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On Laplacian and Signless Laplacian Estrada Indices of Graphs

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Abstract

Let G be a graph with n vertices and $\mu_1, \ldots, \mu_n$ and $q_1, \ldots, q_n$ denote the Laplacian eigenvalues and signless Laplacian eigenvalues of G, respectively. The Laplacian Estrada index and signless Laplacian Estrada index of G is defined as $\mathrm{LEE}(G) = e^{\mu_1} + \cdots + e^{\mu_n}$ and $\mathrm{SLEE}(G) = e^{q_1} + \cdots + e^{q_n}$. We prove that for any graph G, $\mathrm{SLEE}(G) \geq \mathrm{LEE}(G)$, with equality if and only if G is bipartite. Also, we show that if G has m edges and t triangles, then $\mathrm{SLEE}(G) > n+3m+t+\frac{4m^2}{n}+\frac{4m^3}{3n^2}$ and $\mathrm{SLEE}(G) \geq \sqrt{n^2+16m^2+6mn+2nt+\frac{32m^3}{3n}}$.

1 Introduction

Throughout this paper we consider simple graphs, that is finite and undirected graphs without loops and multiple edges. If G is a graph with vertex set $\{1, \ldots, n\}$, the *adjacency matrix* of G is an $n \times n$ matrix $A = A(G) = [a_{ij}]$, where $a_{ij} = 1$ if there is an edge between the vertices i and j, and 0 otherwise. The *Laplacian matrix* of G is the matrix $L = L(G) = D - A$ where D is a diagonal matrix with $(d_1, \ldots, d_n)$ on the main diagonal in which d_i is the degree of the vertex i. The *signless Laplacian matrix* of G is the matrix $Q = Q(G) = D + A$. Since L and Q are real symmetric matrices, their eigenvalues are real numbers. We denote the Laplacian eigenvalues and signless Laplacian eigenvalues of G by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and $q_1 \geq q_2 \geq \cdots \geq q_n$, respectively. The Laplacian and signless Laplacian matrix are positive semi-definite matrix, so $\mu_i, q_i \geq 0$ and the multiplicity of 0 as an eigenvalue of L is equal to the number of connected components of G and the

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multiplicity of 0 as an eigenvalue of Q is equal to the number of bipartite connected components of G (see [7]). For details on Laplacian eigenvalues of graphs we refer the reader to [4, 17, 18] and for signless Laplacian see [4, 6, 7].

The *Estrada index* of G defined by E. Estrada [9, 10, 11] as

$$\mathrm{EE}(G) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. The Estrada index has already found a remarkable variety of applications. Initially it was used to quantify the degree of folding of long-chain molecules, especially proteins [9, 10, 11]; for this purpose the EE-values of pertinently constructed weighted graphs were employed. Another, fully unrelated, application of EE (of simple graphs) was proposed by Estrada and Rodríguez–Velázquez [13, 14]. They showed that EE provides a measure of the centrality of complex (communication, social, metabolic, etc.) networks. In addition to this, in [15] a connection between EE and the concept of extended atomic branching was considered. An application of the Estrada index in statistical thermodynamic has also been reported [12].

Mathematical properties of the Estrada index were studied in a number of recent works [5, 19]; for a survey see [8].

Similar to Estrada index, the *Laplacian Estrada index* of a graph G was introduced in [16] (see also [21]) as

$$\mathrm{LEE}(G) = \sum_{i=1}^{n} e^{\mu_i}. \tag{1}$$

Various properties of LEE were established in [16, 21].

The *signless Laplacian Estrada index* of a graph G was introduced in [1] as

$$\mathrm{SLEE}(G) = \sum_{i=1}^{n} e^{q_i}. \tag{2}$$

In this paper we show that for any graph, SLEE is always greater than or qual to LEE. Moreover, we find two lower bounds for the SLEE of a graph in terms of its number of vertices, the number of edges and the number of triangles.

2 Laplacian Estrada index vs. signless Laplacian Estrada index

In this section, we prove that for any graph G, $\mathrm{SLEE}(G) \geq \mathrm{LEE}(G)$.

We consider the Laplacian and signless Laplacian spectral moments of graphs G which are

$$\sum_{i=1}^{n} \mu_i^k = \mathrm{tr}(L^k), \quad \sum_{i=1}^{n} q_i^k = \mathrm{tr}(Q^k).$$

By the the Taylor expansion of the exponential function e^x, we have

$$\mathrm{LEE}(G) = \sum_{k=0}^{\infty} \frac{\mathrm{tr}(L^k)}{k!}, \tag{3}$$

$$\mathrm{SLEE}(G) = \sum_{k=0}^{\infty} \frac{\mathrm{tr}(Q^k)}{k!}. \tag{4}$$

We need the following well-known result (see [6, 7]).

