A Multivariate CLT for Dissociated Sums with Applications to $U$-Statistics and Random Complexes

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Abstract

Acyclic partial matchings on simplicial complexes play an important role in topological data analysis by facilitating efficient computation of (persistent) homology groups. Here we describe probabilistic properties of critical simplex counts for such matchings on clique complexes of Bernoulli random graphs. In order to accomplish this goal, we generalise the notion of a dissociated sum to a multivariate setting and prove an abstract multivariate central limit theorem using Stein’s method. As a consequence of this general result, we are able to extract central limit theorems not only for critical simplex counts, but also for generalised $U$-statistics (and hence for clique counts in Bernoulli random graphs) as well as simplex counts in the link of a fixed simplex in a random clique complex.

1 Introduction

The task of efficiently computing simplicial homology groups has received considerable attention over the last two decades. Much of the impetus for recent computational advances [31] has come from topological data analysis [8]; here filtered simplicial complexes are built around data sets for the purposes of extracting persistent homology barcodes [17, 32], which serve as multi-scale topological descriptors of the underlying geometry. At their core, all such homology computations reduce to the study of chain complexes, which are sequences of the form

$$\cdots \xrightarrow{d_{i+1}} C_i \xrightarrow{d_i} C_{i-1} \xrightarrow{d_{i-1}} \cdots \xrightarrow{d_2} C_1 \xrightarrow{d_1} C_0.$$ 

Here $C_i$ is a vector space whose dimension equals the number of $i$-simplices in a given simplicial complex $L$, whereas $d_i : C_i \to C_{i-1}$ is an incidence matrix encoding which $(i-1)$-simplices lie in the boundary of a given $i$-simplex. These matrices satisfy the property that every successive composite $d_{i+1} \circ d_i$ equals zero, and the desired homology groups of $L$ are given by the quotient vector spaces $\text{ker} d_i / \text{img} d_{i+1}$.

Computing the homology groups of $L$ in practice amounts to diagonalising the matrices $\{d_i : C_i \to C_{i-1}\}$ via row and column operations, which is a straightforward task in principle. Unfortunately, Gaussian elimination on an $n \times n$ matrix incurs an $O(n^3)$ cost, which becomes prohibitive when facing simplicial complexes built around large data sets. The standard remedy to this conundrum is to try construct a much smaller chain complex which has the same homology groups, and by far the most fruitful mechanism for achieving such homology-preserving reductions is discrete Morse theory [14, 30, 18, 25]. The key structure here is that of an acyclic partial matching, which pairs together certain adjacent simplices of $L$. The unpaired simplices are called critical, and the homology groups of $L$ may be recovered from a chain complex whose vector spaces are spanned by (only the) critical simplices.

Thus, one naturally seeks an optimal acyclic partial matching on $L$ which admits the fewest possible critical simplices. Unfortunately, the optimal matching problem is computationally intractable to solve [20] even approximately [3] for large $L$. Our goal in this paper is to simultaneously quantify the benefit of using discrete Morse theoretic reductions on random simplicial complexes and to provide a robust null model by which to measure their efficacy on general (i.e., not necessarily random) choices of simplicial complex $L$. 

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We accomplish these tasks by carefully analysing the distribution of critical simplex counts of a specific (lexicographical) type of acyclic partial matching defined on clique complexes $X(n,p)$ of Bernoulli random graphs $G(n,p)$.

**This Paper**

From a probabilistic perspective, understanding the number of critical simplices reduces to studying the random vector $(T_2, T_3, \ldots, T_{d+1}) \in \mathbb{Z}^d$ defined as follows. Letting $\{Y_{i,j}\}_{1 \leq i < j \leq n}$ be a sequence of i.i.d. Bernoulli variables, set

$$T_k = \sum_{s \subset \{n\}} \prod_{i \neq j \in s} Y_{i,j} \left[ \prod_{i=1}^{\min(s)-1} \left( 1 - \prod_{j \in s} Y_{i,j} \right) - \prod_{i=1}^{\min(s)-1} \left( 1 - \prod_{j \in s \setminus \{i\}} Y_{i,j} \right) \right].$$

This random variable, which we discuss in Section 6, arises naturally in stochastic topology [7, 6] but has been poorly studied from a distributional approximation perspective. To the best of our knowledge, only the expected value of a closely-related random variable has been calculated (see [4, Section 8] and Remark 32 below). In this work, we prove a multivariate normal approximation theorem for the random vector $(T_2, \ldots, T_{d+1})$.

While there is no shortage of multivariate normal approximation theorems [13, 34, 29, 10], the existing ones are not sufficiently fine-grained for our purposes. We therefore return to the pioneering work of Barbour, Karoński, and Ruciński [2], who proved a univariate central limit theorem (CLT) for a decomposable sum of random variables using Stein’s method, treating the case of dissociated sums as a special case. Here we extend their ideas to the multivariate setting; the resulting multivariate CLT allows us to prove results of interest in stochastic topology and topological data analysis, in both novel and previously studied contexts.

In particular, our CLT provides the promised bound on a multivariate normal approximation for critical simplices of lexicographical acyclic partial matchings on random clique complexes.

We also explore three additional applications of the general CLT in this paper which are of interest across topological data analysis in general and stochastic topology in particular:

1. We are able to prove a normal approximation result for the random vector which counts simplices in the *link* of any given simplex in a random clique complex. The notion of a link generalises the neighbourhood of a given vertex in a graph. Therefore, studying the multivariate distribution of the number of simplices (across different dimensions) that lie in the link of a given simplex forms a natural higher-order counterpart to the study of degree distributions of vertices in random graphs. To the best of our knowledge, this is the first work studying this random variable.

2. We extend results from [19] on generalised $U$-statistics to show not only distributional convergence asymptotically but a stronger result, detailing explicit non-asymptotic bounds on the approximation. Our notion of a generalised $U$-statistic is slightly more general than the one from [19], since we do not require the random variables at hand to be identically distributed. Many interesting problems can be seen as special cases — these include classical $U$-statistics [26, 24], monochromatic subgraph counts of inhomogeneous random graphs with independent random vertex colours, and the number of overlapping patterns in a sequence of independent Bernoulli trials, among others.

3. We study the joint distribution of $k$-clique counts in $G(n,p)$ random graph where $k \in \{2, 3, \ldots, d+1\}$, and we allow $d$ to depend on $n$. This result significantly generalises [35, Proposition 2] beyond the case when $k \in \{2, 3\}$. To the best of our knowledge, this is the first multivariate normal approximation result with explicit bounds where the sizes of the subgraphs can increase with $n$ and the resulting bound still asymptotically goes to 0. Such results on trade-offs between $d, n$, and the Bernoulli success probability $p$, follow naturally through the use of Stein’s method.
Main Results

Let $n$ and $d$ be positive integers. For each $i \in [d] := \{1, 2, \ldots, d\}$, we fix an index set $I_i \subset [n] \times \{i\}$ and consider the union of disjoint sets $I := \bigcup_{i \in [d]} I_i$. Associate to each such $s = (k, i) \in I$ a real centered random variable $X_s$ and form for each $i \in [d]$ the sum

$$W_i := \sum_{s \in I_i} X_s.$$ 

Our interest here is in the resulting random vector $W = (W_1, \ldots, W_d) \in \mathbb{R}^d$. The following notion is a natural multivariate generalisation of the dissociated sum from [28]; see also [2].

**Definition 1.** We call $W$ a vector of dissociated sums if for each $s \in I$ and $j \in [d]$ there exists a dependency neighbourhood $D_j(s) \subset I_j$ satisfying three criteria:

1. the difference $\left( W_j - \sum_{u \in D_j(s)} X_u \right)$ is independent of $X_s$;
2. for each $t \in I$, the quantity $\left( W_j - \sum_{u \in D_j(s)} X_u - \sum_{v \in D_j(t) \setminus D_j(s)} X_v \right)$ is independent of the pair $(X_s, X_t)$;
3. $X_s$ and $X_t$ are independent if $t \not\in \bigcup_{j} D_j(s)$.

Let $W$ be a vector of dissociated sums as defined above. For each $s \in I$, by construction, the sets $D_j(s), j \in [d]$ are disjoint (although for $s \neq t$, the sets $D_j(s)$ and $D_j(t)$ may not be disjoint). We write $D(s) = \bigcup_{j \in [d]} D_j(s)$ for the disjoint union of these of dependency neighbourhoods. With this preamble in place, we state our main result.

**Theorem 2.** Let $h : \mathbb{R}^d \to \mathbb{R}$ be any three times continuously differentiable function whose third partial derivatives are Lipschitz continuous and bounded. Consider a standard $d$-dimensional Gaussian vector $Z \sim \text{MVN}(0, \text{Id}_{d \times d})$. Assume that for all $s \in I$, we have $\mathbb{E} \{ X_s \} = 0$ and $\mathbb{E} \left| X_s^3 \right| < \infty$. Then, for any vector of dissociated sums $W \in \mathbb{R}^d$ with a positive semi-definite covariance matrix $\Sigma$, 

$$\left| \mathbb{E} h(W) - \mathbb{E} h(\Sigma^{1/2} Z) \right| \leq B_2 \sup_{i,j,k \in [d]} \left\| \frac{\partial^3 h}{\partial x_i \partial x_j \partial x_k} \right\|_{\infty},$$

where $B_2 = B_{2.1} + B_{2.2}$ is the sum given by

$$B_{2.1} := \frac{1}{3} \sum_{s \in I} \sum_{t,u \in D(s)} \left( \frac{1}{2} \mathbb{E} |X_s X_t X_u| + \mathbb{E} |X_s X_t| \mathbb{E} |X_u| \right)$$

$$B_{2.2} := \frac{1}{3} \sum_{s \in I} \sum_{t \in D(s)} \sum_{u \in D(t) \setminus D(s)} \left( \mathbb{E} |X_s X_t X_u| + \mathbb{E} |X_s X_t| \mathbb{E} |X_u| \right).$$

In the case that each component of $W$ is a sum of an equal number of i.i.d. random variables and each i.i.d. sequence is independent, then the bound in Theorem 2 is optimal with respect to the size $n$ of the sum in each component. However, compared to the CLT from [13], the bound is not optimal in the length $d$ of the vector $W$.

The desired CLT for critical simplex counts follows as a corollary to Theorem 2. We state a simple version of this result here; the full statement and proof have been recorded as Theorem 37 below. The interpretation of our results and their relevance to TDA is detailed in Remark 38. To this end, let $W \in \mathbb{R}^d$ be an appropriately scaled and centered vector, whose $i$-th component counts the number of critical simplices of dimension $i$ for the lexicographical acyclic partial matching on the random clique complex $X(n, p)$.

**Theorem 3.** Let $Z \sim \text{MVN}(0, \text{Id}_{d \times d})$ and $\Sigma$ be the covariance matrix of $W$. Let $h : \mathbb{R}^d \to \mathbb{R}$ be three times partially differentiable function whose third partial derivatives are Lipschitz continuous and bounded. Then there is a constant $B_3 > 0$ independent of $n$ and a natural number $N_3$ such that for any $n \geq N_3$ we have

$$\left| \mathbb{E} h(W) - \mathbb{E} h(\Sigma^{1/2} Z) \right| \leq B_3 \sup_{i,j,k \in [d]} \left\| \frac{\partial^3 h}{\partial x_i \partial x_j \partial x_k} \right\|_{\infty} n^{-1}.$$
En route to proving Theorem 3, we study the distribution of the number of critical simplices. As a result, we are also establish the following properties, which are of direct interest in computational topology. Here we assume that \( p \in (0, 1) \) and \( k \in \{1, 2, \ldots\} \) are constants and the random simplicial complex model is \( X(n, p) \).

1. The expected number of critical \( k \)-simplices is one order of \( n \) smaller than the expected number of \( k \)-simplices; see Lemma 33.

2. The variance of the number of critical \( k \)-simplices is at least of the order \( n^{2k} \), as shown in Lemma 35. An upper bound of the same order can be proved similarly. The variance of the total number of \( k \)-simplices is also of the same order.

3. Knowing the expected value and the variance one can prove concentration results using different concentration inequalities, for example, Chebyshev’s inequality. This would show that not only the expected value of critical simplices is smaller compared to all simplices but also that large deviations from the mean are unlikely, hence implying that the substantial improvement of one order of \( n \) is not only expected but also likely.

4. To know how many critical simplices there are, it is not necessary to check every simplex. Certain simplices have a very small chance of being critical, and can be safely ignored. The probability of this omission causing an error is vanishingly small asymptotically; see Proposition 36.

More details are provided in Remark 38.

**Related Work**

Theorem 2 is not the first generalisation of the results in [2] to a multivariate setting, see for example [13, 34]. The key advantage of our approach is that it allows for bounds which are non-uniform in each component of the vector \( W \). This is useful when, for example, the number of summands in each component are of different order or when the sizes of dependency neighbourhoods in each component are of different order. The applications considered here are precisely of this type, where the non-uniformity of the bounds is crucial. Moreover, we do not require the covariance matrix \( \Sigma \) to be invertible, and can therefore accommodate degenerate multivariate normal distributions.

Another multivariate central limit theorem for centered subgraph counts in the more general setting of a random graph associated to a graphon can be found in [23]. That proof is based on Stein’s method via a Stein coupling. Translating this result for uncentered subgraph counts would yield an approximation by a function of a multivariate normal. Several univariate normal approximation theorems for subgraph counts are available; recent developments in this area include [33], which uses Malliavin calculus together with Stein’s method, and [12], which uses the Stein-Tikhomirov method.

**Organisation**

This paper is organised as follows. In Section 2 we prove our main approximation theorem using smooth test functions and extend the result to non-smooth test functions using a smoothing technique from [15]. In Section 3 we introduce a slight generalisation of generalised \( U \)-statistics for which Theorem 2 gives a CLT with explicit bounds. In Section 4 we briefly introduce simplicial complexes and the \( X(n, p) \) random simplicial complex. Then we apply the results in Section 2 to clique counts in \( G(n, p) \); these counts can be viewed as simplex counts in the random simplicial complex \( X(n, p) \). In Section 5 we prove an approximation theorem for count variables of simplices that are in the link of a fixed simplex, explaining the relevant notions on the way. Finally, in Section 6 we detail the notion of critical simplices and prove an approximation theorem for critical simplex counts.
2 Multivariate CLT for dissociated sums

Throughout this paper we use the following notation. Given positive integers \( n, m \) we write \([m, n]\) for the set \( \{m, m + 1, \ldots, n\} \) and \([n]\) for the set \( \{1, n\} \). Given a set \( X \) we write \(|X|\) for its cardinality, \( \mathcal{P}(X) \) for its powerset, and given a positive integer \( k \) we write \( \mathcal{C}_k = \{t \in \mathcal{P}([n]) \mid |t| = k\} \) for the collection of subsets of \([n]\) which are of size \( k \). For a function \( f : \mathbb{R}^d \to \mathbb{R} \) we write \( \partial_i f = \frac{\partial f}{\partial x_i} \) and \( \partial_{ij} f = \frac{\partial^2 f}{\partial x_i \partial x_j} \). Also, we write \( |f|_k = \sup_{i_1, i_2, \ldots, i_k \in [d]} \|\partial_{i_1 \ldots i_k} f\|_\infty \) for any integer \( k \geq 1 \), as long as the quantities exist. Here \( \| \cdot \|_\infty \) denotes the supremum norm while \( \| \cdot \|_2 \) denotes the Euclidean norm. The notation \( \nabla \) denotes the gradient operator in \( \mathbb{R}^d \). For a positive integer \( d \) we define a class of test functions \( h : \mathbb{R}^d \to \mathbb{R} \), as follows. We say \( h \in \mathcal{H}_d \) iff \( h \) is three times partially differentiable with third partial derivatives being Lipschitz and \( |h|_3 < \infty \).

