Research Article

Properties and Applications of the Eigenvector Corresponding to the Laplacian Spectral Radius of a Graph

Haizhou Song and Qiufen Wang

College of Mathematical Sciences, Huaqiao University, Quanzhou, Fujian 362021, China

Correspondence should be addressed to Haizhou Song; hzsong@hqu.edu.cn

Received 26 November 2012; Revised 26 February 2013; Accepted 26 February 2013

Academic Editor: Yong-Kui Chang

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We study the properties of the eigenvector corresponding to the Laplacian spectral radius of a graph and show some applications. We obtain some results on the Laplacian spectral radius of a graph by grafting and adding edges. We also determine the structure of the maximal Laplacian spectrum tree among trees with n vertices and k pendant vertices (n, k fixed), and the upper bound of the Laplacian spectral radius of some trees.

1. Introduction

The theory of graph spectra has been established in the 1950s and 1960s. Chung has taken the investigation of the theory of graph spectra to a new level by a 45-minute report [1] presented at the World Congress of Mathematicians in 1994, and in monographs [2]. Applications of the theory of graph spectra have also been found in the fields of electrical networks and vibration theory [3, 4]. The wide range of the applications of the theory of graph spectra has led it to become a very active field of research of graph theory over the last thirty to forty years, and large numbers of results are continuously emerging.

There are many results on the (adjacency) spectral radius for different classes of graphs. Guo et al. [5] have studied the largest and the second largest spectral radius of trees with n vertices and diameter d . Guo and Shao [6] have studied the first $\lfloor d/2 \rfloor + 1$ (where $\lfloor x \rfloor$ represents the maximal integer not more than x) spectral radii of graphs with n vertices and diameter d . Wu et al. [7] have studied the spectral radius of trees on k pendant vertices.

There are also many results on the Laplacian spectral radius for different classes of graphs. Hong and Zhang [8] have studied the upper and lower bounds for the Laplacian spectral radius of trees. Guo [9] has studied the second largest Laplacian eigenvalues of trees. In the paper, we further study the properties of the eigenvector corresponding to

the Laplacian spectral radius of a graph and obtain some applications on the Laplacian spectral radius of trees with k pendant vertices.

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. Let $d_G(v_i)$ denote the degree of vertex v_i ($1 \leq i \leq n$) of graph G sometimes for convenience we denote by $d(v_i)$. If $D(G) = \text{diag}(d(v_1), d(v_2), \dots, d(v_n))$ is the diagonal matrix of the vertex degree and $A(G)$ is the $(0, 1)$ adjacency matrix of G , then the matrix $L(G) = D(G) - A(G)$ is called the Laplacian matrix of graph G . When G is connected, $A(G)$ is irreducible, and, by the Perron-Frobenius theorem [10–12], the spectral radius $\rho(G)$ is simple and there is a unique positive unit eigenvector. We refer to such an eigenvector as the *Perron vector* of G . It is easy to see that $L(G)$ is a positive semidefinite M matrix and its rows sum to 0, $L(G)$ is singular. Hence, the eigenvalues of $L(G)$ can be ordered as $\mu_1(G) \geq \mu_2(G) \geq \dots \geq \mu_n(G) = 0$. The largest eigenvalue $\mu_1(G)$ of $L(G)$ is called the Laplacian spectral radius of the graph G , denoted by $\mu(G)$. This has been used extensively in fields such as theoretical chemistry, combinatorial optimization, and communication networks [13, 14].

A pendant vertex of G is a vertex of degree 1. Let $N_G(v)$ denote the adjacent vertex set of v in G and d_v the degree of v . $\mathcal{T}_{n,k}$ denotes the set of trees for n vertices and k pendant vertices (n, k fixed). The tree $T_{n,k}$ is obtained from a star $K_{1,k}$

FIGURE 1

FIGURE 2

and k paths of almost equal length by joining each pendant vertex of $K_{1,k}$ to an end of one path. Obviously, $2 \leq k \leq n-1$. Assume $q = \lfloor (n-1)/k \rfloor$, $n-1 = kq + r$ ($0 \leq r \leq k-1$); $T_{n,k}$ is shown in Figure 1.

In general, $T_{n,n-1} = K_{1,n-1}$, $T_{n,2} = P_n$, and $T_{n,n-2} = S(1, n-3)$, a tree is obtained from two stars $K_{1,n-3}$ and $K_{1,1}$ by joining their central vertices. For example, $T_{6,5} = K_{1,5}$, $T_{6,4} = S(1, 3)$, and $T_{6,2}$ is a path of length 6 (Figure 2).

In Section 2, we describe some properties of the eigenvector corresponding to the Laplacian spectral radius of a graph. Section 3 presents some applications of the eigenvector corresponding to the Laplacian spectral radius of a graph, including some results on the Laplacian spectral radius of a graph by grafting and adding edges. Then we obtain the structure of the maximal Laplacian spectrum tree among trees with n vertices and k pendant vertices (n, k fixed), and the upper bound of the Laplacian spectral radius for some trees.

2. Properties of the Eigenvector Corresponding to the Laplacian Spectral Radius of a Graph

For convenience, we denote $L(G)$ by L sometimes. Since the Laplacian matrix $L(G)$ is a real symmetric matrix, we have the following theorem.

Theorem 1. Let G be a simple connected graph of n vertices. $L(G)$ is the Laplacian matrix of G , with vector $x \in \mathbb{R}^{n \times 1}$. Then

- (1) $\mu(G) = \max_{1 \leq i \leq n} \mu_i$, where μ_i is the eigenvalue of $L(G)$;
- (2) $\mu(G) = \max_{\|x\|=1} (x' L x)$;
- (3) if $\|x\| = 1$ and $x' L(G)x = \mu(G)$, then $L(G)x = \mu(G)x$.

Proof. (1) It is proved by the definition.

