



On the Estrada and Laplacian Estrada indices of graphs

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ARTICLE INFO

Article history:

Received 15 February 2011

Accepted 28 March 2011

Available online 4 May 2011

Submitted by R.A. Brualdi

AMS classification:

05C35

05C50

Keywords:

Estrada index

Laplacian Estrada index

Spectral moments

Closed walks

Edge grafting operation

Tree

ABSTRACT

The Estrada index of a graph G is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i}$, where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of G . The Laplacian Estrada index of a graph G is defined as $LEE(G) = \sum_{i=1}^n e^{\mu_i}$, where $\mu_1, \mu_2, \dots, \mu_n$ are the Laplacian eigenvalues of G . An edge grafting operation on a graph moves a pendent edge between two pendent paths. We study the change of Estrada index of graph under edge grafting operation between two pendent paths at two adjacent vertices. As the application, we give the result on the change of Laplacian Estrada index of bipartite graph under edge grafting operation between two pendent paths at the same vertex. We also determine the unique tree with minimum Laplacian Estrada index among the set of trees with given maximum degree, and the unique trees with maximum Laplacian Estrada indices among the set of trees with given diameter, number of pendent vertices, matching number, independence number and domination number, respectively.

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1. Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$, where $|V(G)| = n$. Let $\mathbf{A}(G)$ be the adjacency matrix of G . Denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$ the eigenvalues of G (i.e., the eigenvalues of $\mathbf{A}(G)$) [3]. Let $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ be the Laplacian matrix of G , where $\mathbf{D}(G)$ is the diagonal matrix of vertex degrees of G . Denote by $\mu_1, \mu_2, \dots, \mu_n$ the Laplacian eigenvalues of G (i.e., the eigenvalues of $\mathbf{L}(G)$) [31].

The Estrada index is a newly proposed graph-spectrum-based invariant, which is defined as [11]

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

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It found various applications in a large variety of problems. Estrada index gives maximum values for the most folded structures, thus it is useful in the measure of folding of the molecular structures [11], especially protein chain [12,13]. Estrada index is also an effective method to measure the centrality of complex networks [14,15], extended atomic branching [16] and the carbon-atom skeleton [22].

In the last few years, Estrada index has attracted more and more attentions of mathematicians. A number of lower and upper bounds for Estrada index were established. Gutman et al. [21] and de la Peña et al. [17] estimated Estrada index in terms of the numbers of vertices and edges, and established bounds for Estrada index involving graph energy. Bamdad et al. [1] gave a lower bound of Estrada index in terms of the numbers of positive, zero, negative adjacency eigenvalues and graph energy.

Recently, the trees with extremal Estrada indices were characterized. The Estrada indices of trees are maximized by the star [4,5,17,37] and minimized by the path [5]. Ilić and Stevanović [24] determined the unique tree with minimum Estrada index among trees with given maximum degree. Zhang et al. [34] determined the unique trees with maximum Estrada indices among trees with given matching number. Li [27] determined the unique tree with maximum Estrada index among trees with given bipartition. Du and Zhou [9] determined the unique trees with maximum Estrada indices among trees with given number of pendent vertices, independence number and domination number, respectively. More results on Estrada index can be found in [6,10,18,19,26,35,36].

In full analogy with Estrada index, Fath-Tabar et al. [18] proposed the Laplacian Estrada index, which is defined as

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

Independently of [18], Li et al. [28] proposed the Laplacian Estrada index of another form, which is defined as

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

where n and m are, respectively, the numbers of vertices and edges of G . In [28,29], Li et al. established bounds for $LEE_{Li}(G)$ in terms of the numbers of vertices, edges and graph Laplacian energy. Clearly, $LEE(G) = e^{2m/n} LEE_{Li}(G)$. Thus, the two definitions of Laplacian Estrada index are actually equivalent. In the following, we use the definition of Laplacian Estrada index proposed by Fath-Tabar et al. in [18].

Zhou and Gutman [38] established lower and upper bounds of Laplacian Estrada index in terms of the numbers of vertices, edges and the first Zagreb index, they also obtained a relationship between the Laplacian Estrada index of a bipartite graph and the Estrada index of its line graph. Bamdad et al. [1] gave a lower bound of Laplacian Estrada index in terms of the numbers of vertices, edges and connected components.

Ilić and Zhou [25] proved that the Laplacian Estrada indices of trees are maximized by the star and minimized by the path, which showed the use of Laplacian Estrada index as a measure of branching in alkanes. Du [8] determined the tree with maximum Laplacian Estrada index among trees with given bipartition, and characterized the trees with the first six maximum Laplacian Estrada indices. More results on Laplacian Estrada index were reported in [7,39,40].

A latest survey on Estrada index and Laplacian Estrada index can be found in [23]. These results prompt us to study more properties for the two novel graph invariants.

A pendent path at v in a graph G is a path in which no vertex other than v is incident with any edge of G outside the path, where the degree of v is at least three.

An edge grafting operation on a graph moves a pendent edge between two pendent paths at two vertices (not necessarily distinct). Taking the graphs G_1, G_2 shown in Fig. 1 as an example, where G_2 is the graph obtained from G_1 by deleting the edge xy and adding the edge zy , we say G_2 is obtained under an edge grafting operation on G_1 .

The edge grafting operation on graph was often considered and used in the study of various graph invariants, e.g., spectral radius [30], Laplacian spectral radius [20], graph energy [32,33]. Recently, Ilić and Stevanović [24] studied the change of Estrada index of graph under edge grafting operation between two pendent paths at the same vertex.

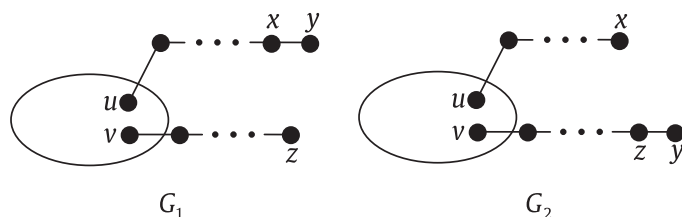


Fig. 1. An example on edge grafting operation.

