Counting loopy graphs with given degrees

Catherine Greenhill
School of Mathematics and Statistics
University of New South Wales
Sydney, Australia 2052
csg@unsw.edu.au

Brendan D. McKay*
Research School of Computer Science
Australian National University
Canberra ACT 0200, Australia
bdm@cs.anu.edu.au

Abstract

Let \( \mathbf{d} = (d_1, d_2, \ldots, d_n) \) be a vector of nonnegative integers. We study the number of symmetric 0-1 matrices whose row sum vector equals \( \mathbf{d} \). While previous work has focussed on the case of zero diagonal, we allow diagonal entries to equal 1. Specifically, for \( D \in \{1, 2\} \) we define the set \( \mathcal{G}_D(\mathbf{d}) \) of all \( n \times n \) symmetric 0-1 matrices with row sums given by \( \mathbf{d} \), where each diagonal entry is multiplied by \( D \) when forming the row sum. We obtain asymptotically precise formulae for \( |\mathcal{G}_D(\mathbf{d})| \) in the sparse range (where, roughly, the maximum row sum is \( o(n^{1/2}) \)), and in the dense range (where, roughly, the average row sum is proportional to \( n \) and the row sums do not vary greatly). The case \( D = 1 \) corresponds to enumeration by the usual row sum of matrices. The case \( D = 2 \) corresponds to enumeration by degree sequence of undirected graphs with loops but no repeated edges, due to the convention that a loop contributes 2 to the degree of its incident vertex. We also analyse the distribution of the trace of a random element of \( \mathcal{G}_D(\mathbf{d}) \), and prove that it is well approximated by a binomial distribution in the dense range, and by a Poisson binomial distribution in the sparse range.

1 Introduction

Let \( \mathbf{d} = (d_1, d_2, \ldots, d_n) \) be a vector of nonnegative integers. Define \( G(\mathbf{d}) \) to be the number of \( n \times n \) symmetric matrices over \( \{0, 1\} \) with zero diagonal, such that row \( j \) sums to \( d_j \), for \( j = 1, \ldots, n \).

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The quantity $G(d)$ has been well studied, as cited below. In this paper we consider the case where the diagonal need not be zero. For $D \in \{1, 2\}$ define $G_D(d)$ to be the set of $n \times n$ symmetric matrices $A = (a_{jk})$ over $\{0, 1\}$ such that

$$Da_{jj} + \sum_{1 \leq k \leq n, k \neq j} a_{jk} = d_j \quad \text{for } j = 1, \ldots, n.$$ 

We wish to find an asymptotic formula for

$$G_D(d) = |G_D(d)|.$$ 

The case of $D = 1$ corresponds to enumeration by row sum of symmetric 0-1 matrices. If we interpret $A$ as the adjacency matrix of a simple undirected graph with loops, then the case of $D = 2$ corresponds to enumeration by degree sequence of simple undirected graphs with loops. Such graphs arise in various applications including the study of graph homomorphisms [9] and sign patterns [4].

Throughout the paper we will refer to a nonzero entry on the diagonal of a 0-1 matrix as a loop. For $\ell = 0, 1, \ldots, n$, let $G_D(d, \ell)$ be the set of matrices in $G_D(d)$ with exactly $\ell$ loops (that is, with trace $\ell$), and let $G_D(d, \ell) = |G_D(d, \ell)|$. Clearly we have $G_D(d, 0) = G(d)$ and $G_D(d) = \sum_{\ell=0}^{n} G_D(d, \ell)$. We also note here that $G_1(d, \ell) = 0$ unless $\sum_{j=1}^{n} d_j$ has the same parity as $\ell$, and $G_2(d, \ell) = 0$ unless $\sum_{j=1}^{n} d_j$ is even.

When $d_j = d$ for $j = 1, \ldots, n$, we write $G_D(d) = G_D(n, d)$ and refer to this as the regular case.

We will use the following parameters frequently:

$$S = \sum_{j=1}^{n} d_j, \quad d = \frac{S}{n},$$

$$\lambda = \frac{d}{n - 1}, \quad d_{\text{max}} = \max_j d_j,$$

$$R = \sum_{j=1}^{n} (d_j - d)^2, \quad S_r = \sum_{j=1}^{n} [d_j]_r \quad (r = 2, 3),$$

where $[a]_r = a(a - 1) \cdots (a - r + 1)$ denotes the falling factorial.

Throughout the paper, the asymptotic notation $O(f(m))$ refers to the passage of the variable $m$ to infinity. (Usually $m = n$ or $m = S$.) In the dense setting we also use a modified notation $\tilde{O}(f(n))$, which is to be taken as a shorthand for $O(f(n)n^{ce})$ with $c$ a numerical constant (perhaps a different constant for each occurrence). We write $\Omega(g(n))$ to indicate any function which is greater than $Cg(n)$ for some constant $C > 0$ and sufficiently large $n.$
It appears that there is very little prior research on $G_D(d)$. The most general result, by Bender and Canfield, dates from 1978.

**Theorem 1.1 ([3]).** Suppose that $1 \leq d_{\text{max}} = O(1)$. Then

$$
G_1(d) = \frac{1}{\sqrt{2}} \left( \frac{S}{e} \right)^{S/2} \left( \prod_{j=1}^{n} d_j! \right)^{-1} \exp \left( \sqrt{S} - \frac{1}{4} - \frac{S}{S} - \frac{S^2}{4S^2} + o(1) \right)
$$

uniformly as $S \to \infty$.

Note that $G_1(n, 1)$ is the number of involutions on $n$ letters (and also the number of Young tableaux with $n$ cells, see [20, A000085]). The asymptotic expansion of $G_1(n, 1)$ was previously known, see [5, 19]. We found no prior asymptotic work on $G_2(d)$ at all.

In the case of $D = 1$, a graph with $n$ vertices and $\ell$ loops can be mapped to a graph with $n+1$ vertices and no loops, by introducing a new vertex and replacing each loop by an edge to this vertex. This mapping is bijective and hence

$$
G_1((d_1, \ldots, d_n, \ell)) = G((d_1, \ldots, d_n, \ell)).
$$

However, this doesn’t seem to be of much use in asymptotic enumeration, since the important values of $\ell$ place the degree sequence $(d_1, \ldots, d_n, \ell)$ out of range of existing explicit estimates.

Our approach to estimating $G_D(d)$ will be to sum over all possible diagonals using the existing estimates for $G(d)$. The main estimates we will use are the following two theorems. The history of previous results on $G(d)$ is summarized in [14] and [16].

McCay and Wormald [17, Theorem 5.2] proved the following asymptotic formula for $G(d)$ in the sparse regime.

**Theorem 1.2 ([17]).** If $1 \leq d_{\text{max}} = o(S^{1/3})$ then

$$
G(d) = \frac{S!}{(S/2)! \prod_{j=1}^{n} d_j!} \exp \left( -\frac{S_2}{2S} - \frac{S_2^2}{4S^2} - \frac{S_2 S_3}{2S^3} + \frac{S_4}{4S^4} + \frac{S_3}{6S^3} + O \left( \frac{d_{\text{max}}^3}{S} \right) \right),
$$

uniformly as $S \to \infty$, with $S$ even.

In the case of dense matrices, the following result was due to McCay and Wormald [16] except that we will use an improved error term from a generalization by McCay [15]. A less explicit formula allowing a wider variation of the degrees was proved by Barvinok and Hartigan [2].
Theorem 1.3 ([15]). Let \(a, b > 0\) be constants such that \(a + b < \frac{1}{2}\). Then there is a constant \(\varepsilon_0 = \varepsilon_0(a, b) > 0\) such that the following holds. Suppose that \(d_j - d\) is uniformly \(O(n^{1/2 + \varepsilon_0})\) for \(j = 1, \ldots, n\) and that
\[
\min\{d, n - d - 1\} \geq \frac{n}{3a\log n}
\]
for sufficiently large \(n\). Then provided \(S\) is even we have
\[
G(d) = \sqrt{2} (\lambda^\lambda (1 - \lambda)^{-\lambda})^{(\ell)} \exp\left(\frac{1}{4} - \frac{R^2}{4\lambda^2(1 - \lambda)^2n^4} + O(n^{-b})\right) \prod_{j=1}^{n} \left(\frac{n-1}{d_j}\right). \tag{1.1}
\]

This formula also matches the sparse case under slightly more restricted conditions than Theorem 1.2 and is conjectured to hold in the intermediate domain as well (see [18, Theorem 2.5] and the conjecture stated immediately thereafter).

Note that Theorem 1.3 remains true if \(\varepsilon_0(a, b)\) is decreased (but is still positive), since the conditions of the theorem become stronger.

We now state our main enumeration theorems, starting with the dense regime.

Theorem 1.4. Let \(a, b > 0\) be constants such that \(a + b < \frac{1}{2}\). Then there is a constant \(\varepsilon = \varepsilon(a, b) > 0\) such that the following holds. Suppose that \(d_j - d\) is uniformly \(O(n^{1/2 + \varepsilon})\) for \(j = 1, \ldots, n\) and that
\[
\min\{d, n - d\} \geq \frac{n}{3a\log n} \tag{1.2}
\]
for sufficiently large \(n\). For \(D \in \{1, 2\}\), define
\[
\mu_D = \frac{d}{n + D - 1},
\]
and let
\[
Q_1(d, \ell) = \frac{1}{4} + \frac{(\ell - d)^2}{4(d(n - d))} - \frac{(\ell - d)^2R}{2d^2(n - d)^2} - \frac{R^2}{4d^2(n - d)^2},
\]
\[
Q_2(d, \ell) = \frac{1}{4} - \frac{\ell(n - \ell)}{\mu_2(1 - \mu_2)n^2} - \frac{R^2}{4\mu_2^2(1 - \mu_2)^2n^4} + \frac{R}{\mu_2(1 - \mu_2)n^2}
+ \frac{(1 - 2\mu_2)(\ell - \mu_2n)R}{\mu_2^2(1 - \mu_2)^2n^3} - \frac{2(\ell - \mu_2n)^2R}{\mu_2^2(1 - \mu_2)^2n^4}.
\]

When \(\ell\) has the same parity as \(S\) we have
\[
G_1(d, \ell) = \sqrt{2} \left(\mu_1^{\ell/2} (1 - \mu_1)^{(n - \ell)/2}\right) \left(\frac{n}{\ell}\right) \mu_1^\ell \left(1 - \mu_1\right)^{(n - \ell)/2}
\times \exp(Q_1(d, \ell) + O(n^{-b})) \prod_{j=1}^{n} \left(\frac{n}{d_j}\right).
\]
while for \( \ell = 0, \ldots, n \) and even \( S \) we have
\[
G_2(d, \ell) = \sqrt{2} \left( \mu_2^\ell (1 - \mu_2)^{1-\mu_2} \right)^{\binom{n+1}{2}} \mu_2^n (1 - \mu_2)^{n-\ell} \times \exp(Q_2(d, \ell) + O(n^{-b})) \prod_{j=1}^{n} \left( \frac{n+1}{d_j} \right).
\]
Defining
\[
\bar{\ell}_1 = \frac{d^{1/2} n}{d^{1/2} + (n-d)^{1/2}}, \quad \bar{\ell}_2 = \mu_2 n = \frac{dn}{n+1},
\]
we have
\[
G_1(d) = \frac{1}{\sqrt{2}} \left( \mu_1^\ell (1 - \mu_1)^{1-\mu_1} \right)^{n^{2/2}} (\mu_1^{1/2} + (1 - \mu_1)^{1/2})^n \times \exp(Q_1(d, \bar{\ell}_1) + O(n^{-b})) \prod_{j=1}^{n} \left( \frac{n}{d_j} \right)
\]
and, for even \( S \),
\[
G_2(d) = \sqrt{2} \left( \mu_2^\ell (1 - \mu_2)^{1-\mu_2} \right)^{\binom{n+1}{2}} \exp(Q_2(d, \bar{\ell}_2) + O(n^{-b})) \prod_{j=1}^{n} \left( \frac{n+1}{d_j} \right).
\]

In Theorem 1.6 we will prove that \( \bar{\ell}_D \) is close to the expected number of loops in a randomly chosen element of \( G_D(d) \). For the reader’s convenience, we note that
\[
Q_2(d, \bar{\ell}_2) = -\frac{1}{4} \left( 1 - \frac{R}{\mu_2(1 - \mu_2)n^2} \right) \left( 3 - \frac{R}{\mu_2(1 - \mu_2)n^2} \right).
\]
Unfortunately, the expression for \( Q_1(d, \bar{\ell}_1) \) does not simplify much. In the case of regular graphs we have \( R = 0 \), so the formulae for \( Q_D(d, \ell) \) simplify greatly and in particular
\[
Q_1(d, \bar{\ell}_1) = \frac{n}{2n + 4\sqrt{d(n-d)}}.
\]

Our main result for the sparse case is the following.

