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Some Results on Laplacian Estrada Index of Graphs

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Abstract

Let G be a simple graph of order n and let $\mu_1(G), \mu_2(G), \ldots, \mu_n(G)$ be its Laplacian eigenvalues. The Laplacian Estrada index of G is defined as

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

In this paper, we present some new bounds for $LEE(G)$ in terms of the number of vertices, the number of edges, the maximum degree, the minimum degree, the clique number, the independence number and the chromatic number of the graph G, and characterize the graphs for which the bounds are attained. In addition, we give an asymptotic property of LEE of iterated line graphs of a regular graph.

1 Introduction

Let $G = (V, E)$ be a simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. The adjacency matrix of G is $A(G) = (a_{ij})$, where $a_{ij} = 1$ if the vertices v_i, v_j are adjacent in G and 0 otherwise. The eigenvalues of $A(G)$, denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$ (arranged in non-increasing order), are also called the eigenvalues of the graph G. The Laplacian matrix of G is defined to be $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of vertex degrees in G. The eigenvalues of $L(G)$, denoted by $\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G) \geq \mu_n(G) = 0$ (arranged in non-increasing order), are also referred to as the Laplacian eigenvalues of the graph G. The Laplacian spectrum of G is a multiset consisting of all its Laplacian eigenvalues, that is,

$$\text{Spec}_L(G) = \{\mu_1(G), \mu_2(G), \ldots, \mu_{n-1}(G), \mu_n(G)\}.$$

It is well known that the second smallest Laplacian eigenvalue $\mu_{n-1}(G) > 0$ if and only if G is connected, and hence it is called the algebraic connectivity of G as well [12]. For more properties concerning the Laplacian eigenvalues of graphs, one can refer to [13, 20].

The Estrada index of a graph G is defined as

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

This graph-spectrum-based graph invariant was put forward by Estrada in [7,8], 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 pointed out in [9] 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 found in [10]. In addition, various mathematical properties of the Estrada index were also investigated, see [14] for a comprehensive survey.

In analogy to the Estrada index, the Laplacian Estrada index of a graph G was introduced in [11] as

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

Independently, in [18], the authors defined the Laplacian Estrada index of G as

$$LEE_{LSC}(G) = \sum_{i=1}^{n} e^{\mu_i(G) - \frac{2m}{n}} \ ,$$

where the graph G has n vertices and m edges. Notice that these two "Laplacian Estrada indices" are essentially equivalent since $LEE(G) = e^{2m/n} LEE_{LSC}(G)$. In this paper, we use the definition (1) which looks simpler in the form than $LEE_{LSC}(G)$.

Various properties of LEE have been established, see [11, 18] for some fundamental properties, and [1, 16, 19, 22, 23] for more (upper and lower) bounds on $LEE(G)$ relating the number of vertices, the number of edges, the maximum degree, the first Zagreb index and the degree sequences of the graph G. In [22], Zhou and Gutman established a nice relation between LEE and EE, which states that if G is a bipartite graph with n vertices and m edges, then

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

where $\mathcal{L}(G)$ is the line graph of G. Using this relation and the corresponding results of Estrada index, Ilić and Zhou [15] proved that the path P_n has minimal, while the star S_n has maximal Laplacian Estrada index among trees on n vertices. In addition, Zhu [24] determined the extremal graphs with given connectivity k or given matching number maximizing the Laplacian Estrada index. For more results on this aspect, we refer the reader to [4–6, 17].

A maximum clique of a graph G is a clique (*i.e.*, complete subgraph) of maximum possible size for G. The size of the maximum clique of G, denoted by $\omega = \omega(G)$, is known as a clique number of G. Given a graph G, a subset S of $V(G)$ is called an independent set of G if any two vertices in S are not adjacent. The independence number of G, denoted by $\alpha = \alpha(G)$, is defined to be the number of vertices in the largest independent set of G. The chromatic number of G, denoted by $\chi = \chi(G)$, is the minimum number of colors used to assign a color to each of its vertices such that any two adjacent vertices in G have different colors.

In this paper, we shall present some new upper and lower bounds for $LEE(G)$ in terms of the number of vertices, the number of edges, the maximum degree, the minimum degree, the clique number, the independence number and the chromatic number of the graph G, and characterize the graphs for which the bounds are attained. We also give an asymptotic property of LEE of iterated line graphs of a regular graph.