(2) Since $L(G)$ is a real symmetric matrix, there exists an orthogonal matrix P for which $P^{-1}LP = \text{diag}(\mu_1, \mu_2, \dots, \mu_n) \triangleq D$, where $P = (W_1, W_2, \dots, W_n)$. Let $x = Py$, so $x' L x = y' P' L P y = y' P^{-1} L P y = y' D y = \sum_{i=1}^n \mu_i y_i^2$.

P is an orthogonal matrix and $x = Py$. Then, when $\|x\| = 1$, we have $\|y\| = 1$. Assume, without loss of generality, that $\mu_1 \leq \mu_2 \leq \dots \leq \mu_n$. Thus,

$$\begin{aligned} \max_{\|x\|=1} (x' L x) &= \max_{\|y\|=1} \sum_{i=1}^n \mu_i y_i^2 \leq \max_{\|y\|=1} \sum_{i=1}^n \mu_n y_i^2 \\ &= \mu_n \max_{\|y\|=1} \sum_{i=1}^n y_i^2 = \mu_n = \mu(G). \end{aligned} \quad (1)$$

Let $y = e_n = (0, 0, \dots, 0, 1)'_{n \times 1}$, so we have $x = Py = W_n$, and then the above equality holds. Therefore, $\mu(G) = \max_{\|x\|=1} (x' L x)$.

(3) Since $L(G)$ is a real symmetric matrix, there exists an orthogonal matrix P for which $P^{-1}LP = \text{diag}(\mu_1, \mu_2, \dots, \mu_n) \triangleq D$, where $P = (W_1, W_2, \dots, W_n)$, and W_i is the eigenvector corresponding to μ_i of $L(G)$. Assume, without loss of generality, that $\mu_1 \leq \mu_2 \leq \dots \leq \mu_n$.

Let $x = Py$, and then $x' L(G)x = y' P' L P y = y' D y$. Since $x' L(G)x = \mu(G)$, we have $x' L(G)x = y' D y = \mu_n = \mu(G)$. Thus, $y = e_n = (0, 0, \dots, 0, 1)'_{n \times 1}$ and then $x = Py = P e_n = W_n$. However, W_n is the eigenvector corresponding to μ_n of $L(G)$, that is, $L(G)W_n = \mu_n W_n$. Thus, $L(G)x = \mu(G)x$. $\square$

Definition 2. Let G be a simple connected graph, $G = (V, E)$. If vector $x \in \mathbb{R}^{n \times 1}$ satisfies $\|x\| = 1$ and $x' L(G)x = \mu(G)$, then we call x the standard Laplacian spectral vector of G .

Theorem 3. Let T be a tree, and $V(T) = \{v_1, v_2, \dots, v_n\}$. Let L be the Laplacian matrix of T and x be the standard Laplacian spectral vector of T . Then

- (1) x is a real vector;
- (2) $|x| > 0$.

Proof. (1) Since L is a real symmetric matrix, we have $\mu(T) \in \mathbb{R}$. Thus, x is a real vector.

(2) Suppose that $|x| > 0$ is not established. Then there exists vertex set $H = \{v_{j_1}, v_{j_2}, \dots, v_{j_t}\}$, which means $x_{j_i} = 0$ ($i = 1, 2, \dots, t$), where x_j corresponds to vertex v_j . Since x is the standard Laplacian spectral vector of T , we have $\|x\| = 1$. Thus, $x \neq 0$ and there exists vertex $v \in V(T)$ that makes $x_v = 0$ and vertex $u \in N_T(v)$ that makes $x_u \neq 0$.

Let T form a root tree with v as its root vertex. $N_T(v) = \{w_1, w_2, \dots, w_s\} \triangleq W$. Let T_i be the subtree of T obtained from vertex w_i and all its descendants. Let $y_v = x_v = 0$, $y_{w_i} = |x_{w_i}|$ ($i = 1, 2, \dots, s$), $y_j = x_j$ when $x_{w_i} \geq 0$, and let v_j be the vertex of subtree T_i , $y_j = -x_j$ when $x_{w_i} < 0$ and v_j be the vertex of subtree T_i ($i = 1, 2, \dots, s$).

Thus, we have $y_{w_i} \geq 0$ ($i = 1, 2, \dots, s$), $\|y\| = 1$ and $y' L y = x' L x = \mu(L(T)) \triangleq \mu(T)$. By Definition 2, we know that y is the standard Laplacian spectral vector of T . Then $(D - A)y = \mu(T)y$. We have $((D - A)y)_v = (\mu(T)y)_v$. Thus, $\sum_{i=1}^s y_{w_i} = 0$.

However, $y_{w_i} \geq 0$ and there exists $i_0 \in \{1, 2, \dots, s\}$ that makes $w_{i_0} = u$, $y_u > 0$. Therefore, $\sum_{i=1}^s y_{w_i} > 0$. This contradiction completes the proof. $\square$

Theorem 4. Let v be a vertex of tree T and $v_1, v_2, \dots, v_s$ be the pendant vertices of T that are adjacent to v . If $x =$

FIGURE 3

FIGURE 4

$(x_1, x_2, \dots, x_n)'$ is the standard Laplacian spectral vector of T , where x_i corresponds to the vertex v_i ($1 \leq i \leq n$). Then $x_{v_j} = x_{v_i}$, $1 \leq i < j \leq s$.

Proof. $x = (x_1, x_2, \dots, x_n)'$ is the standard Laplacian spectral vector of T . By Definition 2 and Theorem 1, we have $L(T)x = \mu(T)x$. $L(T) = D(T) - A(T)$, so $(D(T) - A(T))x = \mu(T)x$, and then we have $(d_T(v_i) - \mu(T))x_{v_i} = x_v$, $1 \leq i \leq s$. Therefore, we have $(1 - \mu(T))x_{v_1} = x_v$, $(1 - \mu(T))x_{v_2} = x_v, \dots, (1 - \mu(T))x_{v_s} = x_v$. Thus, $x_{v_j} = x_{v_i}$, $1 \leq i < j \leq s$. $\square$

Theorem 5. Let $x = (x_1, x_2, \dots, x_n)'$ be the standard Laplacian spectral vector of tree T , where x_i corresponds to vertex v_i ($1 \leq i \leq n$), $T = (V, E)$. Then

(1) for $\forall uv \in E(T)$, we have $x_u x_v < 0$;

(2) $\sum_{i=1}^n x_i = 0$.