The notation \( \mathbb{I}_d \) denotes the disjoint union \( d \times d \) identity matrix. The vertex set of all graphs and simplicial complexes is assumed to be \([n]\). If \( s = (x, i) \in \mathbb{I} \) is an element of the index set in Definition 1, then we denote the second component of the tuple by \(|s|\), that is \(|s| := i\). We also use Bachmann-Landau asymptotic notation: we say \( f(n) = O(g(n)) \) iff \( \lim \sup_{n \to \infty} \frac{|f(n)|}{g(n)} < \infty \) and \( f(n) = \Omega(g(n)) \) iff \( \lim \inf_{n \to \infty} \frac{f(n)}{g(n)} > 0 \).

Throughout this section, \( W \in \mathbb{R}^d \) is a vector of dissociated sums in the sense of Definition 1, with covariance matrix whose entries are \( \Sigma_{ij} = \text{Cov}(W_i, W_j) \) for \((i, j) \in [d]^2\). For each \( s \in \mathbb{I} \) we denote by \( \mathbb{D}(s) \subset \mathbb{I} \) the disjoint union \( \bigcup_{j=1}^d \mathbb{D}_j(s) \). For each triple \((s, t, j) \in \mathbb{I}^2 \times [d]\) we write the set-difference \( \mathbb{D}_j(t) \setminus \mathbb{D}_j(s) \) as \( \mathbb{D}_j(t; s) \subset \mathbb{I} \) denoting the disjoint union of such differences over \( j \in [d]\).

2.1 Smooth test functions

To prove Theorem 2 we use Stein’s method for multivariate normal distributions; for details see for example Chapter 12 in [10]. Our proof of Theorem 2 is based on the Stein characterization of the multivariate normal distribution: \( Z \in \mathbb{R}^d \) is a multivariate normal \( \text{MVN}(0, \Sigma) \) if and only if the identity

\[
E \left\{ \nabla^T \Sigma \nabla f(Z) - Z^T \nabla f(Z) \right\} = 0
\]

holds for all twice continuously differentiable \( f : \mathbb{R}^d \to \mathbb{R} \) for which the expectation exists. In particular, we will use the following result based on [29, Lemma 1 and Lemma 2]. As Lemma 1 and Lemma 2 in [29] are stated there only for infinitely differentiable test functions, we give the proof here for completeness.

Lemma 4 (Lemma 1 and Lemma 2 in [29]). Fix \( n \geq 2 \). Let \( h : \mathbb{R}^d \to \mathbb{R} \) be \( n \)-times continuously differentiable with \( n \)-th partial derivatives being Lipschitz and \( Z \sim \text{MVN}(0, \text{Id}_{d \times d}) \). Then, if \( \Sigma \in \mathbb{R}^{d \times d} \) is symmetric positive semidefinite, there exists a solution \( f : \mathbb{R}^d \to \mathbb{R} \) to the equation

\[
\nabla^T \Sigma \nabla f(w) - w^T \nabla f(w) = h(w) - \mathbb{E} h \left( \Sigma^{1/2} Z \right), \quad w \in \mathbb{R}^d,
\]

such that \( f \) is \( n \)-times continuously differentiable and we have for every \( k = 1, \ldots, n \):

\[
|f|_k \leq \frac{1}{k} |h|_k.
\]

Proof. Let \( h \) be as in the assertion. It is shown in Lemma 2.1 in [9], which is based on a reformulation of Eq. (2.20) in [1], that a solution of (2.2) for \( h \) is given by \( f(x) = f_h(x) = \int_0^1 \frac{1}{2t} \mathbb{E} \{ h(Z_{x,t}) \} \, dt \), with \( Z_{x,t} = \sqrt{t} x + \sqrt{1-t} \Sigma^{1/2} Z \). As \( h \) has \( n \)-th partial derivatives being Lipschitz and hence for differentiating \( f \) we can bring the derivative inside the integral, it is straightforward to see that the solution \( f \) is \( n \)-times continuously differentiable.

The bound on \( |f|_k \) is a consequence of

\[
\frac{\partial^k f}{\partial x_{i_1} \ldots \partial x_{i_k}}(x) = \int_0^1 (2t)^{-1} t^{k/2} \mathbb{E} \left\{ \frac{\partial^k h}{\partial x_{i_1} \ldots \partial x_{i_k}}(Z_{x,t}) \right\} \, dt
\]
Thus, as with the vector of dissociated sums, here we recall that if \( \mathbf{s} \) is a solution to the Stein equation (2.2) for the test function \( h \) we set \( D_s = D_s(h) = \mathbb{E} \{ X_s X_t \} \). Since the variables \( \{ X_s \mid s \in \mathbb{I} \} \) are centered and as \( X_t \) is independent of \( X_s \) if \( t \not\in \mathbb{D}(s) \), for each \((i, j) \in [d]^2\) we have

\[
\Sigma_{ij} = \text{Cov}(W_i, W_j) = \sum_{s \in \mathbb{I}} \sum_{t \in \mathbb{D}(s)} \mathbb{E} \{ X_s X_t \}.
\]

We now use the decomposition of \( \Sigma_{ij} \) from (2.4) in the expression (2.3). For each pair \((s, j) \in \mathbb{I} \times [d]\) and \( t \in \mathbb{D}(s) \) we set \( \mathbb{D}_j(t; s) = \mathbb{D}_j(t) \setminus \mathbb{D}_j(s) \) and

\[
U^s_j := \sum_{u \in \mathbb{D}_j(s)} X_u; \quad W^s_j := W_j - U^s_j, \quad \text{and} \quad V^{s,t}_j := \sum_{v \in \mathbb{D}_j(t; s)} X_v; \quad W^{s,t}_j := W^s_j - V^{s,t}_j.
\]

By Definition 1, \( W^s_j \) is independent of \( X_s \), while \( W^{s,t}_j \) is independent of the pair \((X_s, X_t)\).

Next we decompose the r.h.s. of (2.3):

\[
\left| \mathbb{E} \left\{ \sum_{i=1}^{d} W_i \partial_i f(W) - \sum_{i,j=1}^{d} \partial_i f(W) \Sigma_{ij} \right\} \right| = |R_1 + R_2 + R_3|;
\]

with

\[
R_1 = \sum_{i=1}^{d} \mathbb{E} \{ W_i \partial_i f(W) \} - \sum_{s \in \mathbb{I}} \sum_{j=1}^{d} \mathbb{E} \{ X_s U^s_j \partial_s f(W^s) \}, \quad \text{(2.6)}
\]

\[
R_2 = \sum_{s \in \mathbb{I}} \sum_{j=1}^{d} \mathbb{E} \{ X_s U^s_j \partial_s f(W^s) \} - \sum_{s \in \mathbb{I}} \sum_{t \in \mathbb{D}_j(s)} \mathbb{E} \{ X_s X_t \} \mathbb{E} \partial_s f(W^{s,t}), \quad \text{and} \quad \text{(2.7)}
\]

\[
R_3 = \sum_{s \in \mathbb{I}} \sum_{t \in \mathbb{D}(s)} \mathbb{E} \{ X_s X_t \} \left( \mathbb{E} \partial_s f(W^{s,t}) - \mathbb{E} \partial_s f(W) \right). \quad \text{(2.8)}
\]

Here we recall that if \( s = (k, i) \) then \(|s| = i \in [d]\).

As with the vector of dissociated sums \( W \in \mathbb{R}^d \) itself, we can assemble these differences into random vectors. Thus, \( W^s \in \mathbb{R}^d \) is \((W^s_1, \ldots, W^s_d)\), and similarly \( W^{s,t} = (W^{s,t}_1, \ldots, W^{s,t}_d) \). In the next three claims, we provide bounds on \( R_i \) for \( i \in [3] \).

**Claim 5.** The absolute value of the expression \( R_1 \) from (2.6) is bounded above by

\[
|R_1| \leq \left( \frac{1}{2} \sum_{s \in \mathbb{I}} \sum_{t \in \mathbb{D}(s)} \sum_{u \in \mathbb{D}(s)} \mathbb{E} \{ X_s X_t X_u \} \right) |f|_3.
\]
Proof. Note that

\[
R_1 = \sum_{i=1}^{d} \sum_{s \in I_i} \mathbb{E} \{ X_s \partial_i f(W) \} - \sum_{s \in I} \sum_{j=1}^{d} \mathbb{E} \{ X_s U_j^s \partial_{i,j} f(W^s) \}
\]

\[
= \sum_{i=1}^{d} \sum_{s \in I_i} \left( \mathbb{E} \{ X_s \partial_i f(W) \} - \sum_{j=1}^{d} \mathbb{E} \{ X_s U_j^s \partial_{i,j} f(W^s) \} \right).
\]

For each \( s \in I_i \), it follows from (2.5) that \( W = U^s + W^s \). Using the Lagrange form of the remainder term in Taylor’s theorem, we obtain

\[
\partial_i f(W) = \sum_{j=1}^{d} \partial_{ij} f(W^s) U_j^s + \frac{1}{2} \sum_{j,k=1}^{d} \partial_{ijk} f(W^s + \theta_s U^s) U_j^s U_k^s
\]

for some random \( \theta_s \in (0, 1) \). Using this Taylor expansion in the expression for \( R_1 \), we get the following four-term summand \( S_{i,s} \) for each \( i \in [d] \) and \( s \in I_i \):

\[
S_{i,s} = \mathbb{E} \{ X_s \partial_i f(W^s) \} + \sum_{j=1}^{d} \mathbb{E} \{ X_s \partial_{ij} f(W^s) U_j^s \}
\]

\[
+ \frac{1}{2} \sum_{j,k=1}^{d} \mathbb{E} \{ X_s \partial_{ijk} f(W^s + \theta_s U^s) U_j^s U_k^s \} - \sum_{j=1}^{d} \mathbb{E} \{ X_s \partial_{ij} f(W^s) U_j^s \}.
\]

The second and fourth terms cancel each other. Recalling that \( X_s \) is centered by definition and independent of \( W^s \) by Definition 1, the third term also vanishes and

\[
R_1 = \sum_{i=1}^{d} \sum_{s \in I_i} S_{i,s} = \frac{1}{2} \sum_{i,j,k=1}^{d} \sum_{s \in I_i} \mathbb{E} \{ X_s \partial_{ijk} f(W^s + \theta_s U^s) U_j^s U_k^s \}.
\]

Recalling that \( \| \partial_{ijk} f \|_\infty \leq |f|_3 \) and that \( U_j^s = \sum_{t \in D_j(s)} X_t \), we have:

\[
|R_1| \leq \frac{1}{2} \sum_{i,j,k=1}^{d} \sum_{s \in I_i} \mathbb{E} \left| X_s \partial_{ijk} f(W^s + \theta_s U^s) U_j^s U_k^s \right|
\]

\[
\leq \frac{|f|_3^2}{2} \sum_{i,j,k=1}^{d} \sum_{s \in I_i} \mathbb{E} \left| X_s \sum_{t \in D_j(s)} X_t \sum_{u \in D_k(s)} X_u \right|
\]

\[
\leq \frac{|f|_3^2}{2} \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{u \in \mathbb{D}(s)} \mathbb{E} \left| X_s X_t X_u \right|
\]

as desired. \( \square \)

Claim 6. The absolute value of the expression \( R_2 \) from (2.7) is bounded above by

\[
|R_2| \leq \left( \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{u \in \mathbb{D}(s; t)} \mathbb{E} \left| X_s X_u X_t \right| \right) |f|_3.
\]

Proof. Recalling that \( U_j^s = \sum_{t \in D_j(s)} X_t \) and \( \mathbb{D}(s) = \bigcup_{j=1}^{d} \mathbb{D}_j(s) \),

\[
R_2 = \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \left( \mathbb{E} \{ X_s X_t \partial_{i} f(W^s) \} - \mathbb{E} \{ X_s X_t \} \mathbb{E} \{ \partial_{i} |W^s| \} \right).
\]

7
Fix \( s \in I \) and \( t \in \mathbb{D}_j(s) \). Recall that by (2.5), \( W^s = W^{s,t} + V^{s,t} \). Using the Lagrange form of the remainder term in Taylor’s theorem, we obtain:

\[
\partial_{[s]\|t]} f(W^s) = \partial_{[s]\|t]} f(W^{s,t}) + \sum_{k=1}^d \partial_{[s]\|t]} f(W^{s,t} + \theta_{s,t} V^{s,t}) V^{s,t}_k
\]

for some random \( \theta_{s,t} \in (0,1) \). Using this Taylor expansion in the expression for \( R_2 \), we get the following three-term summand \( S_{s,t} \) for each pair \( (s,t) \in I \times \mathbb{D}_j(s) \):

\[
S_{s,t} = \mathbb{E} \left\{ X_s X_t \partial_{[s]\|t]} f(W^{s,t}) \right\} + \sum_{k=1}^d \mathbb{E} \left\{ X_s X_t \partial_{[s]\|t]} f(W^{s,t} + \theta_{s,t} V^{s,t}) V^{s,t}_k \right\} - \mathbb{E} \left\{ \partial_{[s]\|t]} f(W^{s,t}) \right\}.
\]

Recalling that \( W^{s,t} \) is independent of the pair \( (X_s, X_t) \) the first and the last terms cancel each other and only the sum over \( k \) is left:

\[
R_2 = \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} S_{s,t} = \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{k=1}^d \mathbb{E} \left\{ X_s X_t \partial_{[s]\|t]} f(W^{s,t} + \theta_{s,t} V^{s,t}) V^{s,t}_k \right\}.
\]