The paper is organized as follows. In Section 3, a transformation that increases the Estrada index is presented. Motivated by [24], in Section 4 we study the change of Estrada index of graph under edge grafting operation between two pendent paths at two adjacent vertices. As the application, in Section 5 we give the result on the change of Laplacian Estrada index of bipartite graph under edge grafting operation between two pendent paths at the same vertex. In Sections 6 and 7, we characterize the trees with extremal Laplacian Estrada indices, including the unique tree with minimum Laplacian Estrada index among the set of trees with given maximum degree, and the unique trees with maximum Laplacian Estrada indices among the set of trees with given diameter, number of pendent vertices, matching number, independence number and domination number, respectively.

2. Preliminaries

Denote by $M_k(G)$ the k th spectral moment of the graph G , i.e., $M_k(G) = \sum_{i=1}^n \lambda_i^k$. It is well-known that $M_k(G)$ is equal to the number of closed walks of length k in G (see [3]). Then

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

Let G_1 and G_2 be two graphs. If $M_k(G_1) \leq M_k(G_2)$ for all positive integers k , then $EE(G_1) \leq EE(G_2)$. Moreover, if $M_{k_0}(G_1) < M_{k_0}(G_2)$ for some positive integer k_0 , then $EE(G_1) < EE(G_2)$.

Let $u, v \in V(G)$ (not necessarily $u \neq v$). A walk is said to be a (u, v) -walk if it starts at u and ends at v in G . Let $\mathcal{W}_k(G; u, v)$ be the set of (u, v) -walks of length k in G . Let $M_k(G; u, v) = |\mathcal{W}_k(G; u, v)|$. Clearly, $M_k(G; u, v) = M_k(G; v, u)$ for all positive integers k (see [3]).

Let $u_1, v_1 \in V(G_1)$ and $u_2, v_2 \in V(G_2)$. If $M_k(G_1; u_1, v_1) \leq M_k(G_2; u_2, v_2)$ for all positive integers k , then we write $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$. If $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$ and there is at least one positive integer k_0 such that $M_{k_0}(G_1; u_1, v_1) < M_{k_0}(G_2; u_2, v_2)$, then we write $(G_1; u_1, v_1) \prec (G_2; u_2, v_2)$.

For convenience, let $M_k(G; u) = M_k(G; u, u)$, and

$$(G_1; u_1, u_1) \preceq (G_2; u_2, u_2) \Leftrightarrow (G_1; u_1) \preceq (G_2; u_2),$$

$$(G_1; u_1, u_1) \prec (G_2; u_2, u_2) \Leftrightarrow (G_1; u_1) \prec (G_2; u_2).$$

Let P_n be the path on n vertices. Let $d_G(v)$ be the degree of v in G . Let $d_G(u, v)$ be the distance from u to v in a connected graph G .

For a subset M of the edge set of the graph G , $G - M$ denotes the graph obtained from G by deleting the edges in M , and for a subset M^* of the edge set of the complement of G , $G + M^*$ denotes the graph obtained from G by adding the edges in M^* . For $v \in V(G)$ let $G - v$ be the graph obtained from G by deleting v and its incident edges.

3. Lemmas

Let H be a graph (not necessarily connected) with $u, v \in V(H)$. Suppose that $w_i \in V(H)$, and $uw_i, vw_i \notin E(H)$ for $1 \leq i \leq r$. Let $E_u = \{uw_1, uw_2, \dots, uw_r\}$ and $E_v = \{vw_1, vw_2, \dots, vw_r\}$. Let $H_u = H + E_u$ and $H_v = H + E_v$.

Let $V_u = \{u, w_1, w_2, \dots, w_r\}$ and $V_v = \{v, w_1, w_2, \dots, w_r\}$. Clearly, $V_u \setminus \{u\} = V_v \setminus \{v\}$.

For $x_1, x_2 \in V_u$ ($x_1, x_2 \in V_v$, respectively), let $\mathcal{T}_k(H_u; x_1, x_2)$ ($\mathcal{T}_k(H_v; x_1, x_2)$, respectively) be the set of (x_1, x_2) -walks of length k in H_u (H_v , respectively) starting and ending at the edge(s) in E_u (E_v , respectively).

Lemma 3.1. Suppose that $(H; u) \prec (H; v)$ and $(H; w_i, u) \preceq (H; w_i, v)$ for $1 \leq i \leq r$. Then for any positive integer k ,

- (i) $|\mathcal{T}_k(H_u; u, u)| \leq |\mathcal{T}_k(H_v; v, v)|$;
- (ii) $|\mathcal{T}_k(H_u; u, x_2)| \leq |\mathcal{T}_k(H_v; v, x_2)|$ for $x_2 \in V_u \setminus \{u\}$;
- (iii) $|\mathcal{T}_k(H_u; x_1, u)| \leq |\mathcal{T}_k(H_v; x_1, v)|$ for $x_1 \in V_u \setminus \{u\}$;
- (iv) $|\mathcal{T}_k(H_u; x_1, x_2)| \leq |\mathcal{T}_k(H_v; x_1, x_2)|$ for $x_1, x_2 \in V_u \setminus \{u\}$.

Proof. We only prove (i). The proofs of (ii), (iii) and (iv) are similar.

Let k be any positive integer.

We may decompose any $W \in \mathcal{T}_k(H_u; u, u)$ into five possible types of sections as follows:

- (a) a walk in H_u with all edges in E_u ;
- (b) a (u, u) -walk in H ;
- (c) a (w_i, u) -walk in H , where $1 \leq i \leq r$;
- (d) a (u, w_i) -walk in H , where $1 \leq i \leq r$;
- (e) a (w_i, w_j) -walk in H , where $1 \leq i, j \leq r$ (not necessarily $i \neq j$).