Proof. (1) Since x is the standard Laplacian spectral vector of T , by Definition 2 we have $\mu(T) = x' L(T) x = \sum_{(i,j) \in E} (x_i - x_j)^2$. By Theorem 3, we have $|x_u| > 0$ and $|x_v| > 0$. Thus, $x_u x_v \neq 0$.

Suppose that there exists edge $uv \in E(T)$ such that $x_u x_v > 0$. Let tree T form a root tree with r as its root vertex. Assume, without loss of generality, that vertex u is the parent node of the vertex v (Figure 3). Let T_1 be the subtree of T obtained from vertex v and all its descendants, and let T_1 be a k -layer tree, $T_1 = (V_1, E_1)$ (Figure 4). Without loss of generality, we assume that $x_u > 0$, so $x_v > 0$.

Let $y_i = x_i$ ($v_i \in V \setminus V(T_1)$), $y_v = -x_v$, and $y_{w_1} = |x_{w_1}|$ ($\forall w_1$ are the vertices in the second layer of T_1), $y_{w_2} = (-1)^3 |x_{w_2}|$ ($\forall w_2$ are the vertices in the third layer of

T_1), $\dots$, $y_{w_{k-1}} = (-1)^k |x_{w_{k-1}}|$ ($\forall w_{k-1}$ are the vertices in the k th layer of T_1). Then $\|y\| = \|x\| = 1$ and we have

$$\begin{aligned} & y' L(T) y \\ &= \sum_{(i,j) \in E} (y_i - y_j)^2 \\ &= \sum_{(i,j) \in E \setminus E_1} (x_i - x_j)^2 + \sum_{(i,j) \in E_1 \setminus uv} (y_i - y_j)^2 + (x_u + x_v)^2 \\ &> \sum_{(i,j) \in E \setminus E_1} (x_i - x_j)^2 + \sum_{(i,j) \in E_1 \setminus uv} (x_i - x_j)^2 + (x_u - x_v)^2 \\ &= \sum_{(i,j) \in E} (x_i - x_j)^2 = \mu(T). \end{aligned} \tag{2}$$

Thus, there exists a unit vector $y = (y_1, y_2, \dots, y_n)'$ such that $\mu(T) < y' L(T) y$. This implies a contradiction with Theorem 1. Therefore, $x_u x_v < 0$.

(2) Since x is the standard Laplacian spectral vector of T , we have

$$(D(T) - A(T))x = \mu(T)x. \tag{3}$$

Then

$$(d_T(v_i) - \mu(T))x_i = \sum_{v_j \in N_T(v_i)} x_j. \tag{4}$$

Thus, we have

$$\sum_{i=1}^n (d_T(v_i) - \mu(T))x_i = \sum_{i=1}^n \sum_{v_j \in N_T(v_i)} x_j. \tag{5}$$

Therefore, $\sum_{i=1}^n d_T(v_i)x_i - \mu(T) \sum_{i=1}^n x_i = \sum_{i=1}^n d_T(v_i)x_i$. So $\sum_{i=1}^n x_i = 0$. $\square$

3. Applications of the Eigenvector Corresponding to the Laplacian Spectral Radius

In this section, we present some applications of the eigenvector of the Laplacian spectral radius of a graph.

Theorem 6. Let u and v be the vertices of tree T . Denote the distance of vertices u and v by $d(u, v)$ and $d(u, v) = k$, where k is an odd number and $k \geq 3$. Let G' be the graph obtained from T by adding edge (u, v) . Then $\mu(G') > \mu(T)$.

Proof. Let $x = (x_1, x_2, \dots, x_n)'$ be the standard Laplacian spectral vector of tree T , where x_i corresponds to vertex

v_i ($1 \leq i \leq n$). Since k is an odd number and $k \geq 3$, by Theorem 5 we have $x_u x_v < 0$. Thus,

$$\begin{aligned} \mu(G') &= \max_{\|y\|=1} y' L(G') y \\ &= \max_{\|y\|=1} \sum_{(i,j) \in E(G')} (y_i - y_j)^2 \\ &\geq \sum_{(i,j) \in E(G')} (x_i - x_j)^2 \\ &> \sum_{(i,j) \in E(T)} (x_i - x_j)^2 = \mu(T). \end{aligned} \quad (6)$$

Therefore, $\mu(G') > \mu(T)$. $\square$

According to the well-known Courant-Weyl inequalities, we have the following lemma.

Lemma 7 (see [15]). Let G be a graph with n vertices and let $G' = G + e$ be the graph obtained by inserting a new edge e into G . Let $\mu_i(G)$ and $\mu_i(G')$ be the eigenvalues of the Laplacian matrix of G and G' ($i = 1, 2, \dots, n$), respectively. Then $\mu_1(G') \geq \mu_1(G) \geq \mu_2(G') \geq \mu_2(G) \geq \dots \geq \mu_n(G') = \mu_n(G) = 0$.

Lemma 8 (see [16]). Let G be a connected graph for n vertices with at least one edge. Then $\mu(G) \geq \Delta(G) + 1$, where $\Delta(G)$ is the largest degree of the graph G , and equality holds if and only if $\Delta(G) = n - 1$.

Theorem 9. Let G be a connected graph for n vertices, and let u_j be the vertex of G and $v_1^j, v_2^j, \dots, v_{m_j}^j$ be the pendant vertices of G adjacent to vertex u_j ($1 \leq j \leq k$). Let G_1 be the graph obtained from G by adding $\sum_{j=1}^k q_j$ ($1 \leq q_j \leq m_j(m_j - 1)/2$) edges, where t_j edges are among $v_1^j, v_2^j, \dots, v_{m_j}^j$ ($j = 1, 2, \dots, k$). Then $\mu(G) = \mu(G_1)$.