Recalling that \( ||\partial_{ijk} f||_\infty \leq |f|_3 \) and that \( V^{s,t}_k = \sum_{u \in \mathbb{D}_k(t;s)} X_u \) we have:

\[
|R_2| \leq \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{k=1}^d \sum_{u \in \mathbb{D}_k(t;s)} \mathbb{E} |X_s X_t X_u \partial_{[s]\|t]} f(W^{s,t} + \theta_{s,t} V^{s,t})| \leq |f|_3 \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{u \in \mathbb{D}(t;s)} \mathbb{E} |X_s X_t X_u|,
\]

as required.

\[\square\]

**Claim 7.**

\[
|R_3| \leq \left( \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \left\{ \sum_{u \in \mathbb{D}(s)} \mathbb{E} |X_s X_t| \mathbb{E} |X_u| + \sum_{u \in \mathbb{D}(t;s)} \mathbb{E} |X_s X_t| \mathbb{E} |X_u| \right\} \right) |f|_3.
\]

**Proof.** Fix \( (s,t) \in I \times \mathbb{D}_j(s) \). Recall that by (2.5), \( W^{s,t} = W - U^s - V^{s,t} \). Using the Lagrange form of the remainder term in Taylor’s theorem, we obtain

\[
\partial_{[s]\|t]} f(W^{s,t}) = \partial_{[s]\|t]} f(W) - \sum_{k=1}^d \partial_{[s]\|t]} f(W - \rho_{s,t} (U^s + V^{s,t})) (U^s_k + V^{s,t}_k)
\]

for some random \( \rho_{s,t} \in (0,1) \). Recalling that \( U^s_k = \sum_{t \in \mathbb{D}_k(s)} X_t \) and \( V^{s,t}_k = \sum_{u \in \mathbb{D}_k(t;s)} X_u \),

\[
R_3 = - \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{k=1}^d \mathbb{E} \{ X_s X_t \} \mathbb{E} \{ \partial_{[s]\|t]} f(W - \rho_{s,t} (U^s + V^{s,t})) (U^s_k + V^{s,t}_k) \}
\]

\[
= - \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{u \in \mathbb{D}(s)} \mathbb{E} \{ X_s X_t \} \mathbb{E} \{ X_u \partial_{[s]\|t]} f(W - \rho_{s,t} (U^s + V^{s,t})) \}
\]

\[
- \sum_{s \in I} \sum_{t \in \mathbb{D}(s)} \sum_{u \in \mathbb{D}(t;s)} \mathbb{E} \{ X_s X_t \} \mathbb{E} \{ X_u \partial_{[s]\|t]} f(W - \rho_{s,t} (U^s + V^{s,t})) \}.
\]
Recalling that $\|\partial_{ijk}f\|_\infty \leq |f|_3$ we bound:

$$|R_3| \leq |f|_3 \sum_{s \in \mathcal{D}} \sum_{t \in \mathcal{D}(s)} \sum_{u \in \mathcal{D}(s)} \mathbb{E} |X_s X_t| \mathbb{E} |X_u| + |f|_3 \sum_{s \in \mathcal{D}} \sum_{t \in \mathcal{D}(s)} \sum_{u \in \mathcal{D}(t,s)} \mathbb{E} |X_s X_t| \mathbb{E} |X_u|,$$

as required. \(\square\)

Take any $h \in \mathcal{H}_d$. Let $f : \mathbb{R}^d \to \mathbb{R}$ be the associated solution from Lemma 4. Combining Claims 4 - 7 and using Lemma 4 we have:

$$\left| \mathbb{E} h(W) - \mathbb{E} h(\Sigma^{\frac{1}{2}} Z) \right|$$

$$\leq \left| \mathbb{E} \{ \nabla^T \Sigma \nabla f(W) - W^T \nabla f(W) \} \right| \leq |R_1| + |R_2| + |R_3| + |R_4|$$

$$\leq |f|_3 \sum_{s \in \mathcal{D}} \sum_{t \in \mathcal{D}(s)} \sum_{u \in \mathcal{D}(s)} \left( \frac{1}{2} \mathbb{E} |X_s X_t X_u| + \mathbb{E} |X_s X_t| \mathbb{E} |X_u| \right)$$

$$+ |f|_3 \sum_{s \in \mathcal{D}} \sum_{t \in \mathcal{D}(s)} \sum_{u \in \mathcal{D}(t,s)} \left( \mathbb{E} |X_s X_t X_u| + \mathbb{E} |X_s X_t| \mathbb{E} |X_u| \right)$$

$$\leq \frac{1}{3} |h|_3 B_2.$$

\(\square\)

In most of our applications, the variables $X_s$ are centered and rescaled Bernoulli random variables. Hence, the following lemma is useful.

**Lemma 8.** Let $\xi_1, \xi_2, \xi_3$ be Bernoulli random variables with expected values $\mu_1, \mu_2, \mu_3$ respectively. Let $c_1, c_2, c_3 > 0$ be any constants. Consider variables $X_i := c_i (\xi_i - \mu_i)$ for $i = 1, 2, 3$. Then we have

$$\mathbb{E} |X_1 X_2 X_3| \leq c_1 c_2 c_3 \left\{ \mu_1 \mu_2 (1 - \mu_1)(1 - \mu_2) \right\}^{\frac{1}{2}};$$

$$\mathbb{E} |X_1 X_2| \mathbb{E} |X_3| \leq c_1 c_2 c_3 \left\{ \mu_1 \mu_2 (1 - \mu_1)(1 - \mu_2) \right\}^{\frac{1}{2}}.$$

**Proof.** Note that $X_3$ can take two values: $-c_3 \mu_3$ or $c_3 (1 - \mu_3)$. As $0 \leq \mu_3 \leq 1$, we have

$$\mathbb{E} |X_1 X_2| \mathbb{E} |X_3| \leq c_3 \mathbb{E} |X_1 X_2|;$$

$$\mathbb{E} |X_1 X_2 X_3| \leq c_3 \mathbb{E} |X_1 X_2|.$$

Applying the Cauchy-Schwarz inequality and direct calculation of the second moments gives

$$\mathbb{E} |X_1 X_2| \leq \left\{ \mathbb{E} \{X_1^2\} \mathbb{E} \{X_2^2\} \right\}^{\frac{1}{2}} = c_1 c_2 \left\{ \mu_1 \mu_2 (1 - \mu_1)(1 - \mu_2) \right\}^{\frac{1}{2}},$$

which finishes the proof. \(\square\)

### 2.2 Non-smooth test functions

Here we follow [23, Section 5.3] very closely to derive a bound on the convex set distance between a vector of dissociated sums $W \in \mathbb{R}^d$ with covariance matrix $\Sigma$ and a target multivariate normal distribution $\Sigma^{\frac{1}{2}} Z$, where $Z \sim \text{MVN}(0, \text{Id}_{\sqrt{d}})$. The smoothing technique used here is introduced in [15]. However, a better (polylogarithmic) dependence on $d$ could potentially be achieved using a recent result [16, Proposition 2.6], at the expense of larger constants. Let $\mathcal{K}$ be a class of convex sets in $\mathbb{R}^d$. 


Corollary 10. We have the following two bounds:

1. Under the assumptions of Theorem 2,

   \[ \left| \mathbb{E} h(W) - \mathbb{E} (\Sigma^{1/2} Z) \right| \leq B_{10} |h|_3. \]

2. Assuming the hypotheses of Theorem 9,

   \[ \sup_{A \in \mathcal{K}} |\mathbb{P}(W \in A) - \mathbb{P}(\Sigma^{1/2} Z \in A)| \leq 2^{\frac{7}{2}} 3^{-\frac{3}{4}} \pi^2 B_{10}^{\frac{4}{3}}. \]
Here $B_{10}$ is a sum over $(i,j,k) \in [d]^3$ of the form

$$B_{10} := \frac{1}{3} \sum_{(i,j,k)} |\alpha_{ij}| \left( \frac{3\alpha_{ik}}{2} + 2\alpha_{jk} \right) \beta_{ijk};$$

and $\alpha_{ij}$ is the largest value attained by $|\mathbb{D}_j(s)|$ over $s \in I_i$, and

$$\beta_{ijk} = \max_{s,t,u} \left( \mathbb{E}[X_s X_t X_u], \mathbb{E}[X_s X_t], \mathbb{E}[X_u] \right)$$

as $(s,t,u)$ range over $I_i \times I_j \times I_k$.

### 3 Generalised $U$-statistics

Here we consider the case of generalised $U$-statistics, which were first introduced in [19]. We expand the notion slightly by considering independent but not necessarily identically distributed variables instead of i.i.d. variables.

Let $\{\xi_i\}_{1 \leq i \leq n}$ be a sequence of of independent random variables taking values in a measurable set $\mathcal{X}$ and let $\{Y_{i,j}\}_{1 \leq i < j \leq n}$ be an array of of independent random variables taking values in a measurable set $\mathcal{Y}$ which is independent of $\{\xi_i\}_{1 \leq i \leq n}$. We use the convention that $Y_{i,j} = Y_{j,i}$ for any $i < j$. For example, one can think of $X_i$ as a random label of a vertex $i$ in a random graph where $Y_{i,j}$ is the indicator for the edge connecting $i$ and $j$. Given a subset $s \subseteq [n]$ of size $m$, write $s = \{s_1, s_2, \ldots, s_m\}$ such that $s_1 < s_2 < \ldots < s_m$ and set $\mathcal{X}_s = (\xi_{s_1}, \xi_{s_2}, \ldots, \xi_{s_m})$ and $\mathcal{Y}_s = (Y_{s_1, s_2}, Y_{s_1, s_3}, \ldots, Y_{s_{m-1}, s_m})$. Recall that $C_k$ denotes the collection of subsets of $[n]$ which are of size $k$.

**Definition 11.** Given $1 \leq k \leq n$ and a measurable function $f : \mathcal{X}^k \times \mathcal{Y}^k \to \mathbb{R}$ define the associated generalised $U$-statistic by

\[
S_{n,k}(f) = \sum_{s \in C_k} f(\mathcal{X}_s, \mathcal{Y}_s).
\]

#### 3.1 The first approximation theorem

Let $\{k_i\}_{i \in [n]}$ be a collection of positive integers, each being at most $n$, and for each $i \in [d]$ let $f_i : \mathcal{X}^{k_i} \times \mathcal{Y}^{k_i} \to \mathbb{R}$ be a measurable function. We are interested in the joint distribution of $S_{n,k_1}(f_1), S_{n,k_2}(f_2), \ldots, S_{n,k_d}(f_d)$.

Fix $i \in [d]$. For $s \in I_i := C_k_i \times \{i\}$ define $X_s = \sigma_i^{-1}(f_i(\mathcal{X}_s, \mathcal{Y}_s) - \mu_s)$, where $\mu_s = E \{f_i(\mathcal{X}_s, \mathcal{Y}_s)\}$ and $\sigma_i^2 = \text{Var}(S_{n,k_i}(f_i))$. Now let $W_i = \sum_{s \in I_i} X_s$ be a random variable and write $W = (W_1, W_2, \ldots, W_d) \in \mathbb{R}^d$. By construction, $W_i$ has mean 0 and variance 1.

**Assumption 12.** We assume that

1. For any $i \in [d]$ there is $\alpha_i > 0$ such that for all $s, t \in I_i$ for which $\text{Cov}(f_i(\mathcal{X}_s, \mathcal{Y}_s), f_i(\mathcal{X}_t, \mathcal{Y}_t))$ is non-zero we have $\text{Cov}(f_i(\mathcal{X}_s, \mathcal{Y}_s), f_i(\mathcal{X}_t, \mathcal{Y}_t)) \geq \alpha_i$.
2. There is $\beta \geq 0$ such that for any $i, j, l \in [d]$ and any $s \in I_i$, $t \in I_j$, $u \in I_l$ we have
   \[
   \mathbb{E} \{|f_i(\mathcal{X}_s, \mathcal{Y}_s) - \mu_s| f_j(\mathcal{X}_t, \mathcal{Y}_t) - \mu_t| f_l(\mathcal{X}_u, \mathcal{Y}_u) - \mu_u| \leq \beta
   \]
   as well as
   \[
   \mathbb{E} |f_i(\mathcal{X}_s, \mathcal{Y}_s) - \mu_s| f_j(\mathcal{X}_t, \mathcal{Y}_t) - \mu_t| f_l(\mathcal{X}_u, \mathcal{Y}_u) - \mu_u| \leq \beta.
   \]
3. The random variables $X_s$ have finite absolute third moments.

The first assumption is not necessary but very convenient and we use it to derive a lower bound for the variance $\sigma^2$. It holds in a variety of settings, for example, subgraph counts in a random graph. A normal
approximation theorem can be proven in our framework when the assumption does not hold and a sufficiently large lower bound for the variance is acquired in a different way. Similarly, we use the second assumption to get a convenient bound on mixed moments. However, depending on a particular question at hand, one might want to use a bound on mixed moments, which is not uniform in \( i, j, l \) and sometimes even one that is not uniform in \( s, u, v \). We will discuss such an example (which does not fit into the framework of generalised \( U \)-statistics) in Section 6. In this section, in order to maintain the generality and simplicity of the proofs, we work under Assumption 12. In [19, Theorem 6] it is assumed that all summands in the generalised \( U \)-statistic have finite second moment as well as that the sums admit a particular decomposition which is not easily translatable to our framework. In contrast to [19] we obtain a non-asymptotic bound on the normal approximation, as follows.

**Theorem 13.** Let \( Z \sim \text{MVN}(0, \text{Id}_{d \times d}) \) and let \( W \) with covariance matrix \( \Sigma \) satisfy Assumption 12.

1. Let \( h \in \mathcal{H}_d \). Then
   \[
   \left| \mathbb{E}h(W) - \mathbb{E}h(\Sigma^{1/2}Z) \right| \leq |h|_3 B_{13} n^{-\frac{1}{2}}.
   \]

2. Let \( \mathcal{K} \) be a class of convex sets in \( \mathbb{R}^d \). Then
   \[
   \sup_{A \in \mathcal{K}} \left| \mathbb{P}(W \in A) - \mathbb{P}(\Sigma^{1/2}Z \in A) \right| \leq 2^7 3^{-\frac{3}{2}} d^{\frac{3}{2}} B_{13} n^{-\frac{1}{2}}.
   \]

Here,
\[
B_{13} = \frac{2\psi}{3} \sum_{i,j,l=1}^d k_i^{\min(k_i,k_j)+1} \left( k_i^{\min(k_i,k_l)+1} + k_j^{\min(k_j,k_l)+1} \right) K_i K_j K_l
\]
and
\[
K_i = (2k_i^2 - k_i)^{-\frac{k_i}{2} + \frac{1}{2}}.
\]

**Proof.** Note that if \( s = (\phi, i) \in \mathbb{I}_i \) and \( u = (\psi, j) \in \mathbb{I}_j \) are chosen such that \( \phi \cap \psi = \emptyset \), then the corresponding variables \( X_s \) and \( X_u \) are independent since \( f_i(X_s, Y_i) \) and \( f_j(X_u, Y_u) \) do not share any random variables from the sets \( \{ \xi_i \}_{1 \leq i \leq n} \) and \( \{ Y_{i,j} \}_{1 \leq i < j \leq n} \). Hence, if for any \( s = (\phi, i) \in \mathbb{I}_i \) we set \( \mathbb{D}_j(s) = \{ (\psi, j) \in \mathbb{I}_j \mid |\phi \cap \psi| \geq 1 \} \), then \( W \) satisfies the assumptions of Corollary 10. It remains to bound the quantity \( B_{10} \).