**Theorem 1.5.** Suppose that \( 1 \leq d_{\text{max}} = o(S^{1/3}) \). Then
\[
G_1(d) = \frac{1}{\sqrt{2}} \left( \frac{S}{e} \right)^{S/2} \left( \prod_{j=1}^{n} d_j! \right)^{-1} \exp \left( \sqrt{S} - \frac{1}{4} - \frac{S_2}{S} - \frac{S_2^2}{4S^2} \right.
\]
\[
\left. + \frac{7}{24S^{3/2}} + \frac{S_2}{S^{3/2}} + \frac{S_3}{3S^{3/2}} + \frac{S_2^2}{2S^{5/2}} - \frac{S_2^2S_3}{2S^4} + \frac{S_4}{4S^5} + \frac{S_3^2}{6S^3} + O \left( \frac{d_{\text{max}}^3}{S} \right) \right)
\]
uniformly as \( S \to \infty \), and
\[
G_2(d) = \sqrt{2} \left( \frac{S}{e} \right)^{S/2} \left( \prod_{j=1}^{n} d_j! \right)^{-1} \exp \left( \frac{S_2}{2S} - \frac{S_2^2}{4S^2} - \frac{S^2S_3}{2S^4} + \frac{S_4}{4S^5} + \frac{S_3^2}{6S^3} + O \left( \frac{d_{\text{max}}^3}{S} \right) \right)
\]
uniformly as \( S \to \infty \) with \( S \) even.
If $S$ is even then we may replace the factor $\sqrt{2} \,(S/e)^{S/2}$ by $S!/(S/2)!^{2^{S/2}}$. In the regular case the formulae simplify as follows.

**Corollary 1.1.** Suppose that $1 \leq d = o(n^{1/2})$. Then

$$G_1(n, d) = \frac{1}{\sqrt{2}} \,(d!)^{-n} \left(\frac{nd}{e}\right)^{nd/2} \times \exp\left(\frac{2 - 2d - d^2}{4} + \frac{24(n - 1)d + 20d^2 + 11}{24\sqrt{nd}} - \frac{d^3}{12n} + O\left(\frac{d^2}{n}\right)\right)$$

uniformly as $n \to \infty$, and

$$G_2(n, d) = \sqrt{2} \,(d!)^{-n} \left(\frac{nd}{e}\right)^{nd/2} \exp\left(-\frac{(d - 1)(d - 3)}{4} - \frac{d^3}{12n} + O\left(\frac{d^2}{n}\right)\right)$$

uniformly as $n \to \infty$ with $nd$ even.

Again, if $nd$ is even then the factor $\sqrt{2} \,(nd/e)^{nd/2}$ may be replaced by $(nd)!/(nd/2)!^{2^{nd/2}}$.

Theorems 1.4 and 1.5 are proved in Section 2 and 3, respectively. Along the way we prove some technical results (Lemmas 2.1, 3.2, 3.3) which may be of independent interest. But first, in Section 1.1 we state a theorem on the distribution of the trace of a random element of $G_D(d)$, and discuss some interesting features of this distribution. Theorem 1.6 is proved in Section 4. Finally in Section 5 we state a conjecture regarding the number of regular graphs with loops, for all possible degrees.

### 1.1 The distribution of the trace

The calculations we will give in the process of proving Theorems 1.4 and 1.5 will provide some information on the distribution of the trace of a random element of $G_D(d)$. We summarize that information here.

For $p = (p_1, \ldots, p_n) \in [0, 1]^n$, let $X_1, \ldots, X_n$ be independent random variables with $\text{Prob}(X_j = 0) = 1 - p_j$ and $\text{Prob}(X_j = 1) = p_j$ for each $j$. The **Poisson binomial distribution** $\text{PB}(p)$ is the distribution of $\sum_{j=1}^n X_j$. Define

$$\text{PB}(p, \ell) = \text{Prob}\left(\sum_{j=1}^n X_j = \ell\right).$$

The special case $p = (p, \ldots, p)$ gives the familiar binomial distribution,

$$\text{PB}((p, \ldots, p), \ell) = \text{Bin}(n, p, \ell) = \binom{n}{\ell} p^\ell (1 - p)^{n-\ell}.$$
Theorem 1.6. Let \( Y_D = Y_D(d) \) be the random variable given by the trace of an element of \( G_D(d) \) chosen uniformly at random.

(i) If the conditions of Theorem 1.4 hold then, for \( \ell = 0, \ldots, n \),

\[
\begin{align*}
\text{Prob}(Y_1 = \ell) & = (2 + O(n^{-b})) \text{Bin}(n, \bar{\ell}_1/n, \ell) + O(e^{-n^{O(1)}}), \\
\mathbb{E}(Y_1) & = \bar{\ell}_1(1 + O(n^{-b})), \\
\text{Var}(Y_1) & = \bar{\ell}_1(1 - \bar{\ell}_1/n)(1 + O(n^{-b})), \\
\text{Prob}(Y_2 = \ell) & = (1 + O(n^{-b})) \text{Bin}(n, \bar{\ell}_2/n, \ell) + O(e^{-n^{O(1)}}), \\
\mathbb{E}(Y_2) & = \bar{\ell}_2(1 + O(n^{-b})), \\
\text{Var}(Y_2) & = \bar{\ell}_2(1 - \bar{\ell}_2/n)(1 + O(n^{-b})),
\end{align*}
\]

where \( \ell \) must have the same parity as \( S \) in the \( D = 1 \) case and \( S \) must be even in the \( D = 2 \) case.

(ii) Define \( p' = (p'_1, \ldots, p'_n) \) and \( p'' = (p''_1, \ldots, p''_n) \), where for \( j = 1, \ldots, n \),

\[
\begin{align*}
p'_j & = \frac{d_j}{\sqrt{S}} - \frac{d_j(2d_j - 1)}{2S} + \frac{d_j^3}{S^{3/2}} + \frac{d_j(d_j - 2)S_2}{S^{5/2}} - \frac{d_jS_2^2}{2S^{7/2}}, \\
p''_j & = \frac{d_j(d_j - 1)}{S}.
\end{align*}
\]

If the conditions of Theorem 1.5 hold then, for \( \ell = 0, \ldots, n \),

\[
\begin{align*}
\text{Prob}(Y_1 = \ell) & = \left(2 + O\left(\frac{d_{\max}^3}{S^2} + S^{-1/3}\right)\right) \text{PB}(p', \ell) + O(e^{-S^{O(1)}}), \\
\mathbb{E}(Y_1) & = \sqrt{S} - \frac{S_2}{S} - \frac{1}{2} + O\left(\frac{d_{\max}^3}{S^{11/2}}\right), \\
\text{Var}(Y_1) & = \sqrt{S} - \frac{2S_2}{S} - 1 + O\left(\frac{d_{\max}^3}{S^{11/2}}\right), \\
\text{Prob}(Y_2 = \ell) & = \left(1 + O\left(\frac{d_{\max}^3}{S^{2/3}} + S^{-1/3}\right)\right) \text{PB}(p'', \ell) + O(e^{-S^{O(1)}}), \\
\mathbb{E}(Y_2) & = \left(1 + O\left(\frac{d_{\max}^3}{S}\right)\right) \frac{S_2}{S}, \\
\text{Var}(Y_2) & = \left(1 + O\left(\frac{d_{\max}^3}{S}\right)\right) \frac{S_2}{S},
\end{align*}
\]

where \( \ell \) must have the same parity as \( S \) in the \( D = 1 \) case and \( S \) must be even in the \( D = 2 \) case.
The parameter $\mu_D$ can be thought of as measuring the density of entries equal to 1, while $Y_D/n$ is the density of loops in a randomly chosen element of $G_D(d)$. In the dense range of Theorem 1.6 we see that $Y_2/n$ is concentrated near the same value $\mu_2$, while $Y_1/n$ is concentrated near $\overline{\ell}_1 = \frac{\sqrt{\mu_1}}{\sqrt{\mu_1} + \sqrt{1 - \mu_1}}$.

Figure 1 illustrates this curious difference between $D = 1$ and $D = 2$.

![Figure 1](image-url)  

Figure 1: The expected density of the diagonal as a function of the overall density $\mu_D$.

When $D = 1$, Theorem 1.6 tells us that the most significant term in $\mathbb{E}(Y_D)$ depends only on $S$ and not on $d$, within the range of $d$ values allowed by the theorem. To explore this further, let $A_n(S)$ be the set of all $n \times n$ symmetric 0-1 matrices with exactly $S$ entries equal to 1. The number of matrices in $A_n(S)$ with exactly $\ell$ loops is

$$\binom{n}{\ell} \binom{\binom{n}{2}}{\binom{S-\ell}{2}}$$

when $S$ and $\ell$ have the same parity, and 0 otherwise. For $1 \leq S \leq n^2 - 1$, it can be proved that the maximum value of this function occurs either at $\overline{\ell}_1$ rounded up to an integer of the same parity as $S$ or $\overline{\ell}_1$ rounded down to such an integer. On the basis of experiments, we conjecture that the mean number of loops in $A_n(S)$ always lies in $(\overline{\ell}_1 - \frac{1}{2}, \overline{\ell}_1 + \frac{1}{2})$.

Also note that $\overline{\ell}_1 \sim \sqrt{S}$ for $S = o(n^2)$, matching the leading term of $\mathbb{E}(Y_1)$ in the sparse case.
When $D = 2$ we consider instead the set $B_n(S)$ of all graphs with loops allowed, with $n$ vertices and $S/2$ edges (loops counting twice). Matrices which correspond to graphs in $B_n(S)$ can be formed by choosing $S/2$ entries on or below the main diagonal, setting these equal to 1, then adding this matrix to its transpose. (Nonzero entries on the diagonal all equal 2, which is their contribution to the row sum.) The number of graphs in $B_n(S)$ with exactly $\ell$ loops is
\[
\binom{n}{\ell} \left( \frac{n}{2} \right)^{S/2 - \ell}.
\]
Up to scaling, this is the hypergeometric distribution with parameters $\binom{n+1}{2}, n, S/2$ and mean $S/(n+1) = \mu_2 n$.

The binomial distributions in part (i) of the theorem are asymptotically normal, as is well known. The Poisson binomial distributions in part (ii) of the theorem are asymptotically normal for $Y_1$ (see [8]), and asymptotically Poisson for $Y_2$, by Le Cam’s Theorem [11] (see also [1, Equation 1.1]).

2 The dense case

In this section we prove Theorem 1.4.

2.1 A technical lemma

We will require a technical lemma which might be of some independent interest. If $\beta = (\beta_1, \ldots, \beta_n)$ is a vector of real numbers and $\ell = 0, \ldots, n$, define
\[
U_\ell(\beta) = \sum_{1 \leq j_1 < \cdots < j_\ell \leq n} \prod_{s=1}^{\ell} e^{\beta_{j_s}}.
\]

Lemma 2.1. Define $\bar{\beta} = \frac{1}{n} \sum_{j=1}^{n} \beta_j$ and suppose that $\beta_j - \bar{\beta} = \tilde{O}(n^{-1/2})$ uniformly for $j = 1, \ldots, n$. Then, for sufficiently small $\varepsilon > 0$, we have
\[
U_\ell(\beta) = \binom{n}{\ell} \exp \left( \ell \bar{\beta} + \frac{\ell(n - \ell)}{2n^2} \sum_{j=1}^{n} (\beta_j - \bar{\beta})^2 + \tilde{O}(n^{-1/2}) \right),
\]
uniformly for $\ell = 0, \ldots, n$.

