LAPLACIAN ESTRADA INDEX OF TREES

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(Received August 25, 2009)

Abstract

Let $G$ be a simple graph with $n$ vertices and let $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_{n-1} \geq \mu_n = 0$ be the eigenvalues of its Laplacian matrix. The Laplacian Estrada index of a graph $G$ is defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$. Using the recent connection between Estrada index of a line graph and Laplacian Estrada index, we prove that the path $P_n$ has minimal, while the star $S_n$ has maximal $LEE$ among trees on $n$ vertices. In addition, we find the unique tree with the second maximal Laplacian Estrada index.

1. INTRODUCTION

Let $G$ be a simple graph with $n$ vertices. The spectrum of $G$ consists of the eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ of its adjacency matrix [1]. The Estrada index of $G$ is defined as

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

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This graph–spectrum–based graph invariant was put forward by Estrada in [2, 3], where it was shown that \( EE(G) \) can be used as a measure of the degree of folding of long chain polymeric molecules. Further, it was shown in [4] that the Estrada index provides a measure of the centrality of complex networks, while a connection between the Estrada index and the concept of extended atomic branching was pointed out in [5]. Some mathematical properties of the Estrada index were studied in [6–17].

For a graph \( G \) with \( n \) vertices, let \( \mu_1 \geq \mu_2 \geq \ldots \geq \mu_{n-1} \geq \mu_n = 0 \) be the eigenvalues of its Laplacian matrix [18]. In full analogy with Eq. (1), the Laplacian Estrada index of \( G \) is defined as [19]

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

Bounds for the Laplacian Estrada index may be found in [19–21].

Let \( L(G) \) be the line graph of \( G \). In [21], the authors proved the following relation between Laplacian Estrada index of \( G \) and Estrada index of a line graph of \( G \).

**Theorem 1.** [21] Let \( G \) be a graph with \( n \) vertices and \( m \) edges. If \( G \) is bipartite, then

\[
LEE(G) = n - m + e^2 \cdot EE(L(G)).
\]

Our goal here is to add some further evidence to support the use of \( LEE \) as a measure of branching in alkanes. While the measure of branching cannot be formally defined, there are several properties that any proposed measure has to satisfy [22, 23]. Basically, a topological index \( TI \) acceptable as a measure of branching must satisfy the inequalities

\[
TI(P_n) < TI(T) < TI(S_n) \quad \text{or} \quad TI(P_n) > TI(T) > TI(S_n),
\]

for \( n = 5, 6, \ldots \), where \( P_n \) is the path, \( S_n \) is the star on \( n \) vertices, and \( T \) is any \( n \)-vertex tree, different from \( P_n \) and \( S_n \). For example, the first relation is obeyed by the largest graph eigenvalue [24] and Estrada index [15], while the second relation is obeyed by the Wiener index [25], Hosoya index and graph energy [26].

We show that among the \( n \)-vertex trees, the path \( P_n \) has minimal and the star \( S_n \) maximal Laplacian Estrada index,

\[
LEE(P_n) < LEE(T) < LEE(S_n),
\]

where \( T \) is any \( n \)-vertex tree, different from \( P_n \) and \( S_n \). We also find the unique tree with the second maximal Laplacian Estrada index.
2. LAPLACIAN ESTRADA INDEX OF TREES

In our proofs, we will use a connection between Estrada index and the spectral moments of a graph. For $k \geq 0$, we denote by $M_k$ the $k$th spectral moment of $G$,

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

A walk of length $k$ in $G$ is any sequence of vertices and edges of $G$, $w_0, e_1, w_1, e_2, \ldots, w_{k-1}, e_k, w_k$, such that $e_i$ is the edge joining $w_{i-1}$ and $w_i$ for every $i = 1, 2, \ldots, k$. The walk is closed if $w_0 = w_k$. It is well-known (see [1]) that $M_k(G)$ represents the number of closed walks of length $k$ in $G$. Obviously, for every graph $M_0 = n$, $M_1 = 0$ and $M_2 = 2m$. From the Taylor expansion of $e^x$, we have that the Estrada index and the spectral moments of $G$ are related by

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k}{k!}.$$  \hspace{1cm} (2)

Thus, if for two graphs $G$ and $H$ we have $M_k(G) \geq M_k(H)$ for all $k \geq 0$, then $EE(G) \geq EE(H)$. Moreover, if the strict inequality $M_k(G) > M_k(H)$ holds for at least one value of $k$, then $EE(G) > EE(H)$.