2 Lemmas and results

We first list some lemmas that will be used in our proofs.

Lemma 1 (see [20]) *Let $G' = G + e$ be the graph obtained from G by adding a new edge e. Then*

$$\mu_1(G') \geq \mu_1(G) \geq \mu_2(G') \geq \mu_2(G) \geq \cdots \geq \mu_{n-1}(G') \geq \mu_{n-1}(G) \geq \mu_n(G') = \mu_n(G) = 0 .$$

Moveover, there exists some i such that $\mu_i(G') > \mu_i(G)$.

As a direct consequence of Lemma 1, we have the following result.

Lemma 2 *Let $G' = G + e$ be the graph obtained from a graph G by adding a new edge e. Then $LEE(G+e) > LEE(G)$ and consequently, if H is a subgraph of G, then $LEE(G) \geq LEE(H)$, with equality if and only if $G \cong H$.*

Denote by $\Delta(G)$ and $\delta(G)$ the maximum and the minimum degree of the graph G, respectively. The following are several bounds on the largest Laplacian eigenvalue $\mu_1(G)$ and the algebraic connectivity $\mu_{n-1}(G)$ of a graph G.

Lemma 3 (see [20]) *Let G be a graph of order n. Then $\mu_1(G) \leq n$ with equality if and only if $\overline{G}$ is disconnected, where $\overline{G}$ is the complement of G.*

Lemma 4 (see [13]) *Let G be a graph containing at least one edge. Then $\mu_1(G) \geq \Delta(G)+1$. Moreover, if G is connected, then the equality holds if and only if $\Delta(G) = n-1$.*

Lemma 5 (see [12]) *Let G be a non-complete graph. Then $\mu_{n-1}(G) \leq \delta(G)$.*

Lemma 6 (see [2]) *Let G be a graph of order n with m edges. Then $\mu_{n-1}(G) \geq 2m - (n-2)(\Delta(G)+1)$.*

Let K_n and K_{n_1,n_2} $(n_1 + n_2 = n)$ be the complete graph and the complete bipartite graph on n vertices, respectively. Denote by $G \cup H$ the vertex-disjoint union of graphs G and H. In particular, we write kG for the vertex-disjoint union of k copies of the graph G. Let $G \vee H$ be the graph obtained from $G \cup H$ by adding all possible edges joining the vertices in G with those in H. Recently, a characterization of graphs from Laplacian eigenvalues was obtained in [2].

Lemma 7 (see [2]) *Let G be a non-complete graph with $n > 3$ vertices. Then $\mu_1(G) = \Delta(G) + 1$, $\mu_2(G) = \cdots = \mu_{n-2}(G)$ and $\mu_{n-1}(G) = \delta(G)$ if and only if G is isomorphic to one of the following graphs: $2K_1 \vee K_{n-2}$, $K_{1,n-1}$, $(K_1 \cup K_{n-2}) \vee K_1$, $K_2 \cup (n-2)K_1$, $K_{n-1} \cup K_1$, and $K_{1,n-2} \cup K_1$.*

Now we are ready to present our main results.

Theorem 8 *Let G be a connected non-complete graph with $n > 3$ vertices and m edges. Let $\Delta(G) = \Delta$ and $\delta(G) = \delta$. Then*

$$LEE(G) \geq 1 + e^{\Delta+1} + e^{\delta} + (n-3)e^{\frac{2m-\Delta-\delta-1}{n-3}}, \tag{2}$$

with equality holding in (2) if and only if $G \cong 2K_1 \vee K_{n-2}$, or $G \cong K_{1,n-1}$, or $G \cong (K_1 \cup K_{n-2}) \vee K_1$.