Proof. The factor $e^{\ell \bar{\beta}}$ can be removed by replacing each $\beta_j$ by $\beta_j - \bar{\beta}$, so it suffices to prove the lemma for $\sum_{j=1}^{n} \beta_j = \bar{\beta} = 0$. 

9
We divide the proof into three parts, depending on $\ell$. Let $B = \max j |\beta_j|$. Choose a constant $c \geq 0$ such that $Bn^{1/2-\varepsilon} = o(1)$.

First assume that $n^{1/2-\varepsilon} \leq \ell \leq n - n^{1/2-\varepsilon}$. Since $U_\ell(\beta)$ is the coefficient of $y^\ell$ in $\prod_{j=1}^n (1 + e^{\beta_j}y)$, we can estimate it using the saddle point method. We choose the contour to be a circle of radius $r$ centered at the origin, where

$$r = \frac{\ell}{n - \ell}.$$

For $j = 1, \ldots, n$ let

$$\psi_j = \frac{e^{\beta_j}r}{1 + e^{\beta_j}r}.$$

Changing variable according to $y = re^{i\theta}$ and applying Cauchy’s theorem, we obtain

$$U_\ell(\beta) = P(\beta) \int_{-\pi}^{\pi} F(\theta) d\theta,$$

where

$$P(\beta) = \prod_{j=1}^n \frac{(1 + re^{\beta_j})}{2\pi r^\ell}, \quad F(\theta) = \prod_{j=1}^n \frac{(1 + \psi_j(e^{i\theta} - 1))}{e^{i\theta}}.$$

The coefficient $\psi_j$ satisfies

$$\psi_j = \frac{\ell}{n} + \frac{\ell(n - \ell)}{n^2} \beta_j + \frac{\ell(n - \ell)(n - 2\ell)}{2n^3} \beta_j^2 + \tilde{O}(\beta_j^3) \quad (2.1)$$

$$= \frac{\ell}{n} (1 + \tilde{O}(n^{-1/2})).$$

We now divide the domain of integration into the two subdomains $|\theta| \leq \theta_0$ and $|\theta| > \theta_0$, where

$$\theta_0 = \sqrt{\frac{n}{\ell(n - \ell)}} \log n.$$

Expanding $F(\theta)$ for $|\theta| \leq \theta_0$, we find using (2.1) that

$$F(\theta) = \exp \left( -\frac{\ell(n - \ell)}{2n} \theta^2 + O(1) \frac{\ell(n - \ell)}{n} \theta^3 + \tilde{O}(n^{-1/2}) \right),$$

where the $O(1)$ term is independent of $\theta$. Since the interval $|\theta| \leq \theta_0$ is symmetric about 0, we can instead integrate

$$\frac{1}{2} (F(-\theta) + F(\theta)) = \exp \left( -\frac{\ell(n - \ell)}{2n} \theta^2 + \tilde{O}(n^{-1/2}) \right).$$
Furthermore,
\[ \int_{\theta_0}^{\infty} \exp \left( -\frac{\ell(n-\ell)}{2n} \theta^2 + \tilde{O}(n^{-1/2}) \right) d\theta = n^{-\Omega(\log n)} \]
(and similarly for the lower tail) and hence

\[ \int_{-\theta_0}^{\theta_0} F(\theta) d\theta = \sqrt{\frac{2\pi n}{\ell(n-\ell)}} \exp(\tilde{O}(n^{-1/2})). \]

For the complementary subdomain \(|\theta| > \theta_0\), note that
\[ |1 + \psi_j(e^{i\theta} - 1)| = \sqrt{1 - 2\psi_j(1 - \psi_j)(1 - \cos \theta)}, \]
which is a decreasing function for \(\theta \in (\theta_0, \pi)\). Therefore,
\[ |F(\theta_0)| = \prod_{j=1}^{n} \sqrt{1 - 2\psi_j(1 - \psi_j)(1 - \cos \theta_0)} \leq \exp \left( -\frac{2 \log^2 n}{\pi^2} + \tilde{O}(n^{-1/2}) \right) = n^{-\Omega(\log n)}. \]

Hence
\[ \int_{-\pi}^{\pi} F(\theta) d\theta = n^{-\Omega(\log n)} + \int_{-\theta_0}^{\theta_0} F(\theta) d\theta = \sqrt{\frac{2\pi n}{\ell(n-\ell)}} \exp(\tilde{O}(n^{-1/2})). \]

Finally, we calculate that
\[ P(\beta) = \frac{n^n}{2\pi \ell \ell^\ell (n-\ell)^{n-\ell}} \prod_{j=1}^{n} \frac{1 + re^{\beta_j}}{1 + r} \]
\[ = \frac{n^n}{2\pi \ell \ell^\ell (n-\ell)^{n-\ell}} \exp \left( \frac{\ell(n-\ell)}{2n^2} \sum_{j=1}^{n} \beta_j^2 + \tilde{O}(n^{-1/2}) \right). \]

Therefore
\[ U_\ell(\beta) = \frac{n^{n+1/2}}{\sqrt{2\pi \ell \ell^{\ell+1/2} (n-\ell)^{n-\ell+1/2}}} \exp \left( \frac{\ell(n-\ell)}{2n^2} \sum_{j=1}^{n} \beta_j^2 + \tilde{O}(n^{-1/2}) \right), \]
which equals the expression in the lemma, by Stirling’s formula.

We next consider the case that \(0 \leq \ell < n^{1/2 - \epsilon}\). Expand \(U_\ell(\beta) = \sum_{s \geq 0} T_s / s!\), where
\[ T_s = \sum_{1 \leq j_1 < \cdots < j_s \leq n} (\beta_{j_1} + \cdots + \beta_{j_s})^s. \]
It follows from [7, Lemma 5] that
\[ T_0 = \binom{n}{\ell}, \quad T_1 = 0, \quad T_2 = \binom{n}{\ell} O(\ell B^2) \quad \text{and} \quad T_3 = \binom{n}{\ell} O(\ell B^3). \quad (2.2) \]

We proceed to bound \( T_s \) for \( s \geq 4 \). Let \( \sum_{j_1, \ldots, j_\ell} \) denote the sum over all sequences \((j_1, \ldots, j_\ell) \in \{1, \ldots, n\}^\ell \) with \( \ell \) distinct entries. Applying the multinomial theorem, we have
\[
T_s = \frac{1}{\ell!} \sum_{m_1 + \ldots + m_\ell = s} \binom{s}{m_1, \ldots, m_\ell} B(m_1, \ldots, m_\ell),
\]
where
\[
B(m_1, \ldots, m_\ell) = \sum_{j_1, \ldots, j_\ell} \beta_{m_1}^{j_1} \cdots \beta_{m_\ell}^{j_\ell}.
\]

Let \( \mathcal{M}_1 \) be the set of all compositions \( m = (m_1, \ldots, m_\ell) \) of \( s \) such that \( m_i = 1 \) for some \( i \), and let \( \mathcal{M}_2 \) be the set of all other compositions of \( s \). For all \( m \) we have
\[
|B(m)| \leq [n]_\ell B^s,
\]
using the falling factorial. For \( m \in \mathcal{M}_1 \), suppose as a representative case that \( m_\ell = 1 \). Then
\[
B(m) = \sum_{j_1, \ldots, j_\ell} \beta_{m_1}^{j_1} \cdots \beta_{m_\ell}^{j_\ell}
= \sum_{j_1, \ldots, j_{\ell-1}} \beta_{m_1}^{j_1} \cdots \beta_{m_{\ell-1}}^{j_{\ell-1}} \sum_{j_\ell \notin \{j_1, \ldots, j_{\ell-1}\}} \beta_{j_\ell}
= -\sum_{j_1, \ldots, j_{\ell-1}} \beta_{m_1}^{j_1} \cdots \beta_{m_{\ell-1}}^{j_{\ell-1}} \sum_{j_\ell \in \{j_1, \ldots, j_{\ell-1}\}} \beta_{j_\ell},
\]
where the last step uses the assumption \( \sum_{j=1}^n \beta_j = 0 \). This shows that for \( m \in \mathcal{M}_1 \) we have
\[
|B(m)| \leq \ell [n]_{\ell-1} B^s = O(\ell / n) [n]_\ell B^s.
\]
Consequently
\[
|T_s| \leq \binom{n}{\ell} B^s \left( O(\ell / n) \sum_{m \in \mathcal{M}_1} \binom{s}{m_1, \ldots, m_\ell} + \sum_{m \in \mathcal{M}_2} \binom{s}{m_1, \ldots, m_\ell} \right).
\]
Furthermore
\[
\sum_{m \in \mathcal{M}_1} \binom{s}{m_1, \ldots, m_\ell} \leq \ell^s.
\]
Next, notice that for any fixed integer \( s \geq 4 \),
\[
C_s = \sum_{m \in \mathcal{M}_2} \binom{s}{m_1, \ldots, m_\ell}
\]
is the coefficient of $x^s$ in the Maclaurin expansion of $s!(e^x - x)^\ell$. Since that expansion has nonnegative coefficients, $C_s \leq s!\eta^{-s}(e^\eta - \eta)^\ell$ for any $\eta > 0$. Substituting $\eta = \sqrt{s/\ell}$ and using the fact that $(e^{\sqrt{x}} - \sqrt{x})^{1/2} < 2$ for $x > 0$ gives

$$C_s \leq s!(s/\ell)^{-s/2}(e^{s/\ell} - \sqrt{s/\ell})^\ell \leq s!(2\sqrt{\ell/\ell})^s.$$  

Hence we have, for any fixed integer $s \geq 4$,

$$|T_s| \leq \binom{n}{\ell} \left( O(\ell/n) \ell^s + s! \left(2\sqrt{\ell/\ell}\right)^s \right).$$ (2.3)

Using (2.2) for $s \leq 3$ and (2.3) for $s \geq 4$, gives

$$U_{\ell}(\beta) = \binom{n}{\ell} \left( 1 + \tilde{O}(n^{-1/2}) + O(\ell/n) \sum_{s \geq 4} \frac{1}{s!} B^s \ell^s + O(1) \sum_{s \geq 4} B^s \left(2\sqrt{\ell/\ell}\right)^s \right).$$

Since $B\ell = o(1)$ and $B\sqrt{\ell} = \tilde{O}(n^{-1/4})$, the first sum in the above expression is $O(\ell/n) = \tilde{O}(n^{-1/2})$, while the second sum is at most

$$\sum_{s \geq 4} B^s \ell^{s/2} = O(B^4 \ell^2) = \tilde{O}(n^{-1}).$$

Hence

$$U_{\ell}(\beta) = \binom{n}{\ell} \left( 1 + \tilde{O}(n^{-1/2}) \right),$$

which matches the lemma for this range of $\ell$ values.

For the remaining range $n - n^{1/2 - \varepsilon} < \ell \leq n$, we can apply the identity $U_{\ell}(\beta) = U_{n-\ell}(-\beta)$, which is a consequence of $\sum_j \beta_j = 0$. The lemma is thus proved. \qed

### 2.2 Proof of the dense theorem (Theorem 1.4)

Suppose that $a, b > 0$ are constants such that $a + b < \frac{1}{2}$, and $d$ is such that (1.2) holds and $d_j - d$ is uniformly $O(n^{1/2+\varepsilon})$ for $j = 1, \ldots, n$ and some $\varepsilon > 0$. In the following, we will assume that $\varepsilon$ is sufficiently small. Later in the proof we will infer that we can take $\varepsilon = \varepsilon(a, b)$ for some function $\varepsilon(a, b) > 0$, as required by Theorem 1.4.

