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ON THE LAPLACIAN ESTRADA INDEX OF A GRAPH

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Abstract Let G be a graph of order n. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the adjacency matrix of G, and let $\mu_1, \mu_2, \ldots, \mu_n$ be the eigenvalues of the Laplacian matrix of G. Much studied Estrada index of the graph G is defined as $EE = EE(G) = \sum\limits_{i=1}^{n} e^{\lambda_i}$. We define and investigate the Laplacian Estrada index of the graph G, $LEE = LEE(G) = \sum\limits_{i=1}^{n} e^{(\mu_i - \frac{2m}{n})}$. Bounds for LEE are obtained, as well as some relations between LEE and graph Laplacian energy.

1. INTRODUCTION

Let $G = (V, E)$ be a graph without loops and multiple edges. 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*. For $v \in V(G)$, let $d(v)$ be the degree of v.

In this paper, we are concerned only with undirected simple graphs (loops and multiple edges are not allowed). Let G be a graph with n vertices and the adjacency matrix $A(G)$. Let $D(G)$ be a 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 and the Laplacian eigenvalues of G, respectively. The multiset of eigenvalues of A(G) (L(G)) is called the adjacency (Laplacian) spectrum of G. Other undefined notations may be referred to [**1**].

The basic properties of the eigenvalues and Laplacian eigenvalues of the graph can be found in the book [**2**].

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The *energy* of the graph G is defined in [**8**, **9**] as:

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i|. \tag{1}$$

The *Estrada index* of the graph G is defined in [**4**–**6**] as:

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

Denoting by $M_k = M_k(G)$ the *k-th spectral moment* of the graph G ([**4**] equal to the number of closed walks of length k of the graph G),

$$M_k = M_k(G) = \sum_{i=1}^{n} (\lambda_i)^k,$$

and bearing in mind the power-series expansion of e^x, we have

$$EE = \sum_{k=0}^{\infty} \frac{M_k}{k!}. \tag{3}$$

The quantity defined by (2) or (3) appears in Physics and Chemistry; for details see the surveys [**4**–**6**]. Recently much work on the Estrada index of the graph appeared also in the mathematical literature (see, for instance, [**3**, **10**]).

It is evident from (3) that if graph G can be transformed to another graph G', such that $M_k(G') \geq M_k(G)$ holds for all values of k, and $M_k(G') > M_k(G)$ holds for at least some values of k, then $EE(G') > EE(G)$. We assume that graph transformation $G \to G'$, where $G' = G + e$ be the graph obtained from G by adding a new edge e into G. By adding a new edge e into G, the number of closed walks of length k will certainly not decrease, and in some cases (e.g., for $k = 2$) will strictly increase. Bearing that in mind, we conclude that the n-vertex with as few as possible and as many as possible edges has the minimum and the maximum EE, respectively. From (2), we find that $EE(\overline{K_n}) = n$ and $EE(K_n) = e^{n-1} + (n-1)\,\frac{1}{e}$. Hence, for any graph G of order n, different from the complete graph K_n and from its (edgeless) complement $\overline{K_n}$, we have

$$n = EE(\overline{K_n}) < EE(G) < EE(K_n) = e^{n-1} + (n-1)\,\frac{1}{e}\,.$$

Recently, J. A. de la Peña *et al.* [**3**] established lower and upper bounds for EE in terms of the number of vertices and number of edges, and also obtained some inequalities between EE and the energy of G. Their results are as follows.

Theorem 1. [**3**] *Let G be an (n, m)-graph. Then the Estrada index of G is bounded as*

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

Equality on both sides of (4) *is attained if and only if $G \cong \overline{K_n}$.*

Theorem 2. [**3**] *Let G be a regular graph of degree r and of order n. Then its Estrada index is bounded as*

$$\begin{aligned} &e^r + \sqrt{n + 2nr - (2r^2 + 2r + 1) + (n-1)(n-2)e^{-2r/(n-1)}} \\ &\leq EE(G) \leq n - 2 + e^r + e^{\sqrt{r(n-r)}}. \end{aligned}$$

Theorem 3. [**3**] *Let G be an (n, m)-graph. Then*

$$EE(G) - E(G) \leq n - 1 - \sqrt{2m} + e^{\sqrt{2m}}. \tag{5}$$

Or

$$EE(G) \leq n - 1 + e^{E(G)}. \tag{6}$$

Equality (5) *or* (6) *is attained if and only if $G \cong \overline{K_n}$.*

Theorem 4. [**3**] *Let G be a regular graph of degree r and of order n. Then*

$$EE(G) - E(G) \leq n - 2 + e^r - r - \sqrt{r(n-r)} + e^{\sqrt{r(n-r)}}.$$

In this paper, we define and investigate the Laplacian Estrada index of G as $LEE = LEE(G) = \sum_{i=1}^{n} e^{(\mu_i - \frac{2m}{n})}$, and get some analogy between the properties of $EE(G)$ and $LEE(G)$, but also some significant differences.