Proof. For convenience, we set $\mu_i(G) = \mu_i$, $i = 1, 2, \ldots, n$. Recall that $\sum_{i=1}^{n} \mu_i = 2m$ and $\mu_n = 0$. By the arithmetic-geometric inequality, it follows from (1) that

$$\begin{aligned} LEE(G) &= 1 + e^{\mu_1} + e^{\mu_{n-1}} + \sum_{i=2}^{n-2} e^{\mu_i} \\ &\geq 1 + e^{\mu_1} + e^{\mu_{n-1}} + (n-3)\left(e^{\sum_{i=1}^{n-2} \mu_i}\right)^{\frac{1}{n-3}} \\ &= 1 + e^{\mu_1} + e^{\mu_{n-1}} + (n-3)e^{\frac{2m-x-\mu_{n-1}}{n-3}}, \end{aligned}$$

with equality if and only if $\mu_2 = \mu_3 = \cdots = \mu_{n-2}$.

For $\Delta + 1 \leq x \leq n$, let

$$f(x) = e^x + (n-3)e^{\frac{2m-x-\mu_{n-1}}{n-3}}.$$

Taking the first derivative of $f(x)$ with respect to x, we obtain

$$f'(x) = e^x - e^{\frac{2m-x-\mu_{n-1}}{n-3}}.$$

It is easy to see that if $x \geq \frac{2m-\mu_{n-1}}{n-2}$, then $f'(x) \geq 0$, and hence $f(x)$ is increasing monotonously with respect to x. Moreover, by Lemmas 3, 4 and 6, we get

$$n \geq \mu_1 \geq \Delta + 1 \geq \frac{2m - \mu_{n-1}}{n-2}.$$

Thus, from the above argument, we have

$$\begin{aligned} LEE(G) &\geq 1 + e^{\mu_{n-1}} + f(\mu_1) \\ &\geq 1 + e^{\mu_{n-1}} + f(\Delta + 1) \\ &\geq 1 + e^{\mu_{n-1}} + e^{\Delta+1} + (n-3)e^{\frac{2m-\Delta-1-\mu_{n-1}}{n-3}}. \end{aligned}$$

Further, for $0 < x \leq \delta$, let

$$g(x) = e^x + (n-3)e^{\frac{2m-\Delta-1-x}{n-3}}.$$

Taking the first derivative of $g(x)$ with respect to x, we get

$$g'(x) = e^x - e^{\frac{2m-\Delta-1-x}{n-3}}.$$

One can see easily that if $x \leq \frac{2m-\Delta-1}{n-2}$, then $g'(x) \leq 0$, and so $g(x)$ is decreasing monotonously with respect to x. Moreover, noting that $(n-2)\delta + \Delta + 1 \leq 2m$, we have

$$0 < \mu_{n-1} \leq \delta \leq \frac{2m - \Delta - 1}{n-2},$$

Consequently, it follows from the above argument that

$$\begin{aligned} LEE(G) &\geq 1 + e^{\Delta+1} + g(\mu_{n-1}) \\ &\geq 1 + e^{\Delta+1} + g(\delta) \\ &\geq 1 + e^{\Delta+1} + e^{\delta} + (n-3)e^{\frac{2m-\Delta-\delta-1}{n-3}} , \end{aligned}$$

(2) follows.

Now we discuss the sharpness of (2). If G is isomorphic to one of the graphs mentioned in the theorem, then a simple calculation shows that the equality holds in (2). Conversely, if the equality holds in (2) then all the inequalities in the above argument must be equalities, from which we obtain

$$\mu_1 = \Delta + 1,\ \mu_2 = \mu_3 = \cdots = \mu_{n-2} \text{ and } \mu_{n-1} = \delta .$$

Thus, by Lemma 7 and, noting that G is connected, we have the desired result.

This completes the proof. □

Remark. It should be mentioned that two similar bounds as (2) were reported in [23]. Let G be a connected graph with n vertices, m edges and maximum degree Δ. Then

$$LEE(G) \geq 1 + (n-1)e^{\frac{2m}{n-1}} , \tag{3}$$

with equality holding in (3) if and only if $G \cong K_n$;

$$LEE(G) \geq 1 + e^{\Delta+1} + (n-2)e^{\frac{2m-\Delta-1}{n-2}} , \tag{4}$$

with equality holding in (4) if and only if $G \cong K_n$ or $G \cong K_{1,n-1}$. Notice that our bound (2) are incomparable to the bounds (3) and (4). However, there are more graphs which attain our bound.

In [21], Nordhaus and Gaddum presented lower and upper bounds on the sum of the chromatic numbers of a graph and its complement. Here we deduce a Nordhaus-Gaddum-type result for LEE based on Theorem 8.