First, to find \( \alpha_{ij} \) as in Corollary 10, given \( \phi \in C_{k_i} \) and if \( k_i, k_j \geq m \) then there are \( \binom{k_i}{m} \binom{n-k_i}{n-k_j} \) subsets \( \psi \in C_{k_j} \) such that \( |\phi \cap \psi| = m \). Therefore, we have for any \( i, j \in [d] \) and \( s \in \mathbb{I}_i \)
\[
|\mathbb{D}_j(s)| = \sum_{m=1}^{\min(k_i,k_j)} \binom{k_i}{m} \binom{n-k_i}{k_j-m} \alpha_{ij} \leq k_i^{\min(k_i,k_j)+1} (n-k_i)^{k_j-1}.
\]

Note that
\[
\mathbb{E} |X_s X_t X_u| = (\sigma_i \sigma_j \sigma_k)^{-1} \mathbb{E} |\{ f_i(X_s, Y_s) - \mu_s \} \{ f_j(X_t, Y_t) - \mu_t \} \{ f_l(X_u, Y_u) - \mu_u \}|
\]
as well as
\[
\mathbb{E} |X_s X_t| \mathbb{E} |X_u| = (\sigma_i \sigma_j \sigma_k)^{-1} \mathbb{E} |\{ f_i(X_s, Y_s) - \mu_s \} \{ f_j(X_t, Y_t) - \mu_t \}| \mathbb{E} |f_l(X_u, Y_u) - \mu_u|.
\]

Using Assumption 12, for any \( i, j, l \in [d] \) and \( s \in \mathbb{I}_i, t \in \mathbb{I}_j, u \in \mathbb{I}_l \)
\[
\mathbb{E} |X_s X_t X_u| \leq (\sigma_i \sigma_j \sigma_k)^{-1} \beta \quad \text{and} \quad \mathbb{E} |X_s X_t| \mathbb{E} |X_u| \leq (\sigma_i \sigma_j \sigma_k)^{-1} \beta.
\]

To take care of the variance terms, we lower bound the variance using Assumption 12,
\[
\text{Var}(S_n, k_i(f_i)) = \sum_{s \in C_{k_i}} \sum_{t \in \mathbb{D}_s(s)} \text{Cov}(f_i(X_s, Y_s), f_i(X_t, Y_t))
\]

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Using Equations (3.1) - (3.3) to bound the quantity $B$ so that the sequence $\{B_i\}$ bounds, as follows. For any $s$ we set $D_i(s) = \{(\psi, j) \in I_j \mid |\phi \cap \psi| \geq 2\}$, so that $W$, under the additional Assumption 14, satisfies the assumptions of Corollary 10.

Next we consider the special case that the functions in Definition 11 only depend on the second component, so that the sequence $\{\xi_i\}_{i \in [n]}$ can be ignored. Continuing to use the same notation, we want to understand the joint distribution of $S_{n, k_1}(f_1), S_{n, k_2}(f_2), \ldots, S_{n, k_d}(f_d)$. However, we add an additional assumption.

Assumption 14. We assume that the functions $f_i$ only depend on the variables $\{Y_{i,j}\}_{1 \leq i < j \leq n}$. That is, we can write $f_i : Y^{k_i} \rightarrow \mathbb{R}$.

Such functions arise, for instance, when counting subgraphs in an inhomogeneous Bernoulli random graph. A detailed example of such generalised $U$-statistic is worked out in Section 4.

In this case, we can adapt the previous theorems slightly and get improved bounds. We still work under Assumption 12. The key difference in this case is that the dependency neighbourhoods become smaller: now the subsets need to overlap in at least 2 elements for the corresponding summands to share at least one variable $Y_{i,j}$ and hence become dependent. This makes both the variance and the size of dependency neighbourhoods smaller. In the context of Theorem 2, the trade-off works out in our favour to give smaller bounds, as follows. For any $s = (\phi, i) \in I_i$ we set $D_i(s) = \{(\psi, j) \in I_j \mid |\phi \cap \psi| \geq 2\}$, so that $W$, under the additional Assumption 14, satisfies the assumptions of Corollary 10.
In this case, we can adjust Equations (3.1) and (3.3). The proofs are exactly the same as previously, with the only difference being that when we sum over \( m \), we start at \( m = 2 \) as opposed to \( m = 1 \).

**Theorem 15.** Consider \( W \) that satisfies Assumption 14. Let \( Z \sim \text{MVN}(0, \text{Id}_{d \times d}) \) and \( \Sigma \) be the covariance matrix of \( W \).

1. Let \( h \in \mathcal{H}_d \). Then
   \[
   \left| \mathbb{E}h(W) - \mathbb{E}h(\Sigma^{\frac{1}{2}}Z) \right| \leq \|h\|_3 B_{15} n^{-\frac{1}{2}};
   \]

2. Let \( \mathcal{K} \) be a class of convex sets in \( \mathbb{R}^d \). Then
   \[
   \sup_{A \in \mathcal{K}} |\mathbb{P}(W \in A) - \mathbb{P}(\Sigma^{\frac{1}{2}}Z \in A)| \leq 2^{\frac{5}{2}} 3^{-\frac{1}{2}} d^\frac{3}{4} B_{15}^\frac{1}{2} n^{-\frac{3}{4}}.
   \]

Here
\[
B_{15} = \frac{16 \beta_3}{3}; \sum_{i,j,l=1}^d k_i^{\min(k_i,k_j)+1} k_j^{\min(k_i,k_l)+1} \alpha_i \alpha_j \alpha_l \left( k_i^{\min(k_i,k_l)+1} + k_j^{\min(k_i,k_l)+1} \right) k_i K_j K_l
\]
and
\[
K_i = (2k_i^2 - k_i)^{-\frac{k_i}{2} + \frac{1}{2}}.
\]

**Proof.** Equation (3.1) becomes
\[
|\mathbb{D}_j(s)| \leq k_i^{\min(k_i,k_j)+1} (n - k_i)^{-k_i - 2}.
\]
Equation (3.3) becomes
\[
\sigma_i^{-1} \leq 2n^{-k_i+1} \alpha_i^{-\frac{3}{2}} (2k_i^2 - 2k_i)^{-\frac{3}{2} + 1}.
\]

Using the adjusted bounds in Corollary 10 gives the result. \( \square \)

## 4 Clique counts in \( G(n,p) \)

In this section we apply Theorem 15 to approximate simplex counts. Firstly, we recall the notion of a simplicial complex [36, Ch 3.1]; these provide higher-dimensional generalisations of a graph and constitute data structures of interest across algebraic topology in general and topological data analysis in particular. Then we introduce the random simplicial complex \( X(n,p) \), which is a random model studied in stochastic topology [21, 22]. This provides an alternative interpretation of clique counts in \( G(n,p) \) as simplex counts in \( X(n,p) \). Recall that \( G(n,p) \) is a random graph on \( n \) vertices where each pair of vertices is connected with probability \( p \), independently of any other pair.

**Definition 16.** A simplicial complex \( \mathcal{L} \) on a vertex set \( V \) is a set of nonempty subsets of \( V \) (i.e. \( \emptyset \neq \mathcal{L} \subseteq \mathcal{P}(V) \)) such that the following properties are satisfied:

1. for each \( v \in V \) the singleton \( \{v\} \) lies in \( \mathcal{L} \), and
2. if \( t \in \mathcal{L} \) and \( s \subset t \) then \( s \in \mathcal{L} \).

The **dimension** of a simplicial complex \( \mathcal{L} \) is \( \max_{s \in \mathcal{L}} |s| - 1 \). Elements of a simplicial complex are called **simplices**. If \( s \) is a simplex, then its dimension is \( |s| - 1 \). A simplex of dimension \( k \) can be called a \( k \)-simplex. Note that the notion of one-dimensional simplicial complex is equivalent to the notion of a graph, with the vertex set \( V \) and edges as subsets.

**Definition 17.** Given a graph \( G = (V,E) \) the clique complex \( \mathcal{X} \) of \( G \) is a simplicial complex on \( V \) such that
\[
t \in \mathcal{X} \iff \forall u,v \in t, \{u,v\} \in E.
\]

The \( X(n,p) \) random simplicial complex is the clique complex of the \( G(n,p) \) random graph.
In particular, $t \in \mathcal{X}$ if and only if the vertices of $t$ span a clique in $G$. Thus, elements in $\mathbf{X}(n,p)$ are cliques in $G(n,p)$. Consider $G \sim G(n,p)$. For $1 \leq x < y \leq n$ let $Y_{x,y} := \mathbb{I}(x \sim y)$ be the edge indicator. In this section we are interested in the $(i+1)$-clique count in $G(n,p)$ or, equivalently, the $i$-simplex count in $\mathbf{X}(n,p)$, given by

$$T_i = \sum_{s \in C_i} \prod_{x \neq y \in s} Y_{x,y}. \quad (4.1)$$

Let $\mathcal{Y}^{i+1} = \{0, 1\}^{i+1}$ and let $f_i : \mathcal{Y}^{i+1} \to \mathbb{R}$ be the function

$$f_i(\mathcal{Y}_s) = \prod_{Y_{x,y} \in \mathcal{Y}_s} Y_{x,y}.$$ 

Then the associated generalised U-statistic $S_{n,i+1}(f_i)$ equals the $(i+1)$-clique count $T_i$, as given by Equation (4.1). To apply Theorem 15 we need to center and rescale our variables. It is easy to see that $\mathbb{E}(f_i(\mathcal{Y}_s)) = p^{(i+1)}$ if $\phi \in C_{i+1}$ Just like in Section 3.1, we let $I_i := C_{i+1} \times \{i\}$ and for $s = (\phi, i) \in I_i$ we define $X_s := \sigma^{-1}\left(f_i(\mathcal{Y}_s) - p^{(i+1)}\right)$ and $W_i = \sum_{s \in I_i} X_s$. Now the vector of interest is $W = (W_1, W_2, \ldots, W_d) \in \mathbb{R}^d$.

This brings us to the next approximation theorem.

**Corollary 18.** Let $Z \sim \text{MVN}(0, \text{Id}_{d \times d})$ and $\Sigma$ be the covariance matrix of $W$.

1. Let $h \in \mathcal{H}_d$. Then

$$\left| \mathbb{E}h(W) - \mathbb{E}h(\Sigma^{1/2}Z) \right| \leq |h|_3 B_{18} n^{-1}.$$ 

2. Let $\mathcal{K}$ be a class of convex sets in $\mathbb{R}^d$. Then

$$\sup_{A \in \mathcal{K}} |\mathbb{P}(W \in A) - \mathbb{P}(\Sigma^{1/2}Z \in A)| \leq 2 \sqrt{2} 3^{-2d + \frac{1}{2}} B_{18}^{\frac{3}{2}} n^{-\frac{1}{2}}.$$ 

Here

$$B_{18} = \frac{16}{3} d^{2d+5} p^{-3(d+1)}(1 - p^{(i+1)})(p^{-1} - 1)^{-\frac{1}{2}}.$$ 

**Proof.** Firstly observe that for any $\phi, \psi \in C_{i+1}$ for which $|\phi \cap \psi| \leq 1$ the covariance vanishes, while if $|\phi \cap \psi| \geq 2$ the covariance is non-zero, and we have

$$\text{Cov}(f_i(\mathcal{Y}_\phi), f_i(\mathcal{Y}_\psi)) = p^{(i+1)}(\frac{d}{2} + \frac{1}{2})(\frac{d}{2} - \frac{1}{2}) = p^{(i+1)}(p^{-1} - 1).$$

For $s = (\phi, i) \in I_i$ write $\hat{X}_s = f_i(\mathcal{Y}_\phi) - p^{(i+1)}$. Then by Lemma 8 we get:

$$\mathbb{E}\left| \hat{X}_s \hat{X}_t \right| \mathbb{E} \left| \hat{X}_u \right| \leq \left\{ p^{(i+1)} + (i+1) p^{(i+1)}(1 - p^{(i+1)}) \right\} \frac{1}{2};$$

$$\mathbb{E}\left| \hat{X}_s \hat{X}_t \hat{X}_u \right| \leq \left\{ p^{(i+1)} + (i+1) p^{(i+1)}(1 - p^{(i+1)}) \right\} \frac{1}{2}.$$ 

Since $\left\{ p^{(i+1)} + (i+1) p^{(i+1)}(1 - p^{(i+1)}) \right\} \frac{1}{2} \leq p(1 - p^{(i+1)})$, we see that Assumption 12 holds. Clearly Assumption 14 also holds and therefore we can apply Theorem 15 with $k_i = i + 1$, $K_i = (2(i + 1)^2 - 2(i + 1)^{-\frac{1}{2}}(i+1)+1$, $\alpha_i = p^{(i+1)}(p^{-1} - 1)$, and $\beta = p(1 - p^{(i+1)})$. Using the bounds $K_i \leq 1$ as well as $2 \leq k_i^\alpha \leq d^{d+1}$, and $\sqrt{p^{(d+1)}} \sqrt{p^{-1} - 1}$ finishes the proof. \hfill \Box

**Remark 19.** It is easy to show that with high probability there are no large cliques in $G(n,p)$ for $p < 1$ constant. To see this, the expectation of the number of $k$-cliques is $\binom{n}{k} p^{(\frac{k^2}{2})}$. By Stirling’s approximation, $k = \Omega\left(\ln^{1+\epsilon}(n)\right)$ for any positive $\epsilon$ forces the expectation to go to 0 asymptotically. Hence, by Markov’s
inequality, with high probability there are no cliques of order \( \ln^{1+\epsilon}(n) \) or larger for any \( \epsilon > 0 \). For cliques of order larger than \( \ln^{1/2}(n) \) and fixed \( p \), a Poisson approximation might be more suitable.

Recall that in Corollary 18 the size of the maximal clique we count is \( d + 1 \). Note that if \( d = O(\ln^{1/2-\epsilon}(n)) \) for any \( \epsilon > 0 \), then the bounds in Corollary 18 tend to 0 as \( n \) tends to infinity as long as \( p \in (0, 1) \) stays constant. This might seem quite small but in the light there not being any cliques of order \( \ln^{1+\epsilon}(n) \) with high probability, this is meaningfully large.