2. THE LAPLACIAN ESTRADA INDEX CONCEPT

The *first Zagreb index* of G is defined in [**7**] as $M = M(G) = \sum_{u \in V(G)} d^2(u)$.

Lemma 1. [**12**] *Let G be an (n, m)-graph. Then,*

$$M \leq m\Big(\frac{2m}{n-1} + n - 2\Big),$$

with equality if and only if G is S_n or K_n.

Lemma 2. [**13**] *If G is a triangle-free and a quadrangle-free graph, then*

$$M \leq n(n-1),$$

with equality if and only if G is the star or a Moore graph of diameter 2.

Lemma 3. *Let G be an (n, m)-graph with maximum degree Δ and minimum degree δ, then*

$$\frac{4m^2}{n} \leq M \leq 2m(\Delta + \delta) - n\delta\Delta. \tag{7}$$

Equality on both sides of (7) *is attained if and only if* G *is regular.*

Proof. By the CAUCHY-SCHWARZ inequality, we have

$$M = \sum_{u\in V(G)} d^2(u) \geq \frac{\Big(\sum\limits_{u\in V(G)} d(u)\Big)^2}{n} = \frac{4m^2}{n}\,.$$

Equality holds if and only if G is regular.

Summing the inequality $\big(d(u)-\delta\big)\big(d(u)-\Delta\big) \leq 0$ for every $u \in V(G)$, we have that

$$\sum_{u\in V(G)} d^2(u) - (\Delta+\delta) \sum_{u\in V(G)} d(u) + n\delta\Delta \leq 0.$$

Then,

$$M \leq 2m(\Delta+\delta) - n\delta\Delta.$$

Equality holds if and only if G is regular. This ends the proof. □

The *Laplacian energy* of the graph G is defined in [**11**] as:

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

Definition. *If* G *is an* (n,m)*-graph, and its Laplacian eigenvalues are* $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$*, then the Laplacian Estrada index of* G*, denoted by* $LEE(G)$*, is equal to*

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

And let

$$M'_k = \sum_{i=1}^{n} \Big(\mu_i - \frac{2m}{n}\Big)^k.$$

Then $M'_0 = n$; $M'_1 = 0$; $M'_2 = M + 2m\Big(1 - \frac{2m}{n}\Big)$ (where M is the first Zagreb index of G as above). And bearing in mind the power-series expansion of e^x, we have

(10) $$LEE = \sum_{k=0}^{\infty} \frac{M'_k}{k!}\,.$$

Lemma 4. *If the graph* G *is regular, then* $M_{2k}(G) = M'_{2k}$ $(k \in \mathbb{Z})$*,* $LE(G) = E(G)$*,* $LEE(G) = \sum\limits_{i=1}^{n} e^{-\lambda_i}$*. Further, if the regular graph* G *is bipartite, then* $M_k(G) = M'_k$*,* $LEE(G) = EE(G)$*.*

Proof. If an (n,m)-graph is regular of degree r, then $r = 2m/n$ and [**2**], we have

$$\mu_i - r = -\lambda_{n-i+1}, \qquad i = 1,2,\ldots,n,$$

and from the definition of M_k, M'_k, E, LE, EE and LEE of the graph G, respectively. We have $M_{2k}(G) = M'_{2k}$ $(k \in \mathbb{Z})$, $LE(G) = E(G)$, $LEE(G) = \sum_{i=1}^{n} e^{-\lambda_i}$.

If the regular graph G is a bipartite graph, from [**2**], we have

$$\lambda_i = -\lambda_{n+1-i}, \qquad i = 1,2,\ldots,n$$

Then, $\sum_{i=1}^{n} \lambda_i^k = \sum_{i=1}^{n} (-\lambda_i)^k$ and $\sum_{i=1}^{n} e^{-\lambda_i} = \sum_{i=1}^{n} e^{\lambda_i}$. We have $M_k(G) = M'_k$, $LEE(G) = EE(G)$. □

Theorem 5. *Let G be an (n,m)-graph with maximum degree Δ and minimum degree δ, then the Laplacian Estrada index of G is bounded as*

$$\sqrt{n^2+4m} \le LEE(G) \le n-1+e^{\sqrt{2m(\Delta+\delta+1-\frac{2m}{n})-n\delta\Delta}}. \tag{11}$$

Equality on both sides of (11) *is attained if and only if* $G \cong \overline{K_n}$.

