, the maximum degree of the K -NNG also has the order of at most K , and thus the conditions in Corollary 2 also hold for the K -NNG when $K = O(N^\beta)$, $\beta < 0.5$. To further relax K and/or dimensions, the degree distributions of the K -MST or the K -NNG is needed, which is nontrivial for both fixed and non-fixed dimensions and will be explored in future research.

2.2. Weighted and max-type edge-count test

Theorem 4. *Under Condition C.1, in the usual limiting regime, $Z_w^P \xrightarrow{\mathcal{D}} N(0, 1)$ under the permutation null distribution.*

Theorem 5. *Under Condition C.3, in the usual limit regime, $Z_{diff}^P \xrightarrow{\mathcal{D}} N(0, 1)$ under the permutation null distribution.*

Condition C.3 is equivalent to

$$\frac{\sum_{i=1}^N |\tilde{d}_i|^{2+\delta}}{V_G^{\frac{2+\delta}{2}}} \rightarrow 0, \quad \text{for some } \delta > 0, \tag{3}$$

according to [Hoeffding \(1951\)](#). One condition in [C.2](#) for [Theorem 1](#) is actually setting δ to be 1 in [\(3\)](#). Comparing conditions in [Theorems 1, 4 and 5](#), it is not hard to see that the union of conditions for Z_w^P and Z_{diff}^P separately is less stringent than those in [Theorem 1](#). This is reasonable as [Theorem 1](#) needs the asymptotic normality of the joint distribution of (Z_w^P, Z_{diff}^P) while [Theorem 4 and 5](#) only needs that for one of the marginal distributions.

For the max-type edge-count test, the limiting distribution of test statistic still requires the conditions in [Theorem 1](#). However, if some techniques are used to conservatively estimate the p -value for the max-type statistic, such as the Bonferroni correction, then the union of the conditions in [Theorems 4 and 5](#) would be enough.

Corollary 6. *For graphs with $|G| = O(KN)$ and $1 \lesssim K < N$, if $\text{Var}(Q_G) < K^{1.5}\sqrt{N}$ and $E(Q_G^3) = o(K^2N)$, then, in the usual limiting regime, $Z_w^P \xrightarrow{D} N(0, 1)$ under the permutation null distribution.*

Remark 7. For the K -MST and the K -NNG on the multivariate data with a fixed dimension, the maximum degree has the order of K . Then, $\text{Var}(Q_G)$ has the order at most $K^2/4$, and $E(Q_G^3)$ has the order at most K^3 . Thus, the conditions in [Corollary 6](#) hold for all $K < N$.

Corollary 8. *For graphs with $|G| = O(KN)$ and $1 \lesssim K \lesssim N$, if $1 \lesssim \text{Var}(Q_G)$ and the concentration inequality*

$$P(|Q_G - E(Q_G)| \geq t) \leq 2\exp\left(-\frac{ct^2}{V_G^a}\right), \quad t > 0,$$

holds for all large N with some constants $c > 0$ and $0 < a < 1$, then, in the usual limit regime, $Z_{diff}^P \xrightarrow{D} N(0, 1)$.

Remark 9. For the K -MST and the K -NNG constructed on multivariate data with a fixed dimension, conditions in [Corollary 8](#) hold if $K = O(N^\beta)$, $\beta < 0.5$, because V_G has the order at least N when $1 \lesssim \text{Var}(Q_G)$.

2.3. Original edge-count test

Consider the usual limit region where $\lim_{N \rightarrow \infty} m/N = r \in (0, 1)$. When $r = 0.5$, the original edge-count test is equivalent to the weighted edge-count test asymptotically. Thus, we here study the asymptotic distribution of the original edge-count test statistic when $r \neq 0.5$.

Theorem 10. *In the usual limit region and $\lim_{N \rightarrow \infty} \frac{m}{N} = r$ with r a constant and $r \neq \frac{1}{2}$, under [Condition C.4](#), $Z_o^P \xrightarrow{D} N(0, 1)$ under the permutation null distribution.*

The condition [C.4](#) in [Theorem 10](#) are weaker than the conditions required in [Theorem 1](#) as T has the order of $\max\{|G|, V_G\}$.

Corollary 11. *For graphs with $|G| = O(KN)$ and $1 \lesssim K < N$, in the usual limit regime and $\lim_{N \rightarrow \infty} \frac{m}{N} = r$ with r a constant and $r \neq \frac{1}{2}$, if either of the following conditions*

- $|G|$ and V_G do not have the same order, and

$$P(|Q_G - E(Q_G)| \geq t) \leq 2\exp\left(-\frac{ct^2}{Ta}\right), \quad t > 0,$$

- $|G| \asymp V_G$, and

$$P(|Q_G - E(Q_G)| \geq t) \leq 2\exp\left(-\frac{ct^2}{Na}\right), \quad t > 0,$$

holds for all large N with some constants $c > 0$ and $0 < a < 1$, then $Z_o^P \xrightarrow{D} N(0, 1)$.

Remark 12. For the K -MST and the K -NNG constructed on multivariate data with a fixed dimension, conditions in Corollary 11 hold if $K = O(N^\beta)$ with $\beta < 0.5$ when $|G| \asymp V_G$. When $|G|$ and V_G do not have the same order, these conditions hold as long as $K < N$.

2.4. Some brief comments on the conditions

The sufficient conditions in Theorem 1 are derived using Stein’s method with the first neighbor dependency. One key step is to have the upper bound in the Stein’s inequality

$$\sqrt{\frac{2}{\pi}} E_B \left| \sum_{i \in N} \{\xi_i \eta_i - E_B(\xi_i \eta_i)\} + \sum_{e \in G} \{\xi_e \eta_e - E_B(\xi_e \eta_e)\} \right| + \sum_{i \in N} E_B |\xi_i \eta_i^2| + \sum_{e \in G} E_B |\xi_e \eta_e^2| \quad (4)$$

to go to zero, where E_B , ξ_i , η_i , ξ_e and η_e are defined in Section 4. Condition $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$ ensures that the quantity $\sum_{i \in N} E_B |\xi_i \eta_i^2|$ goes to zero. Conditions $\sum_{i=1}^N \tilde{d}_i^3 = o(V_G \sqrt{|G|})$ and $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ lead to the zero limit of the quantity $\sum_{e \in G} E_B |\xi_e \eta_e^2|$. To ensure the first quantity in (4) to go to zero, under the three previous mentioned conditions ($\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$, $\sum_{i=1}^N \tilde{d}_i^3 = o(V_G \sqrt{|G|})$ and $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$), we need two additional conditions, $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k = o(|G|V_G)$ and $N_{sq} = o(|G|^2)$. Conditions in Theorems 4 and 10 are derived in a similar way.

Theorem 5 is derived in a different way as the test statistic in this case can be expressed into a weighted sum of independent random variables. Then the Lyapunov CLT can be applied.

The locSCB approach used in proving Theorems 1, 4, 10 will be detailed in Section 4. For the moment-based method, it was first proposed in Daniels (1944). Later, Friedman and Rafsky (1983) claimed that Daniels’ conditions can be weakened and provided their new conditions. However, they did not give an explicit proof. Pham, Möcks and Sroka (1989) found that conditions in Friedman and Rafsky (1983) are not sufficient, so they fixed this problem and proposed a new set of weaker conditions. By using the conditions in Pham, Möcks and Sroka (1989), the conditions to ensure the asymptotic distributions of the graph-based tests can be weakened. However, we found that our locSCB approach could result in even weaker conditions. A discussion of the conditions from the moment-based method is detailed in Section S2 of the Supplementary Material (Zhu and Chen, 2024).

3. Discussions on the new conditions

3.1. A comparison to the best existing conditions

For the asymptotic distribution of the generalized edge-count test statistic, [Chu and Chen \(2019\)](#) had the best result that required the following conditions:

$$|G| = O(N^\alpha), 1 \leq \alpha < 1.25, \quad \sum_{e \in G} |A_e||B_e| = o(|G|^{1.5}), \quad \sum_{e \in G} |A_e|^2 = o(|G|\sqrt{N}), \quad V_G = O\left(\sum_{i=1}^N |G_i|^2\right).$$

We here compare our conditions in [Theorem 1](#) with those in [Chu and Chen \(2019\)](#). We first state some propositions with proofs deferred to Section S4 of the Supplementary Material ([Zhu and Chen, 2024](#)).

- P.1** $\sum_{e \in G} |A_e|^2 \asymp \sum_{i=1}^N |G_i|^3$;
- P.2** $\sum_{e \in G} |A_e||B_e| \asymp \sum_{i=1}^N |G_i|^2|G_{i,2}| + \sum_{i=1}^N |G_{i,2}|^2$;
- P.3** $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k \lesssim \sum_{i=1}^N |G_{i,2}|^2 + \frac{|G|^2}{N^2} \sum_{i=1}^N |G_i|^2$;
- P.4** $N_{sq} \lesssim \sum_{i=1}^N |G_i||G_{i,2}|$.