Remark 20. Note that in Corollary 18 we use multivariate normal distribution with covariance \( \Sigma \), which is the covariance of \( W \) when \( n \) is finite and it differs from the limiting covariance, as mentioned in [35]. To approximate \( W \) with the limiting distribution, one could proceed in the spirit of [35, Proposition 3] in two steps: use the existing theorems to approximate \( W \) with \( \Sigma Z \) and then approximate \( \Sigma Z \) with \( \Sigma_L Z \) where \( \Sigma_L \) is the limiting covariance, which is non-invertible, as observed in [19].

Remark 21. Corollary 18 generalises the result [35, Proposition 2] beyond the case when \( d = 2 \) and we get a bound of the same order of \( n \). [23, Theorem 3.1] considers centered subgraph counts in a random graph associated to a graphon. If we take the graphon to be constant, the associated random graph is just \( G(n, p) \). Compared to [23, Theorem 3.1] we place weaker smoothness conditions on our test functions. However, we make use of the special structure of cliques whereas [23, Theorem 3.1] applies to any centered subgraph counts. Translating [23, Theorem 3.1] into a result for uncentered subgraph counts, as we provide here in the special case of clique counts, is not trivial for general \( d \).

However, it should be possible to extend our results, using the same abstract approximation theorem, beyond the random clique complex to Linial-Meshulam random complexes [27] or even more general multiparameter Costa-Farber random complexes [11]. We shall consider this conjecture in future work.

5 Simplex counts in links

Next we use Corollary 10 to provide a multivariate normal approximation for the simplex counts in links of a simplicial complex. Recall Definition 16.

Definition 22. The link of a simplex \( t \) in a simplicial complex \( L \) is the subcomplex

\[
\text{lk}(t) = \{ s \in L \mid s \cup t \in L \text{ and } t \cap s = \emptyset \}
\]

Example 23. If we look at a graph as a one dimensional simplicial complex, then the vertices are sets of the form \( \{i\} \) and edges are sets of the form \( \{i, j\} \). For a vertex \( t = \{v\} \), the edges of the form \( s = \{v, u\} \) will not be in the link of \( t \) because \( t \cap s = \emptyset \) is not satisfied. If we pick \( s = \{i, j\} \) and \( v \notin s \), then \( s \cup t \in L \) is not satisfied. So there will be no edges in the link. However, if \( s = \{u\} \) and \( u \) is a neighbour of \( v \), then \( s \cup t \in L \) and \( s \cap t = \emptyset \). Hence the link of a vertex will be precisely the other vertices that the vertex is connected to; the notion of the link generalises the idea of a neighbourhood in a graph.

Example 24. Now consider the simplicial complex depicted in Figure 1: it has 8 vertices, 12 edges and 3 two-dimensional simplices that are shaded in grey. On the left hand side of the figure we see highlighted in blue the link of the vertex 1, which is highlighted in red. So \( \text{lk}\{1\} = \{\{2\}, \{3\}, \{5\}, \{6\}, \{8\}, \{2, 3\}, \{2, 8\}, \{5, 6\}\} \).

On the right hand side of the figure we see highlighted in blue the link of the edge \( \{1, 2\} \), which is highlighted in red. That is, \( \text{lk}\{1, 2\} = \{\{3\}, \{8\}\} \).

Consider a random simplicial complex \( X(n, p) \). For \( 1 \leq i < j \leq n \) define the edge indicator \( Y_{i,j} := 1 \) \( \{\{i, j\}\} \in X(n, p) \). In this section we study the count of \( (k-1) \)-simplices that would be in the link of a fixed subset \( t \subseteq [n] \) if the subset spanned a simplex in \( X(n, p) \). Given that \( t \) is a simplex, the variable counts the number of \( (k-1) \)-simplices in \( \text{lk}(t) \). Thus, the random variable of interest is

\[
T_k^t = \sum_{s \subseteq \partial_k} \left\{ 1 \left( t \cap s = \emptyset \right) \prod_{i \notin j \subseteq s} Y_{i,j} \prod_{i \in s, j \in t} Y_{i,j} \right\} \quad (5.1)
\]

Note that the product \( \prod_{i \in s, j \in t} Y_{i,j} \) ensures that \( t \cup s \) is a simplex if \( t \) spans a simplex. The random variable \( T_k^t \) does not fit into the framework of generalised \( U \)-statistics because the summands depend not only on the
variables that are indexed by the subset $s$. Moreover, we do not sum over all subsets $s$ but rather only the ones that do not intersect $t$.

### 5.1 Moments

It is easy to see that for any positive integer $k$ and $t \subseteq [n],$

$$E\{T_{t}^{k+1}\} = \binom{n - |t|}{k+1} p^{(k+1)+|t|(k+1)} = \binom{n - |t|}{k+1} \mu_{k+1}^{t}$$

since there are $\binom{n}{k+1}$ choices for $s \in C_{k+1}$ such that $s \cap t = \emptyset$. Next we derive a lower bound on the variance.

**Lemma 25.** For any fixed $1 \leq k \leq n-1$ and $t \subseteq [n]$ we have:

$$\text{Var}(T_{t}^{k+1}) \geq (k+1) \binom{n - |t|}{2k+1} \binom{2k+1}{k} (\mu_{k+1}^{t})^{2} \left\{ p^{\frac{|t|}{2}} - 1 \right\}.$$

**Proof.** First let us calculate $Cov(T_{k+1}^{t}, T_{l+1}^{t})$. For fixed subsets $s \in C_{k+1}$ and $u \in C_{l+1}$ if $|s \cap u| = 0$, then the corresponding variables $\prod_{i \neq j \in s} Y_{i,j} \prod_{i \in s, j \in t} Y_{i,j}$ and $\prod_{i \neq j \in u} Y_{i,j} \prod_{i \in u, j \in t} Y_{i,j}$ are independent and so have zero covariance.

For $1 \leq m \leq l+1$, the number of pairs of subsets $s \in C_{k+1}$ and $u \in C_{l+1}$ such that $s \cap t = \emptyset = u \cap t$ and $|s \cap u| = m$ is $\binom{n-|t|}{k+1} \binom{k+1}{m} \binom{n-|t|-k-1}{l+1-m}$. Since each summand is non-negative, we lower bound by the $m = 1$ summand and get (with $\binom{a}{0} := 0$)

$$Cov(T_{k+1}^{t}, T_{l+1}^{t}) = \sum_{m=1}^{l+1} \binom{n - |t|}{k+1} \binom{k+1}{m} \binom{n - |t| - k - 1}{l + 1 - m} \left\{ \mu_{k+1}^{t} \mu_{l+1}^{t} p^{\frac{|t|}{2}} - |t| \mu_{k+1}^{t} \mu_{l+1}^{t} \right\} \geq \binom{n - |t|}{k+1} \binom{k+1}{l} \left\{ \mu_{k+1}^{t} \mu_{l+1}^{t} p^{\frac{|t|}{2}} - 1 \right\} = (k+1) \binom{n - |t|}{l+k+1} \binom{l+k+1}{l} \mu_{k+1}^{t} \mu_{l+1}^{t} \left\{ p^{\frac{|t|}{2}} - 1 \right\}.$$

Taking $l = k$ completes the proof.

---

Figure 1: Left: the link (highlighted in blue) of the vertex 1 (highlighted in red). Right: the link (highlighted in blue) of the edge $\{1, 2\}$ (highlighted in red). The two-dimensional simplices are shaded in grey.
5.2 Approximation theorem

For a multivariate normal approximation of counts given in Equation (5.1), we write \( \sigma_i = \sqrt{\text{Var}(T_{i+1})} \) and \( C_{i+1}^t = \{ \phi \in C_{i+1} \mid \phi \cap t = \emptyset \} \), as well as \( \mathbb{I}_i := C_{i+1}^t \times \{ i \} \). For \( s = (\phi, i) \in \mathbb{I}_i \) define

\[
X_s = \sigma_i^{-1} \left( \prod_{i \neq j \in \phi} Y_{i,j} \prod_{i \in \phi, j \neq t} Y_{i,j} - \mu_{i+1}^t \right).
\]

It is clear that \( \mathbb{E} \{ X_s \} = 0 \). Let \( W_i^t = \sum_{s \in \mathbb{I}_i} X_s \) and \( W^t = (W_1^t, W_2^t, \ldots, W_d^t) \in \mathbb{R}^d \). Then we have the following approximation theorem.

**Theorem 26.** Let \( Z \sim \text{MVN}(0, \text{Id}_{d \times d}) \) and \( \Sigma \) be the covariance matrix of \( W^t \).

1. Let \( h \in \mathcal{H}_d \). Then

\[
|\mathbb{E}h(W^t) - \mathbb{E}(\Sigma^{\frac{1}{2}} Z)| \leq |h|_3 B_{26}(n - |t|)^{- \frac{1}{2}}.
\]

2. Let \( \mathcal{K} \) be the class of convex sets in \( \mathbb{R}^d \). Then

\[
\sup_{A \in \mathcal{K}} |\mathbb{P}(W^t \in A) - \mathbb{P}(\Sigma^{\frac{1}{2}} Z \in A)| \leq 2^{\frac{7}{2}} 3^{-\frac{3}{2}} d^{\frac{3}{2}} B_{26}^2 (n - |t|)^{- \frac{1}{2}}.
\]

Here

\[
B_{26} = \frac{7}{6}(2d + 1)^{5d + \frac{17}{2}} (p^{-|t|} - 1)^{- \frac{1}{2}} p^{-(d+1)(d+2)|t|}.
\]

**Proof.** It is clear that \( W^t \) satisfies the conditions of Corollary 10 with the dependency neighbourhood \( \mathcal{D}_j(s) = \{ (\psi, j) \in \mathbb{I}_j \mid |\phi \cap \psi| \geq 1 \} \) for any \( s = (\phi, i) \in \mathbb{I}_i \). So we aim to bound the quantity \( B_{10} \) from the corollary.

Given \( \phi \in C_{i+1}^t \) and \( m \leq \min(i + 1, j + 1) \) there are \( \binom{i+1}{m} \binom{n-|t|-i-1}{j+1-m} \) subsets \( \psi \in C_{j+1}^t \) such that \( |\psi \cap \phi| = m \). Therefore, for any \( i, j \in [d] \) and \( s \in \mathbb{I}_i \), we have

\[
|\mathcal{D}_j(s)| = \sum_{m=1}^{\min(i,j)+1} \binom{i+1}{m} \binom{n-|t|-i-1}{j+1-m} \\
\leq (i+1)^{\min(i,j)+2} (n-|t|)^{j} \\
\leq (d+1)^{d+2} (n-|t|)^{j} \quad (5.2)
\]

giving a bound for \( \alpha_{ij} \). For a bound on \( \beta_{ijk} \), applying Lemma 8, for any \( i, j, k \in [d] \) and \( s \in \mathbb{I}_i, u \in \mathbb{I}_j, v \in \mathbb{I}_k \) we get

\[
\mathbb{E} |X_s X_u X_v| \leq (\sigma_i \sigma_j \sigma_k)^{-1} \left\{ \mu_{i+1}^t \mu_{j+1}^t (1 - \mu_{i+1}^t)(1 - \mu_{j+1}^t) \right\}^{\frac{1}{2}}; \quad (5.3)
\]
\[
\mathbb{E} |X_s X_u| \mathbb{E} |X_v| \leq (\sigma_i \sigma_j \sigma_k)^{-1} \left\{ \mu_{i+1}^t \mu_{j+1}^t (1 - \mu_{i+1}^t)(1 - \mu_{j+1}^t) \right\}^{\frac{1}{2}}. \quad (5.4)
\]

Now we apply Corollary 25 and get

\[
\sigma_i^2 \geq (i+1) \binom{n-|t|}{2i+1} \binom{2i+1}{i} \left( \mu_{k+1}^t \right)^2 \left\{ p^{-|t|} - 1 \right\} \\
\geq \frac{(n-|t|)^{2i+1}}{(2d+1)^{d+1} d^d} \left( \mu_{k+1}^t \right)^2 \left\{ p^{-|t|} - 1 \right\}.
\]

Taking both sides of the inequality to the power of \(-\frac{1}{2}\) we get for any \( i \in [d] \)

\[
\sigma_i^{-1} \leq (n-|t|)^{-\frac{i-\frac{1}{2}}{2}} (2d+1)^{\frac{d+1}{2} d^d} \left( \mu_{k+1}^t \right)^{-1} \left\{ p^{-|t|} - 1 \right\}^{-\frac{1}{2}}. \quad (5.5)
\]
Using Equations (5.2) - (5.5) to bound $B_{10}$ from Corollary 10 we get:

$$
B_{10} \leq \frac{7}{6} \sum_{i,j,k=1}^{d} \left( \frac{n - |t|}{i + 1} \right) (d + 1)^{2d+4} (n - |t|)^{i+j+k} (\sigma_i \sigma_j \sigma_k)^{-1} \\
\{ \mu_{i+1}^{t} \mu_{j+1}^{t} (1 - \mu_{i+1}^{t})(1 - \mu_{j+1}^{t}) \}^{\frac{1}{2}} \\
\leq \frac{7}{6} \sum_{i,j,k=1}^{d} (n - |t|)^{i+j+k+1} (d + 1)^{2d+4} (n - |t|)^{-i-j-k-\frac{3}{2}} (2d + 1)^{\frac{3d+3}{2}} d^{\frac{d}{2}} \\
(p^{-|t|} - 1)^{-\frac{1}{2}} (\mu_{k+1}^{t} \mu_{i+1}^{t} \mu_{j+1}^{t})^{-1} \{ \mu_{i+1}^{t} \mu_{j+1}^{t} (1 - \mu_{i+1}^{t})(1 - \mu_{j+1}^{t}) \}^{\frac{1}{2}} \\
\leq (n - |t|)^{-\frac{1}{2}} \frac{7}{6} (2d + 1)^{5d+\frac{1}{2}} (p^{-|t|} - 1)^{-\frac{1}{2}} \sum_{i,j,k=1}^{d} ((\mu_{i+1}^{t} \mu_{j+1}^{t})^{-1} (\mu_{k+1}^{t})^{-2})^{\frac{1}{2}} \\
\leq \left\{ \frac{7}{6} (2d + 1)^{5d+\frac{1}{2}} (p^{-|t|} - 1)^{-\frac{1}{2}} p^{-(d+1)(d+2|t|)} \right\} (n - |t|)^{-\frac{1}{2}}.
$$

**Remark 27.** Recall that $\mathbb{E} \{ T_{k+1}^{t} \} = \frac{(n-|t|)p^{(k+1)}+|t|}{k+1}$. By Stirling’s approximation, if $p \in (0, 1)$ is a constant, then $\max(k, |t|) = \Omega((\ln n)^{1+\epsilon}(n))$ for any positive $\epsilon$ forces the expectation to go to 0 asymptotically. Hence, by Markov’s inequality, with high probability there are no $k$-simplices in the link of $t$ as long as $\max(k, |t|)$ is of order $\ln^{1+\epsilon}(n)$ or larger for any $\epsilon > 0$ for a constant $p$.

