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On extremal trees with respect to their terminal distance spectral radius

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Abstract

Let G be a simple connected graph. The terminal distance matrix of G is the distance matrix between all pendant vertices of G. In this paper, we introduce some general transformations that increase the terminal distance spectral radius of a connected graph and characterize the extremal trees with respect to the terminal distance spectral radius among all trees with a fixed number of pendant vertices. Then we obtain upper and lower bounds for the terminal distance spectral radius of trees with fixed number of pendant vertices.

1 Introduction

Let G be a simple connected graph on n vertices, with its vertices labelled by $\{v_1, v_2, \ldots, v_n\}$. The distance $d_G(v_i, v_j)$ between two vertices v_i and v_j of G is equal to the length (that is, the number of edges) of any shortest path that connects v_i and v_j [1]. The distance matrix of G is an n-square matrix whose (i, j)-entry is $d_G(v_i, v_j)$. Recently, the so-called terminal distance matrix [2, 3] or reduced distance matrix [4] of graphs has been considered. If G has k pendant vertices (that is, vertices of degree one), labelled by $\{v_1, v_2, \ldots, v_k\}$, then its terminal distance matrix, $RD(G)$, is the square matrix of order k whose (i, j)-entry is $d_{ij} = d_G(v_i, v_j)$.

The terminal distance matrix of trees is of special interest, since a tree can be reconstructed by its terminal distance matrix. Concepts based on the distance matrix are intensively employed in mathematical chemistry [5–8]. In particular, one of the oldest topological molecular indices, the Wiener index, is defined as one half of the sum of all elements of the distance matrix of a graph. Also, the terminal Wiener index of a graph G is defined by analogy as one half of a sum of the elements of $RD(G)$.

Spectrum-based indices, which are calculated using the eigenvalues and eigenvectors of various graph matrices, form a yet another family of topological indices, the most famous being the Estrada index. Balaban et al. [9] suggested the distance spectral radius (the largest eigenvalue of the distance matrix) as a molecular descriptor giving rise to the extensive QSPR research and to the studies of mathematical properties of the distance spectral radius (DSR).

Recently, the extremal trees with respect to the distance spectral radius have been studied by many researchers [10–13]. In this paper we will characterize the extremal trees on k pendant vertices with respect to their terminal distance spectral radius. Then the minimum and maximum of the terminal distance spectra radius of trees with a fixed number of pendant vertices will be computed.

2 Trees with the minimum terminal distance spectral radius

In this section, we introduce a general transformation that increases the terminal distance spectral radius of a graph, and then we determine the trees on n vertices with a fixed number of pendant vertices which have the minimum terminal spectral radius. Let ϱ_G denote the spectral radius of $RD(G)$ and let x be a positive eigenvector of $RD(G)$ corresponding to ϱ_G. We will denote by x_i the component of x corresponding to a pedant vertex i of G. The components of x indexed by pendant vertices of G which are joined to a common parent by a pendant path will be studied in the following lemma (see Fig. 1).

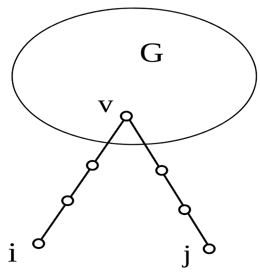

Figure 1: The graph of Lemma 2.1.

Lemma 2.1. *Let i and j be two pendant vertices which are joined to a common parent, v, by a pendant path in G. If $d_G(v,i) \geq d_G(v,j)$, then $x_i \geq x_j$. In particular if $d_G(v,i) = d_G(v,j)$, then $x_i = x_j$.*

Proof. Let $RD(G) = [d_{ij}]$ denote the terminal distance matrix of G and let x be a positive eigenvector of $RD(G)$ corresponding to ϱ_G. From the eigenvalue equation, $\varrho_G x = RD(G)x$ at components x_i and x_j, we obtain

$$\varrho_G x_i = \sum_{r=1}^{k} d_{ir} x_r = \sum_{r \neq i=1}^{k} (d_{iv} + d_{vr}) x_r. \tag{1}$$

$$\varrho_G x_j = \sum_{r=1}^{k} d_{jr} x_r = \sum_{r \neq j=1}^{k} (d_{jv} + d_{vr}) x_r. \tag{2}$$

By subtracting Eq. (2) from Eq. (1) we have $(\varrho_G + d_{vj})x_i = (\varrho_G + d_{vi})x_j$, and hence $x_i \geq x_j$. Therefore the lemma is proved. □