The condition $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ in [Theorem 1](#) can be easily obtained from [Proposition P.1](#) and under the condition $\sum_{e \in G} |A_e||B_e| = o(|G|^{1.5})$ as

$$\sum_{i=1}^N |G_i|^2 \leq \sum_{i=1}^N |G_i|^3 \asymp \sum_{e \in G} |A_e|^2 \lesssim \sum_{e \in G} |A_e||B_e|.$$

For conditions $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$ and $\sum_{i=1}^N \tilde{d}_i^3 = o(V_G \sqrt{|G|})$ in [Theorem 1](#), we have,

$$\sum_{i=1}^N \tilde{d}_i^3 \lesssim \sum_{i=1}^N |\tilde{d}_i|^3 \lesssim \sum_{i=1}^N |G_i|^3 + \frac{|G|}{N} \sum_{i=1}^N |G_i|^2 + \frac{|G|^3}{N^2}. \tag{5}$$

Under conditions in [Chu and Chen \(2019\)](#), the right-hand side in (5) is dominated by $V_G \sqrt{|G|}$, so it is also dominated by $V_G^{1.5}$. For the condition on $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k$, from [Proposition P.3](#), we have

$$\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k \lesssim \sum_{i=1}^N |G_{i,2}|^2 + \frac{|G|^2}{N^2} \sum_{i=1}^N |G_i|^2 \lesssim \sum_{i=1}^N |G_{i,2}|^2 + V_G |G| \frac{|G|}{N^2}. \tag{6}$$

Then, from [Proposition P.2](#), we have $\sum_{i=1}^N |G_{i,2}|^2 \lesssim \sum_{e \in G} |A_e||B_e|$, which is dominated by $|G|^{1.5}$ under [Chu and Chen \(2019\)](#)'s conditions. With the fact that $|G|^{1.5} \lesssim |G|V_G$ and $|G| \lesssim N^2$, the conditions in [Chu and Chen \(2019\)](#) imply the condition $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_j \tilde{d}_k = o(|G|V_G)$.

For the condition on N_{sq} in [Theorem 1](#), from [Propositions P.2](#) and [P.4](#), we have that

$$N_{sq} \lesssim \sum_{i=1}^N |G_i||G_{i,2}| \lesssim \sum_{e \in G} |A_e||B_e|.$$

Hence, the condition $N_{sq} = o(|G|^2)$ is weaker than the condition $\sum_{e \in G} |A_e||B_e| = o(|G|^{1.5})$ in [Chu and Chen \(2019\)](#).

In the above inequalities, many are significantly loosened that the right-hand side could be much larger than the left-hand side. For a graph that satisfies the conditions in [Chu and Chen \(2019\)](#), its maximum size needs to be smaller than the order of $N^{1.25}$. But for our new conditions, the size of graph can be much larger.

For the weighted edge-count test, [Chen, Chen and Su \(2018\)](#) had the best result so far, and required that $\sum_{e \in G} |A_e||B_e| = o(|G|^{1.5})$, $\sum_{e \in G} |A_e|^2 = o(|G|\sqrt{N})$ and $|G| = o(N^{1.5})$. Our conditions in [Theorem 4](#) only require $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ and $N_{sq} \lesssim |G|^2$, and they are much weaker as $\sum_{i=1}^N |G_i|^2 \lesssim \sum_{e \in G} |A_e||B_e|$ and $N_{sq} \lesssim \sum_{e \in G} |A_e||B_e|$.

Existing works have not studied the conditions for Z_{diff}^P directly.

For the original edge-count test, [Chen and Zhang \(2015\)](#) had the best result so far. They require $\sum_{e \in G} |A_e||B_e| = o(\min\{N^{1.5}, |G|^{1.5}\})$ and $|G| = O(N^\alpha)$, $\alpha < 1.125$, which are more stringent than conditions in [Theorem 10](#). For the condition $\sum_{i=1}^N |\tilde{d}_i|^3 = o(T^{1.5})$ in [Theorem 10](#), we have

$$\sum_{i=1}^N |\tilde{d}_i|^3 \lesssim \sum_{i=1}^N |G_i|^3 + \frac{|G|}{N} \sum_{i=1}^N |G_i|^2 + \frac{|G|^3}{N^2},$$

where the right-hand side is dominated by $|G|^{1.5}$ from [Proposition P.2](#) and under [Chen and Zhang \(2015\)](#)'s conditions. For the condition $\sum_{i=1}^N |G_i|^2 = o(T^{1.5})$ in [Theorem 10](#), we have $\sum_{i=1}^N |G_i|^2 \lesssim \sum_{e \in G} |A_e||B_e| < |G|^{1.5}$. For the condition on $\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_i \tilde{d}_j$, from [Propositions P.2](#) and [P.3](#) and under [Chen and Zhang \(2015\)](#)'s condition on $\sum_{e \in G} |A_e||B_e|$, we have

$$\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} \tilde{d}_i \tilde{d}_j \lesssim \sum_{i=1}^N |G_{i,2}|^2 + \frac{|G|^2}{N^2} \sum_{i=1}^N |G_i|^2 < |G|^2 \lesssim T^2.$$

For condition $N_{sq} = o(T_1^2)$, we have $N_{sq} \lesssim \sum_{e \in G} |A_e||B_e|$ from [Proposition P.2](#) and [P.4](#). Under [Chen and Zhang \(2015\)](#)'s condition, $\sum_{e \in G} |A_e||B_e|$ is dominated by $|G|^{1.5}$, so it is also dominated by T^2 .

3.2. How far are the new conditions from being necessary?

The conditions in [Theorems 1, 4, 5](#) and [10](#) are sufficient conditions. One question is how far the new conditions are from being necessary. Here, we focus on the generalized edge-count test and check the validity of the asymptotic χ_2^2 under some synthetic graphs. We repeatedly generate graphs from particular generating rules, obtain the approximate distribution of the test statistic through random permutations, and compare the approximate distribution with the χ_2^2 distribution via Kolmogorov–Smirnov (KS) test. For each simulation setting, we repeat 100 times, the proportion of rejection of the KS test is plotted in [Figure 4](#). We try to construct graphs that violate the conditions in [Theorem 1](#). The following six graph generating rules are considered:

- (i) Fix N ($N = 2000$) nodes indexing from $1, \dots, N$. Connect the first node to N^α nodes that are randomly selected from nodes $2, \dots, N$. Next, randomly select N edges from all pairwise edges of nodes $2, \dots, N$.
- (ii) Fix N ($N = 2000$) nodes indexing from $1, \dots, N$. Connect the first node to N^α nodes that are randomly selected from nodes $2, \dots, N$. Next, connect node i to node $i + 1$ for $i \in \{2, \dots, N - 1\}$ and finally connect nodes N and 2 .
- (iii) Fix N ($N = 2000$) nodes indexing from $1, \dots, N$. Build the complete graph over the first $M = \lceil N^\alpha \rceil$ nodes. Next, randomly select $2(N - M)$ edges from all pairwise edges of nodes $M + 1, \dots, N$. Connect the above two subgraphs by adding one edge.

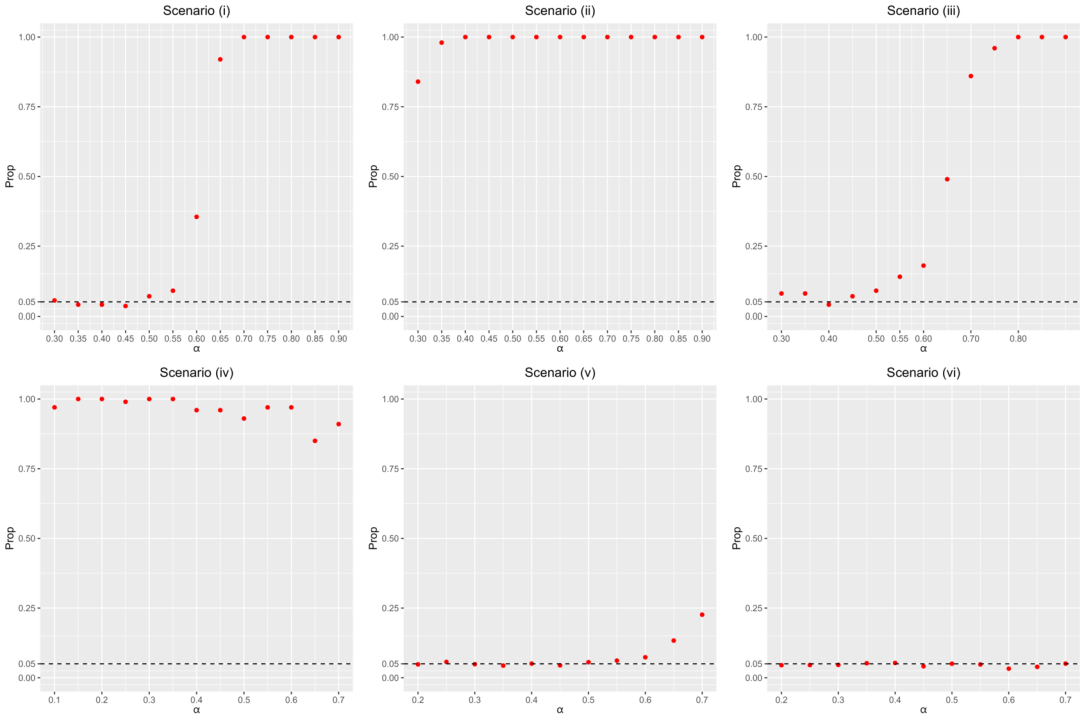


Figure 4. Proportion of rejections from the χ_2^2 distribution under different graph generating rules.

- (iv) Fix N ($N = 1000$) nodes indexing from $1, \dots, N$, and arrange them to be a circle in the sequence of increasing number. Connect the node i to the next $\lceil N^\alpha \rceil$ nodes. Then connect the node 1 to node $2 + \lceil N^\alpha \rceil$.
- (v) Randomly sample N ($N = 2500$) observations from the 2-dimensional standard Gaussian distribution. Build the K -MST on the observations with $K = \lceil N^\alpha \rceil$ and α ranging from 0.2 to 0.7.
- (vi) Randomly sample N ($N = 2500$) observations from the 50-dimensional standard Gaussian distribution. Build the K -MST on the observations with $K = \lceil N^\alpha \rceil$ and α ranging from 0.2 to 0.7.

