## ARTICLE IN PRESS

Discrete Applied Mathematics [ ( ] ] ] .



Contents lists available at ScienceDirect

## **Discrete Applied Mathematics**

journal homepage: www.elsevier.com/locate/dam

## The von Neumann entropy of random multipartite graphs\*

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#### ARTICLE INFO

Article history: Received 29 September 2016 Received in revised form 1 July 2017 Accepted 3 July 2017 Available online xxxx

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

### 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  $\rho_G$ . 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.

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### 1. Introduction

Let *G* be a simple undirected graph with vertex set  $V_G = \{v_1, v_2, ..., v_n\}$  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 on  $v_i$ . 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 [20]. It is defined to be

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

where  $\mu_i$  are the eigenvalues of the  $n \times n$  density matrix describing the quantum-mechanical system (Normally, a density matrix is a positive semidefinite matrix whose trace is equal to 1). It is known [12] that the von Neumann entropy of a quantum state provides a means of characterizing its information content, which is in analogy to the Shannon entropy of a statistical ensemble from classical information theory; and that the von Neumann entropy of a state takes center stage in the burgeoning field of quantum information theory. Up until now, there are lots of studies on the von Neumann entropy, and we refer the reader to [1–3,10,11,13,14,17,18,20,22].

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

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

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http://dx.doi.org/10.1016/j.dam.2017.07.008 0166-218X/© 2017 Elsevier B.V. All rights reserved.

Please cite this article in press as: D. Hu, et al., The von Neumann entropy of random multipartite graphs, Discrete Applied Mathematics (2017), http://dx.doi.org/10.1016/j.dam.2017.07.008.

Supported by NSFC (Nos. 11571135, 11671320 and 11601431), "973" program (No. 2013CB834204), China Postdoctoral Science Foundation (No. 2016M600813) and Natural Science Foundation of Shaanxi Province (No. 2017JQ1019).

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where  $d_G = \sum_{v_i \in V_G} d_G(v_i) = \operatorname{Tr}(D(G))$  is the *degree sum* of *G*, and  $\operatorname{Tr}(D(G))$  means the trace of D(G). Suppose that  $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n = 0$  are the eigenvalues of  $\rho_G$ . 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  $Olog_2 O = O$ . It is known that this quantity can be interpreted as a measure of regularity of graphs [4,15] and also that it can be used as a measure of graph complexity [9].

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 exist two constants  $C_1 > 0$  and  $C_2 > 0$  such that  $C_1 \le |f(n)/g(n)| \le C_2$ , as  $n \to \infty$ . Up until now, lots of results on the von Neumann entropy of a graph have been given. For example, Braunstein et al. [4] proved that, for a graph G on n vertices,  $0 \le S(G) \le \log_2(n-1)$ , 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 [16], 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  $\infty$ . More interesting, in [7], Du et al. considered the von Neumann entropy of the Erdős–Rényi model  $\mathcal{G}_n(p)$ , named after Erdős and Rényi [8]. 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. And recently, in [6], Dairyko et al. conjectured that all connected graphs of order n have von Neumann entropy at least as great as the star  $K_{1,n-1}$ and proved this for almost all graphs of order n. They also showed that adding an edge to a graph can lower its von Neumann entropy.

The purpose of this paper is to study the von Neumann entropy of random multipartite graphs. We use  $K_{n;\beta_1,...,\beta_k}$  to denote the complete k-partite graph with vertex set V (|V| = n), whose parts are  $V_1, \ldots, V_k$  ( $2 \le k = k(n) \le n$ ) satisfying  $|V_i| = n\beta_i = n\beta_i(n), i = 1, 2, \dots, k$ . The random k-partite graph model  $\mathcal{G}_{n;\beta_1,\dots,\beta_k}(p)$  consists of all random k-partite graphs in which the edges are chosen independently with probability p from the set of edges of  $K_{n;\beta_1,...,\beta_k}$ . We denote by  $A_{n,k} := A(G_{n;\beta_1,...,\beta_k}(p)) = (x_{ij})_{n \times n}$  the adjacency matrix of random k-partite graphs  $G_{n;\beta_1,...,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,...,\beta_k}(p)$ , 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  $j \in V \setminus V_l$ ,  $i \neq j$ ,  $1 \le l \le k$ . 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  $j \in V \setminus V_l$ , 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,  $\mathcal{G}_{n;\beta_1,...,\beta_k} = \mathcal{G}_n(p)$ , 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  $S(G_{n;\beta_1,...,\beta_k})$  for almost all  $G_{n;\beta_1,...,\beta_k}(p) \in \mathcal{G}_{n;\beta_1,...,\beta_k}(p)$ by the limiting behavior of the spectra of random symmetric matrices. Our main result is stated as follows:

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

$$\begin{aligned} \frac{1+o(1)}{1-\sum_{i=1}^{k}\beta_{i}^{2}}\log_{2}\left(n\left(1-\sum_{i=1}^{k}\beta_{i}^{2}\right)\right) &\leq S(G_{n;\beta_{1},...,\beta_{k}}(p))\\ &\leq \frac{1-\max_{1\leq i\leq k}\{\beta_{i}\}+o(1)}{1-\sum_{i=1}^{k}\beta_{i}^{2}}\log_{2}\left(\frac{n\left(1-\sum_{i=1}^{k}\beta_{i}^{2}\right)}{1-\max_{1\leq i\leq k}\{\beta_{i}\}}\right),\end{aligned}$$

independently of 0 , where <math>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  $\mathbb{E}(X_{12}) = 0$ ,  $Var(X_{12}) = 1$  and  $\mathbb{E}(X_{12}) < \infty$ . Define  $S := \operatorname{diag}\left(\sum_{i \neq j} X_{ij}\right)_{1 \leq i \leq n}$  and let M = S - X, where  $\operatorname{diag}\{\cdot\}$  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 [21]). Let X, Y and Z be  $n \times n$  Hermitian matrices such that X = Y + Z. Suppose that X, Y, Z have eigenvalues, respectively,  $\lambda_1(X) \geq \cdots \geq \lambda_n(X)$ ,  $\lambda_1(Y) \geq \cdots \geq \lambda_n(Y)$ ,  $\lambda_1(Z) \geq \cdots \geq \lambda_n(Z)$ . Then, for  $i = 1, 2, \ldots, n$ , the following inequalities hold:

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

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