Proof. If $\Delta(G) = n - 1$, by Lemma 8 we have $\mu(G) = \Delta(G) + 1 = n$. However, it is clear that $\mu(G_1) = \Delta(G_1) + 1 = n - 1 + 1 = n$, so $\mu(G) = \mu(G_1)$. We suppose that $\Delta(G) \leq n - 2$.

Let G' be the graph obtained from G by adding $\sum_{j=1}^k t_j$ ($t_j = m_j(m_j - 1)/2$) edges, where t_j edges are among $v_1^j, v_2^j, \dots, v_{m_j}^j$ ($j = 1, 2, \dots, k$). By Lemma 7, we have $\mu(G) \leq \mu(G_1) \leq \mu(G')$. To obtain the result, we only need to prove that $\mu(G) \geq \mu(G')$.

Let $X = (X_1, X_2, \dots, X_n)'$ be the standard Laplacian spectral vector of G' , then $L(G')X = \mu(G')X$. For $L(G') = D(G') - A(G')$, we have

$$\begin{aligned} (d_{G'}(v_i^l) - \mu(G')) X_{v_i^l} &= X_{u_i} + \sum_{j=1, j \neq i}^{m_i} X_{v_j^l}, \\ 1 \leq i \leq m_i, \quad 1 \leq l \leq k. \end{aligned} \quad (7)$$

FIGURE 5

Then, for $1 \leq i < j \leq m_i$ and $1 \leq l \leq k$, we have

$$\begin{aligned} (d_{G'}(v_i^l) - \mu(G')) X_{v_i^l} - (d_{G'}(v_j^l) - \mu(G')) X_{v_j^l} \\ = X_{v_j^l} - X_{v_i^l} \end{aligned} \quad (8)$$

since $d_{G'}(v_1^l) = d_{G'}(v_2^l) = \dots = d_{G'}(v_{m_i}^l) = m_i \leq n - 2$. Thus,

$$\begin{aligned} (m_i - \mu(G')) (X_{v_i^l} - X_{v_j^l}) &= X_{v_j^l} - X_{v_i^l}, \\ 1 \leq i < j \leq m_i, \quad 1 \leq l \leq k. \end{aligned} \quad (9)$$

For $\Delta(G') \leq n - 2$, by Lemma 8 we have $\mu(G') > \Delta(G') + 1 \geq m_i + 1$. So $X_{v_i^l} = X_{v_j^l}$, $1 \leq i < j \leq m_i$, $1 \leq l \leq k$. Thus, we have

$$\begin{aligned} \mu(G) &\geq X' L(G) X = \sum_{(i,j) \in E(G)} (X_i - X_j)^2 \\ &= \sum_{(i,j) \in E(G')} (X_i - X_j)^2 \\ &= X' L(G') X = \mu(G'). \end{aligned} \quad (10)$$

That is, $\mu(G) \geq \mu(G')$. This completes the proof. $\square$

Theorem 10. Let u, v be two vertices of tree T . Suppose that $v_1, v_2, \dots, v_s$ ($1 \leq s \leq d_v$) are some vertices of $N_T(v) \setminus (N_T(u) \cup \{u\})$, and $x = (x_1, x_2, \dots, x_n)'$ is the standard Laplacian spectral vector of T , where x_i corresponds to vertex v_i ($1 \leq i \leq n$). Let T^* be the tree obtained from T by deleting the edges (v, v_i) and adding the edges (u, v_i) ($1 \leq i \leq s$) (Figure 5). If $|x_u| \geq |x_v|$, then $\mu(T) < \mu(T^*)$.

Proof. For tree T , let T form a root tree with vertex v as the parent node of vertex v_i ($1 \leq i \leq s$), $T = (V, E)$. Let T_1 be the subtree of T obtained from the parent node v and $v_1, v_2, \dots, v_s$ and the v_1 descendants, v_2 descendants, $\dots$, v_s descendants, $T_1 = (V_1, E_1)$. For tree T^* , let T^* form a root tree with vertex u as the parent node of vertex v_i ($1 \leq i \leq s$), $T^* = (V^*, E^*)$. Let T_1^* be the subtree of T^* obtained from the parent node u and $v_1, v_2, \dots, v_s$ and the v_1 descendants, v_2 descendants, $\dots$, and v_s descendants. Let subtree T_1^* be a k -layer tree with vertex u as the root node. Consider $E_1' = E_1 \setminus \{vv_1, vv_2, \dots, vv_s\}$.

Let $y_i = x_i$ ($v_i \in V \setminus V(T_1)$), $y_v = x_v$, $y_{w_1} = -(\text{sign } x_u)|x_{w_1}|$ (for all w_1 are the vertices in the second layer of T_1^*), $y_{w_2} = (-1)^2(\text{sign } x_u)|x_{w_2}|$ (for all w_2 are the vertices in the third layer of T_1^*), ..., and $y_{w_{k-1}} = (-1)^{k-1}(\text{sign } x_u)|x_{w_{k-1}}|$ (for all w_{k-1} are the vertices in the k th layer of T_1^*). Then we have $\|y\| = 1$ and

$$\begin{aligned}
 & y' L(T^*) y - x' L(T) x \\
 &= \sum_{(i,j) \in E^*} (y_i - y_j)^2 - \sum_{(i,j) \in E} (x_i - x_j)^2 \\
 &= \left[\sum_{(i,j) \in E'_1} (y_i - y_j)^2 + \sum_{(i,j) \in E^* \setminus E'_1} (y_i - y_j)^2 \right] \\
 &\quad - \left[\sum_{(i,j) \in E'_1} (x_i - x_j)^2 + \sum_{(i,j) \in E \setminus E'_1} (x_i - x_j)^2 \right] \quad (11) \\
 &= \sum_{(i,j) \in E^* \setminus E'_1} (y_i - y_j)^2 - \sum_{(i,j) \in E \setminus E'_1} (x_i - x_j)^2 \\
 &= \sum_{i=1}^s (|x_u| + |x_{v_i}|)^2 - \sum_{i=1}^s (|x_v| + |x_{v_i}|)^2 \\
 &= \sum_{i=1}^s (|x_u|^2 - |x_v|^2) + 2 \sum_{i=1}^s |x_{v_i}| (|x_u| + |x_v|) \geq 0.
 \end{aligned}$$

