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Berry–Esseen bounds for generalized U-statistics*

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Abstract

In this paper, we establish optimal Berry–Esseen bounds for the generalized U-statistics. The proof is based on a new Berry–Esseen theorem for exchangeable pair approach by Stein's method under a general linearity condition setting. As applications, an optimal convergence rate of the normal approximation for subgraph counts in Erdoš–Rényi graphs and graphon-random graph is obtained.

Keywords: generalized U-statistics; Stein's method; exchangeable pair approach; Berry-Esseen bound; graphon-generated random graph; Erdös-Rényi model.
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1 Introduction

Let $\mathcal{X}$ and $\mathcal{Y}$ be two measurable spaces. Let $X = (X_1, \dots, X_n) \in \mathcal{X}^n$ and $Y = (Y_{i,j})_{1 \leqslant i<j \leqslant n} \in \mathcal{Y}^{n(n-1)/2}$ be two independent sequences of i.i.d. random variables; moreover, we set $Y_{j,i} = Y_{i,j}$ for $j > i$. For $k \geqslant 1$, let $f : \mathcal{X}^k \times \mathcal{Y}^{k(k-1)/2} \to \mathbb{R}$ be a function and we say f is symmetric if the value of the function $f(x_{i_1}, \dots, x_{i_k}; y_{i_1,i_2}, \dots, y_{i_{k-1},i_k})$ remains unchanged any permutation of indices $1 \leqslant i_1 \neq i_2 \neq \cdots \neq i_k \leqslant n$ where $(x_{i_1}, \dots, x_{i_k}; y_{i_1,i_2}, \dots, y_{i_{k-1},i_k}) \in \mathcal{X}^k \times \mathcal{Y}^{k(k-1)/2}$. In this paper, we consider the generalized U-statistic defined by

$$S_{n,k}(f) = \sum_{\alpha \in \mathcal{I}_{n,k}} f(X_{\alpha(1)}, \dots, X_{\alpha(k)}; Y_{\alpha(1),\alpha(2)}, \dots, Y_{\alpha(k-1),\alpha(k)}), \tag{1.1}$$

where for every $\ell \geqslant 1$ and $n \geqslant \ell$,

$$\mathcal{I}_{n,\ell} = \{\alpha = (\alpha(1), \dots, \alpha(\ell)) : 1 \leqslant \alpha(1) < \cdots < \alpha(\ell) \leqslant n\}. \tag{1.2}$$

We note that every $\alpha \in \mathcal{I}_{n,\ell}$ is an ℓ-fold ordered index.

As a generalization of the classical U-statistic, generalized U-statistics have been widely applied in the random graph theory as a count random variable. Janson and

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Nowicki [13] studied the limiting behavior of $S_{n,k}(f)$ via a projection method. Specifically, the function f can be represented as an orthogonal sum of terms indexed by subgraphs of the complete graph with k vertices. Janson and Nowicki [13] showed that the limiting behavior of $S_{n,k}(f)$ depends on topology of the principle support graphs (see more details in Subsection 2.1) of f. In particular, the random variable $S_{n,k}(f)$ is asymptotically normally distributed if the principle support graphs are all connected. However, the convergence rate is still unknown.

The main purpose of this paper is to establish a Berry–Esseen bound for S_n by using Stein's method. Stein's method is a powerful tool to estimating convergence rates for distributional approximation. Since introduced by [26] in 1972, Stein's method has shown to be a powerful tool to evaluate distributional distances for dependent random variables. One of the most important techniques in Stein's method is the exchangeable pair approach, which is commonly taken in computing the Berry–Esseen bound for both normal and nonnormal approximations. We refer to [27, 21, 6, 23] for more details on Berry–Esseen bound for bounded exchangeable pairs. It is worth mentioning that Shao and Zhang [24] obtained a Berry–Esseen bound for unbounded exchangeable pairs. Note that generalized U-statistics are also functionals of independent random variables. Lachiéze-Rey and Peccati [16] applied a generalized perturbative approach to develop a Berry–Esseen theorem for functionals of independent random variables; however, the Berry–Esseen bound in [16] involves some terms that are complicated to compute. In this paper, we develop a general exchangeable pair approach to obtain a Berry–Esseen bound for generalized U-statistics $S_{n,k}(f)$.

Let W be the random variable of interest, and we say (W, W') is an exchangeable pair if $(W, W') \stackrel{d.}{=} (W', W)$. For normal approximation, it is often to assume the following condition holds:

$$\mathbb{E}\{W - W' | W\} = \lambda(W + R), \tag{1.3}$$

where $\lambda > 0$ and R is a random variable with a small $\mathbb{E}|R|$. The condition (1.3) can be understood as a linear regression condition. Although an exchangeable pair can be easily constructed, it may be not easy to verify the linearity condition (1.3) in some applications.

In this paper, we aim to establish an optimal Berry–Esseen bound for the generalized U-statistics by developing a new Berry–Esseen theorem for exchangeable pair approach by assuming a more general condition than (1.3). More specifically, we replace $W - W'$ in (1.3) by a random variable D that is an antisymmetric function of (X, X'). The new result is given in Section 4. There are several advantages of our result. Firstly, we propose a new condition more general than (1.3) that may be easy to verify. For instance, the condition can be verified by constructing an antisymmetric random variable by the Gibbs sampling method, embedding method, generalized perturbative approach and so on. Secondly, the Berry–Esseen bound often provides an optimal convergence rate for many practical applications.

The rest of this paper is organized as follows. In Section 2, we give the Berry–Esseen bounds for $S_{n,k}(f)$. Applications to subgraph counts in κ-random graphs are given in Section 3. The new Berry–Esseen theorem for exchangeable pair approach under a new setting is established in Section 4. We give the proofs of our main results in Section 5. The proofs of other results are postponed to Section 6.

2 Main results

Let $k \geqslant 1$ be a fixed integer. Let (X, Y), f and $S_{n,k}(f)$ be defined in Section 1. We now apply Hoeffding's decomposition to rewrite $S_{n,k}(f)$ as a sum of uncorrelated random variables. The Hoeffding decomposition was first introduced by Hoeffding [11], and we follow [13] to give a Hoeffding decomposition of $S_{n,k}(f)$. For any $\ell \geqslant 1$, $[\ell] = \{1, \dots, \ell\}$ and $[\ell]_2 = \{(i,j) : 1 \leqslant i < j \leqslant \ell\}$. Let $A \subset [k]$ and let $B \subset [k]_2$, and let $X_A = (X_i)_{i\in A}$ and $Y_B = (Y_{i,j})_{(i,j)\in B}$. Specially, we can simply write $f(X_1, \dots, X_k; Y_{1,2}, \dots, Y_{k-1,k})$ as $f(X_{[k]}; Y_{[k]_2})$. Let $V(B)$ be the set of vertices which appears in B, that is,

$$V(B) = \{i \in [k] : \text{there exists } j \in [k] \text{ such that } (i,j) \in B\}. \tag{2.1}$$

Let $G_{A,B}$ be the graph with vertex set $A \cup V(B)$ and edge set B, and let $v_{A,B}$ be the number of nodes in $G_{A,B}$.

By the Hoeffding decomposition, we have

$$f(X_{[k]}; Y_{[k]_2}) = \sum_{A\subset[k], B\subset[k]_2} f_{A,B}(X_A; Y_B) \quad a.s.$$

where $f_{A,B} : \mathcal{X}^{|A|} \times \mathcal{Y}^{|B|} \to \mathbb{R}$ is defined as

$$\begin{aligned} f_{A,B}(x_A; y_B) = &\sum_{(A',B'): A'\subset A, B'\subset B} (-1)^{|A|+|B|-|A'|-|B'|} \\ &\qquad \times \mathbb{E}\big\{ f(X_1, \dots, X_k; Y_{1,2}, \dots, Y_{k-1,k}) \bigm| X_{A'} = x_{A'}, Y_{B'} = y_{B'} \big\}, \end{aligned} \tag{2.2}$$

where $x_A = (x_i)_{i\in A}$ and $y_B = (y_{i,j})_{(i,j)\in B}$ for $A \subset [k]$ and $B \subset [k]_2$. We remark that if $A = \varnothing$ and $B = \varnothing$, then $f_{\varnothing,\varnothing}(X_\varnothing; Y_\varnothing) = \mathbb{E}\{f(X_{[k]}; Y_{[k]_2})\}$. For $\ell = 0, 1, \dots, k$, let

$$f_{(\ell)}(X_{[k]}; Y_{[k]_2}) = \begin{cases} \mathbb{E}\{f(X_{[k]}; Y_{[k]_2})\} & \text{if } \ell = 0, \\ \displaystyle\sum_{v_{A,B}=\ell} f_{A,B}(X_A; Y_B) & \text{if } 1 \leqslant \ell \leqslant k, \end{cases} \tag{2.3}$$

where $v_{A,B}$ is the number of nodes in $G_{A,B}$. Let $d = \min\{\ell > 0 : f_{(\ell)} \not\equiv 0\}$, and we call d the *principal degree* of f. We say the function $f_{(d)}(\cdot;\cdot)$ is the *principal part* of function f. Moreover, we say the indices (A, B) satisfying that $v_{A,B} = d$ and $f_{A,B} \not\equiv 0$ are the *principal support indices* of f.

The central limit theorems for $S_{n,k}(f)$ is proved in [13]. We remark that if f has the principal degree d, then $\mathrm{Var}(S_{n,k}(f))$ is of order n^{2k-d}, see Lemmas 2 and 3 in [13]. Janson and Nowicki [13] proved that if all graphs in $\mathcal{G}_{f,d}$ are connected, then

$$\frac{S_{n,k}(f) - \mathbb{E}\{S_{n,k}(f)\}}{(\mathrm{Var}(S_{n,k}(f)))^{1/2}} \xrightarrow{d.} N(0,1).$$

Note that if not all principal support graphs are connected, then the limiting distribution of the scaled version of $S_{n,k}$ is nonnormal (see Theorems 2 and 3 in [13]), and we will consider this case in another paper.

Now, assume that f is a symmetric function having principal degree d ($1 \leqslant d \leqslant k$). In this subsection, we give a Berry–Esseen bound for $S_{n,k}(f)$. For $x \in \mathcal{X}$, by (2.3), we have

$$f_{(1)}(x) \coloneqq f_{\{1\},\varnothing}(x) = \mathbb{E}\{f(X_{[k]}; Y_{[k]_2}) \,|\, X_1 = x\} - \mathbb{E}\{f(X_{[k]}; Y_{[k]_2})\}.$$

If $\|f_{(1)}(X_1)\|_2 > 0$, then it follows that $d = 1$. Here and in the sequel, we denote by $\|Z\|_p \coloneqq (\mathbb{E}\,|Z|^p)^{1/p}$ for $p > 0$ and we denote by $\Phi(\cdot)$ the distribution function of $N(0,1)$. Let $\tau \coloneqq \|f(X_{[k]}; Y_{[k]_2}) - \mathbb{E}\, f(X_{[k]}; Y_{[k]_2})\|_4 < \infty$. The following theorem provides the Berry–Esseen bound for $S_{n,k}(f)$ in the case where $\|f_{(1)}(X_1)\|_2 > 0$. Let $\sigma_{(1)} \coloneqq \|f_{(1)}(X_1)\|_2$.

Theorem 2.1. *If $\sigma_{(1)} > 0$, then*

$$\sup_{z\in\mathbb{R}} \left| \mathbb{P}\left[\frac{S_{n,k}(f) - \mathbb{E}\{S_{n,k}(f)\}}{\sqrt{\mathrm{Var}\{S_{n,k}(f)\}}} \leqslant z \right] - \Phi(z) \right| \leqslant \frac{8k\tau^2}{\sqrt{n}\sigma_{(1)}^2}. \tag{2.4}$$

Remark 2.2. We remark that $\mathrm{Var}(S_{n,k}(f)) = O(n^{2k-1})$ as $n \to \infty$. Typically, the right hand side of (2.4) is of order $n^{-1/2}$. Specially, if $f(X_{[k]}, Y_{[k]_2}) = h(X_{[k]})$ almost surely for some symmetric function $h : \mathcal{X}^k \to \mathbb{R}$, then $S_{n,k}$ is the classical U-statistic. In this case, Chen and Shao [8] obtained a Berry–Esseen bound of order $n^{-1/2}$ under the assumption that $\|h(X_{[k]})\|_3 < \infty$.

If $\sigma_{(1)} = 0$, then $d \geqslant 2$, that is, the principal degree of f is at least 2. For any graph G, let $\mathrm{Aut}(G)$ be the collection of automorphisms of G, and let $|\mathrm{Aut}(G)|$ be its cardinality. Let

$$\pi_\ell = \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|} \quad \text{for } d \leqslant \ell \leqslant k, \tag{2.5}$$

and let

$$\Lambda_{k,d} = \pi_d + \frac{1}{\pi_d} \sum_{\ell=d+1}^{k} \pi_\ell + 1. \tag{2.6}$$

Let $\sigma_{A,B} = \sqrt{\mathbb{E} f_{A,B}(X_A; Y_B)^2}$, and let $\mathcal{J}_{f,\ell} = \{(A,B) : A \subset [\ell], B \subset [\ell]_2, \sigma_{A,B} \neq 0, v_{A,B} = \ell\}$. Moreover, let $\mathcal{G}_{f,\ell} = \{G_{A,B} : (A,B) \in \mathcal{J}_{f,\ell}\}$. Let $\sigma_{\min} \coloneqq \min\{\sigma_{A,B} : (A,B) \in \mathcal{J}_{f,d}\}$.

We have the following theorem.

Theorem 2.3. *Assume that f is a symmetric function having principal degree d for some $2 \leqslant d \leqslant k$, and assume further that all graphs in $\mathcal{G}_{f,d}$ are connected. Then, we have*

$$\sup_{z\in\mathbb{R}} \left| \mathbb{P}\left[\frac{(S_{n,k}(f) - \mathbb{E}\{S_{n,k}(f)\})}{\sqrt{\mathrm{Var}\{S_{n,k}(f)\}}} \leqslant z \right] - \Phi(z) \right| \leqslant C n^{-1/2} \frac{k\Lambda_{k,d}\tau^2}{\sigma_{\min}^2},$$

where $C > 0$ is an absolute constant.

If we further assume that the function f does not depend on X, i.e., $f(X;Y) = g(Y)$ almost surely for some symmetric $g : \mathcal{Y}^{k(k-1)/2} \to \mathbb{R}$, we obtain a sharper convergence rate. To give the theorem, we first introduce some more notation. Let $G^{(r)}$ be the graph generated from G by deleting the node r and all the edges connecting to the node r. We say G is *strongly connected* if G is connected and $G^{(r)}$ is either connected or empty for all $r \in V(G)$. The following theorem provides a sharper Berry–Esseen bound than that in Theorem 2.3.

Theorem 2.4. *Assume that $f(X_{[k]}; Y_{[k]_2}) = g(Y_{[k]_2})$ almost surely for some symmetric $g : \mathcal{Y}^{k(k-1)/2} \to \mathbb{R}$. Let τ and $\sigma_{\min}$ be defined in Theorem 2.3. Assume that the conditions in Theorem 2.3 are satisfied and assume further that all graphs in $\mathcal{G}_{f,d}$ are strongly connected. Then,*

$$\sup_{z\in\mathbb{R}} \left| \mathbb{P}\left[\frac{(S_{n,k}(f) - \mathbb{E}\{S_{n,k}(f)\})}{\sqrt{\mathrm{Var}\{S_{n,k}(f)\}}} \leqslant z \right] - \Phi(z) \right| \leqslant C n^{-1} \frac{k\Lambda_{k,d}\tau^2}{\sigma_{\min}^2},$$

where $C > 0$ is an absolute constant.

3 Applications

3.1 Subgraphs counts in random graphs generated from graphons

A symmetric Lebesgue measurable function $\kappa : [0,1]^2 \to [0,1]$ is called a *graphon*, which was firstly introduced by Lovász and Szegedy [18] to represent the graph limit. Given a graphon κ and $n \geqslant 2$, the κ-random graph $\mathbb{G}(n,\kappa)$ can be generated as follows: Let $X = (X_1, \ldots, X_n)$ be a vector of independent random variables uniformly distributed on $[0,1]$. Given X, we generate the graph $\mathbb{G}(n,\kappa)$ by connecting the node pair (i,j) independently with probability $\kappa(X_i, X_j)$. This construction was firstly introduced by Diaconis and Freedman [9], which can be used to study large dense and sparse random graphs and random trees generated from graphons. We refer to [18, 3, 4, 17, 2] for more details. For any simple graph F, let $E(F)$ be the edge set of F, let $V(F)$ be the vertex set of F, and let $v(F) = |V(F)|$ and $e(F) = |E(F)|$.

Subgraph counts are important statistics in estimating graphons. As a special case, when $\kappa \equiv p$ for some $p \in (0,1)$, the κ-random graph model becomes the classical Erdös–Rényi model $\mathrm{ER}(p)$. The study of asymptotic properties of subgraph counts in $\mathrm{ER}(p)$ dates back to [19, 1, 13] for more details. Recently, Krokowski, Reichenbachs and Thäle [15], Röllin [22] and Privault and Serafin [20] applied Stein's method to obtain an optimal Berry–Esseen bound for triangle counts in $\mathrm{ER}(p)$. For subgraph counts in κ-random graph, Kaur and Röllin [14] proved an upper bound of the Kolmogorov distance for multivariate normal approximations for centered subgraph counts with order $n^{-1/(p+2)}$ for some $p > 0$. However, the Berry–Esseen bounds for subgraph counts of κ-random graph is still unknown so far. In this subsection, we apply Theorems 2.3 and 2.4 to prove sharp Berry–Esseen bounds for subgraph counts statistics.