Under the graph-generating rule (i), the condition $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ holds if $0 < \alpha < 0.75$, the conditions $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$ and $\sum_{i=1}^N \tilde{d}_i^3 = o(V_G \sqrt{|G|})$ hold if $\alpha < 0.5$. The top-left panel in Figure 4 shows that the χ_2^2 distribution approximation starts to be violated at $\alpha = 0.5$, which is consistent with the analytical result. Under the graph-generating rule (ii), the second sufficient condition $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$ does not hold for any $0 < \alpha < 1$, which is consistent with the simulation results. Under the graph-generating rule (iii), the condition $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ holds if $\alpha < 0.5$, the condition $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$ holds with $0 < \alpha < 1$, the condition $\sum_{i=1}^N \tilde{d}_i^3 = o(V_G \sqrt{|G|})$ holds if $0 < \alpha < 0.5$ and the condition $N_{sq} = o(|G|^2)$ holds if $\alpha < 0.5$, which is consistent with the simulation results. Under the graph-generating rule (iv), the condition $\sum_{i=1}^N |\tilde{d}_i|^3 = o(V_G^{1.5})$ does not hold for any $0 < \alpha < 1$, which is also consistent with the simulation results in bottom-left panel.

Under the graph-generating rules (v) and (vi), the K -MST is considered. Remark 3 states that the sufficient conditions in Theorem 1 hold for the K -MST if $K = O(N^\beta)$ with $\beta < 0.5$ under fixed dimensions. We can see that the χ_2^2 approximation works well for $\beta < 0.5$. When $d = 2$, the approximation

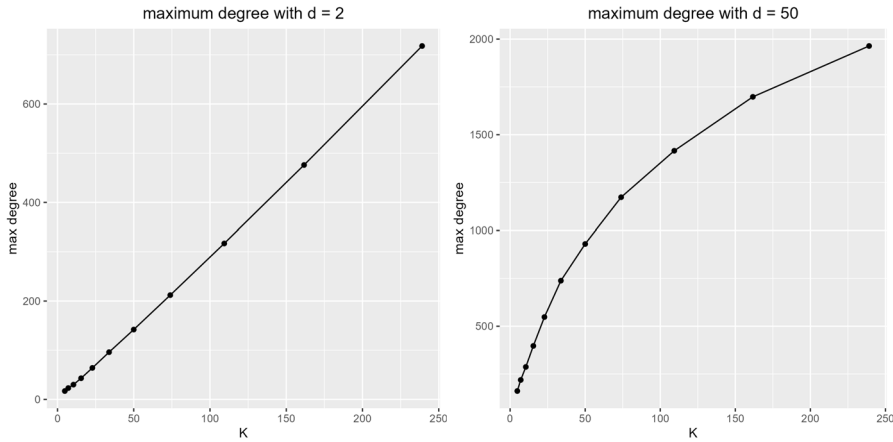


Figure 5. Relationship between the maximum degree of the K -MST and K under both dimensions, $d = 2$ (Scenario (v)) and $d = 50$ (Scenario (vi)).

starts to deviate when α is bigger than 0.55. Interestingly, when the dimension is larger ($d = 50$), the χ^2_2 approximation still works well when α reaches 0.7. One plausible reason is that Remark 3 considers the asymptotics under fixed dimensions, under which the maximum degree of the K -MST is of order K . However, when d is large, the maximum degree of the K -MST is limited to be below the order of K due to the insufficient sample size N . This can be seen from Figure 5 where the maximum degree of K -MST are plotted over K . When $d = 50$, if we approximate the maximum degree by cK^γ , then the estimated value of γ is 0.70. Assume $K = O(N^\beta)$, the conditions in Corollary 6 hold as long as $2\beta\gamma < 1$ that leads to $\beta < 1/(2\gamma) = 0.713$. This result shows that using the χ^2_2 distribution to approximate the distribution of the generalized edge-count statistic on K -MST for data with a relatively large dimension is still a viable option even for K 's larger than the upper bound in Remark 3.

The densities of empirical distributions under these scenarios with specific choices of α 's such that the asymptotic χ^2_2 distribution is violated are plotted in Figure 6. When the asymptotic χ^2_2 distribution is violated, the asymptotic distribution of test statistics under different scenarios can be quite different. However, it seems that the tail probability (on the right) is lighter than the χ^2_2 distribution, which allows us to still use the critical value obtained from the χ^2_2 distribution to control the type I error. Here, the study is through simulations. More systematical investigations will be done in future research.

3.3. Upper bounds of the difference to the limiting distribution

Since Stein's method is used, we could compute the upper bound of the difference between the quantity of interest and the standard normal distribution evaluated by Lipschitz-1 functions for finite samples. Here we focus on Theorem 1. Figure 7 plots this upper bound (to be more specific, the right-hand side of (12) in Section 4) for data in different dimensions and graphs in different densities. We consider three settings: (i) $d = 100$, 5-MST; (ii) $d = 100$, \sqrt{N} -MST; (iii) $d = N$, \sqrt{N} -MST; where data are all generated from the multivariate Gaussian distribution. We see that the upper bound decreases as N increases.

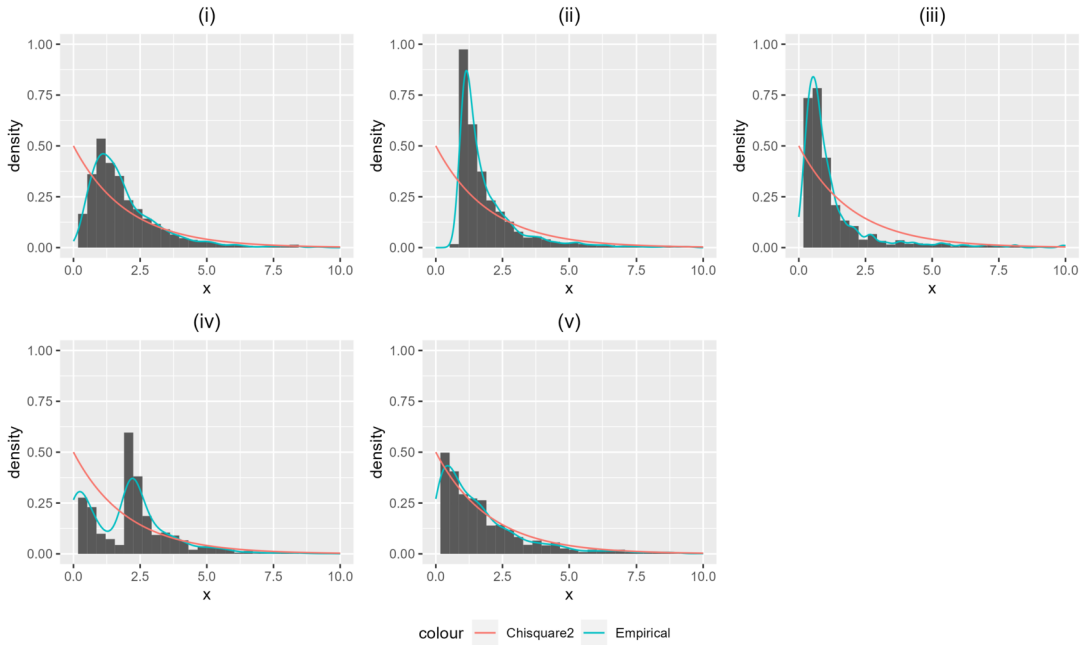


Figure 6. Densities of empirical distributions under scenarios (i) - (v) with specific choices of α 's so that the conditions in Theorem 1 are violated. We set $N = 2000, \alpha = 0.8$ for scenarios (i), (ii), (iii), $N = 1000, \alpha = 0.5$ for scenario (iv), and $N = 2500, \alpha = 0.7$ for scenario (v). The red line is the density of the χ^2_2 distribution.

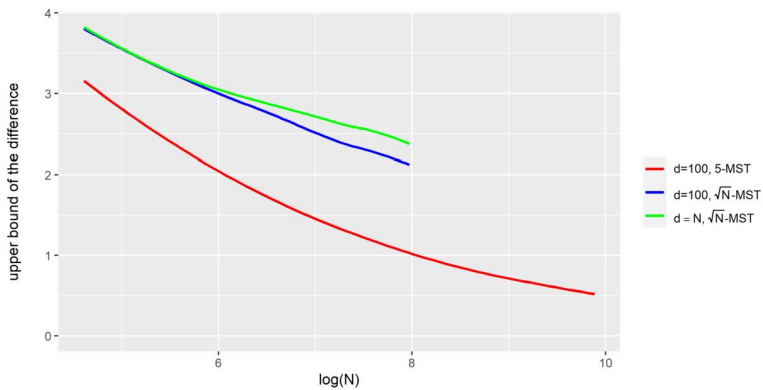


Figure 7. The upper bound under three settings. Each value in the plot takes the average among 100 simulation runs with the setting. The red line is under the setting (i) with N ranging from 100 to 20000. The blue and green lines are under settings (ii) and (iii), respectively, with N only ranging from 100 to 3000 due to their high computation complexity at large N .

3.4. Is a denser graph always more preferable?

Simulation results in Section 1.3 show that GET₅₀ has a large power than GET₅ under multiple scenarios. Here, we study the power of the generalized edge-count test on K -MST in more detail by increasing the order of K continuously from 0 to 0.85. In particular, we set $m = n = 100$ and $K = \lceil N^\beta \rceil$ with β ranging from 0 to 0.85. We consider 8 different scenarios, among which scenarios (i)–(iv) are the same as those in Section 1.3 with a fixed dimension $d = 500$ and scenarios (v)–(ix) are listed below with $\Sigma = (0.5^{|i-j|})_{1 \leq i, j \leq d}$ and $d = 500$. Scenarios (i) and (ii) compare Gaussian distributions with both mean and variance to be different; scenarios (iii) and (iv) compare non-Gaussian distributions with both mean and variance to be different; scenarios (v)–(vii) further compare Gaussian distributions with only mean difference, only scale difference, and only covariance difference, respectively; scenario (viii) compares Gaussian and non-Gaussian distributions; and scenario (ix) compares extremely heavy-tailed distributions with both location and scale to be different.