Proof. Lower bound. Directly from (9), we get

$$LEE^2(G) = \sum_{i=1}^{n} e^{2(\mu_i - \frac{2m}{n})} + 2\sum_{i<j} e^{(\mu_i-\frac{2m}{n})} e^{(\mu_j-\frac{2m}{n})}. \tag{12}$$

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

$$\begin{aligned}
2\sum_{i<j} e^{(\mu_i-\frac{2m}{n})} e^{(\mu_j-\frac{2m}{n})} &\ge n(n-1)\Big(\prod_{i<j} e^{(\mu_i-\frac{2m}{n})} e^{(\mu_j-\frac{2m}{n})}\Big)^{2/[n(n-1)]}\\
&= n(n-1)\Big[\Big(\prod_{i=1}^{n} e^{(\mu_i-\frac{2m}{n})}\Big)^{n-1}\Big]^{2/[n(n-1)]}\\
&= n(n-1)(e^{M'_1})^{2/n}\\
&= n(n-1). \qquad (13)
\end{aligned}$$

By means of a power-series expansion, and $M'_0 = n$, $M'_1 = 0$ and $M'_2 = M + 2\Big(1 - \dfrac{2m}{n}\Big)$, we get

$$\begin{aligned}
\sum_{i=1}^{n} e^{2(\mu_i-\frac{2m}{n})} &= \sum_{i=1}^{n} \sum_{k\ge 0} \frac{\big[2(\mu_i - \frac{2m}{n})\big]^k}{k!}\\
&= n + 2\Big[2m\Big(1-\frac{2m}{n}\Big) + M\Big] + \sum_{i=1}^{n}\sum_{k\ge 3} \frac{\big[2(\mu_i - \frac{2m}{n})\big]^k}{k!}
\end{aligned}$$

We use a multiplier $r \in [0,8]$, as to arrive at,

$$\sum_{i=1}^{n} e^{2(\mu_i - \frac{2m}{n})} \geq n + 2\Big[2m\Big(1 - \frac{2m}{n}\Big) + M\Big] + r\sum_{i=1}^{n}\sum_{k\geq 3}\frac{\big(\mu_i - \frac{2m}{n}\big)^k}{k!}$$
$$= (1-r)n + (4-r)\Big[m\Big(1 - \frac{2m}{n}\Big) + \frac{M}{2}\Big] + rLEE$$

Further, by Lemma 7, we get

$$\sum_{i=1}^{n} e^{2(\mu_i - \frac{2m}{n})} \geq (1-r)n + (4-r)\Big[m\Big(1 - \frac{2m}{n}\Big) + \frac{2m^2}{n}\Big] + rLEE$$

i.e.,

$$\sum_{i=1}^{n} e^{2(\mu_i - \frac{2m}{n})} \geq (1-r)n + (4-r)m + rLEE \tag{14}$$

By substituting (13) and (14) back into (12), and solving for LEE, we have

$$LEE \geq \frac{r}{2} + \sqrt{\Big(n - \frac{r}{2}\Big)^2 + (4-r)m}$$

It is elementary to show that for $n \geq 2$ and $m \geq 1$ the function

$$f(x) := \frac{x}{2} + \sqrt{\Big(n - \frac{x}{2}\Big)^2 + (4-r)m}$$

monotonically decreases in the interval $[0,8]$. Consequently, the best lower bound for LEE is attained for $r = 0$. Then we arrive at the first half of Theorem 5.