Let $\Xi = (\xi_{i,j})_{1\leqslant i<j\leqslant n}$ be the adjacency matrix of $\mathbb{G}(n,\kappa)$, where for each (i,j), the binary random variable $\xi_{i,j}$ indicates the connection of the graph. Formally, let $Y = (Y_{1,1}, \dots, Y_{n-1,n})$ be a vector of independent uniformly distributed random variables on $[0,1]$ that is also independent of X, and then we can write $\xi_{i,j} = \mathbb{1}(Y_{i,j} \leqslant \kappa(X_i, X_j))$. For any nonrandom simple F with $v(F) = k$, the (injective) subgraph counts and induced subgraph counts in $\mathbb{G}(n,\kappa)$ are defined by

$$\begin{aligned}
T_F^{\mathrm{inj}} &\coloneqq T_F^{\mathrm{inj}}(\mathbb{G}(n,\kappa)) = \sum_{\alpha\in\mathcal{I}_{n,k}} \phi_F^{\mathrm{inj}}(\xi_{\alpha(1),\alpha(2)}, \dots, \xi_{\alpha(k-1),\alpha(k)}),\\
T_F^{\mathrm{ind}} &\coloneqq T_F^{\mathrm{ind}}(\mathbb{G}(n,\kappa)) = \sum_{\alpha\in\mathcal{I}_{n,k}} \phi_F^{\mathrm{ind}}(\xi_{\alpha(1),\alpha(2)}, \dots, \xi_{\alpha(k-1),\alpha(k)}),
\end{aligned}$$

respectively, where for $(u_{1,1}, \dots, u_{k-1,k}) \in \mathbb{R}^{k(k-1)/2}$,

$$\begin{aligned}
\phi_F^{\mathrm{inj}}(u_{1,1}, \dots, u_{k-1,k}) &= \sum_{H:H\cong F} \prod_{(i,j)\in E(H)} u_{i,j},\\
\phi_F^{\mathrm{ind}}(u_{1,2}, \dots, u_{k-1,k}) &= \sum_{H:H\cong F} \prod_{(i,j)\in E(H)} u_{i,j} \prod_{(i,j)\notin E(H)} (1-u_{i,j}).
\end{aligned}$$

Here, the summation $\sum_{H:H\cong F}$ ranges over the subgraphs with $v(F)$ nodes that are isomorphic to F and thus contains $v(F)!/|\operatorname{Aut}(F)|$ terms, where $|\operatorname{Aut}(F)|$ is the number of automorphisms of F. Therefore, we have

$$\|\phi_F^{\mathrm{inj}}(\xi_{1,1}, \dots, \xi_{k-1,k})\|_4 \leqslant \frac{k!}{|\mathrm{Aut}(F)|}, \quad \|\phi_F^{\mathrm{inj}}(\xi_{1,1}, \dots, \xi_{k-1,k})\|_4 \leqslant \frac{k!}{|\mathrm{Aut}(F)|}. \tag{3.1}$$

Moreover, we note that both ϕ_F^{inj} and ϕ_F^{ind} are symmetric. For example, if F is the 2-star, then $k = 3$, $|\operatorname{Aut}(F)| = 2$ and

$$\begin{aligned}
\phi_F^{\mathrm{inj}}(\xi_{1,2}, \xi_{1,3}, \xi_{2,3}) &= \xi_{1,2}\xi_{1,3} + \xi_{1,2}\xi_{2,3} + \xi_{1,3}\xi_{2,3},\\
\phi_F^{\mathrm{ind}}(\xi_{1,2}, \xi_{1,3}, \xi_{2,3}) &= \xi_{1,2}\xi_{1,3}(1-\xi_{2,3}) + \xi_{1,2}\xi_{2,3}(1-\xi_{1,3}) + \xi_{1,3}\xi_{2,3}(1-\xi_{1,2}).
\end{aligned}$$

If F is a triangle, then $|\operatorname{Aut}(F)| = 6$ and

$$\phi_F^{\mathrm{inj}}(\xi_{1,2}, \xi_{1,3}, \xi_{2,3}) = \phi_F^{\mathrm{ind}}(\xi_{1,2}, \xi_{1,3}, \xi_{2,3}) = \xi_{1,2}\xi_{1,3}\xi_{2,3}.$$

Let

$$\begin{aligned}
t_F(\kappa) &= \int_{[0,1]^k} \prod_{(i,j)\in E(F)} \kappa(x_i, x_j) \prod_{i\in V(F)} dx_i,\\
t_F^{\mathrm{ind}}(\kappa) &= \int_{[0,1]^k} \prod_{(i,j)\in E(F)} \kappa(x_i, x_j) \prod_{(i,j)\notin E(F)} (1-\kappa(x_i, x_j)) \prod_{i\in V(F)} dx_i.
\end{aligned}$$

Then, we have

$$\mathbb{E}\{\phi_F^{\mathrm{inj}}(\xi_{1,1},\dots,\xi_{k-1,k})\} = \frac{k!}{|\operatorname{Aut}(F)|}t_F(\kappa),$$
$$\mathbb{E}\{\phi_F^{\mathrm{ind}}(\xi_{1,1},\dots,\xi_{k-1,k})\} = \frac{k!}{|\operatorname{Aut}(F)|}t_F^{\mathrm{ind}}(\kappa).$$

As $\xi_{i,j} = \mathbb{1}(Y_{i,j} \leqslant \kappa(X_i, X_j))$, let

$$f_F^{\mathrm{inj}}(X_{[k]}; Y_{[k]_2}) = \phi_F^{\mathrm{inj}}(\xi_{1,1},\dots,\xi_{k-1,k}),$$

Now, as random variables $(\xi_{i,j})_{1\leqslant i<j\leqslant n}$ are conditionally independent given X, we have

$$\mathbb{E}\{f_F^{\mathrm{inj}}(X_{[k]}; Y_{[k]_2}) \,|\, X\} = \sum_{H\cong F} \prod_{(i,j)\in E(H)} \kappa(X_i, X_j),$$
$$\mathbb{E}\{f_F^{\mathrm{ind}}(X_{[k]}; Y_{[k]_2}) \,|\, X\} = \sum_{H\cong F} \prod_{(i,j)\in E(H)} \kappa(X_i, X_j) \prod_{(i,j)\notin E(H)} (1-\kappa(X_i, X_j)).$$

Let

$$\begin{aligned} f_{(1)}^{\mathrm{inj}}(x) &= \mathbb{E}\{f_F^{\mathrm{inj}}(X_{[k]}; Y_{[k]_2}) \,|\, X_1 = x\} \\ &= \sum_{H\cong F} \mathbb{E}\biggl\{ \prod_{(i,j)\in E(H)} \kappa(X_i, X_j) \biggm| X_1 = x \biggr\}, \end{aligned}$$

and similarly, let

$$\begin{aligned} f_{(1)}^{\mathrm{ind}}(x) &= \mathbb{E}\{f_F^{\mathrm{ind}}(X_{[k]}; Y_{[k]_2}) \,|\, X_1 = x\} \\ &= \sum_{H\cong F} \mathbb{E}\biggl\{ \prod_{(i,j)\in E(H)} \kappa(X_i, X_j) \prod_{(i,j)\notin E(H)} (1-\kappa(X_i, X_j)) \biggm| X_1 = x \biggr\}. \end{aligned}$$

We have the following theorem, which follows from Theorem 2.1 and (3.1) directly.

Theorem 3.1. *Let* $\sigma_{(1)}^{\mathrm{inj}} = \|f_{(1)}^{\mathrm{inj}}(X_1) - \mathbb{E}\{f_{(1)}^{\mathrm{inj}}(X_1)\}\|_2$ *and* $\sigma_{(1)}^{\mathrm{ind}} = \|f_{(1)}^{\mathrm{ind}}(X_1) - \mathbb{E}\{f_{(1)}^{\mathrm{ind}}(X_1)\}\|_2$. *Assume that* $\sigma_{(1)}^{\mathrm{inj}} > 0$*, then*

$$\sup_{z\in\mathbb{R}} \biggl| \mathbb{P}\biggl[\frac{\sqrt{n}}{k\sigma_{(1)}^{\mathrm{inj}}} \binom{n}{k}^{-1} (T_F^{\mathrm{inj}} - \mathbb{E}\{T_F^{\mathrm{inj}}\}) \leqslant z \biggr] - \Phi(z) \biggr| \leqslant 8n^{-1/2} \frac{k(k!)^2}{|\operatorname{Aut}(F)|^2 (\sigma_{(1)}^{\mathrm{inj}})^2}.$$

Moreover, assume that $\sigma_{(1)}^{\mathrm{ind}} > 0$*, then*

$$\sup_{z\in\mathbb{R}} \biggl| \mathbb{P}\biggl[\frac{\sqrt{n}}{k\sigma_{(1)}^{\mathrm{ind}}} \binom{n}{k}^{-1} (T_F^{\mathrm{ind}} - \mathbb{E}\{T_F^{\mathrm{ind}}\}) \leqslant z \biggr] - \Phi(z) \biggr| \leqslant 8n^{-1/2} \frac{k(k!)^2}{|\operatorname{Aut}(F)|^2 (\sigma_{(1)}^{\mathrm{ind}})^2}.$$

If $\kappa \equiv p$ for a fixed number $0 < p < 1$, then the random variables $(\xi_{i,j})_{1\leqslant i<j\leqslant n}$ are i.i.d. and the functions f_F^{inj} and f_F^{ind} do not depend on X. We have the following theorem:

Theorem 3.2. *Let* $\kappa \equiv p$ *for* $0 < p < 1$*. Then*

$$\sup_{z\in\mathbb{R}} \biggl| \mathbb{P}\biggl[\frac{T_F^{\mathrm{inj}} - \mathbb{E}\{T_F^{\mathrm{inj}}\}}{(\operatorname{Var}\{T_F^{\mathrm{inj}}\})^{1/2}} \leqslant z \biggr] - \Phi(z) \biggr| \leqslant Cn^{-1},$$

where $C > 0$ *is a constant depending only on* k *and* p*.*

Remark 3.3. For the L_1 bound, Barbour, Karoński and Ruciński [1] proved the same order of $O(n^{-1})$ in the case that p is a constant. For the Berry–Esseen bound, Privault and Serafin [20] proved a general Berry–Esseen bound for subgraph counts for Erdös–Rényi random graph using a different method. Specially, if p is a constant, then Theorem 3.2 provides the same result as in [20].

For induced subgraph counts, we need to consider some separate cases. Let $s(F)$ and $t(F)$ denote the number of 2-stars and triangles in F, respectively. If any of the following conditions holds, then it has been proven in [13] that $(T_F^{\mathrm{ind}} - \mathbb{E}\{T_F^{\mathrm{ind}}\})/(\mathrm{Var}\{T_F^{\mathrm{ind}}\})^{1/2}$ converges to a standard normal distribution:

(G1) If $e(F) \neq p\binom{v(F)}{2}$;

(G2) if $e(F) = p\binom{v(F)}{2}$, $s(F) \neq 3p^2\binom{v(F)}{3}$;

(G3) if $e(F) = p\binom{v(F)}{2}$, $s(F) = 3p^2\binom{v(F)}{3}$ and $t(F) \neq p^3\binom{v(F)}{3}$.

The following theorem gives the Berry–Esseen bounds for induced subgraph counts.

Theorem 3.4. *Let $\kappa \equiv p$ for $0 < p < 1$. If (G1) or (G3) holds, then*

$$\sup_{z\in\mathbb{R}}\left|\mathbb{P}\left[\frac{T_F^{\mathrm{ind}} - \mathbb{E}\{T_F^{\mathrm{ind}}\}}{(\mathrm{Var}\{T_F^{\mathrm{ind}}\})^{1/2}} \leqslant z\right] - \Phi(z)\right| \leqslant Cn^{-1}, \tag{3.2}$$

where $C > 0$ is a constant depending only on k and p. If (G2) holds, then

$$\sup_{z\in\mathbb{R}}\left|\mathbb{P}\left[\frac{T_F^{\mathrm{ind}} - \mathbb{E}\{T_F^{\mathrm{ind}}\}}{(\mathrm{Var}\{T_F^{\mathrm{ind}}\})^{1/2}} \leqslant z\right] - \Phi(z)\right| \leqslant Cn^{-1/2}, \tag{3.3}$$

where $C > 0$ is a constant depending only on k and p.

4 A new Berry–Esseen bound for exchangeable pair approach

4.1 Berry–Esseen bound

In this section, we establish a new Berry–Esseen theorem for exchangeable pair approach under a new setting. Let $X \in \mathcal{X}$ be a random variable valued on a measurable space and let $W = \phi(X)$ be the random variable of interest where $\phi : \mathcal{X} \to \mathbb{R}$. Assume that $\mathbb{E}\{W\} = 0$ and $\mathbb{E}\{W^2\} = 1$. We propose the following condition:

(A) Let (X, X') be an exchangeable pair and let $F : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be an antisymmetric function. Assume that $D := F(X, X')$ is square integrable and satisfies the following condition:

$$\mathbb{E}\{D|X\} = \lambda(W + R), \tag{4.1}$$

where $\lambda > 0$ is a constant and R is an integrable random variable.

We remark that the operator of antisymmetric functions was firstly mentioned in [12], and the condition (A) was considered by Chatterjee [5], who applied the exchangeable pair approach to prove concentration inequalities.

The following theorem provides a uniform Berry–Esseen bound for exchangeable pair approach under the assumption (A).

Theorem 4.1. *Let (X, X') and D satisfy the condition* (A). *Let $W' = \phi(X')$ and $\Delta = W - W'$. Then,*

$$\sup_{z\in\mathbb{R}}|\mathbb{P}[W \leqslant z] - \Phi(z)| \leqslant \mathbb{E}\left|1 - \frac{1}{2\lambda}\mathbb{E}\{D\Delta \,|\, W\}\right| + \frac{1}{\lambda}\mathbb{E}\big|\mathbb{E}\{D^*\Delta \,|\, W\}\big| + \mathbb{E}|R|, \tag{4.2}$$

provided that $D^* := F^*(X, X')$ is a square integrable random variable satisfying that $D^* \geqslant |D|$, where F^* is a symmetric function.

Remark 4.2. Assume that (1.3) is satisfied. Then, we can choose $D = \Delta = W - W'$, and the right hand side of (4.2) reduces to

$$\mathbb{E}\left|1 - \frac{1}{2\lambda}\,\mathbb{E}\{\Delta^2 \,|\, W\}\right| + \frac{1}{\lambda}\,\mathbb{E}\big|\mathbb{E}\{\Delta^*\Delta|W\}\big| + \mathbb{E}\,|R|,$$

where $\Delta^* \coloneqq \Delta^*(W, W')$ is a symmetric function for W and W' satisfying that $\Delta^* \geqslant |\Delta|$ and Δ^* is square integrable. Thus, Theorem 4.1 recovers to Theorem 2.1 in [24].

The following corollary is useful for random variables that can be decomposed as a sum of W and a remainder term. Specifically, let $T \coloneqq T(X)$ be a random variable such that $T = W + U$, where $W = \phi(X)$ is as defined at the beginning of this section, and $U \coloneqq U(X)$ is a square integrable random variable which is usually taken as a remainder term. The following corollary gives a Berry–Esseen bound for T.

Corollary 4.3. *Let $(X, X') \in \mathcal{X} \times \mathcal{X}$ be an exchangeable pair and let $D \coloneqq F(X, X')$ where $F : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is antisymmetric. Assume that D is square integrable and*

$$\mathbb{E}\{D \,|\, X\} = \lambda(W + R) \tag{4.3}$$

for some $\lambda > 0$ and some integrable random variable R. Let $U' \coloneqq U(X')$ and $\Delta = \phi(X) - \phi(X')$. Then, we have

$$\begin{aligned}\sup_{z\in\mathbb{R}}\big|\mathbb{P}[T \leqslant z] - \Phi(z)\big| \leqslant \mathbb{E}&\left|1 - \frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \,|\, X\}\right| \\ &+ \frac{1}{\lambda}\,\mathbb{E}\big|\mathbb{E}\{D^*\Delta \,|\, X\}\big| + \frac{3}{2\lambda}\,\mathbb{E}|D(U - U')| + \mathbb{E}\,|R| + \mathbb{E}\,|U|,\end{aligned}$$

provided that $D^* \coloneqq D^*(X, X')$ is any symmetric function of X and X' satisfying that $D^* \geqslant |D|$ and D^* is square integrable.

Remark 4.4. Assume that $X = (X_1, \dots, X_n)$ is a family of independent random variables. Let $W = \sum_{i=1}^n \xi_i$ be a linear statistic, where $\xi_i = h_i(X_i)$ and h_i is a nonrandom function, such that $\mathbb{E}\,\xi_i = 0$ and $\sum_{i=1}^n \mathbb{E}\,\xi_i^2 = 1$, and let $U = U(X_1, \dots, X_n) \in \mathbb{R}$ be a square integrable random variable. Let $T = W + U$, $\beta_2 = \sum_{i=1}^n \mathbb{E}\{|\xi_i|^2 \mathbb{1}(|\xi_i| > 1)\}$ and $\beta_3 = \sum_{i=1}^n \mathbb{E}\{|\xi_i|^3 \mathbb{1}(|\xi_i| \leqslant 1)\}$. Chen and Shao [8] (see also [25]) proved the following result:

$$\sup_{z\in\mathbb{R}}|\mathbb{P}[T \leqslant z] - \Phi(z)| \leqslant 17(\beta_2 + \beta_3) + 5\,\mathbb{E}\,|U| + 2\sum_{i=1}^n \mathbb{E}|\xi_i(U - U^{(i)})|, \tag{4.4}$$

where $U^{(i)}$ is any random variable independent of ξ_i.

The Berry–Esseen bound in Corollary 4.3 improves Chen and Shao [8]'s result in the sense that the random variable W in our result is not necessarily a partial sum of independent random variables, and our result in Corollary 4.3 can be applied to a general class of random variables.

4.2 Proof of Theorem 4.1

In this subsection, we prove Theorem 4.1 by Stein's method. The proof is similar to that of Theorem 2.1 in [24]. To begin with, we need to prove the following lemma, which is useful in the proof of Theorem 4.1.

Lemma 4.5. *Assume that* (4.1) *is satisfied. Let ψ be a nondecreasing and bounded function. Then,*

$$\frac{1}{2\lambda}\left|\mathbb{E}\left\{D\int_{-\Delta}^{0}\big(\psi(W + u) - \psi(W)\big)\,du\right\}\right| \leqslant \frac{1}{2\lambda}\,\mathbb{E}\big\{D^*\Delta\psi(W)\big\},$$

where D^* is as defined in Theorem 4.1.