- (v) $X_1, \dots, X_m \stackrel{iid}{\sim} N(\mathbf{0}_d, \Sigma)$ and $Y_1, \dots, Y_n \stackrel{iid}{\sim} N(0.6/d^{1/3} \mathbf{1}_d, \Sigma)$.
- (vi) $X_1, \dots, X_m \stackrel{iid}{\sim} N(\mathbf{0}_d, \Sigma)$ and $Y_1, \dots, Y_n \stackrel{iid}{\sim} N(\mathbf{0}_d, (1 + 0.17/d^{1/3})^2 \times \Sigma)$.
- (vii) $X_1, \dots, X_m \stackrel{iid}{\sim} N(\mathbf{0}_d, I_d)$ and $Y_1, \dots, Y_n \stackrel{iid}{\sim} N(\mathbf{0}_d, \Sigma_1)$ where $\Sigma_1 = (0.4^{|i-j|})_{1 \leq i, j \leq d}$.
- (viii) $X_1, \dots, X_m \stackrel{iid}{\sim} N(\mathbf{0}_d, I_d)$ and $Y_i = (Y_{i,1}^T, Y_{i,2}^T)^T$ with $Y_{i,1} \sim N(\mathbf{0}_{d/2}, I_{d/2})$, $Y_{i,2} \sim t_{30}(\mathbf{0}_{d/2}, I_{d/2})$, and $i = 1, \dots, n$.
- (ix) $X_1, \dots, X_m \stackrel{iid}{\sim} t_1(\mathbf{0}_d, I_d)$ and $Y_1, \dots, Y_n \stackrel{iid}{\sim} t_1(0.6/d^{1/3} \mathbf{1}_d, (1 + 0.17/d^{1/3})^2 \times \Sigma)$.

For each scenario and each K , we run 1,000 trials and the power is estimated as the proportion of trials that reject the null hypothesis at 0.05 significance level. Figure 8 plots the estimated power. We see that, when β increases from 0 to 0.25, the power of the test increases for all scenarios. However, the optimal value of β varies across different scenarios. For some scenarios, the power increases till β reaches 0.8 and then decreases; while for some scenarios, the power begins to decrease at a much smaller β . Based on the observation, it is in general safe to consider graphs denser than $O(N)$, while the optimal density of the graph needs further investigation. One plausible way could be to choose a few representative K 's to run the test and then use a multiple testing correction technique, such as the Bonferroni correction, or a p -value combining technique, such as the harmonic mean p -value, to draw the conclusion.

3.5. Checking empirical sizes

Theorems in Section 2 provide theoretical guarantees asymptotically. Here, we check empirical sizes for finite samples under a few distributions. Let

$$X_i = \Sigma^{\frac{1}{2}} U_i, i = 1, \dots, m, \quad Y_j = \Sigma^{\frac{1}{2}} V_j, j = 1, \dots, n$$

with $\Sigma = (0.5^{|i-j|})_{1 \leq i, j \leq d}$. Four distributions for U_i 's and V_j 's are considered:

- (i) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} N(\mathbf{0}_d, I_d)$,
- (ii) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} t_5(\mathbf{0}_d, I_d)$,
- (iii) $U_1, \dots, U_m, V_1, \dots, V_n \stackrel{iid}{\sim} \text{Uniform}[-1, 1]^d$,
- (iv) $U_1, \dots, U_m, V_1, \dots, V_n$ are iid with coordinates of $U_i, V_j \stackrel{iid}{\sim} \text{Exp}(1)$.

Here, $M = \binom{N}{2}$ and we use $\lfloor s \rfloor$ to denote the largest integer that is not larger than s . We consider both the equal sizes ($m = n = 100$) and unequal sizes ($m = 50, n = 100$) cases. Table 2 presents the proportion

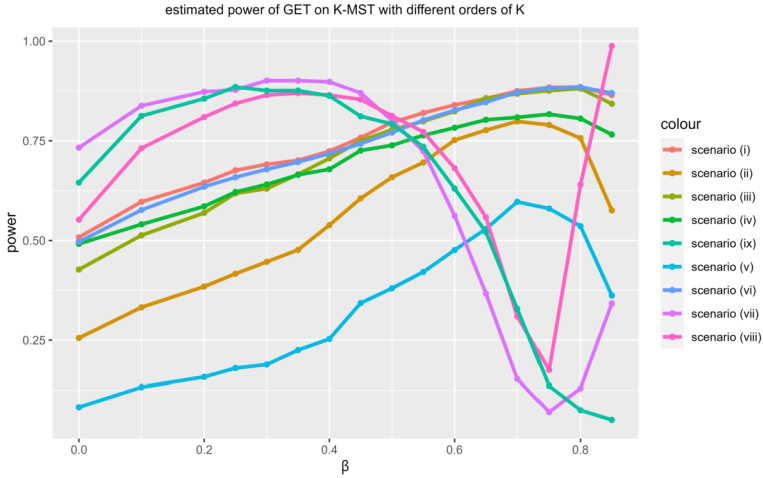


Figure 8. Estimated power at 0.05 significance level of GET on K -MST with $K = \lceil N^\beta \rceil$, $\beta \in [0, 0.85]$.

of trials (out of 1,000) that the generalized edge-count test statistic is greater than the 95% quantile of χ_2^2 under the equal sizes case. We see that the empirical size is quite close to the nominal level for all simulation settings. The results for the generalized edge-count test under the unequal sizes case, the original edge-count test, the weighted edge-count test, and the max-type edge-count test are similar, and are presented in Section S4 of the Supplementary Material (Zhu and Chen, 2024).

Table 2. Empirical size of the generalized edge-count test with $m = n = 100$.

distribution	d \ G	[M ^{0.5}]	[M ^{0.6}]	[M ^{0.7}]	[M ^{0.8}]	[M ^{0.9}]	[M ^{0.95}]	[M ^{0.99}]
		(i) normal	0.5N	0.042	0.046	0.055	0.052	0.046
	N	0.049	0.042	0.052	0.056	0.046	0.042	0.059
	1.5N	0.042	0.047	0.037	0.041	0.045	0.056	0.052
	2N	0.045	0.058	0.049	0.053	0.058	0.051	0.053
(ii) t ₅	0.5N	0.043	0.042	0.055	0.041	0.052	0.054	0.048
	N	0.036	0.04	0.035	0.058	0.055	0.047	0.046
	1.5N	0.034	0.047	0.05	0.06	0.049	0.055	0.047
	2N	0.045	0.044	0.045	0.053	0.039	0.053	0.066
(iii) exp(1)	0.5N	0.046	0.047	0.044	0.059	0.048	0.046	0.051
	N	0.042	0.047	0.053	0.055	0.05	0.047	0.059
	1.5N	0.047	0.049	0.045	0.045	0.055	0.052	0.052
	2N	0.05	0.042	0.051	0.052	0.042	0.052	0.051
(iv) uniform	0.5N	0.049	0.046	0.048	0.056	0.043	0.048	0.053
	N	0.045	0.043	0.042	0.046	0.049	0.047	0.047
	1.5N	0.034	0.056	0.038	0.048	0.048	0.055	0.05
	2N	0.05	0.047	0.048	0.044	0.055	0.049	0.058

4. Proof of Theorem 1

To study the limiting distributions of Z_w^P and Z_{diff}^P jointly, we need to deal with the linear combinations of $\sum_{e \in G} 1_{\{J_e=1\}}$ and $\sum_{e \in G} 1_{\{J_e=2\}}$. It is clear that the items in these summations are dependent. The dependency comes from two sources. One is due to the permutation null distribution – given one node from sample X, the probability of another node coming from sample X is no longer m/N . The other is due to the nature of the graph-based methods that different edges could share one common node. To conquer these two issues, we work under the bootstrap null distribution to remove the dependency caused by the permutation null distribution first, and then link statistics under the bootstrap null distribution and the permutation null distribution together. For the dependency caused by the nature of the graph-based method, we use the following Stein’s method.

Theorem 13 (Chen, Goldstein and Shao (2011) Theorem 4.13). *Let $\{\xi_i, i \in \mathcal{J}\}$ be a random field with mean zero, $W = \sum_{i \in \mathcal{J}} \xi_i$ and $Var(W) = 1$, for each $i \in \mathcal{J}$ there exists $K_i \subset \mathcal{J}$ such that ξ_i and $\xi_{K_i^C}$ are independent, then*

$$\sup_{f \in Lip(1)} |Ef(W) - Ef(Z)| \leq \sqrt{\frac{2}{\pi}} E \left| \sum_{i \in \mathcal{J}} \{\xi_i \eta_i - E(\xi_i \eta_i)\} \right| + \sum_{i \in \mathcal{J}} E \left| \xi_i \eta_i^2 \right|,$$

where $\eta_i = \sum_{j \in K_i} \xi_j$, Z is the standard normal.

The Stein’s method we rely on is different from that used in Chen and Friedman (2017), Chen and Zhang (2015), Chu and Chen (2019). The main difference is that the theorem used in these earlier works considers a second neighbor of the dependency that, for each $i \in \mathcal{J}$, there exists $K_i \subset L_i \subset \mathcal{J}$ such that ξ_i is independent of $\xi_{K_i^C}$ and ξ_{K_i} is independent of $\xi_{L_i^C}$. Then the upper bound involves $\sum_{j \in L_i} \xi_j$ that could easily expand under the graph structure especially when the graph is dense, causing the conditions to be stringent. We here turn to the Stein’s theorem that only considers the first neighbor of dependency and the resulting quantities can be strategically handled to not expand too much to obtain much weaker conditions. One difficulty in using this version of Stein’s method rather than the second-neighbor version is that the summation is inside the absolute value for the first term on the right-hand side, so we need to manipulate the terms carefully to not relax too much; the detailed manipulations are provided in Section S3 of the Supplementary Material (Zhu and Chen, 2024).

