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A note on the Laplacian Estrada index of trees[1]

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Abstract

The Laplacian Estrada index of a graph G is defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$, where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$ are the eigenvalues of its Laplacian matrix. An unsolved problem in [19] is whether $S_n(3, n-3)$ or $C_n(n-5)$ has the third maximal Laplacian Estrada index among all trees on n vertices, where $S_n(3, n-3)$ is the double tree formed by adding an edge between the centers of the stars S_3 and S_{n-3} and $C_n(n-5)$ is the tree formed by attaching $n-5$ pendent vertices to the center of a path P_5. In this paper, we partially answer this problem, and prove that $LEE(S_n(3, n-3)) > LEE(C_n(n-5))$ and $C_n(n-5)$ cannot have the third maximal Laplacian Estrada index among all trees on n vertices.

1 Introduction

The Estrada index of G is defined as

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

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of its adjacency matrix. This graph invariant based on graph-spectrum was put forward by Estrada in [1,2], where it was shown that $EE(G)$ can be used as a measure of the degree of folding of long chain polymeric

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molecules. Further, it was shown in [3] that the Estrada index provides a measure of the centrality of complex networks. Estrada et al. pointed out in [4] a connection between EE and the concept of extended atomic branching. Some mathematical properties of the Estrada index were studied in [5–15].

In analogy to the equation above, the Laplacian Estrada index [16] of G is defined as

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

where $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{n-1} \geq \mu_n = 0$ are the eigenvalues of its Laplacian matrix. Some bounds for the Laplacian Estrada index may be found in [16-18]. Specially, a relation between the Laplacian Estrada index of a bipartite graph G and the Estrada index of its line graph $L(G)$ was proved in [18].

Theorem 1([18]). Let G be a graph with n vertices and m edges. If G is bipartite, then $LEE(G) = n - m + e^2 EE(L(G))$.

The measure of branching is important in chemistry. In order to add some further evidence to support the use of LEE as a measure of branching in alkanes, it is worth to characterize the extremal graph or order the trees on n vertices with respect to LEE. Using the connection between Estrada index of a line graph and Laplacian Estrada index, it was proven in [19] that the path P_n and the star S_n have the minimal and maximal LEE among all trees on n vertices, respectively; while the double star $S_n(2, n-2)$ is the unique tree with the second maximal Laplacian Estrada index, where the double star $S_n(a, b)$ is the tree formed by adding an edge between the centers of the stars S_a and S_b, $a + b = n$. An unsolved problem in [19] is whether $S_n(3, n-3)$ or $C_n(n-5)$ (see Figure 1) has the third maximal Laplacian Estrada index. By their method, the third maximal Laplacian Estrada index of trees on $n \geq 6$ vertices is uniquely achieved by $S_n(3, n-3)$ or the tree with maximum Laplacian Estrada index among all caterpillar trees on n vertices and diameter 4. At the same time, testing by computer, Ilić and Zhou [19] pointed out that $S_n(3, n-3)$ is the unique tree with the third maximal Laplacian Estrada index and $C_n(n-5)$ is the unique tree with the fourth maximal Laplacian Estrada index for $6 \leq n \leq 22$.

In this paper, we partially answer this problem, and prove in a rigorous mathematical manner that the Laplacian Estrada index of $S_n(3, n-3)$ is greater than that of $C_n(n-5)$. This shows that $C_n(n-5)$ cannot have the third maximal Laplacian Estrada index among all trees on n vertices, and $S_n(3, n-3)$ is the unique trees with the third maximal Laplacian Estrada indices for $n \geq 6$ if $C_n(n-5)$ has the maximal Laplacian Estrada index among all trees om n vertices and diameter 4.

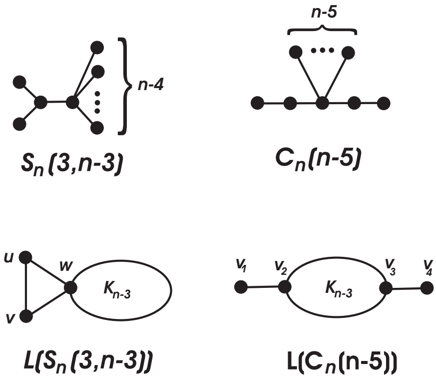

Fig. 1. $S_n(3, n-3)$, $C_n(n-5)$, and their line graphs.

2 $LEE(S_n(3, n-3)) > LEE(C_n(n-5))$

The following formulas can be used to compute the characteristic polynomials of some graphs.

Theorem 2([20]). Let $\phi(G, x)$ be the characteristic polynomial of a graph G.

(i)If v is a vertex of degree 1 in G, and w is the vertex adjacent to v, then

$$\phi(G, x) = x\phi(G - v, x) - \phi(G - v - w, x) \ .$$

(ii)If $e = vw$ is an edge of G, and $\mathcal{C}(e)$ is the set of all cycles containing e, then

$$\phi(G, x) = \phi(G - e, x) - \phi(G - v - w, x) - 2 \sum_{Z \in \mathcal{C}(e)} \phi(G - V(Z), x) \ .$$