Recall that in Theorem 26 we count all simplices up to dimension $d$ in the link of $t$. Note that if $\max(d^2, d|t|) = O(\ln^{1-\epsilon}(n))$ for any $\epsilon > 0$, then the bounds in Theorem 26 tend to 0 as $n$ tends to infinity as long as $p \in (0, 1)$ stays constant. In particular, if $d$ is a constant, Theorem 26 gives an approximation for all sizes of $t$ for which the approximation is needed.

## 6 Critical simplex counts in lexicographical Morse matchings

Finally we attend to our motivating problem, critical simplex counts. We first introduce the relevant notions.

**Definition 28.** A **partial matching** on a simplicial complex $\mathcal{L}$ is $\Sigma = \{ (s, t) \mid s \subseteq t \in \mathcal{L} \text{ and } |t| - |s| = 1 \}$ such that every simplex appears in at most one pair of $\Sigma$. A $\Sigma$-**path** (of length $k \geq 1$) is a sequence of distinct simplices of $\mathcal{L}$ of the following form:

$$(s_1 \subseteq t_1 \supseteq s_2 \subseteq t_2 \supseteq \ldots \supseteq s_k \subseteq t_k)$$

such that $(s_i, t_i) \in \Sigma$ and $|t_i| - |s_{i+1}| = 1$ for all $i \in [k]$. A $\Sigma$-path is called a **gradient path** if $k = 1$ or $s_1$ is not a subset of $t_k$. A partial matching $\Sigma$ on $\mathcal{L}$ is called **acyclic** iff every $\Sigma$-path is a gradient path. Given a partial matching $\Sigma$ on $\mathcal{L}$, we say that a simplex $t \in \mathcal{L}$ is **critical** iff $t$ does not appear in any pair of $\Sigma$.

For a one-dimensional simplicial complex, viewed as a graph, a partial matching $\Sigma$ is comprised of elements $(v; \{u, v\})$ with $v$ a vertex and $\{u, v\}$ an edge. A $\Sigma$-path is then a sequence of distinct vertices and edges $v_1, \{v_1, v_2\}, v_2, \{v_2, v_3\}, \ldots, v_k, \{v_k, v_{k+1}\}$ where each consecutive pair of the form $(v_i, \{v_i, v_{i+1}\})$ is constrained to lie in $\Sigma$.

We refer the interested reader to [14] for an introduction to discrete Morse theory and to [30] for seeing how it is used to reduce computations in the persistent homology algorithm. In this work we aim to understand how much improvement one would likely get on a random input when using a specific type of acyclic partial matching, defined below.
Definition 29. Let $\mathcal{L}$ be a simplicial complex and assume that the vertices are ordered by $[n] = \{1, \ldots, n\}$. For each simplex $s \in \mathcal{L}$ define

$$I_{\mathcal{L}}(s) := \{ j \in [n] \mid j < \min(s) \text{ and } s \cup \{j\} \in \mathcal{L}\}.$$ 

Now consider the pairings

$$s \leftrightarrow s \cup \{i\},$$

where $i = \min I_{\mathcal{L}}(s)$ is the smallest element in the set $I_{\mathcal{L}}(s)$, defined whenever $I_{\mathcal{L}}(s) \neq \emptyset$. We call this the lexicographical matching.

Due to the min $I_{\mathcal{L}}(s)$ construction in the lexicographical matching, the indices are decreasing along any path and hence it will be a gradient path, showing that the lexicographical matching is indeed an acyclic partial matching on $\mathcal{L}$.

Example 30. Consider the simplicial complex $\mathcal{L}$ depicted in Figure 2. The complex has 5 vertices, 6 edges and one two-dimensional simplex that is shaded in grey. The red arrows show the lexicographical matching on this simplicial complex: there is an arrow from a simplex $s$ to $t$ iff the pair $(s,t)$ is part of the matching. More explicitly, the lexicographical matching on $\mathcal{L}$ is

$$\Sigma = \{(\{2\}, \{1,2\}), (\{3\}, \{2,3\}), (\{4\}, \{1,4\}), (\{5\}, \{3,5\}), (\{4,5\}, \{3,4,5\})\}.$$ 

Note that $\{3,4\}$ cannot be matched because the set $I_{\mathcal{L}}(\{3,4\})$ is empty. Also, in any lexicographical matching $\{1\}$ is always critical as there are no vertices with a smaller label and hence the set $I_{\mathcal{L}}(\{1\})$ is empty. So under this matching there are two critical simplices: $\{1\}$ and $\{3,4\}$, highlighted in blue in the figure. Hence, if we were computing the homology of this complex, considering only two simplices would be sufficient instead of all 12 which are in $\mathcal{L}$ - a significant improvement.

The following lemma is an immediate consequence of Definition 29.

Lemma 31. Let $\mathcal{L}$ be a simplicial complex. Consider the lexicographical matching on $\mathcal{L}$. Then $t \in \mathcal{L}$ matches with one of its cofaces (i.e. $s \in \mathcal{L}$ with $|s| - |t| = 1$ and $t \subset s$) iff it is not the case that for all $j < \min(t)$ we have $t \cup \{j\} \notin \mathcal{L}$. Also, $t \in \mathcal{L}$ matches with one of its faces (i.e. $s \in \mathcal{L}$ with $|t| - |s| = 1$ and $s \subset t$) iff for all $j < \min(t)$ we have $t \setminus \{\min(t)\} \cup \{j\} \notin \mathcal{L}$.

Consider a random simplicial complex $X(n,p)$. Here we study the joint distribution of critical simplices in different dimensions with respect to the lexicographical matching on a random clique complex $X(n,p)$. For any pair of integers $1 \leq i < j \leq n$ let $Y_{i,j} := \mathbb{1}(\{i,j\} \in X(n,p))$ be the edge indicator. In this section we study the count of $(k-1)$-simplices that are critical under the lexicographical matching on $X(n,p)$.

Fix $s \in C_k$. Define the variables $X_s^+ = \mathbb{1} (s \text{ matches with its coface given it is a simplex})$ and $X_s^- = \mathbb{1} (s \text{ matches with its face given it is a simplex})$. The events that the two variables indicate are disjoint. By Lemma 31 we can see that $X_s^+ = 1 - \prod_{i=1}^{\min(s)-1} \left(1 - \prod_{j \in s} Y_{i,j}\right)$ and that $X_s^- = \prod_{i=1}^{\min(s)-1} \left(1 - \prod_{j \in s_\ominus} Y_{i,j}\right)$, where $s_\ominus := s \setminus \{\min(s)\}$. Hence,

$$\mathbb{1} (s \text{ is a critical simplex}) = \mathbb{1} (s \in X(n,p)) \left(1 - (X_s^+ + X_s^-)\right)$$
Lemma 33. For any

\[ \text{error after committing it ourselves in an earlier version of this paper.} \]

Proof.

Thus, the random variable of interest is

\[
T_k = \sum_{s \in C_k} \prod_{i \not\in j \in s} \left[ \min(s) - 1 \prod_{i=1}^{\min(s)-1} \left(1 - \prod_{j \in s} Y_{i,j}\right) \right].
\]

(6.1)

Note that this random variable does not fit into the framework of generalised U-statistics because the summands depend not only on the variables that are indexed by the subset s.

Remark 32. The construction of Costa and Farber from [11] provides a more general model for random simplicial complexes than \( X(n, p) \). Their model depends on an underlying vertex set \([n]\) along with a sequence of probabilities \( p := (p_1, p_2, \ldots, p_{n-1}) \). A simplicial complex drawn from this model contains all \( n \) vertices, and each edge appears independently with probability \( p_1 \). The resulting 3-cliques are then filled by 2-simplices again independently with probability \( p_2 \), and so forth. Thus, \( X(n, p) \) is the Costa-Farber complex with probability sequence \((p, 1, 1, \ldots, 1)\).

The authors of [4, Sec 8] have also sought to compute the expected number of critical simplices for the lexicographical Morse matching, but in the more general setting of Costa-Farber random complexes. Their calculation is based on the premise that a simplex \( s \) in such a complex is critical if and only if it admits no cofacets \( t = s \cup \{i\} \) with \( i < \min(s) \). Unfortunately, this premise is flawed. If true, it would force every simplex of maximal dimension to be critical for the simple reason that it admits no cofacets whatsoever, and the simplex \( \{3, 4, 5\} \) from Figure 2 serves as an easy counterexample. The problem with the premise is that it fails to account for the larger simplex \( t \) in the \( \Sigma \)-pair \((s, t)\). In terms of the variables introduced after Lemma 31, the authors of [4] have computed the expected value of the random variable

\[
\sum_{s \in C_k} \prod_{i \not\in j \in s} \left[ \min(s) - 1 \prod_{i=1}^{\min(s)-1} \left(1 - \prod_{j \in s} Y_{i,j}\right) \right],
\]

rather than \( T_k \) from (6.1) above. Although this oversight results in over-counting the expected number of critical simplices, it does not alter the asymptotic behaviour described in [4, Sec 8]. We only spotted this error after committing it ourselves in an earlier version of this paper.

6.1 Moments

Lemma 33. For any \( 1 \leq k \leq n - 1 \) we have:

\[
p^{\binom{k+1}{2} + k} \binom{n - 2}{k} (1 - p) \leq E\{T_{k+1}\} \leq p^{\binom{k+1}{2} - k - 1} \binom{n - 1}{k} (1 - p).
\]

Proof.

\[
E \{T_{k+1}\} = \sum_{l=1}^{n-k} \sum_{s \in C_{k+1}} \prod_{i \not\in j \in s} \left[ \prod_{i=1}^{l-1} \left(1 - \prod_{j \in s} Y_{i,j}\right) - \prod_{i=1}^{l-1} \left(1 - \prod_{j \in s} Y_{i,j}\right) \right]
\]

\[
= p^{\binom{k+1}{2}} \sum_{l=1}^{n-k} \sum_{s \in C_{k+1}} \left\{(1 - p^{k+1})^{l-1} - (1 - p^k)^{l-1}\right\}
\]

\[
= p^{\binom{k+1}{2}} \sum_{l=0}^{n-k-1} \binom{n-1-l}{k} \left\{(1 - p^{k+1})^l - (1 - p^k)^l\right\}
\]

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For any integer \( k \leq n \leq n - 1 \) we have:

\[
\text{Var}(T_{k+1}) = 2p(\frac{k+1}{2})V_1 + 2p(\frac{k}{2})V_2 + p^2(\frac{k+1}{2})V_3 + p(\frac{k}{2})V_4,
\]

where

\[
V_1 = \sum_{i,j=1}^{n-k} \sum_{m=1}^{k} \min(k+1,j-i) \sum_{q=1}^{m} \left( \frac{n-j}{2k+1-m-q} \right) \left( \frac{k}{2k+1-m} \right) \left( \frac{j-i+1}{q-1} \right) \left\{ p^{-\left(\frac{1}{2}\right)}(1-p^{k+1})^{j-i-q}(1-p^{k+1-m})^{q}[(1-2p^{k+1}+p^{2k+2-m})^{i-1} - (1-p^{k+1} - p^{k} + p^{2k+2-m})^{i-1} + p^{-\left(\frac{1}{2}\right)}(1-p^{k})^{j-i-q}(1-p^{k-m})^{q}][(1-2p^{k}+p^{2k+1-m})^{i-1} - (1-p^{k+1} - p^{k} + p^{2k+2-m})^{i-1} - ((1-p^{k+1})^{i-1} - (1-p^{k})^{i-1})((1-p^{k+1})^{j-1} - (1-p^{k})^{j-1})] \right\};
\]

\[
V_2 = \sum_{i,j=1}^{n-k} \sum_{m=1}^{k} \min(k+1,j-i) \sum_{q=1}^{m} \left( \frac{n-j}{2k+1-m-q} \right) \left( \frac{k}{2k+1-m} \right) \left( \frac{j-i+1}{q-1} \right) \left\{ p^{-\left(\frac{1}{2}\right)}(1-p^{k+1})^{j-i-q}(1-p^{k+1-m})^{q}[(1-2p^{k+1}+p^{2k+2-m})^{i-1} - (1-p^{k+1} - p^{k} + p^{2k+2-m})^{i-1} + p^{-\left(\frac{1}{2}\right)}(1-p^{k})^{j-i-q}(1-p^{k-m})^{q}][(1-2p^{k}+p^{2k-m})^{i-1} - (1-p^{k+1} - p^{k} + p^{2k+2-m})^{i-1} - ((1-p^{k+1})^{i-1} - (1-p^{k})^{i-1})((1-p^{k+1})^{j-1} - (1-p^{k})^{j-1})] \right\};
\]

\[
V_3 = \sum_{i=1}^{n-k} \sum_{m=1}^{k} \left( \frac{n-i}{2k+1-m} \right) \left( \frac{k}{2k+1} \right) \left( \frac{m}{m-1} \right) \left\{ p^{-\left(\frac{1}{2}\right)}[(1-2p^{k+1}+p^{2k+2-m})^{i-1} + (1-p^{k} + p^{2k+2-m})^{i-1} - 2(1-p^{k} - p^{k+1} + p^{2k+2-m})^{i-1} - ((1-p^{k+1})^{i-1} - (1-p^{k})^{i-1})^{2}] \right\};
\]

\[
V_4 = \sum_{i=1}^{n-k} \left( \frac{n-i}{k} \right) \left\{ (1-p^{k+1})^{i-1} - (1-p^{k})^{i-1} - p(\frac{k+1}{2})((1-p^{k+1})^{i-1} - (1-p^{k})^{i-1})^{2} \right\}.
\]
Here the notation $\sum_{i<j}^{n-k}$ stands for $\sum_{i=1}^{n-k-1} \sum_{j=i+1}^{n-k}$.

**Lemma 35.** For a fixed integer $1 \leq k \leq n - 1$ and $p \in (0, 1)$ there is a constant $C_{p,k} > 0$ independent of $n$ and a natural number $N_{p,k}$ such that for any $n \geq N_{p,k}$:

$$\Var(T_{k+1}) \geq C_{p,k} n^{2k}.$$  

In Lemma 35 the constant could have been made explicit at the expense of a lengthy calculation. The proofs of Lemmas 34 and 35 are long (and not particularly insightful) calculations, which are deferred to the Appendix.

Just knowing the expectation and the variance can already give us some information about the variable. For example, we obtain the following proposition. This proposition shows that considering only a subset of the simplices already gives a good approximation for the critical simplex counts. We recall the notation that $f(n) = \omega(g(n))$ indicates that $\lim_{n \to \infty} \frac{f(n)}{g(n)} = \infty$.

