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On the von Neumann entropy of a graph

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ABSTRACT

The von Neumann entropy of a nonempty graph provides a mean of characterizing the information content of the quantum state of a physical system. We give sharp upper and lower bounds for the von Neumann entropy of a nonempty graph using graph parameters and characterize the graphs when each bound is attained. These upper (lower, respectively) bounds are shown to be incomparable in general by examples.

1. Introduction

In quantum mechanics, the state of a physical system is represented by a positive semi-definite hermitian matrix with unit trace, called its density matrix. The von Neumann entropy of a quantum state is defined as the Shannon entropy associated with the eigenvalues of its density matrix. It provides a mean of characterizing the information content of the quantum state.

We consider simple graphs. Let G be a graph on n vertices with vertex set $V(G)$ and edge set $E(G)$. The adjacency matrix of G is the $n \times n$ matrix $A(G) = (a_{uv})$, where $a_{uv} = 1$ if u and v are adjacent in G, and 0 otherwise. For $u \in V(G)$, $d_G(u)$ or d_u denotes the degree of u in G. The matrix $L(G) = D(G) - A(G)$ is known as the (combinatorial) Laplacian matrix of G, where $D(G)$ is the degree diagonal matrix of G. For a nonempty graph G, let $\sigma(G) = \frac{1}{d_G}L(G)$, where d_G is the trace of $L(G)$, i.e., the sum of degrees of G, i.e., $2|E(G)|$. Note that $\sigma(G)$ is a positive semi-definite hermitian matrix with unit trace. It may be interpreted as the density matrix of a physical system. We call $\sigma(G)$ the density matrix of G. Let $\rho_1, \ldots, \rho_n$ be the eigenvalues of $\sigma(G)$, arranged in a non-increasing order. Then $\rho_n = 0$ and the multiplicity of eigenvalue 0 for $\sigma(G)$ is equal to the number of components of G. The von Neumann entropy of G is defined as [2]

$$s(G) = -\sum_{i=1}^{n} \rho_i \log_2 \rho_i$$

with convention that $0 \log_2 0 = 0$. Thus, $s(G) = -\sum_{i=1}^{n-1} \rho_i \log_2 \rho_i$.

Braunstein et al. [2] showed that, for a nonempty graph G on n vertices,

$$0 \le s(G) \le \log_2(n-1)$$

with left equality if and only if G has a single edge and with right equality if and only if G is (isomorphic to) the complete graph K_n. For a graph G with n vertices and $m \ge 1$ edges, let $Z = Z(G) = \sum_{u \in V(G)} d_u^2$. Let S_n be the star on n vertices. Among

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others, Dairyko et al. [5] showed that

$$s(G) \geq -\log_2 \frac{2m+Z}{4m^2}, \tag{1.1}$$

and they used this inequality to deduce sufficient conditions that $s(G) \geq s(S_n)$. Recall that, early, it was asked in [16] whether S_n minimizes von Neumann entropy among connected graphs with $n \geq 2$ vertices, which was conjectured to be true in [5]. The von Neumann entropies of the Erdős–Rényi random graphs and multipartite generalizations have been studied in [6,12]. Related work on the von Neumann entropies may be found in [3,10].

In this paper, we find upper and lower bounds for the von Neumann entropy of a nonempty graph in terms of graph parameters that are easy to discern to some extent such as the number of vertices, the number of edges, the maximum degree, the degree sequence, the conjugate degree sequence, and the quantity Z, and determine those graphs that attain the bounds. Particularly, we determine the graphs attaining the bound in (1.1). We also compare these bounds by examples.

2. Preliminaries

For a graph G on n vertices, let $\lambda_1, \ldots, \lambda_n$ be the Laplacian eigenvalues of G (i.e., the eigenvalues of $L(G)$), arranged in a non-increasing order. When more than one graph is under discussion, we may write $\lambda_i(G)$ in place of λ_i. We mention that λ_{n-1} is known as the algebraic connectivity of G, see [7]. Obviously, $\lambda_i = 2m\rho_i$, where $m = |E(G)|$.

Recall that, for a nonempty graph G with n vertices,

$$\sum_{i=1}^{n-1} \rho_i = \operatorname{tr}(\sigma(G)) = 1.$$

This fact will be used frequently.

Lemma 2.1 ([15]). *Let G be a nonempty graph with maximum degree Δ. Then $\lambda_1 \geq \Delta + 1$ with equality when G is connected on n vertices if and only if $\Delta = n - 1$.*

For a graph G, let $\overline{G}$ be its complement.