Theorem 9 *Let G be a connected graph with $n > 3$ vertices and a connected complement $\overline{G}$. Let $\Delta(G) = \Delta$ and $\delta(G) = \delta$. Then*

$$LEE(G) + LEE(\overline{G}) > e^{\Delta+1} + e^{n-1-\Delta} + e^{\delta} + e^{n-\delta} + 2(n-3)e^{\frac{n}{2}} + 2 . \tag{5}$$

Proof. For convenience, we let

$$f(m,\Delta,\delta) = 1 + e^{\Delta+1} + e^{\delta} + (n-3)e^{\frac{2m-\Delta-\delta-1}{n-3}} \,.$$

Observing that $|E(\overline{G})| = \frac{n(n-1)}{2} - m$, $\Delta(\overline{G}) = n-1-\delta$, and $\delta(\overline{G}) = n-1-\Delta$, by Theorem 8, we have

$$\begin{aligned} LEE(G) + LEE(\overline{G}) &> f(m,\Delta,\delta) + f\left(\frac{n(n-1)}{2} - m, n-1-\delta, n-1-\Delta\right) \\ &= 2 + e^{\Delta+1} + e^{\delta} + e^{n-\delta} + e^{n-1-\Delta} \\ &\quad + (n-3)\left(e^{\frac{2m-\Delta-\delta-1}{n-3}} + e^{\frac{(n-1)(n-2)-2m+\Delta+\delta-1}{n-3}}\right) \\ &\geq e^{\Delta+1} + e^{n-1-\Delta} + e^{\delta} + e^{n-\delta} + 2(n-3)e^{\frac{n}{2}} + 2\,, \end{aligned}$$

where the first inequality holds strictly since $\overline{G}$ is required to be connected, while the second inequality follows from the fact that $e^a + e^b \geq 2e^{\frac{a+b}{2}}$ holds for $a, b \geq 0$, which is a direct consequence of the arithmetic-geometric inequality. The proof is completed. □

Remark. Based on (3), Zhou [23] showed that,

$$LEE(G) + LEE(\overline{G}) > (n-1)e^{\frac{n}{2}} + 2\,. \tag{6}$$

Observing that $e^x + e^{n-x} \geq 2e^{\frac{n}{2}}$ holds for $0 \leq x \leq n$, one can see easily that our bound (5) is always better than the bound (6).

For $2 \leq \omega \leq n$, we denote by $KS_{n,\omega}$ the graph obtained from K_ω by attaching $n-\omega$ pendent edges to one of its vertices. It is obvious that $KS_{n,\omega}$ is a graph with n vertices and clique number ω. In particular, $KS_{n,n} \cong K_n$ and $KS_{n,2} \cong K_{1,n-1}$. It is easy to check that (see also [3])

$$\mathrm{Spec}_L(KS_{n,\omega}) = \{n, \underbrace{\omega,\ldots,\omega}_{\omega-2}, \underbrace{1,\ldots,1}_{n-\omega}, 0\}\,. \tag{7}$$

Theorem 10 *Let G be a connected graph with n vertices, maximum degree Δ and clique number ω $(2 \leq \omega \leq n)$. Then*

$$LEE(G) \geq 1 + e^{\Delta+1} + (\omega-2)e^{\omega} + (\Delta-\omega+1)e\,, \tag{8}$$

with equality holding in (8) if and only if $G \cong KS_{n,\omega}$.

Proof. Observe first that K_ω is a subgraph of G. If $\omega = n$, then $G \cong K_n \cong KS_{n,n}$, and hence the equality holds in (8). Otherwise, we have $\omega \leq \Delta \leq n-1$ since G is connected.

In this case, if $\Delta = n-1$, then $KS_{n,\omega}$ is obviously a subgraph of G and hence, by Lemma 2 and (7), we have

$$LEE(G) \geq LEE(KS_{n,\omega}) = 1 + e^{\Delta+1} + (\omega-2)e^{\omega} + (\Delta-\omega+1)e\,,$$

with equality if and only if $G \cong KS_{n,\omega}$.