Proof of Lemma 4.5. Since $\psi(\cdot)$ is nondecreasing, it follows that

$$\Delta\big(\psi(W) - \psi(W')\big) \geqslant 0$$

and

$$\begin{aligned} 0 &\geqslant \int_{-\Delta}^{0} \big(\psi(W+u) - \psi(W)\big)\, du \\ &\geqslant -\Delta\big(\psi(W) - \psi(W')\big), \end{aligned}$$

which yields

$$\begin{aligned} -\mathbb{E}\big\{D\mathbb{1}(D>0)\Delta\big(\psi(W) - \psi(W')\big)\big\} &\leqslant \mathbb{E}\bigg\{D\int_{-\Delta}^{0} \big(\psi(W+u) - \psi(W)\big)\, du\bigg\} \\ &\leqslant -\mathbb{E}\big\{D\mathbb{1}(D<0)\Delta\big(\psi(W) - \psi(W')\big)\big\}. \end{aligned}$$

Recalling that $W = \phi(X)$, $W' = \phi(X')$, $D = F(X, X')$ is antisymmetric and $D^* = F^*(X, X')$ is symmetric, as (X, X') is exchangeable, we have

$$\mathbb{E}\big\{D\mathbb{1}(D>0)\Delta\big\{\psi(W) - \psi(W')\big\}\big\} = -\mathbb{E}\big\{D\mathbb{1}(D<0)\Delta\big(\psi(W) - \psi(W')\big)\big\},$$

and

$$\mathbb{E}\big\{D^*\mathbb{1}(D>0)\Delta\psi(W)\big\} = -\mathbb{E}\big\{D^*\mathbb{1}(D<0)\Delta f(W')\big\}.$$

Moreover, as $\mathbb{E}\big\{D^*\Delta\mathbb{1}(D=0)\big(\psi(W) - \psi(W')\big)\big\} \geqslant 0$ and $\mathbb{E}\big\{D^*\mathbb{1}(D=0)\Delta\psi(W)\big\} = -\mathbb{E}\big\{D^*\mathbb{1}(D=0)\Delta\psi(W')\big\}$, it follows that

$$\mathbb{E}\{D^*\Delta\mathbb{1}(D=0)\psi(W)\} \geqslant 0.$$

Therefore,

$$\begin{aligned} &\frac{1}{2\lambda}\bigg|\mathbb{E}\bigg\{D\int_{-\Delta}^{0} \big\{\psi(W+u) - \psi(W)\big\}\, du\bigg\}\bigg| \\ &\quad\leqslant -\frac{1}{2\lambda}\,\mathbb{E}\big\{D\mathbb{1}(D<0)\Delta\big(\psi(W) - \psi(W')\big)\big\} \\ &\quad\leqslant \frac{1}{2\lambda}\,\mathbb{E}\big\{D^*\mathbb{1}(D<0)\Delta\big(\psi(W) - \psi(W')\big)\big\} \\ &\quad= \frac{1}{2\lambda}\,\mathbb{E}\big\{D^*\Delta\big(\mathbb{1}(D>0) + \mathbb{1}(D<0)\big)\psi(W)\big\} \\ &\quad\leqslant \frac{1}{2\lambda}\,\mathbb{E}\{D^*\Delta\psi(W)\}. \end{aligned}$$

□

Proof of Theorem 4.1. We apply some ideas of Theorem 2.1 in [24] to prove the desired result. Let $z \in \mathbb{R}$ be a fixed real number, and ψ_z the unique bounded solution to the Stein equation:

$$\psi'(w) - w\psi(w) = \mathbb{1}(w \leqslant z) - \Phi(z), \tag{4.5}$$

where $\Phi(\cdot)$ is the distribution function of the standard normal distribution. It is well known that (see, e.g., Lemma 2.2 in [7])

$$\psi_z(w) = \begin{cases} \sqrt{2\pi}e^{w^2/2}\Phi(w)\big\{1 - \Phi(z)\big\} & \text{if } w \leqslant z, \\ \sqrt{2\pi}e^{w^2/2}\Phi(z)\big\{1 - \Phi(w)\big\} & \text{otherwise,} \end{cases} \tag{4.6}$$

Since $\mathbb{E}\{D|W\} = \lambda(W+R)$, and $D = F(X,X')$ is antisymmetric, it follows that

$$\begin{aligned}0 &= \mathbb{E}\big\{D\big(\psi_z(W) + \psi_z(W')\big)\big\}\\ &= 2\,\mathbb{E}\{D\psi_z(W)\} - \mathbb{E}\big\{D\big(\psi_z(W) - \psi_z(W')\big)\big\}\\ &= 2\lambda\,\mathbb{E}\{(W+R)\psi_z(W)\} - \mathbb{E}\left\{D\int_{-\Delta}^{0}\psi_z'(W+u)\,du\right\}.\end{aligned}$$

Rearranging the foregoing equality, we have

$$\mathbb{E}\{W\psi_z(W)\} = \frac{1}{2\lambda}\,\mathbb{E}\left\{D\int_{-\Delta}^{0}\psi_z'(W+u)\,du\right\} - \mathbb{E}\{R\psi_z(W)\}. \tag{4.7}$$

By (4.5) and (4.7),

$$\begin{aligned}\mathbb{P}(W\leqslant z) - \Phi(z) &= \mathbb{E}\big\{\psi_z'(W) - W\psi_z(W)\big\}\\ &= J_1 - J_2 + J_3,\end{aligned} \tag{4.8}$$

where

$$\begin{aligned}J_1 &= \mathbb{E}\left\{\psi_z'(W)\left(1 - \frac{1}{2\lambda}\,\mathbb{E}\left\{D\Delta\,|\,W\right\}\right)\right\},\\ J_2 &= \frac{1}{2\lambda}\,\mathbb{E}\left\{D\int_{-\Delta}^{0}\left(\psi_z'(W+u) - \psi_z'(W)\right)du\right\},\\ J_3 &= \mathbb{E}\big\{R\psi_z(W)\big\}.\end{aligned}$$

We now bound J_1, J_2 and J_3, separately. By [7, Lemma 2.3], we have

$$\sup_{w\in\mathbb{R}}|\psi_z(w)| \leqslant 1, \quad \sup_{w\in\mathbb{R}}|\psi_z'(w)| \leqslant 1, \quad \sup_{w\in\mathbb{R}}\big|w\psi_z(w)\big| \leqslant 1. \tag{4.9}$$

Therefore,

$$\begin{aligned}|J_1| &\leqslant \mathbb{E}\left|1 - \frac{1}{2\lambda}\,\mathbb{E}\left\{D\Delta\,|\,W\right\}\right|,\\ |J_3| &\leqslant \mathbb{E}\,|R|.\end{aligned} \tag{4.10}$$

Now we consider J_2. Rearranging (4.5) yields $\psi_z'(w) = w\psi_z(w) - \mathbb{1}(w > z) + \big\{1 - \Phi(z)\big\}$. Note that both $w\psi_z(w)$ and $\mathbb{1}(w > z)$ are nondecreasing and bounded functions (see, e.g. [7, Lemma 2.3]), by Lemma 4.5,

$$\begin{aligned}|J_2| &\leqslant \frac{1}{2\lambda}\left|\mathbb{E}\left\{D\int_{-\Delta}^{0}\left\{(W+u)\psi_z(W+u) - W\psi_z(W)\right\}du\right\}\right|\\ &\quad + \frac{1}{2\lambda}\left|\mathbb{E}\left\{D\int_{-\Delta}^{0}\left\{\mathbb{1}(W+u>z) - \mathbb{1}(W>z)\right\}du\right\}\right|\\ &\leqslant \frac{1}{2\lambda}\,\mathbb{E}\big\{\big|\mathbb{E}\left\{D^*\Delta\,|\,W\right\}\big|\big(|W\psi_z(W)| + \mathbb{1}(W>z)\big)\big\}\\ &\leqslant J_{21} + J_{22},\end{aligned} \tag{4.11}$$

where

$$\begin{aligned}J_{21} &= \frac{1}{2\lambda}\,\mathbb{E}\Big\{\big|\mathbb{E}\left\{D^*\Delta\,|\,W\right\}\big|\cdot\big|W\psi_z(W)\big|\Big\},\\ J_{22} &= \frac{1}{2\lambda}\,\mathbb{E}\Big\{\big|\mathbb{E}\left\{D^*\Delta\,|\,W\right\}\big|\mathbb{1}(W>z)\Big\}.\end{aligned}$$

Then, by (4.9), $|J_2| \leqslant \frac{1}{\lambda}\,\mathbb{E}\big|\mathbb{E}\left\{D^*\Delta\,|\,W\right\}\big|$. This proves Theorem 4.1 together with (4.10). $\square$

4.3 Proof of Corollary 4.3

In this subsection, we apply Theorem 4.1 to prove Corollary 4.3. By (4.3), we have

$$\mathbb{E}\{D \mid X\} = \lambda(T - U + R).$$

Let $T' = \phi(X') + U(X')$, then we have (T, T') is exchangeable. Let

$$\mathcal{D}^* = \{D^* := F^*(X, X') : D^* \geqslant |D| \text{ and } F^* : \mathcal{X} \times \mathcal{X} \to \mathbb{R} \text{ is a symmetric function}\}.$$

By Theorem 4.1, we have

$$\begin{aligned}
&\sup_{z\in\mathbb{R}}\bigl|\mathbb{P}[T \leqslant z] - \Phi(z)\bigr| \\
&\quad\leqslant \mathbb{E}\Bigl|1 - \frac{1}{2\lambda}\,\mathbb{E}\{D(T - T') \,|\, T\}\Bigr| + \inf_{D^*\in\mathcal{D}^*} \frac{1}{\lambda}\,\mathbb{E}\bigl|\mathbb{E}\{D^*(T - T') \,|\, T\}\bigr| + \mathbb{E}\,|U| + \mathbb{E}\,|R| \\
&\quad\leqslant \mathbb{E}\Bigl|1 - \frac{1}{2\lambda}\,\mathbb{E}\{D(T - T') \,|\, X\}\Bigr| \\
&\qquad + \inf_{D^*\in\mathcal{D}^*} \frac{1}{\lambda}\,\mathbb{E}\bigl|\mathbb{E}\{D^*(T - T') \,|\, X\}\bigr| + \mathbb{E}\,|U| + \mathbb{E}\,|R| \\
&\quad\leqslant \mathbb{E}\Bigl|1 - \frac{1}{2\lambda}\,\mathbb{E}\{D(\phi(X) - \phi(X')) \,|\, X\}\Bigr| \\
&\qquad + \inf_{D^*\in\mathcal{D}^*} \frac{1}{\lambda}\,\mathbb{E}\bigl|\mathbb{E}\{D^*(\phi(X) - \phi(X')) \,|\, X\}\bigr| + \mathbb{E}\,|U| + \mathbb{E}\,|R| + \frac{1}{2\lambda}\,\mathbb{E}\,|D(U - U')| \\
&\qquad + \inf_{D^*\in\mathcal{D}^*} \frac{1}{\lambda}\,\mathbb{E}|D^*(U - U')|,
\end{aligned} \tag{4.12}$$

where the second inequality follows from that fact that T is $\sigma(X)$-measurable and Jenson's inequality. Choosing $D^* = |D|$ in the last term of the right hand side of (4.12) and recalling that $\Delta = \phi(X) - \phi(X')$, we complete the proof.

5 Proofs of Theorems 2.1, 2.3 and 2.4

In this section, we give the proofs of Theorems 2.1, 2.3 and 2.4. To simplify our statements, we assume that $\mathbb{E}\{f(X_{[k]}; Y_{[k]_2})\} = 0$ throughout this section without loss of generality. We denote by C an absolute constant that may take different values in different places.

5.1 Proof of Theorem 2.1

Without loss of generality, we assume that $n \geqslant \max(2, k^2)$, otherwise the inequality is trivial. We use Corollary 4.3 to prove this theorem. Recall that

$$f_{(1)}(x) = \mathbb{E}\{f(X_{[k]}; Y_{[k]_2}) \,|\, X_1 = x\}.$$

For each $\alpha = (\alpha(1), \dots, \alpha(k)) \in \mathcal{I}_{n,k}$, let

$$\begin{aligned}
&r(X_{\alpha(1)}, \dots, X_{\alpha(k)}; Y_{\alpha(1),\alpha(2)}, \dots, Y_{\alpha(k-1),\alpha(k)}) \\
&\quad = f(X_{\alpha(1)}, \dots, X_{\alpha(k)}; Y_{\alpha(1),\alpha(2)}, \dots, Y_{\alpha(k-1),\alpha(k)}) - \sum_{j=1}^{k} f_{(1)}(X_{\alpha(j)}).
\end{aligned} \tag{5.1}$$

Let $\widetilde{\sigma}_n = \sqrt{\mathrm{Var}\{S_{n,k}(f)\}}$, and

$$T = \frac{1}{\widetilde{\sigma}_n} S_{n,k}(f).$$

Then, it follows from (5.1) that T has the following decomposition

$$T = W + U,$$

where

$$\begin{aligned} W &= \frac{1}{\widetilde{\sigma}_n} \binom{n-1}{k-1} \sum_{i=1}^{n} f_{(1)}(X_i), \\ U &= \frac{1}{\widetilde{\sigma}_n} \sum_{\alpha \in \mathcal{I}_{n,k}} r\big(X_{\alpha(1)}, \dots, X_{\alpha(k)}; Y_{\alpha(1),\alpha(2)}, \dots, Y_{\alpha(k-1),\alpha(k)}\big). \end{aligned}$$

By orthogonality we have $\operatorname{Cov}(W, U) = 0$, and thus

$$\widetilde{\sigma}_n^2 \geqslant \operatorname{Var}\bigg(\binom{n-1}{k-1} \sum_{i=1}^{n} f_{(1)}(X_i) \bigg) = \binom{n-1}{k-1}^2 \operatorname{Var}\bigg(\sum_{j=1}^{n} f_{(1)}(X_j) \bigg) = \binom{n}{k}^2 \frac{k^2 \sigma_{(1)}^2}{n}. \tag{5.2}$$

Let $X' = (X_1', \dots, X_n')$ be an independent copy of $(X_1, \dots, X_n)$. For each $i = 1, \dots, n$, define $X^{(i)} = (X_1^{(i)}, \dots, X_n^{(i)})$ where

$$X_j^{(i)} = \begin{cases} X_j & \text{if } j \neq i, \\ X_i' & \text{if } j = i, \end{cases}$$

and let

$$U^{(i)} = \frac{1}{\widetilde{\sigma}_n} \sum_{\alpha \in \mathcal{I}_{n,k}} r\big(X_{\alpha(1)}^{(i)}, \dots, X_{\alpha(k)}^{(i)}; Y_{\alpha(1),\alpha(2)}, \dots, Y_{\alpha(k-1),\alpha(k)}\big).$$

Recall that $\tau \coloneqq \|f(X_{[k]}; Y_{[k]_2})\|_4 < \infty$. The following lemma provides the upper bounds of $\mathbb{E}\{U_1^2\}$ and $\mathbb{E}\{(U_1 - U_1^{(i)})^2\}$.

Lemma 5.1. *For $n \geqslant k^2$ and $k \geqslant 2$,*

$$\mathbb{E}\{U^2\} \leqslant \frac{(k-1)^2 \tau^2}{2(n-1)\sigma_{(1)}^2} \tag{5.3}$$

$$\mathbb{E}\{(U - U^{(i)})^2\} \leqslant \frac{2(k-1)^2 \tau^2}{n(n-1)\sigma_{(1)}^2}. \tag{5.4}$$

The proof of Lemma 5.1 is put in the appendix.

Now, we apply Corollary 4.3 to prove the Berry–Esseen bound for T. Let I be a random index uniformly distributed over $\{1, \dots, n\}$, which is independent of all others. Then, $((X, Y), (X^{(I)}, Y))$ is an exchangeable pair. Let

$$D = \Delta = \frac{1}{\widetilde{\sigma}_n} \binom{n-1}{k-1} \big(f_{(1)}(X_I) - f_{(1)}(X_I') \big).$$

and recall that X and Y are independent, then it follows that

$$\mathbb{E}\{D \,|\, X, Y\} = \frac{1}{n} W.$$

Thus, (4.3) is satisfied with $\lambda = 1/n$ and $R = 0$. Moreover, we have

$$\begin{aligned} \frac{1}{2\lambda} \mathbb{E}\{D\Delta \,|\, X, X', Y\} &= \frac{1}{2\widetilde{\sigma}_n^2} \binom{n-1}{k-1}^2 \sum_{i=1}^{n} \big(f_{(1)}(X_i) - f_{(1)}(X_i') \big)^2, \\ \frac{1}{\lambda} \mathbb{E}\{|D|\Delta \,|\, X, X', Y\} &= \frac{1}{\widetilde{\sigma}_n^2} \binom{n-1}{k-1}^2 \sum_{i=1}^{n} \big(f_{(1)}(X_i) - f_{(1)}(X_i') \big) \big| f_{(1)}(X_i) - f_{(1)}(X_i') \big|. \end{aligned}$$

Also,

$$\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta\} = \mathbb{E}\{W^2\} = 1 - \mathbb{E}\{U^2\}, \quad \mathbb{E}\{|D|\Delta\} = 0.$$

Recall that $\tau = \|f(X_{[k]}; Y_{[k]_2})\|_4$. Note that

$$\frac{k-1}{n-1} \leqslant \frac{2}{\sqrt{n}} \quad \text{for } n \geqslant \max(2, k^2). \tag{5.5}$$

By the Cauchy inequality and Lemma 5.1, we have for $n \geqslant \max(2, k^2)$,

$$\begin{aligned}
&\mathbb{E}\bigg|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \,|\, X, X', Y\} - 1\bigg| \\
&\quad \leqslant \mathbb{E}\bigg|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \,|\, X, X', Y\} - \frac{1}{2\lambda}\,\mathbb{E}\{D\Delta\}\bigg| + \mathbb{E}\{U^2\} \\
&\quad \leqslant \frac{1}{2\widetilde{\sigma}_n^2}\binom{n-1}{k-1}^2 \bigg(\mathrm{Var}\bigg\{\sum_{i=1}^n \big(f_{(1)}(X_i) - f_{(1)}(X_i')\big)^2\bigg\}\bigg)^{1/2} + \frac{(k-1)^2\tau^2}{2(n-1)\sigma_{(1)}^2} \\
&\quad \leqslant \frac{1}{2\widetilde{\sigma}_n^2}\binom{n-1}{k-1}^2 \bigg(\sum_{i=1}^n \mathbb{E}\big\{f_{(1)}(X_i) - f_{(1)}(X_i')\big\}^4\bigg)^{1/2} + \frac{(k-1)^2\tau^2}{2(n-1)\sigma_{(1)}^2} \\
&\quad \leqslant \frac{1}{2\widetilde{\sigma}_n^2}\binom{n-1}{k-1}^2 \bigg(8\sum_{i=1}^n \mathbb{E}\big\{f_{(1)}(X_i)^4\big\} + \mathbb{E}\big\{f_{(1)}(X_i')^4\big\}\bigg)^{1/2} + \frac{(k-1)^2\tau^2}{2(n-1)\sigma_{(1)}^2} \\
&\quad = \frac{2n^{3/2}\tau^2}{k^2\sigma_{(1)}^2}\binom{n-1}{k-1}^2\binom{n}{k}^{-2} + \frac{(k-1)^2\tau^2}{2(n-1)\sigma_{(1)}^2} \\
&\quad = \frac{2\tau^2}{\sqrt{n}\sigma_{(1)}^2} + \frac{(k-1)\tau^2}{\sqrt{n}\sigma_{(1)}^2} \leqslant \frac{(k+1)\tau^2}{\sqrt{n}\sigma_{(1)}^2},
\end{aligned}$$

where we used (5.2) and (5.5) in the last line. Using the same argument, we have for $n \geqslant \max\{2, k^2\}$,

$$\begin{aligned}
&\mathbb{E}\bigg|\frac{1}{\lambda}\,\mathbb{E}\{|D|\Delta \,|\, X, X', Y\}\bigg| \\
&\quad \leqslant \frac{1}{\widetilde{\sigma}_n^2}\binom{n-1}{k-1}^2 \bigg(\mathrm{Var}\bigg\{\sum_{i=1}^n \big(f_{(1)}(X_i) - f_{(1)}(X_i')\big)\big|f_{(1)}(X_i) - f_{(1)}(X_i')\big|\bigg\}\bigg)^{1/2} \\
&\quad \leqslant \frac{1}{\widetilde{\sigma}_n^2}\binom{n-1}{k-1}^2 \bigg(\sum_{i=1}^n \mathbb{E}\big\{f_{(1)}(X_i) - f_{(1)}(X_i')\big\}^4\bigg)^{1/2} \\
&\quad \leqslant \frac{1}{\widetilde{\sigma}_n^2}\binom{n-1}{k-1}^2 \bigg(8\sum_{i=1}^n \mathbb{E}\big\{f_{(1)}(X_i)^4\big\} + \mathbb{E}\big\{f_{(1)}(X_i')^4\big\}\bigg)^{1/2} \\
&\quad = \frac{4n^{3/2}\tau^2}{k^2\sigma_{(1)}^2}\binom{n-1}{k-1}^2\binom{n}{k}^{-2} \\
&\quad \leqslant \frac{4\tau^2}{\sqrt{n}\sigma_{(1)}^2}.
\end{aligned}$$

Now we give the bounds for U and $U^{(i)}$. We have two cases. For the case where $k = 1$, then it follows that $U = 0$ and $U^{(i)} = 0$. Note that $\mathbb{E}\, f_{(1)}(X_i)^2 \leqslant \tau^2$. As for $k \geqslant 2$, noting that $n \leqslant 2(n-1)$ for $n \geqslant 2$, by Lemma 5.1 and the Cauchy inequality, we have

$$\mathbb{E}|U| \leqslant \frac{(k-1)\tau}{\sqrt{2}(n-1)^{1/2}\sigma_{(1)}} \leqslant \frac{(k-1)\tau}{\sqrt{n}\sigma_{(1)}},$$

and

$$\begin{aligned}\frac{1}{\lambda}\,\mathbb{E}|D(U-U')| &= \frac{1}{\widetilde{\sigma}_n}\binom{n-1}{k-1}\sum_{i=1}^{n}\mathbb{E}\{|(f_{(1)}(X_i)-f_{(1)}(X_i'))(U-U^{(i)})|\} \\ &\leqslant \frac{2}{\widetilde{\sigma}_n}\binom{n-1}{k-1}\sum_{i=1}^{n}\mathbb{E}\{|f_{(1)}(X_i)(U-U^{(i)})|\} \\ &\leqslant \frac{2}{\widetilde{\sigma}_n}\binom{n-1}{k-1}\sum_{i=1}^{n}(\mathbb{E}\,f_{(1)}(X_i)^2)^{1/2}(\mathbb{E}\{(U-U^{(i)})^2\})^{1/2} \\ &\leqslant \frac{2}{\widetilde{\sigma}_n}\binom{n-1}{k-1}\frac{\sqrt{2}n^{1/2}(k-1)\tau^2}{(n-1)^{1/2}\sigma_{(1)}}.\end{aligned}$$

By (5.2), we have

$$\widetilde{\sigma}_n \geqslant \binom{n-1}{k-1}n^{1/2}\sigma_{(1)},$$

and thus, using the inequality $n \leqslant 2(n-1)$ again, we obtain

$$\frac{1}{\lambda}\,\mathbb{E}|D(U-U')| \leqslant \frac{2\sqrt{2}(k-1)\tau^2}{(n-1)^{1/2}\sigma_{(1)}^2} \leqslant \frac{4(k-1)\tau^2}{\sqrt{n}\sigma_{(1)}^2}.$$

Here, with a slight abuse of notation, we choose (X,X') in Corollary 4.3 as $((X,Y),(X^{(I)},Y))$ in this theorem. By Corollary 4.3, and noting that $\sigma_{(1)}^2 \leqslant \mathbb{E}\{f(X_{\{\alpha\}};Y_{\{\alpha\}})^2\} \leqslant \tau^2$, we have

$$\begin{aligned}\sup_{z\in\mathbb{R}}\big|\mathbb{P}[T\leqslant z]-\Phi(z)\big| &\leqslant \frac{(k+5)\tau^2}{\sqrt{n}\sigma_{(1)}^2} + \frac{7(k-1)\tau^2}{\sqrt{n}\sigma_{(1)}^2} \\ &\leqslant \frac{8k\tau^2}{\sqrt{n}\sigma_{(1)}^2}.\end{aligned}$$

This proves (2.4).