On the other hand, we may decompose any $W' \in \mathcal{T}_k(H_v; v, v)$ into five possible types of sections as follows:

- (a') a walk in H_v with all edges in E_v ;
- (b') a (v, v) -walk in H ;
- (c') a (w_i, v) -walk in H , where $1 \leq i \leq r$;
- (d') a (v, w_i) -walk in H , where $1 \leq i \leq r$;
- (e') a (w_i, w_j) -walk in H , where $1 \leq i, j \leq r$ (not necessarily $i \neq j$).

By replacing u by v , we may construct an injection $f_s^{(a)}$ mapping a walk of length s in H_u with all edges in E_u into a walk of length s in H_v with all edges in E_v .

Since $(H; u) \prec (H; v)$, we may construct an injection $f_s^{(b)}$ mapping a (u, u) -walk of length s in H into a (v, v) -walk of length s in H .

Since $(H; w_i, u) \preceq (H; w_i, v)$, we may construct an injection $f_s^{(c_i)}$ mapping a (w_i, u) -walk of length s in H into a (w_i, v) -walk of length s in H , where $1 \leq i \leq r$.

Note that $M_s(H; u, w_i) = M_s(H; w_i, u)$ and $M_s(H; v, w_i) = M_s(H; w_i, v)$ for any positive integer s (see [3]), and thus $(H; u, w_i) \preceq (H; v, w_i)$ for $1 \leq i \leq r$. It follows that we may construct an injection $f_s^{(d_i)}$ mapping a (u, w_i) -walk of length s in H into a (v, w_i) -walk of length s in H , where $1 \leq i \leq r$.

Finally, we construct a mapping f^* from $\mathcal{T}_k(H_u; u, u)$ to $\mathcal{T}_k(H_v; v, v)$. Let $W = W_1 W_2 \cdots \in \mathcal{T}_k(H_u; u, u)$, where W_s for $s \geq 1$ is a walk of length l_s of type (a), (b), (c), (d) or (e). Let $f^*(W) = f^*(W_1) f^*(W_2) \cdots$, where $f^*(W_s) = f_s^{(a)}(W_s)$ if W_s is of type (a), $f^*(W_s) = f_s^{(b)}(W_s)$ if W_s is of type (b), $f^*(W_s) = f_s^{(c_i)}(W_s)$ if W_s is of type (c) and starts at w_i , $f^*(W_s) = f_s^{(d_i)}(W_s)$ if W_s is of type (d) and ends at w_i , and $f^*(W_s) = W_s$ if W_s is of type (e). Note that $f^*(W_s)$ for $s \geq 1$ is a walk of length l_s of type (a'), (b'), (c'), (d') or (e'), and thus $f^*(W) \in \mathcal{T}_k(H_v; v, v)$ and f^* is an injection. This implies that $|\mathcal{T}_k(H_u; u, u)| \leq |\mathcal{T}_k(H_v; v, v)|$. \square

The following lemma is a generalization of Lemma 1 in [34] and Lemma 3.2 in [10].

Lemma 3.2. If $(H; u) \prec (H; v)$ and $(H; w_i, u) \preceq (H; w_i, v)$ for $1 \leq i \leq r$, then $EE(H_u) < EE(H_v)$.

Proof. For positive integer k , let $S_u(k)$ ($S_v(k)$, respectively) be the set of closed walks of length k in H_u (H_v , respectively) containing some edges in E_u (E_v , respectively). Then

$$M_k(H_u) = M_k(H) + |S_u(k)|,$$

$$M_k(H_v) = M_k(H) + |S_v(k)|.$$

We need only to show that $|S_u(k)| \leq |S_v(k)|$ for all positive integers k , and it is strict for some positive integer k_0 .

We may uniquely decompose any $W \in S_u(k)$ into three sections, say $W_1 W_2 W_3$, where W_1 is a walk in H whose length may be zero, W_2 is the longest walk of W in H_u starting and ending at the edge(s) in E_u , and W_3 is a walk in H whose length may be zero. By the choice of W_2 , we know that W_2 starts at some vertex in V_u and ends at some vertex in V_u . Let

$$S_u^{(x_1, x_2)}(k) = \{W \in S_u(k) : W_2 \text{ is an } (x_1, x_2)\text{-walk}\},$$

where $x_1, x_2 \in V_u$. Then

$$\begin{aligned} |S_u(k)| &= \sum_{x_1, x_2 \in V_u} |S_u^{(x_1, x_2)}(k)| = |S_u^{(u, u)}(k)| + \sum_{x_2 \in V_u \setminus \{u\}} |S_u^{(u, x_2)}(k)| \\ &\quad + \sum_{x_1 \in V_u \setminus \{u\}} |S_u^{(x_1, u)}(k)| + \sum_{x_1, x_2 \in V_u \setminus \{u\}} |S_u^{(x_1, x_2)}(k)|. \end{aligned}$$

Similarly, let

$$S_v^{(x_1, x_2)}(k) = \{W \in S_v(k) : W_2 \text{ is an } (x_1, x_2)\text{-walk}\},$$

where $x_1, x_2 \in V_v$, and thus

$$\begin{aligned} |S_v(k)| &= \sum_{x_1, x_2 \in V_v} |S_v^{(x_1, x_2)}(k)| = |S_v^{(v, v)}(k)| + \sum_{x_2 \in V_v \setminus \{v\}} |S_v^{(v, x_2)}(k)| \\ &\quad + \sum_{x_1 \in V_v \setminus \{v\}} |S_v^{(x_1, v)}(k)| + \sum_{x_1, x_2 \in V_v \setminus \{v\}} |S_v^{(x_1, x_2)}(k)|. \end{aligned}$$

Now we have

$$\begin{aligned} |S_u^{(u, u)}(k)| &= \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} \sum_{y \in V(H)} M_{k_1}(H; y, u) \cdot |\mathcal{T}_{k_2}(H_u; u, u)| \cdot M_{k_3}(H; u, y) \\ &= \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_u; u, u)| \sum_{y \in V(H)} M_{k_1}(H; y, u) \cdot M_{k_3}(H; u, y) \\ &= \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_u; u, u)| \cdot M_{k_1+k_3}(H; u, u). \end{aligned}$$

Similarly,

$$|S_v^{(v, v)}(k)| = \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_v; v, v)| \cdot M_{k_1+k_3}(H; v, v).$$

By Lemma 3.1 (i), $|\mathcal{T}_s(H_u; u, u)| \leq |\mathcal{T}_s(H_v; v, v)|$ for all positive integers s . Since $(H; u) \prec (H; v)$, we have $M_s(H; u, u) \leq M_s(H; v, v)$ for all positive integers s , and it is strict for some positive integer s_0 . It follows that $|S_u^{(u, u)}(k)| \leq |S_v^{(v, v)}(k)|$, and it is strict for some positive integer k_0 .

