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Sharp Bounds on the Signless Laplacian Estrada Index of Graphs

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Abstract. Let G be a connected graph with n vertices and m edges. Let $q_1, q_2, \dots, q_n$ be the eigenvalues of the signless Laplacian matrix of G, where $q_1 \geq q_2 \geq \cdots \geq q_n$. The signless Laplacian Estrada index of G is defined as $SLEE(G) = \sum_{i=1}^{n} e^{q_i}$. In this paper, we present some sharp lower bounds for $SLEE(G)$ in terms of the k-degree and the first Zagreb index, respectively.

1. Introduction

Let $G = (V, E)$ be a simple connected undirected graph with $V = \{v_1, v_2, \dots, v_n\}$ and $|E(G)| = m$. Sometimes, we refer to G as an (n, m) graph. For $v_i \in V(G)$, $N_G(v_i)$ is the set of all neighbors of the vertex v_i in G and $d_G(v_i) = |N_G(v_i)|$. The average of G is defined as $\overline{d}(G) = \frac{1}{n}\sum_{i=1}^{n} d_G(v_i)$. For $v_i \in V(G)$, the number of walks of length k of G starting at v_i is denoted by $d_k(v_i)$, and also called k-degree of the vertex v_i (see [16]). Clearly, one has $d_0(v_i) = 1$, $d_1(v_i) = d_G(v_i)$ and $d_{k+1}(v_i) = \sum_{w \in N(v_i)} d_k(w)$. For two vertices v_i and v_j $(i \neq j)$, the distance between v_i and v_j is the number of edges in a shortest path joining v_i and v_j. The diameter of a graph, denoted by $\mathrm{diam}(G)$, is the maximum distance between any two vertices of G.

The first Zagreb index is one of the oldest and most used molecular structure-descriptor, defined as the sum of squares of the degrees of the vertices, i.e.,

$$M_1(G) = \sum_{i=1}^{n} d_G^2(v_i).$$

Zagreb index $M_1(G)$ was first introduced in [14] and the survey of properties of M_1 is given in [3], [4].

Let $A(G)$ be the adjacency matrix of G and $D(G) = \mathrm{diag}(d_1, d_2, \dots, d_n)$ be the diagonal matrix of vertex degrees. The Laplacian matrix of G is $L(G) = D(G) - A(G)$. Clearly, $L(G)$ is a real symmetric matrix. From this fact and Geršgorin's Theorem, it follows that its eigenvalues are nonnegative real numbers. The signless Laplacian matrix of G is $Q(G) = D(G) + A(G)$. Sometimes, $Q(G)$ is also called the unoriented Laplacian matrix of G (see [12], [18]). The matrix $Q(G)$ is symmetric and nonnegative, and, when G is connected, it is irreducible. The eigenvalues of an $n \times n$ matrix M are denoted by $\lambda_1(M), \lambda_2(M), \dots, \lambda_n(M)$ and assume that $\lambda_1(M) \geq \lambda_2(M) \geq \cdots \geq \lambda_n(M)$, while for a graph G, we will denote $\lambda_i := \lambda_i(L(G))$, $q_i := \lambda_i(Q(G))$ and

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$\mu_i := \lambda_i(A(G))$, $i = 1, 2, \ldots, n$. Research on signless Laplacian matrix has become popular recently (see [5]-[11]).

Some graph-spectrum-based invariants, put forward [10] and [13], respectively, are defined as

$$EE(G) = \textstyle\sum_{i=1}^{n} e^{\mu_i} \quad \text{and} \quad LEE(G) = \textstyle\sum_{i=1}^{n} e^{\lambda_i}.$$

EE was eventually called the Estrada index [2], *LEE* was called the Laplacian Estrada index, and for details on the theory of *EE* and *LEE* see the reviews [9], [17], [19] and [20]. Ayyaswamy *et al.* [1] defined the signless Laplacian Estrada index of a graph G, denoted by $SLEE(G)$, as

$$SLEE(G) = \sum_{i=1}^{n} e^{q_i}$$

and obtain some upper and lower bounds for it in terms of the number of vertices and number of edges. Although $SLEE(G) = LEE(G)$ for G is a bipartite graph, it is chemically interesting for the fullerenes, fluoranthenes and other non-alternant conjugated species, in which $SLEE$ and $LEE(G)$ differ.

In this paper, we present some lower bounds for $SLEE(G)$ in terms of the k-degree and the first Zagrab index, and characterize the equality cases, respectively.

2. Results

The following results will be useful in the sequel.

