MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **63** (2010) 769-776

ISSN 0340 - 6253

LAPLACIAN ESTRADA INDEX OF TREES

Aleksandar Ilić[a] and Bo Zhou[b‡]

[a] *Faculty of Sciences and Mathematics, University of Niš, Višegradska 33, 18000 Niš, Serbia*
e-mail: aleksandari@gmail.com

[b] *Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China*
e-mail: zhoubo@scnu.edu.cn

(Received August 25, 2009)

Abstract

Let G be a simple graph with n vertices and let $\mu_1 \geqslant \mu_2 \geqslant \ldots \geqslant \mu_{n-1} \geqslant \mu_n = 0$ 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 $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_n$ of its adjacency matrix [1]. The Estrada index of G is defined as

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

‡Corresponding author.

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 $\mu_1 \geqslant \mu_2 \geqslant \ldots \geqslant \mu_{n-1} \geqslant \mu_n = 0$ 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 $\mathcal{L}(G)$ 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*

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

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

$$TI(P_n) < TI(T) < TI(S_n) \qquad \text{or} \qquad TI(P_n) > TI(T) > TI(S_n),$$

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 $k \geqslant 0$, we denote by M_k the kth 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

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

Thus, if for two graphs G and H we have $M_k(G) \geqslant M_k(H)$ for all $k \geqslant 0$, then $EE(G) \geqslant EE(H)$. 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],

$$EE(P_n) < EE(G) < EE(K_n), \tag{3}$$

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

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

and from Theorem 1 we get $LEE(P_n) \leqslant LEE(T) \leqslant LEE(S_n)$ with left equality if and only if $T \cong P_n$ and right equality if and only if $T \cong S_n$. $\square$

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 σ-transform of G.*

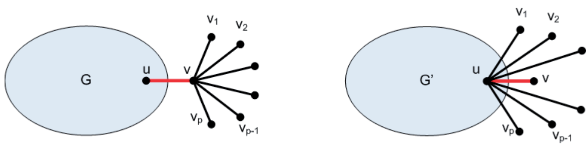

Figure 1: σ-transformation applied to G at vertex v.

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

$$LEE(G) < LEE(G')\,. \tag{4}$$

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

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

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 $uv_1, uv_2, \ldots, uv_p$, vu, $uu_1, uu_2, \ldots, uu_m$. Here, we have one clique of size $m+p+1$.

Since H is a proper subgraph of H', it follows that for every $k \geqslant 0$, $M_k(H') \geqslant M_k(H)$ 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 $LEE(G) < LEE(G')$. $\square$

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 σ-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 $LEE(T) < LEE(S_n)$.*

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 $2 \leqslant a \leqslant \lfloor \frac{n}{2} \rfloor$. 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 $x_1 \geqslant x_2 \geqslant x_3 > 0$ 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 $a \leqslant \frac{n}{2}-1$, we have

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

Next we have

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

Finally we have

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

Thus $x_3 \in [0,1]$, $x_2 \in [a,a+1]$ and $x_1 \in \left[n-a+1, n-a+\frac{3}{2}\right]$ for $2 \leqslant a \leqslant \frac{n}{2}-1$. 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 $a \leqslant \frac{n}{2}-1$ we have

$$h(a) \geqslant h\left(\frac{n}{2}-1\right) = e^{n/2}\left(e^{-1}-e+e^2-e^{3/2}\right)+1-e > \frac{e^{n/2}}{2}+1-e > 0.$$

Thus, for $2 \leqslant a < \lfloor \frac{n}{2} \rfloor - 1$, we have

$$e^0 + e^a + e^{n-a+1} > e^1 + e^{a+2} + e^{n-a+1/2},$$

and then $LEE(S_n(a,b)) > LEE(S_n(a+1,b-1))$. The special case $a = \lfloor \frac{n}{2} \rfloor$ can be handled easily,

$$\begin{aligned} & LEE(S_n(2,n-2)) - LEE\left(S_n\left(\left\lfloor \frac{n}{2} \right\rfloor, \left\lceil \frac{n}{2} \right\rceil\right)\right) \\ > \;& e^{n-1} + e^2 - e^{\lceil n/2 \rceil} - e^{\lceil n/2 \rceil + 2} - e > e^{\lceil n/2 \rceil} \cdot \left(e^{\lfloor n/2 \rfloor - 1} - 1 - e^2\right) - e > 0 \text{ for } n > 7 \end{aligned}$$

and by direct calculation, we also have $LEE(S_n(2,n-2)) - LEE\left(S_n\left(\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\right)\right) > 0$ for $n = 6, 7$. By Theorem 3, the second maximal 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 $n \geqslant 5$ vertices with the second maximal Laplacian Estrada index is a double star $S_n(2, n-2)$.*