That is, $y' L(T^*) y \geq x' L(T) x$. Thus,

$$\mu(T) = x' L(T) x \leq y' L(T^*) y \leq \max_{\|y\|=1} y' L(T^*) y = \mu(T^*). \quad (12)$$

Therefore, $\mu(T) \leq \mu(T^*)$.

If $\mu(T) = \mu(T^*)$, then the equalities in (12) hold. Thus, $\mu(T) = y' L(T^*) y = \mu(T^*)$. By Theorem 1, we have $L(T^*) y = \mu(T^*) y$. Thus,

$$\mu(T^*) y_v = (L(T^*) y)_v = d_{v^*} y_v - \sum_{v_i \in N_{T^*}(v)} y_{v_i}, \quad (13)$$

where d_{v^*} is the degree of vertex v of tree T^* .

In addition, from $L(T)x = \mu(T)x$ we have

$$\begin{aligned}
 \mu(T) x_v &= (L(T) x)_v \\
 &= d_v x_v - \sum_{v_i \in N_T(v)} x_{v_i} \\
 &= d_v y_v - \sum_{v_i \in N_{T^*}(v)} x_{v_i} - \sum_{i=1}^s x_{v_i}, \quad (14)
 \end{aligned}$$

where d_v is the degree of vertex v of tree T .

By (13) and (14), we have

$$(\mu(T^*) - \mu(T)) x_v = \sum_{i=1}^s x_i - s x_v + \sum_{v_i \in N_{T^*}(v)} (x_i - y_i). \quad (15)$$

Assume, without loss of generality, that $x_v > 0$.

FIGURE 6

If $x_u > 0$, by Theorem 5, we have

$$(\mu(T^*) - \mu(T)) x_v = \sum_{i=1}^s x_i - s x_v < 0, \quad (16)$$

which implies the contradiction $\mu(T^*) < \mu(T)$.

If $x_u < 0$, by Theorem 5, we have

$$(\mu(T^*) - \mu(T)) x_v = \sum_{i=1}^s x_i - s x_v + \sum_{v_i \in N_{T^*}(v)} (x_i - |x_i|) < 0, \quad (17)$$

which implies the contradiction $\mu(T^*) < \mu(T)$.

Thus, if $|x_u| \geq |x_v|$, then $\mu(T) < \mu(T^*)$. $\square$

Corollary 11. Suppose that T^* is as defined as in Theorem 10 $y = (y_1, y_2, \dots, y_n)^T$ is the standard Laplacian spectral vector of T^* , and then $|y_u| > |y_v|$.

Proof. Otherwise, if $|y_u| \leq |y_v|$, by Theorem 10, we have $\mu(T^*) < \mu(T)$. This contradiction completes the proof. $\square$

Corollary 12. Let G be a simple connected graph with n vertices. Let r, s , and t be three distinct vertices, where $rs \in E(G)$ and $rt \notin E(G)$. Let G^* be the simple connected graph obtained from G by deleting the edge rs and adding the edge rt . Suppose that $x = (x_1, x_2, \dots, x_n)^T$ is the standard Laplacian spectral vector of G , where x_i corresponds to the vertex v_i ($1 \leq i \leq n$). $x^* = (x_1^*, x_2^*, \dots, x_n^*)^T$ is the standard Laplacian spectral vector of G^* , where x_i^* corresponds to the vertex v_i^* ($1 \leq i \leq n$). If $|x_t| \geq |x_s|$, then $|x_t^*| > |x_s^*|$.

Proof. Obviously, G is obtained from G^* by deleting the edge rt and adding the edge rs . Assume that $|x_t^*| \leq |x_s^*|$. Since G^* is a simple connected graph, by Theorem 10 we have $\mu(G^*) < \mu(G)$. If $|x_t| \geq |x_s|$, by Theorem 10 we have $\mu(G) < \mu(G^*)$. This contradiction completes the proof. $\square$

Lemma 13 (see [17]). Let u be a vertex of tree G , and for positive integers k and l let $G_{k,l}$ denote the tree obtained from G by adding pendant paths of length k and l at u (Figure 6). If $k \geq l \geq 1$, then $\mu(G_{k,l}) > \mu(G_{k+1,l-1})$.

Theorem 14 (see [7, 8]). *Among all the trees for n vertices and k pendant vertices, the maximal Laplacian spectral radius is obtained uniquely at $T_{n,k}$.*

Proof. We have to prove that if $T \in \mathcal{T}_{n,k}$, then $\mu(T) \leq \mu(T_{n,k})$ with equality only when $T = T_{n,k}$. Let t be the cardinality of the vertices of degree 3 or greater.

Case 1. $t = 0$. In this case, T is a path of length n , and hence $T = T_{n,2}$. We have $\mu(T) = \mu(T_{n,2})$.

Case 2. $t = 1$. The result $\mu(T) \leq \mu(T_{n,k})$ follows from repeated use of Lemma 13, and equality holds if and only if $T = T_{n,k}$.

