The von Neumann entropy of random multipartite graphs*

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Abstract

Let G be a graph with n vertices and $L(G)$ its Laplacian matrix. Define $\rho_G = \frac{1}{d_G}L(G)$ to be the *density matrix* of G, where d_G denotes the sum of degrees of all vertices of G. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of ρ_G. The *von Neumann entropy* of G is defined as $S(G) = -\sum_{i=1}^{n} \lambda_i \log_2 \lambda_i$. In this paper, we establish a lower bound and an upper bound to the von Neumann entropy for random multipartite graphs.

Keywords: Random multipartite graphs; von Neumann entropy; Density matrix

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1 Introduction

Let G be a simple undirected graph with vertex set $V_G = \{v_1, v_2, \ldots, v_n\}$ and edge set E_G. The *adjacency matrix* $A(G)$ of G is the symmetric matrix $[A_{ij}]$, where $A_{ij} = A_{ji} = 1$ if vertices v_i and v_j are adjacent, otherwise $A_{ij} = A_{ji} = 0$. Let $d_G(v_i)$ denote the *degree* of the vertex v_i, that is, the number of edges incident to v_i. The *Laplacian matrix* of G is the matrix $L(G) = D(G) - A(G)$, where $D(G)$, called the *degree matrix*, is a diagonal matrix with the diagonal entries the degrees of the vertices of G.

The *von Neumann entropy* was originally introduced by von Neumann around 1927 for proving the irreversibility of quantum measurement processes in quantum mechanics [18]. It is defined to be

$$S = -\sum_{i=1} \mu_i \log_2 \mu_i,$$

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where μ_i are the eigenvalues of the density matrix describing the quantum-mechanical system (Normally, a density matrix is a positive semidefinite matrix whose trace is equal to 1). Up until now, there are lots of studies on the von Neumann entropy, and we refer the reader to [1–3, 9–12, 15, 16, 18, 20].

In [4], Braunstein et al. defined the *density matrix of a graph G* as

$$\rho_G := \frac{1}{d_G} L(G) = \frac{1}{\mathrm{Tr}(D(G))} L(G),$$

where $d_G = \sum_{v_i \in V_G} d_G(v_i) = \mathrm{Tr}(D(G))$ is the *degree sum* of G, and $\mathrm{Tr}(D(G))$ means the trace of $D(G)$. Suppose that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n = 0$ are the eigenvalues of ρ_G. Then

$$S(G) := -\sum_{i=1}^{n} \lambda_i \log_2 \lambda_i,$$

is called the *von Neumann entropy of a graph G*. By convention, define $0 \log_2 0 = 0$. It is known that this quantity can be interpreted as a measure of regularity of graphs [**?**] and also that it can be used as a measure of graph complexity [8].

Up until now, lots of results on the von Neumann entropy of a graph have been given. For examples, Braunstein et al. [4] proved that, for a graph G on n vertices, $0 \leq S(G) \leq \log_2(n-1)$, with the left equality holding if and only if G is a graph with only one edge, and the right equality holding if and only if G is the complete graph K_n. In [14], Passerini and Severini showed that the von Neumann entropy of regular graphs with n vertices tends to $\log_2(n-1)$ as n tends to ∞. More interesting, in [6], Du *et al.* considered the von Neumann entropy of the Erdős-Rényi model $\mathcal{G}_n(p)$, named after Erdős and Rényi [7]. They proved that, for almost all $G_n(p) \in \mathcal{G}_n(p)$, almost surely $S(G_n(p)) = (1 + o(1)) \log_2 n$, independently of p, where an event in a probability space is said to be held asymptotically *almost surely* (*a.s.* for short) if its probability goes to one as n tends to infinity.

The purpose of this paper is to study the von Neumann entropy of random multipartite graphs. We use $K_{n;\beta_1,\ldots,\beta_k}$ to denote the complete k-partite graph with vertex set V ($|V| = n$), whose parts are $V_1, \ldots, V_k$ ($2 \leq k = k(n) \leq n$) satisfying $|V_i| = n\beta_i = n\beta_i(n)$, $i = 1, 2, \ldots, k$. The random k-partite graph model $\mathcal{G}_{n;\beta_1,\ldots,\beta_k}(p)$ consist of all random k-partite graphs in which the edges are chosen independently with probability p from the set of edges of $K_{n;\beta_1,\ldots,\beta_k}$. We denote by $A_{n,k} := A(G_{n;\beta_1,\ldots,\beta_k}(p)) = (x_{ij})_{n\times n}$ the adjacency matrix of random k-partite graphs $G_{n;\beta_1,\ldots,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,\ldots,\beta_k}(p)$, where x_{ij} is a random indicator variable for $\{v_i, v_j\}$ being an edge with probability p, for $i \in V_l$ and $j \in V \backslash V_l$, $i \neq j$, $1 \leq l \leq k$. Then $A_{n,k}$ satisfies the following properties:

- x_{ij}'s, $1 \le i < j \le n$, are independent random variables with $x_{ij} = x_{ji}$;
- $\Pr(x_{ij} = 1) = 1 - \Pr(x_{ij} = 0) = p$ if $i \in V_l$ and $j \in V \backslash V_l$, while $\Pr(x_{ij} = 0) = 1$ if $i \in V_l$ and $j \in V_l$, $1 \le l \le k$.

Note that when $k = n$, $\mathcal{G}_{n;\beta_1,\ldots,\beta_k} = \mathcal{G}_n(p)$, that is, the random multipartite graph model can be viewed as a generalization to the Erdős-Rényi model.

In this paper, we establish a lower bound and an upper bound to $S(G_{n;\beta_1,\ldots,\beta_k})$ for almost all $G_{n;\beta_1,\ldots,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,\ldots,\beta_k}(p)$ by the limiting behavior of the spectra of random symmetric matrices. Our main result is stated as follows:

Theorem 1. *Let $G_{n;\beta_1,\ldots,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,\ldots,\beta_k}(p)$. Then almost surely*

$$\frac{1+o(1)}{1-\sum\limits_{i=1}^{k}\beta_i^2}\log_2\left(n\left(1-\sum_{i=1}^{k}\beta_i^2\right)\right) \le S(G_{n;\beta_1,\ldots,\beta_k}(p))$$

$$\le -\frac{1-\max\limits_{1\le i\le k}\{\beta_i\}+o(1)}{1-\sum\limits_{i=1}^{k}\beta_i^2}\log_2\left(\frac{1-\max\limits_{1\le i\le k}\{\beta_i\}}{n\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)}\right),$$

independently of $0 < p < 1$, where $o(1)$ means a quantity goes to 0 as n goes to infinity.

2 Proof of Theorem 1

Before proceeding, we give some definitions and lemmas.

Lemma 1 (Bryc *et al.* [5])**.** *Let X be a symmetric random matrix satisfying that the entries X_{ij}, $1 \le i < j \le n$, are a collection of independent identically distributed (i.i.d.) random variables with $\mathbb{E}(X_{12}) = 0, \mathrm{Var}(X_{12}) = 1$ and $\mathbb{E}(X_{12}^4) < \infty$. Define $S := \mathrm{diag}\left(\sum_{i\neq j} X_{ij}\right)_{1\le i\le n}$ and let $M = S - X$, where $\mathrm{diag}\{\cdot\}$ denotes a diagonal matrix. Denote by $\| M \|$ the spectral radius of M. Then*

$$\lim_{n\to\infty}\frac{\| M \|}{\sqrt{2n\log n}} = 1 \quad a.s.,$$

i.e., with probability 1, $\frac{\| M \|}{\sqrt{2n\log n}}$ converges weakly to 1 as n tends to infinity.

Lemma 2 (Weyl [19])**.** *Let X, Y and Z be $n\times n$ Hermitian matrices such that $X = Y + Z$. Suppose that X, Y, Z have eigenvalues, respectively, $\lambda_1(X) \ge \cdots \ge \lambda_n(X)$, $\lambda_1(Y) \ge \cdots \ge \lambda_n(Y)$, $\lambda_1(Z) \ge \cdots \ge \lambda_n(Z)$. Then, for $i = 1, 2, \ldots, n$, the following inequalities hold:*

$$\lambda_i(Y) + \lambda_n(Z) \le \lambda_i(X) \le \lambda_i(Y) + \lambda_1(Z).$$