**Proposition 36.** Fix $k \in [n]$. Let $K \leq n-k$ and set the random variable:

$$T_{k+1}^K := \sum_{s \in C_{k+1}} \prod_{i \neq j \in s, \min(s) \leq K} Y_{i,j} \left[ \prod_{i=1}^{\min(s)-1} \left( 1 - \prod_{j \in s} Y_{i,j} \right) - \prod_{i=1}^{\min(s)-1} \left( 1 - \prod_{j \in s^c} Y_{i,j} \right) \right].$$

If $K = K(n) = \omega(\ln^{1+\epsilon}(n))$ for any $\epsilon > 0$, then the variable $T_{k+1} - T_{k+1}^K$ vanishes with high probability, provided that $p$ and $k$ stay constant.

**Proof.** A similar calculation to that for Lemma 33 shows that:

$$\mathbb{E} \left\{ T_{k+1} - T_{k+1}^K \right\} = \sum_{i=K+1}^{n-k} \binom{n-i}{k} \binom{k^{(i+1)}}{2} \{ (1-p^{k+1})^{i-1} - (1-p^k)^{i-1} \} \leq \binom{n}{k} p^{(k+1)} (1-p^{k+1})K \sum_{i=0}^{\infty} (1-p^{k+1})^i \leq p^{(k+1)} - k \frac{n^k}{k!} (1-p^{k+1})^K.$$  

Using Markov’s inequality, we get:

$$\mathbb{P}(T_{k+1} - T_{k+1}^K \geq 1) \leq p^{(k+1)} - k \frac{n^k}{k!} (1-p^{k+1})^K,$$

which asymptotically vanishes as long as $K = \omega(\ln^{1+\epsilon}(n))$.  

### 6.2 Approximation theorem

For $i \in [d]$, recall a random variable counting $i$-simplices in $X(n, p)$ that are critical under the lexicographical matching, as given in (6.1). We write for the $i$-th index set $I_i := C_{i+1} \times \{ i \}$. For $s = (\phi, i) \in I_i$ we write

$$\mu_s = p^{(i+1)} \left( (1-p^{i+1})^{\min(\phi)-1} - (1-p^i)^{\min(\phi)-1} \right)$$

and $\sigma_i = \sqrt{\Var(T_{i+1})}$. Let

$$X_s = \sigma_i^{-1} \left\{ \prod_{i \neq j \in \phi} Y_{i,j} \left[ \prod_{i=1}^{\min(\phi)-1} \left( 1 - \prod_{j \in \phi} Y_{i,j} \right) - \prod_{i=1}^{\min(\phi)-1} \left( 1 - \prod_{j \in \phi^c} Y_{i,j} \right) \right] - \mu_s \right\}.$$  

Let $W_I = \sum_{s \in I} X_s$ and $W = (W_1, W_2, \ldots, W_d) \in \mathbb{R}^d$. For bounds that asymptotically go to zero for this example, we use Theorems 2 and 9 directly: the uniform bounds from Corollary 10 are not fine enough here.

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Theorem 37. Let $Z \sim \text{MVN}(0, \text{Id}_{d \times d})$ and $\Sigma$ be the covariance matrix of $W$.

1. Let $h \in \mathcal{H}_d$. Then there is a constant $B_{37.1} > 0$ independent of $n$ and a natural number $N_{37.1}$ such that for any $n \geq N_{37.1}$ we have

$$|\mathbb{E}h(W) - \mathbb{E}h(\Sigma^{1/2} Z)| \leq B_{37.1} |h|_3 n^{-1}.$$

2. Let $K$ be the class of convex sets in $\mathbb{R}^d$. Then there is a constant $B_{37.2} > 0$ independent of $n$ and a natural number $N_{37.2}$ such that for any $n \geq N_{37.2}$ we have

$$\sup_{A \in K} |\mathbb{P}(W \in A) - \mathbb{P}(\Sigma^{1/2} Z \in A)| \leq B_{37.2} n^{-4/3}.$$

Proof. It is clear that $W$ satisfies the conditions of Theorems 2 and 9 for any $s = (\phi, i) \in \mathbb{I}_i$ setting

$$D_j(s) = \{(\psi, j) \in I_j \mid |\phi \cap \psi| \geq 1\}.$$

We apply Theorems 2 and 9. For the bounds on the quantity $B_2$ from Theorems 2 and 9 we use Lemma 8 and Lemma 35. We write $C$ for an unspecified positive constant that does not depend on $n$. Also, we assume here that $n$ is large enough for the bound in Lemma 35 to apply. We write $\mu(p, i, a) = p^{(a+1)} ((1 - p^{i+1})^{a-1} - (1 - p)^{n-1})$. Then we have:

$$B_2 \leq \frac{1}{3} \sum_{i,j,k=1}^{d} \sum_{a=1}^{n-i} \sum_{b=1}^{n-j} \sum_{\phi, \psi, \phi \cap \psi = a, \min(\phi) = a} 3 \left( \sum_{r \in \mathcal{D}_k((\phi, i))} \frac{1}{2} (\sigma_i \sigma_j \sigma_k)^{-1} \{ \mu(p, i, a) \mu(p, j, b) (1 - \mu(p, i, a)) (1 - \mu(p, j, b)) \}^{1/2} \right)$$

$$+ \sum_{r \in \mathcal{D}_k((\psi, j))} (\sigma_i \sigma_j \sigma_k)^{-1} \{ \mu(p, i, a) \mu(p, j, b) (1 - \mu(p, i, a)) (1 - \mu(p, j, b)) \}^{1/2}$$

$$\leq \sum_{i,j,k=1}^{d} \sum_{a=1}^{n-i} \sum_{b=1}^{n-j} Cn^{i+j-1} n^{-i-j-k} \left( (1 - p^{i+1})^{a-1} (1 - p^{j+1})^{b-1} + (1 - p)^{a-1} (1 - p)^{b-1} \right)^{1/2}$$

$$\leq Cn^{-1} \sum_{i,j,k=1}^{d} \sum_{a=1}^{n-i} \sum_{b=1}^{n-j} \left[ (1 - p^{i+1})^{a-1} (1 - p^{j+1})^{b-1} \right]^{1/2} + \left[ (1 - p)^{a-1} (1 - p)^{b-1} \right]^{1/2}$$

$$\leq Cn^{-1} d^3 \left\{ \frac{1}{(1 - \sqrt{1 - p^{i+1}})^2} + \frac{1}{(1 - \sqrt{1 - p^j})^2} \right\} \leq Cn^{-1}.$$

\[\square\]

Remark 38. The relevance of understanding the number of critical simplices in the context of TDA is as follows. We assume that $p \in (0, 1)$ and $k \in \{1, 2, \ldots\}$ are constants.

1. As seen in Lemma 33, the expected number of critical $k$-simplices under the lexicographical matching is one power of $n$ smaller than the total number of $k$-simplices in $\mathbf{X}(n, p)$.

2. In light of our approximation Theorem 37 we also know that the (rescaled) deviations from the mean are approximately normal and the bounds are of the same order of $n$ compared to the approximation of all simplex counts in $\mathbf{X}(n, p)$ as given in Theorem 18. Knowing the expectation and the variance from Lemmas 34 and 33, one can apply concentration inequalities, for example, Chebyshev’s inequality, to show that the number of critical simplices concentrates around its mean. Hence, because of the concentration of measure, the computational improvements as a result of lexicographical matching are likely substantial in $\mathbf{X}(n, p)$.
3. From Proposition 36, it is very likely that in $X(n,p)$ all $k$-simplices $s \in X(n,p)$ with $\min(s) = \omega(\ln^{1+\epsilon}(n))$ for any fixed $\epsilon > 0$ are not critical.

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Proof of Lemma 34. For \( s \in C_{k+1} \) recall that \( s_\ominus = s \setminus \{ \min(s) \} \). We write:

\[
Y_s^+ = \prod_{i=1}^{\min(s)-1} \left( 1 - \prod_{j \notin s} Y_{i,j} \right), \quad Y_s^- = \prod_{i=1}^{\min(s)-1} \left( 1 - \prod_{j \notin s} Y_{i,j} \right),
\]

\[
Z_s = \prod_{i \neq j \in s} Y_{i,j}, \quad Y_s = Y_s^+ - Y_s^-.
\]
Then $Z_s$ and $Y_s$ are independent and $T_{k+1} = \sum_{s \in C_{k+1}} Z_s Y_s$. Consider the variance:

$$
\text{Var}(T_{k+1}) = \sum_{s \in C_{k+1}} \text{Var}(Z_s Y_s) + \sum_{s \neq t \in C_{k+1}, \min(s) \neq \min(t)} \text{Cov}(Z_s Y_s, Z_t Y_t) + \sum_{s \neq t \in C_{k+1}, \min(s) = \min(t)} \text{Cov}(Z_s Y_s, Z_t Y_t). \tag{A.1}
$$

For the first term in (A.1), writing

$$
P(Z_s Y_s = 1) = \mu(p, k, i) = p^{(k+1)}((1 - p^{k+1})^{i-1} - (1 - p^k)^{i-1})
$$

we see:

$$
\sum_{s \in C_{k+1}} \text{Var}(Z_s Y_s) = \sum_{i=1}^n \sum_{s \in C_{k+1}, \min(s) = i} \left( \mathbb{E} \left\{ (Z_s Y_s)^2 \right\} - \mathbb{E} \left\{ Z_s Y_s \right\}^2 \right) = \sum_{i=1}^{n-k} \binom{n-i}{k} \left( P(Z_s Y_s = 1) - P(Z_s Y_s = 1)^2 \right) = \sum_{i=1}^{n-k} \binom{n-i}{k} \{ \mu(p, k, i) - (\mu(p, k, i))^2 \} = p^{(k+1)} V_4.
$$

Now consider the covariance terms in (A.1), the expansion of the variance. Note that for any $s, t \in C_{k+1}$ if $s \cap t = \emptyset$, then the variables $Z_s Y_s$ and $Z_t Y_t$ can be written as functions of two disjoint sets of independent edge indicators and hence have zero covariance.

Fix $s, t \in C_{k+1}$ and assume $|s \cap t| = m$ where $1 \leq m \leq k$. Note that because $m \neq k + 1$, we have $s \neq t$. There are $2^{(k+1)} - \binom{m}{2}$ distinct edges in $s$ and $t$ combined and hence $P(Z_s Z_t = 1) = p^{2^{(k+1)} - \binom{m}{2}}$. Also, $Y_s Y_t = Y_s^+ Y_t^+ + Y_s^- Y_t^- - Y_s^+ Y_t^- - Y_s^- Y_t^+$. For the rest of the proof when calculating probabilities we assume w.l.o.g. that $\min(s) \leq \min(t)$. Then we have for $Y_s^+ Y_t^+$:

$$
Y_s^+ Y_t^+ = \prod_{i=1}^{\min(t)-1} (1 - \prod_{j \in t} Y_{i,j}) \prod_{i=1}^{\min(s)-1} (1 - \prod_{j \in s} Y_{i,j}).
$$

Fix $i \in [\min(s) - 1]$. Then with $\neg$ denoting the complement

$$
P(1 - \prod_{j \in s} Y_{i,j}, 1 - \prod_{j \in t} Y_{i,j}) = P(\neg(\prod_{j \in s} Y_{i,j} = 1 \cup \prod_{j \in t} Y_{i,j} = 1))
$$

$$
= 1 - \left\{ P(\prod_{j \in s} Y_{i,j} = 1) + P(\prod_{j \in t} Y_{i,j} = 1) - P(\prod_{j \in s} Y_{i,j} = 1 \cap \prod_{j \in t} Y_{i,j} = 1) \right\} = 1 - (2p^{k+1} - p^{k+2-m}).
$$

Moreover, $\prod_{i=1}^{\min(s)-1} (1 - \prod_{j \in s} Y_{i,j}) (1 - \prod_{j \in t} Y_{i,j})$ and $\prod_{i=\min(s)}^{\min(t)-1} (1 - \prod_{j \in t} Y_{i,j})$ are independent of $Z_s Z_t$. Recall the notation $[a, b] = \{a, a + 1, \ldots, b\}$ for two positive integers $a \leq b$. Setting $q_{s,t} := |s \cap [\min(s), \min(t) - 1]|$,

$$
P(Y_s^+ Y_t^+ = 1 | Z_s Z_t = 1)
$$
Using the described strategy we get:

\[ P\left( \prod_{i=1}^{\min(s)-1} (1 - \prod_{j \in s} Y_{i,j}) (1 - \prod_{j \in \ell} Y_{i,j}) = 1 \right) P\left( \prod_{i=\min(s)}^{\min(t)-1} (1 - \prod_{j \in s} Y_{i,j}) = 1 \right) \]

\[ = (1 - 2p^{k+1} + p^{2k+2-m}\min(s) - 1)(1 - p^{k+1})\min(t) - (1 - p^{k+1})\min(a,t) \]

This strategy of splitting the product \( Y_s^+ Y_t^+ \) into three products of independent variables, only one of which is dependent on \( Z_s Z_t \) works exactly in the same way for the variables \( Y_s^+ - Y_t^+ \), \( Y_s^+ Y_t^- \), \( Y_s^- Y_t^- \). We write

\[ i = \min(s), j = \min(t), \text{ and } q \text{ instead of } q_{s,t}. \]

Also, we set

\[ \pi(i, j, a, b, d_1, d_2, q) := (1 - p^a - p^b + p^{a+b-d_1})^{i-1}(1 - p^a)^{j-1-q}(1 - p^{a-d_2})^q. \]

Using the described strategy we get:

\[ P\left( Y_s^- Y_t^- = 1 | Z_s Z_t = 1 \right) = \pi(i, j, k, k, |s \cap t|, |s \cap t|, q) \]
\[ P\left( Y_s^+ Y_t^- = 1 | Z_s Z_t = 1 \right) = \pi(i, j, k, k+1, |s \cap t|, |s \cap t|, q) \]
\[ P\left( Y_s^- Y_t^+ = 1 | Z_s Z_t = 1 \right) = \pi(i, j, k+1, k, |s \cap t|, m, q). \]

Now we are ready to calculate the covariance:

\[\text{Cov}(Z_s Y_s, Z_t Y_t) = \mathbb{E} \left\{ Z_s Z_t Y_s^+ Y_t^+ \right\} - \mathbb{E} \left\{ Z_s Z_t Y_s^- Y_t^- \right\} - \mathbb{E} \left\{ Z_s Z_t Y_s^+ Y_t^- \right\} - \mathbb{E} \left\{ Z_s Z_t Y_s^- Y_t^+ \right\} \]
\[= P(Z_s Z_t = 1) \left[ P(Y_s^+ Y_t^+ = 1 | Z_s Z_t = 1) + P(Y_s^- Y_t^- = 1 | Z_s Z_t = 1) \right] \]
\[= P(Y_s^+ Y_t^- = 1 | Z_s Z_t = 1) - P(Y_s^- Y_t^+ = 1 | Z_s Z_t = 1) \]
\[= p^{2(k+1) - (\min(s) + \min(t))} \pi(i, j, k, 1, k, m, m, q) - \pi(i, j, k, 1, s \cap t, m, q) \]
\[= - \pi(i, j, k, 1, s \cap t, m, q) \]