Now we suppose that $\Delta \leq n-2$. If there is a vertex of (maximum) degree Δ being exactly a vertex of a certain maximum clique of G, then $KS_{\Delta+1,\omega}$ is clearly a proper subgraph of G and hence, by Lemma 2 and (7) again, we get

$$LEE(G) > LEE(KS_{\Delta+1,\omega}) = 1 + e^{\Delta+1} + (\omega-2)e^{\omega} + (\Delta-\omega+1)e\ .$$

Otherwise, let v be any vertex of (maximum) degree Δ and K_{ω} be any maximum clique of G. Assume that v is adjacent to p vertices of K_{ω}. Evidently, $0 \leq p \leq \omega-2$ and hence $\Delta-p-1 \geq \Delta-\omega+1 \geq 1$. On the other hand, $K_{\omega} \cup K_{1,\Delta-p}$ is clearly a proper subgraph of G. Since

$$\mathrm{Spec}_L\,(K_{\omega} \cup K_{1,\Delta-p}) = \{\underbrace{\omega,\ldots,\omega}_{\omega-1}, \Delta-p+1, \underbrace{1,\ldots,1}_{\Delta-p-1}, 0, 0\}\,,$$

by Lemmas 1 and 4, we obtain

$$\mu_1(G) > \Delta+1,\ \ \mu_{\omega}(G) \geq \Delta-p+1\,,\ \ \mu_n(G) = 0,$$
$$\mu_i(G) \geq \omega,\ \ i = 2,3,\ldots,\omega-1\,,$$
$$\mu_j(G) \geq 1,\ \ j = \omega+1, \omega+2, \ldots, \omega+\Delta-p-1\ .$$

Consequently, it follows from (1) that

$$\begin{aligned} LEE(G) &> 1 + e^{\Delta+1} + (\omega-2)e^{\omega} + e^{\Delta-p+1} + (\Delta-p-1)e \\ &> 1 + e^{\Delta+1} + (\omega-2)e^{\omega} + (\Delta-\omega+1)e\ . \end{aligned}$$

This completes the proof. □

A complete split graph $CS(n,\omega)$ is a graph consisting of a clique on ω vertices and a independent set on $n-\omega$ vertices in which each vertex of the clique is adjacent to each vertex of the independent set.

Theorem 11 *Let G be a graph with n vertices and independence number α. Then*

$$LEE(G) \leq 1 + (n-\alpha)e^{n} + (\alpha-1)e^{n-\alpha}\,, \tag{9}$$

with equality holding in (9) if and only if $G \cong CS(n, n-\alpha)$.

Proof. Let S be an arbitrary maximum independent set of G and let $G[V(G)\backslash S]$ be the subgraph of G induced by the vertex set $V(G)\backslash S$. Obviously, $|S| = \alpha$ and hence $|V(G)\backslash S| = n-\alpha$. It is easy to see that G is a subgraph of $CS(n, n-\alpha)$ since $G[V(G)\backslash S]$ is always a subgraph of $K_{n-\alpha}$. On the other hand, a little calculation shows that (see also [3])

$$\mathrm{Spec}_L(CS(n, n-\alpha)) = \{\underbrace{n, \ldots, n}_{n-\alpha}, \underbrace{n-\alpha, \ldots, n-\alpha}_{\alpha-1}, 0\} .$$

Consequently, by Lemma 2, we have

$$LEE(G) \leq LEE(CS(n, n-\alpha)) = 1 + (n-\alpha)e^n + (\alpha-1)e^{n-\alpha} ,$$

with equality if and only if $G \cong CS(n, n-\alpha)$, completing the proof. □

Let $K_{n_1,\ldots,n_r}$ $(n_1 + \cdots + n_r = n)$ be the complete r-partite graph with n_i vertices in the i-th part for $i = 1, 2, \ldots, r$. A direct calculation shows that

$$\mathrm{Spec}_L(K_{n_1,\ldots,n_r}) = (\underbrace{n, \ldots n}_{r-1}, \underbrace{n-n_1, \ldots, n-n_1}_{n_1-1}, \ldots, \underbrace{n-n_r, \ldots, n-n_r}_{n_r-1}, 0) . \tag{10}$$

Theorem 12 *Let G be a graph with n vertices and chromatic number χ, where $2 \leq \chi \leq n$. Write $n = s\chi + t$ with $0 \leq t < \chi$.*

(1) If $n = \chi + t$ with $0 \leq t < \chi$, or $n = 2\chi + t$ with $0 \leq t \leq 3$, or $n = 3\chi$ with $2 \leq \chi \leq 3$, then

$$LEE(G) \leq 1 + (\chi-1)e^n + (\chi-t)(s-1)e^{n-s} + tse^{n-s-1} , \tag{11}$$

with equality holding in (11) if and only if $G \cong K_{\underbrace{s, \ldots, s}_{\chi-t}, \underbrace{s+1, \ldots, s+1}_{t}}$.

