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MORE ON THE LAPLACIAN ESTRADA INDEX

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Let G be a graph with n vertices and let $\mu_1, \mu_2, \ldots, \mu_n$ be its Laplacian eigenvalues. In some recent works a quantity called Laplacian Estrada index was considered, defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$. We now establish some further properties of LEE, mainly upper and lower bounds in terms of the number of vertices, number of edges, and the first Zagreb index.

1. INTRODUCTION

In this paper we are concerned with simple graphs. Let n and m be, respectively, the number of vertices and edges of G. In what follows we say that G is an (n, m)-graph.

The spectrum of the graph G, consisting of the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$, is the spectrum of its adjacency matrix [**2**]. The Laplacian spectrum of the graph G, consisting of the numbers $\mu_1, \mu_2, \ldots, \mu_n$, is the spectrum of its Laplacian matrix [**9**, **10**]. In what follows we assume that the Laplacian eigenvalues are arranged in non-increasing order.

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

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

motivated by its chemical applications, proposed earlier by Ernesto Estrada [**4**–**7**]. The mathematical properties of the Estrada index have been studied in a number of recent works [**1**, **3**, **11**, **13**, **17**].

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In full analogy with Eq. (1), the *Laplacian Estrada index* of a graph G was defined in [**8**] as:

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

Independently of [**8**], another variant of the Laplacian Estrada index was put forward in [**16**], defined as

$$LEE_{[16]}(G) = \sum_{i=1}^{n} e^{\mu_i - 2m/n} \ .$$

Evidently, $LEE_{[16]}(G) = e^{-2m/n} \, LEE(G)$, and therefore results obtained for LEE can be immediately re-stated for $LEE_{[16]}$ and vice versa. As far as we could see, the results communicated in [**16**] are not equivalent to those in this paper or to those in our earlier works [**8**, **19**]. In particular, our Proposition 3.2 improves the bound (18) in [**16**, Theorem 12].

Some basic properties of the Laplacian Estrada index were determined in the papers [**8**], [**16**], and [**19**]. We now establish some further properties, mainly upper and lower bounds. At the outset we note that

$$LEE(G) = \sum_{k \geq 0} \frac{1}{k!} \sum_{i=1}^{n} \mu_i^{\, k}$$

where the standard notational convention that $0^0 = 1$ is used.

2. PRELIMINARIES

Let K_n be the complete graph on n vertices. Let $G_1 \cup G_2$ denote the the vertex-disjoint union of the graphs G_1 and G_2. Let $\overline{G}$ be the complement of the graph G.

Recall that the first Zagreb index of the graph G, denoted by $M_1(G)$, is the sum of the squares of the degrees of vertices of G; for details on this graph invariant see [**12**] and the references cited therein.

For an (n, m)-graph G, if $\mu_2 = \cdots = \mu_{n-1} = \dfrac{2m}{n}$, then $\mu_1 = \dfrac{2m}{n}$. If $m > 0$, then $\mu_1 \geq \dfrac{2m}{n-1} > \dfrac{2m}{n}$. Thus, we have

Lemma 2.1. *Let G be an (n, m)-graph. Then $\mu_2 = \cdots = \mu_{n-1} = \dfrac{2m}{n}$ if and only if $G = \overline{K_n}$.*

Lemma 2.2 [18]. *Let G be a graph on n vertices. Then $\mu_1 = \cdots = \mu_{n-1}$ if and only if $G = K_n$ or $G = \overline{K_n}$.*

3. THE MAIN RESULTS

We first seek upper bounds for the Laplacian Estrada index.

Proposition 3.1. *Let G be an (n,m)-graph. Then*

$$LEE(G) \le n - 1 + 2m - \sqrt{M_1(G) + 2m} + e^{\sqrt{M_1(G)+2m}}$$

with equality if and only if $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$.

Proof. Recall that $\sum_{i=1}^{n} {\mu_i}^2 = M_1(G) + 2m$. For an integer $k \ge 3$,

$$\begin{aligned}\left(\sum_{i=1}^{n} {\mu_i}^2\right)^k &\ge \sum_{i=1}^{n} {\mu_i}^{2k} + k \sum_{1\le i<j\le n} \left({\mu_i}^2 {\mu_j}^{2(k-1)} + {\mu_i}^{2(k-1)} {\mu_j}^2\right) \\ &\ge \sum_{i=1}^{n} {\mu_i}^{2k} + 2k \sum_{1\le i<j\le n} {\mu_i}^k {\mu_j}^k \ge \left(\sum_{i=1}^{n} {\mu_i}^k\right)^2\end{aligned}$$

and then

$$\sum_{i=1}^{n} {\mu_i}^k \le \left(\sum_{i=1}^{n} {\mu_i}^2\right)^{k/2} = \left(M_1(G) + 2m\right)^{k/2}$$

with equality if and only if at most one of $\mu_1, \mu_2, \ldots, \mu_n$ is non-zero, or equivalently $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$.

