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NOTE ON ESTRADA AND L-ESTRADA INDICES OF GRAPHS

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A b s t r a c t. Let G be a graph of order n. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues and $\mu_1, \mu_2, \ldots, \mu_n$ its Laplacian eigenvalues. The Estrada index EE of the graph G is defined as the sum of the terms e^{λ_i}, $i = 1, 2, \ldots, n$. In this paper the notion of Laplacian–Estrada index (L-Estrada index, LEE) of a graph is introduced. It is defined as the sum of the terms e^{μ_i}, $i = 1, 2, \ldots, n$. The basic properties of LEE are established, and compared with the analogous properties of EE. In addition, the Estrada and L-Estrada indices of some important classes of graphs are computed.

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1. *Introduction*

Throughout this paper we are concerned with simple graphs, that is, with graphs having no loops or multiple edges or directed edges. Let G be such a graph and $\{1, 2, \ldots, n\}$ be the set of its vertices. Let $\deg(i)$ be the degree of the vertex i. The diagonal matrix $D(G) = ||d_{ij}||$ is defined by

$d_{ii} = \deg(i)$ and $d_{ij} = 0$ if $i \neq j$. The adjacency matrix of G, denoted by $A(G)$, is the square matrix of order n whose $(i,j)-$entry is equal to the number of edges between the vertices i and j. The Laplacian matrix of G is defined as $L(G) = D(G) - A(G)$. The characteristic polynomial and the Laplacian characteristic polynomial of G are, respectively, the characteristic polynomial of the adjacency matrix and of the Laplacian matrix. We denote them by $\phi(G,\lambda)$ and $\psi(G,\lambda)$, respectively. Thus, $\phi(G,\lambda) = \det(\lambda I_n - A(G))$ and $\psi(G,\lambda) = \det(\lambda I_n - L(G))$, where I_n is the unit matrix of order n.

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ and $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ be, respectively, the ordinary and the Laplacian eigenvalues of G, i.e., the zeros of $\phi(G,\lambda)$ and $\psi(G,\lambda)$. These eigenvalues form the (ordinary) spectrum and the Laplacian spectrum of the underlying graph. Details of the the theory of graph spectra and Laplacian graph spectra can be found in the book [3] and the reviews [21–23].

The Estrada index $EE(G)$ of the graph G is defined as the sum of the terms e^{λ_i}, $i = 1, 2, \ldots, n$. This quantity, introduced by Ernesto Estrada, has noteworthy chemical applications (see [5–7] and the references cited therein). A large number of recent works [1, 2, 4, 9, 10, 12–18, 24, 25] is devoted to the study of its mathematical properties.

We now define the Laplacian–Estrada index, or, shorter, the L-Estrada index of G, denoted by $LEE(G)$, to be the sum of the terms e^{μ_i}, $i = 1, 2, \ldots, n$. In this paper, some basic properties of this new index are established.

* * *

We now introduce some notation that will be used throughout this paper.

The vertex and edge set of the graph G will be denoted by $V(G)$ and $E(G)$, respectively.

An empty graph is a graph without edges, i. e., $E(G) = \emptyset$. The complement of a graph G is denoted by $\overline{G}$, where $e \in E(\overline{G})$ if and only if $e \notin E(G)$.

Suppose that G and H are two graphs with disjoint vertex sets. The disjoint union of G and H is a graph $G \cup H$, such that $V(G \cup H) = V(G) \cup V(H)$ and $E(G \cup H) = E(G) \cup E(H)$.

The join $G + H$ of the above specified graphs G and H is the graph obtained from $G \cup H$ by connecting all vertices from $V(G)$ with all vertices from $V(H)$. If $G_1, G_2, \ldots, G_n$ are graphs with mutually disjoint vertex sets,

then we denote $G_1 + G_2 + \cdots + G_n$ by $\sum_{i=1}^{n} G_i$. In the case that $G_1 = G_2 = \cdots = G_n = G$, we denote $\sum_{i=1}^{n} G_i$ by $n\,G$.

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a, x)(b, y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$. If $G_1, G_2, \ldots, G_n$ are graphs with mutually disjoint vertex sets, then we denote $G_1 \times G_2 \times \cdots \times G_n$ by $\prod_{i=1}^{n} G_i$. In the case that $G_1 = G_2 = \cdots = G_n = G$, we denote $\prod_{i=1}^{n} G_i$ by G^n.

