MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **68** (2012) 835-842

ISSN 0340 - 6253

On the Laplacian Estrada Index of Unicyclic Graphs *

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(Received September 1, 2011)

Abstract

Let G be a simple graph with n vertices. If $\mu_1, \mu_2, \ldots, \mu_n$ are the Laplacian eigenvalues of G, then the Laplacian Estrada index is defined as $LEE(G) = \sum_{i=1}^{n} e^{\mu_i}$. In this paper, the unicyclic graph on n vertices with the maximal Laplacian Estrada index is determined.

1 Introduction

Given a simple graph G with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$, the adjacency matrix $A(G) = [a_{ij}]$ of G is an $n \times n$ symmetric matrix of 0's and 1's with $a_{ij} = 1$ if and only if v_i and v_j are joined by an edge. Denote the degree of vertex v_i by $d_G(v_i)$. Then the Laplacian matrix of G is $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix $diag(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$. Since $A(G), L(G)$ are real symmetric matrices, their eigenvalues $\lambda_1(G), \lambda_2(G), \cdots, \lambda_n(G)$ and $\mu_1(G), \mu_2(G), \cdots, \mu_n(G)$, respectively, are real numbers. The eigenvalues of $A(G)$ and $L(G)$ are called the adjacency eigenvalues and the Laplacian eigenvalues of G, respectively. In what follows we assume that $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G)$ and $\mu_1(G) \geq \mu_2(G) \geq \ldots \mu_{n-1}(G) \geq \mu_n(G) = 0$.

The Laplacian Estrada index of a graph G is defined in [9] as

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

*Supported by NSFC (Grant No.11001089).

(Independently of [9], another variant of the Laplacian Estrada index was put forward in [10], defined as $LEE^*(G) = \sum_{i=1}^{n} e^{\mu_i(G)-2m/n}$). Bounds and various properties of Laplacian Estrada index were found in [9–14]. For a bipartite graph G with n vertices and m edges, it is shown [8] that

$$LEE(G) = n - m + e^2 \cdot EE(\mathcal{L}(G)), \tag{1}$$

where $\mathcal{L}(G)$ is the line graph of G, and $EE(\mathcal{L}(G)) = \sum_{i=1}^{n} e^{\lambda_i(\mathcal{L}(G))}$ is the Estrada index ([5–7]) of $\mathcal{L}(G)$. Using the formal (1) and the results of Estrada index, Allić and Zhou [8] showed that the path P_n has minimal, while the star S_n has maximal Laplacian Estrada index among trees on n vertices. Obviously, this method is not suited to calculate the Laplacian Estrada index of the general graphs. So, it is interesting to consider the index for the non-bipartite graphs.

Let G be a graph with n vertices and m edges. If $n = m$, then we call G an unicyclic graph. Let S_n^3 be the unicyclic graph obtained by adding an edge to the star graph S_n. In this paper, we will show that S_n^3 is the unique unicyclic graph on n vertices with maximal Laplacian Estrada index.

2 Main Results

Let G be a graph with n vertices and let $G^* = G + e$ be the graph obtained from G by inserting a new edge e into G.

Lemma 1 *[1, 3] The Laplacian eigenvalues of G and G^* interlace, that is,*

$$\mu_1(G^*) \geq \mu_1(G) \geq \mu_2(G^*) \geq \mu_2(G) \geq \cdots \geq \mu_n(G^*) = \mu_n(G) = 0.$$

Lemma 2 *[15] Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, and N_u be the set of neighbors of u. Then*

$$\mu_1(G) \leq \max\{d_G(u) + d_G(v) - |N_u \cap N_v| : uv \in E(G)\}.$$

Let $s(G) = \max\{d_G(u)+d_G(v)-|N_u \cap N_v| : uv \in E(G)\}$ and $n(G) = |V(G)|$. Clearly, if G is an unicyclic graph with n vertices, then $s(G) \leq n$.

