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Ordering Trees with Fixed Order and Matching Number by Laplacian Spectral Radius

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Abstract Let $T(n,i)$ be the set of all trees with order n and matching number i. We determine the third to sixth trees in $T(2i+1,i)$ and the third to fifth trees in $T(n,i)$ for $n \geq 2i+2$ with the largest Laplacian spectral radius.

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1. Introduction

Let G be a simple graph with vertex set $\{v_1, v_2, \ldots, v_n\}$. Let $A(G)$ be the adjacency matrix of G and $D(G) = \mathrm{diag}(d(v_1), d(v_2), \ldots, d(v_n))$ be the diagonal matrix of vertex degrees of G, where $d(v_i)$ is the degree of v_i. Then the Laplacian matrix $L(G)$ of G is $L(G) = D(G) - A(G)$. It is well-known that $L(G)$ is real symmetric and positive semi-definite. It follows that its eigenvalues are nonnegative real numbers. The largest eigenvalue of $L(G)$ is called the Laplacian spectral radius of G, denoted by $\mu(G)$.

To classify and order graphs by their eigenvalues is an interesting problem proposed by Cveković [1]. Especially for some types of trees, many results on this problem have been obtained. Zhang determined the tree with the largest Laplacian spectral radius in the set of trees with fixed order and independence number [2]. Hong and Zhang determined the tree with the largest Laplacian spectral radius in the set of trees with fixed order and pendant vertex number [3]. Let $T(n,i)$ be the set of trees with order n and matching number i. According to the largest Laplacian spectral radius, the first eight trees in $T(2i,i)$ were determined in [4–7].

The matrix $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix of G. Let $\rho(G)$ denote the spectral radius of $Q(G)$. If G is connected, then $Q(G)$ is non-negative and irreducible, and by the Perron-Frobenius theorem of non-negative matrices, $\rho(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\rho(G)$. We shall refer to such an eigenvector as the Perron vector of G. Throughout, let $\mathrm{in}(G)$ be the matching number of a graph

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G, dia(G) be the diameter of G and x_w^G be the coordinate corresponding to the vertex w in the Perron vector x of G. Now we give some results used in this paper.

Lemma 1.1 ([8]) *Let G be a simple graph. Then $Q(G)$ and $L(G)$ have the same spectrum if and only if G is a bipartite graph.*

Lemma 1.2 ([9]) *Let $\Delta(G)$ be the maximum degree of a simple connected graph G with at least two vertices. Then $\rho(G) \geq \Delta(G) + 1$, with equality if and only if G is a star.*

Lemma 1.3 ([10]) *Let u be a vertex of a connected graph G with at least two vertices. Suppose that $P = v_1v_2 \cdots v_k$ and $S = u_1u_2 \cdots u_l$ are two new disjoint paths. Let $G^1_{k,l}$ denote the graph obtained from G, P and S by joining u to v_1 with an edge and joining u to u_1 with another edge. If $k \geq l+2$, then $\rho(G^1_{k,l}) < \rho(G^1_{k-1,l+1})$. The procedure from $G^1_{k,l}$ to $G^1_{k-1,l+1}$ is called the first edge transformation of graph, 1.e.t. for short.*

Lemma 1.4 ([10]) *Let vu be an edge of a connected graph G with $d(v) \geq 2$ and $d(u) \geq 2$. Suppose that $P = v_1v_2 \cdots v_k$ and $S = u_1u_2 \cdots u_l$ are two new disjoint paths. Let $G^2_{k,l}$ denote the graph obtained from G, P and S by joining v to v_1 with an edge and joining u to u_1 with another edge. If $k \geq l+2$, then $\rho(G^2_{k,l}) < \rho(G^2_{k-1,l+1})$. The procedure from $G^2_{k,l}$ to $G^2_{k-1,l+1}$ is called the second edge transformation of graph, 2.e.t. for short.*

Lemma 1.5 ([3]) *Let u and v be two vertices of a connected graph G. Let $v_1, v_2, \ldots, v_p (\neq u)$ be some vertices being adjacent to v but not adjacent to u in G. If $x_u^G \geq x_v^G$, then*

$$\rho(G) < \rho(G - \{vv_1, vv_2, \ldots, vv_p\} + \{uv_1, uv_2, \ldots, uv_p\}).$$

The procedure from G to $G - \{vv_1, vv_2, \ldots, vv_p\} + \{uv_1, uv_2, \ldots, uv_p\}$ is called the third edge transformation of graph, 3.e.t. for short.

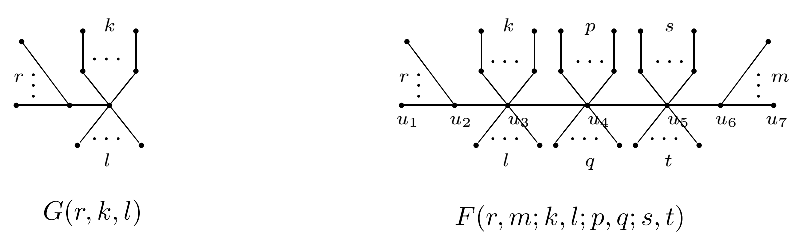

Figure 1 Two special trees

Let $G(r,k,l)$ and $F(r,m;k,l;p,q;s,t)$ be the two trees shown in Figure 1. Write

$T^1_{n,i} = G(1, i-2, n-2i+1)$, $T^2_{n,i} = G(2, i-2, n-2i)$,

$T^3_{n,i} = G(1, i-1, 0)$, $T^4_{n,i} = F(1,0;0,1;i-4,n-2i+1;0,0)$,

$T^5_{n,i} = F(1,0;0,0;i-3,n-2i;0,0)$, $T^6_{n,i} = F(1,1;i-4,n-2i+1;0,0;0,0)$,

$T^7_{n,i} = G(3, i-2, n-2i-1)$, $T^8_{n,i} = F(1,0;0,2;i-4,n-2i;0,0)$,

$T^9_{n,i} = F(1,0;1,1;i-5,n-2i+1;0,0)$, $\qquad T^{10}_{n,i} = F(2,0;i-4,n-2i;0,1;0,0)$,

$T^{11}_{n,i} = F(1,1;0,1;i-5,n-2i+1,0,1)$.