Let P_n denote a path on n vertices. We say lengths of P_n and P_m are almost the same if $|n - m| \leq 1$. A tree in which exactly one vertex has degree greater than 2 is said to be starlike. By $T_{n,k}$ we denote the starlike tree which is obtained from a star S_{k+1} together with k paths of almost equal lengths by joining each pendant vertex of S_{k+1} to an end vertex of one path (Fig. 2). Also, if $T_{n,k}$ has r pendant vertices at distance $q + 1$ and $t = k - r$ pendant vertices at distance q from its central vertex, then we will denote this tree by $T_{q,r,t}$. Obviously $n - 1 = kq + r$.

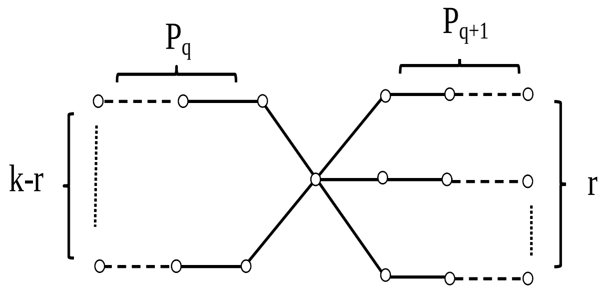

Figure 2: The graph of $T_{n,k}$

Now let G be a simple graph and v ibe one of its vertices. If q_i, r_i and t_i for $i = 1, 2$ are non negative integers, then we denote by $G(l_1, r_1, t_1, l_2, r_2, t_2)$ the graph obtained from $G \cup T_{q_1,r_1,t_1} \cup T_{q_2,r_2,t_2}$ by joining v to both the central vertices of T_{q_1,r_1,t_1} and T_{q_2,r_2,t_2} by a path of order $l_1 - q_1$ and a path of order $l_2 - q_2$, respectively (see Fig. 3).

Assume that $\bar{G} = G(l_1, r_1, t_1, l_2, r_2, t_2)$ and let x be a positive eigenvector of $\bar{G}$ corresponding to $\varrho_{\bar{G}}$. By use of Lemma 2.1, we denote by x_{r_i} and x_{t_i} the components of x corresponding to the further pendant vertices and the closer pendant vertices of T_{q_i,r_i,t_i} to its central vertex, respectively, for $i = 1, 2$. In the following lemma, we will study the variation of $\varrho_{\bar{G}}$ when the distance between the central vertex of T_{q_1,r_1,t_1} and v is increased, but the distance between the central vertex of T_{q_2,r_2,t_2} and v is decreased (using the previous notation).

Lemma 2.2. *Let G be a simple graph with at least one pendant vertex. If $r_2x_{r_2} + t_2x_{t_2} \leq r_1x_{r_1} + t_1x_{t_1}$, then $\varrho_{G(l_1,r_1,t_1,l_2,r_2,t_2)} < \varrho_{G(l_1+1,r_1,t_1,l_2-1,r_2,t_2)}$.*

Proof. Let $RD = [d_{ij}]$ denote the terminal distance matrix of $\bar{G} = G(l_1, r_1, t_1, l_2, r_2, t_2)$ and $RD^* = [d^*_{ij}]$ denote the terminal distance matrix of $G^* = G(l_1 + 1, r_1, t_1, l_2 - 1, r_2, t_2)$. As above, suppose x is an eigenvector of RD corresponding to $\varrho_{\bar{G}}$ and x_{r_1} is a component of x corresponding to a pendant vertex of T_{r_1,r_1,t_1} in $\bar{G}$. Obviously, if i is a pendant vertex of G, then $d^*_{r_1 i} > d_{r_1 i}$. Now we consider the following two cases.

In the first case, let x be an eigenvector of RD^* corresponding to ϱ_{G^*}. From the eigenvalue equation $\varrho_{G^*}x = RD^*x$ at x_{r_1}, we obtain

$$\varrho_{G^*}x_{r_1} = \sum_{j=1}^{k} d^*_{r_1 j}x_j > \sum_{j=1}^{k} d_{r_1 j}x_j = \varrho_{\bar{G}}x_{r_1}.$$

Thus $\varrho_{G^*} > \varrho_{\bar{G}}$ and lemma is proved in this case.