2. *The Estrada index of graphs*

This section is concerned with the use of algebraic techniques in the study of the Estrada index of graphs. We begin with the following simple:

Proposition 1. *Let G be a graph with exactly n vertices. Then $EE(G) \geq n$, with equality if and only if G is the empty graph.*

P r o o f. From the inequality between the arithmetic and geometric means,

$$\frac{EE(G)}{n} \geq \sqrt[n]{\prod_{i=1}^{n} e^{\lambda_i}} = \sqrt[n]{e^{\sum_{i=1}^{n} \lambda_i}} = \sqrt[n]{e^0} = 1$$

with equality if and only if for all $1 \leq i, j \leq n$, $e^{\lambda_i} = e^{\lambda_j}$, that is if and only if $\lambda_i = \lambda_j$. This implies that all λ_i's are zero, as desired. □

Proposition 2. *([1]) If G is an r-regular graph with n vertices and $m = rn/2$ edges, and $L(G)$ is its line graph, then $EE(L(G)) = e^{r-2}EE(G) + (m - n)e^{-2}$.*

By Proposition 2, if G is a connected r-regular graph, then $EE(L(G)) = EE(G)$ if and only if $r = 1, 2$ and G is a cycle or a path with two vertices. To see this, we assume that $EE(L(G)) = EE(G)$ and $r \geq 3$. Then $m > n$ and

$$EE(G) = \frac{(n - m)e^{-2}}{e^{r-2} - 1}\ .$$

This would imply that $EE(G) < 0$, a contradiction.

Proposition 3. *Let G and H be r– and s-regular graphs with p and q vertices, respectively. Then*

$$EE(G+H) = EE(G)+EE(H)-(e^r+e^s)+2e^{(r+s)/2}\,cosh\left(\frac{\sqrt{(r-s)^2+4pq}}{2}\right).$$

P r o o f. It is known that [3]

$$\phi(G+H,\lambda) = \frac{\phi(G,\lambda)\,\phi(H,\lambda)}{(x-r)(x-s)}[(x-r)(x-s)-pq]\,.$$

Since

$$x_1 = \frac{(r+s)+\sqrt{(r-s)^2+4pq}}{2} \quad \text{and} \quad x_2 = \frac{(r+s)-\sqrt{(r-s)^2+4pq}}{2}$$

are the roots of $x^2-(r+s)x+rs-pq=0$, the eigenvalues of $G+H$ are those of G and H in which r and s are exchanged by x_1 and x_2. Hence

$$EE(G+H) = EE(G)+EE(H)-(e^r+e^s)+e^{x_1}+e^{x_2}$$

proving the result. □

Corollary 3.1. *If G is an r-regular n-vertex graph then*

$$EE(2G) = 2EE(G)-2e^r+2e^r\,cosh(n)\,.$$

Corollary 3.2. $EE(K_{m,n}) = m+n-2+2cosh(\sqrt{mn})$.

Corollary 3.3. *If G is r-regular then*

$$EE(3G) = 3EE(G)-3e^r+2e^r\,cosh(n)+2e^{(2r+n)/2}\,cosh\left(\frac{3n}{2}\right)-e^{r+n}\,.$$

The n-vertex star graph S_n is a tree with one vertex having degree $n-1$ and the other $n-1$ vertices having degree 1.

Corollary 3.4. $EE(S_{n+1}) = n-1+2\,cosh(\sqrt{n})$.

The wheel W_n is a graph of order n containing a cycle of order $n-1$, and a vertex to which all other vertices are connected.

Corollary 3.5. $EE(W_{n+1}) = EE(C_n) - e^2 + 2e\,cosh(\sqrt{n+1})$.