Lemma 2.1 [15]. *Let A be a nonnegative symmetric matrix and x be a unit vector of $\mathfrak{R}^n$. If $\rho(A) = x^T A x$, then $Ax = \rho(A)x$.*

Lemma 2.2 [6]. *Let G be a connected graph. If $Q(G)$ has exactly k distinct eigenvalues, then $diam(G) + 1 \le k$.*

In the following, we denote $M_k = \sum_{i=1}^{n} d_k^2(v_i)$, $N_k = \sum_{i=1}^{n} (d_1(v_i)d_k(v_i) + d_{k+1}(v_i))^2$ for $k \ge 1$. Then $M_1 = \sum_{i=1}^{n} d_1(v_i)^2$ is the first Zagreb index.

Lemma 2.3. *Let G be a connected graph with n vertices and k-degree sequence $d_k(v_1), d_k(v_2), \ldots, d_k(v_n)$. Then*

$$q_1(G) \ge \sqrt{\frac{N_k}{M_k}}, \tag{1}$$

with equality holds in (1) if and only if $Q^{k+2}(G)\mathbf{J} = q_1^2(G)Q^k(G)\mathbf{J}$.

Proof. Let $X = (x_1, x_2, ..., x_n)^T$ be the unit positive eigenvector of $Q(G)$ corresponding to $q_1(G)$. Take

$$C = \sqrt{\frac{1}{\sum_{i=1}^{n} d_k^2(v_i)}}\,(d_k(v_1), d_k(v_2), ..., d_k(v_n))^T.$$

Noting that C is a unit positive vector, and hence we have

$$q_1(G) = \sqrt{\rho\,(Q^2(G))} = \sqrt{X^T Q^2(G) X} \ge \sqrt{C^T Q^2(G) C}.$$

Since

$$\begin{aligned} & Q(G)C \\ = & \sqrt{\frac{1}{\sum\limits_{i=1}^{n} d_k^2(v_i)}}\left(d_1(v_1)d_k(v_1) + \sum_{j=1}^{n} a_{1j}d_k(v_j), \ldots, d_1(v_n)d_k(v_n) + \sum_{j=1}^{n} a_{nj}d_k(v_j)\right)^T \\ = & \sqrt{\frac{1}{\sum_{i=1}^{n} d_k^2(v_i)}}\,(d_1(v_1)d_k(v_1) + d_{k+1}(v_1), \ldots, d_1(v_n)d_k(v_n) + d_{k+1}(v_n))^T, \end{aligned}$$

we have

$$q_1(G) \geq \sqrt{C^T Q^2(G) C} = \sqrt{\frac{\sum_{i=1}^n (d_1(v_i)d_k(v_i) + d_{k+1}(v_i))^2}{\sum_{i=1}^n d_k^2(v_i)}}.$$

If the equality holds in (1), then

$$\rho\left(Q^2(G)\right) = C^T Q^2(G) C.$$

By Lemma 2.1, we have $\rho\left(Q^2(G)\right)C = Q^2(G)C$. Since $Q(G)$ is a nonnegative irreducible positive semidefinite matrix, all eigenvalues of $Q(G)$ are nonnegative. By Perron-Frobenius Theorem, the multiplicity of $\rho\left(Q(G)\right)$ is one. Since $\rho\left(Q^2(G)\right) = (\rho(Q(G))^2$, we have the multiplicity of $\rho\left(Q^2(G)\right)$ is one. Hence, if the equality holds, if and only if $C = X$ is the eigenvector of $Q^2(G)$ corresponding to the eigenvector $\rho\left(Q(G)\right)^2$, that is, if and only if $Q^{k+2}(G)\mathbf{J} = q_1^2(G)Q^k(G)\mathbf{J}$. ■

Remark 1. A known lower bound

$$q_1 \geq \frac{4m}{n} \tag{2}$$

was given in [5], where the equality holds if and only if G is a regular graph. Note that

$$\begin{aligned}
N_k M_{k-1} &= \sum_{i=1}^n (d_1(v_i)d_k(v_i) + d_{k+1}(v_i))^2 \sum_{i=1}^n d_{k-1}^2(v_i) \\
&\geq \left(\sum_{i=1}^n (d_1(v_i)d_{k-1}(v_i)d_k(v_i) + d_{k-1}(v_i)d_{k+1}(v_i))\right)^2 \\
&= \left(\sum_{i=1}^n d_1(v_i)d_{k-1}(v_i)d_k(v_i) + \sum_{i=1}^n d_{k-1}(v_i)\sum_{j=1}^n a_{ij}d_k(v_j)\right)^2 \\
&= \left(\sum_{i=1}^n d_1(v_i)d_{k-1}(v_i)d_k(v_i) + \sum_{j=1}^n d_k(v_j)\sum_{i=1}^n a_{ji}d_{k-1}(v_i)\right)^2 \\
&= \left(\sum_{i=1}^n d_1(v_i)d_{k-1}(v_i)d_k(v_i) + \sum_{i=1}^n d_k(v_i)\sum_{j=1}^n d_k(v_j)\right)^2 \\
&= \sum_{i=1}^n (d_1(v_i)d_{k-1}(v_i) + d_k(v_i))^2 \sum_{i=1}^n d_k^2(v_i) = N_{k-1}M_k
\end{aligned}$$