Lemma 1. *For any graph G, $L(G)$ and $Q(G)$ are similar (have the same eigenvalues) if and only if G is bipartite.*

We know that a graph G is non-bipartite if and only if there exists some closed walk of odd length in G. Also the number of closed walks of length k in G is equal to $\mathrm{tr}(A^k)$ (see [4]). So we have the following lemma.

Lemma 2. *A graph G is non-bipartite if and only if there exits some odd integer s such that* $\mathrm{tr}(A^s) > 0$.

Theorem 1. *For any graph G,*

$$\mathrm{SLEE}(G) \geq \mathrm{LEE}(G),$$

equality holds if and only if G is bipartite.

Proof. The terms appearing in the expansion of $(D + A)^k$ are the same as those in the expansion of $(D - A)^k$, the only difference is that all the signs of the terms in the expansion of $(D + A)^k$ are positive, but some of the terms in the expansion of $(D - A)^k$ have negative signs. Since D and A are matrices with non-negative entries, for any $k \geq 0$ we have

$$\mathrm{tr}(Q^k) = \mathrm{tr}\left((D + A)^k\right) \geq \mathrm{tr}\left((D - A)^k\right) = \mathrm{tr}(L^k).$$

Therefore,

$$\mathrm{SLEE}(G)=\sum_{k=0}^{\infty}\frac{\mathrm{tr}(Q^k)}{k!}\geq\sum_{k=0}^{\infty}\frac{\mathrm{tr}(L^k)}{k!}=\mathrm{LEE}(G).$$

If G is bipartite, then by Lemma 1, L and Q are similar and so $\mathrm{SLEE}(G)=\mathrm{LEE}(G)$. If G is not bipartite, by Lemma 2, there is an odd integer s such that $\mathrm{tr}(A^s)>0$. Hence,

$$\mathrm{tr}(Q^s)=\mathrm{tr}\left((D+A)^s\right)=\mathrm{tr}(D^s)+\cdots+\mathrm{tr}(A^s)>\mathrm{tr}(D^s)+\cdots-\mathrm{tr}(A^s)=\mathrm{tr}\left((D-A)^s\right)=\mathrm{tr}(L^s).$$

Therefore, by (3) and (4), $\mathrm{SLEE}(G)>\mathrm{LEE}(G)$. □

3 Lower bounds for signless Laplacian Estrada index

In this section we obtain two lower bounds for the $\mathrm{SLEE}(G)$ in terms of the number of vertices, the number of edges and the number of triangles of G.

We recall Holder inequality. Let $a_1,\ldots,a_n,b_1,\ldots,b_n$ be non-negative real numbers, $p,q>1$ and $\frac{1}{p}+\frac{1}{q}=1$. Then

$$\sum_{i=1}^{n}a_ib_i\leq\left(\sum_{i=1}^{n}a_i^p\right)^{\frac{1}{p}}\left(\sum_{i=1}^{n}b_i^q\right)^{\frac{1}{q}}.$$

Lemma 3. *(See [6, 7]) Let G be graph with n vertices, m edges, t triangles and degree sequence $d_1,\ldots,d_n$. Then*

$$\mathrm{tr}(Q)=2m, \tag{5}$$

$$\mathrm{tr}(Q^2)=2m+\sum_{i=1}^{n}d_i^2, \tag{6}$$

$$\mathrm{tr}(Q^3)=6t+3\sum_{i=1}^{n}d_i^2+\sum_{i=1}^{n}d_i^3. \tag{7}$$

Theorem 2. *Let G be graph with n vertices, $m\geq 1$ edges and t triangles. Then*

$$\mathrm{SLEE}(G)>n+3m+t+\frac{4m^2}{n}+\frac{4m^3}{3n^2}.$$

Proof. Let $d_1,\ldots,d_n$ be the degree sequence of G. Since $m\geq 1$, for all k, $\mathrm{tr}(Q^k)>0$, so by (4),

$$\mathrm{SLEE}(G)>n+\mathrm{tr}(Q)+\frac{\mathrm{tr}(Q^2)}{2}+\frac{\mathrm{tr}(Q^3)}{6}. \tag{8}$$