Next we consider the two covariance sums in (A.1) separately. First assume that \( \min(s) \neq \min(t) \). Given \( i, j \in [n - k], m \in [k] \), and \( q \in [\min(k + 1, j - i)] \) define the set

\[ \Gamma_{k+1}(i, j, m, q) = \{ (s, t) | s, t \in C_{k+1}, \min(s) = i, \min(t) = j, |s \cap t| = m, \max(q_{s,t}, q_{t,s}) = q \} \]

as well as

\[ \Gamma_{k+1}^+(i, j, m, q) = \{ (s, t) \in \Gamma_{k+1}(i, j, m, q) | \min(t) \in s \} \]

and

\[ \Gamma_{k+1}^-(i, j, m, q) = \{ (s, t) \in \Gamma_{k+1}(i, j, m, q) | \min(t) \notin s \}. \]

Next we argue that

\[ |\Gamma_{k+1}^+(i, j, m, q)| = \binom{n-j}{2k+1-m-q} \binom{2k+1-m-q}{k} \binom{k}{m-1} \binom{j-i+1}{q-1}. \]

To see this, assume \( i < j \). Note that to pick a pair \( (s, t) \in \Gamma_{k+1}^+(i, j, m, q) \) with \( \min(s) = i \) and \( \min(t) = j \) we need to pick the \( 2k - m \) vertices in \( s \cup t \). Firstly, we pick the vertices that are not included in \( s \cap [\min(s), \min(t) - 1] = s \cap [i, j - 1] \). Since \( \min(s) \in s \cap [\min(s), \min(t) - 1] \), this amounts to choosing \( 2k - m - (q - 1) \) vertices out of \( n - j \). Then we decide which of the vertices that we have just picked will
lie in \( t \). This means we further need to choose \( k \) out of \( 2k + 1 - m - q \) vertices. Then we choose \( m - 1 \) out of \( k \) vertices of \( t \) to lie in \( s \cap t \) (under the assumption that we already have \( \min(t) \in s \)). Finally, we choose the set \( s \cap [\min(s), \min(t) - 1] \), which amounts to picking \( q - 1 \) vertices out of \( j - i + 1 \) possible choices. If any of the binomial coefficients are negative, we set them to 0. The case \( j < i \) is analogous.

An analogous argument shows that

\[
|\Gamma_{k+1}^-(i, j, m, q)| = \binom{n-j}{2k+1-m-q} \binom{2k+1-m-q}{k} \binom{j-i+1}{q-1}.
\]

Now using the covariance expression we have just derived, we get

\[
\sum_{s \neq i \in C_{k+1} \setminus \min(s) \neq \min(t)} \Cov(Z_s Y_s, Z_t Y_t)
\]

\[
= \sum_{i=1}^{n-k} \sum_{j=i+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} \Cov(Z_s Y_s, Z_t Y_t)
\]

\[
+ \sum_{i=1}^{n-k} \sum_{j=i+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} \Cov(Z_s Y_s, Z_t Y_t)
\]

\[
+ \sum_{j=1}^{n-k} \sum_{i=j+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} \Cov(Z_s Y_s, Z_t Y_t)
\]

\[
+ \sum_{j=1}^{n-k} \sum_{i=j+1}^{n-k} \sum_{q=1}^{\min(k+1,j-i)} \Cov(Z_s Y_s, Z_t Y_t)
\]

\[
= \sum_{i=1}^{n-k} \sum_{j=i+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} |\Gamma_{k+1}^+(i, j, m, q)| p^2(\frac{k+1}{2}) - \binom{m}{2} (\pi(i, j, k+1, k+1, m, m, q)
\]

\[ + \pi(i, j, k, m-1, m-1, q) - \pi(i, j, k, k+1, m-1, m-1, q)
\]

\[ - \pi(i, j, k+1, k, m, m, q) - \mu(p, k, i)\mu(p, k, j)\}
\]

\[
+ \sum_{i=1}^{n-k} \sum_{j=i+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} |\Gamma_{k+1}^+(i, j, m, q)| p^2(\frac{k+1}{2}) - \binom{m}{2} (\pi(i, j, k+1, k+1, m, m, q)
\]

\[ + \pi(i, j, k, m, m, q) - \pi(i, j, k, k+1, m, m, q)
\]

\[ - \pi(i, j, k+1, k, m, m, q) - \mu(p, k, i)\mu(p, k, j)\}
\]

\[
+ \sum_{j=1}^{n-k} \sum_{i=j+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} |\Gamma_{k+1}^+(j, i, m, q)| p^2(\frac{k+1}{2}) - \binom{m}{2} (\pi(j, i, k+1, k+1, m, m, q)
\]

\[ + \pi(j, i, k, m-1, m-1, q) - \pi(j, i, k, k+1, m-1, m-1, q)
\]

\[ - \pi(j, i, k+1, k, m, m, q) - \mu(p, k, i)\mu(p, k, j)\}
\]

\[
+ \sum_{j=1}^{n-k} \sum_{i=j+1}^{n-k} \sum_{m=1}^{k} \sum_{q=1}^{\min(k+1,j-i)} |\Gamma_{k+1}^+(j, i, m, q)| p^2(\frac{k+1}{2}) - \binom{m}{2} (\pi(j, i, k+1, k+1, m, m, q)
\]

\[ + \pi(j, i, k, m, m, q) - \pi(j, i, k, k+1, m, m, q)
\]

\[ - \pi(j, i, k+1, k, m, m, q) - \mu(p, k, i)\mu(p, k, j)\}
\]

\[
= 2p(\frac{k+1}{2})V_1 + 2p(\frac{k+1}{2})V_2.
\]
Similarly, we calculate the remaining term in the expansion of the variance (A.1). We notice that if \( i = j \), then \( q = 0 \) and we have \( \Gamma_{k+1}(i, i, m, 0) = \Gamma_{k+1}^*(i, i, m, 0) \). Hence, \(|\Gamma_{k+1}(i, i, m, 0)| = (\binom{n-1}{2k+1-m} \binom{2k+1-m}{k} \binom{k}{m-1}) \), and

\[
\sum_{s \neq t \in \mathbb{C}_{k+1}} \sum_{m=1}^{n-k} \sum_{(s, t) \in \Gamma_{k+1}(i, i, m, 0)} \text{Cov}(Z_s Y_s, Z_t Y_t) = \sum_{i=1}^{n-k} \sum_{m=1}^{k} \sum_{(s, t) \in \Gamma_{k+1}(i, i, m, 0)} \text{Cov}(Z_s Y_s, Z_t Y_t)
\]

\[
= \sum_{i=1}^{n-k} \sum_{m=1}^{k} \left( \frac{n-i}{2k+1-m} \right) \binom{2k+1-m}{k} \binom{k}{m-1} \left\{ p^{-\binom{m}{2}} \left[ \left(1 - 2p^{k+1} + p^{2k+2-m}\right)^{i-1} + \left(1 - 2p^{k+1} + p^{2k+1-m}\right)^{i-1} \right] - 2(1 - p^k - p^{k+1} + p^{2k+2-m})^{i-1} \right\} \left[ - (1 - p^{k+1})^{i-1} - (1 - p^k)^{i-1} \right]
\]

\[= p^{2(k+1)} V_3. \]

**Proof of Lemma 35.** Fix \( 1 \leq k \leq n - 1 \) and \( p \in (0, 1) \), and consider the variance. From Lemma 34 we have \( \text{Var}\{T_{k+1}\} = 2p^{2(k+1)} V_1 + 2p^{2(k+1)} V_2 + p^{2(k+1)} V_3 + p^{(k+1)} V_4 \). First we lower bound \( V_1 \) and \( V_2 \) by just the negative part of the sum:

\[
V_1 \geq \sum_{i<j} \sum_{m=1}^{n-k} \sum_{q=1}^{\min(k+1,j-i)} \left( \frac{n-j}{2k+1-m-q} \right) \binom{2k+1-m-q}{k} \binom{k}{m-1} \left( j-i+1 \right)^2
\]

\[
+ \left( 1 - p^{k+1} \right)^{i+j-2} + (1 - p^k)^{i+j-2}
\]

\[
+ p^{-\binom{m}{2}} \left( 1 - p^{k+1} \right)^{j-i-q} (1 - p^{k+1-m})^q (1 - p^{k+1} - p^k + p^{2k+1-m})^{i-1}
\]

\[
+ p^{-\binom{m}{2}} (1 - p^{k+1})^{j-i-q} (1 - p^{k-m})^q (1 - p^{k+1} - p^k + p^{2k+2-m})^{i-1}
\].

\[
V_2 \geq \sum_{i<j} \sum_{m=1}^{n-k} \sum_{q=1}^{\min(k+1,j-i)} \left( \frac{n-j}{2k+1-m-q} \right) \binom{2k+1-m-q}{k} \binom{k}{m} \left( j-i+1 \right)^2
\]

\[
+ \left( 1 - p^{k+1} \right)^{i+j-2} + (1 - p^k)^{i+j-2}
\]

\[
+ p^{-\binom{m}{2}} \left( 1 - p^{k+1} \right)^{j-i-q} (1 - p^{k+1-m})^q (1 - p^{k+1} - p^k + p^{2k+2-m})^{i-1}
\]

\[
+ p^{-\binom{m}{2}} (1 - p^{k+1})^{j-i-q} (1 - p^{k-m})^q (1 - p^{k+1} - p^k + p^{2k+1-m})^{i-1}
\].

Now using that \( \binom{k}{m} + \binom{k}{m-1} = \binom{k+1}{m} \) and \( (1 - p^{k+1}) \geq (1 - p^{k-m}) \) for \( m \geq 0 \) it is easy to see that \( V_1 + V_2 \geq -4R_1 - 4R_2 \), where

\[
R_1 := \sum_{i<j} \sum_{m=1}^{n-k} \sum_{q=1}^{\min(k+1,j-i)} \left( \frac{n-j}{2k+1-m-q} \right) \binom{2k+1-m-q}{k} \binom{k+1}{m} \left( j-i+1 \right)^2
\]

\[
(1 - p^{k+1})^{i+j-2};
\]

\[
R_2 := \sum_{i<j} \sum_{m=1}^{n-k} \sum_{q=1}^{\min(k+1,j-i)} \left( \frac{n-j}{2k+1-m-q} \right) \binom{2k+1-m-q}{k} \binom{k+1}{m} \left( j-i+1 \right)^2
\]

\[
p^{-\binom{m}{2}} (1 - p^{k+1})^{j-i-q} (1 - p^{k+1-m})^q (1 - p^{k+1} - p^k + p^{2k+1-m})^{i-1}.
\]

For \( V_3 \) we lower bound by terms with \( m = 1 \) and the negative parts of the other terms:

\[
V_3 \geq \sum_{i=1}^{n-k} \binom{n-i}{2k} \binom{2k}{k} \left\{ \left( 1 - 2p^{k+1} + p^{2k+1} \right)^{i-1} - (1 - p^{k+1})^{2i-2} \right\}
\]

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\[
- \sum_{i=1}^{n-k} \sum_{m=2}^{k} \binom{n-i}{2k+1-m} \binom{2k+1-m}{k} \binom{k}{m-1} \sum_{q=1}^{\min(k+1,j-i)} \frac{(n-j)^{2k+1-m-q}}{(2k+1-m-q)!} \frac{(2k+1-m-q)^k}{k!} \frac{(k+1)^m}{m!} \frac{(j-i+1)^{q-1}}{(q-1)!} \left( (1-p^{k+1})^{i+j} \right) + 1
\]

here we call the positive part of the lower bound \( R_4 \) and the negative part \( R_3 \). For \( V_4 \) we use the trivial lower bound \( V_4 \geq 0 \). Hence, we have:

\[
\text{Var}(T_{k+1}) \geq p^{2(k+1)} (R_4 - 8R_1 - 8R_2 - R_3).
\]

Let us now upper bound \( R_1 \):

\[
R_1 \leq \sum_{i<j} \sum_{m=1}^{n-k} \sum_{q=1}^{\min(k+1,j-i)} \frac{(n-j)^{2k+1-m-q}}{(2k+1-m-q)!} \frac{(2k+1-m-q)^k}{k!} \frac{(k+1)^m}{m!} \frac{(j-i+1)^{q-1}}{(q-1)!} \left( (1-p^{k+1})^{i+j} \right) + 1
\]

Noting that \((1-p^{k+1})^{i+j}(1-p^{k+1} - p^{k+1-m})^{i-1} \leq (1-p^{k+1})^{i-1} \), we can bound \( R_2 \) in an identical way:

\[
R_2 \leq \frac{n^{2k-1}(2k-1)^k(k+1)^{k+1}}{(k-1)!} p^{-\binom{k}{2}} \sum_{i<j} (1-p^{k+1})^{i+j} - 1
\]

Noting that \((1-p^{k+1} + p^{2k+2-m})^{i-1} \leq (1-p^{k+1})^{i-1} \) and \((1-p^{k+1})^{2i-2} \leq (1-p^{k+1})^{i-1} \) we proceed to bound \( R_3 \):

\[
R_3 \leq \sum_{i=1}^{n-k} \sum_{m=2}^{k} \binom{n-i}{2k+1-m} \binom{2k+1-m}{k} \binom{k}{m-1} 2(p^{-\binom{k}{2}} + 1)(1-p^{k+1})^{i-1}
\]

To lower bound \( R_4 \) we just take the \( i = 2 \) term:

\[
R_4 \geq \binom{n-2}{2k} \binom{2k}{k} \left\{ (1-2p^{k+1} + p^{2k+1})^2 - (1-2p^{k+1} + p^{2k+2}) \right\}
\]
\[ \geq \frac{(n - 2)^{2k}}{(2k)^2} \binom{2k}{k} p^{2k+1}(1 - p). \]

Since \( R_1, R_2, R_3 \) are all at most of the order \( n^{2k-1} \) and \( R_2 \) is at least of the order \( n^{2k} \), we have that for any fixed \( k \geq 1 \) and \( p \in (0, 1) \) there exists a constant \( C_{p,k} > 0 \) independent of \( n \) and a natural number \( N_{p,k} \) such that for any \( n \geq N_{p,k} \):

\[ \text{Var}(T_{k+1}) \geq p^2 \left( \frac{1}{2} \right) (4R_4 - 8R_1 - 8R_2 - R_3) \geq C_{p,k} n^{2k}. \]