Similarly, by Lemma 3.1 (ii), (iii) and (iv), we have

$$\begin{aligned}
 & \sum_{x_2 \in V_u \setminus \{u\}} |S_u^{(u, x_2)}(k)| \\
 &= \sum_{x_2 \in V_u \setminus \{u\}} \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_u; u, x_2)| \cdot M_{k_1+k_3}(H; x_2, u) \\
 &\leq \sum_{x_2 \in V_v \setminus \{v\}} |S_v^{(v, x_2)}(k)| = \sum_{x_2 \in V_v \setminus \{v\}} \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_v; v, x_2)| \cdot M_{k_1+k_3}(H; x_2, v), \\
 &\quad \sum_{x_1 \in V_u \setminus \{u\}} |S_u^{(x_1, u)}(k)| = \sum_{x_1 \in V_u \setminus \{u\}} \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_u; x_1, u)| \cdot M_{k_1+k_3}(H; u, x_1) \\
 &\leq \sum_{x_1 \in V_v \setminus \{v\}} |S_u^{(x_1, v)}(k)| = \sum_{x_1 \in V_v \setminus \{v\}} \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_v; x_1, v)| \cdot M_{k_1+k_3}(H; v, x_1), \\
 &\quad \sum_{x_1, x_2 \in V_u \setminus \{u\}} |S_u^{(x_1, x_2)}(k)| = \sum_{x_1, x_2 \in V_u \setminus \{u\}} \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_u; x_1, x_2)| M_{k_1+k_3}(H; x_2, x_1) \\
 &\leq \sum_{x_1, x_2 \in V_v \setminus \{v\}} |S_v^{(x_1, x_2)}(k)| = \sum_{x_1, x_2 \in V_v \setminus \{v\}} \sum_{\substack{k_1+k_2+k_3=k \\ k_1, k_3 \geq 0, k_2 \geq 1}} |\mathcal{T}_{k_2}(H_v; x_1, x_2)| M_{k_1+k_3}(H; x_2, x_1).
 \end{aligned}$$

Therefore $|S_u(k)| \leq |S_v(k)|$ for all positive integers k , and it is strict for some positive integer k_0 . \square

4. The change of Estrada index of graph under edge grafting operation

Let G be a connected graph with at least two vertices, and u and v be two adjacent vertices in G .

For integers a, b with $a, b \geq 0$, let $G_u(a, b)$ be the graph obtained from G by attaching two pendent paths $P_a: x_1x_2 \cdots x_a$ and $P_b: y_1y_2 \cdots y_b$ at end vertices x_1 and y_1 to u , and let $G_{u,v}(a, b)$ be the graph obtained from G by attaching two pendent paths $P_a: x_1x_2 \cdots x_a$ and $P_b: y_1y_2 \cdots y_b$ at end vertices x_1 and y_1 , respectively, to u and v , see Fig. 2. For $G_u(a, b)$, we require that $a \geq b \geq 0$.

Ilić and Stevanović [24] considered the change of Estrada index of graph under edge grafting operation between two pendent paths at the same vertex, and gave the following result.

Lemma 4.1 [24]. For integers s, t with $s \geq t + 2 \geq 2$, $EE(G_u(s, t)) < EE(G_u(s - 1, t + 1))$.

In this section, we consider the change of Estrada index of graph under edge grafting operation between two pendent paths at two adjacent vertices.

Since the Estrada index of a disconnected graph is equal to the sum of Estrada indices of its connected components, thus we need only to consider the connected graphs.

Let s, t be integers with $s \geq t + 2 \geq 2$. If $d_G(u) = d_G(v) = 1$ (i.e., $G = uv \cong P_2$), then both $G_{u,v}(s, t)$ and $G_{u,v}(t + 1, s - 1)$ are the paths on $s + t + 2$ vertices, and thus $EE(G_{u,v}(s, t)) =$

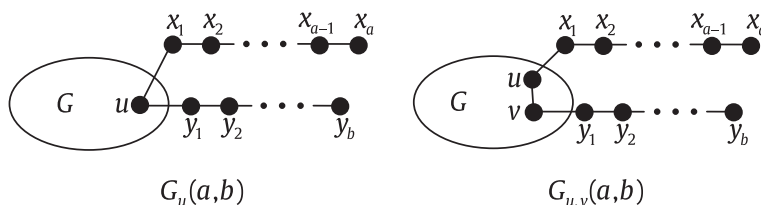


Fig. 2. The graphs $G_u(a, b)$ and $G_{u,v}(a, b)$.

$EE(G_{u,v}(t+1, s-1))$. If $d_G(u) > 1$ and $d_G(v) = 1$, then $G_{u,v}(s, t) \cong G_{u,v}(t+1, s-1)$, and thus $EE(G_{u,v}(s, t)) = EE(G_{u,v}(t+1, s-1))$. If $d_G(u) = 1$ and $d_G(v) > 1$, then by Lemma 4.1, $EE(G_{u,v}(s, t)) < EE(G_{u,v}(t+1, s-1))$. Suppose in the following that $d_G(u), d_G(v) > 1$, and we will show that $EE(G_{u,v}(s, t)) < EE(G_{u,v}(t+1, s-1))$.