It is easily seen that

$$\begin{aligned}LEE(G) &= n + 2m + \sum_{k\ge 2} \frac{1}{k!} \sum_{i=1}^{n} {\mu_i}^k \le n + 2m + \sum_{k\ge 2} \frac{1}{k!} \left(\sqrt{M_1(G) + 2m}\right)^k \\ &= n + 2m - 1 - \sqrt{M_1(G) + 2m} + e^{\sqrt{M_1(G)+2m}}\end{aligned}$$

with equality if and only if $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$. □

Let n_1 be the number of non-isolated vertices of G. Then $2m \ge n_1$. Since $M_1(G) \le (n_1 - 1)2m$, we have $\sqrt{M_1(G) + 2m} \le \sqrt{2mn_1} \le 2m$ with equality if and only if $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$. Thus

$$e^{2m} - e^{\sqrt{M_1(G)+2m}} \ge \sum_{k=0}^{2} \frac{(2m)^k - \left(\sqrt{M_1(G) + 2m}\right)^k}{k!}$$

and then from Proposition 3.1 we arrive at a previously communicated bound [**8**]:

$$LEE(G) \le n - 1 + m - 2m^2 + \frac{1}{2} M_1(G) + e^{2m}$$

in which equality is attained if and only if $G = K_2 \cup \overline{K_{n-2}}$ or $G = \overline{K_n}$.

Recall that the Laplacian energy of an (n,m)-graph is defined in [14] as:

$$LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| .$$

Proposition 3.2. *Let G be an (n,m)-graph. Then*

$$LEE(G) \le e^{\frac{2m}{n}} \left(n - 1 - LE(G) + e^{LE(G)} \right)$$

with equality if and only if $G = \overline{K_n}$.

Proof. Note that $\sum_{i=1}^{n} \left(\mu_i - \frac{2m}{n} \right) = 0$ and $\mu_1 \ge \frac{2m}{n}$. Then

$$\begin{aligned} e^{-\frac{2m}{n}} LEE(G) &= \sum_{i=1}^{n} e^{\mu_i - \frac{2m}{n}} = n + \sum_{k \ge 2} \frac{1}{k!} \sum_{i=1}^{n} \left(\mu_i - \frac{2m}{n} \right)^k \\ &\le n + \sum_{k \ge 2} \frac{1}{k!} \left(\sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| \right)^k = n + \sum_{k \ge 2} \frac{1}{k!} LE(G)^k \\ &= n - 1 - LE(G) + e^{LE(G)} \end{aligned}$$

with equality if and only if $\sum_{i=1}^{n} \left(\mu_i - \frac{2m}{n} \right)^k = \left(\sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right| \right)^k$ holds for all integers $k \ge 2$, i. e., if and only if at most one of $\mu_i - \frac{2m}{n}$ for $i = 1, 2, \ldots, n$, is positive and all others are equal to zero, i. e., $\mu_2 = \cdots = \mu_{n-1} = \frac{2m}{n}$. By Lemma 2.1, this latter condition is equivalent to $G = \overline{K_n}$. □

By a similar, but somewhat more detailed consideration we obtain

$$LEE(G) \le e^{\frac{2m}{n}} \left(n - 1 - LE(G) - \frac{1}{2} LE(G)^2 + \frac{1}{2} M_1(G) + m - \frac{2m^2}{n} + e^{LE(G)} \right)$$

with equality if and only if $G = \overline{K_n}$.

We now deduce a few lower bounds for the Laplacian Estrada index.

Proposition 3.3. *Let G be an (n,m)-graph with $n \ge 2$. Then*

$$LEE(G) \ge 2 + \sqrt{n(n-1)e^{4m/n} + 4 - 3n - 4m}$$

with equality if and only if $G = \overline{K_n}$.