Lemma 2.2 ([15]). *Let G be a graph with n vertices. Then the Laplacian eigenvalues of $\overline{G}$ are $n - \lambda_{n-1}(G), \ldots, n - \lambda_1(G), 0$.*

Lemma 2.3 ([15]). *Let G be a connected graph with diameter d. Suppose that G has exactly k distinct Laplacian eigenvalues. Then $d + 1 \leq k$.*

Lemma 2.4 ([15]). *Let G be a graph on n vertices with minimum degree δ and $G \ncong K_n$. Then $\lambda_{n-1} \leq \delta$.*

For a graph G on n vertices, let μ_1 be the largest eigenvalue of $A(G)$, and q_1 the largest eigenvalue of $Q(G) = D(G)+A(G)$. It is known that $\mu_1 \geq \sqrt{\frac{Z}{n}}$ with equality when G is connected if and only if G is regular or bipartite semiregular (i.e., bipartite and vertices in the same color class have equal degrees), see [11]. Let x be the nonnegative unit eigenvector of $A(G)$ corresponding to μ_1. Then $q_1 \geq x^\top Q(G)x = \sum_{uv\in E(G)}(x_u + x_v)^2 \geq 2 \cdot 2\sum_{uv\in E(G)} x_u x_v = 2\mu_1$ with equalities if and only if $Q(G)x = q_1 x$ and $x_u = x_v$ for any $uv \in E(G)$ [4]. Thus $q_1 \geq 2\mu_1$ with equality when G is connected if and only if G is regular. If G is bipartite, then $\lambda_1 = q_1$ (see [15]), and thus $\lambda_1 \geq 2\sqrt{\frac{Z}{n}}$ with equality when G is connected if and only if G is regular. Thus, we have the following lemma.

Lemma 2.5. *Let G be a bipartite graph on n vertices. Then $\lambda_1 \geq 2\sqrt{\frac{Z}{n}}$ with equality when G is connected if and only if G is regular.*

For non-increasing sequences $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{y} = (y_1, \ldots, y_n)$, $\mathbf{x}$ is majorized by $\mathbf{y}$, denoted by $x \preceq y$, if $\sum_{i=1}^{j} x_i \leq \sum_{i=1}^{j} y_i$ for $j = 1, \ldots, n$, and equality holds when $j = n$.

Lemma 2.6 ([8]). *Let G be a graph with non-increasing degree sequence $(d_1, \ldots, d_n)$, where $d_n \geq 1$. Then*

$$(d_1 + 1, d_2, \ldots, d_{n-1}, d_n - 1) \preceq (\lambda_1, \ldots, \lambda_n).$$

For the (non-increasing) degree sequence $(d_1, \ldots, d_n)$ of a graph G, its conjugate degree sequence is $(d_1^*, \ldots, d_n^*)$, where $d_i^* = |\{j : d_j \geq i\}|$. The following lemma was conjectured in [9] and was confirmed in [1].

Lemma 2.7. *Let G be a graph with conjugate degree sequence $(d_1^*, \ldots, d_n^*)$. Then*

$$(\lambda_1, \ldots, \lambda_n) \preceq (d_1^*, \ldots, d_n^*).$$

For vertex-disjoint graphs G and H, $G \cup H$ denotes the vertex-disjoint union of G and H, and sH denotes the vertex-disjoint union of s copies of H for a positive integer s. Let $G \cup 0H = G$.

For vertex-disjoint graphs G and H, the join $G \vee H$ is the graph obtained from $G \cup H$ by adding edges between each vertex of G and each vertex of H. Let $\Gamma_1 = \{K_p : p \geq 1\}$, and for $i \geq 1$, $\Gamma_{i+1} = \{\overline{G} \vee K_q : G \in \Gamma_i, q \geq 1\}$. Let $\Gamma = \cup_{i \geq 1} \Gamma_i$. Let $\Gamma^{(n)}$ be the set of graphs in Γ of order n.

Lemma 2.8 ([14]). *Let G be a connected graph with conjugate degree sequence $(d_1^*, \ldots, d_n^*)$. Then $(\lambda_1, \ldots, \lambda_n) = (d_1^*, \ldots, d_n^*)$ if and only if G is isomorphic to a graph in $\Gamma^{(n)}$.*

A real function F defined on a set on $\mathbb{R}^n$ is said to be strictly Schur-convex if $F(\mathbf{x}) < F(\mathbf{y})$ whenever $\mathbf{x} \preceq \mathbf{y}$ but $\mathbf{x} \neq \mathbf{y}$. From [13, p. 64, C.1.a], if a real function f defined on an interval in $\mathbb{R}$ is strictly convex, then $\sum_{i=1}^{n} f(x_i)$ is strictly Schur-convex.

3. Upper bounds and extremal graphs

In this section, we give upper bounds for the von Neumann entropy of a nonempty graph and characterize the extremal graphs.