P r o o f. $W_{n+1} = K_1 + C_n$. □

Example 1. A Möbius ladder L_n of order $2n$ is a simple graph obtained by introducing a twist in a prism graph of order n that is isomorphic to the circulant graph. In this example the Estrada index of a Möbius graph is computed. By [3], the eigenvalues of L_n are $\lambda_k = (-1)^k + 2\cos(k\pi/n)$, where $0 \leq k \leq 2n-1$. So,

$$\begin{aligned} EE(L_n) &= e \sum_{k=0,k \text{ even}}^{2n-2} e^{2\cos(k\pi/n)} + e^{-1} \sum_{k=1,k \text{ odd}}^{2n-1} e^{2\cos(k\pi/n)} \\ &= e \sum_{k=0}^{n-1} e^{2\cos(2k\pi/n)} + e^{-1} \sum_{k=0}^{n-1} e^{2\cos((2k+1)\pi/n)} \\ &= e\,EE(C_n) + e^{-1} \sum_{k=0}^{n-1} e^{2\cos((2k+1)\pi/n)} \ . \end{aligned}$$

In what follows we denote $\frac{1}{2\pi}\int_0^{2\pi} e^{2\cos(x)}dx$ by I_0. Then a similar argument as in [14] shows that $EE(L_n) \approx eEE(C_n)+e^{-1}EE(C_n) = 2n\,cosh(1)\,I_0$.

Example 2. Take the star graph S_{n+1} and add a new edge to each of its $n+1$ vertices to get an star-like graph T_{2n+2}. By [3], $\phi(T_{2n+2},\lambda) = (\lambda^2-1)^{n-1}[(\lambda^2-1)^2 - n\lambda^2]$ and so

$$Spec(T_{2n+2}) = \begin{pmatrix} 1 & -1 & [\sqrt{n} \pm \sqrt{n+4}]/2 & [-\sqrt{n} \pm \sqrt{n+4}]/2 \\ n-1 & n-1 & 1 & 1 \end{pmatrix} .$$

Therefore,

$$EE(T_{2n+2}) = 2(n-1)\,cosh(1) + 4\,cosh\left(\frac{\sqrt{n+4}}{2}\right) cosh\left(\frac{\sqrt{n}}{2}\right) .$$

Proposition 4. Let G be an r-regular graph. Then

$$EE(\overline{G}) = e^{n-r-1} - e^{-r-1} + e^{-1}\sum_{i=1}^{n} e^{-\lambda_i} \ .$$

In particular, if G is bipartite then $EE(\overline{G}) = e^{-1}\,EE(G) + e^{n-r-1} - e^{-r-1}$.

P r o o f. The first formula is a direct consequence of [3]

$$\phi(\overline{G},\lambda) = (-1)^n \, \frac{\lambda - n + r + 1}{\lambda + r + 1} \, \phi(G, -\lambda - 1) \ .$$

In order to arrive at the second equality, it is enough to note that the eigenvalues of bipartite graphs are symmetric around zero. □

Let $R(G)$ be the graph obtained from G by adding a new vertex to each edge of G, see [3, p. 63].

Example 3. $EE(R(C_n)) \approx 8.57594154\, n$, for large n.
In order to obtain this result, notice that by [3]

$$\phi(R(C_n),\lambda) = (\lambda+1)^n \, \phi\left(C_n, \frac{\lambda^2-2}{\lambda+1}\right) \ .$$

The eigenvalues of $R(C_n)$ are the roots of $(\lambda^2-2)/(\lambda+1) = 2\cos(2k\pi/n)$, $1 \le k \le n$. This yields

$$\lambda_k = \pm\sqrt{\cos^2\left(\frac{2k\pi}{n}\right) + 2\cos\left(\frac{2k\pi}{n}\right) + 2} + \cos\left(\frac{2k\pi}{n}\right)$$

and thus

$$\begin{aligned} EE(R(C_n)) &= \sum_{k=1}^{n} e^{\cos(\frac{2k\pi}{n}) + \sqrt{\cos^2(\frac{2k\pi}{n}) + 2\cos(\frac{2k\pi}{n}) + 2}} \\ &+ \sum_{k=1}^{n} e^{\cos(\frac{2k\pi}{n}) - \sqrt{\cos^2(\frac{2k\pi}{n}) + 2\cos(\frac{2k\pi}{n}) + 2}} \\ &\approx 8.57594154\, n \ . \end{aligned}$$

Proposition 5.

$$EE\left(\prod_{i=1}^{r} G_i\right) = \prod_{i=1}^{r} EE(G_i) \ .$$

In particular, $EE(G^r) = EE(G)^r$.