Upper bound. Starting from the following inequality, we get

$$\begin{aligned}
LEE = n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{\big(\mu_i - \frac{2m}{n}\big)^k}{k!} &\leq n + \sum_{i=1}^{n}\sum_{k\geq 1}\frac{\big|\mu_i - \frac{2m}{n}\big|^k}{k!} \\
&= n + \sum_{k\geq 1}\frac{1}{k!}\sum_{i=1}^{n}\Big[\Big(\mu_i - \frac{2m}{n}\Big)^2\Big]^{k/2} \\
&\leq n + \sum_{k\geq 1}\frac{1}{k!}\Big[\sum_{i=1}^{n}\Big(\mu_i - \frac{2m}{n}\Big)^2\Big]^{k/2} \\
&= n + \sum_{k\geq 1}\frac{1}{k!}\Big[M + 2m\Big(1 - \frac{2m}{n}\Big)\Big]^{k/2} \\
&= n - 1 + \sum_{k\geq 0}\frac{\Big(\sqrt{M + 2m(1 - \frac{2m}{n})}\Big)^k}{k!} \\
&= n - 1 + e^{\sqrt{M + 2m(1 - \frac{2m}{n})}}. \qquad (15)
\end{aligned}$$

By Lemma 3, we have

$$LEE \leq n-1+e^{\sqrt{2m(\Delta+\delta+1-\frac{2m}{n})-n\delta\Delta}},$$

which directly leads to the right-hand side inequality in (11).

From the derivation of (11) it is evident that equality will be attained if and only if the graph G has all zero eigenvalues. This happens only in the case of the edgeless graph $\overline{K_n}$, [**2**].

The proof is completed. □

Remark. If in inequality (15) we utilize the upper bound of M in Lemma 1, we have the upper bound for LEE in terms of the number of vertices and number of edges as follows,

$$LEE \leq n-1+e^{\sqrt{m(n+\frac{2m}{n-1}-\frac{4m}{n})}}.$$

Further, if the (n,m)-graph is a triangle-free and a quadrangle-free graph, by Lemma 2, we have,

$$LEE \leq n-1+e^{\sqrt{n(n-1)+2m(1-\frac{2m}{n})}}.$$

Since $\mu_n = 0$, if we consider $LEE - e^{2m/n} = \sum_{i=1}^{n-1} e^{(\mu_i - 2m/n)}$ in the same way as in Theorem 5, we have the following bounds of $LEE(G)$:

Theorem 6. *Let G be an (n,m)-graph with maximal degree Δ and minimal degree δ, then the Laplacian Estrada index of G is bounded as*

$$\begin{aligned} & e^{-2m/n} + \sqrt{(n-1)\left[1+(n-2)e^{\frac{4m}{n(n-1)}}\right] + 4m\left(1+\frac{1}{n}-\frac{2m}{n^2}\right)} \\ & \leq LEE(G) \leq n-2+e^{\frac{-2m}{n}} + e^{\sqrt{2m(1+\Delta+\delta-\frac{2m}{n}-\frac{2m}{n^2})-n\Delta\delta}}. \end{aligned} \tag{16}$$

Equality on both sides of (16) *is attained if and only if $G \cong \overline{K_n}$.*

If G is regular, by Lemma 4, Theorem 2 and Theorem 6, the following result is obviously.

Theorem 7. *Let G be a regular graph of degree r and of order n. Then its Laplacian Estrada index is bounded as*

$$\begin{aligned} & e^{-r} + \sqrt{n+2nr-(2r^2-2r+1)+(n-1)(n-2)e^{2r/(n-1)}} \\ & \leq LEE(G) \leq n-2+e^{-r}+e^{\sqrt{r(n-r)}}. \end{aligned}$$

Further, if the regular graph G is a bipartite graph, then its Laplacian Estrada index is bounded as

$$\begin{aligned} & e^{r} + \sqrt{n+2nr-(2r^2+2r+1)+(n-1)(n-2)e^{-2r/(n-1)}} \\ & \leq LEE(G) \leq n-2+e^{r}+e^{\sqrt{r(n-r)}}. \end{aligned}$$

3. BOUNDS FOR THE LAPLACIAN ESTRADA INDEX INVOLVING GRAPH LAPLACIAN ENERGY

Theorem 8. *Let G be an (n,m)-graph with maximum degree Δ and minimum degree δ, then*

$$LEE-LE \le n-1-\sqrt{2m\Big(\Delta+\delta+1-\frac{2m}{n}\Big)-n\delta\Delta}+e^{\sqrt{2m(\Delta+\delta+1-\frac{2m}{n})-n\delta\Delta}}, \tag{17}$$

or

$$LEE(G) \le n-1+e^{LE(G)}. \tag{18}$$

Equality (17) *or* (18) *is attained if and only if* $G \cong \overline{K_n}$.