Theorem 3.1. *Let G be a graph with n vertices, k components, m edges and maximum degree Δ, where $n \geq k+2$. Then*

$$s(G) \leq -\frac{\Delta+1}{2m}\log_2\frac{\Delta+1}{2m} - \left(1-\frac{\Delta+1}{2m}\right)\log_2\frac{1-\frac{\Delta+1}{2m}}{n-k-1} \tag{3.1}$$

with equality if and only if $G \cong S_{n-k+1} \cup (k-1)K_1$, or $G \cong aK_{\Delta+1} \cup (k-a)K_1$ for some positive integer $a = \frac{n-k}{\Delta}$.

Proof. Since G has k components, we have $\rho_{n-k+1} = \cdots = \rho_n = 0$ and $\sum_{i=1}^{n-k} \rho_i = 1$. Note that $f(x) = -x\log_2 x$ for $x > 0$ is a strictly concave function. By Jensen's inequality, we have

$$\sum_{i=2}^{n-k} \frac{1}{n-k-1} \cdot (-\rho_i \log_2 \rho_i) \leq -\frac{\sum_{i=2}^{n-k}\rho_i}{n-k-1}\log_2\frac{\sum_{i=2}^{n-k}\rho_i}{n-k-1},$$

i.e.,

$$-\sum_{i=2}^{n-k}\rho_i\log_2\rho_i \leq -\sum_{i=2}^{n-k}\rho_i\log_2\frac{\sum_{i=2}^{n-k}\rho_i}{n-k-1} = -(1-\rho_1)\log_2\frac{1-\rho_1}{n-k-1},$$

with equality if and only if $\rho_2 = \cdots = \rho_{n-k}$. Therefore

$$s(G) \leq -\rho_1\log_2\rho_1 - (1-\rho_1)\log_2\frac{1-\rho_1}{n-k-1}$$

with equality if and only if $\lambda_2 = \cdots = \lambda_{n-k}$.

Let $g(x) = -x\log_2 x - (1-x)\log_2\frac{1-x}{n-k-1}$ for $0 < x \leq 1$. Obviously, $g'(x) = -\log_2\frac{(n-k-1)x}{1-x}$, which is negative for $\frac{1}{n-k} \leq x < 1$. Thus $g(x)$ is strictly decreasing for $\frac{1}{n-k} \leq x \leq 1$. By Lemma 2.1, $\lambda_1 \geq \Delta+1$. Note that $2m \leq (\Delta+1)(n-k)$, which is obvious if $k=1$, and follows by considering its components if $k \geq 2$. Then $\rho_1 = \frac{\lambda_1}{2m} \geq \frac{\Delta+1}{2m} \geq \frac{1}{n-k}$. Thus

$$s(G) \leq g(\rho_1) \leq g\left(\frac{\Delta+1}{2m}\right) = -\frac{\Delta+1}{2m}\log_2\frac{\Delta+1}{2m} - \left(1-\frac{\Delta+1}{2m}\right)\log_2\frac{1-\frac{\Delta+1}{2m}}{n-k-1}.$$

This proves (3.1).

Suppose that equality holds in (3.1). By the above argument, we have $\lambda_1 = \Delta+1$, $\lambda_2 = \cdots = \lambda_{n-k}$. Obviously, there is a component G_1 of G with maximum degree Δ. Since $\lambda_1 = \Delta+1$, we have by Lemma 2.1 that $\lambda_1 \geq \lambda_1(G_1) \geq \Delta+1 = \lambda_1$, and then $\lambda_1(G_1) = \Delta+1$, implying that $\Delta = |V(G_1)| - 1$. Thus $\overline{G_1} = K_1 \cup H$ for a graph H on Δ vertices. By Lemma 2.2, the Laplacian eigenvalues of $\overline{G_1}$ are $\underbrace{\Delta+1-\lambda_2, \ldots, \Delta+1-\lambda_2}_{\Delta-1 \text{ times}}, 0, 0$, and thus the Laplacian eigenvalues of H are $\underbrace{\Delta+1-\lambda_2, \ldots, \Delta+1-\lambda_2}_{\Delta-1 \text{ times}}, 0$. If $\Delta+1-\lambda_2 = 0$, then H is empty, and if $\Delta+1-\lambda_2 > 0$, then by Lemma 2.3, H is complete. Therefore $G_1 \cong S_{\Delta+1}$ or $G_1 \cong K_{\Delta+1}$.

Case 1. $G_1 \cong S_{\Delta+1}$ with $\Delta \geq 2$. Note that the Laplacian eigenvalues of $S_{\Delta+1}$ are $\Delta+1, \underbrace{1, \ldots, 1}_{\Delta-1 \text{ times}}, 0$. Then $\lambda_2 = \cdots = \lambda_{n-k} = 1$. Let $G_1' = G - V(G_1)$ when $G \neq G_1$. Then the largest Laplacian eigenvalue G_1' is at most 1. If G_1' is not an empty graph, then by

Lemma 2.1, its largest Laplacian eigenvalue is at least 2, a contradiction. Thus each component of G except G_1 (when $k > 1$) is trivial. Thus G_1 is the only nontrivial component of G. Therefore $G \cong S_{\Delta+1} \cup (k-1)K_1$ with $\Delta = n - k$.