Among the $n$-vertex connected graphs, the path $P_n$ has minimal and the complete graph $K_n$ maximal Estrada index [8, 15],

$$EE(P_n) < EE(G) < EE(K_n),$$  \hspace{1cm} (3)

where $G$ is any $n$-vertex connected graph, different from $P_n$ and $K_n$.

**Theorem 2.** Among the $n$-vertex trees, the path $P_n$ has minimal and the star $S_n$ maximal Laplacian Estrada index,

$$LEE(P_n) < LEE(T) < LEE(S_n),$$

where $T$ is any $n$-vertex tree, different from $P_n$ and $S_n$.

**Proof.** The line graph of a tree $T$ is a connected graph with $n-1$ vertices. The line graph of a path $P_n$ is also a path $P_{n-1}$, while the line graph of a star $S_n$ is a complete graph $K_{n-1}$. Using the relation (3) it follows that

$$EE(\mathcal{L}(P_n)) \leq EE(\mathcal{L}(T)) \leq EE(\mathcal{L}(S_n)),$$

and from Theorem 1 we get $LEE(P_n) \leq LEE(T) \leq LEE(S_n)$ with left equality if and only if $T \cong P_n$ and right equality if and only if $T \cong S_n$.  \hspace{1cm} □
3. SECOND MAXIMAL LAPLACIAN ESTRADA OF TREES

**Definition 1.** Let $v$ be a vertex of degree $p+1$ in a graph $G$, which is not a star, such that $vv_1, vv_2, \ldots, vv_p$ are pendent edges incident with $v$ and $u$ is the neighbor of $v$ distinct from $v_1, v_2, \ldots, v_p$. We form a graph $G' = \sigma(G, v)$ by removing edges $vv_1, vv_2, \ldots, vv_p$ and adding new edges $uv_1, uv_2, \ldots, uv_p$. We say that $G'$ is $\sigma$-transform of $G$.

![Figure 1: $\sigma$-transformation applied to $G$ at vertex $v$.](image)

**Theorem 3.** Let $G' = \sigma(G, v)$ be a $\sigma$-transform of a bipartite graph $G$. Then

$$\text{LEE}(G) < \text{LEE}(G'). \quad (4)$$

**Proof.** The graphs $G$ and $G'$ are both bipartite and have the same number of vertices and edges. Using Theorem 1, it is enough to prove inequality

$$\text{EE}(\mathcal{L}(G)) < \text{EE}(\mathcal{L}(G')).$$

Let $u_1, u_2, \ldots, u_m$ be the neighbors of $u$ in $G$, different from $v$. Consider the induced subgraph $H$ of $\mathcal{L}(G)$ formed using vertices $vv_1, vv_2, \ldots, vv_p, vu, uu_1, uu_2, \ldots, uu_m$. It is easy to see that these vertices are grouped in two cliques of sizes $p + 1$ and $m + 1$ with the vertex $uv$ in common. Similarly, consider the induced subgraph $H'$ of $\mathcal{L}(G')$ formed using corresponding vertices $uw_1, uw_2, \ldots, uw_p, vu, uu_1, uu_2, \ldots, uu_m$. Here, we have one clique of size $m + 1$.

Since $H$ is a proper subgraph of $H'$, it follows that for every $k \geq 0$, $M_k(H') \geq M_k(H)$ and then $M_k(\mathcal{L}(G')) \geq M_k(\mathcal{L}(G))$, which is strict for some $k$. Finally, using the relation (2), we have $\text{LEE}(G) < \text{LEE}(G'). \quad \square$

Let $T$ be an arbitrary tree on $n$ vertices with root $v$. We can find a vertex $u$ that is the parent of the leaf on the deepest level and apply $\sigma$-transformation at $u$ to strictly increase the Laplacian Estrada index.
Corollary 1. Let $T$ be a tree on $n$ vertices. If $T \not\cong S_n$, then $\text{LEE}(T) < \text{LEE}(S_n)$.

Let $S_n(a, b)$ be the tree formed by adding an edge between the centers of the stars $S_a$ and $S_b$, where $a + b = n$ and $2 \leq a \leq \lfloor \frac{n}{2} \rfloor$. We call $S_n(a, b)$ the double star. By direct calculation, the characteristic polynomial of the Laplacian matrix of the double star $S_n(a, b)$ is equal to

$$P(x) = (-1)^n x(x-1)^{n-4} \left(x^3 - (n+2)x^2 + (n+2 + ab)x - n\right).$$

We may assume that $n > 5$. The Laplacian spectra of $S_n(a, b)$ consists of three real roots of polynomial $f_{n,a}(x) = x^3 - (n+2)x^2 + (n+2 + a(n-a))x - n$, $1$ with multiplicity $n-4$, and $0$ with multiplicity one. In order to establish the ordering of double stars with $n$ vertices by LEE values it is enough to consider the following function $g_{n,a}(x_1, x_2, x_3) = e^{x_1} + e^{x_2} + e^{x_3}$, where $x_1 \geq x_2 \geq x_3 > 0$ are the roots of $f_{n,a}(x)$.