For $n \geq 2i+1$, [4,7] have shown that $T^1_{n,i}$ and $T^2_{n,i}$ are the first two trees in $T(n,i)$ with the largest Laplacian spectral radius, respectively. In this paper, we will determine the third to sixth trees in $T(2i+1,i)$ and the third to fifth trees in $T(n,i)$ for $n \geq 2i+2$ by the largest Laplacian spectral radius, namely we obtain the following main results.

Theorem 1.6 *Let $i \geq 6$.*

(1) If $n = 2i+1$, then in $T(n,i)$, $T^3_{n,i}, T^4_{n,i}, T^5_{n,i}$ and $T^6_{n,i}$ are the four trees with the third largest value to the sixth largest value of Laplacian spectral radius, respectively.

(2) If $n \geq 2i+2$, then in $T(n,i)$, $T^4_{n,i}, T^5_{n,i}$ and $T^6_{n,i}$ are the three trees with the third largest value to the fifth largest value of Laplacian spectral radius, respectively.

Where $\mu(T^3_{n,i}) = \frac{1}{2}(i+3+\sqrt{i^2-2i+5})$, $\mu(T^4_{n,i}), \mu(T^5_{n,i}), \mu(T^6_{n,i})$ are the largest roots of following three equations, respectively.

$$\lambda^7 - (n-i+10)\lambda^6 + (10n-10i+36)\lambda^5 - (36n-35i+56)\lambda^4 + (57n-50i+30)\lambda^3$$
$$-(39n-25i-8)\lambda^2 + (11n-3i-8)\lambda - n = 0.$$

$$\lambda^6 - (n-i+8)\lambda^5 + (8n-8i+22)\lambda^4 - (22n-21i+23)\lambda^3 + (24n-19i+4)\lambda^2$$
$$-(9n-3i-4)\lambda + n = 0.$$

$$\lambda^6 - (n-i+9)\lambda^5 + (9n-9i+28)\lambda^4 - (28n-27i+32)\lambda^3 + (34n-28i)\lambda^2$$
$$-(12n-3i-16)\lambda + n = 0.$$

2. Some lemmas

Write $\theta(k,l) = \lambda^2 - k\lambda + l$, $\delta(k,l) = \theta(3,1)\theta(k+l+3,k+2) - k\theta(2,1)$. By an elementary calculation, we obtain the characteristic polynomials of signless Laplacian matrices of $G(r,k,l)$ and $F(r,m;k,l;p,q;s,t)$ as follows:

$$\phi(G(r,k,l)) = (\lambda-1)^{r+l-2}(\theta(3,1))^{k-1}g(r,k,l),$$
$$\phi(F(r,m;k,l;p,q;s,t)) = (\lambda-1)^{r+m+l+q+t-5}(\theta(3,1))^{k+p+s-3}f(r,m;k,l;p,q;s,t),$$

where

$$g(r,k,l) = \theta(r+2,1)[\theta(3,1)\theta(k+l+2,k+1) - k\theta(2,1)] - \theta(2,1)\theta(3,1),$$
$$f(r,m;k,l;p,q;s,t) = \theta(r+2,1)\theta(m+2,1)\delta(k,l)\delta(p,q)\delta(s,t) -$$
$$\theta(r+2,1)\theta(m+2,1)\theta(2,1)\theta^2(3,1)[\delta(k,l)+\delta(s,t)] -$$
$$\theta(2,1)\theta(3,1)\delta(p,q)[\theta(r+2,1)\delta(k,l) + \theta(m+2,1)\delta(s,t) - \theta(2,1)\theta(3,1)] +$$
$$\theta^2(2,1)\theta^3(3,1)[\theta(r+2,1)+\theta(m+2,1)].$$

Lemma 2.1 *Let $i \geq 6$.*

(1) When $n \geq 2i+2$, $\rho(T^4_{n,i}) > \rho(T^5_{n,i}) > \rho(T^6_{n,i}) > \rho(T^j_{n,i})$, $j \geq 7$.

(2) When $n = 2i+1$, $\rho(T^3_{n,i}) > \rho(T^4_{n,i}) > \rho(T^5_{n,i}) > \rho(T^6_{n,i}) > \rho(T^j_{n,i})$, $j \geq 8$.

Proof For $j = 3,4,5,6$, by Lemma 1.2, we have $\rho(T^j_{n,i}) \geq \Delta(T^j_{n,i}) + 1 = n - i$. Let

$$\xi_{k,l} = \lambda^2(\lambda-1)^{n-2i}(\lambda-2)^k(\lambda^2-3\lambda+1)^{i-4-l}.$$

(1) By using 2.e.t, $T^5_{n,i}$ can be transformed into $T^4_{n,i}$. Again by applying 1.e.t, $T^6_{n,i}$ can be transformed into $T^5_{n,i}$. So by Lemmas 1.4 and 1.3, we have $\rho(T^4_{n,i}) > \rho(T^5_{n,i}) > \rho(T^6_{n,i})$.