Case 3. $t > 1$. Let $x = (x_1, x_2, \dots, x_n)^T$ be the standard Laplacian spectral vector of T , where x_i corresponds to the vertex v_i ($1 \leq i \leq n$). Suppose that u, v are two vertices of T of degree 3 or greater, and $|x_u| \geq |x_v|$. Since T is a tree, there is a unique path between u and v , and only one of the neighbors of v , say w , is on the path. Assume $\{v_1, v_2, \dots, v_{d_v-2}\} \subset N_T(v) \setminus \{w\}$. Delete the edges (v, v_i) and add the edges (u, v_i) ($1 \leq i \leq d_v-2$). Then we obtain a new tree T_1^* . Obviously, T_1^* still has k pendant vertices. By Theorem 10, we have $\mu(T) < \mu(T_1^*)$ and the cardinality of the vertices of degree 3 or greater decreases to $t-1$.

If $t-1 > 1$, repeat the above step to T_1^* until the cardinality is only 1. Thus, we obtain trees $T_2^*, T_3^*, \dots, T_{t-1}^*$ and $\mu(T_1^*) < \mu(T_2^*) < \dots < \mu(T_{t-1}^*)$. Moreover, each T_i^* has k pendant vertices. Referring to Case 2, we have $\mu(T_{t-1}^*) \leq \mu(T_{n,k})$. Therefore, $\mu(T) < \mu(T_{n,k})$.

The cases complete the proof. $\square$

Theorem 15 (see [8]). $\mu(T_{n,k-1}) < \mu(T_{n,k})$, $3 \leq k \leq n-1$.

Proof. The proof is obvious from Lemma 13. $\square$

For the sake of clarity, we identify a graph by its characteristic polynomial. Let $\Phi(L(G))$ be the characteristic polynomial of graph G . For convenience, we denote $\Phi(L(G))$ by $\Phi(G)$ sometimes. First, we require some lemmas.

Lemma 16 (see [9]). *Let $e = uv$ be a cut edge of the simple connected graph G . G_1 and G_2 are two connected branches of $G - uv$, where $u \in V(G_1)$, $v \in V(G_2)$. Then $\Phi(G) = \Phi(G_1)\Phi(G_2) - \Phi(G_1)\Phi(L_v(G_2)) - \Phi(G_2)\Phi(L_u(G_1))$. Here, $\Phi(L_v(G_2))$ denotes the determinant obtained by deleting the row and column for vertex v of G_2 from the determinant for $L(G_2)$, and $\Phi(L_u(G_1))$ denotes the determinant obtained by deleting the row and column for vertex u of G_1 from the determinant for $L(G_1)$.*

Lemma 17 (see [18]). *Let P_n be a path with n vertices, let P_n^0 be the path obtained by adding a loop on a pendant vertex in P_n , and let P_n^{00} be the path obtained by adding loops on the two pendant vertices in P_n . Suppose that the degree of contribution corresponding to each loop is 1 and $\Phi(P_0) = 0$, $\Phi(P_0^0) = 1$, $\Phi(P_0^{00}) = 1$. Then*

$$(1) \Phi(P_{n+1}) = (x-2)\Phi(P_n) + \Phi(P_{n-1}), \quad (n \geq 1),$$

$$(2) x\Phi(P_n^0) = \Phi(P_{n+1}) + \Phi(P_n),$$

$$(3) \Phi(P_n) = x\Phi(P_{n-1}^{00}), \quad (n \geq 1),$$

$$(4) \Phi(P_n) = (x/\sqrt{x^2-4x})(a^n - b^n), \text{ where } a = (x-2 + \sqrt{x^2-4x})/2 \text{ and } b = (x-2 - \sqrt{x^2-4x})/2.$$

From Lemma 16, by induction we can obtain the following lemma.

Lemma 18. *Let $G_1, G_2, \dots, G_s$, G be $s+1$ disjoint simple connected graphs, where $v_i \in G_i$ ($i = 1, 2, \dots, s$) and $v \in G$. Let H_s be the graph obtained from $G_1, G_2, \dots, G_s$ and G by adding new edges $vv_1, vv_2, \dots, vv_s$. Then*

$$\begin{aligned} \Phi(H_s) &= \Phi(G) \prod_{i=1}^s [\Phi(G_i) - \Phi(L_{v_i}(G_i))] \\ &\quad - \Phi(L_v(G)) \\ &\quad \times \sum_{i=1}^s \left[\Phi(G_i) \prod_{j=1, j \neq i}^s (\Phi(G_j) - \Phi(L_{v_j}(G_j))) \right]. \end{aligned} \quad (18)$$

From Lemmas 16, 17, and 18, we have the following theorem.

Theorem 19. *The characteristic polynomial of $T_{n,k}$ ($2 \leq k \leq n-1$) is*

$$\begin{aligned} \Phi(T_{n,k}) &= [\Phi(P_{q+1}) - \Phi(P_q^0)]^{r-1} [\Phi(P_q) - \Phi(P_{q-1}^0)]^{k-r-1} \\ &\quad \times \{x[\Phi(P_{q+1}) - \Phi(P_q^0)][\Phi(P_q) - \Phi(P_{q-1}^0)] \\ &\quad - r[\Phi(P_q) - \Phi(P_{q-1}^0)]\Phi(P_{q+1}) \\ &\quad - (k-r)\Phi(P_q)[\Phi(P_{q+1}) - \Phi(P_q^0)]\}, \end{aligned} \quad (19)$$

where $q = [(n-1)/k]$, $n-1 = kq + r$ ($0 \leq r \leq k-1$), and P_q is a path of length q .

As for the Laplacian spectral radius of $T_{n,k}$, we only need to consider the greatest root of

$$\begin{aligned} &x[\Phi(P_{q+1}) - \Phi(P_q^0)][\Phi(P_q) - \Phi(P_{q-1}^0)] \\ &- r[\Phi(P_q) - \Phi(P_{q-1}^0)]\Phi(P_{q+1}) \\ &- (k-r)\Phi(P_q)[\Phi(P_{q+1}) - \Phi(P_q^0)] = 0. \end{aligned} \quad (20)$$

In general, the Laplacian spectral radius is difficult to calculate although the characteristic polynomial can be identified by Chebyshev polynomials. Thus, we only give some results in some cases.