In the second case, suppose x is not an eigenvector of RD^* corresponding to ϱ_{G^*}. If G^1 denotes the pendant vertices of G, then

$$\begin{aligned} x^T RD^* x - x^T RDx &= 2r_1 \sum_{u \in G^1} (l_1 + d_{vu}) x_{r_1} x_u + 2t_1 \sum_{u \in G^1} (l_1 - 1 + d_{vu}) x_{t_1} x_u \\ &\quad + 2r_2 \sum_{u \in G^1} (l_2 - 2 + d_{vu}) x_{r_2} x_u + 2t_2 \sum_{u \in G^1} (l_2 - 3 + d_{vu}) x_{r_1} x_u \\ &\quad - \Big(2r_1 \sum_{u \in G^1} (l_1 - 1 + d_{vu}) x_{r_1} x_u + 2t_1 \sum_{u \in G^1} (l_1 - 2 + d_{vu}) x_{t_1} x_u \\ &\quad + 2r_2 \sum_{u \in G^1} (l_2 - 1 + d_{vu}) x_{r_2} x_u + 2t_2 \sum_{u \in G^1} (l_2 - 2 + d_{vu}) x_{t_2} x_u \Big) \\ &= 2 \sum_{u \in G^1} (r_1 x_{r_1} + t_1 x_{t_1} - r_2 x_{r_2} - t_2 x_{t_2}) x_u. \end{aligned}$$

Hence $x^T RD^* x \geq x^T RDx$. From the Rayleigh quotient we get

$$\varrho_{G^*} = \sup_{y \neq 0} \frac{y^T RD^* y}{y^T y} > \frac{x^T RD^* x}{x^T x} \geq \frac{x^T RDx}{x^T x} = \varrho_{\bar{G}}.$$

Therefore the lemma is proved. $\square$

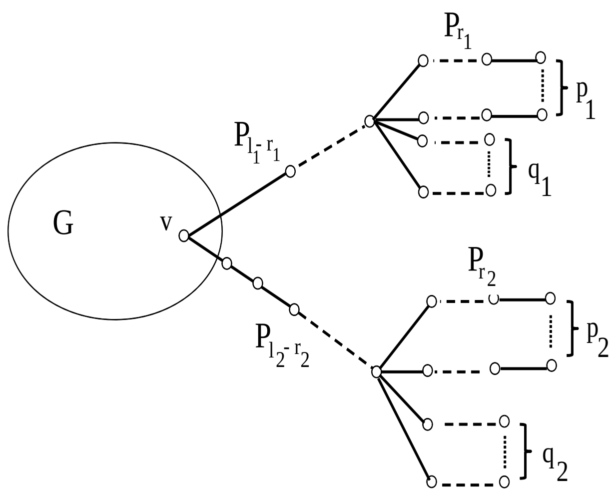

Figure 3: The graph of $G(l_1, p_1, q_1, l_2, p_2, q_2)$.

Now the main result of this section can be obtained as an immediate consequence of Lemma 2.2 in the following theorem.

Theorem 2.3. *Among n-vertex trees with a fixed number k of pendant vertices, $T_{n,k}$ has minimal terminal distance spectral radius.*

Proof. Let T be a tree with the minimum terminal distance spectral radius among n-vertex trees with a fixed number k of pendant vertices. If for positive integers $l_2 - 1 > l_1 > 1$, there exist two pendant paths P_{l_1} and P_{l_2} at a vertex v of T, then for $G = T - V(P_{l_1} \cup P_{l_2}) \cup \{v\}$, we have $T = G(l_1 - 1, 1, 0, l_2 - 1, 1, 0)$. By use of Lemma 2.2, $\varrho_T > \varrho_{G(l_1,1,0,l_2-2,1,0)}$ which contradicts the choice of T. Therefore the lengths of pendant paths at any vertex of T are almost the same.

Now we show that T must be a starlike tree. If T is not a starlike tree, then T contains two vertices v_1 and v_2 with degree greater than two that are furthest from a center vertex of T with minimal distance from each other. For non negative integers q_i, r_i t_i, let T_{q_i,r_i,t_i} denote the induced subtree of T, rooted at v_i for $i = 1, 2$. If v_i is joined by P_{n_i}, a path of order n_i, to a vertex (say v) with degree greater than 2, and G is the connected component of $T - V(P_{n_1} \cup P_{n_2}) \cup \{v\}$ which contains v, then $T = G(l_1, r_1, t_1, l_2, r_2, t_2)$ where $l_i = d_T(v, v_i) + q_i + 1$ for $i = 1, 2$. Now by using Lemma 2.2, we can obtain a new n-vertex tree with k pendant vertices from T with the terminal distance spectral radius less than ϱ_T, contradicting the choice of T.