Proof. In the proof of Theorem 5, we have the following inequality,

$$LEE = n+\sum_{i=1}^{n}\sum_{k\ge 1}\frac{\big(\mu_i-\frac{2m}{n}\big)^k}{k!} \le n+\sum_{i=1}^{n}\sum_{k\ge 1}\frac{\big|\mu_i-\frac{2m}{n}\big|^k}{k!}.$$

Taking into account the definition of graph Laplacian energy (8), we have

$$LEE \le n+LE+\sum_{i=1}^{n}\sum_{k\ge 2}\frac{\big|\mu_i-\frac{2m}{n}\big|^k}{k!},$$

which, as in Theorem 5, leads to

$$\begin{aligned} LEE-LE &\le n+\sum_{i=1}^{n}\sum_{k\ge 2}\frac{\big|\mu_i-\frac{2m}{n}\big|^k}{k!} \\ &\le n-1-\sqrt{M+2m\Big(1-\frac{2m}{n}\Big)}+e^{\sqrt{M+2m(1-\frac{2m}{n})}}. \end{aligned} \tag{19}$$

It is elementary to show that the function $f(x) := e^x - x$ monotonically increases in the interval $[0,+\infty]$. Consequently, the best upper bound for $LEE - LE$ is attained for $M = 2m(\Delta+\delta) - n\delta\Delta$ by Lemma 3. Then we have

$$LEE-LE \le n-1-\sqrt{2m\Big(\Delta+\delta+1-\frac{2m}{n}\Big)-n\delta\Delta}+e^{\sqrt{2m(\Delta+\delta+1-\frac{2m}{n})-n\delta\Delta}}.$$

This inequality holds for all (n,m)-graphs. Equality is attained if and only if $G \cong \overline{K_n}$.

Another route to connect LEE and LE, is the following:

$$\begin{aligned} LEE \le n+\sum_{i=1}^{n}\sum_{k\ge 1}\frac{\big|\mu_i-\frac{2m}{n}\big|^k}{k!} &\le n+\sum_{k\ge 1}\frac{1}{k!}\Big(\sum_{i=1}^{n}\Big|\mu_i-\frac{2m}{n}\Big|\Big)^k \\ &= n+\sum_{k\ge 1}\frac{LE^k}{k!} = n-1+\sum_{k\ge 0}\frac{LE^k}{k!} \end{aligned}$$

implying, $LEE(G) \leq n-1+e^{LE(G)}$.

Also on this formula equality occurs if and only if $G \cong \overline{K_n}$. □

Remark. If in inequality (19) we utilize the upper bound of M in Lemma 1, we have the upper bound for $LEE - LE$ in terms of the number of vertices and number of edges as follows,

$$LEE - LE \leq n-1-m\Big(n+\frac{2m}{n-1}-\frac{4m}{n}\Big)+e^{\sqrt{m(n+\frac{2m}{n-1}-\frac{4m}{n})}}.$$

Further, if the (n,m)-graph is a triangle-free and a quadrangle-free graph, by Lemma 6, we have,

$$LEE - LE \leq n-1-n(n-1)+2m\Big(1-\frac{2m}{n}\Big)+e^{\sqrt{n(n-1)+2m(1-\frac{2m}{n})}}.$$

Since $\mu_n = 0$, if we consider $LEE - e^{2m/n} = \sum_{i=1}^{n-1} e^{(\mu_i - 2m/n)}$ in the same way as in Theorem 8, we have the following results:

Theorem 9. *Let G be an (n,m)-graph with maximum degree Δ and minimum degree δ, then*

$$\begin{aligned} LEE - LE \leq\; & n-2+e^{-\frac{2m}{n}}-\frac{2m}{n}-\sqrt{2m\Big(\Delta+\delta+1-\frac{2m}{n}-\frac{2m}{n^2}\Big)-n\delta\Delta} \\ & + e^{\sqrt{2m(\Delta+\delta+1-\frac{2m}{n}-\frac{2m}{n^2})-n\delta\Delta}}, \end{aligned} \tag{20}$$

or

$$LEE(G) \leq n-2+e^{-\frac{2m}{n}}(1+e^{LE(G)}). \tag{21}$$

Equality (20) *or* (21) *is attained if and only if $G \cong \overline{K_n}$.*

By Lemma 4 and Theorem 9, a similar formula is deduced for regular graphs,

Theorem 10. *Let G be a regular graph of degree r and of order n. Then*

$$LEE - LE \leq n-2+e^{-r}-r-\sqrt{r(n-r)}+e^{\sqrt{r(n-r)}},$$

or

$$LEE(G) \leq n-2+e^{-r}(1+e^{LE(G)}).$$

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