Case 2. $G_1 \cong K_{\Delta+1}$. If $\Delta = 1$, then $G \cong mK_2 \cup (n-2m)K_1$ with $k = n - m$. Suppose that $\Delta \geq 2$. If G has another nontrivial component G_1' except G_1, then $\lambda_2 = \cdots = \lambda_{n-k} = \Delta + 1$, and by Lemma 2.3, the diameter of G_1' is 1, and thus $G_1' \cong K_{\Delta+1}$. Thus $G \cong aK_{\Delta+1} \cup (k-a)K_1$ for some positive integer $a = \frac{n-k}{\Delta}$ whether $\Delta = 1$ or $\Delta \geq 2$.

Combining Cases 1 and 2, $G \cong S_{\Delta+1} \cup (k-1)K_1$ with $\Delta = n-k$, or $G \cong aK_{\Delta+1} \cup (k-a)K_1$ for some positive integer $a = \frac{n-k}{\Delta}$.

Conversely, if $G \cong S_{n-k+1} \cup (k-1)K_1$, or $G \cong aK_{\Delta+1} \cup (k-a)K_1$ for some positive integer $a = \frac{n-k}{\Delta}$, then $\lambda_2 = \cdots = \lambda_{n-k}$, and for any nontrivial component of G, it has $\Delta + 1$ vertices and its maximum degree is Δ, and thus it is easily seen that equality holds in (3.1). □

In Theorem 3.1, we need to know the number of components, which is eliminated in the following theorem with a weaker but still useful upper bound.

Theorem 3.2. *Let G be a graph with $n \geq 3$ vertices, $m \geq 1$ edges and maximum degree Δ. Then*

$$s(G) \leq -\frac{\Delta+1}{2m}\log_2\frac{\Delta+1}{2m} - \left(1 - \frac{\Delta+1}{2m}\right)\log_2\frac{1-\frac{\Delta+1}{2m}}{n-2} \tag{3.2}$$

with equality if and only if $G \cong S_n$ or $G \cong K_n$.

Proof. Let k be the number of components of G. Note that $f(x) = \log_2 x$ is strictly increasing for $x \geq 0$. We have $\log_2\frac{1-\frac{\Delta+1}{2m}}{n-k-1} \geq \log_2\frac{1-\frac{\Delta+1}{2m}}{n-2}$, which is strict when $k > 1$. Thus, by Theorem 3.1, we have (3.2), and equality holds in (3.2) if and only if $G \cong S_n$ or $G \cong K_n$. □

Theorem 3.3. *Let G be a graph with m edges and non-increasing degree sequence $(d_1, \ldots, d_n)$, where $d_n \geq 1$. Then*

$$s(G) \leq \log_2(2m) - \frac{d_1+1}{2m}\log_2(d_1+1) - \sum_{i=2}^{n-1}\frac{d_i}{2m}\log_2 d_i - \frac{d_n-1}{2m}\log_2(d_n-1) \tag{3.3}$$

with equality if and only if $G \cong S_n$.

Proof. Let $f(x) = x\log_2 x$ for $x \geq 0$. Obviously, $f(x)$ is strictly convex. From [13, p. 64, C.1.a], $\sum_{i=1}^{n} f(x_i)$ is strictly Schur-convex. By Lemma 2.6, we have

$$\sum_{i=1}^{n}\lambda_i\log_2\lambda_i \geq (d_1+1)\log_2(d_1+1) + \sum_{i=2}^{n-1} d_i\log_2 d_i + (d_n-1)\log_2(d_n-1)$$

with equality if and only if $(\lambda_1, \ldots, \lambda_n) = (d_1+1, d_2, \ldots, d_{n-1}, d_n-1)$. Note that $\sum_{i=1}^{n}\lambda_i\log_2\lambda_i = 2m\log_2(2m) + 2m\sum_{i=1}^{n}\rho_i\log_2\rho_i$. Thus

$$2ms(G) \leq 2m\log_2(2m) - (d_1+1)\log_2(d_1+1) - \sum_{i=2}^{n-1} d_i\log_2 d_i - (d_n-1)\log_2(d_n-1),$$

from which (3.3) follows.

