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Note on the Laplacian Estrada Index of a Graph*

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Abstract

Let G be a simple graph of order n with m edges. The Laplacian Estrada index of G is defined as $LEE = LEE(G) = \sum_{i=1}^{n} e^{(\mu_i - 2m/n)}$, where $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of G. In this note, we present two sharp lower bounds for LEE and characterize the graphs for which the bounds are attained.

1 Introduction

Let $G = (V, E)$ be a simple graph. Let n and m be the number of vertices and edges of G, respectively. Such a graph will be referred to as an (n, m)-*graph*.

Let $A(G)$ be the adjacency matrix of G and $D(G)$ be the diagonal matrix with degrees of the corresponding vertices of G on the main diagonal and zero elsewhere. The matrix $L(G) = D(G) - A(G)$ is called the *Laplacian matrix* of G. Since $A(G)$ and $L(G)$ are real symmetric matrices, their eigenvalues are real numbers. So, we can assume that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$, and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ are the adjacency eigenvalues and the Laplacian eigenvalues of G, respectively. The multiset of eigenvalues of $A(G)$ $(L(G))$ is called the *adjacency (Laplacian) spectrum* of G.

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The *Estrada index* of the graph G was defined in [3] as:

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i} . \tag{1.1}$$

Motivated by its chemical applications proposed by Ernesto Estrada [7], the mathematical properties of the Estrada index have been studied in a number of recent works [1,3–5,13,15–18], for details see the review [11].

In analogy with Eq. (1.1), the *Laplacian Estrada index* of a graph G was defined in [14] as:

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i - 2m/n} . \tag{1.2}$$

Independently of [14], another variant of the Laplacian Estrada index was put forward in [8], defined as

$$LEE_{[8]}(G) = \sum_{i=1}^{n} e^{\mu_i}. \tag{1.3}$$

Evidently, $LEE_{[8]}(G) = e^{2m/n}\, LEE(G)$, and therefore results obtained for LEE can be immediately re-stated for $LEE_{[8]}$ and vice versa.

Some basic properties of the Laplacian Estrada index were determined in the papers [6,8,12,14,19,20]. In particular, the appropriate relations between the Laplacian Estrada index and the Laplacian energy, the first Zagreb index, the Estrada index of the graph and the Estrada index of its line graph were established in [8,14,20]. So, it is significant and necessary to further investigate the relation between the Laplacian Estrada index of a graph and its graph-theoretic properties.

In this note, we present two lower bounds for the Laplacian Estrada index of a graph in terms of its maximum degree and characterize the graphs for which the bounds are attained.

2 Preliminaries

For any $e \in E(G)$, we use $G - e$ to denote the graph obtained by deleting e from G. Let $\overline{G}$ be the complement of the graph G. The vertex-disjoint union of the graphs G_1 and G_2 is denoted by $G_1 \cup G_2$. Let $G_1 \vee G_2$, the join graph of G_1 and G_2, be the graph obtained from $G_1 \cup G_2$ by adding all possible edges from vertices of G_1 to vertices of G_2, i. e., $G_1 \vee G_2 = \overline{\overline{G_1} \cup \overline{G_2}}$. The following result describes the relation between the Laplacian spectrum of G and the Laplacian spectrum of its complement $\overline{G}$.

Proposition 2.1. (**[9, p.280]**) *Let G be a graph of order n. Then $\mu_i(G) = n - \mu_{n-i}(\overline{G})$ for $1 \le i \le n-1$.*

Let K_n, S_n and $K_{a,b}$ $(a+b=n)$ be the complete graph, the star, and the complete bipartite graph, of order n, respectively. The maximum degree of G is denoted by Δ. The lower bound on the Laplacian spectral radius of G in terms of its maximum degree was described as follows.