Every vector $z = (z_1, \ldots, z_n) \in \{0, 1\}^n$ is a potential diagonal of one of our matrices. Define $|z| = \sum_{j=1}^n z_j$ and for $\ell = 0, \ldots, n$ let

$$A_{\ell} = \{ z \in A : |z| = \ell \}. \quad (2.4)$$
If $D\ell$ and $S$ have the same parity then

$$G_D(d, \ell) = \sum_{z \in A_\ell} G(d - Dz). \quad (2.5)$$

We proceed by applying Theorem 1.3 to estimate $G(d - Dz)$ and then summing the result over all $z \in A_\ell$. Note that the average entry of $d - Dz$ is $d - D\ell/n$.

Let $\hat{a}$ be any constant such that $a < \hat{a} < \frac{1}{2} - b$ and let $\varepsilon_0 = \varepsilon_0(\hat{a}, b)$ be the positive constant guaranteed by Theorem 1.3. Then for $\ell = 0, \ldots, n$ we have

$$\min \left\{ \frac{d - D\ell}{n}, n - d + \frac{D\ell}{n} \right\} \geq \frac{n}{3\hat{a} \log n}$$

for sufficiently large $n$. Provided $\varepsilon \leq \varepsilon_0$, we have that $(d_j - Dz_j) - (d - D\ell/n)$ is uniformly $O(n^{1/2 + \varepsilon_0})$ for $j = 1, \ldots, n$. So Theorem 1.3 with the constants $(\hat{a}, b)$ applies to every vector $d - Dz$, using the value $\varepsilon_0 = \varepsilon_0(\hat{a}, b)$ guaranteed by that theorem.

Next we will compare factors from the expression for $G(d - Dz)$ given by (1.1) with corresponding factors from the formula for $G_D(d, \ell)$ given in Theorem 1.4. Let $\lambda_\ell$ denote the density of $d - Dz$ for any $z \in A_\ell$. That is,

$$\lambda_\ell = \frac{d - D\ell}{n} - \frac{D\ell}{n(n-1)} = \mu_D - \frac{D(\ell - \mu_D n)}{n(n-1)}.$$

Also let $\delta_j = d_j - d$ for $j = 1, \ldots, n$, which allows us to write $R = \sum_{j=1}^n \delta_j^2$. Then

$$\frac{(\lambda_\ell^n(1 - \lambda_\ell)^{1-n})^n}{(\mu_D^n(1 - \mu_D)^{1-n})^n} = \mu_D^{D\ell/2}(1 - \mu_D)^{-D(n-\ell)/2} \exp\left(\frac{D^2(\ell - \mu_D n)^2}{4\mu_D(1 - \mu_D)n^2} + \tilde{O}(n^{-1})\right).$$

Using the expansion $[m]_k = m^k \exp\left(-\frac{k(k-1)}{2m} + O(k^3/m^2)\right)$, valid when $m \to \infty$ such that $k = o(m^{2/3})$, we find that

$$\frac{\binom{n-1}{d_j-Dz_j}}{\binom{n-D-1}{d_j}} = \mu_D^{Dz}(1 - \mu_D)^{D(1-z_j)} \exp\left(-\frac{D(D-1)(\mu_D - z_j)^2}{2\mu_D(1 - \mu_D)n} - \frac{D(\mu_D - z_j)\delta_j^2}{\mu_D(1 - \mu_D)n} - \frac{D(\mu_D - z_j)^2\delta_j^2}{2\mu_D^2(1 - \mu_D)^2n^2} + \tilde{O}(n^{-3/2})\right).$$
Since \( z_j^2 = z_j \) and \( \sum_{j=1}^{n} z_j = \ell \), we obtain

\[
\prod_{j=1}^{n} \left( \frac{n-1}{d_j-Dz_j} \right) = \mu_D^{D}(1 - \mu_D)^{D(n-\ell)}
\times \exp\left( -\frac{D(D-1)}{2} - \frac{D(D-1)(1 - 2\mu_D)(\ell - \mu_Dn)}{2\mu_D(1 - \mu_D)n} - \frac{DR}{2(1 - \mu_D)^2n^2} \right)
\times \sum_{j=1}^{n} \left( \frac{D\delta_j}{\mu_D(1 - \mu_D)n} - \frac{D(1 - 2\mu_D)\delta_j^2}{2\mu_D^2(1 - \mu_D)^2n^2} \right) z_j + \tilde{O}(n^{-1/2}).
\]

Finally, apart from the \( O(n^{-b}) \) error term, the expression inside the exponential in (1.1) for \( \mathbf{d} - Dz \) is

\[
\frac{1}{4} - \frac{\left( \sum_{j=1}^{n}(d_j - Dz_j - \lambda_{\ell}(n-1))^2 \right)^2}{4\lambda_{\ell}^2(1 - \lambda_{\ell})^2n^4} = \frac{1}{4} - \frac{R^2}{4\mu_D^2(1 - \mu_D)^2n^4} + \tilde{O}(n^{-1/2}).
\]

Combining these expressions gives

\[
G(\mathbf{d} - Dz) = A \ V(\ell) \ \exp\left( \sum_{j=1}^{n} \beta_j z_j \right) \quad (2.6)
\]

where

\[
A = \sqrt{2} \left( \mu_D^{D} (1 - \mu_D)^{1 - \mu_D} \right)^{n^2 + \mu_Dn/2} \prod_{j=1}^{n} \left( \frac{n + D - 1}{d_j} \right) \exp(O(n^{-b}) + \tilde{O}(n^{-1/2})), \quad (2.7)
\]

\[
V(\ell) = \mu_D^{\ell D/2} (1 - \mu_D)^{(n-\ell)D/2} \exp\left( \frac{1}{4} - \frac{D(D-1)}{2} - \frac{D(D-1)(1 - 2\mu_D)(\ell - \mu_Dn)}{2\mu_D(1 - \mu_D)n} \right)
\times \frac{D^2(\ell - \mu_Dn)^2}{4\mu_D^2(1 - \mu_D)^2n^2} - \frac{DR}{2(1 - \mu_D)^2n^2} - \frac{R^2}{4\mu_D^2(1 - \mu_D)^2n^4},
\]

\[
\beta_j = \frac{D\delta_j}{\mu_D(1 - \mu_D)n} - \frac{D(1 - 2\mu_D)\delta_j^2}{2\mu_D^2(1 - \mu_D)^2n^2} \quad \text{for } j = 1, \ldots, n.
\]

Next we must sum over all \( z \in A_{\ell} \). Note that \( \beta_j = \tilde{O}(n^{-1/2}) \) for \( j = 1, \ldots, n \), and the average of \( \beta_1, \ldots, \beta_n \) is

\[
\bar{\beta} = -\frac{D(1 - 2\mu_D)R}{2\mu_D^2(1 - \mu_D)^2n^3} = \tilde{O}(n^{-1}).
\]

Hence Lemma 2.1 applies and shows that

\[
\sum_{z \in A_{\ell}} \exp\left( \sum_{j=1}^{n} \beta_j z_j \right) = \binom{n}{\ell} \ \exp\left( \ell \bar{\beta} + \frac{\ell(n - \ell)}{2n^2} \sum_{j=1}^{n} (\beta_j - \bar{\beta})^2 + \tilde{O}(n^{-1/2}) \right)
\]

\[
= \binom{n}{\ell} \ \exp\left( \frac{D^2(\ell^2 - \ell)R}{2\mu_D^2(1 - \mu_D)^2n^4} - \frac{D(1 - 2\mu_D)\ell R}{2\mu_D^2(1 - \mu_D)^2n^3} + \tilde{O}(n^{-1/2}) \right). \quad (2.8)
\]
Combining (2.5) and (2.6)–(2.8) gives

\[ G_D(d, \ell) = A \left( \binom{n}{\ell} \mu_D^{\ell/2} (1 - \mu_D)^{(n-\ell)/2} \exp(Q_D(d, \ell) + \tilde{O}(n^{-1/2})) \right) \tag{2.9} \]

where \( Q_D(d, \ell) \) is defined in the statement of Theorem 1.4 for \( D \in \{1, 2\} \).

Next we will estimate \( G_D(d) \) by summing (2.9) over allowable values of \( \ell \). Recall the definition of \( \bar{\ell}_D \) given in the theorem statement. Ignoring the factor \( A \) which is independent of \( \ell \), we calculate

\[
\sum_{\ell=0}^{n} \left( \binom{n}{\ell} \mu_D^{\ell/2} (1 - \mu_D)^{(n-\ell)/2} \exp(Q_D(d, \ell) + \tilde{O}(n^{-1/2})) \right) \\
= (1 - \mu_D)^{Dn/2} \sum_{\ell=0}^{n} \left( \binom{n}{\ell} \left( \frac{\mu_D}{1 - \mu_D} \right)^{\ell/2} \exp(Q_D(d, \bar{\ell}_D) + \tilde{O}(n^{-1}(\ell - \bar{\ell}_D) + n^{-1/2})) \right) \\
= (1 - \mu_D)^{Dn/2} \exp(Q_D(d, \bar{\ell}_D)) \sum_{\ell=0}^{n} \left( \binom{n}{\ell} \left( \frac{\mu_D}{1 - \mu_D} \right)^{\ell/2} \exp(\tilde{O}(n^{-1}(\ell - \bar{\ell}_D) + n^{-1/2})) \right). 
\tag{2.10} \]

If \( |\ell - \bar{\ell}_D| \leq n^{1/2+\eta} \) for some constant \( \eta > 0 \) then the error term in the corresponding summand is \( \tilde{O}(n^{-1/2}) \), so these summands are essentially terms from a binomial expansion. If \( |\ell - \bar{\ell}_D| > n^{1/2+\eta} \) then

\[
\left( \binom{n}{\ell} \left( \frac{\mu_D}{1 - \mu_D} \right)^{\ell/2} \right) \leq \exp(-\Omega(n^{2\eta})), \quad \exp(\tilde{O}(n^{-1}(\ell - \bar{\ell}_D))) = \exp(\tilde{O}(1)), 
\tag{2.11} \]

so the contribution from the tails of the sum is negligible. Therefore

\[
\sum_{\ell=0}^{n} \left( \binom{n}{\ell} \left( \frac{\mu_D}{1 - \mu_D} \right)^{\ell/2} \exp(\tilde{O}\left(\frac{\ell - \bar{\ell}_D}{n} + n^{-1/2}\right)) \right) \\
= \exp(\tilde{O}(n^{-1/2})) \sum_{\ell=0}^{n} \left( \binom{n}{\ell} \left( \frac{\mu_D}{1 - \mu_D} \right)^{\ell/2} \right) \\
= \left( 1 + \left( \frac{\mu_D}{1 - \mu_D} \right)^{D/2} \right)^n \exp(\tilde{O}(n^{-1/2})). 
\tag{2.12} \]

The preceding calculations hold for any sufficiently small \( \varepsilon > 0 \), so in particular they hold for some \( \varepsilon = \varepsilon(a, b) \) such that \( \varepsilon \leq \varepsilon_0 \) and the \( \tilde{O}(n^{-1/2}) \) error terms in (2.7), (2.9) and (2.13) are all \( O(n^{-b}) \). Then the claimed formulae for \( G_D(d, \ell) \) follow immediately from (2.7) and (2.9).

Furthermore, multiplying (2.13) by \( A (1 - \mu_D)^{Dn/2} \exp(Q_D(d, \bar{\ell}_D)) \) using (2.7) and substituting \( D = 2 \) gives the desired formula for \( G_2(d) \).
For $D = 1$, we must sum over only those values of $\ell$ with the same parity as $S$. That is, we must replace (2.12) with a sum over just the even (or just the odd) values of $\ell$. By standard properties of the binomial distribution, the parity-restricted sum is half the full sum, within additive error $O(n^{-b})$, say. (This also follows from Lemma 3.3 when $\mu_1 \neq \frac{1}{2}$, and hence when $\mu_1 = 1/2$ by analytic continuation.) The additive error can be absorbed into the relative error in (2.13), since the main factor there is $\Omega(1)$. This gives the desired formula for $G_1(d)$, completing the proof.