The bootstrap null distribution places probability $1/2^N$ on each of the 2^N assignments of N observations to either of the two samples, i.e., each observation is assigned to sample X with probability m/N and to sample Y with probability n/N , independently from any other observations. Let E_B, Var_B, Cov_B be expectation, variance and covariance under the bootstrap null distribution. It is not hard to see that the number of observations assigned to sample X may not be m . Let n_X be this number and $Z_X = (n_X - m)/\sigma^B$ where σ^B is the standard deviation of n_X under the bootstrap null distribution. Notice that the bootstrap null distribution becomes the permutation null distribution conditioning on $n_X = m$. We express (Z_w^P, Z_{diff}^P) in the following way:

$$\begin{pmatrix} Z_w^P \\ Z_{diff}^P \end{pmatrix} = \begin{bmatrix} \sigma_w^B/\sigma_w^P & 0 \\ 0 & \phi_N \end{bmatrix} \begin{pmatrix} Z_w^B \\ \sqrt{T_G} Z_{diff}^B/\sqrt{V_G} \end{pmatrix} + \begin{pmatrix} (\mu_w^B - \mu_w^P)/\sigma_w^P \\ (\mu_{diff}^B - \mu_{diff}^P)/\sigma_{diff}^P \end{pmatrix}, \tag{7}$$

where $Z_w^B = (R_w - \mu_w^B)/\sigma_w^B$, $Z_{diff}^B = (R_{diff} - \mu_{diff}^B)/\sigma_{diff}^B$, $\phi_N = \sqrt{(N - 1)/N}$, $T_G = \sum_{i=1}^N |G_i|^2$ and

$$\mu_w^B = E_B(R_w) = \frac{mnN - m^2 - n^2}{N^2(N - 2)} |G|, \quad \mu_{diff}^B = E_B(R_{diff}) = \frac{m - n}{N} |G|,$$

$$\begin{aligned} \sigma_{\text{diff}}^B &= \sqrt{\text{Var}_B(R_{\text{diff}})} = \sqrt{\frac{mn}{N^2} \sum |G_i|^2}, \quad \sigma_w^B = \sqrt{\text{Var}_B(R_w)} = \sqrt{\frac{m^2 n^2}{N^4} |G| + \frac{mn(m-n)^2}{N^4(N-2)^2} \sum_{i=1}^N |G_i|^2}, \\ \mu_w^P &= \text{E}_P(R_w) = \frac{(n-1)(m-1)}{(N-1)(N-2)} |G|, \quad \mu_{\text{diff}}^P = \text{E}_P(R_{\text{diff}}) = \frac{m-n}{N} |G|, \\ \sigma_{\text{diff}}^P &= \sqrt{\frac{m(m-1)n(n-1)}{N(N-1)(N-2)(N-3)} \left(\frac{m-2}{n-1} + \frac{n-2}{m-1} + 2 \right) \left(\sum |G_i|^2 - \frac{4|G|^2}{N} \right)}, \\ \sigma_w^P &= \sqrt{\frac{m(m-1)n(n-1)}{N(N-1)(N-2)(N-3)} \left(|G| - \frac{2}{N(N-1)} |G|^2 - \frac{1}{N-2} \left(\sum |G_i|^2 - \frac{4|G|^2}{N} \right) \right)}. \end{aligned}$$

Here we deal with Z_w^B and $\sqrt{T_G/V_G} Z_{\text{diff}}^B$ rather than Z_w^B and Z_{diff}^B directly to get rid of the condition $V_G = O(\sum_{i=1}^N |G_i|^2)$ appeared in [Chen and Friedman \(2017\)](#) and [Chu and Chen \(2019\)](#). Since the distribution of $(Z_w^B, \sqrt{T_G/V_G} Z_{\text{diff}}^B)$ under the permutation null distribution is equivalent to the distribution of $(Z_w^B, \sqrt{T_G/V_G} Z_{\text{diff}}^B) | Z_X = 0$ under the bootstrap null distribution, we only need to show the following two statements for proving [Theorem 1](#):

- S.1** $\left(Z_w^B, \sqrt{T_G/V_G} \left(Z_{\text{diff}}^B - \sqrt{1 - V_G/T_G} Z_X \right), Z_X \right)$ is asymptotically multivariate Gaussian distributed under the bootstrap null distribution and the covariance matrix of the limiting distribution is of full rank.
- S.2** $\sigma_w^B/\sigma_w^P \rightarrow c_w; (\mu_w^B - \mu_w^P)/\sigma_w^P \rightarrow 0; (\mu_{\text{diff}}^B - \mu_{\text{diff}}^P)/\sigma_{\text{diff}}^P \rightarrow 0$ where c_w is a positive constant.

From statement **S.1**, the asymptotic distribution of $(Z_w^B, \sqrt{T_G/V_G} (Z_{\text{diff}}^B - \sqrt{1 - V_G/T_G} Z_X))$ conditioning on $Z_X = 0$ is a bivariate Gaussian distribution under the bootstrap null distribution, which further implied that the asymptotic distribution of $(Z_w^B, \sqrt{T_G/V_G} Z_{\text{diff}}^B)$ under the permutation null distribution is a bivariate Gaussian distribution. Then, with statement **S.2**, $\phi_N \rightarrow 1$ and equation (7), we have $(Z_w^P, Z_{\text{diff}}^P)$ asymptotically bivariate Gaussian distributed under the permutation null distribution. Finally, plus the fact that $\text{Var}_P(Z_w^P) = \text{Var}_P(Z_{\text{diff}}^P) = 1$ and $\text{Cov}_P(Z_w^P, Z_{\text{diff}}^P) = 0$, we have that $S \xrightarrow{D} \chi_2^2$.

The statement **S.2** is easy to prove. It is clear that $\mu_{\text{diff}}^B - \mu_{\text{diff}}^P = 0$. It is also not hard to see that, under condition $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$, in the usual limit regime, σ_w^B, σ_w^P are of the same order of $\sqrt{|G|}$ and $(\mu_w^B - \mu_w^P)/\sigma_w^P$ goes to zero as $|G| = o(N^2)$ and $\sum_{i=1}^N |G_i|^2 = o(|G|N)$.

Next we prove the statement **S.1**. Let

$$\begin{aligned} W &= a_1 Z_w^B + a_2 \sqrt{\frac{T_G}{V_G}} \left(Z_{\text{diff}}^B - \sqrt{1 - \frac{V_G}{T_G}} Z_X \right) + a_3 Z_X \\ &= a_1 Z_w^B + a_2 \sqrt{\frac{T_G}{V_G}} Z_{\text{diff}}^B + \left(a_3 - a_2 \sqrt{\frac{T_G}{V_G}} - 1 \right) Z_X. \end{aligned} \tag{8}$$

Firstly we show that, in the usual limit regime,

$$\lim_{N \rightarrow \infty} \text{Var}_B(W) > 0 \text{ when at least one of } a_1, a_2, a_3 \text{ is not zero.} \tag{9}$$

Since g_i 's are independent under the bootstrap null distribution, It is not hard to derive that

$$\text{Cov}_B(R_1, n_X) = 2|G|p^2q, \quad \text{Cov}_B(R_2, n_X) = -2|G|pq^2.$$

Then we have,

$$\begin{aligned} \text{Cov}_B(Z_w^B, Z_{\text{diff}}^B) &= pq \frac{(n-m)}{(N-2)} \frac{\sum_{i=1}^N |G_i|^2}{N\sigma_w^B \sigma_{\text{diff}}^B}, & \text{Cov}_B(Z_w^B, Z_X) &= pq \frac{2(n-m)}{(N-2)} \frac{|G|}{N\sigma_w^B \sigma^B}, \\ \text{Cov}_B(Z_{\text{diff}}^B, Z_X) &= \frac{2pq|G|}{\sigma_{\text{diff}}^B \sigma^B}, & (\sigma^B)^2 &= Npq, \end{aligned}$$

where $p = m/N, q = n/N$.

Then the variance of W under the bootstrap null distribution can be computed as

$$\begin{aligned} \text{Var}_B(W) &= a_1^2 + a_2^2 + a_3^2 + 2a_1 a_2 pq \frac{n-m}{N-2} \sqrt{\frac{T_G}{V_G}} \frac{\sum_{i=1}^N |G_i|^2}{N\sigma_w^B \sigma_{\text{diff}}^B} \\ &\quad + 4pqa_1 \frac{n-m}{N-2} \left(a_3 - a_2 \sqrt{\frac{T_G}{V_G} - 1} \right) \frac{|G|}{N\sigma_w^B \sigma^B}, \\ &= a_1^2 + a_2^2 + a_3^2 + 4a_1 a_3 \sqrt{pq} \frac{n-m}{N-2} \frac{|G|}{N^{1.5} \sigma_w^B} + 2a_1 a_2 pq \frac{n-m}{N-2} \frac{\sqrt{V_G}}{\sigma_w^B N}. \end{aligned} \tag{10}$$

Note that $\sigma_w^B \asymp \sqrt{|G|}$, so

$$\frac{|G|}{N^{1.5} \sigma_w^B} \asymp \frac{\sqrt{|G|}}{N^{1.5}} \rightarrow 0 \text{ and } \frac{\sqrt{V_G}}{\sigma_w^B N} \lesssim \sqrt{\frac{\sum_{i=1}^N |G_i|^2}{|G|N^2}} \rightarrow 0.$$

Thus, we have

$$\lim_{N \rightarrow \infty} \text{Var}_B(W) = a_1^2 + a_2^2 + a_3^2.$$

This implies that the covariance matrix of the joint limiting distribution is of full rank. Then by Cramér-Wold device, statement **S.1** holds if W is asymptotically Gaussian distributed under the bootstrap null distribution for any combinations of a_1, a_2, a_3 such that at least one of them is nonzero.