For $j = 7,8,9,10,11$, according to $\phi(F(r,m;k,l;p,q;s,t))$ and $\phi(G(r,k,l))$, by a calculation,

$$\phi(T^j_{n,i}) - \phi(T^6_{n,i}) = a_j\{[(i-6)\theta(3,2) + (n-2i)\theta(3,1)]\varphi^{(1)}_j + \varphi^{(2)}_j\},$$

where

$$a_7 = \xi_{0,0},\ \varphi^{(1)}_7 = \theta(2,-2),\ \varphi^{(2)}_7 = 4\lambda^3 - 19\lambda^2 + 28\lambda - 16;$$
$$a_8 = \xi_{0,0},\ \varphi^{(1)}_8 = \theta(2,-1),\ \varphi^{(2)}_8 = 4\lambda^3 - 19\lambda^2 + 28\lambda - 13;$$
$$a_9 = \xi_{1,0},\ \varphi^{(1)}_9 = \lambda,\ \varphi^{(2)}_9 = 4\lambda^2 - 11\lambda + 6;$$
$$a_{10} = \xi_{0,1},\ \varphi^{(1)}_{10} = \theta(3,1)\theta(3,-1) - \lambda,\ \varphi^{(2)}_{10} = (\lambda-1)[\lambda^3\theta(6,7) + 13\theta(2,1) - 4];$$
$$a_{11} = \xi_{1,2},\ \varphi^{(1)}_{11} = \lambda\theta(3,1)\theta(4,2) - \theta(1,0),\ \varphi^{(2)}_{11} = (\lambda-2)[\lambda^4\theta(6,8) + 6\lambda\theta(\frac{13}{6},1) - 1].$$

When $\lambda \geq \rho(T^6_{n,i})$, since a_j, $\varphi^{(1)}_j$ and $\varphi^{(2)}_j$ are positive, we have

$$\phi(T^j_{n,i}) - \phi(T^6_{n,i}) > a_j\varphi^{(2)}_j > 0.$$

This implies that $\rho(T^6_{n,i}) > \rho(T^j_{n,i})$, $j = 7,8,9,10,11$.

(2) From $\phi(G(r,k,l))$ and $\phi(F(r,m;k,l;p,q;s,t))$, we get

$$\phi(T^3_{n,i}) = \lambda(\lambda^2-3\lambda+1)^{i-1}\theta(i+3,2i+1),\quad \phi(T^4_{n,i}) = \lambda(\lambda-1)(\lambda^2-3\lambda+1)^{i-4}\omega(\lambda),$$

where $\rho(T^3_{n,i})$ is the largest positive root of $\theta(i+3,2i+1)$, $\rho(T^4_{n,i})$ is the largest positive root of $\omega(\lambda)$ and

$$\begin{aligned}\omega(\lambda) =& [\lambda^3\theta(8,15) + 3\lambda^2(2\lambda-7) + (i+3)(\lambda-i) + 2i(i-1) - 1]\theta(i+3,2i+1) + \\ & [(i-6)(i^2+2i+8) + 45](\lambda-2) + i(i-6) + 3(i-2).\end{aligned}$$

For $\lambda \geq \rho(T^3_{n,i})$, we have $\omega(\lambda) > 0$, i.e., $\phi(T^4_{n,i}) > 0$. This implies that $\rho(T^3_{n,i}) > \rho(T^4_{n,i})$. In the similar way to (1), we can show the other inequalities. □

Lemma 2.2 *Let* $r \neq 0$, $k \neq 0$ *and* $\max\{r-k-l, 1\} \leq j \leq r$. *Then*

$$\rho(G(r,k,l)) < \rho(G(r-j,k,l+j)).$$

The procedure from $G(r,k,l)$ *to* $G(r-j,k,l+j)$ *is called the fourth edge transformation of graph, 4.e.t. for short.*

Proof By calculation, we have

$$g(r,k,l) - g(r-j,k,l+j) = j\lambda^2[(k+l+j-r)\theta(3,1) + k].$$

By Lemma 1.2, we have $\rho(G(r-j,k,l+j)) \geq 3$. So for $\lambda \geq \rho(G(r-j,k,l+j))$, $\theta(3,1) > 0$. It follows that $g(r,k,l) > g(r-j,k,l+j)$, namely $\phi(G(r,k,l)) > \phi(G(r-j,k,l+j))$. Thus the required result holds. □

Lemma 2.3 *(1) Let $r \neq 0$ and $\max\{r-k-l-1, 1\} \leq j \leq r$. Then*

$$\rho(F(r,m;k,l;p,q;s,t)) < \rho(F(r-j,m;k,l+j;p,q;s,t)).$$

The procedure from $F(r,m;k,l;p,q;s,t)$ to $F(r-j,m;k,l+j;p,q;s,t)$ is called the fifth edge transformation of graph, 5.e.t. for short.

(2) Let $p+q \neq 0$, $l \neq 0$ and $k+l \geq 2$. Then

$$\rho(F(1,1;k,l;p,q;s,t)) < \rho(F(1,1;0,1;p+k,q+(l-1);s,t)).$$

The procedure from $F(1,1;k,l;p,q;s,t)$ to $F(1,1;0,1;p+k,q+(l-1);s,t)$ is called the sixth edge transformation of graph, 6.e.t. for short.