\section{The sparse case}

In this section we prove Theorem 1.5.

\subsection{Some useful results}

First, we present two lemmas involving the Poisson binomial distribution, which we introduced in Section 1.1. Let $\mathbf{p} = (p_1, \ldots, p_n)$ satisfy $0 \leq p_1, \ldots, p_n \leq 1$ and let $X$ be a random variable with distribution $\text{PB}(\mathbf{p})$. The mean of $X$ is $\bar{X} = \mathbb{E}(X) = \sum_{j=1}^{n} p_j$. The following tail bounds are standard.

**Lemma 3.1.** If $X$ is a Poisson binomial random variable then, for any $s \geq 0$, we have

\[
\Pr(X - \bar{X} \leq -s) \leq \exp\left(-\frac{s^2}{2\bar{X}}\right),
\]

\[
\Pr(X - \bar{X} \geq s) \leq \exp\left(-\bar{X}\varphi\left(\frac{s}{\bar{X}}\right)\right),
\]

where $\varphi(x) = (1 + x) \log(1 + x) - x$.

**Proof.** These bounds are attributed to Chernoff, see [10, Theorems 2.1 and 2.8] and [6, Theorem 3.2].

**Lemma 3.2.** Let $X$ be a random variable with Poisson binomial distribution $\text{PB}(\mathbf{p})$ and mean $\bar{X} \leq n/(\log n)^2$. For a fixed constant $C > 0$, let $f : \mathbb{R} \to \mathbb{R}$ be a function such that

\[
|f(x)| \leq C\left(\frac{x^2}{n} + \frac{|x|}{n^{1/2}}\right) \quad \text{for} \quad |x| \leq n.
\]

Then

\[
\mathbb{E}(\exp(f(X - \bar{X}))) = 1 + \mathbb{E}(f(X - \bar{X})) + O(\mathbb{E}(f(X - \bar{X})^2)) + n^{-\Omega(\log n)}
\]

\[
= \exp\left(\mathbb{E}(f(X - X)) + O(\mathbb{E}(f(X - X)^2)) + n^{-\Omega(\log n)}\right).
\]
In particular, the contribution to this expectation from values of $X$ with $|X - \bar{X}| > n^{1/2}$ is

$$\sum_{\ell, |\ell - X| > n^{1/2}} \Pr(X = \ell) \exp(f(\ell - \bar{X})) = n^{-\Omega(\log n)}. \quad (3.2)$$

**Proof.** Define $g(x) = e^{f(x)} - f(x)$. Note that $|g(x)| \leq e^{|f(x)|}$ for all $x$, which implies that

$$|g(x)| \leq \exp\left(\frac{C x^2}{n} + \frac{C |x|}{n^{1/2}}\right) \quad \text{for } |x| \leq n. \quad (3.3)$$

We write

$$\mathbb{E}(g(X - \bar{X})) = \Sigma_1 + \Sigma_2 + \Sigma_3$$

where

$$\Sigma_1 = \sum_{\ell, |\ell - X| \leq n^{1/2}} \Pr(X = \ell) g(\ell - \bar{X}),$$

$$\Sigma_2 = \sum_{\ell, |\ell - X| > n^{1/2}} \Pr(X = \ell) g(\ell - \bar{X}),$$

$$\Sigma_3 = \sum_{\ell, \ell - \bar{X} < -n^{1/2}} \Pr(X = \ell) g(\ell - \bar{X}).$$

In each of these sums, $\ell$ is a nonnegative integer in $\{0, \ldots, n\}$ which satisfies the additional constraint given. We now bound these three sums in turn.

For $\Sigma_1$, note that when $|\ell - \bar{X}| \leq n^{1/2}$ we have $f(\ell - \bar{X}) \leq 2C = O(1)$. Hence

$$g(\ell - \bar{X}) = O\left(f(\ell - \bar{X})^2\right)$$

uniformly for all $\ell$ in this range. It follows that $\sum_{\ell, |\ell - X| \leq n^{1/2}} \Pr(X = \ell) f(\ell - \bar{X})^2 \leq \mathbb{E}(f(X - \bar{X})^2)$, and hence

$$\Sigma_1 = O\left(\mathbb{E}(f(X - \bar{X})^2)\right). \quad (3.4)$$

Now we consider $\Sigma_2$. Since $\bar{X} \varphi(s/\bar{X})$ is a decreasing function of $\bar{X}$, and $\bar{X} \leq n/(\log n)^2$ by assumption, Lemma 3.1 shows that

$$\Pr(X - \bar{X} \geq s) \leq \exp\left(-\frac{n}{\log^2 n} \varphi\left(\frac{s \log^2 n}{n}\right)\right).$$

Applying (3.3) shows that $\Sigma_2$ is bounded above by

$$n \max_{n^{1/2} < s \leq n} \exp(L_1(s));$$

where

$$L_1(s) = \frac{Cs^2}{n} + \frac{Cs}{n^{1/2}} - \frac{n}{\log^2 n} \varphi\left(\frac{s \log^2 n}{n}\right).$$
Now
\[ L_1'(s) = \frac{2Cs}{n} + \frac{C}{n^{1/2}} - \log \left( 1 + \frac{s \log^2 n}{n} \right), \]
which is negative for sufficiently large \( n \) for \( s \in \{n^{1/2}, n\} \). Also \( L'''_1(s) > 0 \) for all \( s \geq 0 \), so it must be that \( L_1'(s) < 0 \) for \( n^{1/2} \leq s \leq n \) when \( n \) is sufficiently large. It follows that the maximum of \( L_1 \) on the interval \([n^{1/2}, n]\) occurs at \( s = n^{1/2} \). Since \( L_1(n^{1/2}) = -\frac{1}{2} \log^2 n + O(1) \), we deduce that
\[ \Sigma_2 = n \exp(-\Omega(\log^2 n)) = n^{-\Omega(\log n)}. \]  
(3.5)

A bound on \( \Sigma_3 \) can be obtained similarly. Using the first bound in Lemma 3.1, we find
\[ \Sigma_3 \leq n \max_{n^{1/2} < s \leq n} \exp(L_2(s)), \]
where
\[ L_2(s) = \frac{Cs^2}{n} + \frac{Cs}{n^{1/2}} - \frac{s^2 \log^2 n}{2n}. \]
By the same argument as before, the maximum of \( L_2(s) \) occurs at \( s = n^{1/2} \) for sufficiently large \( n \), and we conclude that \( \Sigma_3 = n^{-\Omega(\log n)} \), which together with (3.5) implies (3.2). Combining (3.2) and (3.4) establishes (3.1), completing the proof. \( \square \)

For a given function \( f : \{0, 1, \ldots, n\} \rightarrow \mathbb{R} \), define the polynomial \( \hat{f} : \mathbb{R}^n \rightarrow \mathbb{R} \) by
\[ \hat{f}(y_1, \ldots, y_n) = \sum_{(x_1, \ldots, x_n) \in \{0, 1\}^n} f(x_1 + \cdots + x_n) \prod_{j=1}^n y_j^{x_j} (1 - y_j)^{1-x_j}. \]
(Note that this is indeed a polynomial in \( y_1, \ldots, y_n \), since \( 1 - x_j \in \{0, 1\} \).) In the case that \( 0 \leq y_1, \ldots, y_n \leq 1 \), we have
\[ \hat{f}(y_1, \ldots, y_n) = \mathbb{E}(f(Y)), \]  
(3.6)
where \( Y \) is a random variable with distribution \( \text{PB}((y_1, \ldots, y_n)) \).

The following lemma will be used when \( D = 1 \) to handle the parity restriction on the number of loops.

**Lemma 3.3.** Fix \((p_1, \ldots, p_n) \in [0, 1]^n\) such that \( p_j \neq \frac{1}{2} \) for \( j = 1, \ldots, n \). Define
\[ r_j = -\frac{p_j}{1 - 2p_j} \]
for \( j = 1, \ldots, n \), and let
\[ Z = \prod_{j=1}^n (1 - 2p_j). \]
Then for \( \rho = 0, 1 \),

\[
\sum_{(x_1, \ldots, x_n) \in \{0, 1\}^n \atop x_1 + \cdots + x_n \equiv \rho \pmod{2}} f(x_1 + \cdots + x_n) \prod_{j=1}^{n} p_j^{x_j} (1 - p_j)^{1-x_j} = \frac{1}{2} \hat{f}(p_1, \ldots, p_n) + (-1)^\rho \frac{1}{2} Z \hat{f}(r_1, \ldots, r_n).
\]

**Proof.** Let \( X \) be a random variable with Poisson binomial distribution \( \text{PB}((p_1, \ldots, p_n)) \). The probability generating function for \( X \) is

\[
P(w) = \sum_{t=0}^{n} w^t \Pr(X = t) = \prod_{j=1}^{n} (1 - p_j + p_j w).
\]

Note that

\[
\hat{f}(p_1, \ldots, p_n) = \sum_{t=0}^{n} f(t) \Pr(X = t) = \sum_{t=0}^{n} f(t) [w^t] P(w). \tag{3.7}
\]

Now

\[
P(-w) = \prod_{j=1}^{n} (1 - p_j - p_j w) = Z \prod_{j=1}^{n} (1 - r_j + r_j w).
\]

This expression has the same algebraic form as \( P(w) \), but with \( r_j \) in place of \( p_j \) for \( j = 1, \ldots, n \). Therefore, by comparison with (3.7) we have

\[
\sum_{t=0}^{n} f(t) [w^t] P(-w) = Z \hat{f}(r_1, \ldots, r_n).
\]

Hence we calculate that

\[
\sum_{(x_1, \ldots, x_n) \in \{0, 1\}^n \atop x_1 + \cdots + x_n \equiv \rho \pmod{2}} f(x_1 + \cdots + x_n) \prod_{j=1}^{n} p_j^{x_j} (1 - p_j)^{1-x_j} = \sum_{t=0}^{n} f(t) \Pr(X = t) = \sum_{t=0}^{n} f(t) [w^t] P(-w) + (-1)^\rho \frac{1}{2} Z \hat{f}(r_1, \ldots, r_n)
\]

as claimed. \( \square \)
3.2 Proof of the sparse theorem (Theorem 1.5)

We now prove Theorem 1.5. Assume throughout this section that $1 \leq d_{\text{max}} = o(S^{1/3})$ and that $S$ is even if $D = 2$. Furthermore, note that deleting vertices of degree zero does not affect either the value of $G_D(d)$ or the formulae for it given in Theorem 1.5. Hence we assume without loss of generality that $d_j \geq 1$ for $j = 1, \ldots, n$.

Let

$$H(d) = \sqrt{2} \left( \frac{S}{e} \right)^{S/2} \left( \prod_{j=1}^{n} d_j ! \right)^{-1} \exp \left( - \frac{S_2}{2S} - \frac{S_2^2}{4S^2} - \frac{S_2 S_3}{2S^3} + \frac{S_2^4}{4S^5} + \frac{S_3^2}{6S^3} \right).$$

Using Stirling’s approximation, Theorem 1.2 can be restated as follows: when $S$ is even and $1 \leq d_{\text{max}} = o(S^{1/3})$, then

$$G(d) = H(d) \exp(O(d_{\text{max}}^3/S)), \quad (3.8)$$

uniformly as $S \to \infty$. We proceed to estimate $G_D(d)/H(d)$.

Define

$$A^{(1)} = \{ z \in \{0, 1\}^n : \text{for } j = 1, \ldots, n, \text{ if } d_j < D \text{ then } z_j = 0 \},$$

$$A^{(2)} = \{ z \in \{0, 1\}^n : |z| \equiv S \pmod{2} \}$$

and let

$$A = \begin{cases} 
A^{(1)} \cap A^{(2)} & \text{if } D = 1, \\
A^{(1)} & \text{if } D = 2.
\end{cases}$$

(Recall that $|z|$ denotes the number of entries of $z$ equal to 1.) Then

$$G_D(d) = H(d) \sum_{z \in A} \frac{G(d - Dz)}{H(d)}. \quad (3.9)$$

Our strategy is to compare the ratio $G(d - Dz)/H(d)$ to the ratio $H(d - Dz)/H(d)$, which we now investigate.