Lemma 4.2. *Let $\mathcal{G} = G - v$. Suppose that a, b are two integers with $a > b \geq 1$. Then*

- (i) $(\mathcal{G}_u(a, b); y_1) < (\mathcal{G}_u(a, b); x_1)$;
- (ii) $(\mathcal{G}_u(a, b); z, y_1) \leq (\mathcal{G}_u(a, b); z, x_1)$ for $z \in V(\mathcal{G}) \setminus \{u\}$.

Proof. (i) Let k be any positive integer. For two distinct vertices $x, y \in V(\mathcal{G}_u(a, b))$, let $\mathcal{W}_k(\mathcal{G}_u(a, b); x, [y])$ be the set of (x, x) -walks of length k in $\mathcal{G}_u(a, b)$ containing y , and let $M_k(\mathcal{G}_u(a, b); x, [y]) = |\mathcal{W}_k(\mathcal{G}_u(a, b); x, [y])|$.

Note that

$$M_k(\mathcal{G}_u(a, b); y_1) = M_k(P_b; y_1) + M_k(\mathcal{G}_u(a, b); y_1, [u])$$

and

$$M_k(\mathcal{G}_u(a, b); x_1) = M_k(P_a; x_1) + M_k(\mathcal{G}_u(a, b); x_1, [u]).$$

Since $a > b \geq 1$, P_b is a proper subgraph of P_a , and then $(P_b; y_1) < (P_a; x_1)$. Thus we need only to show that $M_k(\mathcal{G}_u(a, b); y_1, [u]) \leq M_k(\mathcal{G}_u(a, b); x_1, [u])$.

We construct a mapping f from $\mathcal{W}_k(\mathcal{G}_u(a, b); y_1, [u])$ to $\mathcal{W}_k(\mathcal{G}_u(a, b); x_1, [u])$. For $W \in \mathcal{W}_k(\mathcal{G}_u(a, b); y_1, [u])$, we may uniquely decompose W into three sections, say $W_1W_2W_3$, where W_1 is the shortest (y_1, u) -section of W (for which the internal vertices, if exist, are only possible to be y_1, y_2, \dots, y_b), W_2 is the longest (u, u) -section of W whose length may be zero, and W_3 is the remaining (u, y_1) -section of W (for which the internal vertices, if exist, are only possible to be y_1, y_2, \dots, y_b). Let $f(W) = f(W_1)f(W_2)f(W_3)$, where $f(W_1)$ is an (x_1, u) -walk obtained from W_1 by replacing y_i by x_i for $i = 1, 2, \dots, b$, $f(W_2) = W_2$, and $f(W_3)$ is a (u, x_1) -walk obtained from W_3 by replacing y_i by x_i for $i = 1, 2, \dots, b$. Obviously, $f(W) \in \mathcal{W}_k(\mathcal{G}_u(a, b); x_1, [u])$ and f is an injection. Thus $M_k(\mathcal{G}_u(a, b); y_1, [u]) \leq M_k(\mathcal{G}_u(a, b); x_1, [u])$.

(ii) Let $z \in V(\mathcal{G}) \setminus \{u\}$, and k be any positive integer. We construct a mapping f from $\mathcal{W}_k(\mathcal{G}_u(a, b); z, y_1)$ to $\mathcal{W}_k(\mathcal{G}_u(a, b); z, x_1)$. For $W \in \mathcal{W}_k(\mathcal{G}_u(a, b); z, y_1)$, we may uniquely decompose W into two sections, say W_1W_2 , where W_1 is the longest (z, u) -section of W , and W_2 is the remaining (u, y_1) -section of W (for which the internal vertices, if exist, are only possible to be y_1, y_2, \dots, y_b). Let $f(W) = f(W_1)f(W_2)$, where $f(W_1) = W_1$, and $f(W_2)$ is a (u, x_1) -walk obtained from W_2 by replacing y_i by x_i for $i = 1, 2, \dots, b$. Obviously, $f(W) \in \mathcal{W}_k(\mathcal{G}_u(a, b); z, x_1)$ and f is an injection. Thus $M_k(\mathcal{G}_u(a, b); z, y_1) \leq M_k(\mathcal{G}_u(a, b); z, x_1)$. \square

Theorem 4.1. *Suppose that G is a connected graph. Let u, v be two adjacent vertices in G , where $d_G(u), d_G(v) > 1$. For integers s, t with $s \geq t+2 \geq 2$, $EE(G_{u,v}(s, t)) < EE(G_{u,v}(t+1, s-1))$.*

Proof. Denote by w_1, w_2, \dots, w_r the neighbors of v in G different from u , where $r = d_G(v) - 1$. Let $\mathcal{G} = G - v$. Since $s > t+1 \geq 1$, by Lemma 4.2 (i) and (ii), we have $(\mathcal{G}_u(s, t+1); y_1) < (\mathcal{G}_u(s, t+1); x_1)$, and $(\mathcal{G}_u(s, t+1); w_i, y_1) \leq (\mathcal{G}_u(s, t+1); w_i, x_1)$ for $1 \leq i \leq r$.

Let $E_{y_1} = \{y_1w_1, y_1w_2, \dots, y_1w_r\}$ and $E_{x_1} = \{x_1w_1, x_1w_2, \dots, x_1w_r\}$. Note that

$$G_{u,v}(s, t) \cong \mathcal{G}_u(s, t+1) + E_{y_1}$$

and

$$G_{u,v}(t+1, s-1) \cong \mathcal{G}_u(s, t+1) + E_{x_1}.$$

Then the result follows from Lemma 3.2. \square

For $x \in V(G)$, let $N_G(x)$ be the set of neighbors of x in G .

If $N_G(u) \setminus \{v\} = N_G(v) \setminus \{u\}$, then $G_{u,v}(a, b) \cong G_{u,v}(b, a)$ for integers a, b with $a, b \geq 0$, and thus we have

Corollary 4.1. Suppose that G is a connected graph. Let u, v be two adjacent vertices in G , where $d_G(u), d_G(v) > 1$. Suppose that $N_G(u) \setminus \{v\} = N_G(v) \setminus \{u\}$. For integers s, t with $s \geq t + 2 \geq 2$, $EE(G_{u,v}(s, t)) < EE(G_{u,v}(t + 1, s - 1)) = EE(G_{u,v}(s - 1, t + 1))$.