Proof (1) By calculation, we have

$$f(r,m;k,l;p,q;s,t) - f(r-j,m;k,l+j;p,q;s,t) = j\lambda(c\alpha+\beta),$$

where

$$\begin{aligned}
c &= [(j+k+l+1-r)\lambda - 1]\theta(3,1) + k\lambda, \\
\alpha &= \theta(m+2,1)[\delta(p,q)\delta(s,t) - \theta(2,1)\theta^2(3,1)] - \theta(2,1)\theta(3,1)\delta(p,q), \\
\beta &= [\theta(m+2,1)\delta(s,t) - \theta(2,1)\theta(3,1)]\theta(2,1)\theta^2(3,1).
\end{aligned}$$

Now assume $\lambda \geq \rho(F(r-j,m;k,l+j;p,q;s,t))$. Since $F(0,m;0,0;p,q;s,t)$ and $G(m,s+1,t)$ are the proper subgraphs of $F(r-j,m;k,l+j;p,q;s,t)$, we have from Perron-Frobenius theorem that

$$\rho(F(r-j,m;k,l+j;p,q;s,t)) > \max\{\rho(F(0,m;0,0;p,q;s,t)), \rho(G(m,s+1,t))\}.$$

It follows that

$$f(0,m;0,0;p,q;s,t) > 0, \quad g(m,s+1,t) > 0.$$

On the other hand, from Lemma 1.2, we have

$$\rho(F(r-j,m;k,l+j;p,q;s,t)) \geq \max\{m+2, 3\}.$$

Therefore, by $\phi(G(r,k,l))$ and $\phi(F(r,m;k,l;p,q;s,t))$, we have

$$\alpha = \frac{f(0,m;0,0;p,q;s,t)}{\theta(2,1)\theta^2(3,1)} + \theta(2,1)[g(m,s+1,t) + \theta(2,1)\theta(m+2,1)] > 0.$$

Note that $c \geq -\theta(3,1)$. So we get

$$\begin{aligned}
c\alpha+\beta &\geq -\theta(3,1)\alpha + \beta > \theta(3,1)[\theta(m+2,1)\delta(s,t) - \theta(2,1)\theta(3,1)][\theta(2,1)\theta(3,1) - \delta(p,q)] \\
&= \theta(3,1)[g(m,s+1,t) + \theta(2,1)\theta(m+2,1)] \times \\
&\qquad \{\theta(3,1)[(p+q+1)\lambda - (p+1)] + p\theta(2,1)\} > 0.
\end{aligned}$$

It follows that

$$\phi(F(r,m;k,l;p,q;s,t)) > \phi(F(r-j,m;k,l+j;p,q;s,t)).$$

This implies the required result.

(2) By calculation, we get

$$\frac{f(1,1;k,l;p,q;s,t) - f(1,1;0,1;p+k,q+(l-1);s,t)}{\lambda\theta^2(3,1)[(k+l-1)\theta(3,1)+k]} = \Omega,$$

where

$$\Omega = [\delta(s,t) - \theta(2,1)]\{[(p+q-1)\lambda - 1]\theta(3,1) + (p-1)\lambda\} + \theta(2,1)\theta^2(3,1).$$

From Lemma 1.2, we have

$$\rho(F(1,1;0,1;p+k,q+(l-1);s,t)) \geq \max\{m+2,3\}.$$

First, assume $p+q \geq 2$. For $\lambda \geq \rho(F(1,1;0,1;p+k,q+(l-1);s,t))$, we have

$$\delta(s,t) - \theta(2,1) = \frac{g(m,s+1,t) + \theta(2,1)\theta(3,1)}{\theta(m+2,1)} > 0,$$

$$\{[(p+q-1)\lambda - 1]\theta(3,1) + (p-1)\lambda\} + \theta(2,1)\theta^2(3,1) > \theta(3,1) - \lambda + \theta(2,1) > 0.$$

These indicate that $\Omega > 0$.

Next, assume $p+q = 1$. Since $(p,q) \in \{(1,0),(0,1)\}$, we get

$$\Omega = \lambda[p\theta(3,1) + q\theta(2,1)][(s+t+p)\theta(3,1) + s + 1].$$

Therefore, for $\lambda \geq \rho(F(1,1;0,1;p+k,q+(l-1);s,t))$, we have $\Omega > 0$.

The above discussions indicate that for $\lambda \geq \rho(F(1,1;0,1;p+k,q+(l-1);s,t))$, we always have $\Omega > 0$, that is

$$\phi(F(1,1;k,l;p,q;s,t)) > \phi(F(1,1;0,1;p+k,q+(l-1);s,t)).$$

This implies the required result. $\square$

Let u be a vertex of a simple connected graph H. Suppose that two nonnegative integers k, s satisfy $H - u = kP_2 \bigcup sP_1 \bigcup G$, where G is a connected graph with at least three vertices. Then u is called an end-branch vertex if $s \geq 2$ or $k \neq 0$. In particular, u is called a star end-branch vertex if $s \geq 2$ and $k = 0$.

Let $\tilde{G}(s_1,\ldots,s_k;l)$ be the graph obtained by joining the center of K_{1,s_j} $(j = 1,\ldots,k)$ to the center of $K_{1,l}$ with an edge, where the center of $K_{1,l}$ is called the center of $\tilde{G}(s_1,\ldots,s_k,l)$. Let $\tilde{H} = \tilde{H}(s_1,\ldots,s_k,l;t_1,\ldots,t_p,q)$ be the graph obtained by joining the center u of $\tilde{G}(s_1,\ldots,s_k;l)$ to the center v of $\tilde{G}(t_1,\ldots,t_p;q)$ with an edge. Let

$$\tilde{F} = \tilde{F}(s_1^{(1)},\ldots,s_{k_1}^{(1)},l_1;\ldots;s_1^{(p)},\ldots,s_{k_p}^{(p)},l_p;t_1,\ldots,t_r,q)$$

be the graph obtained by joining the center of $\tilde{G}(s_1^{(j)},\ldots,s_{k_j}^{(j)},l_j)$ $(j = 1,\ldots,p)$ to the center of $\tilde{G}(t_1,\ldots,t_r,q)$ with an edge. Let $T(n,i,d)$ be the set of trees with fixed order n, matching number i and diameter d. Then each tree of $T(n,i,4)$ can be denoted by $\tilde{G}(s_1,\ldots,s_k;l)$; each tree of $T(n,i,5)$ can be denoted by $\tilde{H}$ and each tree of $T(n,i,6)$ can be denoted by $\tilde{F}$.