and equality holds if and only if all the $\frac{d_1(v_i)d_k(v_i)+d_{k+1}(v_i)}{d_{k-1}(v_i)}$ $(i = 1, 2, \ldots, n)$ are equal. Hence

$$q_1 \geq \sqrt{\frac{N_k}{M_k}} \geq \cdots \geq \sqrt{\frac{N_1}{M_1}} \geq \sqrt{\frac{4M_1}{n}} \geq \frac{4m}{n}$$

as $nN_1 = n\sum_{i=1}^n (d^2(v_i) + d_2(v_i))^2 \geq (\sum_{i=1}^n (d^2(v_i) + d_2(v_i)))^2 = (\sum_{i=1}^n d^2(v_i) + \sum_{i=1}^n d_2(v_i)))^2 = (2\sum_{i=1}^n d^2(v_i))^2 = 4M_1^2$ and $nM_1 = n\sum_{i=1}^n d^2(v_i) \geq (\sum_{i=1}^n d(v_i))^2 = 4m^2$. This shows that (1) is better than (2). ■

Remark 2. Another lower bound

$$q_1(G) \geq \frac{M_1}{m} \tag{3}$$

was given in [6], where the equality holds if and only if G is a regular graph or a bipartite semi-regular graph. Recall that (3) is better than (2). ■

Remark 3. Let G_1 and G_2 be the graph obtained from K_3 by attaching a pendant edge and three pendant edges to one vertex of K_3, respectively. For G_1, the bound (1) is 4.5 when $k = 1$ and the bound (3) is 3.8842, and so (1) is better than (3); and for G_2, the bound (1) is 6 when $k = 1$ and the bound (3) is 6.1779, and so (3) is better than (1). Hence, the bounds (1) and (3) are incomparable. ■

Lemma 2.4 [6]. *Let h be a nonnegative. Then (i, j)-entry of $A(G)^h$ is the number of walks of length h from v_i to v_j.*

In the following, we present our main results. The idea of the following proofs comes from [1] and [2].

Theorem 2.5. *If G is a connected (n, m) graph with the k-degree sequence $d_k(v_1), d_k(v_2), \ldots, d_k(v_n)$. Then*

$$SLEE(G) \geq e^{\sqrt{\frac{N_k}{M_k}}} + (n-1)e^{\left(2m-\sqrt{\frac{N_k}{M_k}}\right)/(n-1)} \tag{4}$$

with equality in (4) holds if and only if $G \cong K_n$.

Proof. First we note that if $G \cong K_n$, then $q_1 = 2n - 2$ and $q_2 = q_3 = \cdots = q_n = n - 2$, and then $SLEE(G) = e^{2n-2} + (n-1)e^{n-2}$. Also, we have $M_k = n(n-1)^{2k}, N_k = 4n(n-1)^{2k+2}$ by Lemma 2.4. Then $e^{\sqrt{\frac{N_k}{M_k}}} + (n-1)e^{\left(2m-\sqrt{\frac{N_k}{M_k}}\right)/(n-1)} = e^{2n-2} + (n-1)e^{n-2}$. Hence (4) holds.

Since $q_1 \geq q_2 \geq \cdots \geq q_n \geq 0$ and $\operatorname{tr}(Q(G)) = \sum_{i=1}^{n} q_i = 2m$, we have

$$\begin{aligned} SLEE(G) &= e^{q_1} + e^{q_2} + \cdots + e^{q_n} \\ &\geq e^{q_1} + (n-1)\left(e^{q_2+\cdots+e^{q_n}}\right)^{1/(n-1)} \\ &= e^{q_1} + (n-1)\left(e^{2m-q_1}\right)^{1/(n-1)}. \end{aligned} \tag{5}$$

Let $f(x) = e^x + (n-1)\left(e^{2m-x}\right)^{1/(n-1)}$ and it is easy to see that $f(x)$ is an increasing function when $x > 0$. By Lemma 2.2, we have

$$SLEE(G) \geq e^{\sqrt{\frac{N_k}{M_k}}} + (n-1)e^{\left(2m-\sqrt{\frac{N_k}{M_k}}\right)/(n-1)}.$$

If equality holds in (4), then equality must be taken in inequality (5). So, we have $q_2 = q_3 = \cdots = q_n$, and hence, by Lemma 2.3, $\operatorname{diam}(G) = 1$. Thus, $G \cong K_n$. ■

Now we give another lower bound on $SLEE(G)$ in terms of the Zagrab index M_1 of G.