(2) If $n = 2\chi + t$ with $4 \leq t < \chi$, or $n = 3\chi$ with $\chi \geq 4$, or $n > 3\chi$, then

$$LEE(G) \leq 1 + (\chi-1)(e^n + e^{n-2}) + (n-2\chi+1)e^{2\chi-2} , \tag{12}$$

with equality holding in (12) if and only if $G \cong K_{\underbrace{2, \ldots, 2}_{\chi-1}, n-2\chi+2}$,

Proof. Without loss of generality, we may suppose that G is the graph having the maximum value of LEE. Clearly, $V(G)$ can be partitioned into χ independent vertex subsets, say $V_1, V_2, \ldots, V_\chi$. Let $|V_i| = n_i$ for $i = 1, 2, \ldots, \chi$, and without loss of generality, assume that $1 \leq n_1 \leq n_2 \leq \cdots \leq n_\chi$. Then from Lemma 2 and the maximality of G, it follows that $G \cong K_{n_1,n_2,\ldots,n_\chi}$. Moreover, by (10), we have

$$LEE(G) = 1 + (\chi - 1)e^n + \sum_{i=1}^{\chi}(n_i - 1)e^{n-n_i} \,. \tag{13}$$

Next, we further determine the structure of $G\,(\cong K_{n_1,n_2,\ldots,n_\chi})$. For any $1\leq j < k \leq \chi$, consider the pair (n_j, n_k):

(i) If $(n_j, n_k) = (1, p)$ with $p \geq 3$, then replaying (n_j, n_k) by $(2, p-1)$ in (13) would yield that

$$\begin{aligned} & (p-1)e^{n-p} - \left[e^{n-2} + (p-2)e^{n-p+1}\right] \\ = \;& (e^{n-p} - e^{n-2}) + (p-2)(e^{n-p} - e^{n-p+1}) < 0\,, \end{aligned}$$

contradicting the maximality of G.

(ii) If $(n_j, n_k) = (3, p)$ with $p \geq 4$, then replaying (n_j, n_k) by $(2, p+1)$ in (13), we would get

$$\begin{aligned} & 2e^{n-3} + (p-1)e^{n-p} - \left(e^{n-2} + pe^{n-p-1}\right) \\ = \;& e^{n-p}\left[\frac{e-1}{e}p - (e-2)e^{p-3} - 1\right] \\ \leq \;& e^{n-p}\left[\frac{4(e-1)}{e} - (e-2)e - 1\right] \approx -0.4240e^{n-p} < 0\,, \end{aligned}$$

contradicting the maximality of G as well. Note that the first inequality follows from the fact that the function

$$\frac{e-1}{e}x - (e-2)e^{x-3}$$

is decreasing monotonously when $x \geq 4$.

(iii) If $(n_j, n_k) = (p, q)$ with $q \geq p \geq 4$, then replaying (n_j, n_k) by $(2, p+q-2)$ in (13), we have

$$\begin{aligned} & (p-1)e^{n-p} + (q-1)e^{n-q} - \left[e^{n-2} + (p+q-3)e^{n-p-q+2}\right] \\ = \;& e^{n-q}\left[(p-1)e^{q-p} + (q-1) - e^{q-2} - (p+q-3)e^{2-p}\right] \\ < \;& e^{n-q}\left[q - (e^{p-2} - p + 1)e^{q-p} - 1\right] \\ \leq \;& e^{n-q}\left(2p - e^{p-2} - 2\right) \\ \leq \;& e^{n-q}\left(6 - e^2\right) \approx -1.3891e^{n-q} < 0\,, \end{aligned}$$

which contradicts the maximality of G. Note that the second inequality follows from the fact that $x - (e^{p-2} - p + 1)e^{x-p}$ is decreasing monotonously when $x \geq p \geq 4$, while the third inequality follows from the fact that $2x - e^{x-2}$ is decreasing monotonously when $x \geq 4$.