For convenience, let $G \xrightarrow{\text{j.e.t}} W$ denote the procedure that a graph G is transformed into another graph W by using j.e.t.

Lemma 2.4 *Let $i \geq 6$ and $T \in T(n,i,4)\backslash\{T^1_{n,i}, T^2_{n,i}, T^3_{n,i}\}$. Then $\rho(T) < \rho(T^6_{n,i})$.*

Proof Since $T(2i,i,4) \bigcup T(2i+1,i,4) = \{T^1_{2i,i}, T^1_{2i+1,i}, T^2_{2i+1,i}, T^3_{2i+1,i}\}$, by $T \notin \{T^1_{n,i}, T^2_{n,i}, T^3_{n,i}\}$ we have that $n \geq 2i+2$. There are nonnegative integers $k, l, s_1 \geq \cdots \geq s_{k+1} \geq 1$ such that $T = \tilde{G}(s_1, \ldots, s_{k+1}, l)$. By Lemmas 2.1, 1.4, 1.5 and 2.2, we need show that T can be transformed into $G(3, i-2, n-2i-1) = T^7_{n,i}$ by applying 2.e.t, 3.e.t and 4.e.t. Let $r = \sum_{j=1}^{k+1}(s_j - 1) + 1$. Then $r + l = n - 2k - 2$.

Case 1 Let $l \neq 0$. Then $k = i-2$ and $r \geq 3$ from $T \notin \{T^1_{n,i}, T^2_{n,i}\}$. Set $j = r-3$. We have

$$T \xrightarrow{\text{3.e.t}} G(r,k,l) \xrightarrow{\text{4.e.t}} G(r-j, k, l+j) = T^7_{n,i}.$$

Case 2 Let $l = 0$. Then $k = i-1$ and $r \geq 2$ from $n \geq 2i+2$. Set $m = k-1, j = r-2$. We have

$$T \xrightarrow{\text{3.e.t}} G(r,k,l) \xrightarrow{\text{2.e.t}} G(r+1, m, l+1) \xrightarrow{\text{4.e.t}} G(r+1-j, m, l+1+j) = T^7_{n,i}.$$

The proof is completed. $\square$

Lemma 2.5 *Let $i \geq 6$ and $T \in T(n,i,5)\backslash\{T^4_{n,i}, T^5_{n,i}\}$. Then $\rho(T) < \rho(T^6_{n,i})$.*

Proof Write $H(r;k,l;p,q) = F(r,0;k,l;p,q;0,0)$. By Lemmas 2.1, 2.3(1), 1.4 or 1.5, we need show that T can be transformed into one of $T^8_{n,i}, T^9_{n,i}$ or $T^{10}_{n,i}$ by using 5.e.t, 2.e.t or 3.e.t. There are nonnegative integers $k, l, p, q, s_1, \ldots, s_{k+1}, t_1, \ldots, t_{p+1}$ with

$$s_1 \geq \cdots \geq s_{k+1} \geq 1, t_1 \geq \cdots \geq t_{p+1} \geq 1$$

such that

$$T = \tilde{H}(s_1, \ldots, s_{k+1}, l; t_1, \ldots, t_{p+1}, q) \xrightarrow{\text{3.e.t}} H(r;k,l;p,q) = H',$$

where

$$\text{in}(H') = i, r = \sum_{j=1}^{k+1}(s_j - 1) + \sum_{j=1}^{p+1}(t_j - 1) + 1,\ r + l + q = n - 2(k+p) - 5.$$

Case 1 Let $lq \neq 0$. Then $k + p = i - 4 \geq 2, r + l + q = n - 2i + 3$.

Case 1.1 Let $r = 1$. Without loss of generality, assume $x^{H'}_{u_3} \leq x^{H'}_{u_4}$.

If $k \neq 0$, then

$$H(r;k,l;p,q) \xrightarrow{\text{3.e.t}} H(r;1,1;p+(k-1), q+(l-1)) = T^9_{n,i}.$$

If $k = 0$, then from $T \notin \{T^4_{n,i}, T^5_{n,i}\}$, we have $l \geq 2$. So

$$H(r;k,l;p,q) \xrightarrow{\text{3.e.t}} H(r;0,2;p+k, q+(l-2)) = T^8_{n,i}.$$

Case 1.2 Let $r \geq 2$. Note that $k \geq 2$ when $p = 0$.

If $p \neq 0$, write $j = r-1$, then

$$H(r;k,l;p,q) \xrightarrow{\text{5.e.t}} H(r-j;k,l+j;p,q) \xrightarrow{\text{Method of Case 1.1}} T^8_{n,i} \text{ or } T^9_{n,i}.$$

If $p=0$ and $x_{u_3}^{H'} \geq x_{u_4}^{H'}$, write $j=r-2, \alpha=k+p, \beta=l+(q-1)$, then

$$H(r;k,l;p,q) \xrightarrow{3.\text{e.t}} H(r;\alpha,\beta;0,1) \xrightarrow{5.\text{e.t}} H(r-j;\alpha,\beta+j;0,1)=T_{n,i}^{10}.$$

If $p=0$ and $x_{u_3}^{H'} < x_{u_4}^{H'}$, write $j=r-1, \alpha=k-1, \beta=p+1$, then

$$H(r;k,l;p,q) \xrightarrow{3.\text{e.t}} H(r;\alpha,l;\beta,q) \xrightarrow{5.\text{e.t}} H(r-j;\alpha,l+j;\beta,q) \xrightarrow{3.\text{e.t}} T_{n,i}^{9}.$$

Case 2 Let $lq=0$. Then $k+p=i-3 \geq 3$. Without loss of generality, assume $k \geq p$. So $k \geq 2$.