Suppose equality holds in (3.3). Then $(\lambda_1, \ldots, \lambda_n) = (d_1+1, d_2, \ldots, d_{n-1}, d_n-1)$, and thus $\lambda_{n-1} = d_{n-1} \geq 1$ (implying that G is connected) and $\lambda_1 = d_1 + 1$. Now by Lemma 2.1, $d_1 = n-1$. Thus $\overline{G} = K_1 \cup H$ for a graph H on $n-1$ vertices. By Lemma 2.2, the Laplacian eigenvalues of $\overline{G}$ are $n - d_{n-1}, \ldots, n - d_2, 0, 0$, and thus the Laplacian eigenvalues of H are $n - d_{n-1}, \ldots, n - d_2, 0$, implying that the Laplacian eigenvalues of $\overline{H}$ are $d_2 - 1, \ldots, d_{n-1} - 1, 0$. Obviously, the degree sequence of $\overline{H}$ is $(d_2 - 1, \ldots, d_n - 1)$. By Lemma 2.1, $\overline{H} = \overline{K_{n-1}}$. Thus $G \cong S_n$.

Conversely, the Laplacian eigenvalues of S_n are n, 1 (with multiplicity $n-2$) and 0. It is easily seen that equality holds in (3.3). □

Note that the upper bound is attained for K_n in Theorem 3.2 and is not attained in Theorem 3.3. Let G be the 5-vertex graph obtained from S_5 by adding two edges with one common vertex. Then $m = 6$, $n = 5$ and $(d_1, \ldots, d_5) = (4, 3, 2, 2, 1)$. For this graph, the upper bounds in Theorems 3.2 and 3.3 are respectively $\frac{5}{12}\log_2\frac{12}{5} + \frac{7}{12}\log_2\frac{36}{7} \approx 1.90443$ and $\log_2 12 - \frac{5}{12}\log_2 5 - \frac{1}{4}\log_2 3 - \frac{1}{3} \approx 1.887918$, and thus the upper bound in Theorem 3.3 is better than the one in Theorem 3.2. Therefore the upper bounds in Theorems 3.3 and 3.2 are incomparable in general.

In previous theorem we need to know the degree sequence. If only the two largest degrees are known, then we have the following result.

Theorem 3.4. *Let G be a graph with n vertices and $m \geq 1$ edges, where $n \geq 5$. Let d_1 and d_2 be the maximum degree and second maximum degree of G, respectively. Then*

$$s(G) \leq 1 + \frac{d_1+d_2+1}{2m} + \frac{2m-(d_1+d_2+1)}{2m}\log_2(n-3) \tag{3.4}$$

with equality if and only if $G \cong K_5$.

Proof. Note that $f(x) = -x\log_2 x$ for $x \geq 0$ is a strictly concave function. By Jensen's inequality, we have

$$-\sum_{i=3}^{n-1}\rho_i \log_2 \rho_i \leq -\left(\sum_{i=3}^{n-1}\rho_i\right)\log_2 \sum_{i=3}^{n-1}\frac{\rho_i}{n-3},$$

and thus

$$\begin{aligned} s(G) &\leq -\rho_1\log_2\rho_1 - \rho_2\log_2\rho_2 - \left(\sum_{i=3}^{n-1}\rho_i\right)\log_2\sum_{i=3}^{n-1}\frac{\rho_i}{n-3} \\ &= -\rho_1\log_2\rho_1 - \rho_2\log_2\rho_2 - (1-\rho_1-\rho_2)\log_2\frac{1-\rho_1-\rho_2}{n-3} \end{aligned}$$

with equality if and only if $\rho_3 = \cdots = \rho_{n-1}$. Similarly, by Jensen's inequality,

$$-\rho_1\log_2\rho_1 - \rho_2\log_2\rho_2 \leq -(\rho_1+\rho_2)\log_2\frac{\rho_1+\rho_2}{2}$$

with equality if and only if $\rho_1 = \rho_2$, and

$$-\frac{(\rho_1+\rho_2)\log_2(\rho_1+\rho_2)}{2} - \frac{(1-\rho_1-\rho_2)\log_2(1-\rho_1-\rho_2)}{2} \leq -\frac{1}{2}\log_2\frac{1}{2} = \frac{1}{2},$$

i.e.,

$$-(\rho_1+\rho_2)\log_2(\rho_1+\rho_2) - (1-\rho_1-\rho_2)\log_2(1-\rho_1-\rho_2) \leq 1$$

with equality if and only if $\rho_1+\rho_2 = 1-\rho_1-\rho_2$. Therefore

$$\begin{aligned} s(G) &\leq -(\rho_1+\rho_2)\log_2\frac{\rho_1+\rho_2}{2} - (1-\rho_1-\rho_2)\log_2\frac{1-\rho_1-\rho_2}{n-3} \\ &= -(\rho_1+\rho_2)(\log_2(\rho_1+\rho_2)-1) \\ &\quad -(1-\rho_1-\rho_2)(\log_2(1-\rho_1-\rho_2)-\log_2(n-3)) \\ &= -(\rho_1+\rho_2)\log_2(\rho_1+\rho_2) - (1-\rho_1-\rho_2)\log_2(1-\rho_1-\rho_2) \\ &\quad +(\rho_1+\rho_2) + (1-\rho_1-\rho_2)\log_2(n-3) \\ &\leq 1 + (\rho_1+\rho_2) + (1-\rho_1-\rho_2)\log_2(n-3). \end{aligned}$$

If $n = 5$, then $s(G) \leq 2$ with equality if and only if $\lambda_1 = \cdots = \lambda_4 = \frac{m}{2}$, which, by Lemma 2.3, is equivalently to the fact that $G \cong K_5$. The result for $n = 5$ follows.