5.2 Proof of Theorem 2.3

In this subsection, we give the proof of Theorem 2.3. Recall that $2 \leqslant d \leqslant k$. Without loss of generality, we assume that $n \geqslant k^2$, otherwise the proof is trivial. In this subsection, we denote by C an absolute constant that may take different values in different places.

We first prove a proposition for the Hoeffding decomposition.

Proposition 5.2. *For $A\subset[n], B\subset[n]_2$ such that $(A,B)\neq(\varnothing,\varnothing)$, and for any $\widetilde{A},\widetilde{B}$ such that $\widetilde{A}\subset A$ and $\widetilde{B}\subset B$ but $(\widetilde{A},\widetilde{B})\neq(A,B)$, we have*

$$\mathbb{E}\big\{f_{A,B}(X_A;Y_B)\bigm| X_{\widetilde{A}},Y_{\widetilde{B}}\big\}=0. \tag{5.6}$$

Proof of Proposition 5.2. If $|A|+|B|=1$, then for $(\widetilde{A},\widetilde{B})=(\varnothing,\varnothing)$, by definition,

$$\begin{aligned}\mathbb{E}\big\{f_{A,B}(X_A;Y_B)\bigm| X_{\widetilde{A}},Y_{\widetilde{B}}\big\} &= \mathbb{E}\big\{f_{A,B}(X_A;Y_B)\big\} \\ &= \mathbb{E}\{f(X_{[k]};Y_{[k]_2})\}-\mathbb{E}\{f(X_{[k]};Y_{[k]_2})\}=0.\end{aligned}$$

We prove the proposition by induction. Let $m\geqslant 2$. Assume that (5.6) holds for $1\leqslant |A|+|B|\leqslant m-1$.

Now, we assume that $|A|+|B|=m$. Let $\mathcal{A}_{\widetilde{A},\widetilde{B}}=\{(A',B'):A'\subset\widetilde{A},B'\subset\widetilde{B},\}$ and let $\mathcal{A}^c_{\widetilde{A},\widetilde{B}}=\{(A',B'):A'\subset A,B'\subset B,(A',B')\neq(A,B)\}\setminus\mathcal{A}_{\widetilde{A},\widetilde{B}}$. Reordering (2.2) by the inclusive-exclusive formula we have

$$
\begin{aligned}
&f_{A,B}(X_A;Y_B)\\
&\quad=\mathbb{E}\{f(X_{[k]};Y_{[k]_2})|X_A,Y_B\}-\sum_{|A'|+|B'|<|A|+|B|}f_{A',B'}(X_{A'};Y_{B'})\\
&\quad=\mathbb{E}\{f(X_{[k]};Y_{[k]_2})|X_A,Y_B\}-\sum_{(A',B')\in\mathcal{A}_{\widetilde{A},\widetilde{B}}}f_{A',B'}(X_{A'};Y_{B'})-\sum_{(A',B')\in\mathcal{A}^c_{\widetilde{A},\widetilde{B}}}f_{A',B'}(X_{A'};Y_{B'})\\
&\quad=\mathbb{E}\{f(X_{[k]};Y_{[k]_2})|X_A,Y_B\}-\mathbb{E}\{f(X_{[k]};Y_{[k]_2})|X_{\widetilde{A}},Y_{\widetilde{B}}\}-\sum_{(A',B')\in\mathcal{A}^c_{\widetilde{A},\widetilde{B}}}f_{A',B'}(X_{A'};Y_{B'}).
\end{aligned}
$$

By the induction assumption, we have

$$\sum_{(A',B')\in\mathcal{A}^c_{\widetilde{A},\widetilde{B}}}\mathbb{E}\{f_{A',B'}(X_{A'};Y_{B'})|X_{\widetilde{A}},Y_{\widetilde{B}}\}=0.$$

Then, the desired result follows. □

Let

$$\mathcal{A}_{n,\ell}=\{\alpha=(\alpha(1),\dots,\alpha(\ell)):1\leqslant\alpha(1)\neq\cdots\neq\alpha(\ell)\leqslant n\}.$$

Then, $\mathcal{I}_{n,\ell}\subset\mathcal{A}_{n,\ell}$. For $A\subset[\ell]$ and $B\in[\ell]_2$ and $\alpha=(\alpha(1),\dots,\alpha(\ell))\in\mathcal{A}_{n,\ell}$, write

$$
\begin{aligned}
\alpha(A)&=(\alpha(i))_{i\in A}, & \alpha(B)&=\big((\alpha(i),\alpha(j))\big)_{(i,j)\in B},\\
X_{\alpha(A)}&=(X_i)_{i\in\alpha(A)}, & Y_{\alpha(B)}&=(Y_{i,j})_{(i,j)\in\alpha(B)}.
\end{aligned}
$$

Moreover, for any $f_{A,B}:\mathcal{X}^{|A|}\times\mathcal{Y}^{|B|}\to\mathbb{R}$, let

$$\widetilde{S}_{n,\ell}(f_{A,B})=\sum_{\alpha\in\mathcal{A}_{n,\ell}}f_{A,B}(X_{\alpha(A)};Y_{\alpha(B)}),$$

and similarly, $S_{n,\ell}(f_{A,B})$ can be represented as $\sum_{\alpha\in\mathcal{I}_{n,\ell}}f_{A,B}(X_{\alpha(A)};Y_{\alpha(B)})$.

Let $(Y'_{1,1},\dots,Y'_{n-1,n})$ be an independent copy of $Y=(Y_{1,1},\dots,Y_{n-1,n})$. For any $(i,j)\in\mathcal{A}_{n,2}$, let $Y^{(i,j)}=(Y^{(i,j)}_{1,1},\dots,Y^{(i,j)}_{n-1,n})$ with

$$Y^{(i,j)}_{p,q}=\begin{cases}Y_{p,q} & \text{if } \{p,q\}\neq\{i,j\},\\ Y'_{p,q} & \text{if } \{p,q\}=\{i,j\},\end{cases}\quad\text{for } (p,q)\in\mathcal{I}_{n,2}.$$

Then, it follows that for each $(i,j)\in\mathcal{A}_{n,2}$, $((X,Y),(X,Y^{(i,j)}))$ is an exchangeable pair. For any $B\subset[n]_2$, let $Y^{(i,j)}_B=(Y^{(i,j)}_{p,q})_{(p,q)\in B}$. For any $A\subset[\ell]$, $B\subset[\ell]_2$, $\alpha=(\alpha(1),\dots,\alpha(\ell))\in\mathcal{I}_{n,\ell}$ and $f_{A,B}:\mathcal{X}^{|A|}\times\mathcal{Y}^{|B|}\to\mathbb{R}$, define

$$
\begin{aligned}
Y^{(i,j)}_{\alpha(B)}&=(Y^{(i,j)}_{\alpha(p),\alpha(q)})_{(p,q)\in B},\\
S^{(i,j)}_{n,\ell}(f_{A,B})&=\sum_{\alpha\in\mathcal{I}_{n,\ell}}f_{A,B}(X_{\alpha(A)};Y^{(i,j)}_{\alpha(B)}),\\
\widetilde{S}^{(i,j)}_{n,\ell}(f_{A,B})&=\sum_{\alpha\in\mathcal{A}_{n,\ell}}f_{A,B}(X_{\alpha(A)},Y^{(i,j)}_{\alpha(B)}).
\end{aligned}
$$

Let $f_{(\ell)}$ be defined as in (2.3), and it follows that

$$f = \sum_{\ell=0}^{k} f_{(\ell)}, \quad f_{(0)} = \mathbb{E}\{f(X_{[k]}; Y_{[k]_2})\}, \quad S_{n,k}(f_{(0)}) = \mathbb{E}\{S_{n,k}(f)\}.$$

Moreover, by assumption, as f has principal degree d, and it follows that $f_{(\ell)} \equiv 0$ for $\ell = 1, \ldots, d-1$. Let $\widetilde{\sigma}_n = (\mathrm{Var}\{S_{n,k}(f)\})^{1/2}$ and $\widetilde{\sigma}_{n,\ell} = (\mathrm{Var}\{S_{n,k}(f_{(\ell)})\})^{1/2}$. For any $A \subset [k]$ and $B \subset [k]_2$, let

$$\begin{aligned} \mu_{A,B} &:= \frac{1}{|\mathrm{Aut}(G_{A,B})||B|} \binom{n - v_{A,B}}{n-k}, \\ \nu_{A,B} &:= |B| \times \mu_{A,B} = \frac{1}{|\mathrm{Aut}(G_{A,B})|} \binom{n - v_{A,B}}{n-k}, \end{aligned} \tag{5.7}$$

and for any $\alpha \in \mathcal{A}_{n,\ell}$ ($\ell = 1, \ldots, k$), let

$$\xi^{(i,j)}_{\alpha(A,B)} = f_{A,B}(X_{\alpha(A)}; Y_{\alpha(B)}) - f_{A,B}(X_{\alpha(A)}; Y^{(i,j)}_{\alpha(B)}). \tag{5.8}$$

The next lemma estimates the upper and lower bounds of $\widetilde{\sigma}_n^2$ and $\widetilde{\sigma}_{n,d}^2$. The proof is similar to that of Lemma 4 of [13]. Recall that $\mathcal{J}_{f,\ell} = \{(A,B) : A \subset [\ell], B \subset [\ell]_2, \sigma_{A,B} > 0, v_{A,B} = \ell\}$ for $d \leqslant \ell \leqslant k$ and π_ℓ was defined in (2.5).

Lemma 5.3. *Assume that $n \geqslant 2k^2$ and $k \geqslant 2$. We have for each $(i,j) \in \mathcal{A}_{n,2}$ and $d \leqslant \ell \leqslant k$,*

$$\widetilde{\sigma}_{n,\ell}^2 = \sum_{(A,B) \in \mathcal{J}_{f,\ell}} \frac{n!(n-\ell)!\sigma_{A,B}^2}{(n-k)!^2(k-\ell)!^2|\mathrm{Aut}(G_{A,B})|} \leqslant \frac{\pi_\ell n^{2k-\ell}\tau^2}{(k-\ell)!^2}, \tag{5.9}$$

$$\widetilde{\sigma}_n^2 = \sum_{\ell=d}^{k} \widetilde{\sigma}_{n,\ell}^2 \leqslant \left(\sum_{\ell=d}^{k} \frac{n^{d-\ell}\pi_\ell}{(k-\ell)!^2} \right) n^{2k-d}\tau^2, \tag{5.10}$$

$$\mathbb{E}\{(S_{n,k}(f_{(\ell)}) - S^{(i,j)}_{n,k}(f_{(\ell)}))^2\} \leqslant \frac{2\pi_\ell n^{2k-\ell-2}\tau^2}{(k-\ell)!^2}, \tag{5.11}$$

$$\mathbb{E}\left\{ \left(\sum_{\alpha \in \mathcal{A}_{n,\ell}} \sum_{(A,B) \in \mathcal{J}_{f,\ell}} \mu_{A,B} \xi^{(i,j)}_{\alpha(A,B)} \right)^2 \right\} \leqslant \frac{2\pi_\ell n^{2k-\ell-2}\tau^2}{(k-\ell)!^2}, \tag{5.12}$$

and

$$\widetilde{\sigma}_n^2 \geqslant \widetilde{\sigma}_{n,d}^2 \geqslant \frac{\pi_d \sigma_{\min}^2}{e^2(k-d)!^2} n^{2k-d}, \tag{5.13}$$

where $|\mathrm{Aut}(G)|$ is the number of the automorphisms of G, and $C > 0$ is an absolute constant.

Proof. Recall that $\mathrm{Aut}(G)$ is the collection of automorphisms of G. For any $d \leqslant \ell \leqslant k$ and $(A,B) \in \mathcal{J}_{f,\ell}$, by symmetry of f, we have $f_{A,B} = f_{A',B'}$ for all $G_{A',B'} \in \mathrm{Aut}(G_{A,B})$, and $\widetilde{S}_{n,k}(f_{A,B}) = \widetilde{S}_{n,k}(f_{A',B'})$ for all $G_{A,B} \cong G_{A',B'}$. Note that for each $(A,B) \in \mathcal{J}_{f,\ell}$, there are exactly $k!/((k-\ell)!|\mathrm{Aut}(G_{A,B})|)$ subgraphs of $K(k)$ isomorphic to $G_{A,B}$, where $K(k)$ is the complete graph with k vertices. We then have for each $d \leqslant \ell \leqslant k$ and $(A,B) \in \mathcal{J}_{f,\ell}$, by symmetry,

$$\widetilde{S}_{n,k}(f_{A,B}) = \frac{(n-\ell)!}{(n-k)!} \widetilde{S}_{n,\ell}(f_{A,B}),$$

and

$$\begin{aligned} S_{n,k}(f_{(\ell)}) &= \frac{1}{k!}\widetilde{S}_{n,k}(f_{(\ell)}) \\ &= \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{(k-\ell)!|\mathrm{Aut}(G_{A,B})|}\widetilde{S}_{n,k}(f_{A,B}) \\ &= \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-\ell}{n-k}\widetilde{S}_{n,\ell}(f_{A,B}). \end{aligned} \tag{5.14}$$

By Lemma 4 of [13], we have

$$\mathrm{Var}\big(\widetilde{S}_{n,\ell}(f_{A,B})\big) = \frac{n!|\mathrm{Aut}(G_{A,B})|\sigma^2_{A,B}}{(n-\ell)!},$$

and thus, the variance of $S_{n,k}(f_{(\ell)})$ is given by

$$\begin{aligned} \widetilde{\sigma}^2_{n,\ell} &:= \mathrm{Var}\big(S_{n,k}(f_{(\ell)})\big) \\ &= \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|^2}\binom{n-\ell}{k-\ell}^2 \mathrm{Var}(\widetilde{S}_{n,\ell}(f_{A,B})) \\ &= \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|^2}\binom{n-\ell}{k-\ell}^2 \frac{n!}{(n-\ell)!}|\mathrm{Aut}(G_{A,B})|\sigma^2_{A,B} \\ &= \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{n!(n-\ell)!\sigma^2_{A,B}}{(n-k)!^2(k-\ell)!^2|\mathrm{Aut}(G_{A,B})|}. \end{aligned} \tag{5.15}$$

For any $(A,B)\ncong(A',B')$, by orthogonality,

$$\begin{aligned} &\mathrm{Cov}\big\{\widetilde{S}_{n,k}(f_{A,B}),\widetilde{S}_{n,k}(f_{A',B'})\big\} \\ &= \sum_{\alpha\in\mathcal{A}_{n,k}}\sum_{\alpha'\in\mathcal{A}_{n,k}} \mathrm{Cov}\big\{f_{A,B}(X_{\alpha(A)};Y_{\alpha(B)}), f_{A',B'}(X_{\alpha'(A')};Y_{\alpha'(B')})\big\} = 0, \end{aligned}$$

and it follows that

$$\mathrm{Cov}\big\{\widetilde{S}_{n,k}(f_{(\ell)}),\widetilde{S}_{n,k}(f_{(\ell')})\big\} = 0, \text{ for } d\leqslant\ell\neq\ell'\leqslant k.$$

Hence,

$$\widetilde{\sigma}^2_n = \mathrm{Var}\{S_{n,k}(f)\} = \sum_{\ell=d}^{k}\widetilde{\sigma}^2_{n,\ell}. \tag{5.16}$$

The inequalities (5.9) and (5.10) follows from (5.15) and (5.16) and the fact that

$$\frac{n!(n-\ell)!}{(n-k)!^2} \leqslant n^{2k-\ell} \quad \text{for } d\leqslant\ell\leqslant k.$$

As for (5.13), by (5.15) and (5.16), we have

$$\begin{aligned} \widetilde{\sigma}_n &\geqslant \widetilde{\sigma}^2_{n,d} \\ &= \frac{n!(n-d)!}{(n-k)!^2(k-d)!^2}\sum_{(A,B)\in\mathcal{J}_{f,d}}\frac{\sigma^2_{A,B}}{|\mathrm{Aut}(G_{A,B})|} \\ &\geqslant \frac{n!(n-d)!}{(n-k)!^2(k-d)!^2}\sigma^2_{\min}\sum_{(A,B)\in\mathcal{J}_{f,d}}\frac{1}{|\mathrm{Aut}(G_{A,B})|} \\ &= \frac{n!(n-d)!}{(n-k)!^2(k-d)!^2}\pi_d\sigma^2_{\min}, \end{aligned} \tag{5.17}$$

where in the last line we used the definition that

$$\pi_d = \sum_{(A,B)\in\mathcal{J}_{f,d}} \frac{1}{|\mathrm{Aut}(G_{A,B})|}.$$

Using a famous inequality

$$e^{-\frac{k^2}{2(n-k)}} \leqslant n^{-k}\frac{n!}{(n-k)!} \leqslant 1, \tag{5.18}$$

and using the assumption that $n \geqslant k^2$ and $k \geqslant d \geqslant 2$, we have

$$\frac{(k-d)^2}{2(n-k)} \leqslant \frac{k^2}{2(n-k)} \leqslant 1.$$

Therefore,

$$\frac{n!}{(n-k)!}\frac{(n-d)!}{(n-k)!} \geqslant n^{2k-d}e^{-\frac{k^2}{2(n-k)}-\frac{(k-d)^2}{2(n-k)}} \geqslant e^{-2}n^{2k-d}. \tag{5.19}$$

Combining (5.17) and (5.19) yields (5.13).