Thus v_1 must be joined to v_2 by P_l, a path of order l. Now suppose that P_{r_1} is one of the pendant paths at v_1 and $G = T - V(T_{q_2,r_2,t_2} \cup P_{r_1} \cup P_l) \cup \{v\}$; then $T = G(r_1 - 1, 1, 0, l + r_2, r_2, t_2)$. By use of Lemma 2.2, $\varrho_T > \varrho_{G(r_1,1,0,l+r_2-1,r_2,t_2)}$ which contradicts the choice of T. Therefore T is a starlike tree. Since the lengths of pendant paths at a vertex of T are almost the same, the theorem is proved. □

Corollary 2.3.1. *Let T be an n-vertex tree with k pendant vertices and let $n - 1 = kq + r$ $(0 \le r < k)$. Then $\varrho_T \ge q(k-2) + r - 1 + \sqrt{r(k-2)(2q+1) + (qk+1)^2}$.*

Proof. Let x be a positive eigenvector of $RD(T_{n,k})$ corresponding to $\varrho = \varrho_{T_{n,k}}$. If x_1 and x_2 denote the components of x corresponding to the further pendant vertices and the closer pendant vertices of $T_{n,k}$ from its central vertex, then the eigenvalue equation $\varrho x = RD(T_{n,k})x$ gives the system

$$\varrho x_1 = 2(q+1)(r-1)x_1 + (2q+1)(k-r)x_2,$$

$$\varrho x_2 = (2q+1)rx_1 + 2q(k-r-1)x_2,$$

which, after eliminating x_1 and x_2, yields a quadratic equation in ϱ, whose positive solution is

$$q(k-2) + r - 1 + \sqrt{r(k-2)(2q+1) + (qk+1)^2}.$$

By use of Theorem 2.3, $\varrho_T \ge \varrho_{T_{n,k}}$. Therefore the corollary is proved. □

3 Trees with the maximum terminal distance spectral radius

In this section, first we introduce some general transformations that increase the terminal distance spectral radius of a graph, and then we determine the n-vertex trees with k pendant vertices with maximal terminal distance spectral radius. Let $S^*(r, t, l)$ be the graph obtained from $S_{r+1} \cup S_{t+1}$ by joining the central vertices of the stars S_{r+1} and S_{t+1} by a path of length l (see Fig. 4). In the following lemma, we study the variation of the terminal distance spectral radius of $S^*(r, t, l)$ when the number of the pendant vertices adjacent to end vertices of its central path changes.

Lemma 3.1. *If* $r-1>t\geq 1$, *then* $\varrho_{S^*(r,t,l)} < \varrho_{S^*(r-1,t+1,l)}$.

Proof. Let RD and RD^* denote the terminal distance matrix of $S^*(r,t,l)$ and $S^*(r-1,t+1,l)$, respectively, and let x be a positive eigenvector of RD corresponding to $\varrho=\varrho_{S^*(r,t,l)}$. If x_i and x_j denote the components of x corresponding to the pendant vertices of S_{r+1} and S_{t+1} respectively, by using the eigenvalue equation at components x_i and x_j, we obtain

$$\varrho x_i = 2(r-1)x_i + t(l+2)x_j. \tag{3}$$

$$\varrho x_j = 2(t-1)x_j + r(l+2)x_i. \tag{4}$$

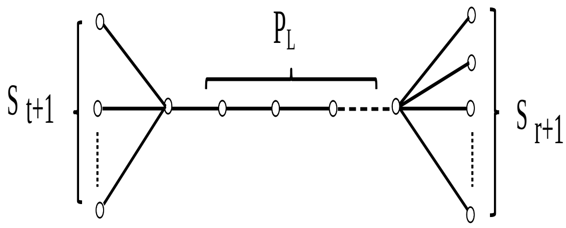

Figure 4: The graph of $S^*(r,t,l)$.