5. The change of Laplacian Estrada index of bipartite graph under edge grafting operation

Let $\mathcal{L}(G)$ be the line graph of a graph G . Zhou and Gutman [38] gave the following relationship between the Laplacian Estrada index of a bipartite graph and the Estrada index of its line graph.

Lemma 5.1 [38]. Let G be a bipartite graph with n vertices and m edges. Then

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

Now we consider the change of Laplacian Estrada index of bipartite graph under edge grafting operation between two pendent paths at the same vertex.

Theorem 5.1. Let G be a nontrivial bipartite connected graph with $u \in V(G)$. For integers s, t with $s \geq t + 2 \geq 2$, $LEE(G_u(s, t)) < LEE(G_u(s - 1, t + 1))$.

Proof. By Lemma 5.1, we need only to show that $EE(\mathcal{L}(G_u(s, t))) < EE(\mathcal{L}(G_u(s - 1, t + 1)))$.

Denote by z_1 (z_2 , respectively) the vertex in $\mathcal{L}(G_u(1, 1))$ corresponding to the edge ux_1 (uy_1 , respectively) in $G_u(1, 1)$. Obviously, z_1 and z_2 are adjacent in $\mathcal{L}(G_u(1, 1))$, and $N_{\mathcal{L}(G_u(1, 1))}(z_1) \setminus \{z_2\} = N_{\mathcal{L}(G_u(1, 1))}(z_2) \setminus \{z_1\}$. Since G is a nontrivial connected graph, we have $\mathcal{L}(G_u(1, 1))$ is also a connected graph, and $d_{\mathcal{L}(G_u(1, 1))}(z_1), d_{\mathcal{L}(G_u(1, 1))}(z_2) > 1$.

For integers a, b with $a \geq b \geq 1$, it is easily seen that $\mathcal{L}(G_u(a, b))$ can be obtained from $\mathcal{L}(G_u(1, 1))$ by attaching two pendent paths on $a - 1$ and $b - 1$ vertices, respectively, to z_1 and z_2 , i.e., $\mathcal{L}(G_u(a, b)) \cong \mathcal{L}(G_u(1, 1))_{z_1, z_2}(a - 1, b - 1)$.

If $t \geq 1$, then by Corollary 4.1,

$$EE(\mathcal{L}(G_u(1, 1))_{z_1, z_2}(s - 1, t - 1)) < EE(\mathcal{L}(G_u(1, 1))_{z_1, z_2}(s - 2, t)),$$

i.e., $EE(\mathcal{L}(G_u(s, t))) < EE(\mathcal{L}(G_u(s - 1, t + 1)))$.

Suppose that $t = 0$. Let $\mathcal{L}(G_u(1, 0)) = \mathcal{L}(G_u(1, 1)) - z_2$. Then $\mathcal{L}(G_u(s, 0))$ can be obtained from $\mathcal{L}(G_u(1, 0))$ by attaching a pendent path on $s - 1$ vertices to z_1 , i.e., $\mathcal{L}(G_u(s, 0)) \cong \mathcal{L}(G_u(1, 0))_{z_1}(s - 1, 0)$. Recall that $\mathcal{L}(G_u(s - 1, 1)) \cong \mathcal{L}(G_u(1, 1))_{z_1, z_2}(s - 2, 0)$. Let

$$N_{\mathcal{L}(G_u(1, 1))}(z_1) \setminus \{z_2\} = N_{\mathcal{L}(G_u(1, 1))}(z_2) \setminus \{z_1\} = \{w_1, w_2, \dots, w_r\}.$$

It is easily seen that

$$\mathcal{L}(G_u(1, 0))_{z_1}(s - 1, 0) \cong \mathcal{L}(G_u(1, 1))_{z_1, z_2}(s - 2, 0) - \{z_1 w_1, z_1 w_2, \dots, z_1 w_r\},$$

and thus

$$EE(\mathcal{L}(G_u(1, 0))_{z_1}(s - 1, 0)) < EE(\mathcal{L}(G_u(1, 1))_{z_1, z_2}(s - 2, 0)),$$

i.e., $EE(\mathcal{L}(G_u(s, 0))) < EE(\mathcal{L}(G_u(s - 1, 1)))$. \square

6. Minimum Laplacian Estrada index of trees with given maximum degree

Let $D_{n,\Delta}$ be the tree obtained by attaching $\Delta - 1$ pendent vertices to one end vertex of the path $P_{n-\Delta+1}$, where $2 \leq \Delta \leq n - 1$.

Theorem 6.1. *Let G be an n -vertex tree with maximum degree Δ , where $2 \leq \Delta \leq n - 1$. Then $LEE(G) \geq LEE(D_{n,\Delta})$ with equality if and only if $G \cong D_{n,\Delta}$.*

Proof. The case $\Delta = 2$ is trivial. Suppose in the following that $3 \leq \Delta \leq n - 1$. Let G be a tree with minimum Laplacian Estrada index among n -vertex trees with a vertex, say x , of maximum degree Δ . If there is another vertex in G different from x with degree at least three, then by Theorem 5.1, we may get a tree of maximum degree Δ with smaller Laplacian Estrada index, a contradiction. Thus, x is the unique vertex in G with degree at least three, i.e., G is a tree obtained by attaching Δ paths to a single vertex x . Now by Theorem 5.1, we have $G \cong D_{n,\Delta}$. \square

Ilić and Zhou [25] showed that the path is the unique tree with minimum Laplacian Estrada index.