Lemma 3 *Let G be an unicyclic graph with $n \geq 8$ vertices and $s(G) \leq n(G) - 2$. Then $LEE(G) \leq LEE(S_n^3)$ with equality if and only if $G \cong S_n^3$.*

Proof. By induction on n to prove it. From the Appendix table of [2], there are 57 unicyclic graphs on 8 vertices of $s(G)$ not greater than 6. We give Table 1 for the LEE of these graphs, in which we use the same graph labels as the Appendix table of [2]. It implies that the result holds for $n = 8$.

· Table 1

Label	LEE	Label	LEE	Label	LEE	Label	LEE
1	134.7549405	16	186.9609149	36	262.8445145	59	196.5311973
2	160.1365435	17	196.4996349	40	375.5477041	60	198.9603315
3	162.8695473	18	194.0249743	46	148.2025007	61	255.6831930
4	161.8648960	19	197.9591155	47	171.0874842	63	255.6831930
5	185.7913581	20	196.4996349	48	173.6518698	66	223.4725411
6	167.0367695	21	200.5709879	49	177.5303031	67	255.6831930
7	189.8493511	22	273.2900119	50	180.1005287	68	260.1511708
8	188.8062398	24	221.0273062	51	171.2213615	69	262.4925186
9	187.0786847	25	225.1518983	52	173.6518698	70	266.9692919
10	191.1401409	26	262.3182544	53	204.5253414	72	282.6953428
11	166.9377926	27	229.4185558	54	194.2417996	74	285.1677715
12	249.2718699	28	229.5574315	55	200.5944661	75	289.5528217
13	213.8760808	29	269.3384290	56	232.4648707		
14	217.8548022	31	285.4480880	57	200.4566498		
15	254.8865204	33	289.9865503	58	239.4760009	S_8^3	3015.6384933

We now suppose that $n \geq 9$ and the result is true for graphs with vertex number less than n. Let G be a graph with n vertices. Suppose $G \cong C_n$. Then $\mu_1(C_n) \leq 4$ and $LEE(G) \leq ne^4$. Note that $LEE({S_n}^3) = e^n + e^3 + e^1 + \cdots + e^1 + e^0 > e^n$. Let $f(n) = e^n - n \cdot e^4$. Note that $f'(n) = e^n - n > 0$, and $f(7) = e^7 - 7e^4 > e^4 > 0$. Hence, $LEE(S_n^3) > e^n > ne^4 \geq LEE(G)$. Suppose $G \ncong C_n$. Then G must have a pendent vertex. Let $wt \in E(G)$ with $d_G(w) = 1$ and $G' = G - w$, then $s(G') \leq s(G) \leq n-2$ and $G = G' \cup \{w\} + wt$. Let $Spec(G') = \{\mu_1, \mu_2, \cdots, \mu_{n-1}\}$ be the Laplacian spectra of G', then

$$LEE(G' \cup \{w\}) = e^{\mu_1} + e^{\mu_2} + \cdots + e^{\mu_{n-1}} + e^0.$$

Note that $\mu_1(H) + \mu_2(H) + \ldots + \mu_n(H) = 2m$ for any graph H and m denotes the number of edges in H. By Lemma 1, then we can assume that the Laplacian spectra of G, is

$$Spec(G) = \{\mu_1 + x_1, \mu_2 + x_2, \cdots, \mu_{n-1} + x_{n-1}, 0\},$$

where $x_i \geq 0$ and $\sum_{i=1}^{n-1} x_i = 2$.

Case 1. $s(G') \leq n(G') - 2 = n - 3$. Then

$$\begin{aligned} LEE(G) &= \sum_{i=1}^{n-1} e^{\mu_i + x_i} + e^0 < e^{\mu_1 + 2} + \sum_{i=2}^{n-1} e^{\mu_i} + e^0 \\ &= e^{\mu_1+2} - e^{\mu_1} + e^0 + \sum_{i=1}^{n-1} e^{\mu_i} \\ &= e^{\mu_1+2} - e^{\mu_1} + e^0 + LEE(G'). \end{aligned}$$