Suppose that $n \geq 6$.

Let $g(x) = 1 + x + (1-x)\log_2(n-3)$. Then $g'(x) = 1 - \log_2(n-3) < 0$, and thus $g(x)$ is strictly decreasing. Now by Lemma 2.6, we have $\rho_1 + \rho_2 \geq \frac{d_1+d_2+1}{2m}$, and thus

$$\begin{aligned} s(G) &\leq g\left(\frac{d_1+d_2+1}{2m}\right) \\ &= 1 + \frac{d_1+d_2+1}{2m} + \left(1 - \frac{d_1+d_2+1}{2m}\right)\log_2(n-3), \end{aligned}$$

from which (3.4) follows.

Suppose that equality holds in (3.4). Then by the above argument, we have $\lambda_1 = \lambda_2 = \frac{m}{2}$, $\lambda_3 = \cdots = \lambda_{n-1} = \frac{m}{n-3}$, and $\lambda_1 + \lambda_2 = d_1 + d_2 + 1$. By Lemma 2.1, $d_1 + d_2 + 1 = \lambda_1 + \lambda_2 = 2\lambda_1 \geq 2d_1 + 2 \geq d_1 + d_2 + 2$, a contradiction. Thus, (3.4) is strict for $n \geq 6$. □

For S_n, the upper bound in Theorem 3.2 is better than the one in Theorem 3.4. For the graph obtained from S_6 and S_5 by adding an edge between a pendant vertex of S_6 and a pendant vertex of S_5, the upper bound in Theorem 3.4 is 3, which is better than the upper bound in Theorem 3.2, which is $\frac{3}{10}\log_2\frac{10}{3} + \frac{7}{10}\log_2\frac{7}{90} \approx 3.1002384$. Thus the upper bounds in Theorems 3.4 and 3.2 are incomparable in general.

Theorem 3.5. *Let G be a graph with n vertices, $m \ge 1$ edges and minimum degree δ. Suppose that $G \ncong K_n$. Then*

$$s(G) \le -\left(1-\frac{\delta}{2m}\right)\log_2 \frac{1-\frac{\delta}{2m}}{n-2} - \frac{\delta}{2m}\log_2 \frac{\delta}{2m} \tag{3.5}$$

with equality if and only if $G \cong K_{n-1} \cup K_1$ or $G \cong S_3$.

Proof. Since $f(x) = -x\log_2 x$ for $x \ge 0$ is a strictly concave function, we have by Jensen's inequality that

$$-\sum_{i=1}^{n-2} \rho_i \log_2 \rho_i \le -\left(\sum_{i=1}^{n-2}\rho_i\right)\log_2 \sum_{i=1}^{n-2}\frac{\rho_i}{n-2},$$

and thus

$$\begin{aligned} s(G) &\le -\left(\sum_{i=1}^{n-2}\rho_i\right)\log_2 \sum_{i=1}^{n-2}\frac{\rho_i}{n-2} - \rho_{n-1}\log_2\rho_{n-1} \\ &= -(1-\rho_{n-1})\log_2\frac{1-\rho_{n-1}}{n-2} - \rho_{n-1}\log_2\rho_{n-1} \end{aligned}$$

with equality if and only if $\rho_1 = \cdots = \rho_{n-2}$.

Suppose first that $\delta = 0$. Then $\rho_{n-1} = 0$, and thus $s(G) \le \log_2(n-2)$ with equality if and only if $\lambda_1 = \cdots = \lambda_{n-2}$. Now (3.5) follows and by Lemma 2.3, equality holds in (3.5) if and only if $G \cong K_{n-1} \cup K_1$.

Next suppose that $\delta > 0$.

Let $g(x) = -(1-x)\log_2 \frac{1-x}{n-2} - x\log_2 x$ for $0 < x < 1$. Obviously, $g'(x) = \log_2 \frac{1-x}{x(n-2)}$, which is positive for $0 < x \le \frac{1}{n-1}$. Thus $g(x)$ is strictly increasing for $0 < x \le \frac{1}{n-1}$. By Lemma 2.4, we have $\rho_{n-1} \le \frac{\delta}{2m} < \frac{1}{n-1}$, and thus $s(G) \le g\left(\frac{\delta}{2m}\right)$, from which (3.5) follows.

