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Signless Laplacian Estrada Index

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Abstract

Let G be a simple (n,m)-graph. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ and $q_1, q_2, \ldots, q_n$ be, respectively, the eigenvalues of the adjacency matrix, and the signless Laplacian matrix of G. The Estrada index of the graph G is $\sum_{i=1}^{n} e^{\lambda_i}$. We define and investigate the signless Laplacian Estrada index, $\sum_{i=1}^{n} e^{q_i}$ and establish lower and upper bounds for it in terms of the number of vertices and number of edges.

1 Introduction

Let G be a simple graph with n vertices and m edges. Such a graph will be referred to as an (n,m)-graph. The eigenvalues of G are the eigenvalues of the adjacency matrix $\mathbf{A}(G)$ of G, and will be denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The Laplacian matrix of G is $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$, where $\mathbf{D}(G) = diag(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees of G. Its eigenvalues are denoted by $\mu_1, \mu_2, \ldots, \mu_n$. The matrix $\mathbf{L}^+(G) = \mathbf{D}(G) + \mathbf{A}(G)$ is called the signless Laplacian matrix of G, and its eigenvalues will be denoted by $q_1, q_2, \ldots, q_n$.

The basic properties of the graph eigenvalues can be found in the books [5, 8], whereas the elements of the Laplacian spectral graph theory in the reviews [19,20,32, 33]. Studies of the spectral properties of the matrix $\mathbf{L}^+(G)$ started only a few years ago, but already a large number of results has been obtained [1,4,6,7,9,10,27,35,37].

A graph–spectrum–based invariant, recently put forward [17], is defined as

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

and was eventually named [11] the *Estrada index*. For details on the theory of the Estrada index see the reviews [14, 21], the recent papers [3, 12, 13, 30, 34, 38] and the references cited therein.

The Laplacian–spectral counterpart of the Estrada index was defined in full analogy with Eq. (1) as [18]

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

and independently as [31]

$$LEE_{LSC}(G) = \sum_{i=1}^{n} e^{(\mu_i - 2m/n)} \ .$$

These two definitions are, of course, essentially equivalent, since $LEE_{LSC} = e^{-2m/n} \times LEE$. For details on the theory of the Laplacian Estrada index see the recent papers [3, 15, 29, 39, 40] and the references cited therein.

We now define the signless Laplacian Estrada index as

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

Remark 1. $SLEE$ and LEE coincide in the case of bipartite graphs. This is an immediate consequence of the well known fact [19,20] that the Laplacian and signless Laplacian spectra of bipartite graphs coincide. Since the vast majority of molecular graphs are bipartite, for them $SLEE$ gives nothing new relative to the previously studied LEE. Chemically interesting case in which $SLEE$ and LEE differ are the fullerenes, fluoranthenes and other non-alternant conjugated species [2, 16, 22–24].

2 $(\mathbf{n}, \mathbf{m})$-Type estimates of the signless Laplacian Estrada index of general graphs

Theorem: 1. *Let G be an (n,m)-graph. Then the signless Laplacian Estrada index of G is bounded as*

$$\sqrt{n+4m+n(n-1)\,e^{4m/n}} \leq SLEE(G) \leq n-1+e^{\sqrt{(n^2-n+2m)m}}\ . \tag{3}$$

Equality on both sides of (3) is attained if and only if $G \cong \overline{K}_n$.

Proof: Denoting $\sum\limits_{i=1}^{n} q_i^k$ by $T_k = T_k(G)$, and bearing in mind the power–series expansion of e^x , we have

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

In the proof of Theorem 1 and of the subsequent estimates we shall frequently use the following results for the first few moments of the signless Laplacian spectrum of an (n,m)-graph [6]:

$$T_0 = n \quad ; \quad T_1 = 2m \quad ; \quad T_2 = 2m + \sum_{i=1}^{n} d_i^2\ . \tag{5}$$

Lower bound.

The considerations that follow emulate the proof technique used in Ref. [11]. Directly from the definition of the signless Laplacian Estrada index, Eq.(2), we get

$$SLEE(G)^2 = \sum_{i=1}^{n} e^{2q_i} + 2\sum_{i<j} e^{q_i} e^{q_j}\ . \tag{6}$$

In view of the inequality between the arithmetic and geometric means,

$$\begin{aligned} 2\sum_{i<j} e^{q_i}\, e^{q_j} \ &\geq\ n(n-1)\left(\prod_{i<j} e^{q_i} e^{q_j}\right)^{\frac{2}{n(n-1)}} = n(n-1)\left[\left(\prod_{i=1}^{n} e^{q_i}\right)^{n-1}\right]^{\frac{2}{n(n-1)}} \\ &=\ n(n-1)\left(e^{T_1}\right)^{2/n} = n(n-1)\,e^{4m/n}\ . \end{aligned} \tag{7}$$