Lemma 20. For a univariate cubic equation $x^3 + kx^2 + mx + n = 0$, we can obtain the roots as follows:

$$\begin{aligned}
 x_1 &= \sqrt[3]{-\frac{q}{2} + \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}} \\
 &\quad + \sqrt[3]{-\frac{q}{2} - \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}} - \frac{k}{3}, \\
 x_2 &= \omega \sqrt[3]{-\frac{q}{2} + \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}} \\
 &\quad + \omega^2 \sqrt[3]{-\frac{q}{2} - \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}} - \frac{k}{3}, \\
 x_3 &= \omega^2 \sqrt[3]{-\frac{q}{2} + \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}} \\
 &\quad + \omega \sqrt[3]{-\frac{q}{2} - \sqrt{\left(\frac{q}{2}\right)^2 + \left(\frac{p}{3}\right)^3}} - \frac{k}{3},
 \end{aligned} \tag{21}$$

where $p = -(1/3)k^2 + m$, $q = (2/27)k^3 - (1/3)km + n$ and $\omega = e^{2\pi i/3}$.

Proof. The lemma is easy to prove. $\square$

Theorem 21. If $[n/2] \leq k \leq n-1$, then

$$\begin{aligned}
 \mu(T_{n,k}) &= \frac{k+4}{3} + \frac{2\sqrt{k^2-k+4}}{3} \cos \frac{\theta}{3}, \\
 \theta &= \arccos \frac{2k^3 - 3k^2 - 48k + 27n - 16}{2(k^2 - k + 4)^{3/2}}, \\
 (0 < \theta < \pi).
 \end{aligned} \tag{22}$$

Moreover, if $k = n-1$, then $\mu(T_{n,n-1}) = n$.

Proof. In this case, for $[n/2] \leq k \leq n-1$, $q = 1$. By (20), we have

$$\begin{aligned}
 &x [\Phi(P_{q+1}) - \Phi(P_q^0)] [\Phi(P_q) - \Phi(P_{q-1}^0)] \\
 &\quad - r [\Phi(P_q) - \Phi(P_{q-1}^0)] \Phi(P_{q+1}) \\
 &\quad - (k-r) \Phi(P_q) [\Phi(P_{q+1}) - \Phi(P_q^0)] = 0.
 \end{aligned} \tag{23}$$

Hence, $x^3 - (k+4)x^2 + (3k+4)x - (k+r+1) = 0$.

Let $f(x) = x^3 - (k+4)x^2 + (3k+4)x - (k+r+1)$, and then we have

1° for $f(0) = -(k+r+1) < 0$ and $f(1) = k-r > 0$, and thus $f(x)$ has a root in $(0, 1)$,

2° for $f(1) > 0$ and $f(k) = -k(k-3) - r - 1 < 0$, and thus $f(x)$ has a root in $(1, k)$,

3° for $f(k) < 0$ and $f(+\infty) > 0$, and thus $f(x)$ has a root in $(k, +\infty)$.

Therefore, the equation has three different real roots.

Let $x = y + (k+4)/3$, and then the equation can translate to $y^3 + py + q = 0$, where $p = -(1/3)(k^2 - k + 4)$ and $q = -(1/27)(2k^3 - 3k^2 - 21k + 27r + 11)$.

Let $s = -q/2 + \sqrt{-\Delta}i = \|s\|e^{i\theta}$, where $\Delta = (q/2)^2 + (p/3)^3 < 0$. Then

$$\begin{aligned}
 \|s\| &= \left\| -\frac{q}{2} + \sqrt{-\Delta}i \right\| \\
 &= \sqrt{\left(-\frac{q}{2}\right)^2 + (-\Delta)} = \sqrt{\frac{q^2}{4} - \frac{q^2}{4} - \frac{p^3}{27}} \\
 &= \frac{1}{27}(k^2 - k + 4)^{3/2},
 \end{aligned} \tag{24}$$

$$\begin{aligned}
 \theta &= \arccos \frac{-q/2}{\|s\|} = \arccos \frac{2k^3 - 3k^2 - 21k + 27r + 11}{2(k^2 - k + 4)^{3/2}}, \\
 (0 < \theta < \pi).
 \end{aligned}$$

Thus, based on the Lemma 20, we can obtain three roots:

$$\begin{aligned}
 x_1 &= \sqrt[3]{-\frac{q}{2} + \sqrt{-\Delta}i} + \sqrt[3]{-\frac{q}{2} - \sqrt{-\Delta}i} + \frac{k+4}{3} \\
 &= \sqrt[3]{\|s\| e^{i\theta}} + \sqrt[3]{\|s\| e^{-i\theta}} + \frac{k+4}{3} \\
 &= \frac{\sqrt{k^2-k+4}}{3} e^{i\theta/3} + \frac{\sqrt{k^2-k+4}}{3} e^{-i\theta/3} + \frac{k+4}{3} \\
 &= \frac{k+4}{3} + \frac{2\sqrt{k^2-k+4}}{3} \cos \frac{\theta}{3},
 \end{aligned} \tag{25}$$

$$\begin{aligned}
 x_2 &= \omega \sqrt[3]{-\frac{q}{2} + \sqrt{-\Delta}i} + \omega^2 \sqrt[3]{-\frac{q}{2} - \sqrt{-\Delta}i} + \frac{k+4}{3} \\
 &= \omega \sqrt[3]{\|s\| e^{i\theta}} + \omega^2 \sqrt[3]{\|s\| e^{-i\theta}} + \frac{k+4}{3} \\
 &= \frac{\sqrt{k^2-k+4}}{3} e^{i\theta/3} e^{2i\pi/3} \\
 &\quad + \frac{\sqrt{k^2-k+4}}{3} e^{-i\theta/3} e^{4i\pi/3} + \frac{k+4}{3} \\
 &= \frac{k+4}{3} + \frac{2\sqrt{k^2-k+4}}{3} \cos \left(\frac{\theta}{3} + \frac{2\pi}{3} \right),
 \end{aligned} \tag{26}$$