Proof. Observe that for $k \geq 2$, $\sum\limits_{i=1}^{n}(2\mu_i)^k \geq 4\sum\limits_{i=1}^{n}\mu_i^k$ with equality for all $k \geq 2$ if and only if $\mu_1 = \cdots = \mu_n = 0$, i. e., $G = \overline{K_n}$. Then

$$\sum_{i=1}^{n} e^{2\mu_i} = \sum_{i=1}^{n}\sum_{k\geq 0}\frac{(2\mu_i)^k}{k!} = n + 4m + \sum_{k\geq 2}\frac{\sum\limits_{i=1}^{n}(2\mu_i)^k}{k!} \geq n + 4m + 4\sum_{k\geq 2}\frac{\sum\limits_{i=1}^{n}\mu_i^k}{k!}$$
$$= n + 4m + 4\,[LEE(G) - n - 2m] = 4LEE(G) - 3n - 4m.$$

In [**8**] it was shown that $2\sum\limits_{1\leq i<j\leq n} e^{\mu_i}e^{\mu_j} \geq n(n-1)e^{4m/n}$. Thus

$$LEE(G)^2 = \sum_{i=1}^{n} e^{2\mu_i} + 2\sum_{1\leq i<j\leq n} e^{\mu_i}e^{\mu_j}$$
$$\geq 4LEE - 3n - 4m + n(n-1)e^{4m/n}\ .$$

Note that $n(n-1)e^{4m/n} + 4 - 3n - 4m \geq n(n-1)\left(1 + \frac{4m}{n}\right) + 4 - 3n - 4m = (n-2)(4m+n-2) \geq 0$. Therefore

$$LEE(G) \geq 2 + \sqrt{n(n-1)e^{4m/n} + 4 - 3n - 4m}$$

with equality if and only if $G = \overline{K_n}$. □

Since

$$LEE(G) \geq \sum_{k=0}^{2}\frac{1}{k!}\sum_{i=1}^{n}\mu_i^k = n + 3m + \frac{1}{2}\,M_1(G)$$

the bound in Proposition 3.3 is an improvement of a bound in [**8**], namely of

$$LEE(G) \geq \sqrt{n(n-1)e^{4m/n} + n + 8m + 2M_1(G)}\ .$$

Let G be an (n,m)-graph with $n \geq 4$. Let

$$F(G) = n(n-1)e^{4m/n} + 16 - 7n - 16m - 2M_1(G)\ .$$

Then $F(G) \geq n(n-1)\left(1 + \frac{4m}{n} + \frac{8m^2}{n^2}\right) + 16 - 7n - 16m - 2M_1(G) = (n-4)^2 + 2\big(2(n-1)m - M_1(G)\big) + 8m\left(m - \frac{m}{n} - 2\right) \geq 0$ for $m \neq 1, 2$. It is easily checked that $F(G) \geq 0$ for $m = 1, 2$. Indeed, if $m = 1$, then $F(G) = n(n-1)e^{4/n} - 7n - 4$, then $F(G) > 0$ for $n = 4, 5$ by direct checking and $F(G) \geq n(n-1)\left(1 + \frac{4}{n}\right) - 7n - 4 = n^2 - 4n - 8 > 0$ for $n \geq 6$. Similarly, if $m = 2$, then $F(G) \geq n(n-1)e^{8/n} - 7n - 28 > 0$. Thus, $F(G) \geq 0$ in any case. By a similar, but somewhat more complicated consideration, we conclude that (for $n \geq 4$)

$$\sum_{i=1}^{n} e^{2\mu_i} \geq n + 8m + 2M_1(G) + 8\left(LEE(G) - n - 3m - \frac{1}{2}\,M_1(G)\right)$$

and then

$$LEE(G) \geq 4 + \sqrt{n(n-1)e^{4m/n} + 16 - 7n - 16m - 2M_1(G)}$$

holds, with equality if and only if $G = \overline{K_n}$.

Proposition 3.4. *Let G be an (n, m)-graph. Then*

$$LEE(G) \geq 1 + 2m - \sqrt{(n-1)\big(M_1(G) + 2m\big)} + (n-1)e^{\sqrt{\left(M_1(G)+2m\right)/(n-1)}}$$

with equality if and only if $G = K_n$ or $G = \overline{K_n}$.