Suppose that equality holds in (3.5). By the above argument, $\lambda_1 = \cdots = \lambda_{n-2}$ and $\lambda_{n-1} = \delta$. By Lemma 2.2, the Laplacian eigenvalues of $\overline{G}$ are $n-\delta, n-\lambda_1, \ldots, n-\lambda_1, 0$. Let $\Delta(\overline{G})$ be the maximum degree of $\overline{G}$. If $\overline{G}$ is connected, then, since $\lambda_1(\overline{G}) = n-\delta = \Delta(\overline{G})+1$, we have by Lemma 2.1 that $\Delta(\overline{G}) = n-1$, implying that $\delta = 0$, which is impossible. Thus $\overline{G}$ is not connected. Then $n - \lambda_1 = 0$, implying that $\overline{G}$ has $n-1$ components, i.e., $\overline{G} \cong K_2 \cup (n-2)K_1$ with $n-\delta = 2$. Thus $\overline{G} \cong K_2 \cup K_1$, i.e., $G \cong S_3$.

Conversely, if $G \cong S_3$, then it is easy to see that (3.5) is an equality. □

From the graphs that attain the bounds, it is easily seen that the upper bound in Theorem 3.5 is incomparable with the ones in Theorems 3.2–3.4.

Let $K_{r,r}$ be the complete bipartite graph with size r for both color classes.

Theorem 3.6. *Let G be a bipartite graph with n vertices and $m \ge 1$ edges, where $n \ge 2$. Then*

$$s(G) \le -\frac{1}{m}\sqrt{\frac{Z}{n}}\log_2\frac{1}{m}\sqrt{\frac{Z}{n}} - \left(1-\frac{1}{m}\sqrt{\frac{Z}{n}}\right)\log_2\frac{1-\frac{1}{m}\sqrt{\frac{Z}{n}}}{n-2} \tag{3.6}$$

with equality if and only if $G \cong K_{n/2,n/2}$.

Proof. By similar argument as in the proof of Theorem 3.1, we have

$$s(G) \le g(\rho_1)$$

with equality if and only if $\rho_2 = \cdots = \rho_{n-1}$, where $g(x) = -x\log_2 x - (1-x)\log_2\frac{1-x}{n-2}$ is strictly decreasing for $x \ge \frac{1}{n-1}$. By Cauchy–Schwarz inequality, we have $Z \ge \frac{\left(\sum_{u\in V(G)} d_u\right)^2}{n} = \frac{4m^2}{n}$. Then by Lemma 2.5, we have $\rho_1 = \frac{\lambda_1}{2m} \ge \frac{1}{m}\sqrt{\frac{Z}{n}} \ge \frac{1}{n-1}$. Thus

$$s(G) \le g(\rho_1) \le g\left(\frac{1}{m}\sqrt{\frac{Z}{n}}\right),$$

from which (3.6) follows.

Suppose that equality holds in (3.6). By the above argument, $\lambda_2 = \cdots = \lambda_{n-1}$. If $\lambda_2 = \cdots = \lambda_{n-1} > 0$, then $n \ge 3$, G is connected, and by Lemmas 2.3 and 2.5, G is a regular complete bipartite graph, i.e., $G \cong K_{n/2,n/2}$. If $\lambda_2 = \cdots = \lambda_{n-1} = 0$, then $G = K_{1,1} \cup (n-2)K_1$, and by Lemma 2.5, n can only be 2, i.e., $G \cong K_{1,1}$.

Conversely, if $G \cong K_{n/2,n/2}$, then $\lambda_2 = \cdots = \lambda_{n-1}$. Since G is a bipartite regular graph, we have by Lemma 2.5 that $\lambda_1 = 2\sqrt{\frac{Z}{n}}$. Thus equality holds in (3.6). □

We remark that for bipartite graphs, the upper bound in Theorem 3.6 is incomparable with the ones in Theorems 3.2, 3.3 and 3.5.

Note the upper bound is attained in Theorem 3.6 by $K_{n/2,n/2}$, but it is not in Theorem 3.4. For the graph obtained from S_6 and S_5 by adding an edge between a pendant vertex of S_6 and a pendant vertex of S_5, the upper bound in Theorem 3.4 is 3, which is better than the upper bound in Theorem 3.6, which is $-\frac{1}{10}\sqrt{\frac{56}{11}}\log_2\frac{1}{10}\sqrt{\frac{56}{11}}-\left(1-\frac{1}{10}\sqrt{\frac{56}{11}}\right)\log_2\frac{1-\frac{1}{10}\sqrt{\frac{56}{11}}}{9}\approx 3.2250095$. Thus the upper bounds in Theorems 3.6 and 3.4 are incomparable in general.