P r o o f. Let $\lambda_0^i, \ldots, \lambda_{n_i}^i$ be the eigenvalues of G_i, $1 \le i \le r$. Then [3] the eigenvalues of $G_1 \times G_2 \times \cdots \times G_r$ are of the form of $\lambda_{i_1}^1 + \cdots + \lambda_{i_r}^r$,

where $1 \leq i_j \leq n_j$. So,

$$EE\left(\prod_{i=1}^{r} G_i\right) = \sum_{i_1,i_2,\ldots,i_r} e^{\lambda_{i_1}^1 + \cdots + \lambda_{i_r}^r} = \sum_{i_1,\ldots,i_r} e^{\lambda_{i_1}^1} \cdots e^{\lambda_{i_r}^r} = \prod_{i=1}^{r} EE(G_i) \ .$$

□

Consider the graph G whose vertices are the N-tuples $b_1\, b_2 \cdots b_N$ with $b_i \in \{0, 1, \cdots, n_i - 1\}$, $n_i \geq 2$, and let two vertices be adjacent if the corresponding tuples differ in precisely one place. Such a graph is called a Hamming graph and is denoted by $H_{n_1,n_2,\cdots,n_N}$. A Hamming graph with $b_1 = b_2 = \cdots = b_N = 2$ is called a hypercube of dimension N and is denoted by Q_N. As well-known, a graph G is a Hamming graph if and only if it can be written in the form $G = \prod_{i=1}^{N} K_{n_i}$.

By Proposition 5, it is possible to compute the Estrada index of a Hamming graph: Since $EE(K_{n_i}) = (n_i - 1)e^{-1} + e^{n_i - 1}$, we get

$$EE(H_{n_1,n_2,\cdots,n_N}) = \prod_{i=1}^{N} [(n_i - 1)e^{-1} + e^{n_i - 1}] \ .$$

Corollary 5.1. *Let Q_n be a hypercube on 2^n vertices. Then*

$$EE(Q_n) = EE((K_2)^n) = [2\, cosh(1)]^n \ .$$

The graphs $R = C_n \times C_m$ and $S = P_n \times C_m$ correspond to what in the theory of nanomaterials is called a C_4–nanotorus and a C_4-nanotube, respectively. In the following corollary, Proposition 5 and the results from [14] are used to compute the Estrada index of R and S.

Corollary 5.2. *$EE(R) \approx mn\, I_0^2$ and $EE(S) \approx m(n+1)\, I_0^2 - m\, cosh(2) I_0$.*

P r o o f. By the main result of [14],

$$EE(C_n) = \sum_{i=1}^{n} e^{\lambda_i} = \sum_{i=1}^{n} e^{2\cos(\frac{2i\pi}{n})} \approx \frac{n}{2\pi} \int_0^{2\pi} e^{2\cos(x)} dx = n\, I_0$$

and

$$EE(P_n) = \sum_{i=1}^{n} e^{2\cos(\frac{k\pi}{n+1})} \approx (n+1) I_0 - cosh(2) \ .$$

The formulas given in Corollary 5.2 follow now straightforwardly from Proposition 5.

Corollary 5.3. *If $T = P_m \times P_n$, for some positive integers m and n, then $EE(T) \approx [(m+1)I_0 - cosh(2)][(n+1)I_0 - cosh(2)]$.*

3. *The L-Estrada index of graphs*

Let G be a graph without loops and multiple edges. Let n and m be, respectively, the number of vertices and edges of G. Such a graph will be referred to as an (n, m)-graph.

Proposition 6. *The following properties of the L-Estrada index hold:*

(a) $LEE(G) \geq ne^{2m/n}$ with equality if and only if $G = \overline{K}_n$,

(b) Suppose that G_1 and G_2 are graphs with $|V(G_i)| = n_i$, $i = 1, 2$. Then

$$LEE(G_1 + G_2) = e^{n_2}\, LEE(G_1) + e^{n_1}\, LEE(G_2) + e^{n_1+n_2} - e^{n_1} - e^{n_2} + 1 \ .$$

(c) Suppose that $G_1, G_2, \ldots, G_k$ are graphs with mutually disjoint vertex sets. Then

$$LEE\left(\prod_{i=1}^{k} G_i\right) = \prod_{i=1}^{k} LEE(G_i) \ .$$

In particular, $LEE(G^k) = LEE(G)^k$.