Lemma 3 (Shiryaev [17]). *Let $X_1, X_2, \dots$ be an infinite sequence of i.i.d. random variables with expected value $\mathbb{E}(X_1) = \mathbb{E}(X_2) = \dots = \mu$, and $\mathbb{E}|X_j| < \infty$. Then*

$$\overline{X}_n := \frac{1}{n}(X_1 + X_2 + \dots + X_n) \to \mu \quad a.s.$$

Proof of Theorem 1. Note that the parts $V_1, \dots, V_k$ of the random k-partite graph $G_{n;\beta_1,\dots,\beta_k}(p)$ satisfy $|V_i| = n\beta_i$, $i = 1, 2, \dots, k$. Then the adjacency matrix $A_{n,k}$ of $G_{n;\beta_1,\dots,\beta_k}(p)$ satisfies

$$A_{n,k} + A'_{n,k} = A_n,$$

where

$$A'_{n,k} = \begin{pmatrix} A_{n\beta_1} & & & \\ & A_{n\beta_2} & & \\ & & \ddots & \\ & & & A_{n\beta_k} \end{pmatrix}_{n\times n,}$$

$A_n := A(G_n(p))$, and $A_{n\beta_i} := A(G_{n\beta_i}(p))$ for $i = 1, 2, \dots, k$.

The degree matrix $D_{n,k} := D(G_{n;\beta_1,\dots,\beta_k}(p))$ of $G_{n;\beta_1,\dots,\beta_k}(p)$ satisfies

$$D_{n,k} + D'_{n,k} = D_n,$$

where

$$D'_{n,k} = \begin{pmatrix} D_{n\beta_1} & & & \\ & D_{n\beta_2} & & \\ & & \ddots & \\ & & & D_{n\beta_k} \end{pmatrix}_{n\times n,}$$

$D_n := D(G_n(p))$, and $D_{n\beta_i} := D(G_{n\beta_i}(p))$ for $i = 1, 2, \dots, k$.

The Laplacian matrix $L_{n,k} := L(G_{n;\beta_1,\dots,\beta_k}(p))$ of $G_{n;\beta_1,\dots,\beta_k}(p)$ satisfies

$$L_{n,k} + L'_{n,k} = L_n,$$

where

$$L'_{n,k} = \begin{pmatrix} L_{n\beta_1} & & & \\ & L_{n\beta_2} & & \\ & & \ddots & \\ & & & L_{n\beta_k} \end{pmatrix}_{n\times n,}$$

$L_n := L(G_n(p))$, and $L_{n\beta_i} := L(G_{n\beta_i}(p))$ for $i = 1, 2, \dots, k$.

Let

$$S = \frac{1}{\sqrt{p(1-p)}}[D_n - p(n-1)I_n]$$

and

$$X = \frac{1}{\sqrt{p(1-p)}}[A_n - p(J_n - I_n)],$$

where J_n is the $n \times n$ all-ones matrix, and I_n is the $n \times n$ identity matrix. Define an auxiliary matrix

$$\begin{aligned}\widetilde{L_n} :=& L_n - p(n-1)I_n + p(J_n - I_n)\\ =& (D_n - p(n-1)I_n) - (A_n - p(J_n - I_n))\\ =& \sqrt{p(1-p)}(S - X).\end{aligned}$$

Note that $\mathbb{E}(X_{12}) = 0, \mathrm{Var}(X_{12}) = 1$, and

$$\mathbb{E}(X_{12}^4) = \frac{1}{p^2(1-p)^2}(p - 4p^2 + 6p^3 - 3p^4) < \infty.$$

By Lemma 1, we have

$$\lim_{n\to\infty} \frac{\| \widetilde{L_n} \|}{\sqrt{2p(1-p)n\log n}} = 1 \quad a.s.$$

Then

$$\lim_{n\to\infty} \frac{\| \widetilde{L_n} \|}{n} = 0 \quad a.s.,$$

i.e.,

$$\| \widetilde{L_n} \| = o(1)n \quad a.s.$$

Let $R_n := p(n-1)I_n - p(J_n - I_n)$. Then

$$\widetilde{L_n} + R_n = L_n.$$

Suppose that $L_n, \widetilde{L_n}, R_n$ have eigenvalues, respectively, $\mu_1(L_n) \geq \cdots \geq \mu_n(L_n)$, $\lambda_1(\widetilde{L_n}) \geq \cdots \geq \lambda_n(\widetilde{L_n})$, $\lambda_1(R_n) \geq \cdots \geq \lambda_n(R_n)$. It follows from Lemma 2 that

$$\lambda_i(R_n) + \lambda_n(\widetilde{L_n}) \leq \mu_i(L_n) \leq \lambda_i(R_n) + \lambda_1(\widetilde{L_n}), \text{ for } i = 1, 2, \ldots, n.$$

Note that $\lambda_i(R_n) = pn$ for $i = 1, 2, \ldots, n-1$ and $\lambda_n(R_n) = 0$. We have

$$\mu_i(L_n) = (p + o(1))n \quad a.s. \text{ for } 1 \leq i \leq n-1, \tag{2.1}$$

and

$$\mu_n(L_n) = o(1)n \ \ a.s. \tag{2.2}$$

In the following, we evaluate the eigenvalues of $L_{n,k}$ according to the spectral distribution of L_n and $L'_{n,k}$.