Lemma 3.4. For $j = 1, \ldots, n$, define

$$a_j = \frac{[d_j]_D}{S^{D/2}} \exp(\Delta + \gamma_j),$$

where

$$\gamma_j = -\frac{D(D + 1)}{2S} - \frac{D(D + 2)S_2}{2S^2} - \frac{DS^3_2}{2S^3} + \left( \frac{D}{S} + \frac{DS_2}{S^2} \right) d_j$$
for \( j = 1, \ldots, n \), and \( \Delta \) is defined by

\[
\Delta = \begin{cases} 
\frac{1}{2S^{1/2}} - \frac{S_3}{2S^3} & \text{if } D = 1, \\
0 & \text{if } D = 2.
\end{cases}
\]

Define \( K(z) \) by

\[
\frac{H(d - Dz)}{H(d)} = \exp(K(z)) \prod_{j=1}^n a_j^z.
\] (3.10)

Then there are functions \( K', K'' : \{0, 1, \ldots, n\} \to \mathbb{R} \) which satisfy

\[
K'(\ell), K''(\ell) = -\Delta \ell + \frac{D^2 \ell^2}{4S} + \frac{D^3 \ell^3}{12S^2} + O\left(\frac{\ell^4}{S^3} + \frac{\ell^3}{S^{3/2}}\right)
\] (3.11)

such that

\[
K'(|z|) \leq K(z) \leq K''(|z|)
\] (3.12)

for all \( z \in \Lambda \) with \( |z| \leq S/3 \).

**Proof.** Define the function

\[
M(d, z) = -\frac{S_2(z)}{2S_1(z)} + \frac{S_2}{2S} - \frac{S_2(z)^2}{4S_1(z)^2} + \frac{S_2}{4S} - \frac{S_2(z)^2 S_3(z)}{2S_1(z)^4} + \frac{S_2 S_3}{2S^4} + \frac{S_2(z)^4}{4S_1(z)^5} - \frac{S_2}{4S^3} + \frac{S_3(z)^2}{6S_1(z)^3} - \frac{S_3}{6S^3},
\]

where \( S_r(z) = \sum_{j=1}^n [d_j - Dz_j]_r \) for \( r = 1, 2, 3 \). Then

\[
\frac{H(d - Dz)}{H(d)} = \exp(M(d, z)) \left(\frac{e}{S}\right)^{D\ell/2} \left(1 - \frac{D\ell}{S}\right)^{(S-D\ell)/2} \prod_{j=1}^n ([d_j]_D)^{z_j} = \exp(M(d, z)) \exp\left(\frac{D^2 \ell^2}{4S} + \frac{D^3 \ell^3}{12S^2} + O\left(\frac{\ell^4}{S^3} + \frac{\ell^3}{S^{3/2}}\right)\right) \prod_{j=1}^n ([d_j]_D)^{z_j}.
\]

Now

\[
S_1(z) = S - D\ell,
\]
\[
S_2(z) = S_2 - 2DW_1 + D(D + 1)\ell,
\]
\[
S_3(z) = S_3 - 3DW_2 + 3D(D + 1)W_1 - D(D + 1)(D + 2)\ell,
\]

where \( W_r = \sum_{j=1}^n [d_j]_r z_j \) for \( r = 1, 2 \). Making these substitutions gives

\[
M(d, z) = O\left(\frac{d_3^\max}{S} + \frac{d_2^\max \ell^2}{S^2}\right) + \sum_{j=1}^n \gamma_j z_j.
\]

Since the terms involving \( \Delta \) cancel, this completes the proof. The lemma is in fact true for any \( \Delta \), but the value we have chosen will be useful in proving Lemma 3.6. \(\square\)
We now calculate some important quantities which will be needed later.

**Lemma 3.5.** When $D = 1$,

\[
\sum_{j=1}^{n} \frac{a_j}{1 + a_j} = \sqrt{S} - \frac{1}{2} + \frac{1}{8S^{1/2}} - \frac{S_2}{S} + \frac{2S_2}{S^{3/2}} + \frac{S_3}{S^{3/2}} + \frac{S_2^2}{2S^{5/2}} + O\left(\frac{d_{\max}^3}{S}\right),
\]

\[
\sum_{j=1}^{n} \log(1 + a_j) = \sqrt{S} - \frac{1}{24S^{1/2}} - \frac{S_2}{2S} + \frac{S_2}{2S^{3/2}} + \frac{S_3}{3S^{3/2}} + \frac{S_2^2}{2S^{5/2}} + O\left(\frac{d_{\max}^3}{S}\right).
\]

When $D = 2$,

\[
\sum_{j=1}^{n} \frac{a_j}{1 + a_j} = \frac{S_2}{S} \exp\left(O\left(\frac{d_{\max}^2}{S}\right)\right),
\]

\[
\sum_{j=1}^{n} \log(1 + a_j) = \frac{S_2}{S} \exp\left(O\left(\frac{d_{\max}^2}{S}\right)\right).
\]

**Proof.** For $D = 1$ we have

\[
\Delta = O(S^{-1/2}), \quad \gamma_j = O\left(\frac{d_{\max}^2}{S}\right) + O\left(\frac{d_{\max}}{S}\right) d_j,
\]

and find that

\[
\sum_{j=1}^{n} a_j = \sqrt{S} + \frac{1}{2} + \frac{1}{8S^{1/2}} + \frac{S_2^2}{2S^{5/2}} + O\left(\frac{d_{\max}^3}{S}\right),
\]

\[
\sum_{j=1}^{n} a_j^2 = \frac{S_2}{S} + \frac{S_2}{S^{3/2}} + 1 + \frac{1}{S^{1/2}} + O\left(\frac{d_{\max}^2}{S}\right),
\]

\[
\sum_{j=1}^{n} a_j^3 = \frac{S_3}{S^{3/2}} + \frac{3S_2}{S^{3/2}} + \frac{1}{S^{1/2}} + O\left(\frac{d_{\max}^2}{S}\right),
\]

\[
\sum_{j=1}^{n} a_j^4 = O\left(\frac{d_{\max}^3}{S}\right),
\]

from which the result follows. When $D = 2$ we have

\[
\sum_{j=1}^{n} a_j = \frac{S_2}{S} + O\left(\frac{d_{\max}^2}{S^2}\right), \quad \sum_{j=1}^{n} a_j^2 = O\left(\frac{d_{\max}^2}{S^2}\right),
\]

which imply the result in this case.

Next we calculate the sum of the right hand side of (3.10) over all $z \in \{0, 1\}^n$ (subject to a parity constraint if $D = 1$), after dividing by the factor $\prod_{j=1}^{n} (1 + a_j)$. 

23
Lemma 3.6. Let $K^*$ be either of the functions $K', K''$ defined in Lemma 3.4. If $D = 1$ then for $\rho \in \{0, 1\}$,
\[
\sum_{z \in \{0, 1\}^n \mid \|z\| \equiv \rho \mod 2} \exp(K^*(|z|)) \prod_{j=1}^n \frac{a_j^{z_j}}{1 + a_j} = \frac{1}{2} \exp \left( -\frac{1}{4} + \frac{1}{3S^{1/2}} + \frac{S_2}{2S^{3/2}} + O \left( \frac{d_{\max}^3}{S} \right) \right).
\]
If $D = 2$ then
\[
\sum_{z \in \{0, 1\}^n} \exp(K^*(|z|)) \prod_{j=1}^n \frac{a_j^{z_j}}{1 + a_j} = \exp(O(d_{\max}^3/S)).
\]

Proof. Define $p = (p_1, \ldots, p_n)$ where $p_j = a_j/(1 + a_j)$ for $j = 1, \ldots, n$, and let $X$ be a random variable with Poisson binomial distribution $\text{PB}(p)$. Then
\[
\sum_{z \in \{0, 1\}^n} \exp(K^*(|z|)) \prod_{j=1}^n \frac{a_j^{z_j}}{1 + a_j} = \mathbb{E}(\exp(K^*(X))).
\]
The expectation of $X$ is $\bar{X} = \sum_{j=1}^n p_j$, which has been calculated for $D = 1, 2$ in Lemma 3.5.

First suppose that $D = 1$. Recall from Lemma 3.5 that
\[
\sum_{j=1}^n p_j = \sqrt{S} + O(d_{\max}) = \sqrt{S} + o(S^{1/3}).
\]
From (3.2) we know that
\[
\sum_{|z| > 3\sqrt{S}} \exp(K^*(|z|)) \prod_{j=1}^n \frac{a_j^{z_j}}{1 + a_j} = n^{-\Omega(\log n)}.
\]
Next we observe that by Lemma 3.1,
\[
\sum_{|\sqrt{S} - |z|| > S^{1/3}} \prod_{j=1}^n \frac{a_j^{z_j}}{1 + a_j} = O(e^{-S^{1/6}}).
\]
For $\ell - \sqrt{S} = O(S^{1/3})$ we have, using (3.11),
\[
\exp(K^*(\ell)) = \exp \left( -\frac{1}{4} + O(d_{\max}^3/S) \right) f(\ell), \quad (3.14)
\]
where
\[
f(\ell) = \frac{\ell^4}{32S^2} - \frac{\ell^3}{8S^{3/2}} + \left( \frac{7}{16S} + \frac{S_2}{8S^{5/2}} + \frac{13}{48S^{3/2}} \right) \ell^2 \\
+ \left( -\frac{5}{8S^{1/2}} + \frac{S_2}{4S^2} - \frac{7}{24S} \right) \ell + \frac{41}{32} + \frac{S_2}{8S^{3/2}} + \frac{5}{48S^{1/2}}.
\]
Since $K^*(\ell) = O(1)$ for $\ell = O(\sqrt{S})$, it follows that
\[
\sum_{|z| \equiv \rho \pmod{2}} \exp(K^*(|z|)) \prod_{j=1}^{n} \frac{a_j^{z_j}}{1 + a_j} = n^{-\Omega(\log n)} + \exp\left(-\frac{1}{4} + O(d_{\max}^3/S)\right) \sum_{|z| \equiv \rho \pmod{2}} f(|z|) \prod_{j=1}^{n} \frac{a_j^{z_j}}{1 + a_j}. \tag{3.15}
\]

We now apply Lemma 3.3 to estimate the sum on the right hand side. The small order moments of $X$ are
\[
\begin{align*}
\mathbb{E}(X^2) &= \bar{X}^2 + \sum_{j=1}^{n} p_j (1 - p_j), \\
\mathbb{E}(X^3) &= \bar{X} + 3\bar{X}^2 + X^3 - 3 \sum_{j=1}^{n} p_j^2 - 3\bar{X} \sum_{j=1}^{n} p_j^2 + 2 \sum_{j=1}^{n} p_j^3, \\
\mathbb{E}(X^4) &= \bar{X} + 7\bar{X}^2 + 6\bar{X}^3 + \bar{X}^4 - (6\bar{X}^2 - 18\bar{X} + 7) \sum_{j=1}^{n} p_j^2 \\
&\quad + 3 \left(\sum_{j=1}^{n} p_j^2\right)^2 + (8\bar{X} + 12) \sum_{j=1}^{n} p_j^3 - 6 \sum_{j=1}^{n} p_j^4.
\end{align*}
\tag{3.16}
\]
Substituting (3.13) into these expressions gives
\[
\mathbb{E}(X^k) = \begin{cases} 
1 & \text{if } k = 0; \\
\sqrt{S} - S_2/S - \frac{1}{2} + O(d_{\max}^3/S^{1/2}) & \text{if } k = 1; \\
S - 2S_2/S^{1/2} + O(d_{\max}^3) & \text{if } k = 2; \\
S^{3/2} - 3S_2 + \frac{3}{2}S + O(d_{\max}^3S^{1/2}) & \text{if } k = 3; \\
S^2 + 4S^{3/2} - 4S^{1/2}S_2 + O(d_{\max}^3S) & \text{if } k = 4.
\end{cases}
\]