$$\begin{aligned}
x_3 &= \omega^2 \sqrt[3]{-\frac{q}{2} + \sqrt{-\Delta}i} + \omega \sqrt[3]{-\frac{q}{2} - \sqrt{-\Delta}i} + \frac{k+4}{3} \\
&= \omega^2 \sqrt[3]{\|s\| e^{i\theta}} + \omega \sqrt[3]{\|s\| e^{-i\theta}} + \frac{k+4}{3} \\
&= \frac{\sqrt{k^2 - k + 4}}{3} e^{i\theta/3} e^{4i\pi/3} \\
&\quad + \frac{\sqrt{k^2 - k + 4}}{3} e^{-i\theta/3} e^{2i\pi/3} + \frac{k+4}{3} \\
&= \frac{k+4}{3} + \frac{2\sqrt{k^2 - k + 4}}{3} \cos\left(\frac{2\pi}{3} - \frac{2\theta}{3}\right).
\end{aligned} \tag{27}$$

For $0 < \theta < \pi$, then $\cos(\theta/3) > \cos(\theta/3 + 2\pi/3)$ and $\cos(\theta/3) > \cos(2\pi/3 - \theta/3)$. Thus, $x_1 > x_2, x_1 > x_3$. So the largest root of the univariate cubic equation is

$$\begin{aligned}
\mu(T_{n,k}) &= \frac{k+4}{3} + \frac{2\sqrt{k^2 - k + 4}}{3} \cos \frac{\theta}{3}, \\
\theta &= \arccos \frac{2k^3 - 3k^2 - 21k + 27r + 11}{2(k^2 - k + 4)^{3/2}}, \\
(0 < \theta < \pi).
\end{aligned} \tag{28}$$

For $r = n - 1 - k$, we have

$$\begin{aligned}
\mu(T_{n,k}) &= \frac{k+4}{3} + \frac{2\sqrt{k^2 - k + 4}}{3} \cos \frac{\theta}{3}, \\
\theta &= \arccos \frac{2k^3 - 3k^2 - 48k + 27n - 16}{2(k^2 - k + 4)^{3/2}}, \\
(0 < \theta < \pi).
\end{aligned} \tag{29}$$

If $k = n - 1$, then it is easy to prove that $f(n) = 0$. Thus, $\mu(T_{n,n-1}) = n$. $\square$

From Theorems 14, 15, and 21, we have the following corollaries.

Corollary 22. Let T be a tree for n vertices. Then $\mu(T) \leq n$ and equality holds if and only if $T = T_{n,n-1}(K_{1,n-1})$, the star with n vertices.

Corollary 23. Let T be a tree for n vertices with $n \geq 4$ and $T \neq T_{n,n-1}$. Then

$$\begin{aligned}
\mu(T) &\leq \frac{n+2}{3} + \frac{2\sqrt{n^2 - 5n + 10}}{3} \cos \frac{\theta}{3}, \\
\theta &= \arccos \frac{2n^3 - 15n^2 + 15n + 52}{2(n^2 - 5n + 10)^{3/2}}, \\
(0 < \theta < \pi)
\end{aligned} \tag{30}$$

and equality holds if and only if $T = T_{n,n-2}(S(1, n-3))$.

FIGURE 7

Corollary 24. Let T be a tree for n vertices. Let $M(T)$ denote one maximum matching of T and suppose that $|M(T)| = i$. Then

$$\begin{aligned}
\mu(T) &\leq \frac{n+4-i}{3} + \frac{2\sqrt{n^2 - (2i+1)n + i^2 + i + 4}}{3} \cos \frac{\theta}{3}, \\
\theta &= \arccos \frac{2n^3 - (6i+3)n^2 + (6i^2 + 6i - 21)n - 2i^3 - 3i^2 + 48i - 16}{2[n^2 - (2i+1)n + i^2 + i + 4]^{3/2}}, \\
(0 < \theta < \pi),
\end{aligned} \tag{31}$$

and equality holds if and only if $T = T_{n,n-i}$.

Proof. Let k denote the cardinality of the pendant vertices of T . For $|M(T)| = i$, we have $k \leq i + n - 2i = n - i$. By Theorems 14 and 15, we have $\mu(T) \leq \mu(T_{n,k}) \leq \mu(T_{n,n-i})$, and equality holds if and only if $T = T_{n,n-i}$.

$T_{n,n-i}$ is shown in Figure 7. Since $i \leq n/2$, $n - i \geq n/2 \geq [n/2]$, by Theorem 21 we have

$$\begin{aligned}
\mu(T) &\leq \frac{n+4-i}{3} + \frac{2\sqrt{n^2 - (2i+1)n + i^2 + i + 4}}{3} \cos \frac{\theta}{3}, \\
\theta &= \arccos \frac{2n^3 - (6i+3)n^2 + (6i^2 + 6i - 21)n - 2i^3 - 3i^2 + 48i - 16}{2[n^2 - (2i+1)n + i^2 + i + 4]^{3/2}}, \\
(0 < \theta < \pi).
\end{aligned} \tag{32}$$

$\square$

Corollary 25. Let T be any tree for $n = 2i$ vertices and $|M(T)| = i$. Then

$$\begin{aligned}
\mu(T) &\leq \frac{i+4}{3} + \frac{2\sqrt{i^2 - i + 4}}{3} \cos \frac{\theta}{3}, \\
\theta &= \arccos \frac{2i^3 - 3i^2 + 6i - 16}{2(i^2 - i + 4)^{3/2}}, \\
(0 < \theta < \pi)
\end{aligned} \tag{33}$$

and equality holds if and only if $T = T_{n,n-i}$.

Acknowledgments

The authors would like to thank the anonymous referees for valuable suggestions and corrections, which have improved

the paper. This research was supported by the Scientific Research Foundation of Huaqiao University (10HZR26) and the Natural Science Foundation of Fujian Province (Z0511028).

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