We reorganized W in the following way

$$\begin{aligned} W &= \frac{a_1 \left(\frac{n-1}{N-2} (R_1 - |G|p^2) + \frac{m-1}{N-2} (R_2 - |G|q^2) \right)}{\sigma_w^B} + a_2 \sqrt{\frac{T_G}{V_G}} \frac{(R_1 - R_2 - |G|p^2 + |G|q^2)}{\sigma_{\text{diff}}^B} \\ &\quad + \left(a_3 - a_2 \sqrt{\frac{T_G}{V_G} - 1} \right) \frac{(n_X - m)}{\sigma^B} \\ &= \sum_{e \in G} \left(\frac{a_1}{\sigma_w^B} \frac{N}{N-2} (I_{\{g_{e^+}=1\}} - p)(I_{\{g_{e^-}=1\}} - p) - \frac{a_1}{\sigma_w^B} \frac{I_{\{J_e=1\}} + I_{\{J_e=2\}} - p^2 - q^2}{N-2} \right) \\ &\quad + \sum_{e \in G} a_2 \sqrt{\frac{T_G}{V_G}} \frac{1}{\sigma_{\text{diff}}^B} \left(I_{\{g_{e^+}=1\}} + I_{\{g_{e^-}=1\}} - 2p \right) + \sum_{i \in N} \left(a_3 - a_2 \sqrt{\frac{T_G}{V_G} - 1} \right) \frac{(I_{\{g_i=1\}} - p)}{\sigma^B}. \end{aligned}$$

Define a function $h : \mathcal{N} \rightarrow \mathbb{R}$ and $h(i) = I_{\{g_i=1\}} - p, i \in \mathcal{N}$. Then,

$$\begin{aligned} (I_{\{g_{e^+}=1\}} - p)(I_{\{g_{e^-}=1\}} - p) &= h(e^+)h(e^-), \\ I_{\{J_e=1\}} + I_{\{J_e=2\}} - p^2 - q^2 &= 2h(e^+)h(e^-) + (p - q)(h(e^+) + h(e^-)), \\ I_{\{g_{e^+}=1\}} + I_{\{g_{e^-}=1\}} - 2p &= h(e^+) + h(e^-). \end{aligned}$$

Thus, W can be expressed as

$$\begin{aligned} W &= \sum_{e \in G} \frac{a_1}{\sigma_w^B} h(e^+)h(e^-) + \left(\frac{a_2}{\sigma_{\text{diff}}^B} \sqrt{\frac{T_G}{V_G}} - \frac{a_1(p - q)}{\sigma_w^B(N - 2)} \right) \sum_{i=1}^N |G_i| h(i) + \sum_{i \in \mathcal{N}} \left(a_3 - a_2 \sqrt{\frac{T_G}{V_G} - 1} \right) \frac{h(i)}{\sigma^B} \\ &= \sum_{e \in G} \frac{a_1}{\sigma_w^B} h(e^+)h(e^-) + \sum_{i=1}^N \left(\frac{a_2}{\sqrt{pqV_G}} \left(|G_i| - \frac{2|G|}{N} \right) - \frac{a_1(p - q)|G_i|}{\sigma_w^B(N - 2)} + \frac{a_3}{\sqrt{pqN}} \right) h(i). \end{aligned}$$

Let $\xi_e = b_0 h(e^+)h(e^-)$ and $\xi_i = b_i h(i)$ with

$$b_0 = \frac{a_1}{\sigma_w^B}, \quad b_i = \frac{a_2}{\sqrt{pqV_G}} \left(|G_i| - \frac{2|G|}{N} \right) - \frac{a_1(p - q)|G_i|}{\sigma_w^B(N - 2)} + \frac{a_3}{\sqrt{pqN}},$$

for $i = 1, \dots, N$. Then

$$W = \sum_{e \in G} \xi_e + \sum_{i \in \mathcal{N}} \xi_i. \tag{11}$$

Plugging in the expressions of σ_w^B , It is not hard to see that

$$|b_0| \lesssim \frac{1}{\sqrt{|G|}}, \quad |b_i| \lesssim \frac{1}{\sqrt{V_G}} \left| |G_i| - \frac{2|G|}{N} \right| + \frac{1}{\sqrt{N}}.$$

Next, we apply the Stein’s method to $\tilde{W} = W/\sqrt{\text{Var}_B(W)}$. Let $\mathcal{J} = G \cup \mathcal{N}$, $K_e = A_e \cup \{e^+, e^-\}$ for each edge $e = (e^+, e^-) \in G$ and $K_i = G_i \cup \{i\}$ for each node $i \in \mathcal{N}$. These K_e ’s and K_i ’s satisfy the assumptions in Theorem 13 under the bootstrap null distribution. Then, we define η_e ’s and η_i ’s as follows:

$$\eta_e = \xi_{e^+} + \xi_{e^-} + \sum_{e \in A_e} \xi_e, \text{ for each edge } e \in G, \text{ and } \eta_i = \xi_i + \sum_{e \in G_i} \xi_e, \text{ for each node } i \in \mathcal{N}.$$

By theorem 13, we have

$$\begin{aligned} \sup_{h \in \text{Lip}(1)} |\mathbb{E}_B h(\tilde{W}) - \mathbb{E}_B h(Z)| &\leq \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{\text{Var}_B(W)}} \mathbb{E}_B \left| \sum_{i \in \mathcal{N}} \{\xi_i \eta_i - \mathbb{E}_B(\xi_i \eta_i)\} + \sum_{e \in \mathcal{G}} \{\xi_e \eta_e - \mathbb{E}_B(\xi_e \eta_e)\} \right| \\ &\quad + \frac{1}{\text{Var}_B^{1.5}(W)} \left(\sum_{i \in \mathcal{N}} \mathbb{E}_B |\xi_i \eta_i^2| + \sum_{e \in G} \mathbb{E}_B |\xi_e \eta_e^2| \right). \end{aligned} \tag{12}$$

Our next goal is to find some conditions under which the RHS² of inequality (12) can go to zero. Since the limit of $\text{Var}_B(W)$ is bounded above zero when a_1, a_2, a_3 are not all zeros, the RHS of inequality (12) goes to zero if the following three terms go to zero:

²RHS: right-hand side; LHS: left-hand side.

$$(A1) \mathbb{E}_B \left| \sum_{i \in N} \{ \xi_i \eta_i - \mathbb{E}_B(\xi_i \eta_i) \} + \sum_{e \in G} \{ \xi_e \eta_e - \mathbb{E}_B(\xi_e \eta_e) \} \right|,$$

$$(A2) \sum_{i \in N} \mathbb{E}_B | \xi_i \eta_i^2 |,$$

$$(A3) \sum_{e \in G} \mathbb{E}_B | \xi_e \eta_e^2 |.$$

For (A1), we have

$$\begin{aligned} & \mathbb{E}_B \left| \sum_{i \in N} \{ \xi_i \eta_i - \mathbb{E}_B(\xi_i \eta_i) \} + \sum_{e \in G} \{ \xi_e \eta_e - \mathbb{E}_B(\xi_e \eta_e) \} \right| \\ & \leq \mathbb{E}_B \left| \sum_{i \in N} \{ \xi_i \eta_i - \mathbb{E}_B(\xi_i \eta_i) \} \right| + \mathbb{E}_B \left| \sum_{e \in G} \{ \xi_e \eta_e - \mathbb{E}_B(\xi_e \eta_e) \} \right| \\ & \leq \sqrt{\sum_{i \in N} \text{Var}_B(\xi_i \eta_i) + \sum_{i,j}^{i \neq j} \text{Cov}_B(\xi_i \eta_i, \xi_j \eta_j)} + \sqrt{\sum_{e \in G} \text{Var}_B(\xi_e \eta_e) + \sum_{e,f}^{e \neq f} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f)} \\ & = \sqrt{\sum_{i \in N} \text{Var}_B(\xi_i \eta_i) + \sum_{i=1}^N \sum_{j \in \text{node}_{G_{i,2}}} \text{Cov}_B(\xi_i \eta_i, \xi_j \eta_j)} \\ & \quad + \sqrt{\sum_{e \in G} \text{Var}_B(\xi_e \eta_e) + \sum_{e \in G} \sum_{f \in C_e \setminus \{e\}} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f)}. \end{aligned}$$

The last equality holds as $\xi_i \eta_i$ and $\{\xi_j \eta_j\}_{j \in \text{node}_{G_{i,2}}}$ are uncorrelated and $\xi_e \eta_e$ and $\{\xi_f \eta_f\}_{f \in C_e}$ are uncorrelated under the bootstrap null distribution. The covariance part of edges is a bit complicated to handle directly, so we decompose it into three parts based on the relationship of e and f :

$$\begin{aligned} \sum_{e \in G} \sum_{f \in C_e \setminus \{e\}} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f) &= \sum_{e \in G} \sum_{f \in A_e \setminus \{e\}} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f) + \sum_{e \in G} \sum_{f \in B_e \setminus A_e} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f) \\ & \quad + \sum_{e \in G} \sum_{f \in C_e \setminus B_e} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f). \end{aligned}$$

By carefully examining these quantities, we can show the following inequalities (13)–(20). Here, we only need to consider the worst case, i.e. b_0 and b_i 's take the largest possible orders, denoted by c_0 and c_i 's, i.e.

$$c_0 = \frac{1}{\sqrt{|G|}}, \text{ and } c_i = \frac{1}{\sqrt{V_G}} \left| |G_i| - \frac{2|G|}{N} \right| + \frac{1}{\sqrt{N}}.$$

The details of obtaining (13)–(20) are provided in Section S3 of the Supplementary Material (Zhu and Chen, 2024).