Proof. We may assume that $n > 1$. We start with an inequality from [**15**, p. 26]: for non-negative numbers $a_1, a_2, \ldots, a_p$ and $\ell \leq k$ with $\ell, k \neq 0$,

$$\left(\frac{1}{p}\sum_{i=1}^{p} {a_i}^{\ell}\right)^{1/\ell} \leq \left(\frac{1}{p}\sum_{i=1}^{p} {a_i}^{k}\right)^{1/k} .$$

Equality is attained if and only if $a_1 = a_2 = \cdots = a_p$. Then, for $k \geq 2$, $p = n-1$, $\ell = 2$, and $a_i = \mu_i$ with $i = 1, 2, \ldots, n-1$, we have

$$\sum_{i=1}^{n-1} {\mu_i}^{k} \geq (n-1)\left(\frac{1}{n-1}\sum_{i=1}^{n-1} {\mu_i}^{2}\right)^{k/2} = (n-1)\left(\sqrt{\frac{M_1(G)+2m}{n-1}}\right)^{k},$$

which is an equality for $k = 2$ whereas equality holds for $k \geq 3$ if and only if $\mu_1 = \mu_2 = \cdots = \mu_{n-1}$. By Lemma 2.2, this is equivalent to $G = K_n$ or $G = \overline{K_n}$.

It is easily seen that

$$\begin{aligned} LEE(G) &= n + 2m + \sum_{k\geq 2} \frac{1}{k!} \sum_{i=1}^{n} {\mu_i}^{k} \\ &\geq n + 2m + (n-1)\sum_{k\geq 2} \frac{1}{k!}\left(\sqrt{\frac{M_1(G)+2m}{n-1}}\right)^{k} \\ &= n + 2m + (n-1)\left(-1 - \sqrt{\frac{M_1(G)+2m}{n-1}} + e^{\sqrt{\frac{M_1(G)+2m}{n-1}}}\right) \\ &= 1 + 2m - \sqrt{(n-1)\left(M_1(G)+2m\right)} + (n-1)e^{\sqrt{\frac{M_1(G)+2m}{n-1}}} \end{aligned}$$

with equality if and only if the lower bound for $\sum_{i=1}^{n-1} {\mu_i}^{k}$ above is attained for $k = 3, 4, \ldots$, i. e., if and only if $G = K_n$ or $G = \overline{K_n}$. □

Proposition 3.5. *Let G be an r-regular graph with n vertices. Then*

$$LEE(G) \geq 1 + (n-1)e^{nr/(n-1)} \tag{2}$$

with equality if and only if $G = K_n$ *or* $G = \overline{K_n}$.

Proof. Note that the Laplacian spectrum of the graph G consists of $r - \lambda_n, r - \lambda_{n-1}, \ldots, r - \lambda_2, 0$, where $\lambda_1 = r, \lambda_2, \ldots, \lambda_n$ are the ordinary eigenvalues of G, arranged in non-increasing order. Then $LEE(G) = 1 + \sum_{i=2}^{n} e^{r-\lambda_i}$ and thus by the arithmetic–geometric–mean inequality,

$$\big(LEE(G) - 1\big)e^{-r} = \sum_{i=2}^{n} e^{-\lambda_i} \geq (n-1)e^{-\frac{1}{n-1}\sum_{i=2}^{n}\lambda_i} = (n-1)e^{r/(n-1)}$$

from which we arrive at the inequality (2), with equality if and only if $\lambda_2 = \cdots = \lambda_n$, that is, $G = K_n$ or $G = \overline{K_n}$. □

Let $\mathcal{L}(G)$ be the line graph of G . In [**8**] it was shown that if G is an r-regular graph with n vertices then

$$LEE(\mathcal{L}(G)) = LEE(G) + \frac{n(r-2)}{2}\, e^{2r}.$$

Proposition 3.6. *Let* G *be an* (n, m)*-graph. If* G *is bipartite, then*

$$LEE(G) = n - m + e^2\, EE\big(\mathcal{L}(G)\big).$$

Proof. It is known that $\prod_{i=1}^{n}(x - \mu_i) = x^{n-m}\prod_{i=1}^{m}(x - 2 - \gamma_i)$ where $\gamma_1, \gamma_2, \ldots, \gamma_m$ are the eigenvalues of $\mathcal{L}(G)$ (see [**2**]). Thus

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i} = (n-m) + \sum_{i=1}^{m} e^{2+\gamma_i} = n - m + e^2 \sum_{i=1}^{m} e^{\gamma_i}$$

$$= n - m + e^2\, EE(\mathcal{L}(G))$$

as desired. □

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