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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,

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

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*

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