Therefore, from the above (i), (ii) and (iii), we can deduce that all the possible values taken by (n_j, n_k) are the following:

$$(1,1),\ (1,2),\ (3,3),\ (2,N) \text{ with } N \geq 2\ . \tag{14}$$

Recall (the assumption) that $1 \leq n_1 \leq n_2 \leq \cdots \leq n_\chi$. It follows easily from (14) that $n_1 = 1$, or 2, or 3. We now consider the following cases:

Case 1. $n = \chi + t$ with $0 \leq t < \chi$ (*i.e.*, $n < 2\chi$). Then $n_1 = 1$ and hence, by (14), we have $n_i = 1$ or 2 for $i = 2, 3, \ldots, \chi$, that is, $G \cong K_{\underbrace{1,\ldots,1}_{\chi-t},\underbrace{2,\ldots,2}_{t}}$.

Case 2. $n = 2\chi + t$ with $0 \leq t < \chi$ (*i.e.*, $2\chi \leq n < 3\chi$). Then it is easy to see that $n_1 \leq 2$. If $n_1 = 1$, then $n_\chi \geq 3$, contradicting (14). Hence, $n_1 = 2$. Further, by (14), we can deduce easily that either $n_i = 2$ or 3 for $i = 2, 3, \ldots, \chi$, or $n_2 = n_3 = \cdots = n_{\chi-1} = 2$ and $n_\chi = n - 2\chi + 2 = t + 2$. Observe that $K_{\underbrace{2,\ldots,2}_{\chi-t},\underbrace{3,\ldots,3}_{t}} \cong K_{\underbrace{2,\ldots,2}_{\chi-1},n-2\chi+2}$ for $t = 0, 1$, and for $t \geq 2$, by (13), we have

$$\begin{aligned}
& LEE(K_{\underbrace{2,\ldots,2}_{\chi-t},\underbrace{3,\ldots,3}_{t}}) - LEE(K_{\underbrace{2,\ldots,2}_{\chi-1},n-2\chi+2}) \\
= \ & (\chi - t)e^{n-2} + 2te^{n-3} - \left[(\chi-1)e^{n-2} + (n - 2\chi + 1)e^{2\chi-2}\right] \\
= \ & 2te^{n-3} - (t-1)e^{n-2} - (t+1)e^{2\chi-2} \quad \text{(recall that } n = 2\chi + t) \\
= \ & e^{2\chi-2}\left\{e^{t-1}[e - (e-2)t] - (t+1)\right\}\ .
\end{aligned}$$

We now consider the function $f(x) = e^{x-1}[e-(e-2)x]-(x+1)$ with $2 \leq x < \chi$. A direct computation shows that $f(2) \approx 0.4841 > 0$, $f(3) \approx 0.1633 > 0$, and $f(x) < 0$ when $x \geq 4$. Thus, from the above argument, we can conclude that if $t \leq 3$, then $G \cong K_{\underbrace{2,\ldots,2}_{\chi-t},\underbrace{3,\ldots,3}_{t}}$, while if $t \geq 4$, then $G \cong K_{\underbrace{2,\ldots,2}_{\chi-1},n-2\chi+2}$.

Case 3. $n = 3\chi$. Observe that if $n_1 = 3$, then $n_i = 3$ for $i = 2, 3, \ldots, \chi$. Otherwise, again by (14), we may deduece that $n_1 = n_2 = \cdots = n_{\chi-1} = 2$ and $n_\chi = n-2\chi+2 = \chi+2$. As in Case 2, by (13), we get

$$\begin{aligned}
& LEE(K_{\underbrace{3,3,\ldots,3}_{\chi}}) - LEE(K_{\underbrace{2,\ldots,2}_{\chi-1},n-2\chi+2}) \\
= \ & 2\chi e^{n-3} - \left[(\chi-1)e^{n-2} + (n-2\chi+1)e^{2\chi-2}\right] \quad \text{(recall that } n = 3\chi) \\
= \ & e^{2\chi-2}\left\{e^{\chi-1}[e - (e-2)\chi] - (\chi+1)\right\}\ ,
\end{aligned}$$

from which we can also conclude that if $\chi = 2$ or 3, then $G \cong K_{\underbrace{3,3,\dots,3}_{\chi}}$, while if $\chi \geq 4$, then $G \cong K_{\underbrace{2,\dots,2}_{\chi-1},n-2\chi+2}$.