(d) If G is an r-regular bipartite graph, then $LEE(G) = e^r\, EE(G)$.

P r o o f. (a) Proposition 6(a) is deduced in a manner analogous to the proof of Proposition 1.

(b) Let $\mu_1, \mu_2, \ldots, \mu_{n_1}$ and $\mu'_1, \mu'_2, \ldots, \mu'_{n_2}$ be the Laplacian eigenvalues of G_1 and G_2, respectively. Then by [3], the Laplacian eigenvalues of $G_1 + G_2$ are of the form $n_2 + \mu_i$, $2 \leq i \leq n$; $n_1 + \mu'_j$, $2 \leq j \leq n$ or 0 or $n_1 + n_2$. This leads to the proof of (b).

(c) In order to prove Proposition 6(c), we assume that G_i, $1 \leq i \leq k$, has n_i vertices. Then by a result of Fiedler [8], the Laplacian eigenvalues of $\prod_{i=1}^{k} G_i$ are of the form $\sum_{i=1}^{k} \mu_{j_i}(G_i)$, $1 \leq j_i \leq n_i$. Therefore,

$$LEE(G) = \sum_{t=1}^{n} e^{\sum_{j_t=1}^{n_t} \mu_{j_t}} = \sum_{i=1}^{n} \prod_{k=1}^{n} e^{\mu_{j_i}} = \prod_{i=1}^{n} LEE(G_i) \ .$$

(d) Finally, we assume that G is an r-regular bipartite graph and λ_i, μ_i, $1 \le i \le n$, are its eigenvalues and Laplacian eigenvalues. Then $\mu_i = r - \lambda_i$ and

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

Since G is bipartite, the eigenvalues of G are symmetric around zero. This implies (d). □

Corollary 6.1. *Let $G_1, G_2, \ldots, G_k$ be n-vertex graphs. Then*

$$LEE\left(\sum_{i=1}^{k} G_i\right) = e^{(k-1)n} \sum_{i=1}^{k} LEE(G_i) + (k-1)\, e^{kn} - k\, e^{n(k-1)} + 1 \ .$$

In particular, $LEE(k\,G) = k\, e^{n(k-1)} LEE(G) + (k-1)\, e^{kn} - k\, e^{n(k-1)} + 1$.

P r o o f. follows by induction on k. □

Example 4. By Proposition 6(c), it is possible to compute the L-Estrada index of a Hamming graph. To do this, note that $LEE(K_{n_i}) = 1 + (n_i - 1)\, e^{n_i}$ and so

$$LEE(H_{n_1,n_2,\ldots,n_N}) = \prod_{i=1}^{N} [1 + (n_i - 1) e^{n_i}] \ .$$

In particular, for a hypercube Q_N, $LEE(Q_N) = (1 + e^2)^N = e^N\, EE(Q_N)$.

Example 5. Let R, S, and T be same as in Corollaries 5.2 and 5.3. In order to apply Proposition 6(d), we first compute the L-Estrada indices of P_n and C_n:

$$LEE(P_n) = \sum_{k=0}^{n-1} e^{4\sin^2(k\pi/(2n))} \approx n \int_0^1 e^{4\sin^2(\pi\, x/2)} dx = n\, J_0 \ (\approx 16.84398368\, n)$$

and

$$LEE(C_n) = \sum_{k=1}^{n} e^{4\sin^2(k\pi/n)} \approx n \int_0^1 e^{4\sin^2(\pi x)} dx = n\, J_0 \ .$$

By Proposition 6(c),

$$LEE(R) = LEE(P_n)\, LEE(C_m) \approx nm\, J_0^2\, LEE(S) \approx km\, J_0^2$$

and $LEE(T) \approx mn\, J_0^2$.

Example 6. Let S_n be the n-vertex star. Then by Proposition 6(b),

$$LEE(S_n) = LEE(K_1 + \overline{K}_{n-1}) = (n-2)e + e^{n+2} + 1 \ .$$

Example 7. Let W_n be the n-vertex wheel. By Theorem 5(b),

$$LEE(W_{n+1}) = LEE(K_1 + C_n) = e\, LEE(C_n) + e^{n+1} - e + 1 \ .$$

Example 8. $LEE(K_{m,n}) = (n-1)e^m + (m-1)e^n + e^{m+n} + 1$.