Lemma 2.2 ([10]). *Let G be a graph containing at least one edge. Then $\mu_1(G) \ge \Delta + 1$. Moreover, if G is connected of order $n > 1$, then the equality holds if and only if $\Delta = n-1$.*

Lemma 2.3 ([2]). *Let G be a simple connected graph of order n. Then $\mu_2 = \mu_3 = \cdots = \mu_{n-1}$ if and only if $G \cong S_n$, $G \cong K_n$ or $G \cong K_{n/2,\,n/2}$ (n is even).*

Lemma 2.4 ([2]). *Let G be a simple connected graph of order n. Then $\mu_1 = \mu_2 = \cdots = \mu_{n-2}$ if and only if $G \cong K_n$ or $G \cong K_n - e$, where e is any edge of K_n.*

Note that for each graph G of order n, $\mu_1 \le n$, and the equality holds if and only if $\overline{G}$ is disconnected. Therefore, it is easy to check that $\mu_1(S_n) = \mu_1(K_n) = \mu_1(K_{a,b}) = \mu_1(K_n - e) = n$, where $a+b=n$ and e is any edge of K_n. Lemmas 2.3 and 2.4 give a characterization for the special case that the graphs with at most three distinct Laplacian eigenvalues. In what follows, we will extend the results just mentioned.

Lemma 2.5. *Let G be a simple graph of order n. Then $\mu_1 = n$ and $\mu_2 = \cdots = \mu_{n-2}$ if and only if $G \cong K_n$, $G \cong K_n - e$, $G \cong S_n$, $G \cong K_1 \vee (K_1 \cup K_{n-2})$, $G \cong K_{n/2,\,n/2}$ (n is even), $G \cong K_1 \vee (K_{(n-1)/2} \cup K_{(n-1)/2})$ (n is odd) or $G \cong \overline{K_{n/3}} \vee (K_{n/3} \cup K_{n/3})$ ($n \equiv 0$ mod 3).*

Proof. G is connected since $\mu_1 = n$. Let $\mu_2 = \cdots = \mu_{n-2} = a$.

If $a = \mu_1 = n$, then Lemma 2.4 implies that $G \cong K_n$ or $G \cong K_n - e$.

If $a = \mu_{n-1}$, then Lemma 2.3 implies that $G \cong S_n$, $G \cong K_n$ or $G \cong K_{n/2,\,n/2}$ (n is even).

If $\mu_{n-1} < a < \mu_1 = n$, then $\overline{G}$ is disconnected with two components since n is a Laplacian eigenvalue of G with multiplicity 1. We may write $\overline{G}$ as $G_1 \cup G_2$, where G_1 and G_2 are two components of $\overline{G}$, and assume that $|G_i| = n_i$ for $i = 1, 2$ $(n_1 \le n_2)$. By Proposition 2.1, the Laplacian eigenvalues of $\overline{G}$ are: $n - \mu_{n-1}, \underbrace{n-a, \ldots, n-a}_{n-3}, 0, 0$. We consider the following two cases.

Case 1. $n_1 = 1$. The Laplacian eigenvalues of G_2 are $n - \mu_{n-1}, \underbrace{n-a, \ldots, n-a}_{n-3}, 0$. Since $n - a < n - \mu_{n-1}$, by Lemma 2.3, we have $G_2 \cong S_{n-1}$ or $G_2 \cong K_{(n-1)/2,\,(n-1)/2}$

(n is odd). Hence $G \cong K_1 \vee \overline{S_{n-1}} = K_1 \vee (K_1 \cup K_{n-2})$ or $G \cong K_1 \vee \overline{K_{(n-1)/2,\,(n-1)/2}} = K_1 \vee (K_{(n-1)/2} \cup K_{(n-1)/2})$ (n is odd).

Case 2. $n_1 > 1$. Since $\overline{G}$ has only two distinct nonzero Laplacian eigenvalues and one of them is of multiplicity 1; thus at least one of G_1 or G_2 is complete. Following, we will show that only G_1 is complete. It is easy to see that the case that both G_1 and G_2 are complete is impossible (otherwise, it contradicts the fact that only one nonzero Laplacian eigenvalue is of multiplicity 1 in $\overline{G}$). So, it suffices to show that G_2 is not complete. Suppose that G_2 is complete. Then $n - a = n_2$ and $n - \mu_{n-1} \leq n_1 \leq n_2$, i. e., $\mu_{n-1} \geq a$, which is a contradiction. Hence G_2 has only two distinct nonzero Laplacian eigenvalues and one of them is of multiplicity 1. By Lemma 2.3, we have $G_2 \cong S_{n_2}$ or $G_2 \cong K_{n_2/2,\,n_2/2}$ (n_2 is even). Recall that G_1 is complete, i. e., $n-a = n_1$. If $G_2 \cong S_{n_2}$, then $n_1 = 1$. It is a contradiction. Thus $G_2 \cong K_{n_2/2,\,n_2/2}$ (n_2 is even). Hence $n-a = n_1 = n_2/2$, i. e., $n_2 = 2n_1$. Therefore $n_1 = n/3$ and $n_2 = 2n/3$. Hence $G \cong \overline{K_{n/3}} \vee \overline{K_{n/3,\,n/3}} = \overline{K_{n/3}} \vee (K_{n/3} \cup K_{n/3})$ ($n \equiv 0 \mod 3$).