Note that as above, $LEE(S_n(3,n-3)) - LEE\left(S_n\left(\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil\right)\right) > 0$ for $n \geqslant 8$ (the cases for $n = 8, 9$ need direct calculation). By Theorem 3 and discussions above, the third maximal Laplacian Estrada index for trees on $n \geqslant 6$ 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 $n \geqslant 6$.

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

[1] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980.

[2] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.* **319** (2000) 713–718.

[3] E. Estrada, Characterization of the folding degree of proteins, *Bioinformatics* **18** (2002) 697–704.

[4] E. Estrada, Topological structural classes of complex networks, *Phys. Rev. E* **75** (2007) 016103-1–016103-12.

[5] E. Estrada, J. A. Rodríguez-Valázquez, M. Randić, Atomic branching in molecules, *Int. J. Quantum Chem.* **106** (2006) 823–832.

[6] I. Gutman, B. Furtula, V. Marković, B. Glišić, Alkanes with greatest Estrada index, *Z. Naturforsch.* **62a** (2007) 495–498.

[7] I. Gutman, A. Graovac, Estrada index of cycles and paths, *Chem. Phys. Lett.* **436** (2007) 294–296.

[8] I. Gutman, E. Estrada, J. A. Rodríguez-Valázquez, On a graph–spectrum–based structure descriptor, *Croat. Chem. Acta* **80** (2007) 151–154.

[9] I. Gutman, S. Radenković, A. Graovac, D. Plavšić, Monte Carlo approach to Estrada index, *Chem. Phys. Lett.* **447** (2007) 233–236.

[10] J. A. de la Peña, I. Gutman, J. Rada, Estimating the Estrada index, *Linear Algebra Appl.* **427** (2007) 70–76.

[11] I. Gutman, Lower bounds for Estrada index, *Publ. Inst. Math.* (*Beograd*) (*N.S.*) **83** (2008) 1–7.

[12] B. Zhou, On Estrada index, *MATCH Commun. Math. Comput. Chem.* **60** (2008) 485–492.

[13] B. Zhou, N. Trinajstić, Estrada index of bipartite graphs, *Int. J. Chem. Model.* **1** (2008) 387–394.

[14] M. Robbiano, R. Jiménez, L. Medina, The energy and an approximation to Estrada index of some trees, *MATCH Commun. Math. Comput. Chem.* **61** (2009) 369–382.

[15] H. Deng, A proof of a conjecture on the Estrada index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 599–606.

[16] H. Deng, A note on the Estrada index of trees, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 607–610.

[17] A. Ilić, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.* (2009), doi:10.1007/s10910-009-9570-0.

[18] R. Merris, Laplacian matrices of graphs: a survey, *Linear Algebra Appl.* **197–198** (1994) 143–176.

[19] G. H. Fath-Tabar, A. R. Ashrafi, I. Gutman, Note on Estrada and L-Estrada indices of graphs, *Bull. Cl. Sci. Math. Nat. Sci. Math.*, in press.

[20] B. Zhou, On sum of powers of Laplacian eigenvalues and Laplacian Estrada index of graphs, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 611–619.

[21] B. Zhou, I. Gutman, More on the Laplacian Estrada index, *Appl. Anal. Discrete Math.* **3** (2009) 371–378.

[22] Z. Marković, V. Ivanov-Petrović, I. Gutman, Extremely branched alkanes, *J. Mol. Struct.* (*Theochem*) **629** (2003) 303–306.

[23] M. Fischermann, I. Gutman, A. Hoffmann, D. Rautenbach, D. Vidović, L. Volkmann, Extremal chemical trees, *Z. Naturforsch.* **57a** (2002) 49–52.

[24] L. Lovász, J. Pelikán, On the eigenvalues of trees, *Period. Math. Hung.* **3** (1973) 175–182.

[25] R. C. Entringer, D. E. Jackson, D. A. Snyder, Distance in graphs, *Czech. Math. J.* **26** (1976) 283–296.

[26] I. Gutman, Acyclic systems with extremal Hückel π-electron energy, *Theor. Chim. Acta* **45** (1977) 79–87.