By Holder inequality for $p = q = 2$, we have $2m = \sum_{i=1}^{n} d_i \leq \sqrt{n}\,(\sum_{i=1}^{n} d_i^2)^{\frac{1}{2}}$. Hence,

$$\sum_{i=1}^{n} d_i^2 \geq \frac{4m^2}{n}. \tag{9}$$

Again, by Holder inequality for $p = 3$ and $q = \frac{3}{2}$, we have $2m = \sum_{i=1}^{n} d_i \leq n^{\frac{2}{3}}\,(\sum_{i=1}^{n} d_i^3)^{\frac{1}{3}}$. Hence,

$$\sum_{i=1}^{n} d_i^3 \geq \frac{8m^3}{n^2}. \tag{10}$$

By (8), (9), (10) and Lemma 3 we have

$$\begin{aligned}\mathrm{SLEE}(G) &\geq n + 2m + \frac{1}{2}\left(2m + \frac{4m^2}{n}\right) + \frac{1}{6}\left(6t + 3\frac{4m^2}{n} + \frac{8m^3}{n^2}\right)\\ &= n + 3m + t + \frac{4m^2}{n} + \frac{4m^3}{3n^2}.\end{aligned}$$

□

For a graph with signless Laplacian eigenvalues $q_1, q_2, \ldots, q_n$, with m edges and t triangles, from the above proof we see that

$$\sum_{i=1}^{n} q_i^2 \geq 2m + \frac{4m^2}{n}, \tag{11}$$

$$\sum_{i=1}^{n} q_i^3 \geq 6t + \frac{12m^2}{n} + \frac{8m^3}{n^2}. \tag{12}$$

By the Taylor's theorem, for any real $x \neq 0$, there is a real η between x and 0 such that $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + e^{\eta}\frac{x^4}{4!}$. So we have the following.

Lemma 4. *For any real $x \neq 0$, one has $e^x > 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}$.*

Theorem 3. *Let G be graph with n vertices, m edges and t triangles. Then*

$$\mathrm{SLEE}(G) > \sqrt{n^2 + 16m^2 + 6mn + 2nt + \frac{32m^3}{3n}}.$$

Proof. Suppose that $q_1, q_2, \ldots, q_n$ are the signless Laplacian eigenvalues of G. Using Lemma 4 we have

$$\begin{aligned}\mathrm{SLEE}(G)^2 &= \sum_{i=1}^{n}\sum_{j=1}^{n} e^{q_i+q_j}\\ &> \sum_{i=1}^{n}\sum_{j=1}^{n}\left(1 + q_i + q_j + \frac{(q_i+q_j)^2}{2} + \frac{(q_i+q_j)^3}{6}\right)\\ &= \sum_{i=1}^{n}\sum_{j=1}^{n}\left(1 + q_i + q_j + q_i^2/2 + q_j^2/2 + q_iq_j + q_i^3/6 + q_j^3/6 + q_i^2q_j/2 + q_iq_j^2/2\right).\end{aligned}$$

Now, by (5),

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(q_i+q_j) = n\sum_{i=1}^{n} q_i + n\sum_{j=1}^{n} q_j = 4mn,$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} q_i q_j = \left(\sum_{i=1}^{n} q_i\right)^2 = 4m^2.$$

By (11),

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(q_i^2/2+q_j^2/2) = \frac{n}{2}\sum_{i=1}^{n} q_i^2 + \frac{n}{2}\sum_{j=1}^{n} q_j^2 \geq 2mn+4m^2,$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(q_i^2 q_j/2+q_i q_j^2/2) = \frac{1}{2}\sum_{i=1}^{n} q_i^2 \cdot \sum_{j=1}^{n} q_j + \frac{1}{2}\sum_{i=1}^{n} q_i \cdot \sum_{j=1}^{n} q_j^2 \geq 4m^2+\frac{8m^3}{n}.$$

Similarly by (12),

$$\sum_{i=1}^{n}\sum_{j=1}^{n}(q_i^3/6+q_j^3/6) \geq 2nt+4m^2+\frac{8m^3}{3n}.$$

Combining the above relations, we have

$$\begin{aligned}\mathrm{SLEE}(G)^2 &> n^2+4mn+4m^2+2mn+4m^2+4m^2+\frac{8m^3}{n}+2nt+4m^2+\frac{8m^3}{3n}\\ &= n^2+16m^2+6mn+2nt+\frac{32m^3}{3n}.\end{aligned}$$

□

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