Since $L_{n,k} = L_n - L'_{n,k}$, Lemma 2 implies that for $1 \leq i \leq n$,

$$\mu_i(L_n) + \mu_n(-L'_{n,k}) \leq \mu_i(L_{n,k}) \leq \mu_i(L_n) + \mu_1(-L'_{n,k}), \tag{2.3}$$

where $\mu_n(-L'_{n,k})$ and $\mu_1(-L'_{n,k})$ are the minimum and maximum eigenvalues of $-L'_{n,k}$ respectively. By (2.1), (2.2) and (2.3), we have

$$np(1-\max_{1\le i\le k}\{\beta_i\})+o(1)n \le \mu_i(L_{n,k}) \le np+o(1)n \quad a.s., \text{ for } 1\le i\le n-1, \tag{2.4}$$

and

$$-np\max_{1\le i\le k}\{\beta_i\}+o(1)n \le \mu_n(L_{n,k}) \le o(1)n \quad a.s. \tag{2.5}$$

Consider the trace $\mathrm{Tr}(D_{n,k})$ of $D_{n,k}$. Note that $\mathrm{Tr}(D_{n,k}) = 2\sum_{i>j}(A_{n,k})_{ij}$. Since $(A_n)_{ij}$ $(i>j)$ are *i.i.d.* with mean p and variance $p(1-p)$, according to Lemma 3, we obtain that with probability 1,

$$\lim_{n\to\infty}\frac{\sum_{i>j}(A_n)_{ij}}{\frac{n(n-1)}{2}} = p,$$

i.e.,

$$\sum_{i>j}(A_n)_{ij} = (p/2+o(1))n^2 \quad a.s.$$

Then

$$\mathrm{Tr}(D_n) = (p+o(1))n^2 \quad a.s.$$

Similarly, for $i=1,2,\ldots,k$,

$$\mathrm{Tr}(D_{n\beta_i}) = (p+o(1))n^2\beta_i^2 \quad a.s.$$

Thus,

$$\begin{aligned}
\mathrm{Tr}(D_{n,k}) &= 2\sum_{i>j}(A_{n,k})_{ij} = 2\sum_{i>j}(A_n - A'_{n,k})_{ij} \\
&= 2\sum_{i>j}(A_n)_{ij} - 2\sum_{i>j}(A'_{n,k})_{ij} \\
&= 2\sum_{n\ge i>j\ge 1}(A_n)_{ij} - 2\left(\sum_{n\beta_1\ge i>j\ge 1}(A_{n\beta_1})_{ij} + \cdots + \sum_{n\beta_k\ge i>j\ge 1}(A_{n\beta_k})_{ij}\right) \\
&= (p+o(1))n^2 \left((p+o(1))(n\beta_1)^2 + \cdots + (p+o(1))(n\beta_k)^2\right) \\
&= p\left(1-\sum_{i=1}^k \beta_i^2\right)n^2 + o(1)n^2 \quad a.s.
\end{aligned} \tag{2.6}$$

By (2.4), (2.5) and (2.6), the eigenvalues of $\rho_{G_{n,k}} = \dfrac{L_{n,k}}{\mathrm{Tr}(D_{n,k})}$ satisfy that, for $1\le i\le n-1$,

$$\frac{p\left(1-\max\limits_{1\le i\le k}\{\beta_i\}\right)+o(1)}{p\left(1-\sum\limits_{i=1}^k\beta_i^2\right)n+o(1)n} \le \lambda_i(\rho_{G_{n,k}}) \le \frac{p+o(1)}{p\left(1-\sum\limits_{i=1}^k\beta_i^2\right)n+o(1)n} \quad a.s., \tag{2.7}$$

and

$$\frac{-p\max\limits_{1\le i\le k}\{\beta_i\}+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\le\lambda_n(\rho_{G_{n,k}})\le\frac{o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\quad a.s. \tag{2.8}$$