It is easy to check that the converse holds. Hence the proof is completed. ■

3 Main results

In this section, we present two lower bounds for the Laplacian Estrada index of G in terms of its maximum degree Δ, and characterize the graphs for which equalities are attained.

Theorem 3.1. *Let G be a connected $(n,\, m)$-graph with maximum degree Δ. Then*

$$LEE(G) \geq e^{\Delta+1-2m/n} + (n-2)(e^{4m/n-\Delta-1})^{1/(n-2)} + e^{-2m/n}. \tag{3.4}$$

Moreover, the equality holds if and only if $G \cong K_n$ or $G \cong S_n$.

Proof. Since $\mu_n = 0$, we have

$$\begin{aligned} LEE(G) &= e^{\mu_1-2m/n} + e^{\mu_2-2m/n} + \cdots + e^{\mu_{n-1}-2m/n} + e^{-2m/n} \\ &\geq e^{\mu_1-2m/n} + (n-2)(\prod_{i=2}^{n-1} e^{\mu_i-2m/n})^{1/(n-2)} + e^{-2m/n} \end{aligned}$$

by the arithmetic–geometric mean inequality, and thus

$$LEE(G) = e^{\mu_1-2m/n} + (n-2)(e^{4m/n-\mu_1})^{1/(n-2)} + e^{-2m/n}$$

as $\sum_{i=1}^{n}(\mu_i - 2m/n) = 0$.

Now we consider the function

$$f(x) = e^x + (n-2)(e^{2m/n-x})^{1/(n-2)} + e^{-2m/n}, \text{ for } x \geq 1 \ .$$

We have

$$f'(x) = e^x - (e^{2m/n-x})^{1/(n-2)} \ .$$

It is easy to see that, for any $(n,\, m)$-graph, $2m \leq n(n-1)$. Thus $f'(x) \geq 0$ and $f(x)$ is an increasing function for $x \geq 1 \geq 2m/[n(n-1)]$. By Lemma 2.2, we have $\mu_1 - 2m/n \geq \Delta + 1 - 2m/n \geq 1$. Hence we have

$$\begin{aligned} LEE(G) &= f(\mu_1 - 2m/n) \geq f(\Delta + 1 - 2m/n) \\ &= e^{\Delta+1-2m/n} + (n-2)(e^{4m/n-\Delta-1})^{1/(n-2)} + e^{-2m/n} \ . \end{aligned}$$

This completes the proof of (3.4).

Suppose that the equality in (3.4) holds. Then all inequalities in the above argument must be equalities, i. e., $\mu_1 = \Delta + 1$ and $\mu_2 = \cdots = \mu_{n-1}$. Hence by Lemmas 2.2 and 2.3, we have $G \cong K_n$ or $G \cong S_n$.

Conversely, it is easy to check that the equality in (3.4) holds for K_n and S_n, and so the proof is completed. ■

Theorem 3.2. *Let G be a connected (n,m)-graph with maximum degree Δ. Then*

$$LEE(G) \geq e^{-2m/n}\left(e^{\Delta+1} + e^{4m/(n-1)-\Delta-1} + (n-3)\, e^{2m/(n-1)} + 1\right). \qquad (3.5)$$

Moreover, the equality holds if and only if $G \cong K_n$ or $G \cong K_1 \vee (K_{(n-1)/2} \cup K_{(n-1)/2})$ (n is odd).