$$\sum_{i=1}^N \text{Var}_B(\xi_i \eta_i) \lesssim \sum_{i=1}^N c_i^4 + c_0^2 \sum_{i=1}^N c_i^2 |G_i|, \tag{13}$$

$$\sum_{e \in G} \text{Var}_B(\xi_e \eta_e) \lesssim c_0^2 \sum_{i=1}^N c_i^2 |G_i| + c_0^3 \sum_{i=1}^N c_i |G_i| + c_0^4 \sum_{i=1}^N |G_i|^2 \tag{14}$$

$$\sum_{i=1}^N \sum_{j \in \text{node}_{G_{i,2}}} \text{Cov}_B(\xi_i \eta_i, \xi_j \eta_j) \lesssim \sum_{i=1}^N \sum_{j \in \text{node}_{G_i}} (c_0 c_i^2 c_j + c_0^2 c_i c_j) \tag{15}$$

$$+ \left| c_0^2 \sum_{i=1}^N \sum_{j \in \text{node}_{G_{i,2}}} b_i b_j N_{i,j} \right|$$

$$\sum_{e \in G} \sum_{f \in A_e \setminus \{e\}} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f) \lesssim \sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} (c_0^3 c_j + c_0^3 c_k + c_0^3 c_i 1_{\{(j,k) \text{ exists}\}}) \tag{16}$$

$$+ c_0^4 N_{sq} + \left| \sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} c_0^2 b_j b_k \right|$$

$$\sum_{e \in G} \sum_{f \in B_e \setminus A_e} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f) \lesssim c_0^4 N_{sq} \tag{17}$$

$$\sum_{e \in G} \sum_{f \in C_e \setminus B_e} \text{Cov}_B(\xi_e \eta_e, \xi_f \eta_f) = 0, \tag{18}$$

$$\sum_{i=1}^N \mathbb{E}_B[|\xi_i \eta_i^2|] \lesssim \sum_{i=1}^N c_i^3 + c_0^2 \sum_{i=1}^N c_i |G_i|, \tag{19}$$

$$\sum_{e \in G} \mathbb{E}_B[|\xi_e \eta_e^2|] \lesssim |G| c_0^3 + c_0 \sum_{i=1}^N |G_i| c_i^2 + c_0^3 \sum_{i=1}^N |G_i|^2. \tag{20}$$

Based on facts that $c_i \lesssim 1$ for all i 's, (A1), (A2) and (A3) going to zero as long as the following conditions hold.

$$\sum_{i=1}^N c_i^3 \rightarrow 0, \tag{21} \quad \sum_{i=1}^N \sum_{j \in \text{node}_{G_i}} (c_0 c_i^2 c_j + c_0^2 c_i c_j) \rightarrow 0, \tag{26}$$

$$c_0^2 \sum_{i=1}^N c_i |G_i| \rightarrow 0, \tag{22} \quad c_0^2 \sum_{i=1}^N \sum_{j \in \text{node}_{G_{i,2}}} b_i b_j N_{i,j} \rightarrow 0, \tag{27}$$

$$|G| c_0^3 \rightarrow 0, \tag{23}$$

$$c_0 \sum_{i=1}^N |G_i| c_i^2 \rightarrow 0, \tag{24} \quad c_0^2 \sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} b_i b_j \rightarrow 0, \tag{28}$$

$$c_0^3 \sum_{i=1}^N |G_i|^2 \rightarrow 0, \tag{25} \quad c_0^4 (N_{sq} + \sum_{i=1}^N |G_i|^2) \rightarrow 0, \tag{29}$$

$$\sum_{i=1}^N \sum_{j,k \in \text{node}_{G_i}}^{j \neq k} (c_0^3 c_j + c_0^3 c_k + c_0^3 c_i 1_{\{(j,k) \text{ exists}\}}) \rightarrow 0. \tag{30}$$

Next, we show that the conditions in Theorem 1 can ensure (21)–(30).

For condition (21), we have

$$\sum_{i=1}^N c_i^3 = \sum_{i=1}^N \left(\frac{1}{\sqrt{V_G}} \left| |G_i| - \frac{2|G|}{N} \right| + \frac{1}{\sqrt{N}} \right)^3 \lesssim \sum_{i=1}^N \frac{||G_i| - \frac{2|G|}{N}|^3}{V_G^{1.5}} + \frac{1}{\sqrt{N}},$$

so condition (21) holds when $\sum_{i=1}^N |\tilde{d}_i|^3 / V_G^{1.5} \rightarrow 0$.

For condition (22), we have

$$c_0^2 \sum_{i=1}^N c_i |G_i| = c_0^2 \sum_{i=1}^N |G_i| \frac{1}{\sqrt{V_G}} \left| |G_i| - \frac{2|G|}{N} \right| + c_0^2 \frac{1}{\sqrt{N}} \sum_{i=1}^N |G_i|.$$

It is easy to check that the second term has the order of $1/\sqrt{N}$, so it goes to zero as $N \rightarrow \infty$. The first term is dominated by $\max |\tilde{d}_i|/\sqrt{V_G}$, which goes to zero under condition $\sum_{i=1}^N |\tilde{d}_i|^3 / V_G^{1.5} \rightarrow 0$ from Theorem 1 in Hoeffding (1951) with r taking 3. Thus, condition (22) holds when $\sum_{i=1}^N |\tilde{d}_i|^3 / V_G^{1.5} \rightarrow 0$.

Condition (23) holds trivially as $|G|c_0^3 = 1/\sqrt{|G|}$.

For condition (24), we have

$$c_0 \sum_{i=1}^N |G_i| c_i^2 = c_0 \sum_{i=1}^N |G_i| \left(\frac{1}{\sqrt{V_G}} \left| |G_i| - \frac{2|G|}{N} \right| + \frac{1}{\sqrt{N}} \right)^2 \lesssim c_0 \sum_{i=1}^N |G_i| \frac{\left(|G_i| - \frac{2|G|}{N} \right)^2}{V_G} + c_0 \frac{1}{N} \sum_{i=1}^N |G_i|.$$

The second term has the order of $\sqrt{|G|}/N$, so it goes to zero when $|G| = o(N^2)$. The first term can be written as

$$c_0 \sum_{i=1}^N |G_i| \frac{\left(|G_i| - \frac{2|G|}{N} \right)^2}{V_G} = c_0 \frac{\sum_{i=1}^N \left(|G_i| - \frac{2|G|}{N} \right)^3}{V_G} + c_0 \frac{2|G|}{N},$$

so it goes to zero under conditions $\sum_{i=1}^N \tilde{d}_i^3 / (V_G \sqrt{|G|}) \rightarrow 0$ and $|G| = o(N^2)$.

For condition (25), it is directly equivalent to $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$. Note that condition $|G| = o(N^2)$ also holds under condition $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ as $\sum_{i=1}^N |G_i|^2 \geq 4|G|^2/N$.

For condition (26), we have with the fact $c_i \lesssim 1$ for all i 's

$$\begin{aligned} \sum_{i=1}^N \sum_{j \in \text{node}_{G_i}} c_0 c_i^2 c_j &\lesssim \sum_{i=1}^N \sum_{j \in \text{node}_{G_i}} c_0 c_i^2 = c_0 \sum_{i=1}^N |G_i| c_i^2, \\ \sum_{i=1}^N \sum_{j \in \text{node}_{G_i}} c_0^2 c_i c_j &\lesssim \sum_{i=1}^N \sum_{j \in \text{node}_{G_i}} c_0^2 c_i = c_0^2 \sum_{i=1}^N |G_i| c_i, \end{aligned}$$

where both the right-hand sides go to zero from (22) and (24).

For condition (27), we have

$$\begin{aligned} \sum_{i=1}^N \sum_{j \in \text{node}_{G_{i,2}}} b_i b_j N_{ij} &= \sum_{i=1}^N \sum_{j \in \text{node}_{G_{i,2}}} b_i b_j \sum_{k=1}^N 1_{\{k \text{ connects } i, j \text{ simultaneously}\}} \\ &= \sum_{k=1}^N \sum_{i \in \text{node}_{G_k}} \sum_{j \in \text{node}_{G_k} \setminus \{i\}} b_i b_j = \sum_{k=1}^N \sum_{i, j \in \text{node}_{G_k}}^{i \neq j} b_i b_j, \end{aligned}$$

so the left-hand side of condition (27) is equal to the term in condition (28).

For condition (28), we have

$$\begin{aligned} c_0^2 \sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} b_j b_k &\lesssim \left| \frac{1}{|G|V_G} \sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} \left(|G_j| - \frac{2|G|}{N} \right) \left(|G_k| - \frac{2|G|}{N} \right) \right| \\ &\quad + \frac{\sum_{i=1}^N |G_i|^{1.5}}{|G|\sqrt{N}} + \frac{\sum_{i=1}^N |G_i|^2}{|G|N}. \end{aligned}$$

It is not hard to see that the second and the third term would go to zero as $N \rightarrow \infty$ under condition $\sum |G_i|^2 / |G|^{1.5} \rightarrow 0$ as

$$\frac{\sum_{i=1}^N |G_i|^{1.5}}{|G|\sqrt{N}} \lesssim \frac{\sqrt{|G| \sum_{i=1}^N |G_i|^2}}{|G|N}, \quad \frac{\sum_{i=1}^N |G_i|^2}{|G|N} \lesssim \frac{\sum_{i=1}^N |G_i|^2}{|G|^{1.5}} \frac{\sqrt{|G|}}{N}.$$

Thus condition (28) holds if conditions $\sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} \left(|G_j| - \frac{2|G|}{N} \right) \left(|G_k| - \frac{2|G|}{N} \right) = o(|G|V_G)$ and $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ hold.

For condition (29), it directly requires $N_{sq} = o(|G^2|)$ as $c_0^3 \sum_{i=1}^N |G_i|^2 \rightarrow 0$.