By the induction hypothesis, $LEE(G') \leq LEE(S^3_{n-1})$ with equality if and only if $G' \cong S^3_{n-1}$. Now by Lemma 2, $\mu_1 \leq s(G') \leq n-3$, and we have

$$\begin{aligned} LEE(G) &\leq e^{\mu_1+2} - e^{\mu_1} + e^0 + LEE(S^3_{n-1}) \\ &= e^{\mu_1+2} - e^{\mu_1} + e^0 + (e^{n-1} + e^3 + (n-4)e^1 + e^0) \\ &= LEE(S^3_n) - [e^n - e^{n-1} + e^1 - e^0 - (e^{\mu_1+2} - e^{\mu_1}] \\ &\leq LEE(S^3_n) - [e^n - e^{n-1} + e^1 - e^0 - (e^{n-2} - e^{n-3})] \\ &= LEE(S^3_n) - (e-1)e^{n-3}(e^2 - e - 1) \\ &< LEE(S^3_n). \end{aligned}$$

Case 2. For any pendent vertex w, $s(G-w) = n-2$. Then $s(G) = n-2$ since $n-2 = s(G-w) \leq s(G) \leq n-2$. *That is,* $s(G-w) = s(G) = n-2$ *for any pendent vertex* w.

Suppose that $uv \in E(G)$ such that $d_G(u) + d_G(v) - |N_u \cap N_v| = s(G)$.

Subcase 2.1. u, v have no common neighbor. Suppose without loss of generality that $d_G(u) = y+1 \geq x+1 = d_G(v)$. Then $d_G(u) + d_G(v) = s(G) = n-2$, $x+y = n-4$, and G can be viewed as the connected graph obtained from a double star $S(x+1, y+1)$ and two isolated vertices by adding three edges to them such that each of the three edges is not incident to u and v, where a double star $S(a,b)$ is the tree obtained from the stars S_a and S_b by joining their centers an edge. Let $d_G(z_1) = \max\{d_G(z)|z \in V(G) \setminus \{u,v\}\}$. Then $d_G(z_1) \leq 4$.

Suppose $x \geq 4$. Then $d_G(u) \geq d_G(v) \geq 5$, and there must exists a pendent vertex adjacent to u in G. Let w_1 be an any pendent vertex at u, then $s(G-w_1) = s(G) - 1 = n-3$, a contradiction.

Suppose $x = 3$. If $d_G(z_1) = 4$, then $z_1 \in V(S(x+1, y+1)) \setminus \{u,v\}$ and the new three edges are all incident to z_1. Suppose that z_1 is adjacent to v, there must exist a pendent vertex, say w_2, adjacent to v, and then $s(G-w_2) = s(G) - 1 = n-3$, a contradiction. If $d_G(z_1) \leq 3$, then $d_G(u) \geq d_G(v) \geq 4 > d_G(z_1)$, and there must exist a pendent vertex, say w_3, that incident to u or v. Clearly, $s(G-w_3) < s(G) = n-2$, a contradiction again.

Suppose $x = 2$. Then $y = n-6 \geq 3 > x$. Clearly, there is no pendent vertex w_4 adjacent to u in G. Otherwise, $s(G-w_4) = s(G) - 1$. A contradiction. If $n \geq 11$, then $y = n-6 \geq 5$ and there must exist a pendent vertex w_5 adjacent to v, and consequently $s(G-w_5) = s(G) - 1$, a contradiction. So $9 \leq n \leq 10$. If $n = 10$, then $y = 4$. Since there are no pendent vertices adjacent to u, there exists at least a pendent vertex w_6

adjacent to v. Clearly, $s(G-w_6)=s(G)-1$, a contradiction. If $n=9$, note the condition $s(G-w)=s(G)=7$ for any pendent vertex w of G, then G must be H_1 or H_2 in fig.1. By direct computation, the result follows.

Suppose $x=1$. Then $y=n-4-1\geq 4$. If $n\geq 10$, then there exists a pendent vertex w_7 at u in G. Clearly, $s(G-w_7)<s(G)$, a contradiction. Thus $n=9$ and $G\cong H_3$, where H_3 is shown as in Fig.1. It is easy to prove the result by direct computation.