Then (2.7) and (2.8) imply that

$$\begin{aligned} S(G_{n;\beta_1,\ldots,\beta_k}(p)) &\ge -\sum_{i=1}^{n-1}\left(\frac{p+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\log_2\left(\frac{p+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\right)\right)\\ &\quad-\frac{o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\log_2\left(\frac{o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\right)\\ &=\frac{1+o(1)}{1-\sum\limits_{i=1}^{k}\beta_i^2}\log_2\left(n\left(1-\sum_{i=1}^{k}\beta_i^2\right)\right) \end{aligned}\tag{2.9}$$

and

$$\begin{aligned} S(G_{n;\beta_1,\ldots,\beta_k}(p)) &\le -\sum_{i=1}^{n-1}\left(\frac{p\left(1-\max\limits_{1\le i\le k}\{\beta_i\}\right)+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\log_2\left(\frac{p\left(1-\max\limits_{1\le i\le k}\{\beta_i\}\right)+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\right)\right)\\ &\quad-\frac{-p\max\limits_{1\le i\le k}\{\beta_i\}+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\log_2\left(\frac{-p\max\limits_{1\le i\le k}\{\beta_i\}+o(1)}{p\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)n+o(1)n}\right)\\ &=-\frac{1-\max\limits_{1\le i\le k}\{\beta_i\}+o(1)}{1-\sum\limits_{i=1}^{k}\beta_i^2}\log_2\left(\frac{1-\max\limits_{1\le i\le k}\{\beta_i\}}{n\left(1-\sum\limits_{i=1}^{k}\beta_i^2\right)}\right). \end{aligned}\tag{2.10}$$

This completes the proof. □

At last, we present some results implied by Theorem 1.

Corollary 1. *Let* $G_{n;\beta_1,\ldots,\beta_k}(p)\in\mathcal{G}_{n;\beta_1,\ldots,\beta_k}(p)$. *Then*

$$S(G_{n;\beta_1,\ldots,\beta_k}(p))=(1+o(1))\log_2 n\quad a.s.$$

if and only if $\max\{n\beta_1,\ldots,n\beta_k\}=o(1)n$.

Note that if $k=n$, then $G_{n;\beta_1,\ldots,\beta_k}(p)=G_n(p)$, that is, $\beta_i=\frac{1}{n}$, $1\le i\le k$. By Corollary 1, we have the following result immediately.

Corollary 2. ([6]) *Let $G_n(p) \in \mathcal{G}_n(p)$ be a random graph. Then almost surely $S(G_n(p)) = (1+o(1))\log_2 n$.*

Corollary 3. *Let $G_{n;\beta_1,\dots,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,\dots,\beta_k}(p)$ satisfying $\lim\limits_{n\to\infty} \max_{1\le i\le k}\{\beta_i\} > 0$ and $\lim\limits_{n\to\infty} \frac{\beta_i}{\beta_j} = 1$. Then*

$$\frac{1+o(1)}{1-\frac{1}{k}} \log_2 \left(n \left(1 - \frac{1}{k} \right) \right) \le S(G_{n;\beta_1,\dots,\beta_k}(p)) \le \left(1 + \frac{k-1}{k} o(1) \right) \log_2 n.$$

Let $f(n), g(n)$ be two functions of n. Then $f(n) = o(g(n))$ means that $f(n)/g(n) \to 0$, as $n \to \infty$; and $f(n) = O(g(n))$ means that there exists a constant C such that $|f(n)| \le Cg(n)$, as $n \to \infty$.

Corollary 4. *Let $G_{n;\beta_1,\dots,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,\dots,\beta_k}(p)$ satisfying $\lim\limits_{n\to\infty} \max_{1\le i\le k}\{\beta_i\} > 0$, and there exist β_i and β_j such that $\lim\limits_{n\to\infty} \frac{\beta_i}{\beta_j} < 1$, that is, there exists an integer $r \ge 1$ such that $|V_1|, \dots, |V_r|$ are of order $O(n)$ and $|V_{r+1}|, \dots, |V_k|$ are of order $o(n)$. Then almost surely*

$$\frac{1+o(1)}{1-\sum\limits_{i=1}^{r}\beta_i^2} \log_2 \left(n \left(1 - \sum_{i=1}^{r} \beta_i^2 \right) \right) \le S(G_{n;\beta_1,\dots,\beta_k}(p))$$

$$\le -\frac{1-\max\limits_{1\le i\le r}\{\beta_i\}+o(1)}{1-\sum\limits_{i=1}^{r}\beta_i^2} \log_2 \left(\frac{1-\max\limits_{1\le i\le r}\{\beta_i\}}{n\left(1-\sum\limits_{i=1}^{r}\beta_i^2\right)} \right).$$

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