It remains to prove (5.11) and (5.12). For any $(i,j)\in\mathcal{A}_{n,2}$, we have

$$\begin{aligned}
S_{n,k}(f_{(\ell)}) - S_{n,k}^{(i,j)}(f_{(\ell)}) &= \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-\ell}{n-k}\big(\widetilde{S}_{n,\ell}(f_{A,B}) - \widetilde{S}_{n,\ell}^{(i,j)}(f_{A,B})\big)\\
&= \sum_{\alpha\in\mathcal{A}_{n,\ell}}\sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-\ell}{n-k}\xi_{\alpha(A,B)}^{(i,j)},
\end{aligned}$$

where $\xi_{\alpha(A,B)}^{(i,j)}$ is given in (5.8), and we have

$$\mathrm{Var}(\xi_{\alpha(A,B)}^{(i,j)}) \leqslant 2\tau^2.$$

By orthogonality, and recalling that $|\mathrm{Aut}(G_{A,B})| \geqslant 1$,

$$\begin{aligned}
&\mathrm{Var}\bigg(\sum_{\alpha\in\mathcal{A}_{n,\ell}}\sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-\ell}{n-k}\xi_{\alpha(A,B)}^{(i,j)}\bigg)\\
&\quad= \sum_{\alpha\in\mathcal{A}_{n,\ell}}\sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|^2}\binom{n-\ell}{n-k}^2 \mathrm{Var}(\xi_{\alpha(A,B)}^{(i,j)})\\
&\quad\leqslant 2\tau^2 \sum_{(A,B)\in\mathcal{J}_{f,\ell}}\sum_{\alpha\in\mathcal{A}_{n,\ell}} \frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-\ell}{n-k}^2\\
&\quad= 2\tau^2 \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{n!}{(n-\ell)!}\frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-\ell}{n-k}^2\\
&\quad= 2\tau^2 \sum_{(A,B)\in\mathcal{J}_{f,\ell}} \frac{n!(n-\ell)!}{(n-k)!^2(k-\ell)!^2}\frac{1}{|\mathrm{Aut}(G_{A,B})|}\\
&\quad\leqslant \frac{2\tau^2\pi_\ell n^{2k-\ell}}{(k-\ell)!^2},
\end{aligned}$$

where we used the inequality (5.18) in the last line.

This completes the proof of (5.11). The inequality (5.12) can be shown in a similar way. □

Recall that $G_{A,B}$ is the graph generated by (A,B). For any (A_j,B_j) for $j=1,2$, we simply write $v_j = v_{A_j,B_j}$ as the number of nodes of the graph G_{A_j,B_j}. Recall that $\mathcal{J}_{f,d} = \{(A,B) : A \subset [d], B \subset [d]_2, \sigma_{A,B} > 0, v_{A,B} = d\}$ and $\mathcal{J}_{f,d+1} = \{(A,B) : A \subset [d+1], B \subset [d+1]_2, \sigma_{A,B} > 0, v_{A,B} = d+1\}$. We have the following lemmas, whose proofs are given in the appendix.

Lemma 5.4. *For all (A_1,B_1), $(A_2,B_2) \in \mathcal{G}_{f,d}$ such that G_{A_1,B_1} and G_{A_2,B_2} are connected, we have*

$$\mathrm{Var}\biggl\{\sum_{(i,j)\in\mathcal{A}_{n,2}}\biggl(\sum_{\alpha_1\in\mathcal{A}_{n,d}^{(i,j)}}\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\biggr)\biggl(\sum_{\alpha_2\in\mathcal{A}_{n,d}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\biggr)\biggr\} \leqslant Ck^2n^{2d-1}\tau^4.$$

Lemma 5.5. *Assume that $k \geqslant d+1$. For all (A_1,B_1), $(A_2,B_2) \in \mathcal{G}_{f,d} \cup \mathcal{G}_{f,d+1}$, we have*

$$\mathrm{Var}\biggl\{\sum_{(i,j)\in\mathcal{A}_{n,2}}\biggl(\sum_{\alpha_1\in\mathcal{A}_{n,v_1}^{(i,j)}}\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\biggr)\biggl|\sum_{\alpha_2\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\biggr|\biggr\} \leqslant Ck^2n^{2\max\{v_1,v_2\}-2}\tau^4.$$

We are now ready to give the proof of Theorem 2.3.

Proof of Theorem 2.3. As we mentioned at the beginning of this subsection, we assume that $n \geqslant k^2$ without loss of generality, otherwise the result is trivial. Recall that $f_{(d)}$ is defined in (2.3). Write $T = \widetilde{\sigma}_n^{-1}S_{n,k}(f)$, and

$$W = \widetilde{\sigma}_n^{-1}S_{n,k}(f_{(d)}), \quad U = T - W = \widetilde{\sigma}_n^{-1}\sum_{\ell=d+1}^{k}S_{n,k}(f_{(\ell)}). \tag{5.20}$$

Here, if $d+1>k$, then set $\sum_{\ell=d+1}^{k}S_{n,k}(f_{(\ell)}) = 0$. We have

$$\begin{aligned}
W &= \frac{1}{\widetilde{\sigma}_n}\sum_{\alpha\in\mathcal{A}_{n,k}}\sum_{A\subset[k],B\subset[k]_2,v_{A,B}=d} f_{A,B}(X_{\alpha(A)};Y_{\alpha(B)}) \\
&= \frac{1}{\widetilde{\sigma}_n}\sum_{\alpha\in\mathcal{A}_{n,d}}\sum_{A\subset[d],B\subset[d]_2,v_{A,B}=d}\binom{n-d}{k-d}\frac{f_{A,B}(X_{\alpha(A)};Y_{\alpha(B)})}{|\mathrm{Aut}(G_{A,B})|} \\
&= \frac{1}{\widetilde{\sigma}_n}\sum_{\alpha\in\mathcal{A}_{n,d}}\sum_{(A,B)\in\mathcal{J}_{f,d}}\binom{n-d}{k-d}\frac{f_{A,B}(X_{\alpha(A)};Y_{\alpha(B)})}{|\mathrm{Aut}(G_{A,B})|},
\end{aligned}$$

where the second equality follows from symmetry and the last equality follows from the assumption that $f_{A,B} \equiv 0$ for all $(A,B) \in \{(A,B) : A \subset [d], B \subset [d]_2\} \setminus \mathcal{J}_{f,d}$.

For each $(i,j) \in \mathcal{A}_{n,2}$, let

$$W^{(i,j)} = \frac{1}{\widetilde{\sigma}_n}S_{n,k}^{(i,j)}(f_{(d)}), \quad U^{(i,j)} = \widetilde{\sigma}_n^{-1}\sum_{\ell=d+1}^{k}S_{n,k}^{(i,j)}(f_{(\ell)}).$$

Let (I,J) be a random 2-fold index uniformly chosen in $\mathcal{A}_{n,2}$, which is independent of all others. Then, $((X,Y),(X,Y^{(I,J)}))$ is an exchangeable pair. Let

$$\Delta = W - W^{(I,J)} = \frac{1}{\widetilde{\sigma}_n}\sum_{\alpha\in\mathcal{A}_{n,d}}\sum_{(A,B)\in\mathcal{J}_{f,d}}\nu_{A,B}\xi_{\alpha(A,B)}^{(I,J)}.$$

Also, define

$$D = \frac{1}{\widetilde{\sigma}_n} \sum_{\alpha \in \mathcal{A}_{n,d}} \sum_{(A,B) \in \mathcal{J}_{f,d}} \mu_{A,B} \xi^{(I,J)}_{\alpha(A,B)}. \tag{5.21}$$

Then, we have D is antisymmetric with respect to (X, Y) and $(X, Y^{(I,J)})$.

Let $\mathcal{A}^{(i,j)}_{n,d} = \{\alpha \in \mathcal{A}_{n,d} : \{i, j\} \subset \{\alpha\}\}$. Then,

$$\mathbb{E}\{D \,|\, X, Y\} = \frac{1}{n(n-1)\widetilde{\sigma}_n} \sum_{(i,j) \in \mathcal{A}_{n,2}} \sum_{\alpha \in \mathcal{A}^{(i,j)}_{n,d}} \sum_{(A,B) \in \mathcal{J}_{f,d}} \mu_{A,B} \, \mathbb{E}\big\{\xi^{(i,j)}_{\alpha(A,B)} \,|\, X, Y\big\}.$$

By (5.6),

$$\begin{aligned}
\mathbb{E}\{f_{A,B}(X_{\alpha(A)}; Y^{(i,j)}_{\alpha(B)}) \,|\, X, Y\} &= \mathbb{E}\{f_{A,B}(X_{\alpha(A)}; Y_{\alpha(B)}) \,|\, X_A, Y_B \setminus \{Y_{i,j}\}\} \\
&= \begin{cases} 0 & \text{if } (i,j) \in B, \\ f_{A,B}(X_{\alpha(A)}; Y_{\alpha(B)}) & \text{otherwise.} \end{cases}
\end{aligned}$$

Moreover, note that for $\alpha \in \mathcal{A}_{n,d}$,

$$\sum_{(i,j) \in \mathcal{A}_{n,2}} \mathbb{1}((i,j) \in \alpha(B)) = |\alpha(B)| = |\{(\alpha(i), \alpha(j)) : (i,j) \in B, \alpha(i) \neq \alpha(j)\}| = 2|B|,$$

and thus

$$\begin{aligned}
\mathbb{E}\{D \,|\, X, Y\} &= \frac{1}{n(n-1)\widetilde{\sigma}_n} \sum_{\alpha \in \mathcal{A}_{n,d}} \sum_{(A,B) \in \mathcal{J}_{f,d}} \mu_{A,B} f_{A,B}(X_{\alpha(A)}; Y_{\alpha(B)}) \sum_{(i,j) \in \mathcal{A}_{n,2}} \mathbb{1}((i,j) \in \alpha(B)) \\
&= \frac{2}{n(n-1)\widetilde{\sigma}_n} \sum_{\alpha \in \mathcal{A}_{n,d}} \sum_{(A,B) \in \mathcal{J}_{f,d}} \nu_{A,B} f_{A,B}(X_{\alpha(A)}; Y_{\alpha(B)}) \\
&= \frac{2}{n(n-1)} W.
\end{aligned} \tag{5.22}$$

Thus, (4.3) is satisfied with $\lambda = 2/(n(n-1))$ and $R = 0$. Moreover, by exchangeability,

$$\mathbb{E}\{D\Delta\} = 2\,\mathbb{E}\{DW\} = 2\lambda\,\mathbb{E}\{W^2\} = 2\lambda \widetilde{\sigma}^2_{n,d}/\widetilde{\sigma}^2_n. \tag{5.23}$$

Then, we have

$$\begin{aligned}
\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \,|\, X, Y, Y'\} = \frac{1}{4\widetilde{\sigma}^2_n} &\sum_{(A_1,B_1) \in \mathcal{J}_{f,d}} \sum_{(A_2,B_2) \in \mathcal{J}_{f,d}} \mu_{A_1,B_1} \nu_{A_2,B_2} \\
&\times \sum_{(i,j) \in \mathcal{A}_{n,2}} \bigg(\sum_{\alpha \in \mathcal{A}^{(i,j)}_{n,d}} \xi^{(i,j)}_{\alpha(A_1,B_1)} \bigg) \bigg(\sum_{\alpha \in \mathcal{A}^{(i,j)}_{n,d}} \xi^{(i,j)}_{\alpha(A_2,B_2)} \bigg).
\end{aligned}$$

Now, by the Cauchy inequality, (5.7) and (5.23) and Lemmas 5.3 and 5.4, we have

$$
\begin{aligned}
&\mathbb{E}\bigg|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \mid X,Y,Y'\} - 1\bigg| \\
&\quad \leqslant \mathbb{E}\bigg|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \mid X,Y,Y'\} - \frac{1}{2\lambda}\,\mathbb{E}\{D\Delta\}\bigg| + \frac{\widetilde{\sigma}_n^2 - \widetilde{\sigma}_{n,d}^2}{\widetilde{\sigma}_n^2} \\
&\quad \leqslant \frac{1}{4\widetilde{\sigma}_n^2} \sum_{(A_1,B_1)\in\mathcal{J}_{f,d}} \sum_{(A_2,B_2)\in\mathcal{J}_{f,d}} \binom{n-d}{n-k}^2 \frac{1}{|\mathrm{Aut}(G_{A_1,B_1})||\mathrm{Aut}(G_{A_2,B_2})|} \\
&\qquad \times \Bigg(\mathrm{Var}\Bigg\{\sum_{(i,j)\in\mathcal{A}_{n,2}} \Bigg(\sum_{\alpha\in\mathcal{A}_{n,d}^{(i,j)}} \xi_{\alpha(A_1,B_1)}^{(i,j)}\Bigg)\Bigg(\sum_{\alpha\in\mathcal{A}_n^{(i,j)}} \xi_{\alpha(A_2,B_2)}^{(i,j)}\Bigg)\Bigg\}\Bigg)^{1/2} \\
&\qquad + \frac{\sum_{\ell=d+1}^{k} \widetilde{\sigma}_{n,\ell}^2}{\widetilde{\sigma}_n^2} \\
&\quad \leqslant \frac{Ck(k-d)!^2 n^{d-1/2}\tau^2}{\pi_d n^{2k-d}\sigma_{\min}^2} \Bigg(\sum_{(A,B)\in\mathcal{J}_{f,d}} \frac{n^{k-d}}{(k-d)!|\mathrm{Aut}(G_{A,B})|}\Bigg)^2 \\
&\qquad + C\frac{(k-d)!^2}{\pi_d n^{2k-d}\sigma_{\min}^2} \sum_{\ell=d+1}^{k} \frac{\pi_\ell n^{2k-\ell}\tau^2}{(k-\ell)!^2}.
\end{aligned}
\tag{5.24}
$$

For the first term of (5.24), we have

$$
\frac{k(k-d)!^2 n^{d-1/2}\tau^2}{\pi_d n^{2k-d}\sigma_{\min}^2} \Bigg(\sum_{(A,B)\in\mathcal{J}_{f,d}} \frac{n^{k-d}}{(k-d)!|\mathrm{Aut}(G_{A,B})|}\Bigg)^2 \leqslant \frac{k\pi_d n^{-1/2}\tau^2}{\sigma_{\min}^2}.
$$

For the second term of (5.24), we have for $d+1 \leqslant \ell \leqslant k$, by (5.18), and recalling that $n \geqslant k^2$,

$$
\frac{(k-d-1)!^2 n^{d+1-\ell}}{(k-\ell)!^2} \leqslant \left(\frac{(k-d-1)^2}{n}\right)^{(\ell-d-1)} \leqslant 1,
$$

then we have

$$
\frac{(k-d)!^2}{\pi_d n^{2k-d}\sigma_{\min}^2} \sum_{\ell=d+1}^{k} \frac{\pi_\ell n^{2k-\ell}\tau^2}{(k-\ell)!^2} \leqslant \frac{k^2\tau^2}{\pi_d n\sigma_{\min}^2} \sum_{\ell=d+1}^{k} \pi_\ell \leqslant \frac{k\tau^2}{\pi_d n^{1/2}\sigma_{\min}^2} \sum_{\ell=d+1}^{k} \pi_\ell. \tag{5.25}
$$

Therefore, we have

$$
\mathbb{E}\bigg|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \mid X,Y,Y'\} - 1\bigg| \leqslant Cn^{-1/2}\frac{k\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}, \tag{5.26}
$$

where $\Lambda_{k,d}$ is as defined in (2.6). Taking $D^* = |D|$, by Lemma 5.5,

$$
\begin{aligned}
&\frac{1}{\lambda}\,\mathbb{E}\big|\mathbb{E}\{D^*\Delta \mid X,Y,Y'\}\big| \\
&\quad \leqslant \frac{1}{4\widetilde{\sigma}_n^2} \sum_{(A_1,B_1)\in\mathcal{J}_{f,d}} \sum_{(A_2,B_2)\in\mathcal{J}_{f,d}} \mu_{A_1,B_1}\nu_{A_2,B_2} \\
&\qquad \times \Bigg(\mathrm{Var}\Bigg\{\sum_{(i,j)\in\mathcal{A}_{n,2}} \Bigg|\sum_{\alpha\in\mathcal{A}_{n,d}^{(i,j)}} \xi_{\alpha(A_1,B_1)}^{(i,j)}\Bigg|\Bigg(\sum_{\alpha\in\mathcal{A}_{n,d}^{(i,j)}} \xi_{\alpha(A_2,B_2)}^{(i,j)}\Bigg)\Bigg\}\Bigg)^{1/2} \\
&\quad \leqslant Cn^{-1/2}\frac{k\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}.
\end{aligned}
\tag{5.27}
$$

Now, by (5.20) and (5.25), Lemma 5.3, and the orthogonality property, we have

$$
\begin{aligned}
\mathbb{E}\,|U|^2 &\leqslant C\widetilde{\sigma}_{n,d}^{-2}\sum_{\ell=d+1}^{k}\widetilde{\sigma}_{n,\ell}^2\\
&\leqslant C\frac{(k-d)!^2}{\pi_d n^{2k-d}\sigma_{\min}^2}\sum_{\ell=d+1}^{k}\frac{\pi_\ell n^{2k-\ell}\tau^2}{(k-\ell)!^2}\\
&\leqslant Cn^{-1}\frac{k^2\tau^2}{\sigma_{\min}^2}\biggl(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\biggr),\\
\mathbb{E}(U-U^{(i,j)})^2 &\leqslant C\widetilde{\sigma}_{n,d}^{-2}\sum_{\ell=d+1}^{k}\mathbb{E}\{(S_{n,k}(f_{(\ell)})-S_{n,k}^{(i,j)}(f_{(\ell)}))^2\}\\
&\leqslant Cn^{-3}\frac{k^2\tau^2}{\sigma_{\min}^2}\biggl(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\biggr).
\end{aligned}
$$

Thus, noting that $\tau\geqslant\sigma_{\min}$ and by (5.12) and (5.21), we have

$$
\begin{aligned}
\mathbb{E}\,|U| &\leqslant Cn^{-1/2}\frac{k\tau}{\sigma_{\min}}\biggl(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\biggr)^{1/2},\\
&\leqslant Cn^{-1/2}\frac{k\tau^2}{\sigma_{\min}^2}\biggl(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\biggr)^{1/2}\leqslant Cn^{-1/2}\frac{k\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}, \qquad (5.28)\\
\frac{1}{\lambda}\,\mathbb{E}\bigl|D(U-U^{(I,J)})\bigr| &= \frac{1}{\widetilde{\sigma}_n}\sum_{(i,j)\in\mathcal{I}_{n,2}}\mathbb{E}\biggl\{\biggl|\biggl(\sum_{\alpha\in\mathcal{A}_{n,d}}\sum_{(A,B)\in\mathcal{J}_{f,d}}\mu_{A,B}\xi_{\alpha(A,B)}^{(i,j)}\biggr)(U-U^{(i,j)})\biggr|\biggr\}\\
&\leqslant Cn^{-1/2}\frac{k\tau^2}{\sigma_{\min}^2}\biggl(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\biggr)^{1/2}\leqslant Cn^{-1/2}\frac{k\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}. \qquad (5.29)
\end{aligned}
$$

Applying Corollary 4.3, and combining (5.26)–(5.29) we obtain the desired result. □

5.3 Proof of Theorem 2.4

The proof of Theorem 2.4 is similar to that of Theorem 2.3. Without loss of generality, we assume that $k\geqslant d+1$, otherwise the proof is even simpler. Again, let C denote a positive absolute constant, which might take different values in different places.