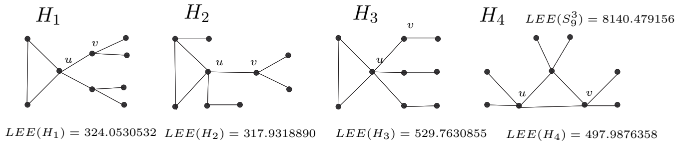

Figure 1 Graphs H_1, H_2, H_3 and H_4.

Subcase 2.2. u, v have a common neighbor. Then $d_G(u)+d_G(v)-1=n-2$. Suppose that $d_G(v)=x+1\leq y+1=d_G(u)$. Then $x+y=n-3$, and G can be viewed as the connected graph obtained from H and two isolated vertices by adding two edges to them such that the two new edges are not incident to u and v, where H is a graph obtained from a triangle $C_3=uvlu$ by attaching $x-1$ pendent vertices to v and $y-1$ pendent vertices to u.

Suppose $y\geq 4$. Then $y-1\geq 3$, and there exists a pendent vertex w_8 adjacent to u in G. It is easy to see that $s(G-w_8)=s(G)-1$, which is a contradiction.

Suppose $y\leq 3$. If $x=3$, then $y=3$ and $n=9$. By the conditions of case 2, $G\cong H_4$ (see Fig.1). So the result is true from the Fig.1. If $x\leq 2$, then $n=x+y+3\leq 8$, it contradict to the condition $n\geq 9$.

By combing Cases 1 and 2, the result follows. □

Lemma 4 *Let G be an unicyclic graph with $n\geq 8$ vertices and $s(G)=n-1$. Then $LEE(G)\leq LEE(S_n^3)$ with equality if and only if $G\cong S_n^3$.*

Proof. Suppose that uv be the edges such that $d_G(u)+d_G(v)-|N_u\cap N_v|=n-1$.

If u and v have no common neighbors, then G can be viewed as the connected graph obtained from a double star $S(a,b)$($a+b=n-1$) and an isolated vertex by adding two

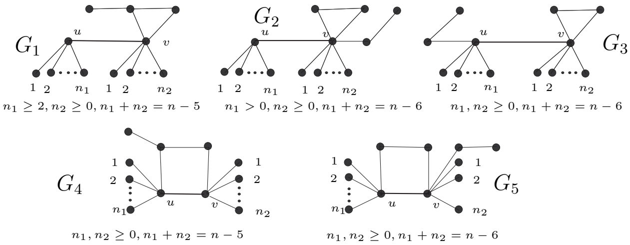

Figure 2 Graphs G_1, G_2, G_3, G_4 and G_5.

edges such that the two new edges are not incident to both u and v. Then G must be one of graphs in Fig.2 and Fig.3.

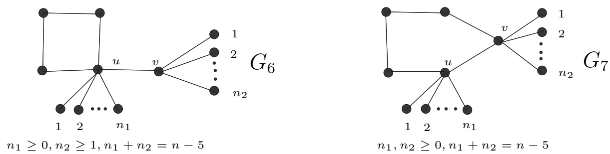

Figure 3 Graphs G_6 and G_7.

If u and v have a common neighbor, then G can be viewed as the connected graph obtained by G' and an isolated vertex by adding two edges such that the two new edges are not incident to both u and v, where G' is the graph obtained from a triangle $C_3 = zuvz$ by joining respectively x and y isolated vertices to u and v, where $x + y = n - 4$. Thus G must be one of graphs in Fig.4.

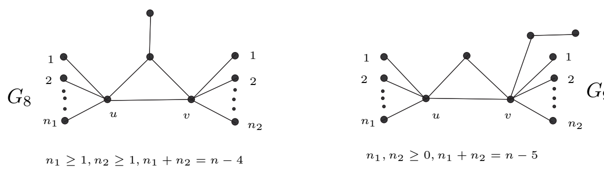

Figure 4 Graphs G_8 and G_9.