We locate $x_1$, $x_2$ and $x_3$. First we have

$$f_{n,a}(n-a+1) = 1-a < 0$$

and

$$f_{n,a}\left(n-a+\frac{3}{2}\right) = \frac{15}{8} + a^2 + n + \frac{n^2}{2} - \frac{11a}{4} - \frac{3na}{2}.$$ 

The last function (considered as a quadratic function of $a$) is decreasing for $a < \frac{11}{8} + \frac{3n}{4}$, and then for $a \leq \frac{n}{2} - 1$, we have

$$f_{n,a}\left(n-a+\frac{3}{2}\right) > f_{n,a}\left(n-\frac{n}{2}+1+\frac{3}{2}\right) = \frac{45+n}{8} > 0.$$

Next we have

$$f_{n,a}(a) = (a-1)(n-2a) \geq 0 \text{ and } f_{n,a}(a+1) = 1 + a - n < 0.$$ 

Finally we have

$$f_{n,a}(0) = -n < 0 \text{ and } f_{n,a}(1) = (a-1)(n-1-a) > 0.$$ 

Thus $x_3 \in [0, 1]$, $x_2 \in [a, a+1]$ and $x_1 \in [n-a+1, n-a+\frac{3}{2}]$ for $2 \leq a \leq \frac{n}{2} - 1$. The function

$$h(a) = e^0 + e^a + e^{n-a+1} - e^1 - e^{a+2} - e^{n-a+1/2}$$

is decreasing for $a > 0$ (since $h'(a) < 0$), and then for $a \leq \frac{n}{2} - 1$ we have

$$h(a) \geq h\left(\frac{n}{2} - 1\right) = e^{n/2} (e^{-1} - e + e^2 - e^{3/2}) + 1 - e > \frac{e^{n/2}}{2} + 1 - e > 0.$$
Thus, for $2 \leq a < \lfloor n/2 \rfloor - 1$, we have
\[ e^0 + e^a + e^{n-a+1} > e^1 + e^{a+2} + e^{n-a+1/2}, \]
and then $\text{LEE}(S_n(a, b)) > \text{LEE}(S_n(a + 1, b - 1))$. The special case $a = \lfloor n/2 \rfloor$ can be handled easily,
\[
\text{LEE}(S_n(2, n - 2)) - \text{LEE} \left( S_n \left( \left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil \right) \right) \\
> e^{n-1} + e^2 - e^{\lfloor n/2 \rfloor} - e^{\lfloor n/2 \rfloor+2} - e > e^{\lfloor n/2 \rfloor-1} - e^2 - e > 0 \quad \text{for } n > 7
\]
and by direct calculation, we also have $\text{LEE}(S_n(2, n - 2)) - \text{LEE} \left( S_n \left( \left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil \right) \right) > 0$ for $n = 6, 7$. By Theorem 3, the second maximal $\text{LEE}$ for $n$-vertex trees is a double star $S_n(a, b)$, and then from discussions above, we have

**Corollary 2.** The unique tree on $n \geq 5$ vertices with the second maximal Laplacian Estrada index is a double star $S_n(2, n - 2)$.

Note that as above, $\text{LEE}(S_n(3, n - 3)) - \text{LEE} \left( S_n \left( \left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil \right) \right) > 0$ for $n \geq 8$ (the cases for $n = 8, 9$ need direct calculation). By Theorem 3 and discussions above, the third maximal Laplacian Estrada index for trees on $n \geq 6$ vertices is uniquely achieved by $S_n(3, n - 3)$ or a caterpillar of diameter four. Tested by computer on trees with at most 22 vertices, $S_n(3, n - 3)$ is the unique tree with the third and the caterpillar formed by attaching $n - 5$ pendent vertices to the center of a path $P_5$ is the unique tree with the fourth maximal Laplacian Estrada index for $n \geq 6$.

**Acknowledgement.** This work is supported by Research Grant 144007 of Serbian Ministry of Science and Technological Development, and the Guangdong Provincial Natural Science Foundation of China (Grant No. 8151063101000026).

**References**