For any $A\subset[k]$ and $B\subset[k]_2$, recall that

$$
\begin{aligned}
\mu_{A,B} &\coloneqq \frac{1}{|\mathrm{Aut}(G_{A,B})||B|}\binom{n-v_{A,B}}{n-k},\\
\nu_{A,B} &\coloneqq |B|\mu_{A,B} = \frac{1}{|\mathrm{Aut}(G_{A,B})|}\binom{n-v_{A,B}}{n-k}.
\end{aligned}
$$

By (2.2) and Proposition 5.2, we have there exists a Hoeffding decomposition of g as follows:

$$
g(y)=\sum_{B\subset[k]_2}g_B(y_B),
$$

where $g_B:\mathcal{Y}^{|B|}\to\mathbb{R}$ is defined as

$$
g_B(y_B)=\sum_{B':B'\subset B}(-1)^{|B|-|B'|}\,\mathbb{E}\bigl\{g(Y_{1,2},\dots,Y_{k-1,k})\bigm| Y_{B'}=y_{B'}\bigr\}, \qquad (5.30)
$$

and where $y = (y_{1,2}, \ldots, y_{k-1,k})$ and $y_B = (y_{i,j} : (i,j) \in B)$. Also, for any $B \subset [\ell]_2$ and $\alpha \in \mathcal{A}_{n,\ell}$ ($\ell = 1, \ldots, k$), let

$$\eta_{\alpha(B)}^{(i,j)} = g_B(Y_{\alpha(B)}) - g_B(Y_{\alpha(B)}^{(i,j)}),$$

and let $V(B)$ be the node set of the graph with edge set B, as defined in (2.1). Recall that from the condition of Theorem 2.4, it follows that $f(X_{[k]}; Y_{[k]_2}) = g(Y_{[k]_2})$ almost surely for some symmetric function g. For any $r \in V(B)$, let $B^{(r)} = \{(i,j) : (i,j) \in B, i \neq r, j \neq r\}$. Recall that $\mathcal{J}_{f,d+1} = \{(A,B) : A \subset [k], B \subset [k]_2, v_{A,B} = d+1, \sigma_{A,B} > 0\}$ and we define $\widetilde{\mathcal{J}}_{f,d} = \{(A,B) \in \mathcal{J}_{f,d} : G_{A,B}$ is strongly connected.$\}$.

We need to apply the following lemma in the proof of Theorem 2.4.

Lemma 5.6. *Assume that* $k \geqslant d+1$. *For all* $(A_j, B_j) \in \widetilde{\mathcal{J}}_{f,d} \cup \mathcal{J}_{f,d+1}, j = 1,2$, *let* $v_j = v_{A_j,B_j}$, *we have*

$$\mathrm{Var}\Bigg\{ \sum_{(i,j)\in\mathcal{A}_{n,2}} \Bigg(\sum_{\alpha_1 \in \mathcal{A}_{n,v_1}^{(i,j)}} \eta_{\alpha_1(B_1)}^{(i,j)} \Bigg) \Bigg(\sum_{\alpha_2 \in \mathcal{A}_{n,v_2}^{(i,j)}} \eta_{\alpha_2(B_2)}^{(i,j)} \Bigg) \Bigg\} \leqslant C k^2 n^{2d-2} \tau^4.$$

Now, we are ready to prove Theorem 2.4.

Proof of Theorem 2.4. Let C denote a positive absolute constant that may take different values in different places. Recall that without loss of generality, we assume that $\mathbb{E}\{f(X_{[k]}, Y_{[k]_2})\} = 0$. Write $T = \widetilde{\sigma}_n^{-1} S_{n,k}(f)$, and let

$$W = \widetilde{\sigma}_n^{-1}(S_{n,k}(f_{(d)}) + S_{n,k}(f_{(d+1)})), \quad U = \widetilde{\sigma}_n^{-1} \sum_{\ell=d+2}^{k} S_{n,k}(f_{(\ell)}). \tag{5.31}$$

Here, if $d+1 > k$, then set $\sum_{\ell=d+1}^{k} S_{n,k}(f_{(\ell)}) = 0$. Then, $T = W + U$. Now we apply Corollary 4.3 again to prove the desired result. To this end, we need to construct an exchangeable pair. For each $(i,j) \in \mathcal{A}_{n,2}$, let

$$W^{(i,j)} = \frac{1}{\widetilde{\sigma}_n}(S_{n,k}^{(i,j)}(f_{(d)}) + S_{n,k}^{(i,j)}(f_{(d+1)})), \quad U^{(i,j)} = \widetilde{\sigma}_n^{-1} \sum_{\ell=d+2}^{k} S_{n,k}^{(i,j)}(f_{(\ell)}).$$

By assumption and recall that $f(X_{[k]}; Y_{[k]_2}) = g(Y_{[k]_2})$ almost surely, W can be rewritten as

$$W = \frac{1}{\widetilde{\sigma}_n} \sum_{(A,B)\in\widetilde{\mathcal{J}}_{f,d}\cup\mathcal{J}_{f,d+1}} \sum_{\alpha\in\mathcal{A}_{n,v_{A,B}}} \nu_{A,B}\, g_B(Y_{\alpha(B)}).$$

Let (I,J) be a random 2-fold index uniformly chosen in $\mathcal{A}_{n,2}$, which is independent of all others. Then, $((X,Y),(X,Y^{(I,J)}))$ is an exchangeable pair. Let

$$\Delta = W - W^{(I,J)} = \frac{1}{\widetilde{\sigma}_n} \Bigg(\sum_{(A,B)\in\widetilde{\mathcal{J}}_{f,d}\cup\mathcal{J}_{f,d+1}} \sum_{\alpha\in\mathcal{A}_{n,v_{A,B}}} \nu_{A,B}\, \eta_{\alpha(B)}^{(I,J)} \Bigg).$$

Also, define

$$D = \frac{1}{\widetilde{\sigma}_n} \Bigg(\sum_{(A,B)\in\widetilde{\mathcal{J}}_{f,d}\cup\mathcal{J}_{f,d+1}} \sum_{\alpha\in\mathcal{A}_{n,v_{A,B}}} \mu_{A,B}\, \eta_{\alpha(B)}^{(I,J)} \Bigg).$$

Then, D is antisymmetric with respect to (X,Y) and $(X,Y^{(I,J)})$.

Following a similar argument leading to (5.22),

$$\mathbb{E}\{D \mid X, Y\} = \frac{2}{n(n-1)} W. \tag{5.32}$$

Thus, (4.3) is satisfied with $\lambda = 2/(n(n-1))$ and $R = 0$. Moreover, by exchangeability,

$$\mathbb{E}\{D\Delta\} = 2\,\mathbb{E}\{DW\} = 2\lambda\,\mathbb{E}\{W^2\} = 2\lambda(\widetilde{\sigma}_{n,d}^2 + \sigma_{n,d+1}^2)/\widetilde{\sigma}_n^2. \tag{5.33}$$

Now, by the Cauchy inequality, (5.33) and Lemmas 5.3 and 5.6, and using a similar argument to the proof of (5.26), we have

$$\begin{aligned}
&\mathbb{E}\left|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \mid X, Y, Y'\} - 1\right| \\
&\quad \leqslant \mathbb{E}\left|\frac{1}{2\lambda}\,\mathbb{E}\{D\Delta \mid X, Y, Y'\} - \frac{1}{2\lambda}\,\mathbb{E}\{D\Delta\}\right| + \frac{\widetilde{\sigma}_n^2 - \widetilde{\sigma}_{n,d}^2 - \sigma_{n,d+1}^2}{\widetilde{\sigma}_n^2} \\
&\quad \leqslant Cn^{-1}\frac{k^2\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}.
\end{aligned}$$

With $D^* = |D|$, and by Lemma 5.5 again,

$$\frac{1}{\lambda}\,\mathbb{E}\big|\mathbb{E}\{D^*\Delta \mid X, Y, Y'\}\big| \leqslant Cn^{-1}\frac{k^2\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}.$$

Now, by (5.31) and Lemma 5.3, and similar to (5.28) and (5.29), we have

$$\begin{aligned}
\mathbb{E}\,|U|^2 &\leqslant C\widetilde{\sigma}_n^{-2}\sum_{\ell=d+2}^{k}\mathbb{E}(S_{n,k}^2(f_{(\ell)})) \leqslant Cn^{-2}\frac{k^4\tau^2}{\sigma_{\min}^2}\bigg(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\bigg), \\
\mathbb{E}(U - U^{(i,j)})^2 &\leqslant C\widetilde{\sigma}_n^{-2}\sum_{\ell=d+2}^{k}\mathbb{E}\{(S_{n,k}(f_{(\ell)}) - S_{n,k}^{(i,j)}(f_{(\ell)}))^2\} \leqslant Cn^{-4}\frac{k^4\tau^2}{\sigma_{\min}^2}\bigg(\frac{1}{\pi_d}\sum_{\ell=d+1}^{k}\pi_\ell\bigg).
\end{aligned}$$

Thus,

$$\begin{aligned}
&\mathbb{E}\,|U| \leqslant Cn^{-1}\frac{k^2\Lambda_{k,d}\tau^2}{\sigma_{\min}^2}, \\
&\frac{1}{\lambda}\,\mathbb{E}\big|D(U - U^{(I,J)})\big| \\
&\quad = \frac{1}{\widetilde{\sigma}_n}\sum_{(i,j)\in\mathcal{I}_{n,2}}\mathbb{E}\bigg\{\bigg|\bigg(\sum_{(A,B)\in\mathcal{J}_{f,d}\cup\mathcal{J}_{f,d+1}}\ \sum_{\alpha\in\mathcal{A}_{n,v_{A,B}}}\mu_{A,B}\eta_{\alpha(A,B)}^{(i,j)}\bigg)(U - U^{(i,j)})\bigg|\bigg\} \\
&\quad \leqslant Cn^{-1}\frac{k^2\Lambda_{k,d}\tau^2}{\sigma_{\min}^2},
\end{aligned}$$

where the last inequality follows from (5.12). Applying Corollary 4.3, we obtain the desired result. □

6 Proof of other results

6.1 Proof of Theorem 3.2

Note that there is no X involved in the function g, and it follows that the principle degree is at least 2. As f_F^{inj} does not dependent on X if $\kappa \equiv p$ for some $0 < p < 1$. Fix F. Define

$$g^{\mathrm{inj}}(Y) = f_F^{\mathrm{inj}}(X; Y)$$

and by Proposition 5.2, we have g^{inj} has the following decomposition:

$$g^{\mathrm{inj}}(Y) = \sum_{B\subset[k]_2} g^{\mathrm{inj}}_B(Y_B). \tag{6.1}$$

By [13, p. 361], we have

$$\begin{aligned} g^{\mathrm{inj}}_{\{(1,2)\}}(y_{1,2}) &= \mathbb{E}\{g^{\mathrm{inj}}(Y)|Y_{1,2} = y_{1,2}\} \\ &= \frac{2e(F)(v(F)-2)!}{|\mathrm{Aut}(G)|} p^{e(F)-1}(\mathbb{1}(y_{1,2} \leqslant p) - p) \neq 0. \end{aligned}$$

Therefore, by Theorem 2.4 with $d = 2$, we complete the proof.

6.2 Proof of Theorem 3.3

Again, let

$$g^{\mathrm{ind}}(Y) = f^{\mathrm{ind}}_F(X;Y),$$

and similar to (6.1), we have

$$g^{\mathrm{ind}}(Y) = \sum_{B\subset[k]_2} g^{\mathrm{ind}}_B(Y_B).$$

Recall that $s(F)$ is the number of 2-stars in F and $t(F)$ is the number of triangles in F. Let

$$\bar{e}(F) = \binom{v(F)}{2}^{-1} e(F), \quad \bar{s}(F) = \binom{v(F)}{3}^{-1} \frac{s(F)}{3}, \quad \bar{t}(F) = \binom{v(F)}{3}^{-1} t(F).$$

Let

$$N(F) = \frac{v(F)!}{|\mathrm{Aut}(F)|} p^{e(F)}(1-p)^{\binom{v(F)}{2}-e(F)}.$$

By Section 9 of [13], letting $B_1 = \{(1,2)\}$, $B_2 = \{(1,2),(1,3)\}$ and $B_3 = \{(1,2),(1,3),(2,3)\}$, we have

$$\begin{aligned} g^{\mathrm{ind}}_{B_1}(y_{1,2}) &= \mathbb{E}\{g^{\mathrm{ind}}(Y)|Y_{1,2} = y_{1,2}\} \\ &= \frac{N(F)}{p(1-p)}(\bar{e}(F) - p)\big(\mathbb{1}(y_{1,2} \leqslant p) - p\big), \\ g^{\mathrm{ind}}_{B_2}(y_{1,2}, y_{1,3}) &= \mathbb{E}\{g^{\mathrm{ind}}(Y)|Y_{1,2} = y_{1,2}, Y_{1,3} = y_{1,3}\} \\ &= \frac{N(F)}{p^2(1-p)^2}(\bar{s}(F) - 2p\bar{e}(F) + p^2)\big(\mathbb{1}(y_{1,2} \leqslant p) - p\big)\big(\mathbb{1}(y_{1,3} \leqslant p) - p\big), \\ g^{\mathrm{ind}}_{B_3}(y_{1,2}, y_{1,3}, y_{2,3}) &= \mathbb{E}\{g^{\mathrm{ind}}(Y)|Y_{1,2} = y_{1,2}, Y_{1,3} = y_{1,3}, Y_{2,3} = y_{2,3}\} \\ &= \frac{N(F)}{p^3(1-p)^3}(\bar{t}(F) - 3p\bar{s}(F) + 3p^2\bar{e}(F) - p^3) \\ &\qquad \times \big(\mathbb{1}(y_{1,2} \leqslant p) - p\big)\big(\mathbb{1}(y_{1,3} \leqslant p) - p\big)\big(\mathbb{1}(y_{2,3} \leqslant p) - p\big). \end{aligned}$$

We now consider the following three cases.

Case 1. If $e(F) \neq p\binom{v(F)}{2}$. In this case, we have $g^{\mathrm{ind}}_{B_1} \not\equiv 0$. Then, by Theorem 2.4, we have (3.2) holds.

Case 2. If $\bar{e}(F) = p$ and $\bar{s}(F) \neq p^2$. In this case, we have

$$g^{\mathrm{ind}}_{B_1} \equiv 0, \quad g^{\mathrm{ind}}_{B_2} \not\equiv 0.$$

However, the graph generated by B_2 is a 2-star, which is not strongly connected. Then, by Theorem 2.3, we have (3.3) holds.

Case 3. If $\bar{e}(F) = p$, $\bar{s}(F) = p^2$ and $\bar{t}(F) \neq p^3$. In this case, we have

$$g_{B_1}^{\mathrm{ind}} \equiv 0, \quad g_{B_2}^{\mathrm{ind}} \equiv 0, \quad g_{B_3}^{\mathrm{ind}} \not\equiv 0.$$

Because the graph generated by B_3 is a triangle, which is strongly connected. Then, by Theorem 2.4, we have (3.2) holds.

A Proofs of some lemmas

A.1 Proof of Lemma 5.1

Proof of Lemma 5.1. We write $\{\alpha\} = \{\alpha(1), \ldots, \alpha(k)\}$ for any $\alpha = (\alpha(1), \ldots, \alpha(k)) \in \mathcal{A}_{n,k}$. Also, write $r_\alpha = r(X_{\alpha(1)}, \ldots, X_{\alpha(k)}; Y_{\alpha(1),\alpha(2)}, \ldots, Y_{\alpha(k-1),\alpha(k)})$. Now, observe that

$$\operatorname{Var}\Big\{\sum_{\alpha \in \mathcal{I}_{n,k}} r_\alpha\Big\} = \sum_{\alpha \in \mathcal{I}_{n,k}} \sum_{\alpha' \in \mathcal{I}_{n,k}} \operatorname{Cov}\big(r_\alpha, r_{\alpha'}\big). \tag{A.1}$$

Note that if $\{\alpha\} \cap \{\alpha'\} = \varnothing$, then r_α and $r_{\alpha'}$ are independent, then clearly it follows that

$$\operatorname{Cov}\big(r_\alpha, r_{\alpha'}\big) = 0 \tag{A.2}$$

if $\{\alpha\} \cap \{\alpha'\} = \varnothing$. If there exists $i \in \{1, \ldots, n\}$ such that $\{\alpha\} \cap \{\alpha'\} = \{i\}$, then

$$\operatorname{Cov}\big(r_\alpha, r_{\alpha'}\big) = \mathbb{E}\Big\{\operatorname{Cov}\big(r_\alpha, r_{\alpha'} \;\big|\; X_i\big)\Big\} + \operatorname{Cov}\big(\mathbb{E}\{r_\alpha | X_i\}, \mathbb{E}\{r_{\alpha'} | X_i\}\big). \tag{A.3}$$

By independence, we have the first term of (A.3) is 0. For the second term, note that for any $i \in \{\alpha\}$, then $\mathbb{E}\{r_\alpha | X_i\} = 0$, and thus the second term of (A.3) is also 0. Therefore,

$$\operatorname{Cov}\big(r_\alpha, r_{\alpha'}\big) = 0, \text{ if } |\{\alpha\} \cap \{\alpha'\}| = 1. \tag{A.4}$$

For any α and α' such that $|\{\alpha\} \cap \{\alpha'\}| \geqslant 2$, by the Cauchy inequality, we have

$$\operatorname{Cov}\big(r_\alpha, r_{\alpha'}\big) \leqslant \sqrt{\operatorname{Var}\big(r_\alpha\big) \operatorname{Var}\big(r_{\alpha'}\big)} = \operatorname{Var}\big(r_\alpha\big),$$

where the equality follows from the fact that $r_\alpha \overset{d.}{=} r_{\alpha'}$. Recall that r_α and $f_1(X_j)$ are orthogonal for every $j \in \{\alpha\}$. By (5.1), we have

$$\operatorname{Var}\big(r_\alpha\big) = \operatorname{Var}\big(\psi(X_{\alpha(1)}, \ldots, X_{\alpha(k)}; Y_{\alpha(1),\alpha(2)}, \ldots, Y_{\alpha(k-1),\alpha(k)})\big) - \sum_{j \in \{\alpha\}} \mathbb{E}\{f_1(X_j)^2\} \leqslant \tau^2.$$

Thus, it follows that

$$\big|\operatorname{Cov}\big(r_\alpha, r_{\alpha'}\big)\big| \leqslant \tau^2, \text{ if } |\{\alpha\} \cap \{\alpha'\}| \geqslant 2. \tag{A.5}$$

Moreover, note that

$$\begin{aligned}
&\sum_{\alpha\in\mathcal{I}_{n,k}}\sum_{\alpha'\in\mathcal{I}_{n,k}}\mathbb{1}(|\{\alpha\}\cap\{\alpha'\}|\geqslant 2)\\
&\quad=\sum_{t=2}^{k}\sum_{\alpha\in\mathcal{I}_{n,k}}\sum_{\alpha'\in\mathcal{I}_{n,k}}\mathbb{1}(|\{\alpha\}\cap\{\alpha'\}|=t)\\
&\quad=\sum_{t=2}^{k}\binom{n}{k}\binom{n-k}{k-t}\binom{k}{t}\\
&\quad=\sum_{u=0}^{k-2}\binom{n}{k}\binom{n-k}{k-u-2}\binom{k}{u+2}\\
&\quad=\sum_{u=0}^{k-2}\binom{n}{k}\frac{k(k-1)}{(u+2)(u+1)}\binom{n-k}{k-u-2}\binom{k-2}{u}\\
&\quad\leqslant\binom{k}{2}\binom{n}{k}\sum_{u=0}^{k-2}\binom{n-k}{k-u-2}\binom{k-2}{u}=\binom{k}{2}\binom{n}{k}\binom{n-2}{k-2},
\end{aligned}\tag{A.6}$$

where in the last line we used the fact that

$$\binom{n}{k}=\sum_{t=0}^{k}\binom{n-k}{k-t}\binom{k}{t}\quad\text{for all } n\geqslant k.$$

Combining (5.2), (A.1), (A.2) and (A.4)–(A.6), we have

$$\begin{aligned}
\mathbb{E}\{U^2\}&\leqslant\frac{\tau^2}{\widetilde{\sigma}_n^2}\sum_{\alpha\in\mathcal{I}_{n,k}}\sum_{\alpha'\in\mathcal{I}_{n,k}}\mathbb{1}(|\{\alpha\}\cap\{\alpha'\}|\geqslant 2)\\
&=\frac{n\tau^2}{k^2\sigma_1^2}\binom{k}{2}\binom{n}{k}^{-1}\binom{n-2}{k-2}\\
&=\frac{(k-1)^2\tau^2}{2(n-1)\sigma_1^2}.
\end{aligned}\tag{A.7}$$

This proves (5.3).