Note the fact that $G_i (i = 1, 2, \ldots 9)$ has Laplacian eigenvalues 1 with multiplicity at least $n_1 + n_2 - 2$ and 0 with multiplicity 1. If $n_1 + n_2 = n - 6$, then we suppose that $\mu_1, \mu_2, \mu_3, \mu_4, \mu_5, \mu_6, \mu_7$ are the remaining Laplacian eigenvalues of G, then $\mu_1 + \mu_2 + \mu_3 + \mu_4 + \mu_5 + \mu_6 + \mu_7 = 2n - (n-8) \cdot 1 - 0 = n + 8$. By Lemma 2, it follows that $\mu_1 \leq s(G) = n - 1$. So, we have that for $n - 1 \geq 9$,

$$\begin{aligned} LEE(G_i) &= e^{\mu_1} + e^{\mu_2} + e^{\mu_3} + e^{\mu_4} + e^{\mu_5} + e^{\mu_6} + e^{\mu_7} + (n-8)e^1 + e^0 \\ &\leq e^{n-1} + e^9 + 5e^0 + (n-8)e^1 + e^0 \\ &< e^n + e^3 + 5e^1 + (n-8)e^1 + e^0 \\ &= LEE(S_n^3) \end{aligned}$$

and for $n - 1 \leq 9$,

$$\begin{aligned} LEE(G_i) &\leq e^{n-1} + e^{n-1} + e^{10-n} + 4e^0 + (n-8)e^1 + e^0 \\ &< e^n + e^3 + e^1 + 4e^1 + (n-8)e^1 + e^0 \\ &= LEE(S_n^3) \end{aligned}$$

Similarly, we can prove the result for the cases $n_1 + n_2 = n - 4$ and $n_1 + n_2 = n - 5$, and then complete the proof. □

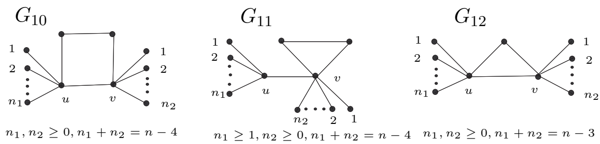

Figure 5 Graphs G_{10}, G_{11} and G_{12}.

Lemma 5 *Let G be the unicyclic graph with $n \geq 9$ vertices and $s(G) = n$. Then $LEE(G) \leq LEE(S_n^3)$ with equality if and only if $G \cong S_n^3$.*

Proof. Since $s(G) = n$, G is a type of graphs in Fig.5. By direct computation we can obtain that the Laplacian characteristic polynomials of G_{10}, G_{11} and G_{12} are respectively

$$\begin{aligned} L_{G_{10}}(x) &= x(x-1)^{n-5}[x^4 - (n+5)x^3 + (n_1n_2 + 6n + 4)x^2 - (3n_1n_2 + 10n - 4)x + 4n] \\ L_{G_{11}}(x) &= x(x-1)^{n-4}[x^3 - (n+2)x^2 + (n + 1 + n_1n_2 + 2n_1)x - n] \\ L_{G_{12}}(x) &= x(x-1)^{n-5}[x^4 - (n+5)x^3 + (5n + n_1n_2 + 7)x^2 - (7n + 2n_1n_2 + 3)x + 3n]. \end{aligned}$$

Then we can obtain that G_{10} has Laplacian eigenvalues 1 with multiplicity $n-5$, 0 with multiplicity 1, and the largest Laplacian eigenvalue less than $n-1$. By a similar proof of Lemma 4, it follows that $LEE(G_{10}) < LEE(S_n^3)$. Similarly, we also can prove that $LEE(G_{11}) < LEE(S_n^3)$ for $n_1 \geq 1, n_2 \geq 0$, and $LEE(G_{12}) < LEE(S_n^3)$ for $n_1, n_2 \geq 1$ and $n \geq 9$. If $n_1 = 0$, then $G_{12} \cong S_n^3$. Thus we complete the proof. □

By Lemmas 3, 4 and 5 it follows

Theorem 1 *Let G be a connected graph with n vertices and n edges, where $n \geq 9$. Then*

$$LEE(G) \leq e^n + e^3 + (n-3)e + 1$$

with equality if and only if $G \cong S_n^3$.

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