By means of a power series expansion, and bearing in mind the properties of T_0 , T_1 , and T_2 , we get

$$\sum_{i=1}^{n} e^{2q_i} = \sum_{i=1}^{n}\sum_{k\geq 0} \frac{(2q_i)^k}{k!} = n + 4m + \sum_{i=1}^{n}\sum_{k\geq 2} \frac{(2q_i)^k}{k!}\ .$$

We use a multiplier $\gamma \in [0,4]$, so as to arrive at

$$\begin{aligned}\sum_{i=1}^{n} e^{2q_i} &\geq n+4m+\gamma\sum_{i=1}^{n}\sum_{k\geq 2}\frac{(q_i)^k}{k!}\\ &= n+4m-\gamma n-2m\gamma+\gamma\sum_{i=1}^{n}\sum_{k\geq 0}\frac{q_i^k}{k!}\end{aligned}$$

which implies

$$\sum_{i=1}^{n} e^{2q_i} \geq (1-\gamma)n+(4-2\lambda)m+\gamma\, SLEE\ . \tag{8}$$

By substituting (7) and (8) back into (6), and solving for $SLEE$ we obtain

$$SLEE \geq \frac{\gamma}{2}+\sqrt{\frac{\gamma^2}{4}+n(1-\gamma)+(4-2\gamma)m+n(n-1)\,e^{4m/n}}\ . \tag{9}$$

It is elementary to show for $n \geq 2$, the function

$$f(x) \geq \frac{x}{2}+\sqrt{\frac{x^2}{4}+n(1-x)+(4-2x)m+n(n-1)\,e^{4m/n}}$$

monotonically decreases in the interval $[0,4]$. Consequently, the best lower bound for SLEE is attained for $\gamma=0$. Setting $\gamma=0$ in (9), we arrive at the first half of Theorem 1.

Upper bound.

Starting with equation (4), we get

$$\begin{aligned}SLEE &= n+\sum_{i=1}^{n}\sum_{k\geq 1}\frac{(q_i)^k}{k!} = n+\sum_{k\geq 1}\frac{1}{k!}\sum_{i=1}^{n}[(q_i)^2]^{k/2}\\ &= n+\sum_{k\geq 1}\frac{1}{k!}(T_2^{k/2}) = n+\sum_{k\geq 1}\frac{1}{k!}\left(2m+\sum_{i=1}^{n}d_i^2\right)^{k/2}\\ &= n+\sum_{k\geq 1}\frac{1}{k!}\left[2m+m\left(\frac{2m}{n-1}+n-2\right)\right]^{k/2}\\ &= n-1+\sum_{k\geq 0}\frac{1}{k!}[(n^2-n+2m)m]^{k/2}\\ &= n-1+\sum_{k\geq 0}e^{\sqrt{(n^2-n+2m)m}}\end{aligned}$$

which leads to the right hand side inequality in (3). ■

Remark 2. The expressions for the first spectral moments of the Laplacian eigenvalues are exactly same as those stated in Eq. (5). Therefore, any result for $SLEE$, based on Eq. (5), will automatically hold also for LEE. However, in the case of Laplacian Estrada index one may use the additional condition $\mu_n = 0$ (which has no counterpart in the case of signless Laplacian eigenvalues). With this additional condition, bounds for LEE can be deduced that are better than those reported in this paper.

3 Lower bound on the signless Laplacian Estrada index of graphs

In this section we establish another lower bound on the signless Laplacian Estrada index. A lower bound on the spectral radius in terms of chromatic number k is given by the following:

Lemma: 1. [36] *Let G be simple graph with chromatic number k. Then*

$$\lambda_1 \geq k - 1 \; . \tag{10}$$

For a connected graph G, $\lambda_1 = k - 1$ if and only if $G \cong K_n$ or G is the cycle C_n of odd length.

The next result gives a relationship between the largest eigenvalue of the adjacency matrix and of the signless Laplacian matrix.

Lemma: 2. [7] *Let G be graph on n vertices. Then $2\lambda_1 \leq q_1$. Equality holds if and only if G is regular.*

Combining Lemmas 1 and 2 we arrive at:

Lemma: 3. *Let G be a graph on n vertices. Then $q_1 \geq 2(k-1)$. Equality holds if and only if $G \cong K_n$ or G is the cycle C_n of odd length.*

Theorem: 2. *Let G be simple connected (n,m)-graph with chromatic number k. Then*

$$SLEE(G) \geq e^{2(k-1)} + (n-1)\, e^{-[2(k-1)-2m]/(n-1)} \; . \tag{11}$$

Equality in (11) holds if and only if $G \cong K_n$.

Proof: Since G is connected, $q_1 \geq 0$. Then by the arithmetic–geometric–mean inequality,

$$SLEE(G) = e^{q_1} + e^{q_2} + \cdots + e^{q_n} \geq e^{q_1} + (n-1)\left(\prod_{i=2}^{n} e^{q_i}\right)^{1/(n-1)} \tag{12}$$

which in view of $\sum_{i=1}^{n} q_i = 2m$ implies

$$SLEE(G) \geq e^{q_1} + (n-1)(e^{2m-q_1})^{1/(n-1)} . \tag{13}$$

Consider the function $f(x) = e^x + (n-1)\, e^{-(x-2m)/(n-1)}$. Since for $x > 0$ $f'(x) = e^x - e^{(2m-x)/(n-1)} > 0$, this is a monotonically increasing function for $x > 0$. From (10) and (13) we arrive at (11).