If $q \neq 0$ and $l=0$, then

$$H(r;k,l;p,q) \xrightarrow{2.\text{e.t}} H(r;k-1,l+1;p,q+1)=H_1.$$

If $q=0$ and $p=0$, then from $T \notin \{T_{n,i}^4, T_{n,i}^5\}$, we have $r \geq 2$. So

$$H(r;k,l;p,q) \xrightarrow{2.\text{e.t}} H(r;k-1,l+1;p,q+1)=H_2.$$

If $q=0$ and $p \neq 0$, then

$$H(r;k,l;p,q) \xrightarrow{2.\text{e.t}} H(r;k-1,l+1;p,q+1)=H_3.$$

It is obvious that $H_j \notin \{T_{n,i}^4, T_{n,i}^5\}$, $\text{in}(H_j)=i$ and H_j $(j=1,2,3)$ satisfy the assumptions of Case 1. Therefore, the results in this case hold by the results of Case 1. $\Box$

Lemma 2.6 *Let $i \geq 6$ and $T \in T(n,i,6) \backslash \{T_{n,i}^6\}$. Then $\rho(T) < \rho(T_{n,i}^6)$.*

Proof There are nonnegative integers

$$r,q,p \geq 2, l_1 \geq \cdots \geq l_p \geq 1, s_1^{(j)} \geq \cdots \geq s_{k_j}^{(j)} \geq 1, \quad j=1,\dots,p$$

such that

$$T=\tilde{F}(s_1^{(1)},\dots,s_{k_1}^{(1)},l_1;\dots;s_1^{(p)},\dots,s_{k_p}^{(p)},l_p;t_1,\dots,t_r,q).$$

Let u_4 be the midpoint of a longest path in T.

(1) Let w and v be two star end-branch vertices with a distance 2 to u_4. Without loss of generality, assume $x_w^T \geq x_v^T$. Let $v_1, v_2, \dots, v_\alpha$ be all pendant vertices at v. Set

$$B_1=T-\{vv_2,\dots,vv_\alpha\}+\{wv_2,\dots,wv_\alpha\}.$$

By Lemma 1.5, we have $\rho(T) < \rho(B_1)$. To B_1 repeat the above procedure until we get a tree B_κ such that it has at most a star end-branch vertex with a distance 2 to u_4 (If there is such a vertex, then denote it by u_2). So we get trees $T, B_1, \dots, B_\kappa$ such that

$$\text{in}(T)=\text{in}(B_1)=\cdots=\text{in}(B_\kappa),\ \rho(T)<\rho(B_1)<\cdots<\rho(B_\kappa).$$

(2) Let $P=u_1u_2u_3\cdots u_7$ be a longest path of B_κ. Let v be an end-branch vertex of B_κ which is not on P and is adjacent to u_4. Let $u_4, v_1, v_2, \dots, v_\alpha, y_1, y_2, \dots, y_\beta$ be all adjacent vertices of v in B_κ, where all of $v_1, v_2, \dots, v_\alpha$ are pendant vertices while all of $y_1, y_2, \dots, y_\beta$ have degree 2. Let $v, u_3, u_5, a_1, a_2, \dots, a_m, b_1, b_2, \dots, b_z$ be all adjacent vertices of u_4 in B_κ, where all of $a_1, a_2, \dots, a_m$ are pendant vertices while all of $b_1, b_2, \dots, b_z$ are not pendant vertices.

Case 2.1 Let $x_v^{B_\kappa} \geq x_{u_4}^{B_\kappa}$. If $m \neq 0$, then set

$$\begin{aligned} C_1 =& B_\kappa - \{u_4u_3, u_4u_5, u_4a_2, \ldots, u_4a_m, u_4b_1, \ldots, u_4b_z\} + \\ & \{vu_3, vu_5, va_2, \ldots, va_m, vb_1, \ldots, vb_z\}. \end{aligned}$$

If $m = 0$, then set

$$C_1 = B_\kappa - \{u_4u_3, u_4u_5, u_4b_1, \ldots, u_4b_z\} + \{vu_3, vu_5, vb_1, \ldots, vb_z\}.$$

Denote the vertex v of C_1 by u_4.

Case 2.2 Let $x_v^{B_\kappa} < x_{u_4}^{B_\kappa}$. If $\alpha \neq 0$, then set

$$C_1 = B_\kappa - \{vv_2, \ldots, vv_\alpha, vy_1, \ldots, vy_\beta\} + \{u_4v_2, \ldots, u_4v_\alpha, u_4y_1, \ldots, u_4y_\beta\}.$$

If $\alpha = 0$, then set

$$C_1 = B_\kappa - \{vy_1, \ldots, vy_\beta\} + \{u_4y_1, \ldots, u_4y_\beta\}.$$

It is obvious that $\mathrm{in}(B_\kappa) \leq \mathrm{in}(C_1)$, and by Lemma 1.5, we have $\rho(B_\kappa) < \rho(C_1)$. To C_1 repeat the above procedure until we obtain a tree C_η such that all vertices adjacent to u_4 and not on P are not end-branch vertices. So we obtain a sequence of trees $B_\kappa, C_1, \ldots, C_\eta = F(r, 1; k, \bar{l}; p, q; s, t)(r \geq 1)$ such that

$$\mathrm{in}(B_\kappa) \leq in(C_1) \leq \cdots \leq \mathrm{in}(C_\eta),\ \rho(B_\kappa) < \rho(C_1) < \cdots < \rho(C_\eta).$$

(3) By applying 5.e.t, C_η can be transformed into $F(1, 1; k, l; p, q; s, t) = F'$, where $l = \bar{l} + (r-1)$.