Theorem 2.6. *If G is a connected (n, m) graph with the Zagrab index M_1. Then*

$$SLEE(G) \geq e^{\frac{M_1}{m}} + e^{\frac{4m}{n}-\frac{M_1}{m}} + (n-2)e^{\frac{2m}{n}} \tag{6}$$

with equality in (6) holds if and only if $G \cong K_{n/2,n/2}$.

Proof. Since $q_1 \geq q_2 \geq \cdots \geq q_n \geq 0$ and $\operatorname{tr}(Q(G)) = \sum_{i=1}^{n} q_i = 2m$, we have

$$\begin{aligned} SLEE(G) &= e^{q_1} + e^{q_2} + \cdots + e^{q_{n-1}} + e^{q_n} \\ &\geq e^{q_1} + e^{q_n} + (n-2)\left(e^{q_2+\cdots+e^{q_{n-1}}}\right)^{\frac{1}{n-2}} \\ &= e^{q_1} + e^{q_n} + (n-2)e^{\frac{2m-q_1-q_m}{n-2}}. \end{aligned} \tag{7}$$

Let $f(x, y) = e^x + e^y + (n-2)e^{\frac{2m-x-y}{n-2}}$, where $x > 0$ and $y \geq 0$. Then $f(x, y)$ has a minimum value $e^x + e^{4m/n-x} + (n-2)e^{\frac{2m-4m/n}{n-2}}$ at $x + y = 4m/n$ (see [1]). Note that $e^x + e^{4m/n-x} + (n-2)e^{\frac{2m-4m/n}{n-2}}$ is an increasing function for $x > 0$, and hence, by (2), we have

$$e^{q_1} + e^{4m/n-q_1} + (n-2)e^{\frac{2m-4m/n}{n-2}} \geq e^{\frac{M_1}{m}} + e^{\frac{4m}{n}-\frac{M_1}{m}} + (n-2)e^{\frac{2m-4m/n}{n-2}}. \tag{8}$$

Thus (6) holds.

If equality holds in (6), then the above inequalities would be equalities. From (3) and (7), we have that G is regular or bipartite semi-regular. From (8) and $\sum_{i=1}^{n} q_i = 2m$, we have $q_2 = \cdots = q_{n-1} = (2m-q_1-q_n)/(n-2)$. Since $q_1 + q_n = 4m/n$, $q_1 = 4m/n$, $q_n = 0$ and $q_2 = \cdots = q_{n-1} = 2m/n$. Hence $G \cong K_{n/2,n/2}$. ■

Remark 4. From Remark 2 and the proof of Theorem 2.6, we have the bound (6) is better that the bound (15) of [1]. ■

Next we establish a lower bound for $SLEE(G)$ in terms of n and m.

Theorem 2.7. *Let G be an (n, m)-graph. Then*

$$SLEE(G) > \sqrt{e^{\frac{8m}{n}} + 1 + (n^2 - 2)e^{\frac{4m}{n}}}. \tag{9}$$

Proof. Note that $\sum_{i=1}^{n} q_i = 2m$ and

$$SLEE(G)^2 = \sum_{i=1}^{n} e^{2q_i} + 2\sum_{i<j} e^{q_i}e^{q_j}. \tag{10}$$

By the arithmetic-geometric inequality, we have

$$\begin{aligned} 2\sum_{i<j} e^{q_i}e^{q_j} &\geq n(n-1)\left(\prod_{i<j} e^{q_i}e^{q_j}\right)^{\frac{2}{n(n-1)}} \qquad (11)\\ &= n(n-1)\left((\prod_{i=1}^{n} e^{q_i})^{n-1}\right)^{\frac{2}{n(n-1)}}\\ &= n(n-1)\left(e^{\sum_{i=1}^{n} q_i}\right)^{\frac{2}{n}} = n(n-1)e^{4m/n}. \end{aligned}$$

On the other hand, by an argument similar to the proof of Theorem 2.6, we have

$$\begin{aligned} \sum_{i=1}^{n} e^{2q_i} &\geq e^{2q_1} + e^{2q_n} + (n-2)\left(e^{2q_2+\cdots+2e^{q_{n-1}}}\right)^{\frac{1}{n-2}}\\ &= e^{2q_1} + e^{2q_n} + (n-2)e^{\frac{4m-2q_1-2q_m}{n-2}}\\ &\geq e^{2q_1} + e^{8m/n-2q_1} + (n-2)e^{\frac{4m}{n}}\\ &\geq e^{8m/n} + e^0 + (n-2)e^{\frac{4m}{n}} \qquad (12) \end{aligned}$$

and the equality in (12) holds if and only $G \cong K_{n/2,n/2}$. But if $G \cong K_{n/2,n/2}$, then the inequality (11) should be strict. Hence, by (10)

$$SLEE(G) > \sqrt{e^{\frac{8m}{n}} + 1 + (n^2 - 2)e^{\frac{4m}{n}}}.$$

■

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