By Theorem 5.1, $LEE(D_{n,\Delta-1}) < LEE(D_{n,\Delta})$ for $4 \leq \Delta \leq n - 1$. Together with Theorem 6.1, we have

Theorem 6.2. *Let G be an n -vertex tree different from $D_{n,3}$ and P_n , where $n \geq 5$. Then $LEE(G) > LEE(D_{n,3}) > LEE(P_n)$.*

7. Maximum Laplacian Estrada indices of trees with given parameters

First we give some lemmas which will be used in our proof.

Lemma 7.1. *Let G and G_1 be two trees shown in Fig. 3, where the path from v to w in G is a pendent path at v , and all neighbors of v in Q of G are switched to be neighbors of u in Q of G_1 . If $d_G(v, w) \leq \max\{d_G(u, x) : x \in V(S)\}$ and S is not a path with an end vertex u , then $LEE(G) < LEE(G_1)$.*

Proof. By Lemma 5.1, we need only to show that $EE(\mathcal{L}(G)) < EE(\mathcal{L}(G_1))$.

Let P be the path from v to w in G . Since $d_G(v, w) \leq \max\{d_G(u, x) : x \in V(S)\}$, there is a vertex $z \in V(S)$ such that $d_G(v, w) \leq d_G(u, z)$, i.e., $d_P(v, w) \leq d_S(u, z)$. Since S is not a path with an end vertex u , P is a proper subgraph of S .

Let v_1 be the neighbor of v in G lying on P ($v_1 = w$ if v and w are adjacent in G), and u_1 be the neighbor of u in G lying on the unique path connecting u and z ($u_1 = z$ if u and z are adjacent in G). Denote by w_1, w_2, \dots, w_t the neighbors of v in Q of G .

For $y_1 y_2 \in E(G)$, let $x_{y_1 y_2}$ be the vertex in $\mathcal{L}(G)$ corresponding to $y_1 y_2 \in E(G)$. Let

$$E_{x_{vv_1}} = \{x_{vv_1}x_{vw_1}, x_{vv_1}x_{vw_2}, \dots, x_{vv_1}x_{vw_t}\},$$

$$E_{x_{uu_1}} = \{x_{uu_1}x_{vw_1}, x_{uu_1}x_{vw_2}, \dots, x_{uu_1}x_{vw_t}\}.$$

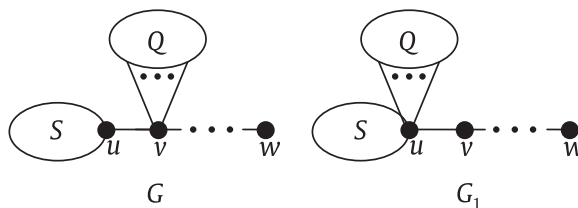


Fig. 3. The trees G and G_1 in Lemma 7.1.

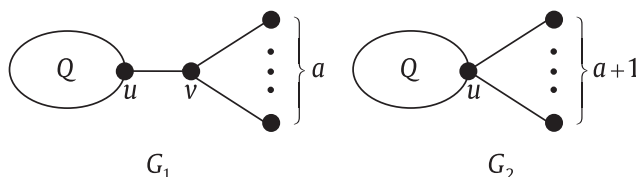


Fig. 4. The trees G_1 and G_2 in Lemma 7.2.

Consider $H = \mathcal{L}(G) - E_{x_{vv_1}}$. By similar proof of Lemma 4.2 (i) and (ii), we have $(H; x_{vv_1}) < (H; x_{uu_1})$, and $(H; x_{vw_i}, x_{vv_1}) \leq (H; x_{vw_i}, x_{uu_1})$ for $1 \leq i \leq t$.

Note that $\mathcal{L}(G) = H + E_{x_{vv_1}}$. Let $G^* = H + E_{x_{uu_1}}$. It follows from Lemma 3.2 that $EE(\mathcal{L}(G)) < EE(G^*)$. It is easily seen that G^* is a subgraph of $\mathcal{L}(G_1)$, and thus $EE(G^*) \leq EE(\mathcal{L}(G_1))$, implying that $EE(\mathcal{L}(G)) < EE(\mathcal{L}(G_1))$. \square

Lemma 7.2 [25]. Let u be a vertex of a tree Q with at least two vertices. For integer $a \geq 1$, let G_1 be the tree obtained by attaching a star S_{a+1} at its center v to u of Q , and G_2 be the tree obtained by attaching $a + 1$ pendent vertices to u of Q , see Fig. 4. Then $LEE(G_1) < LEE(G_2)$.

Let $D^{n,d}$ be the tree obtained from $P_{d+1} = v_0 v_1 \cdots v_d$ by attaching $n - d - 1$ pendent vertices to $v_{\lfloor d/2 \rfloor}$, where $2 \leq d \leq n - 1$.

Theorem 7.1. Let G be an n -vertex tree with diameter d , where $2 \leq d \leq n - 1$. Then $LEE(G) \leq LEE(D^{n,d})$ with equality if and only if $G \cong D^{n,d}$.

Proof. The case $d = n - 1$ is trivial. Suppose that $d < n - 1$. Let G be a tree with maximum Laplacian Estrada index among the n -vertex trees with diameter d , and $P = v_0 v_1 \cdots v_d$ be a diametrical path of G .

By Lemma 7.2, every vertex outside P is a pendent vertex. Let $V_1(G)$ be the set of vertices on P with degree at least three in G . Obviously, $|V_1(G)| \geq 1$ since $d < n - 1$.