For condition (30), we have, by symmetry,

$$\sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} c_0^3 c_j = \sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} c_0^3 c_k.$$

Thus we only need to deal with two components $\sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} c_0^3 c_i 1_{\{(j,k) \text{ exists}\}}$ and $\sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} c_0^3 c_j$. It is not hard to see that they would go to zero under condition $\sum_{i=1}^N |G_i|^2 = o(|G|^{1.5})$ as

$$\begin{aligned} \sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} c_0^3 c_j &\leq c_0^3 \sum_{i=1}^N |G_i| \sum_{j \in \text{node}_{G_i}} c_j \leq c_0^3 \sum_{i=1}^N |G_i| \sqrt{|G_i| \sum_{j \in \text{node}_{G_i}} c_j^2} \lesssim c_0^3 \sum_{i=1}^N |G_i|^{1.5}, \\ \sum_{i=1}^N \sum_{j, k \in \text{node}_{G_i}}^{j \neq k} c_0^3 c_i 1_{\{(j,k) \text{ exists}\}} &\leq c_0^3 \sum_{i=1}^N c_i |G_i|^2 \lesssim c_0^3 \sum_{i=1}^N |G_i|^2. \end{aligned}$$

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Supplementary Material

Supplementary Material to “Limiting distributions of graph-based test statistics” (DOI: [10.3150/23-BEJ1616SUPP](https://doi.org/10.3150/23-BEJ1616SUPP); .pdf). It contains proofs of theorems and technical results, a comparison of the moment method and the locSCB method, and tables of the empirical size of the original, weighted, and max-type edge-count tests.

References

- Beckmann, N.D., Comella, P.H., Cheng, E., Lepow, L., Beckmann, A.G., Tyler, S.R., Mouskas, K., Simons, N.W., Hoffman, G.E., Francoeur, N.J. et al. (2021). Downregulation of exhausted cytotoxic T cells in gene expression networks of multisystem inflammatory syndrome in children. *Nat. Commun.* **12** 1–15.
- Bickel, P.J. (1968). A distribution free version of the Smirnov two sample test in the p -variate case. *Ann. Math. Stat.* **40** 1–23. [MR0256519 https://doi.org/10.1214/aoms/1177697800](https://doi.org/10.1214/aoms/1177697800)
- Biswal, B.B., Mennes, M., Zuo, X.-N., Gohel, S., Kelly, C., Smith, S.M., Beckmann, C.F., Adelstein, J.S., Buckner, R.L., Colcombe, S. et al. (2010). Toward discovery science of human brain function. *Proc. Natl. Acad. Sci.* **107** 4734–4739.
- Bullmore, E. and Sporns, O. (2009). Complex brain networks: Graph theoretical analysis of structural and functional systems. *Nat. Rev. Neurosci.* **10** 186–198. <https://doi.org/10.1038/nrn2575>
- Chen, H., Chen, X. and Su, Y. (2018). A weighted edge-count two-sample test for multivariate and object data. *J. Amer. Statist. Assoc.* **113** 1146–1155. [MR3862346 https://doi.org/10.1080/01621459.2017.1307757](https://doi.org/10.1080/01621459.2017.1307757)
- Chen, H. and Friedman, J.H. (2017). A new graph-based two-sample test for multivariate and object data. *J. Amer. Statist. Assoc.* **112** 397–409. [MR3646580 https://doi.org/10.1080/01621459.2016.1147356](https://doi.org/10.1080/01621459.2016.1147356)
- Chen, L.H.Y., Goldstein, L. and Shao, Q.-M. (2011). *Normal Approximation by Stein’s Method. Probability and Its Applications (New York)*. Heidelberg: Springer. [MR2732624 https://doi.org/10.1007/978-3-642-15007-4](https://doi.org/10.1007/978-3-642-15007-4)
- Chen, H. and Zhang, N.R. (2013). Graph-based tests for two-sample comparisons of categorical data. *Statist. Sinica* **23** 1479–1503. [MR3222245](https://doi.org/10.1007/s11464-013-0479-1)
- Chen, H. and Zhang, N. (2015). Graph-based change-point detection. *Ann. Statist.* **43** 139–176. [MR3285603 https://doi.org/10.1214/14-AOS1269](https://doi.org/10.1214/14-AOS1269)
- Chu, L. and Chen, H. (2019). Asymptotic distribution-free change-point detection for multivariate and non-Euclidean data. *Ann. Statist.* **47** 382–414. [MR3910545 https://doi.org/10.1214/18-AOS1691](https://doi.org/10.1214/18-AOS1691)
- Daniels, H.E. (1944). The relation between measures of correlation in the universe of sample permutations. *Biometrika* **33** 129–135. [MR0010941 https://doi.org/10.2307/2334112](https://doi.org/10.2307/2334112)
- Feigenson, K.A., Gara, M.A., Roché, M.W. and Silverstein, S.M. (2014). Is disorganization a feature of schizophrenia or a modifying influence: Evidence of covariation of perceptual and cognitive organization in a non-patient sample. *Psychiatry Res.* **217** 1–8.
- Friedman, J.H. and Rafsky, L.C. (1979). Multivariate generalizations of the Wald-Wolfowitz and Smirnov two-sample tests. *Ann. Statist.* **7** 697–717. [MR0532236](https://doi.org/10.1214/aos/1177697800)
- Friedman, J.H. and Rafsky, L.C. (1983). Graph-theoretic measures of multivariate association and prediction. *Ann. Statist.* **11** 377–391. [MR0696054](https://doi.org/10.1214/aos/1177697800)
- Gretton, A., Borgwardt, K.M., Rasch, M.J., Schölkopf, B. and Smola, A. (2012). A kernel two-sample test. *J. Mach. Learn. Res.* **13** 723–773. [MR2913716](https://doi.org/10.1214/aos/1177697800)
- Henze, N. (1988). A multivariate two-sample test based on the number of nearest neighbor type coincidences. *Ann. Statist.* **16** 772–783. [MR0947577 https://doi.org/10.1214/aos/1177697800](https://doi.org/10.1214/aos/1177697800)
- Henze, N. and Penrose, M.D. (1999). On the multivariate runs test. *Ann. Statist.* **27** 290–298. [MR1701112 https://doi.org/10.1214/aos/1018031112](https://doi.org/10.1214/aos/1018031112)

- Hoeffding, W. (1951). A combinatorial central limit theorem. *Ann. Math. Stat.* **22** 558–566. [MR0044058 https://doi.org/10.1214/aoms/1177729545](https://doi.org/10.1214/aoms/1177729545)
- Li, H., Aue, A., Paul, D., Peng, J. and Wang, P. (2020). An adaptable generalization of Hotelling's T^2 test in high dimension. *Ann. Statist.* **48** 1815–1847. [MR4124345 https://doi.org/10.1214/19-AOS1869](https://doi.org/10.1214/19-AOS1869)
- Mann, H.B. and Whitney, D.R. (1947). On a test of whether one of two random variables is stochastically larger than the other. *Ann. Math. Stat.* **18** 50–60. [MR0022058 https://doi.org/10.1214/aoms/1177730491](https://doi.org/10.1214/aoms/1177730491)
- Network, C.G.A. et al. (2012). Comprehensive molecular portraits of human breast tumours. *Nature* **490** 61.
- Pham, D.T., Möcks, J. and Sroka, L. (1989). Asymptotic normality of double-indexed linear permutation statistics. *Ann. Inst. Statist. Math.* **41** 415–427. [MR1032590 https://doi.org/10.1007/BF00050659](https://doi.org/10.1007/BF00050659)
- Robins, G. and Salowe, J.S. (1994). On the maximum degree of minimum spanning trees. In *Proceedings of the Tenth Annual Symposium on Computational Geometry* 250–258.
- Rosenbaum, P.R. (2005). An exact distribution-free test comparing two multivariate distributions based on adjacency. *J. R. Stat. Soc. Ser. B. Stat. Methodol.* **67** 515–530. [MR2168202 https://doi.org/10.1111/j.1467-9868.2005.00513.x](https://doi.org/10.1111/j.1467-9868.2005.00513.x)
- Schilling, M.F. (1986). Multivariate two-sample tests based on nearest neighbors. *J. Amer. Statist. Assoc.* **81** 799–806. [MR0860514](https://doi.org/10.1080/01621459.1986.10477059)
- Smirnov, N.V. (1939). On the estimation of the discrepancy between empirical curves of distribution for two independent samples. *Bull. Math. Univ. Moscou* **2** 3–14.
- Wald, A. and Wolfowitz, J. (1940). On a test whether two samples are from the same population. *Ann. Math. Stat.* **11** 147–162. [MR0002083 https://doi.org/10.1214/aoms/1177731909](https://doi.org/10.1214/aoms/1177731909)
- Weiss, L. (1960). Two-sample tests for multivariate distributions. *Ann. Math. Stat.* **31** 159–164. [MR0119305 https://doi.org/10.1214/aoms/1177705995](https://doi.org/10.1214/aoms/1177705995)
- Zhang, J. and Chen, H. (2022). Graph-based two-sample tests for data with repeated observations. *Statist. Sinica* **32** 391–415. [MR4359638 https://doi.org/10.5705/ss.202019.0116](https://doi.org/10.5705/ss.202019.0116)
- Zhang, J.-T., Guo, J., Zhou, B. and Cheng, M.-Y. (2020). A simple two-sample test in high dimensions based on L^2 -norm. *J. Amer. Statist. Assoc.* **115** 1011–1027. [MR4107696 https://doi.org/10.1080/01621459.2019.1604366](https://doi.org/10.1080/01621459.2019.1604366)
- Zhu, Y. and Chen, H. (2024). Supplement to “Limiting distributions of graph-based test statistics on sparse and dense graphs.” <https://doi.org/10.3150/23-BEJ1616SUPP>

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