Suppose now that equality holds in (11). Then equality must hold also in (12) and (13). From equality in (12) and by the arithmetic–geometric–mean inequality, we get $q_2 = q_3 = q_4 = \cdots = q_n$. From equality in (11), we get $q_1 = 2(k-1)$. Since $q_2 = q_3 = q_4 = \cdots = q_n$ and $q_1 = 2(k-1)$, by Lemma 3, $G \cong K_n$.

Conversely, one can easily see that equality in (11) holds for the complete graph K_n. ■

A lower bound on the signless Laplacian spectral radius in terms of n and m of a connected graph G is the following:

Lemma: 4. [6] *Let G be a connected (n,m)-graph. Then*

$$q_1 \geq \frac{4m}{n} \tag{14}$$

with equality if and only if G is a regular graph.

Theorem: 3. *Let G be a simple connected (n,m)-graph. Then*

$$SLEE(G) \geq e^{4m/n} + (n-2)\, e^{2m/n} + 1 . \tag{15}$$

Equality holds in (15) if and only if $G \cong K_{p,p}$.

Proof: Since G is connected, $q_1 > 0$ and $q_n \geq 0$. Then,

$$\begin{aligned} SLEE(G) &= e^{q_1} + e^{q_2} + \cdots + e^{q_n} \\ &\geq e^{q_1} + e^{q_n} + (n-2)\left(\prod_{i=2}^{n-1} e^{q_i}\right)^{1/(n-2)} \qquad (16) \\ &= e^{q_1} + e^{q_n} + (n-2)\, e^{(2m-q_1-q_n)/(n-2)} \end{aligned}$$

as $\sum_{i=1}^{n} q_i = 2m$.

Now we consider the function $f(x,y) = e^x + e^y + (n-2)\, e^{(2m-x-y)/(n-2)}$, for $x > 0$, $y \geq 0$. In order to find its minimum we calculate

$$\begin{aligned}
f_x &= e^x - e^{(2m-x-y)/(n-2)} \\
f_y &= e^y - e^{(2m-x-y)/(n-2)} \\
f_{xx} &= e^x + \frac{1}{n-2}\, e^{(2m-x-y)/(n-2)} \\
f_{xy} &= f_{yx} = \frac{1}{n-2}\, e^{(2m-x-y)/(n-2)} \\
f_{yy} &= e^y + \frac{1}{n-2}\, e^{(2m-x-y)/(n-2)} \; .
\end{aligned}$$

We further have

$$f_x = f_y = 0 \;\Rightarrow\; (n-1)x + y = 2m$$

and

$$x + (n-1)y = 2m \;\Rightarrow\; x + y = \frac{4m}{n} \; .$$

For $x + y = 4m/n$, it is $f_{xx} > 0$ and

$$f_{xx}\, f_{yy} - f_{xy}^2 = e^{4m/n} + \frac{1}{n-2}\, e^{2m/n} \left[e^x + e^{4m/n-x} \right] > 0 \; .$$

From the above, we conclude that $f(x,y)$ has a minimum value at $x + y = 4m/n$ and that the minimum value is $e^x + e^{4m/n-x} + (n-2)\, e^{(2m-4m/n)/(n-2)}$. Therefore, $e^x + e^{4m/n-x} + (n-2)\, e^{(2m-4m/n)/(n-2)}$ is an increasing function for $x > 0$. By Lemma 4, $q_1 \geq 4m/n$. Thus,

$$\begin{aligned}
& e^{q_1} + e^{4m/n-q_1} + (n-2)\, e^{(2m-4m/n)/(n-2)} \\
\geq\; & e^{4m/n} + e^{(4m/n)-(4m/n)} + (n-2)\, e^{(2m-4m/n)/(n-2)} \; . \qquad (17)
\end{aligned}$$

Inequality (15) follows.

Suppose now that equality holds in (15). Then all inequalities in the above argument must be equalities. From equality in (17) and Lemma 4, we get that G is regular.

From equality in (16) and $\sum_{i=1}^{n} q_i = 2m$, we get $q_2 = q_3 = q_4 = \cdots = q_{n-1} = 2m/n$ as $q_1 + q_n = 4m/n$. Thus, $q_1 = 4m/n$, $q_n = 0$, $q_2 = q_3 = q_4 = \cdots = q_{n-1} = 2m/n$. Hence G is the complete bipartite graph $K_{p,p}$, where $n = 2p$. Conversely, one can easily see that equality holds in (15) for the complete bipartite graph $K_{p,p}$. This completes the proof. ■

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