The Zagreb index (or more precisely: the first Zagreb group index) is defined as [11, 19] $Zg(G) = \sum_{i \in V(G)} deg(i)^2$. In what follows, relations between the L-Estrada and Zagreb indices are found.

Proposition 7. *Let G be an (n, m)-graph. Then the L-Estrada index of G is bounded as:*

$$\begin{aligned} \sqrt{n(n-1)e^{4m/n} + n + 8m + 2\, Zg(G)} \ &\leq \ LEE(G) \\ &\leq \ n - 1 + e^{2m} + m - 2m^2 + \frac{1}{2}\, Zg(G) \ . \end{aligned}$$

Equality on both sides of the above inequality is attained if and only if $G \cong \overline{K_n}$.

P r o o f. Using a similar method as in [20], we have

$$\begin{aligned} LEE(G) \ &= \ \sum_{i=1}^{n} e^{\mu_i} = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\mu_i^k}{k!} = n + \sum_{i=1}^{n} \mu_i + \sum_{i=1}^{n} \frac{\mu_i^2}{2!} + \sum_{i=1}^{n} \sum_{k \geq 3} \frac{\mu_i^k}{k!} \\ &= \ n + 3m + \frac{1}{2} Zg(G) + \sum_{i=1}^{n} \sum_{k \geq 3} \frac{\mu_i^k}{k!} = n + 3m + \frac{1}{2} Zg(G) + \sum_{k \geq 3} \frac{1}{k!} \sum_{i=1}^{n} \mu_i^k \\ &\leq \ n + 3m + \frac{1}{2} Zg(G) + \sum_{k \geq 3} \frac{1}{k!} \left(\sum_{i=1}^{n} \mu_i \right)^k \\ &= \ n + 3m + \frac{1}{2} Zg(G) + \sum_{k \geq 3} \frac{1}{k!} (2m)^k \\ &= \ n + 3m + \frac{1}{2} Zg(G) + e^{2m} - 2m^2 - 2m - 1 \end{aligned}$$

resulting in the upper bound.

On the other hand, $LEE(G)^2 = \sum\limits_{i=1}^{n} e^{2\mu_i} + 2\sum\limits_{i<j} e^{\mu_i}\, e^{\mu_j}$ and so,

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

By means of a power–series expansion, we get

$$\begin{aligned} \sum_{i=1}^{n} e^{2\mu_i} &= \sum_{i=1}^{n}\sum_{k\geq 0}\frac{(2\mu_i)^2}{k!} = n + 4m + \sum_{i=1}^{n}\sum_{k\geq 2}\frac{(2\mu_i)^2}{k!} \\ &\geq n + 8m + 2\,Zg(G)\ . \end{aligned}$$

Therefore, $LEE(G)^2 \geq n(n-1)e^{4m/n} + n + 8m + 2Zg(G)$. This implies the lower bound.

If $G \cong \overline{K}_n$ then obviously $m = 0$ and equality on both sides of the above inequality holds. Conversely, we assume that

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

Then $\sum\limits_{k\geq 4}(2\mu_i)^k/k! = 0$, which implies that $\mu_i = 0, 1 \leq i \leq n$, as desired. If

$$LEE(G) = n - 1 + e^{2m} + m - 2m^2 + \frac{1}{2}\,Zg(G)$$

then

$$\sum_{i=1}^{n}\mu_i^k = \left(\sum_{i=1}^{n}\mu_i\right)^k\ .$$

Thus $\mu_i = 0$, $2 \leq i \leq n$. This completes the proof. □

Corollary 7.1. *If G is an r-regular bipartite graph, then*

$$e^r\sqrt{n^2 + 2nr} \leq LEE(G) \leq e^r\,[n - 2 + 2\,cosh(\sqrt{nr})]\ .$$

P r o o f. Apply Proposition 6(d) and Proposition 2 from [4]. □

Proposition 8. *If G is an r-regular graph, then*

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

In particular, for r-regular graphs, $LEE(L(G)) = LEE(G)$ if and only if $r = 2$.