(4) Suppose there are nonnegative integers a, b such that $F' \cong F(1, 1; a, b; 0, 0; 0, 0)$. If $F' \cong T_{n,i}^6$, then we see by $T \ncong T_{n,i}^6$ that 3.e.t or 5.e.t perform at least once. By Lemma 1.5 or Lemma 2.3(1), we have $\rho(T) < \rho(T_{n,i}^6)$. If $F' \ncong T_{n,i}^6$, then $\mathrm{in}(F') > i$, or $\mathrm{in}(F') = i$ and $b = 0$. By using 1.e.t at least once, F' can be transformed into $T_{n,i}^6$. From Lemmas 1.5, 2.3(1) and 1.3, we have $\rho(T) \leq \rho(F') < \rho(T_{n,i}^6)$.

Now suppose that $F' \ncong F(1, 1; a, b; 0, 0; 0, 0)$ for all nonnegative integers a, b, i.e.,

$$(k + l + p + q)(s + t + p + q) \neq 0.$$

According to Lemmas 2.1, 2.3(2), 1.3 or 1.4, we need show that $F(1, 1; k, l; p, q; s, t)$ can be transformed into $T_{n,i}^{11}$ by using 6.e.t, 1.e.t or 2.e.t.

Case 4.1 Let $lqt \neq 0$. Set $a = k + p + s$. Then $a = \mathrm{in}(F(1, 1; k, l, ; p, q; s, t)) - 5 \geq i - 5$.

$$F(1, 1; k, l; p, q; s, t) \xrightarrow{\text{6.e.t}} F(1, 1; 0, 1; a, q + (l-1) + (t-1); 0, 1) \xrightarrow{\text{1.e.t}} T_{n,i}^{11}.$$

Case 4.2 Let $lqt = 0$.

Case 4.2.1 Let $k + s = 0$. Without loss of generality, assume $l \geq t$.

If $l = 0$, then $p = in(F(1, 1; k, l; p, q; s, t)) - 3 \geq i - 3 \geq 3$.

$$F(1, 1; k, l; p, q; s, t) \xrightarrow{\text{2.e.t}} F(1, 1; k, l + 1; p - 2, q + 2; s, t + 1) = H_1.$$

If $l \neq 0$, then $p = \text{in}(F(1,1;k,l;p,q;s,t)) - 4 \geq i - 4 \geq 2$.

$$F(1,1;k,l;p,q;s,t) \xrightarrow{\text{2.e.t}} F(1,1;k,l;p-1,q+1;s,t+1) = H_2.$$

Case 4.2.2 Let $k + s \neq 0$. Without loss of generality, assume $k \neq 0$.

Assume $t \neq 0$. Then

$$F(1,1;k,l;p,q;s,t) \xrightarrow{\text{2.e.t}} F(1,1;k-1,l+1;p,q+1;s,t) = H_3.$$

Next assume $t = 0$. Let $p + s \neq 0$, for instance, $p \neq 0$.

If $l = 0$, then

$$F(1,1;k,l;p,q;s,t) \xrightarrow{\text{2.e.t}} F(1,1;k-1,l+1;p-1,q+2;s,t+1) = H_4.$$

If $l \neq 0$, then

$$F(1,1;k,l;p,q;s,t) \xrightarrow{\text{2.e.t}} F(1,1;k,l;p-1,q+1;s,t+1) = H_5.$$

Next let $p + s = 0$. By $p + q + s + t \neq 0$, we have $q \neq 0$.

If $l = 0$, then $k = \text{in}(F(1,1;k,l;p,q;s,t)) \geq i - 3 \geq 3$. So

$$\begin{aligned} F(1,1;k,l;p,q;s,t) &\xrightarrow{\text{2.e.t}} F(1,1;k-1,l+1;p,q+1;s,t) \\ &\xrightarrow{\text{6.e.t}} F(1,1;0,1;p+(k-1),q+l+1;s,t) \\ &\xrightarrow{\text{2.e.t}} F(1,1;0,1;p+(k-1)-1,q+l+2;s,t+1) = H_6. \end{aligned}$$

If $l \neq 0$, then $k = \text{in}(F(1,1;k,l;p,q;s,t)) \geq i - 4 \geq 2$. So

$$\begin{aligned} F(1,1;k,l;p,q;s,t) &\xrightarrow{\text{6.e.t}} F(1,1;0,1;p+k,q+(l-1);s,t) \\ &\xrightarrow{\text{2.e.t}} F(1,1;0,1;p+k-1,q+l;s,t+1) = H_7. \end{aligned}$$

Obviously, $H_j \ncong F(1,1;a,b;0,0;0,0)$, $\text{in}(H_j) \geq i$ and H_j $(1 \leq j \leq 7)$ satisfy the assumptions of Case 4.1. So the results in this case hold by the results of Case 4.1. $\Box$

Let uv be a nonpendant edge of a tree G. Let $G_{u,v}$ be the graph obtained from G in the following way:

1) Delete the edge uv and identify u and v;

2) Add a new pendant edge to the vertex $u(=v)$.

The procedure from G to $G_{u,v}$ is called an edge-growing transformation of G for the edge uv. By Lemma 1.5, we have $\rho(G) < \rho(G_{u,v})$.