Proof. Since $\mu_n = 0$, we have

$$\begin{aligned} LEE(G) &= e^{\mu_1-2m/n} + e^{\mu_2-2m/n} + \cdots + e^{\mu_{n-1}-2m/n} + e^{-2m/n} \\ &\geq e^{\mu_1-2m/n} + e^{\mu_{n-1}-2m/n} + (n-3)\left(\prod_{i=2}^{n-2} e^{\mu_i-2m/n}\right)^{1/(n-3)} + e^{-2m/n} \\ &= e^{\mu_1-2m/n} + e^{\mu_{n-1}-2m/n} + (n-3)\left(e^{6m/n-(\mu_1+\mu_{n-1})}\right)^{1/(n-3)} + e^{-2m/n} \end{aligned}$$

as $\sum_{i=1}^{n}(\mu_i - 2m/n) = 0$.

Consider the function

$$f(x,\, y) = e^x + e^y + e^{-2m/n} + (n-3)(e^{2m/n-(x+y)})^{1/(n-3)}, \text{ for } x \geq 1,\ y \leq 0 \ .$$

We have

$$\begin{aligned} f_x &= e^x - (e^{2m/n-(x+y)})^{1/(n-3)} \\ f_y &= e^y - (e^{2m/n-(x+y)})^{1/(n-3)} \\ f_{xx} &= e^x + 1/(n-3)(e^{2m/n-(x+y)})^{1/(n-3)} \\ f_{xy} &= 1/(n-3)(e^{2m/n-(x+y)})^{1/(n-3)} \quad \text{and} \\ f_{yy} &= e^y + 1/(n-3)(e^{2m/n-(x+y)})^{1/(n-3)} \ . \end{aligned}$$

Now suppose that $f_x = f_y = 0$. We have $x + y = 4m/[n(n-1)]$. For this case, we have

$$f_{xx} > 0 \ , \quad f_{yy} > 0 \ \text{ and } \ f_{xx} f_{yy} - f_{xy}^2 > 0 \ .$$

Hence we see that $f(x, y)$ has a minimum value at $x + y = 4m/[n(n-1)]$ and the minimum value is $e^x + e^{4m/[n(n-1)]-x} + (n-3)(e^{2m/[n(n-1)]}) + e^{-2m/n}$. Since $4m/[n(n-1)] \leq 2$, it is easy to show that

$$g(x) = e^x + e^{4m/[n(n-1)]-x} + (n-3)\, e^{2m/[n(n-1)]} + e^{-2m/n}$$

is an increasing function for $x \geq 1$. By Lemma 2.2, we have $\mu_1 - 2m/n \geq \Delta + 1 - 2m/n \geq 1$. Hence we have

$$\begin{aligned} LEE(G) &= f\left(\mu_1 - \frac{2m}{n}, \, \mu_{n-1} - \frac{2m}{n}\right) \\ &\geq f\left(\Delta + 1 - \frac{2m}{n}, \, \frac{4m}{n(n-1)} - \Delta - 1 + \frac{2m}{n}\right) \\ &= e^{-2m/n}\left(e^{\Delta+1} + e^{4m/(n-1)-\Delta-1} + (n-3)\, e^{2m/(n-1)} + 1\right) \ . \end{aligned}$$

This completes the proof of (3.5).

Now, suppose that the equality in (3.5) holds. Then all inequalities in the above argument must be equalities, i. e.,

$$\mu_1 = \Delta + 1, \ \mu_1 + \mu_{n-1} = \frac{4m}{n(n-1)} + \frac{4m}{n} \ \text{ and } \ \mu_2 = \cdots = \mu_{n-2} \ .$$

Lemma 2.2 implies that $\Delta = n - 1$ and $\mu_1 = n$. Hence by Lemma 2.5, we can check easily that only $G \cong K_n$ and $G \cong K_1 \vee (K_{(n-1)/2} \cup K_{(n-1)/2})$ (n is odd) satisfy the condition that

$$\mu_1 + \mu_{n-1} = \frac{4m}{n(n-1)} + \frac{4m}{n} = \frac{4m}{n-1} \ .$$

Conversely, it is easy to check that the equality in (3.5) holds for the graphs in Theorem 3.2. Hence the proof is completed. ■

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