P r o o f is analogous to the proof of Proposition 2 [1]. □

Corollary 8.1. *Let $L(G) \equiv L^1(G)$ and for $k \leq 1$, $L^{k+1}(G) = L(L^k(G))$. If G is r-regular then*

$$LEE(L^{k+1}(G)) = LEE(L^k(G)) + n_k\, \frac{r_k - 2}{2}\, e^{2r_k}$$

where $L^k(G)$ is r_k-regular with n_k vertices,

$$r_k = (r-2)2^k + 2 \qquad \textit{and} \qquad n_k = \frac{n}{2^k} \prod_{i=0}^{k-1} (2^i\, r - 2^{i-1} + 2) \ .$$

Proposition 9. If G is an r-regular graph with n vertices then

$$1 + \sqrt{n - 2 + 2nr + 4r - 4r^2 + e^{-2r} + (n-1)(n-2)e^{2r/(n-1)}}$$

$$\leq \quad e^{-r}\, LEE(G) \leq n - 1 - r^2 + \frac{nr}{2} + e^r \ .$$

P r o o f. In order to obtain the lower bound, we consider $(e^{-r} LEE(G) - 1)^2$ and proceed in the same manner as in Proposition 7. In this case,

$$(e^{-r} LEE(G) - 1)^2 = \left(\sum_{\lambda_i \neq r} e^{-\lambda_i} \right)^2 = 2 \sum_{\lambda_i \neq r \neq \lambda_j} e^{-\lambda_i}\, e^{-\lambda_j} + \sum_{\lambda_i \neq r} e^{-2\lambda_i} \ .$$

Now,

$$2 \sum_{\lambda_i \neq r \neq \lambda_j,\ i \neq j} e^{-\lambda_i}\, e^{-\lambda_j} \quad \geq \quad (n-1)(n-2) \left(\prod_{\lambda_i \neq r \neq \lambda_j,\ i \neq j} e^{-\lambda_i}\, e^{-\lambda_j} \right)^{2/[(n-1)(n-2)]}$$

$$
\begin{aligned}
&= (n-1)(n-2)\left(\prod_{\lambda_i \neq r} e^{-\lambda_i}\right)^{2/(n-1)} \\
&= (n-1)(n-2)(e^r)^{2/(n-1)} \\
&= (n-1)(n-2)e^{2r/(n-1)}
\end{aligned}
$$

$$
\begin{aligned}
\sum_{\lambda_i \geq 0} e^{-2\lambda_i} &= \sum_{\lambda_i \neq r} \sum_{k \geq 0} e^{-2\lambda_i} \\
&\geq n - 1 + \sum_{\lambda_i \neq r} (-2\lambda_i) + \sum_{\lambda_i \neq r} \frac{(-2\lambda_i)^2}{2!} + \sum \frac{(-2\lambda_i)^3}{3!} + \cdots \\
&= n - 2 + 2rn - 4r^2 + e^{-2r} + 4r \ .
\end{aligned}
$$

Therefore,

$$
\frac{LEE(G)}{e^r} \geq 1 + \sqrt{n - 2 + 4r + 2nr - 4r^2 + e^{-2r} + (n-1)(n-2)e^{2r/(n-1)}} \ .
$$

We now prove the right–hand side inequality:

$$
e^{-r}\, LEE(G) = 1 + \sum_{\lambda_i \neq r} e^{-\lambda_i} = n + r + \frac{nr - r^2}{2} + \sum_{k \geq 3} \frac{(\lambda_i)^k}{k!} \leq n - 1 + \frac{nr}{2} - r^2 + e^r \ .
$$

□

Corollary 9.1. *Let G be an r-regular bipartite graph. Then,*

$$
\begin{aligned}
2\, cosh(r) + \sqrt{(n-2)^2 + 2nr - 4r^2} \ &\leq \ \frac{LEE(G)}{e^r} = EE(G) \\
&\leq \ n - 4 + 2\, cosh(r) + 2\, cosh\left(\sqrt{\frac{nr}{2} - r^2}\right) \ .
\end{aligned}
$$

P r o o f. Corollary 9.1 follows from Theorem 4 in [4] and Proposition 6(d). □

Proposition 10. *$LEE(G) \leq e^{2m/n}(n-1+e^{LE(G)})$ with equality if and only if $G \cong \overline{K}_n$.*

P r o o f.