Now we prove (5.4). Let $\mathcal{I}_{n,k}^{(i)}=\{\alpha=\{\alpha(1),\dots,\alpha(k)\}:\alpha(1)<\cdots<\alpha(k), i\in\{\alpha\}\}$. Note that

$$U-U^{(i)}=\frac{1}{\widetilde{\sigma}_n}\sum_{\alpha\in\mathcal{I}_{n,k}^{(i)}}r_{\{\alpha\}}^{(i)}.$$

where

$$r_\alpha^{(i)}=r_\alpha-r(X_{\alpha(1)}^{(i)},\dots,X_{\alpha(k)}^{(i)};Y_{\alpha(1),\alpha(2)},\dots,Y_{\alpha(k-1),\alpha(k)}).$$

For each $\alpha\in\mathcal{I}_{n,k}^{(i)}$, by independence and the definition of $r_\alpha^{(i)}$, we have

$$\mathbb{E}\{r_\alpha^{(i)}|X_j,j\in\{\alpha\}\setminus\{i\},Y_{\alpha(1),\alpha(2)},\dots,Y_{\alpha(k-1),\alpha(k)}\}=0.$$

Therefore, for $\alpha\in\mathcal{I}_{n,k}^{(i)}$, we have

$$\begin{aligned}
\operatorname{Var}\bigl(r_\alpha^{(i)}\bigr)&=\mathbb{E}\bigl\{\operatorname{Var}\bigl(r_\alpha^{(i)}\bigm| X_j,j\in\{\alpha\}\setminus\{i\},Y_{\alpha(1),\alpha(2)},\dots,Y_{\alpha(k-1),\alpha(k)}\bigr)\bigr\}\\
&\quad+\operatorname{Var}\bigl(\mathbb{E}\bigl\{r_\alpha^{(i)}\bigm| X_j,j\in\{\alpha\}\setminus\{i\},Y_{\alpha(1),\alpha(2)},\dots,Y_{\alpha(k-1),\alpha(k)}\bigr\}\bigr)\\
&=2\,\mathbb{E}\bigl\{\operatorname{Var}\bigl(r_\alpha\bigm| X_j,j\in\{\alpha\}\setminus\{i\},Y_{\alpha(1),\alpha(2)},\dots,Y_{\alpha(k-1),\alpha(k)}\bigr)\bigr\}\\
&\leqslant 2\operatorname{Var}\bigl(r_\alpha\bigr)\leqslant 2\tau^2.
\end{aligned}$$

Similar to (A.4), we have

$$\mathrm{Cov}\big(r_\alpha^{(i)}, r_{\alpha'}^{(i)}\big) = 0 \quad \text{if } |\{\alpha\} \cap \{\alpha'\}| = 1.$$

Moreover, we have for fixed i,

$$\begin{aligned}
&\sum_{\alpha \in \mathcal{I}_{n,k}^{(i)}} \sum_{\alpha' \in \mathcal{I}_{n,k}^{(i)}} \mathbb{1}(|\{\alpha\} \cap \{\alpha'\}| \geqslant 2) \\
&\quad = \sum_{t=2}^{k} \sum_{\alpha \in \mathcal{I}_{n,k}^{(i)}} \sum_{\alpha' \in \mathcal{I}_{n,k}^{(i)}} \mathbb{1}(|\{\alpha\} \cap \{\alpha'\}| = t) \\
&\quad = \sum_{t=2}^{k} \binom{n-1}{k-1}\binom{n-k}{k-t}\binom{k-1}{t-1} \\
&\quad = \sum_{u=0}^{k-2} \binom{n-1}{k-1}\binom{n-k}{k-u-2}\binom{k-1}{u+1} \\
&\quad = \sum_{u=0}^{k-2} \frac{k-1}{u+1}\binom{n-1}{k-1}\binom{n-k}{k-u-2}\binom{k-2}{u} \\
&\quad \leqslant (k-1)\binom{n-1}{k-1}\binom{n-2}{k-2}.
\end{aligned}$$

Similar to (A.7), we have

$$\begin{aligned}
\mathbb{E}\{(U - U^{(i)})^2\} &= \frac{1}{\widetilde{\sigma}_n^2} \sum_{\alpha \in \mathcal{I}_{n,k}^{(i)}} \sum_{\alpha' \in \mathcal{I}_{n,k}^{(i)}} \mathrm{Cov}\big(r_\alpha^{(i)}, r_{\alpha'}^{(i)}\big) \\
&\leqslant \frac{2n\tau^2}{k^2\sigma_1^2}\binom{n}{k}^{-2} \sum_{\alpha \in \mathcal{I}_{n,k}^{(i)}} \sum_{\alpha' \in \mathcal{I}_{n,k}^{(i)}} \mathbb{1}(|\{\alpha\} \cap \{\alpha'\}| \geqslant 2) \\
&\leqslant \frac{2n(k-1)\tau^2}{k^2\sigma_1^2}\binom{n}{k}^{-2}\binom{n-1}{k-1}\binom{n-2}{k-2} \\
&= \frac{2(k-1)^2\tau^2}{n(n-1)\sigma_1^2}.
\end{aligned}$$

This completes the proof. □

A.2 Proof of Lemmas 5.4 and 5.5

Recall that $\{\alpha\} = \{\alpha(1), \dots, \alpha(\ell)\}$ for $\alpha \in \mathcal{A}_{n,\ell}$. To prove Lemma 5.4, we need the following lemma. In this subsection, we denote by C a positive absolute constant that may take different values in different places.

Lemma A.1. *Let $(A_1, B_1), (A_2, B_2) \in \mathcal{J}_{f,d}$, $(i,j), (i',j') \in \mathcal{A}_{n,2}$, $\alpha_1, \alpha_2 \in \mathcal{A}_{n,d}^{(i,j)}$ and $\alpha_1', \alpha_2' \in \mathcal{A}_{n,d}^{(i',j')}$. Let*

$$s = |\{\alpha_1\} \cap \{\alpha_2\}|, \quad t = |\{\alpha_1'\} \cap \{\alpha_2'\}|.$$

If $|(\{\alpha_1\} \cup \{\alpha_2\}) \cap (\{\alpha_1'\} \cap \{\alpha_2'\})| \leqslant 2d - (s+t)$, then

$$\mathrm{Cov}\Big\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}, \xi_{\alpha_1'(A_1,B_1)}^{(i',j')}\xi_{\alpha_2'(A_2,B_2)}^{(i',j')}\Big\} = 0. \tag{A.8}$$

Proof of Lemma A.1. Let

$$\begin{aligned}
V_0 &= \{\alpha_1\} \cap \{\alpha_2\}, \quad V_1 = \{\alpha_1\} \setminus V_0, \quad V_2 = \{\alpha_2\} \setminus V_0, \quad s = |V_0|, \\
V_0' &= \{\alpha_1'\} \cap \{\alpha_2'\}, \quad V_1' = \{\alpha_1'\} \setminus V_0', \quad V_2' = \{\alpha_2'\} \setminus V_0', \quad t = |V_0'|.
\end{aligned} \tag{A.9}$$

Then, we have $V_1 \cap V_2 = \varnothing$, $V_1' \cap V_2' = \varnothing$, $2 \leqslant s, t \leqslant d$. Without loss of generality, assume that $s \leqslant t$.

If $2d - (s+t) = 0$, which is equivalent to $s = d, t = d$, then $\{\alpha_1\} = \{\alpha_2\}$ and $\{\alpha_1'\} = \{\alpha_2'\}$. If $\{a_1\} \cap \{a_1'\} = \varnothing$, then $(\xi^{(i,j)}_{\alpha_1(A_1,B_1)}, \xi^{(i,j)}_{\alpha_2(A_2,B_2)})$ and $(\xi^{(i',j')}_{\alpha_1'(A_1,B_1)}, \xi^{(i',j')}_{\alpha_2'(A_2,B_2)})$ are independent, which implies that (A.8) holds.

If $2d - (s+t) > 0$ and $|(\{\alpha_1\} \cup \{\alpha_2\}) \cap (\{\alpha_1'\} \cup \{\alpha_2'\})| < 2d - (s+t)$, then there exists $r \in [n]$ such that $r \in (V_1' \cup V_2') \setminus (\{\alpha_1, \alpha_2\})$. Now, assume that $r \in V_2' \setminus (\{\alpha_1, \alpha_2\})$ without loss of generality. Let

$$\mathcal{F}_r = \sigma(X_p, Y_{p,q}, p, q \in [n] \setminus \{r\}) \vee \sigma(Y'_{i',j'}). \tag{A.10}$$

Therefore, we have $\xi^{(i,j)}_{\alpha_1(A_1,B_1)}, \xi^{(i,j)}_{\alpha_2(A_2,B_2)}, \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \in \mathcal{F}_r$. Then, by (5.6),

$$\begin{aligned}
&\mathbb{E}\{\xi^{(i',j')}_{\alpha_2'(A_2,B_2)} \,|\, \mathcal{F}_r\} \\
&= \mathbb{E}\Big\{ f_{A_2,B_2}\big(X_{\alpha_2'(A_2,B_2)}; Y_{\alpha_2'(A_2,B_2)}\big) - f_{A_2,B_2}\big(X_{\alpha_2'(A_2,B_2)}; Y^{(i',j')}_{\alpha_2'(A_2,B_2)}\big) \;\Big|\; \mathcal{F}_r \Big\} \\
&= 0.
\end{aligned} \tag{A.11}$$

Hence,

$$\mathbb{E}\Big\{\xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)} \,|\, \mathcal{F}_r\Big\} = 0,$$

which further implies that

$$\mathbb{E}\Big\{\xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)}\Big\} = 0,$$

and

$$\begin{aligned}
&\mathrm{Cov}\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)}, \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)}\} \\
&\quad = \mathbb{E}\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)}\} \\
&\quad = \mathbb{E}\Big\{\mathbb{E}\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)} \,|\, \mathcal{F}_r\}\Big\} \\
&\quad = \mathbb{E}\Big\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \,\mathbb{E}\{\xi^{(i',j')}_{\alpha_2'(A_2,B_2)} \,|\, \mathcal{F}_r\}\Big\} \\
&\quad = 0.
\end{aligned} \tag{A.12}$$

If $2d-(s+t) > 0$ and $|(\{\alpha_1\} \cup \{\alpha_2\}) \cap (\{\alpha_1'\} \cap \{\alpha_2'\})| = 2d-(s+t)$, then either the following two conditions holds: (a) there exists $r \in V_1' \cup V_2' \setminus (\{\alpha_1\} \cup \{\alpha_2\})$ or (b) $V_0 \cap V_0' = \varnothing$. If (a) holds, then following a similar argument that leading to (A.12), we have (A.8) holds.

If (b) is true, letting $\mathcal{F} = \sigma(X, \{Y_{p,q} : p, q \in V_1 \cup V_2 \cup V_1' \cup V_2'\})$, we have conditional on $\mathcal{F}$, $(\xi^{(i,j)}_{\alpha_1(A_1,B_1)}, \xi^{(i,j)}_{\alpha_2(A_2,B_2)})$ is conditionally independent of $(\xi^{(i',j')}_{\alpha_1'(A_1,B_1)}, \xi^{(i',j')}_{\alpha_2'(A_2,B_2)})$, and thus,

$$\begin{aligned}
&\mathrm{Cov}\Big\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)}, \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)}\Big\} \\
&\qquad = \mathrm{Cov}\Big\{\mathbb{E}\Big\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \,|\, \mathcal{F}\Big\}, \mathbb{E}\Big\{\xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)} \,|\, \mathcal{F}\Big\}\Big\}.
\end{aligned}$$

Without loss of generality, we assume that $V_1 \cup V_2 \cup V_1' \cup V_2' \neq \varnothing$, otherwise the argument is even simpler. Moreover, we may assume that $V_1 \neq \varnothing$. Let $\mathcal{F}_0 = \sigma(Y'_{i,j}, Y_{p,q} : p, q \in V_0)$, and we have $\xi^{(i,j)}_{\alpha_1(A_1,B_1)}$ and $\xi^{(i,j)}_{\alpha_2(A_2,B_2)}$ are conditionally independent given $\mathcal{F} \vee \mathcal{F}_0$. Moreover, by (5.6), $\mathbb{E}\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \,|\, \mathcal{F} \vee \mathcal{F}_0\} = \mathbb{E}\{\xi^{(i,j)}_{\alpha_2(A_2,B_2)} \,|\, \mathcal{F} \vee \mathcal{F}_0\} = 0$, and thus $\mathbb{E}\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \,|\, \mathcal{F}\} = 0$. Therefore, we have under the condition (b),

$$\mathrm{Cov}\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)} \xi^{(i,j)}_{\alpha_2(A_2,B_2)}, \xi^{(i',j')}_{\alpha_1'(A_1,B_1)} \xi^{(i',j')}_{\alpha_2'(A_2,B_2)}\} = 0. \tag{A.13}$$

Combining (A.12) and (A.13) we prove that (A.8) holds for $|\{\alpha_1,\alpha_2\}\cap\{\alpha_1',\alpha_2'\}| = 2d-(s+t)$. This completes the proof. $\square$

Proof of Lemma 5.4. In this proof, we denote by C a constant depending on k and d, which may take different values in different places. For $\alpha_1,\alpha_2,\alpha_1',\alpha_2' \in \mathcal{A}_{n,d}^{(i,j)}$, let s,t be defined as in Lemma A.1, and note that $\{\alpha_1\}$ and $\{\alpha_2\}$ has at least one common element $\{i,j\}$, and $\{\alpha_1'\}$ and $\{\alpha_2'\}$ has at least one two common elements $\{i',j'\}$, we have $2\leqslant s,t\leqslant d$. and

$$
\begin{aligned}
&\operatorname{Var}\Big\{\sum_{(i,j)\in\mathcal{A}_{n,2}}\Big(\sum_{\alpha_1\in\mathcal{A}_{n,d}^{(i,j)}}\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\Big)\Big(\sum_{\alpha_2\in\mathcal{A}_{n,d}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\Big)\Big\}\\
&= \sum_{\substack{(i,j)\in\mathcal{A}_{n,2}\\(i',j')\in\mathcal{A}_{n,2}}}\ \sum_{\substack{\alpha_1\in\mathcal{A}_{n,d}^{(i,j)}\\ \alpha_2\in\mathcal{A}_{n,d}^{(i,j)}}}\ \sum_{\substack{\alpha_1'\in\mathcal{A}_{n,d}^{(i',j')}\\ \alpha_2'\in\mathcal{A}_{n,d}^{(i',j')}}}\operatorname{Cov}\big\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_2(A_2,B_2)}^{(i,j)},\xi_{\alpha_1'(A_1,B_1)}^{(i',j')}\xi_{\alpha_2'(A_2,B_2)}^{(i',j')}\big\}\\
&= \sum_{s,t=2}^{d}\ \sum_{\substack{(i,j)\in\mathcal{A}_{n,2}\\(i',j')\in\mathcal{A}_{n,2}}}\ \sum_{\substack{\alpha_1\in\mathcal{A}_{n,d}^{(i,j)}\\ \alpha_2\in\mathcal{A}_{n,d}^{(i,j)}}}\ \sum_{\substack{\alpha_1'\in\mathcal{A}_{n,d}^{(i',j')}\\ \alpha_2'\in\mathcal{A}_{n,d}^{(i',j')}}} \qquad\qquad\qquad\qquad (A.14)\\
&\quad\times\operatorname{Cov}\big\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_2(A_2,B_2)}^{(i,j)},\xi_{\alpha_1'(A_1,B_1)}^{(i',j')}\xi_{\alpha_2'(A_2,B_2)}^{(i',j')}\big\}\mathbb{1}(O_{s,t}), \qquad\qquad (A.15)
\end{aligned}
$$

where $O_{s,t}=\{|\{\alpha_1\}\cap\{\alpha_2\}|=s\}\cap\{|\{\alpha_1'\}\cap\{\alpha_2'\}|=t\}$. If $|(\{\alpha_1\}\cup\{\alpha_2\})\cap(\{\alpha_1'\}\cap\{\alpha_2'\})|\leqslant 2d-(s+t)$, by (A.8) in Lemma A.1, we have

$$
\operatorname{Cov}\big\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_2(A_2,B_2)}^{(i,j)},\xi_{\alpha_1'(A_1,B_1)}^{(i',j')}\xi_{\alpha_2'(A_2,B_2)}^{(i',j')}\big\}=0.
$$

If $|(\{\alpha_1\}\cup\{\alpha_2\})\cap(\{\alpha_1'\}\cap\{\alpha_2'\})|>2d-(s+t)$, then, recalling that $(\xi_{\alpha_1(A_1,B_1)}^{(i,j)},\xi_{\alpha_2(A_2,B_2)}^{(i,j)})\overset{d.}{=}(\xi_{\alpha_1'(A_1,B_1)}^{(i',j')},\xi_{\alpha_2'(A_2,B_2)}^{(i',j')})$, we have

$$
\begin{aligned}
&\big|\operatorname{Cov}\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_2(A_2,B_2)}^{(i,j)},\xi_{\alpha_1'(A_1,B_1)}^{(i',j')}\xi_{\alpha_2'(A_2,B_2)}^{(i',j')}\}\big|\\
&\leqslant\mathbb{E}\{(\xi_{\alpha_1(A_1,B_1)}^{(i,j)})^2(\xi_{\alpha_2(A_2,B_2)}^{(i,j)})^2\}\\
&\leqslant C\big(\mathbb{E}\{\psi_{A_1,B_1}^4(X_{\alpha_1(A_1,B_1)};Y_{\alpha_1(A_1,B_1)})\}+\mathbb{E}\{\psi_{A_1,B_1}^4(X_{\alpha_2(A_2,B_2)};Y_{\alpha_2(A_2,B_2)})\}\big)\\
&\leqslant C\tau^4. \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (A.16)
\end{aligned}
$$

Therefore, with

$$
O_1=\{|(\{\alpha_1\}\cup\{\alpha_2\})\cap(\{\alpha_1'\}\cup\{\alpha_2'\})|>2d-(s+t)\},
$$

we have

$$
\begin{aligned}
&\operatorname{Var}\Big\{\sum_{(i,j)\in\mathcal{A}_{n,2}}\Big(\sum_{\alpha\in\mathcal{A}_{n,d}^{(i,j)}}\xi_{\alpha(A_1,B_1)}^{(i,j)}\Big)\Big(\sum_{\alpha\in\mathcal{A}_{n,d}^{(i,j)}}\xi_{\alpha(A_1,B_1)}^{(i,j)}\Big)\Big\}\\
&\leqslant C\tau^4\sum_{s,t=0}^{d}\ \sum_{\substack{(i,j)\in\mathcal{A}_{n,2}\\(i',j')\in\mathcal{A}_{n,2}}}\ \sum_{\substack{\alpha_1\in\mathcal{A}_{n,d}^{(i,j)}\\ \alpha_2\in\mathcal{A}_{n,d}^{(i,j)}}}\ \sum_{\substack{\alpha_1'\in\mathcal{A}_{n,d}^{(i',j')}\\ \alpha_2'\in\mathcal{A}_{n,d}^{(i',j')}}}\mathbb{1}(O_1\cap O_{s,t})\\
&\leqslant C\tau^4\sum_{s,t=0}^{d}n^{(2d-s)+(2d-t)-(2d-s-t+1)}\\
&\leqslant Ck^2n^{2d-1}\tau^4.
\end{aligned}
$$

$\square$

Proof of Lemma 5.5. If $k < d+1$, then it follows that $\xi_{\alpha(G)} = 0$ for all $G \in \Gamma_{d+1}$ and $\alpha \in \mathcal{A}_{n,d+1}$. Therefore, we assume $k \geqslant d+1$ without loss of generality.