Lemma 2.7 *Let $\rho(n,i,d) = \max\{\rho(T) : T \in T(n,i,d)\}$. Then $\rho(n,i,d)$ is strictly decreasing in $d(4 \leq d \leq n-1)$.*

Proof For $5 \leq d \leq n-1$, we need prove that $\rho(n,i,d) < \rho(n,i,d-1)$. Assume that $T \in T(n,i,d)$ such that $\rho(n,i,d) = \rho(T)$. Assume that T has two star end-branch vertices u and v. Without loss of generality, assume that $x_u^T \geq x_v^T$. Let $v_1, v_2, \ldots, v_p$ be all pendant vertices at v and let

$$T' = T - \{vv_2, \ldots, vv_p\} + \{uv_2, \ldots, uv_p\}.$$

Then $T' \in T(n,i,d)$, and by Lemma 1.5, $\rho(T') > \rho(T)$, a contradiction to the assumption of T. Therefore, T has at most one star end-branch vertex. Let $u_1u_2\cdots u_du_{d+1}$ be a longest path of T, where u_2 is the unique star end-branch vertex of T if such vertex exists. Let M be a maximum matching of T including edges u_1u_2 and u_du_{d+1}.

Case 1 Suppose that there is a vertex u_j $(3 \leq j \leq d-1)$ not saturated by M.

If u_{j-1} is not saturated by M, then $\{u_{j-1}u_j\} \bigcup M$ is a matching of T, a contradiction with the maximum matching M. Therefore, u_{j-1} is saturated by M. Let G be the tree obtained from T by an edge-growing transformation of T for the edge $u_{j-1}u_j$. Then $\mathrm{in}(G) = i$, $d-1 \leq \mathrm{dia}(G) \leq d$ and $\rho(T) < \rho(G)$. If $\mathrm{dia}(G) = d$, then $G \in J(n,i,d)$, so

$$\rho(n,i,d) = \rho(T) < \rho(G) \leq \rho(n,i,d)$$

a contradiction. Therefore, $\mathrm{dia}(G) = d-1$, i.e., $G \in J(n,i,d-1)$. So

$$\rho(n,i,d) = \rho(T) < \rho(G) \leq \rho(n,i,d-1).$$

Case 2 Suppose that each u_j $(j = 1,2,\ldots,d+1)$ is saturated by M.

Case 2.1 Suppose that there is a j $(3 \leq j \leq d-2)$ such that $u_ju_{j+1} \in M$.

Let G denote the tree obtained from T by an edge-growing transformation of T for the edge u_ju_{j+1}. In the similar way to Case 1, we can prove that the results hold.

Case 2.2 Suppose that $u_ju_{j+1} \notin M$ for each j $(3 \leq j \leq d-2)$.

If there are not pendant edges at u_3 or u_{d-1}, without loss of generality, suppose that there are not pendant edges at u_3. Then there must be a pendant path u_3ab of length 2 at u_3 such that $u_3a \in M$ and b is not saturated by M. Let $G = T - ab + u_3b$. Then $G \in T(n,i,d)$. So by Lemma 1.3, we have

$$\rho(n,i,d) = \rho(T) < \rho(G) \leq \rho(n,i,d),$$

a contradiction. Therefore, there are pendant edges at u_3 and u_{d-1}. Without loss of generality, assume $x^T_{u_3} \geq x^T_{u_{d-1}}$. Let $v_1, v_2, \ldots, v_p, u_{d-2}, u_d$ be all adjacent vertices of u_{d-1}, where v_1 is a pendant vertex. Set

$$G = T - \{u_{d-1}v_2, \ldots, u_{d-1}v_p, u_{d-1}u_d\} + \{u_3v_2, \ldots + u_3v_p, u_3u_d\}.$$

Then $\mathrm{in}(G) = i$, $d-1 \leq \mathrm{dia}(G) \leq d$, and by Lemma 1.5, we have $\rho(T) < \rho(G)$. In the similar way to Case 1, we have $\mathrm{dia}(G) = d-1$, i.e., $G \in J(n,i,d-1)$. So

$$\rho(n,i,d) = \rho(T) < \rho(G) \leq \rho(n,i,d-1).$$

The proof is completed. $\Box$

3. Proof of Theorem 1.6

By Lemma 1.1, we only show that the results hold for the signless Laplacian spectral radius of trees. By Lemma 2.1, for $T \in T(n,i) \backslash \{T^j_{n,i} : 1 \leq j \leq 6\}$, we need show that $\rho(T) < \rho(T^6_{n,i})$. From $i \geq 6$, we have $\mathrm{dia}(T) \geq 4$.

If $\mathrm{dia}(T) = 4$, then by $T \notin \{T^1_{n,i}, T^2_{n,i}, T^3_{n,i}\}$ and Lemma 2.4, we get $\rho(T) < \rho(T^6_{n,i})$.

If $\mathrm{dia}(T) = 5$, then by $T \notin \{T^4_{n,i}, T^5_{n,i}\}$ and Lemma 2.5, we get $\rho(T) < \rho(T^6_{n,i})$.

If $\mathrm{dia}(T) = 6$, then by $T \notin \{T^6_{n,i}\}$ and Lemma 2.6, we get $\rho(T) < \rho(T^6_{n,i})$.

If $\mathrm{dia}(T) \geq 7$, then by Lemmas 2.6 and 2.7, we get

$$\rho(T) \leq \rho(n, i, \mathrm{dia}(T)) \leq \rho(n, i, 7) < \rho(n, i, 6) = \rho(T^6_{n,i}).$$

The proof is completed. □

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