4. Lower bounds and extremal graphs

In this section, we discuss lower bounds for the von Neumann entropy of a nonempty graph and determine the extremal graphs. First we give an alternative proof for (1.1) in the following theorem.

Theorem 4.1. *Let G be a graph with n vertices and $m \geq 1$ edges. Then we have (1.1) with equality if and only if $G \cong rK_s \cup (n-rs)K_1$, where some integers r and s with $r \geq 1$, $s \geq 2$, and $rs \leq n$.*

Proof. Let $f(x) = -\log_2 x$ for $x > 0$. Since $f''(x) = \frac{1}{x^2 \ln 2} > 0$, $f(x)$ is a strictly convex function. Note that $\sum_{i=1}^{n-1}\rho_i = 1$. By Jensen's inequality, we have

$$-\log_2\left(\sum_{i=1}^{n-1}\rho_i\cdot\rho_i\right)\leq-\sum_{i=1}^{n-1}\rho_i\log_2\rho_i,$$

i.e.,

$$s(G)\geq-\log_2\sum_{i=1}^{n-1}\rho_i^2$$

with equality if and only if all nonzero eigenvalues of $\sigma(G)$ are equal. Note that

$$\sum_{i=1}^{n-1}\rho_i^2=\mathrm{tr}(\sigma(G)^2)=\frac{2m+Z}{4m^2}.$$

Thus, (1.1) follows. Equality holds in (1.1) if and only if $\rho_1 = \cdots = \rho_k > 0$ and $\rho_{k+1} = 0$ for some positive integer k, which, by Lemma 2.3, is equivalent to the fact that all nontrivial components are complete with the same number of vertices, i.e., $G \cong rK_s \cup (n-rs)K_1$ for some integers r and s with $r \geq 1$, $s \geq 2$ and $rs \leq n$. □

Note that if G is a connected graph that achieves the equality in (1.1), then $G \cong K_n$.

Theorem 4.2. *Let G be a graph on n vertices with $m \geq 1$ edges and conjugate degree sequence $(d_1^*, \ldots, d_n^*)$. Then*

$$s(G)\geq\log_2(2m)-\frac{1}{2m}\sum_{i=1}^{n-1}d_i^*\log_2 d_i^* \tag{4.1}$$

with equality when G is connected if and only if G is isomorphic to a graph in $\Gamma^{(n)}$.

Proof. Let $f(x) = x\log_2 x$ for $x \geq 0$. Obviously, $f(x)$ is strictly convex. From [13, p. 64, C.1.a], $\sum_{i=1}^{n} f(x_i)$ is strictly Schur-convex. By Lemma 2.7, we have

$$\sum_{i=1}^{n-1}\lambda_i\log_2\lambda_i\leq\sum_{i=1}^{n-1}d_i^*\log_2 d_i^*$$

with equality if and only if $(\lambda_1, \ldots, \lambda_n) = (d_1^*, \ldots, d_n^*)$, which, by Lemma 2.8, is equivalent to the fact that G is isomorphic to a graph in $\Gamma^{(n)}$. Note that $\sum_{i=1}^{n}\lambda_i\log_2\lambda_i = 2m\log_2(2m) + 2m\sum_{i=1}^{n}\rho_i\log_2\rho_i$. Thus

$$2ms(G)\geq 2m\log_2(2m)-\sum_{i=1}^{n-1}d_i^*\log_2 d_i^*,$$

from which (4.1) follows and equality holds in (4.1) if and only if G is isomorphic to a graph in $\Gamma^{(n)}$. □

Note that, for $n \geq 3$, besides K_n, there are other graphs, say S_n, in $\Gamma^{(n)}$. For these graphs in $\Gamma^{(n)} \setminus \{K_n\}$, the bound in Theorem 4.2 is better than the one in (1.1). Let $G = K_{4,4}$. In notation in Theorem 4.2, $n = 8$, $m = 16$, $Z = 128$ and $(d_1^*, \ldots, d_8^*) = (8, 8, 8, 8, 0, 0, 0, 0)$. Then the lower bound in Theorem 4.2 is 2, which is worse than the lower bound in (1.1), which is $\log_2 6.4 \approx 2.67807$. Thus the upper bound in Theorem 4.2 and the early known one in (1.1) are incomparable in general.

5. Concluding remark

The density matrix of a graph was introduced to represent the quantum state of a graph, and the von Neumann entropy measures the 'mixedness' of this quantum state as a convex combination of several pure states. We obtain upper bounds and lower bounds (one was known) for the von Neumann entropy using degree information and gives characterizations for those graphs when each bound is attained. Examples show that any two upper bounds in Theorems 3.2–3.6 (or 3.1, 3.3–3.6) as well as the lower bounds Theorem 4.2 and (1.1) are incomparable in general.

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