Suppose that $|V_1(G)| \geq 2$. Assume that $V_1(G) \cap \{v_1, v_2, \dots, v_{\lfloor \frac{d-1}{2} \rfloor}\} \neq \emptyset$. Choose $v_i \in V_1(G)$ such that $d_G(v_i, v_0)$ is as small as possible. Then $d_G(v_{i+1}, v_d) \geq d_G(v_i, v_0)$. Note that the component of $G - v_i v_{i+1}$ containing v_{i+1} is not a path with an end vertex v_{i+1} since $|V_1(G)| \geq 2$. Now applying Lemma 7.1 to G by setting $u = v_{i+1}$, $v = v_i$ and $w = v_0$, we may get another n -vertex tree with diameter d with larger Laplacian Estrada index, a contradiction. Thus, $|V_1(G)| = 1$, i.e., G is a tree obtained by attaching $n - d - 1$ pendent vertices to v_s for $1 \leq s \leq \lfloor \frac{d}{2} \rfloor$. It follows from Theorem 5.1 that $s = \lfloor \frac{d}{2} \rfloor$, i.e., $G \cong D^{n,d}$. \square

Let n, p be positive integers. Let $s = \lfloor \frac{n-1}{p} \rfloor, r = n - 1 - ps$. Let $T_{n,p}$ be the tree obtained by attaching $p - r$ paths on s vertices and r paths on $s + 1$ vertices to a single vertex, where $2 \leq p \leq n - 1$.

Theorem 7.2. Let G be an n -vertex tree with p pendent vertices, where $2 \leq p \leq n - 1$. Then $LEE(G) \leq LEE(T_{n,p})$ with equality if and only if $G \cong T_{n,p}$.

Proof. The cases $p = 2, n - 1$ are trivial. Suppose in the following that $3 \leq p \leq n - 2$. Let G be a tree with maximum Laplacian Estrada index among the n -vertex trees with p pendent vertices. Let $V_1(G)$ be the set of vertices in G with degree at least three. Let P be a pendent path with minimum length in G at a vertex $v \in V_1(G)$, and w be the pendent vertex in P .

Suppose that $|V_1(G)| \geq 2$. Choose a vertex $y \in V_1(G)$ such that $d_G(v, y)$ is as small as possible. Then the internal vertices (if exist) of the unique path connecting v and y in G are all of degree two. Denote by u the neighbor of v in G lying on the unique path connecting v and y ($u = y$ if v and y are adjacent in G). Let S be the component of $G - uv$ containing u . Obviously, S is not a path with an end vertex u

since $y \in V(S)$. By the choice of P , we have $d_G(v, w) \leq \max\{d_G(u, x) : x \in V(S)\}$. Applying Lemma 7.1 to G , we may get another n -vertex tree G_1 with p pendent vertices such that $LEE(G) < LEE(G_1)$, a contradiction. Thus $|V_1(G)| = 1$, i.e., G is a tree obtained by attaching p pendent paths to a single vertex. It follows from Theorem 5.1 that $G \cong T_{n,p}$. \square

Lemma 7.3. For $2 \leq p \leq n - 2$, $LEE(T_{n,p}) < LEE(T_{n,p+1})$.

Proof. Let u be the pendent vertex of a longest pendent path in $T_{n,p}$. Let v be the neighbor of u , and w be the neighbor of v different from u in $T_{n,p}$. Let $G = T_{n,p} - uv + uw$. By Theorem 5.1, $LEE(T_{n,p}) < LEE(G)$. Note that there are $p + 1$ pendent vertices in G , and thus by Theorem 7.2, $LEE(G) \leq LEE(T_{n,p+1})$. Then the result follows easily. \square

A matching of a graph is an edge subset in which no pair shares a common vertex.

The matching number of G , denoted by $m(G)$, is the maximum cardinality of a matching of G .

For $1 \leq r \leq \lfloor n/2 \rfloor$, let $T^{n,r}$ be the tree obtained by attaching $r - 1$ paths on two vertices to the center of the star S_{n-2r+2} .

Corollary 7.1. Let G be a tree with n vertices and matching number $m = m(G)$, where $2 \leq m \leq \lfloor n/2 \rfloor$. Then $LEE(G) \leq LEE(T^{n,m})$ with equality if and only if $G \cong T^{n,m}$.

Proof. Let M be a maximum matching of G . Let p be the number of pendent vertices in G . Obviously, there is at most one pendent end vertex for an edge of M . Then $p \leq m + (n - 2m) = n - m$. If $p = n - m$, then by Theorem 7.2 (with $s = 1$ and $r = m - 1$), we have $T^{n,m} \cong T_{n,n-m}$ is the unique tree with maximum Laplacian Estrada index. If $p < n - m$, then by Theorem 7.2 and Lemma 7.3,

$$LEE(G) \leq LEE(T_{n,p}) < \cdots < LEE(T_{n,n-m}) = LEE(T^{n,m}).$$

Then the result follows easily. \square

An independent set of a graph is a vertex subset in which no pair is adjacent. The independence number of a graph G , denoted by $\alpha(G)$, is the maximum cardinality of an independent set of G . It is well-known that for any bipartite graph G , $\alpha(G) + m(G) = |V(G)|$, see [2]. From Corollary 7.1, we have

Corollary 7.2. Let G be a tree with n vertices and independence number $\alpha = \alpha(G)$, where $\lceil n/2 \rceil \leq \alpha \leq n - 2$. Then $LEE(G) \leq LEE(T^{n,n-\alpha})$ with equality if and only if $G \cong T^{n,n-\alpha}$.

A dominating set of a graph is a vertex subset whose closed neighborhood contains all vertices of the graph. The domination number of a graph G , denoted by $\gamma(G)$, is the minimum cardinality of a dominating set of G .

A covering of a graph G is a vertex subset K such that every edge of G has at least one end vertex in K .

Let G be a tree. By König's theorem [2], the matching number of G is equal to the minimum cardinality of a covering of G . It is easily seen that a covering of G is also a dominating set of G . It follows that $m(G) \geq \gamma(G)$. By Theorem 5.1, $LEE(T^{n,m}) < LEE(T^{n,m-1})$ for $2 \leq m \leq \lfloor n/2 \rfloor$. Together with Corollary 7.1, we have

Corollary 7.3. Let G be a tree with n vertices and domination number $\gamma = \gamma(G)$, where $2 \leq \gamma \leq \lfloor n/2 \rfloor$. Then $LEE(G) \leq LEE(T^{n,\gamma})$ with equality if and only if $G \cong T^{n,\gamma}$.

Acknowledgements

The authors are grateful for the useful comments and suggestions of the reviewers, which have helped to improve the paper.

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