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

Clearly, equality holds if and only if G is an empty graph. □

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REFERENCES

[1] T. A l e k s ić, I. G u t m a n, M. P e t r o v i ć, *Estrada index of line graphs*, Bull. Acad. serbe sci. arts (Cl. Math. Natur.) **134** (2007) 33–41.

[2] R. C a r b ó – D o r c a, *Smooth function topological structure descriptors based on graph spectra*, J. Math. Chem. **44** (2008) 373–378.

[3] D. C v e t k o v i ć, M. D o o b, H. S a c h s, *Spectra of Graphs – Theory and Application*, Barth, Heidelberg, 1995.

[4] J. A. d e l a P e ñ a, I. G u t m a n, J. R a d a, *Estimating the Estrada index*, Lin. Algebra Appl. **427** (2007) 70–76.

[5] E. E s t r a d a, *Characterization of 3D molecular structure*, Chem. Phys. Lett. **319** (2000) 713–718.

[6] E. E s t r a d a, *Characterization of the folding degree of proteins*, Bioinformatics **18** (2002) 697-704.

[7] E. E s t r a d a, *Topological structural classes of complex networks*, Phys. Rev. E **75** (2007) 016103.

[8] M. F i e d l e r, *Algebraic connectivity of graphs*, Czech. Math. J. **23** (1973) 298–305.

[9] Y. G i n o s a r, I. G u t m a n, T. M a n s o u r, M. S c h o r k, *Estrada index and Chebyshev polynomials*, Chem. Phys. Lett. **454** (2008) 145–147.

[10] I. G u t m a n, *Lower bounds for Estrada index*, Publ. Inst. Math. (Beograd) **83** (2008) 1–7.

[11] I. G u t m a n, K. C. D a s, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50** (2004) 83–92.

[12] I. G u t m a n, E. E s t r a d a, J. A. R o d r í g u e z – V e l á z q u e z, *On a graph spectrum based structure descriptor*, Croat. Chem. Acta **80** (2007) 151–154.

[13] I. G u t m a n, B. F u r t u l a, B. G l i š i ć, V. M a r k o v i ć, A. V e s e l, *Estrada index of acyclic molecules*, Indian J. Chem. **A46** (2007) 723–728.

[14] I. G u t m a n, A. G r a o v a c, *Estrada index of cycles and paths*, Chem. Phys. Lett. **436** (2007) 294–296.

[15] I. G u t m a n, S. R a d e n k o v i ć, *Estrada index of benzenoid hydrocarbons*, Z. Naturforsch. **62a** (2007) 254–258.

[16] I. G u t m a n, S. R a d e n k o v i ć, *A lower bound for the Estrada index of bipartite molecular graphs*, Kragujevac J. Sci. **29** (2007) 67–72.

[17] I. G u t m a n, S. R a d e n k o v i ć, B. F u r t u l a, T. M a n s o u r, M. S c h o r k, *Relating Estrada index with spectral radius*, J. Serb. Chem. Soc. **72** (2007) 1321–1327.

[18] I. Gutman, S. Radenković, A. Graovac, D. Plavšić, *Monte Carlo approach to Estrada index*, Chem. Phys. Lett. **446** (2007) 233–236.

[19] I. G u t m a n, N. T r i n a j s t i ć, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972) 535–538.

[20] I. G u t m a n, B. Z h o u, *Laplacian energy of a graph*, Lin. Algebra Appl. **414** (2006) 29–37.

[21] R. M e r r i s, *Laplacian matrices of graphs: A survey*, Lin. Algebra Appl. **197–198** (1994) 143–176.

[22] R. M e r r i s, *A survey of graph Laplacians*, Lin. Multilin. Algebra **39** (1995) 19–31.

[23] B. M o h a r, *The Laplacian spectrum of graphs*, in: Y. Alavi, G. Chartrand, O. R. Oellermann, A. J. Schwenk (Eds.), *Graph Theory, Combinatorics, and Applications*, Wiley, New York, 1991, pp. 871–898.

[24] M. R o b b i a n o, J. J i m é n e z, L. M e d i n a, *The energy and an approximation to Estrada index of some trees*, MATCH Commun. Math. Comput. Chem. **61** (2009) 369–382.

[25] H. Z h a o, Y. J i a, *On the Estrada index of bipartite graphs*, MATCH Commun. Math. Comput. Chem. **61** (2009) 495–501.

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