Observe that

$$\begin{aligned}
&\mathrm{Var}\left\{ \sum_{(i,j)\in\mathcal{A}_{n,2}} \left(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}} \xi^{(i,j)}_{\alpha_1(A_1,B_1)} \right) \left| \sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \right| \right\} \\
&\quad = \sum_{(i,j)\in\mathcal{A}_{n,2}} \sum_{(i',j')\in\mathcal{A}_{n,2}} \mathrm{Cov}\left\{ \left(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}} \xi^{(i,j)}_{\alpha_1(A_1,B_1)} \right) \left| \sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \right|, \right. \\
&\qquad\qquad \left. \left(\sum_{\alpha'_1\in\mathcal{A}^{(i',j')}_{n,v_1}} \xi^{(i',j')}_{\alpha'_1(A_1,B_1)} \right) \left| \sum_{\alpha'_2\in\mathcal{A}^{(i',j')}_{n,v_2}} \xi^{(i',j')}_{\alpha'_2(A_2,B_2)} \right| \right\}.
\end{aligned} \tag{A.17}$$

Letting

$$\mathcal{F}_1 = \sigma(X) \vee \sigma(Y_{p,q}, Y'_{p,q} : \{p,q\} \neq \{i,j\}),$$

and noting that

$$\left(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}} \xi^{(i,j)}_{\alpha_1(A_1,B_1)} \right) \left| \sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \right|$$

is anti-symmetric with respect to (Y_{ij}, Y'_{ij}), we have

$$\mathbb{E}\left\{ \left(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}} \xi^{(i,j)}_{\alpha_1(A_1,B_1)} \right) \left| \sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \right| \right\} = 0.$$

Now, we consider the following two cases. First, if $\{i,j\} \neq \{i',j'\}$, we have

$$\left(\sum_{\alpha'_1\in\mathcal{A}^{(i',j')}_{n,v_1}} \xi^{(i',j')}_{\alpha'_1(A_1,B_1)} \right) \left| \sum_{\alpha'_2\in\mathcal{A}^{(i',j')}_{n,v_2}} \xi^{(i',j')}_{\alpha'_2(A_2,B_2)} \right| \quad \text{is } \mathcal{F}_1 \text{ measurable}$$

and by anti-symmetry again,

$$\mathbb{E}\left\{ \left(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}} \xi^{(i,j)}_{\alpha_1(A_1,B_1)} \right) \left| \sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \right| \;\middle|\; \mathcal{F}_1 \right\} = 0.$$

Therefore,

$$\begin{aligned}
&\mathrm{Cov}\left\{ \left(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}} \xi^{(i,j)}_{\alpha_1(A_1,B_1)} \right) \left| \sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}} \xi^{(i,j)}_{\alpha_2(A_2,B_2)} \right|, \right. \\
&\qquad \left. \left(\sum_{\alpha'_1\in\mathcal{A}^{(i',j')}_{n,v_1}} \xi^{(i',j')}_{\alpha'_1(A_1,B_1)} \right) \left| \sum_{\alpha'_2\in\mathcal{A}^{(i',j')}_{n,v_2}} \xi^{(i',j')}_{\alpha'_2(A_2,B_2)} \right| \right\} = 0
\end{aligned} \tag{A.18}$$

for $\{i,j\} \neq \{i',j'\}$.

It suffices to consider the case where $\{i,j\}=\{i',j'\}$. Observe that

$$\begin{aligned}
&\mathrm{Cov}\Bigg\{\Bigg(\sum_{\alpha_1\in\mathcal{A}_{n,v_1}^{(i,j)}}\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\Bigg)\Bigg|\sum_{\alpha_2\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\Bigg|,\Bigg(\sum_{\alpha_1'\in\mathcal{A}_{n,v_1}^{(i,j)}}\xi_{\alpha_1'(A_1,B_1)}^{(i,j)}\Bigg)\Bigg|\sum_{\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\Bigg|\Bigg\}\\
&\quad=\mathbb{E}\Bigg\{\Bigg(\sum_{\alpha_1\in\mathcal{A}_{n,v_1}^{(i,j)}}\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\Bigg)\Bigg(\sum_{\alpha_1'\in\mathcal{A}_{n,v_1}^{(i,j)}}\xi_{\alpha_1'(A_1,B_1)}^{(i,j)}\Bigg)\\
&\quad\Bigg|\Bigg(\sum_{\alpha_2\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\Bigg)\Bigg(\sum_{\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\Bigg)\Bigg|\Bigg\}\\
&\quad=\sum_{\alpha_1\in\mathcal{A}_{n,v_1}^{(i,j)}}\sum_{\alpha_1'\in\mathcal{A}_{n,v_1}^{(i,j)}}\mathbb{E}\Bigg\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_1'(A_1,B_1)}^{(i,j)}\Bigg|\sum_{\alpha_2\in\mathcal{A}_{n,v_2}^{(i,j)}}\sum_{\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\Bigg|\Bigg\}.
\end{aligned}\tag{A.19}$$

Let $H_1=\{\alpha_1\}\setminus\{\alpha_1'\}$ and $H_1'=\{\alpha_1'\}\setminus\{\alpha_1\}$. Let $t=|\alpha_1\cap\alpha_1'|$, and then we have $2\leqslant t\leqslant v_1$. Now, as

$$\begin{aligned}
\sum_{\alpha_2\in\mathcal{A}_{n,v_2}^{(i,j)}}\sum_{\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}&=\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_1}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\\
&\quad+\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_2}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\\
&\quad+\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_3}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)},
\end{aligned}$$

where $\mathcal{A}_1=\{\alpha_2,\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}:(H_1\cup H_1')\setminus\{\alpha_2,\alpha_2'\}\neq\varnothing\}$, $\mathcal{A}_2=\{\alpha_2,\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}:(H_1\cup H_1')\setminus\{\alpha_2,\alpha_2'\}=\varnothing,\{\alpha_1\}\cap\{\alpha_1'\}\subset\{\alpha_2\}\cap\{\alpha_2'\}\}$, and $\mathcal{A}_3=\{\alpha_2,\alpha_2'\in\mathcal{A}_{n,v_2}^{(i,j)}:(H_1\cup H_1')\setminus\{\alpha_2,\alpha_2'\}=\varnothing,(\{\alpha_1\}\cap\{\alpha_1'\})\setminus(\{\alpha_2\}\cap\{\alpha_2'\})=\varnothing\}$. Given α_1 and α_1'. We have we have to choose at most another $2(t-2)+\{(v_2-v_1)\vee 0\}$ elements to form α_2 and α_2', and then

$$|\mathcal{A}_2|\leqslant Cn^{2(t-2)}(n^{v_2-v_1}\vee 1).$$

If there exists $r\in(H_1\cup H_1')\setminus\{\alpha_2,\alpha_2'\}$, letting $\mathcal{F}_r=\sigma(X_p,Y_{p,q},Y_{p,q}':p,q\in[n]\setminus\{r\})$, then we have

$$\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_1}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\in\mathcal{F}_r,$$

and by orthogonality, we have

$$\mathbb{E}\big\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_1'(A_1,B_1)}^{(i,j)}|\mathcal{F}_r\big\}=0.$$

Therefore, we have

$$\mathbb{E}\Bigg\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_1'(A_1,B_1)}^{(i,j)}\Bigg|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_1}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\Bigg|\Bigg\}=0.$$

Similarly, by independence, we have

$$\mathbb{E}\Bigg\{\xi_{\alpha_1(A_1,B_1)}^{(i,j)}\xi_{\alpha_1'(A_1,B_1)}^{(i,j)}\Bigg|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_3}\xi_{\alpha_2(A_2,B_2)}^{(i,j)}\xi_{\alpha_2'(A_2,B_2)}^{(i,j)}\Bigg|\Bigg\}=0.$$

Hence, by Cauchy's inequality, we have

$$\begin{aligned}&\left|\mathbb{E}\left\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)}\xi^{(i,j)}_{\alpha_1'(A_1,B_1)}\left|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}^{(i,j)}_{n,v_2}}\xi^{(i,j)}_{\alpha_2(A_2,B_2)}\xi^{(i,j)}_{\alpha_2'(A_2,B_2)}\right|\right\}\right|\\&\qquad\leqslant\mathbb{E}\left\{\left|\xi^{(i,j)}_{\alpha_1(A_1,B_1)}\xi^{(i,j)}_{\alpha_1'(A_1,B_1)}\right|\left|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_2}\xi^{(i,j)}_{\alpha_2(A_2,B_2)}\xi^{(i,j)}_{\alpha_2'(A_2,B_2)}\right|\right\}\\&\qquad\leqslant C\tau^2\sqrt{\mathbb{E}\left\{\left|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_2}\xi^{(i,j)}_{\alpha_2(A_2,B_2)}\xi^{(i,j)}_{\alpha_2'(A_2,B_2)}\right|^2\right\}}.\end{aligned}$$

Following the similar argument in the proof of Lemma 5.4, and recalling that $\{\alpha_1\cap\alpha_1'\}=t$ and $|\mathcal{A}_2|\leqslant Cn^{2(t-2)}(n^{v_2-v_1}\vee 1)$, we have

$$\mathbb{E}\left\{\left|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}_2}\xi^{(i,j)}_{\alpha_2(A_2,B_2)}\xi^{(i,j)}_{\alpha_2'(A_2,B_2)}\right|^2\right\}\leqslant Ck^2n^{2(t-2)}(n^{v_2-v_1}\vee 1)\tau^4.$$

Therefore, we have

$$\left|\mathbb{E}\left\{\xi^{(i,j)}_{\alpha_1(A_1,B_1)}\xi^{(i,j)}_{\alpha_1'(A_1,B_1)}\left|\sum_{\alpha_2,\alpha_2'\in\mathcal{A}^{(i,j)}_{n,v_2}}\xi^{(i,j)}_{\alpha_2(A_2,B_2)}\xi^{(i,j)}_{\alpha_2'(A_2,B_2)}\right|\right\}\right|\leqslant Ck^2n^{2(t-2)}(n^{v_2-v_1}\vee 1)\tau^4.$$

Substituting the foregoing inequality to (A.19), we have

$$\begin{aligned}\sum_{(i,j)\in\mathcal{A}_{n,2}}\mathrm{Cov}\Bigg\{&\Bigg(\sum_{\alpha_1\in\mathcal{A}^{(i,j)}_{n,v_1}}\xi^{(i,j)}_{\alpha_1(A_1,B_1)}\Bigg)\Bigg|\sum_{\alpha_2\in\mathcal{A}^{(i,j)}_{n,v_2}}\xi^{(i,j)}_{\alpha_2(A_2,B_2)}\Bigg|,\\&\qquad\Bigg(\sum_{\alpha_1'\in\mathcal{A}^{(i,j)}_{n,v_1}}\xi^{(i,j)}_{\alpha_1'(A_1,B_1)}\Bigg)\Bigg|\sum_{\alpha_2'\in\mathcal{A}^{(i,j)}_{n,v_2}}\xi^{(i,j)}_{\alpha_2'(A_2,B_2)}\Bigg|\Bigg\}\\&\qquad\qquad\leqslant Ck^2n^{2\max\{v_1,v_2\}-2}\tau^4.\end{aligned}\tag{A.20}$$

By (A.17), (A.18) and (A.20), we complete the proof. □

A.3 Proof of Lemma 5.6

Lemma 5.6 follows from a similar argument as that in the proof of Lemma 5.4 and the following lemma. Recall that $\widetilde{\mathcal{J}}_{f,\ell}=\{(A,B)\in\mathcal{J}_{f,\ell}:G_{A,B}\text{ is strongly connected}\}$. Now, as the function g does not depend on X, we set $A_m=\varnothing$ in the following lemma. With a slight abuse of notation, For $j=1,2$ and for $B_m\subset[k]_2$, let G_m be the graph generated by B_m and let v_m be the number of nodes of G_m.

Lemma A.2. *Let $B_m\in\widetilde{\mathcal{J}}_{f,d}\cup\mathcal{J}_{f,d+1}$ for $m=1,2$. Let $(i,j),(i',j')\in\mathcal{A}_{n,2}$, and let $\alpha_m\in\mathcal{A}^{(i,j)}_{n,v_m}$, $\alpha_m'\in\mathcal{A}^{(i',j')}_{n,v_m}$ for $m=1,2$. Let $s=|\{\alpha_1\}\cap\{\alpha_2\}|$ and $t=|\{\alpha_1'\}\cap\{\alpha_2'\}|$. For $m=1,2$, let γ_m indicate that $B_m\in\widetilde{\mathcal{J}}_{f,d}\cup\widetilde{\mathcal{J}}_{f,d+1}$. Then*

$$\mathrm{Cov}\left\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)},\eta^{(i',j')}_{\alpha_1'(B_1)}\eta^{(i',j')}_{\alpha_2'(B_2)}\right\}=0\tag{A.21}$$

for $|\{\alpha_1,\alpha_2\}\cap\{\alpha_1',\alpha_2'\}|<v_1+v_2+\gamma_1+\gamma_2-(s+t)$.

Proof. The proof is similar to that of Lemma A.1.

Let $V_0,V_0',V_1,V_1',V_2,V_2'$ be defined as in (A.9). Note that if G_B has isolated nodes, then $\eta_{\alpha(B)}=0$ for all $\alpha\in\mathcal{A}_{n,v_B}$, where v_B is the number of nodes of the graph generated by the index set B. If $v_1+v_2=s+t$, then it follows that $\{\alpha_1\}=\{\alpha_2\}$ and $\{\alpha'_1\}=\{\alpha'_2\}$. If $|\{\alpha_1\}\cap\{\alpha'_1\}|<2$, then $\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}$ and $\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}$ are independent, which further implies that (A.21) holds.

Now we consider the case where $v_1+v_2>s+t$. If $|\{\alpha_1,\alpha_2\}\cap\{\alpha'_1,\alpha'_2\}|<v_1+v_2-(s+t)$, then following the same argument as that leading to (A.12), we have (A.21) holds.

If G_1 is connected and $|\{\alpha_1,\alpha_2\}\cap\{\alpha'_1,\alpha'_2\}|=v_1+v_2-(s+t)$, then either the following two conditions holds: (a) there exists $r\in V'_2\setminus(\{\alpha_1\}\cup\{\alpha_2\}\cup V'_0\cup V'_1)$ or (b) $V_0\cap V'_0=\varnothing$. If (a) holds, then following a similar argument as before, we have (A.21) holds. Now we consider that the case where (b) holds. Let $H_1=\{(p,q):p\in V_0,q\in V_1\}$ and

$$\mathcal{F}_1=\sigma(Y_{p,q},Y'_{p,q},:\mathcal{A}_{n,2}\setminus H_1).$$

By orthogonality, we have $\mathbb{E}\{\eta^{(i,j)}_{\alpha_1(B_1)}|\mathcal{F}_1\}=0$.

Note that $\eta_{\alpha_2(B_2)},\eta_{\alpha'_1(B_1)},\eta_{\alpha'_2(B_2)}\in\mathcal{F}_1$, we have

$$\begin{aligned}\mathbb{E}\Big\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}\Big\}&=\mathbb{E}\Big\{\eta^{(i,j)}_{\alpha_2(B_2)}\,\mathbb{E}\Big\{\eta^{(i,j)}_{\alpha_1(B_1)}\;\Big|\;\mathcal{F}_1\Big\}\Big\}=0,\\ \mathrm{Cov}\Big\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)},\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}\Big\}&=\mathbb{E}\Big\{\mathbb{E}\Big\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}\;\Big|\;\mathcal{F}_1\Big\}\\&=\mathbb{E}\Big\{\eta^{(i,j)}_{\alpha_2(B_2)}\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}\,\mathbb{E}\Big\{\eta^{(i,j)}_{\alpha_1(B_1)}\;\Big|\;\mathcal{F}_1\Big\}\Big\}=0.\end{aligned}$$

This proves (A.21) for the case where $|\{\alpha_1,\alpha_2\}\cap\{\alpha'_1,\alpha'_2\}|=v_1+v_2-(s+t)$.

Now, we further assume that $\gamma_1=\gamma_2=1$. If G_1 or G_2 is a graph containing one single edge, then the proof is even simpler. Without loss of generality, we now assume that $G^{(r)}_m$ is connected for every $r\in[n]$ for $m=1,2$. We then prove that (A.21) holds when $|\{\alpha_1,\alpha_2\}\cap\{\alpha'_1,\alpha'_2\}|=v_1+v_2-(s+t)+1$. Under this condition, additional to (a) and (b), there is still another event that may happen: (c) there exists $r\in[n]$ such that $\{r\}=V_0\cap V'_0$. As the cases (a) and (b) have been discussed, we only need to prove that (A.21) holds under (c).

As $\{i,j\}\subset V_0$, we have $s\geqslant 2$, and $V_0\setminus\{r\}$ is not empty. Let

$$\mathcal{F}_2=\sigma\{Y_{p,q},Y'_{p,q}:p\in V_1\cup V_2\cup V'_1\cup V'_2,q\in V_1\cup V_2\cup V'_1\cup V'_2\cup\{r\}\}.$$

Then, conditional on $\mathcal{F}_2$, we have $\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}$ and $\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}$ are conditionally independent. Hence,

$$\begin{aligned}&\mathrm{Cov}\Big\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)},\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}\Big\}\\&\quad=\mathrm{Cov}\Big\{\mathbb{E}\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}|\mathcal{F}_2\},\mathbb{E}\{\eta^{(i',j')}_{\alpha'_1(B_1)}\eta^{(i',j')}_{\alpha'_2(B_2)}|\mathcal{F}_2\}\Big\}.\end{aligned}$$

Letting

$$\mathcal{F}_3=\sigma\{Y_{p,q},Y_{p,q}:p\in V_0\setminus\{r\},q\in V_2\cup\{r\}\}.$$

Now, if $G^{(r)}_1$ is connected for every $r\in[n]$, there is at least one edge in G_1 connecting $V_0\setminus\{r\}$ and V_1, and thus

$$\mathbb{E}\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}|\mathcal{F}_2\vee\mathcal{F}_3\}=\eta^{(i,j)}_{\alpha_2(B_2)}\,\mathbb{E}\{\eta^{(i,j)}_{\alpha_1(B_1)}|\mathcal{F}_2\vee\mathcal{F}_3\}=0,$$

where the last equality follows from orthogonality. Noting that $\mathcal{F}_2\subset\mathcal{F}_3$, then $\mathbb{E}\{\eta^{(i,j)}_{\alpha_1(B_1)}\eta^{(i,j)}_{\alpha_2(B_2)}|\mathcal{F}_2\}=0$ and thus (A.21) holds. $\square$

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