By subtracting Eq. (4) from Eq. (3) we have

$$(\varrho+2+rl)x_i = (\varrho+2+tl)x_j. \tag{5}$$

Hence $x_i<x_j$, and from Eq. (3) we have $\varrho+2>tl$. Thus $(r-1)(\varrho+2+lt) > t(\varrho+2+rl)$. By using this inequality and Eq. (5) we have

$$(r-1)x_i > tx_j. \tag{6}$$

Recall that x is a positive eigenvector of RD corresponding to $\varrho=\varrho_{S^*(r,t,l)}$. Thus we get

$$\begin{aligned} x^TRD^*x - x^TRDx &= 2(l+2)(r-1)x_ix_i + 4tx_ix_j - (4(r-1)x_ix_i + 2t(l+2)x_ix_j) \\ &= 2lx_i((r-1)x_i - tx_j) > 0. \end{aligned}$$

Hence by using Eq. (7), $x^TRD^*x > x^TRDx$. Since x is an eigenvector of $S^*(r,t,l)$, from the Rayleigh quotient we get

$$\varrho_{S^*(r-1,t+1,l)} = \sup_{y\neq 0}\frac{y^TRD^*y}{y^Ty} \geq \frac{x^TRD^*x}{x^Tx} > \frac{x^TRDx}{x^Tx} = \varrho_{S^*(r,t,l)}.$$

Therefore the lemma is proved. □

A caterpillar tree is a tree in which there is a (central) path P such that all vertices are either on P or adjacent to a vertex on P. In the following lemma, the variation of the terminal distance spectral radius of a graph to which a caterpillar tree is attached to one of its vertices is studied (see Fig. 5).

Lemma 3.2. *Let G be a connected graph of order n with k pendant vertices, and let v be one of its vertices. If one of the connected components of $G - v$ is a caterpillar tree with at least one pendant vertex that is not furthest from v, then there exists a connected graph of order n with k pendant vertices, having terminal distance spectral radius greater than ϱ_G.*

Proof. Let T denote the caterpillar tree rooted at v and let P_l denote its central path. If x is a positive eigenvector of G corresponding to ϱ_G, then we denote by x_i the n_i equal components of x corresponding to the pendant vertices of T adjacent to the i-th vertex along P_l, for $1 \leq i \leq l$.

Let G^* denote the graph obtained from G by deleting a pendant vertex adjacent to the i-th vertex along P_l and adding a new pendant vertex to the $(i+1)$-th vertex along P_l for some $1 \leq i < l$. Obviously G^* is a graph on n vertices with k pendant vertices. If RD and RD^* denote the terminal distance matrices of G and G^* respectively and G^1 denotes the pendant vertices of $G - V(T)$, then

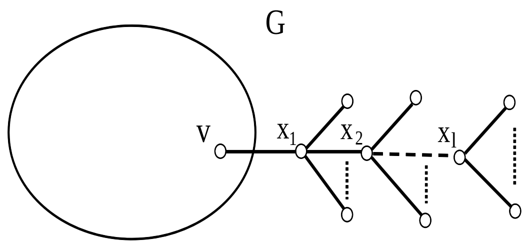

Figure 5: The graph of Lemma 3.2.

$$\begin{aligned} x^T RD^* x - x^T RDx \;=\;& \Big(\sum_{r=1}^{i-1} n_i(r-i+3)x_r x_i + 6(n_i-1)x_i x_i + 4n_{i+1}x_{i+1}x_i \\ & +2\sum_{r=i+2}^{l} n_i(i-r+1)x_i x_r + 2\sum_{u\in G^1}(i+2+d_{vu})x_i x_u\Big) \\ & -\Big(\sum_{r=1}^{i-1} n_i(r-i+2)x_r x_i + 4(n_i-1)x_i x_i + 6n_{i+1}x_{i+1}x_i \\ & +2\sum_{r=i+2}^{l} n_i(i-r+2)x_i x_r + 2\sum_{u\in G^1}(i+1+d_{vu})x_i x_u\Big) \\ =\;& 2(n_i-1)x_i x_i + 2x_i\Big(\sum_{r=1}^{i-1} n_r x_r - \sum_{r=i+1}^{l} n_r x_r - \sum_{u\in G^1} x_u\Big). \qquad (7) \end{aligned}$$

Now let G^{**} denote the graph obtained from G by deleting a pendant vertex adjacent to the i-th vertex along P_l and adding a new pendant vertex to the $(i-1)$-th vertex along P_l, for some $1 < i \leq l$. If RD^{**} denotes the terminal distance matrix of G^{**}, then

$$x^T RD^{**}x - x^T RDx \;=\; 2(n_i-1)x_i x_i - 2x_i\Big(\sum_{r=1}^{i-1} n_r x_r - \sum_{r=i+1}^{l} n_r x_r - \sum_{u\in G^1} x_u\Big). \quad (8)$$