Hence
\[
\hat{f}(p_1, \ldots, p_n) = \mathbb{E}(f(X)) = \exp\left(\frac{1}{3S^{1/2}} + \frac{S_2}{2S^{3/2}} + O\left(\frac{d_{\max}^3}{S}\right)\right)
\]
where $\hat{f}$ is the function obtained from $f$ as in (3.6). Let $f_k$ be the polynomial defined by $f_k(t) = t^k$ for all $t \in \mathbb{R}$, for $k = 1, 2, 3, 4$. Since $\mathbb{E}(X^k) = \hat{f}_k(p_1, \ldots, p_n)$, replacing each $p_j$ with $r_j$ in (3.16) leads to the following (abusing notation slightly to define the abbreviation
\( \hat{f}_1 \) in the first line):

\[
\hat{f}_1 = \hat{f}_1(r_1, \ldots, r_n) = \sum_{j=1}^{n} r_j = O(\sqrt{S}),
\]

\[
\hat{f}_2(r_1, \ldots, r_n) = \hat{f}_1^2 + \sum_{j=1}^{n} r_j(1 - r_j) = O(S),
\]

\[
\hat{f}_3(r_1, \ldots, r_n) = \hat{f}_1 + 3\hat{f}_1^2 + \hat{f}_1^3 - 3\sum_{j=1}^{n} r_j^2 - 3\hat{f}_1 \sum_{j=1}^{n} r_j^2 + 2 \sum_{j=1}^{n} r_j^3 = O(S^{3/2}),
\]

\[
\hat{f}_4(r_1, \ldots, r_n) = \hat{f}_1 + 7\hat{f}_1^2 + 6\hat{f}_1^3 + \hat{f}_1^4 - (6\hat{f}_1^2 - 18\hat{f}_1 + 7) \sum_{j=1}^{n} r_j^2
\]

\[
+ 3\left( \sum_{j=1}^{n} r_j^2 \right)^2 + (8\hat{f}_1 + 12) \sum_{j=1}^{n} r_j^3 - 6 \sum_{j=1}^{n} r_j^4 = O(S^4).
\]

From this we conclude that \( \hat{f}(r_1, \ldots, r_n) = O(1) \). Furthermore,

\[
Z = \exp\left( -\Omega\left( \sum_{j=1}^{n} p_j \right) \right) = e^{-\Omega(\sqrt{S})}.
\]

Thus by Lemma 3.3 we obtain

\[
\sum_{|z| \equiv \rho \pmod{2}} f(|z|) \prod_{j=1}^{n} \frac{a_j^{z_j}}{1 + a_j} = \frac{1}{2} \exp\left( \frac{1}{3S^{1/2}} + \frac{S_2}{2S^{3/2}} + O\left( \frac{d_{\max}}{S} \right) \right).
\]

Combining this with (3.15) establishes the lemma when \( D = 1 \).

Next suppose that \( D = 2 \). Expanding \( K^* \) around \( \bar{X} \) gives

\[
K^*(X) = h(X - \bar{X}) + O(d_{\max}^3/S)
\]

where \( h : \mathbb{R} \to \mathbb{R} \) is a function which satisfies

\[
h(y) = O\left( \frac{d_{\max}}{S} \right) y + O\left( \frac{1}{S} \right) y^2
\]

for \( |y| \leq S \). Recall our assumption that \( d_j \geq 1 \) for \( j = 1, \ldots, n \), which implies that \( S \geq n \). Hence the function \( h \) satisfies the conditions of Lemma 3.2 for some constant \( C > 0 \). We proceed to apply this lemma, specifically (3.1).

The second and fourth central moments of \( X \) are

\[
\mathbb{E}\left( (X - \bar{X})^2 \right) = \sum_{j=1}^{n} p_j(1 - p_j) = O(\bar{X}),
\]

\[
\mathbb{E}\left( (X - \bar{X})^4 \right) = 3 \mathbb{E}\left( (X - \bar{X})^2 \right)^2 + \sum_{j=1}^{n} p_j(1 - p_j)(1 - 6p_j + 6p_j^2) = O(\bar{X} + \bar{X}^2).
\]
Recall from Lemma 3.5 that $\bar{X} = O(d_{\text{max}})$, and also note that $|y| \leq 1 + y^2$. From (3.18) and (3.19), we have

$$\mathbb{E}(h(X - \bar{X})) = O(d_{\text{max}}/S) (1 + \mathbb{E}((X - \bar{X})^2)) = O(d_{\text{max}}^2/S).$$

Similarly, from (3.18) by applying (3.19) and using the inequality $(u + v)^2 \leq 2(u^2 + v^2)$, we obtain

$$\mathbb{E}(h(X - \bar{X})^2) = O(d_{\text{max}}^2/S^2) \mathbb{E}((X - \bar{X})^2) + O(S^{-2}) \mathbb{E}((X - \bar{X})^4) = O(d_{\text{max}}^3/S^2).$$

Therefore (3.1) gives

$$\mathbb{E}(\exp(h(X - \bar{X}))) = \exp(O(d_{\text{max}}^3/S)).$$

This completes the proof when $D = 2$, using (3.17).

We may now prove our main result in the sparse case.

**Proof of Theorem 1.5.** First suppose that $S > n \log n$. Then Lemma 3.4 applies for all values of $\ell$. Furthermore,

$$d_{\text{max}}^3 = o(S - Dn)$$

since $S - Dn = \Omega(S)$, so (3.8) can be applied to $d - Dz$, for all $z \in \Lambda$. Notice also that $a_j = 0$ whenever $d_j < D$, so the sum of the right hand side of (3.10) over $z \in \Lambda$ is equal to the sum over $\{0, 1\}^n$ when $D = 2$, or over $\Lambda^{(2)}$ when $D = 1$. Hence the result follows from (3.9) using (3.8) and Lemmas 3.4–3.6.

Now suppose that $n \leq S \leq n \log n$. We show that terms with $|z| > S/3$ give a negligible contribution to $G_D(d)$.

It is well known that when $S$ is even, we can write

$$G(d) = \frac{S!}{(S/2)! 2^{S/2}} \left( \prod_{j=1}^n d_j! \right)^{-1} P(d)$$

where $P(d)$ is a probability, and hence is at most 1. (Indeed, the $\exp(\cdot)$ factor in (3.8) is an approximation to $P(d)$ when $d_{\text{max}} = o(S^{1/3})$, as proved in [17].) It follows by Stirling’s approximation that

$$G(d) = O(1) \left( \frac{S}{e} \right)^{S/2} \left( \prod_{j=1}^n d_j! \right)^{-1}$$

for any even value of $S$. Recall the definition of $\Lambda_\ell$ from (2.4). For $z \in \Lambda_\ell$ we have

$$G(d - Dz) = O(1) \left( \frac{S - D\ell}{e} \right)^{(S - D\ell)/2} \left( \prod_{j=1}^n (d_j - Dz_j)! \right)^{-1}.$$
Furthermore,

\[ H(d)^{-1} = \exp(O(d_{\max}^2)) \left( \frac{e}{S} \right)^{S/2} \prod_{j=1}^{n} d_j! \]

Hence

\[ \frac{G(d - Dz)}{H(d)} = O(1) \exp(O(d_{\max}^2)) \left( \frac{d_{\max}^2\ell}{S} \right)^{DL/2} . \]

Therefore, recalling that \( \ell \leq n \) and ignoring parity for an upper bound,

\[ \sum_{\ell=S/3}^{n} \sum_{z \in A_{\ell}} \frac{G(d - Dz)}{H(d)} = O(1) \exp(O(d_{\max}^2)) \sum_{\ell=S/3}^{n} \left( \frac{n}{\ell} \right) \left( \frac{d_{\max}^2\ell}{S} \right)^{DL/2} \]

\[ = O(1) \exp(O(d_{\max}^2)) \sum_{\ell=S/3}^{n} \left( \frac{n}{\ell} \right) S^{-DL/6} \]

\[ = O(1) \exp(O(d_{\max}^2)) 2^n S^{-DS/18} \]

\[ = O(S^{-\Omega(S)}) . \tag{3.20} \]

Recall that (3.8) applies when \( \ell < S/3 \). Therefore, using (3.8) and Lemma 3.4,

\[ \frac{G_D(d)}{H(d)} = S^{-\Omega(S)} + \sum_{\ell=0}^{S/3} \sum_{z \in A_{\ell}} \frac{G(d - Dz)}{H(d)} \]

\[ = O(S^{-\Omega(S)}) + \exp(O(d_{\max}^3/S)) \sum_{\ell=0}^{S/3} \sum_{z \in A_{\ell}} \exp(K(z)) \prod_{j=1}^{n} a_{j}^{z_{j}} . \]

Hence, by (3.12),

\[ O(S^{-\Omega(S)}) + \exp(O(d_{\max}^3/S)) \sum_{\ell=0}^{S/3} \exp(K'(\ell)) \sum_{z \in A_{\ell}} \prod_{j=1}^{n} a_{j}^{z_{j}} \]

\[ \leq \frac{G_D(d)}{H(d)} \]

\[ \leq O(S^{-\Omega(S)}) + \exp(O(d_{\max}^3/S)) \sum_{\ell=0}^{S/3} \exp(K''(\ell)) \sum_{z \in A_{\ell}} \prod_{j=1}^{n} a_{j}^{z_{j}} . \tag{3.21} \]

Next we would like to show that, in either the lower or upper bound in (3.21), the sum over \( \ell \) can be extended up to \( \ell = n \) without affecting the answer significantly. Since every term is positive, zero is a lower bound for the tail of the sum. Again, we ignore the parity issue for an upper bound. Let \( K^* \) be either \( K' \) or \( K'' \). Firstly, note that since \( n \leq S \) we have
$K^*(\ell) = O(\ell)$ uniformly for $S/3 \leq \ell \leq n$. Furthermore $a_j = o(S^{-D/6})$ for $j = 1, \ldots, n$. Therefore

$$
\sum_{\ell=S/3}^n \exp(K^*(\ell)) \sum_{z \in A_{\ell}} \prod_{j=1}^n a_j^z \leq \sum_{\ell=S/3}^n \left(\begin{array}{c} n \\ \ell \end{array}\right) (e^{O(1)} S^{-D/6})^\ell \\
\leq \sum_{\ell=S/3}^n \left(\begin{array}{c} n \\ \ell \end{array}\right) S^{-D\ell/7} \\
= O(S^{-\Omega(S)})
$$

(3.22)
as in (3.20). Combining this with (3.21) gives

$$
O(S^{-\Omega(S)}) + \exp(O(d_{\text{max}}^3/S)) \sum_{z \in A} \exp(K'(|z|)) \prod_{j=1}^n a_j^z \\
\leq \frac{G_D(d)}{H(d)} \\
\leq O(S^{-\Omega(S)}) + \exp(O(d_{\text{max}}^3/S)) \sum_{z \in A} \exp(K''(|z|)) \prod_{j=1}^n a_j^z.
$$

The result now follows from Lemma 3.5 and Lemma 3.6.

\[\square\]

4 Proof of Theorem 1.6

Part (i). Under the conditions of Theorem 1.4, the distribution of $Y_D$ follows directly from (2.10) and (2.11), noting in the case of $D = 1$ that the restriction of $\ell$ to the same parity as $S$ changes the normalizing factor by 2 to high precision, as explained in the last paragraph of Section 2.2. The formula for the expectation follows on summing $\ell \operatorname{Prob}(Y_D = \ell)$, since the error term $O(e^{-n\Omega(1)})$ contributes negligibly. To see that the same is true for the variance, it helps to use the cancellation-free formula

$$
\operatorname{Var}(Z) = \sum_{k<\ell} \operatorname{Prob}(Z = k) \operatorname{Prob}(Z = \ell) (k - \ell)^2,
$$

(4.1)

which is true for all discrete random variables $Z$ of finite variance (see for example [12, p. 8]).