Case 4. $n > 3\chi$. If $n_1 = 1$ or 3, then $n_\chi \geq 4$, contradicting (14). Hence, $n_1 = 2$ and by (14), we have $n_2 = n_3 = \cdots = n_{\chi-1} = 2$ and $n_\chi = n - 2\chi + 2$, that is, $G \cong K_{\underbrace{2,\dots,2}_{\chi-1},n-2\chi+2}$.

The proof is completed. □

Using Theorem 12 and the fact that G is a bipartite graph if and only if $\chi(G) = 2$, we have the following corollary immediately.

Corollary 13 *Let G be a bipartite graph with $n \geq 3$ vertices. If $n \neq 6$, then*

$$LEE(G) \leq 1 + e^n + e^{n-2} + (n-3)e^2 \,,$$

with equality if and only if $G \cong K_{2,n-2}$. If $n = 6$, then $LEE(G) \leq 1 + e^6 + 4e^3$, with equality if and only if $G \cong K_{3,3}$.

The iterated line graphs of a graph G are defined recursively as $\mathcal{L}^k(G) = \mathcal{L}(\mathcal{L}^{k-1}(G))$ for $k = 2, 3, \dots$, and it is both consistent and convenient to set $G = \mathcal{L}^0(G)$. Let G be an r-regular graph with n vertices. Obviously, $\mathcal{L}^k(G)$ is also a regular graph. Observe that if $r = 2$, then $\mathcal{L}^k(G) \cong G$ for $k = 1, 2, \dots$. So in what follows we may assume that $r \geq 3$. For $k = 0, 1, \dots$, we also let n_k and r_k be the order and the degree of $\mathcal{L}^k(G)$ respectively, where $n_0 = n$ and $r_0 = r$. In [11], Fath-Tabar, Ashrafi and Gutman established the following recurrence:

Theorem 14 (see [11]) *If G is an r-regular graph, then for $k = 0, 1, \dots$,*

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

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

We now present an asymptotic property of the Laplacian Estrada index of iterated line graphs of a regular graph.

Theorem 15 *Let G be an r-regular graph with n vertices. Then*

$$LEE(\mathcal{L}^k(G)) \sim n e^{4(2^{k-2}r - 2^{k-1} + 1)} \prod_{i=0}^{k-1}(2^{i-1}r - 2^i + 1) \,, \quad (k \to \infty) \,.$$

Proof. For $k = 0, 1, 2, \ldots$, let m_k denote the number of edges in $\mathcal{L}^k(G)$. Noting that $\mathcal{L}^k(G)$ is an r_k-regular graph with n_k vertices, we then have $m_k = n_k r_k/2$. Moreover, from the definition of iterated line graphs of a graph, it follows easily that $m_k = n_{k+1}$ for $k = 0, 1, 2, \ldots$. Now, by applying Theorem 14 repeatedly, we obtain

$$LEE(\mathcal{L}^k(G)) = LEE(G) + \sum_{i=0}^{k-1} \frac{n_i(r_i - 2)}{2} e^{2r_i} = LEE(G) + \sum_{i=0}^{k-1} (m_i - n_i) e^{2r_i} ,$$

from which we can deduce that

$$LEE(G) + e^{2r_{k-1}}(m_{k-1} - n_{k-1}) \leq LEE(\mathcal{L}^k(G)) \leq LEE(G) + e^{2r_{k-1}}(m_{k-1} - n_0) .$$

Consequently, it is not difficult to check that

$$\lim_{k \to \infty} \frac{LEE(\mathcal{L}^k(G))}{e^{2r_{k-1}} m_{k-1}} = 1 ,$$

which would yield the theorem, completing the proof. □

Remark. From Theorem 15, we can see that the asymptotic behavior of the Laplacian Estrada index of iterated line graphs of a regular graph only depends on the number of vertices and regularity of the initial graph, and has nothing to do with its structure.

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