Note that the characteristic polynomial of the complete graph K_n is

$$\phi(K_n, x) = (x + 1 - n)(x + 1)^{n-1} \ .$$

Let $G = L(S_n(3,n-3))$ and $H = L(C_n(n-5))$. By Theorem 2, we have

$$\begin{aligned}
\phi(G,x) = &\ \phi(G-uw,x) - \phi(K_{n-3},x) - 2\phi(K_{n-4},x) \\
= &\ x\phi(G-v,x) - x\phi(K_{n-4},x) - \phi(K_{n-3},x) - 2\phi(K_{n-4},x) \\
= &\ x(x\phi(K_{n-3},x) - \phi(K_{n-4},x)) - x\phi(K_{n-4},x) \\
- &\ \phi(K_{n-3},x) - 2\phi(K_{n-4},x) \\
= &\ (x^2-1)\phi(K_{n-3},x) - (2x+1)\phi(K_{n-4},x) \\
= &\ (x+1)^{n-4}(x^3-(n-4)x^2-3x+(3n-14))
\end{aligned}$$

and

$$\begin{aligned}
\phi(H,x) = &\ x\phi(H-v_1,x) - \phi(H-v_1-v_2,x) \\
= &\ x(x\phi(H-v_1-v_4,x) - \phi(H-v_1-v_4-v_3,x)) \\
- &\ (x\phi(H-v_1-v_2-v_4,x) - \phi(H-v_1-v_2-v_4-v_3,x) \\
= &\ x(x\phi(K_{n-3},x) - \phi(K_{n-4},x)) - (x\phi(K_{n-4},x) - \phi(K_{n-5},x)) \\
= &\ x^2\phi(K_{n-3},x) - 2x\phi(K_{n-4},x) + \phi(K_{n-5},x) \\
= &\ (x+1)^{n-6}(x^2+x-1)(x^3-(n-5)x^2-(n-3)x+(n-6))\ .
\end{aligned}$$

The spectrum of $L(S_n(3,n-3))$ consists of three real roots $a_1 \le a_2 \le a_3$ of polynomial $f(x) = x^3-(n-4)x^2-3x+(3n-14)$ and -1 with multiplicity $n-4$, while the spectrum of $L(C_n(n-5))$ consists of three real roots $b_1 \le b_2 \le b_3$ of polynomial $g(x) = x^3-(n-5)x^2-(n-3)x+(n-6)$, two real roots $c_1 \le c_2$ of x^2+x-1 and -1 with multiplicity $n-6$, where $c_1 = \frac{-1-\sqrt{5}}{2}$ and $c_2 = \frac{-1+\sqrt{5}}{2}$.

Theorem 3. $LEE(S_n(3,n-3)) > LEE(C_n(n-5))$.

Proof. It is true for $n \le 22$ in [19] tested by computer. We prove that $LEE(S_n(3,n-3)) > LEE(C_n(n-5))$ for $n \ge 9$. By Theorem 1, it is enough to show that $EE(L(S_n(3,n-3))) > EE(L(C_n(n-5)))$ for $n \ge 9$.

From the discussion above, we know that the spectra of $L(S_n(3,n-3))$ consists of three real roots $a_1 \le a_2 \le a_3$ of polynomial $f(x)$ and -1 with multiplicity $n-4$, while the spectra of $L(C_n(n-5))$ consists of three real roots $b_1 \le b_2 \le b_3$ of polynomial $g(x)$, two real roots $c_1 \le c_2$ of x^2+x-1 and -1 with multiplicity $n-6$. So, we only need to show that $R_1 > R_2$, where

$$R_1 = e^{a_1} + e^{a_2} + e^{a_3} + 2e^{-1}$$

$$R_2 = e^{b_1} + e^{b_2} + e^{b_3} + e^{c_1} + e^{c_2} \ .$$

For $n \geq 9$, we have

$$\begin{cases} f(-2) = -n < 0 \\ f(-1) = 2n - 8 > 0 \end{cases} \qquad \begin{cases} f(\frac{3}{2}) = \frac{3}{4}n - \frac{49}{8} > 0 \\ f(2) = 4 - n > 0 \end{cases}$$

$$\begin{cases} f(n-4) = -2 < 0 \\ f(n-3) = n^2 - 6n + 4 > 0 \end{cases} \qquad \begin{cases} g(-2) = -n < 0 \\ g(-1) = n - 5 > 0 \end{cases}$$

$$\begin{cases} g(0) = n - 6 > 0 \\ g(1) = 3 - n < 0 \end{cases} \qquad \begin{cases} g(n-4) = -2 < 0 \\ g(n-3) = n^2 - 5n + 3 > 0 \ . \end{cases}$$

And $a_1 \in [-2, -1]$, $a_2 \in [\frac{3}{2}, 2]$, $a_3 \in [n-4, n-3]$; $b_1 \in [-2, -1]$, $b_2 \in [0, 1]$, $b_3 \in [n-4, n-3]$.

Since $e^{-2} + e^{\frac{3}{2}} + 2e^{-1} \approx 5.35278$, $e^{-1} + e^{1} + e^{c_1} + e^{c_2} \approx 5.13973$,

$$e^{a_1} + e^{a_2} + 2e^{-1} \geq e^{-2} + e^{\frac{3}{2}} + 2e^{-1} > e^{-1} + e^{1} + e^{c_1} + e^{c_2} \geq e^{b_1} + e^{b_2} + e^{c_1} + e^{c_2} \ .$$

Now, $a_3 > n - 4$, $b_3 > n - 4$ and $f(x) - g(x) = -x^2 + (n-6)x + (2n-8) < 0$ for $x \geq n - 4$, i.e., $f(x) < g(x)$ for $x \geq n - 4$. We have $a_3 \geq b_3$ and $e^{a_3} \geq e^{b_3}$. So, $R_1 > R_2$.

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