Part (ii). Now suppose that the conditions of Theorem 1.5 hold and consider the case $D = 1$. Let $X$ be a random variable with the Poisson binomial distribution $\text{PB}(p_j)$, where $p_j = a_j/(1+a_j)$ and $a_j$ is defined in Lemma 3.4. From (3.10), (3.14), we find that for $\ell = \sqrt{S} + O(S^{1/3})$, the distribution of $Y_1$ is proportional to $\text{PB}(p)$ to relative error $O(d_{\text{max}}^3/S + S^{-1/3})$.  

29
Moreover, the weight of both $Y_1$ and $X$ from $|\ell - \sqrt{S}| > S^{1/3}$ is $e^{-S^{\Omega(1)}}$, and restriction of $\ell$ to the same parity as $S$ contributes a factor of 2 to high precision as in the proof of Lemma 3.6. This gives, for $\ell = 0, \ldots, n$,

$$\text{Prob}(Y_1 = \ell) = (2 + O(d_{\text{max}}^3/S + S^{-1/3})) \text{PB}(p, \ell) + O(e^{-S^{\Omega(1)}}).$$

Next we show that the parameters $p'$ in the theorem are sufficiently close to the parameters $p$. For each $j$, we find that

$$p_j = \exp(O(d_{\text{max}}^3/S^{3/2} + S^{-1})) p'_j. \quad (4.2)$$

By definition,

$$\text{PB}(p, \ell) = \sum_{|W| = \ell} \left( \prod_{j \in W} p_j \prod_{j \notin W} (1 - p_j) \right),$$

where the sum is over subsets $W \subseteq \{1, 2, \ldots, n\}$ of size $\ell$. Applying (4.2), we find that

$$\text{PB}(p, \ell) = \exp(O(d_{\text{max}}^3/S + S^{-1/2})) \text{PB}(p', \ell)$$

for $\ell = O(\sqrt{S})$. The tail past $\sqrt{S}$ is $e^{-S^{\Omega(1)}}$ for both $\text{PB}(p)$ and $\text{PB}(p')$, by Lemma 3.1. This completes the proof of the distribution for $D = 1$.

The mean and variance follow as for part (i) to the same relative precision as the distribution, but we can do better by using the more accurate distribution analysed in the proof of Lemma 3.6. As we have shown in (3.14), for $\ell = \sqrt{S} + O(S^{1/3})$, which excludes only exponentially small tails,

$$\text{Prob}(Y_1 = \ell) \propto \exp(O(d_{\text{max}}^3/S)) \text{Prob}(X = \ell) f(\ell) \quad (4.3)$$

if $\ell$ has the same parity as $S$. Define the discrete random variable $Z$ by

$$\text{Prob}(Z = t) \propto \text{Prob}(X = \bar{X} + t) f(\bar{X} + t),$$

whenever $\bar{X} + t$ is an integer in $[0, n]$ with the same parity as $S$; and $\text{Prob}(Z = t) = 0$ otherwise. By (4.3) and the argument used in part (i) of this proof,

$$\mathbb{E}(Y_1) = \exp(O(d_{\text{max}}^3/S)) (\bar{X} + \mathbb{E}(Z)),
\quad \text{Var}(Y_1) = \exp(O(d_{\text{max}}^3/S)) \text{Var}(Z).$$

For $m \geq 0$, define the central moment $\mu_m = \mathbb{E}((X - \bar{X})^m)$ and the cumulant $\kappa_m$ by

$$\log \phi(t) = \sum_{m=1}^{\infty} \kappa_m (it)^m/m!,$$

30
where $\phi(t) = \prod_{j=1}^{n}(p_j e^{it} + 1 - p_j)$ is the characteristic function of $X$. We find that $\kappa_m = O(\sqrt{S})$ for $2 \leq m \leq 6$. Using the well-known expressions for the central moments in terms of the cumulants, and the explicit formulae (3.19), we find that

$$
\begin{align*}
\mu_2 &= \sqrt{S} - \frac{2S_2}{S} - \frac{3}{2} + O(d_{\max}^3 / S^{1/2}), \\
\mu_3 &= \kappa_3 = O(\sqrt{S}), \\
\mu_4 &= 3S + O(d_{\max} S^{1/2}), \\
\mu_5 &= \kappa_5 + 10\kappa_3\kappa_2 = O(S), \\
\mu_6 &= \kappa_6 + 15\kappa_4\kappa_2 + 10\kappa_3^2 + 15\kappa_2^3 = O(S^{3/2}).
\end{align*}
$$

Thus we calculate

$$
\begin{align*}
M_0 &= \sum_{\ell=0}^{n} \text{Prob}(X = \ell) f(\ell) = \frac{1}{2} + \frac{1}{6S^{1/2}} + \frac{S_2}{4S^{3/2}} + O(d_{\max}^3 / S), \\
M_1 &= \sum_{\ell=0}^{n} \text{Prob}(X = \ell) f(\ell) (\ell - \bar{X}) = O(d_{\max}^2 / S + S^{-1/2}), \\
M_2 &= \sum_{\ell=0}^{n} \text{Prob}(X = \ell) f(\ell) (\ell - \bar{X})^2 = \frac{\sqrt{S}}{2} - \frac{3S_2}{4S} - \frac{1}{3} + O(d_{\max}^3 / S^{1/2}),
\end{align*}
$$

where the primes indicate that the sums are restricted to $\ell$ having the same parity as $S$. The effect of the parity restriction is handled in the same way as in the proof of Lemma 3.6, and in fact the first summation is equivalent to Lemma 3.6. Now we have that $\mathbb{E}(Z) = M_1 / M_0$ and $\text{Var}(Z) = M_2 / M_0 - \mathbb{E}(Z)^2$. From these the mean and variance of $Y_1$ follow.

Finally we consider part (ii) in the case $D = 2$. Define $X$ as before, with $a_j$ as in Lemma 3.4. By Lemma 3.1, $\text{Prob}(X \geq S^{1/3}) = O(e^{-S^{\Omega(1)}})$. The same bound holds for $\text{Pr}(Y_2 > S/3)$, using the argument leading to (3.20). Combining this with (3.2) and Lemma 3.4 shows that $\text{Pr}(Y_2 \geq 2S^{1/2}) = O(e^{-S^{\Omega(1)}})$. Finally, since $K''(\ell) = O(1)$ for $\ell = O(S^{1/2})$, we conclude that $\text{Pr}(Y_2 \geq S^{1/3}) = O(e^{-S^{\Omega(1)}})$.

Lemma 3.4 shows that for $\ell \leq S^{1/3}$,

$$
\text{Prob}(Y_2 = \ell) = \exp\left(O\left(d_{\max}^3 / S + S^{-1/3}\right)\right) \text{Prob}(X = \ell).
$$

By the argument above, the ratio of $\text{PB}(p)$ to $\text{PB}(p'')$ for $\ell \leq S^{1/3}$ is $\exp\left(O(d_{\max}^2 / S^{2/3})\right)$, since $p_j = \exp\left(O(d_{\max}^3 / S)\right)p_j''$ for all $j$. The given estimate of the distribution of $Y_2$ follows.

To obtain the mean and variance of $Y_2$, we use the sharper estimate

$$
\text{Prob}(Y_2 = \ell) \propto \exp\left(O(d_{\max}^3 / S)\right) \text{Prob}(X = \ell) \left(1 + \ell^2 / S\right),
$$

31
valid for $\ell \leq d_{\max}^{3/4}S^{1/4}$ by Lemma 3.4, with the weight of the tail $\ell > d_{\max}^{3/4}S^{1/4}$ being exponentially small as usual. Using (3.16) we find that $\mathbb{E}(X^2) = O(d_{\max}^2)$, $\mathbb{E}(X^3) = O(d_{\max}^2S_2/S)$ and $\mathbb{E}(X^4) = O(d_{\max}^3S_2S_2/S)$, and so

$$\sum_{\ell=0}^{n} \text{Prob}(X = \ell) (1 + \ell^2/S) = 1 + O\left(\frac{d_{\max}^2}{S}\right),$$

$$\sum_{\ell=0}^{n} \text{Prob}(X = \ell) (1 + \ell^2/S) \ell = \frac{S_2}{S} + O\left(\frac{d_{\max}^2S_2}{S^2}\right),$$

$$\sum_{\ell=0}^{n} \text{Prob}(X = \ell) (1 + \ell^2/S) \ell^2 = \frac{S_2^2}{S^2} + \frac{S_2}{S} + O\left(\frac{d_{\max}^3S_2}{S^2}\right),$$

and from these the expressions for $\mathbb{E}(Y_2)$ and $\text{Var}(Y_2)$ follow, recalling the cancellation-free variance formula (4.1).

5 A conjecture for regular graphs with loops

In the case of $D = 2$ and $d = (d, d, \ldots, d)$, an informal computation provides motivation for the sparse and dense enumeration formulae and suggests a more general conjecture. Since $D = 2$ we have $d \in \{0, 1, \ldots, n + 1\}$. Recall the notations $G_2(n, d) = G_2(d, d, \ldots, d)$ and $\mu_2 = d/(n + 1)$.

Generate a random $n$-vertex graph by independently choosing each of the $\binom{n+1}{2}$ possible edges (including loops) with probability $\mu_2$. Each $d$-regular graph has exactly $nd/2$ edges, so it occurs with probability

$$\mu_2^{nd/2} (1 - \mu_2)^{\binom{n+1}{2} - nd/2}. \tag{5.1}$$

The event that a particular vertex has degree $d$ has probability

$$\binom{n-1}{d} \mu_2^d (1 - \mu_2)^{n-d} + \binom{n-1}{d-2} \mu_2^{d-1} (1 - \mu_2)^{n-d+1} = \binom{n+1}{d} \frac{n-1}{n} \mu_2^d (1 - \mu_2)^{n-d+1}. \tag{5.2}$$

If the vertex degrees were independent (which of course they are not), the number of graphs would be the $n$-th power of (5.2) divided by (5.1). Noting that $(1 - 1/n)^n \to e^{-1}$, this gives a “naïve” estimate

$$\hat{G}_2(n, d) = e^{-1} \binom{n+1}{d} (\mu_2^{m_2}(1 - \mu_2)^{1-m_2})^{\binom{n+1}{2}}.$$
We can see from Theorem 1.4 that $G_2(n, d)$ is larger than $\hat{G}_2(n, d)$ by a factor close to $\sqrt{2} e^{1/4}$ whenever $\min\{d, n - d\} > cn/\log n$ for some constant $c > 2/3$. Less obviously, the same is true for $1 \leq d = o(n^{1/2})$ by Theorem 1.5. Recall that the same constant $\sqrt{2} e^{1/4}$ appears in a similar context for regular graphs without loops [16]. This leads us to investigate the region between the coverage of our sparse and dense theorems.

Using the method described in [13], we computed the exact values of $G_2(n, d)$ for about 150 nontrivial values of $(n, d)$ up to $n = 35$. For example,

$$G_2(22, 10) = 7789744323722189254716829156528211234980743220762340514888.$$

Numerical analysis of these values suggests the following analogue of [16, Conj. 2].

**Conjecture 1.** Let $d = d(n)$ satisfy $1 \leq d \leq n$ with $nd$ even. Then

$$G_2(n, d) = \sqrt{2} \left( \frac{n+1}{d} \right)^n \left( \mu_2^2 (1 - \mu_2)^{1-\mu_2} \right)^{n+1} \exp \left( -\frac{3}{4} + \frac{3c+1}{12cn} + O(n^{-2}) \right)$$

uniformly as $n \to \infty$, where $\mu_2 = d/(n+1)$ and $c = \mu_2(1-\mu_2)(n+1)$.

The numerical evidence suggests that in fact the term $O(n^{-2})$ always lies in the interval $(-2/n^2, 0)$ for $n \geq 4$.

**References**