If $n_i > 1$ for some $1 \leq i \leq l$ or $\sum_{r=1}^{i-1} n_r x_r - \sum_{r=i+1}^{l} n_r x_r - \sum_{u\in G^1} x_u \neq 0$, then the right-hand of Eq. (7) or the right-hand of Eq. (8) is positive, and hence $x^T RD^* x > x^T RDx$ or $x^T RD^{**}x > x^T RDx$. If $x^T RD^* x > x^T RDx$, then by use of the Rayleigh quotient we get

$$\varrho_{G^*} = \sup_{y\neq 0} \frac{y^T RD^* y}{y^T y} \geq \frac{x^T RD^* x}{x^T x} > \frac{x^T RDx}{x^T x} = \varrho_G.$$

Similarly, if $x^T RD^{**}x > x^T RDx$, we have $\varrho_{G^{**}} > \varrho_G$. Thus the lemma is proved in this case.

Otherwise, if $n_i = 1$ for each $1 \leq i \leq l$ and $\sum_{r=1}^{i-1} n_r x_r - \sum_{r=i+1}^{l} n_r x_r - \sum_{u\in G^1} x_u = 0$, then $x^T RD^* x = x^T RD^{**}x = x^T RDx$, and from the Rayleigh quotient we have $\varrho_{G^*}, \varrho_{G^{**}} \geq \varrho_G$. By repeating the processes which are used to construct G^* or G^{**} for enough numbers, a new graph on n vertices with k pendant vertices, denoted by G', is obtained from G such that $n_i > 1$ for some $1 \leq i \leq l$ and $\varrho_G \leq \varrho_{G'}$.

Now, if G' is used instead of G in the above argument, the right-hand of Eq. (7) or the right-hand of Eq. (8) is positive, and hence $x^T RD^* x > x^T RDx$ or $x^T RD^{**}x > x^T RDx$ for G'. By using the Rayleigh quotient we get $\varrho_{G^*} > \varrho_G$ or $\varrho_{G^{**}} > \varrho_G$. Therefore the lemma is proved. □

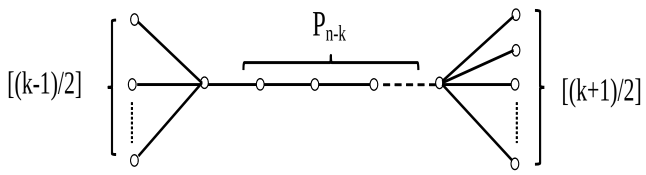

Figure 6: The graph of $T^*_{n,k}$

We now begin the search for trees with k pendant vertices and maximal terminal distance spectral radius. For this purpose we introduce a special case of caterpillar trees. Denote by $T^*_{n,k}$ an n-vertex tree obtained from the path P_{n-k} by attaching to one of its terminal vertices $\lfloor \frac{k}{2} \rfloor$ new pendant vertices and to another terminal vertex $\lceil \frac{k}{2} \rceil$ new pendant vertices (see Fig. 6). We will show that $T^*_{n,k}$ has maximal terminal distance spectral radius.

Theorem 3.3. *Among n-vertex trees with a fixed number k of pendant vertices, $T^*_{n,k}$ has maximal terminal distance spectral radius.*

Proof. Let T be an n-tree with k pendant vertices with maximum terminal distance spectral radius. If for positive integers $l_1 \geq l_2 > 2$ there exist two pendant paths P_{l_1} and P_{l_2} at a vertex v of T, then for $G = T - V(P_{l_1} \cup P_{l_2}) \cup \{v\}$ we have $T = G(l_1 - 1, 1, 0, l_2 - 1, 1, 0)$. By use of Lemma 2.2, $\varrho_T < \varrho_{G(l_1,1,0,l_2-2,1,0)}$ which is a contradiction with the choice of T. Thus all the pendant paths of T are pendant edges.

Suppose T is not a caterpillar tree. Since all of the pendant paths at each vertex of T are pendant edges, there exists a vertex v with $T - v$ containing at least two disjoint caterpillar trees denoted by T_1 and T_2. By using Lemma 3.2, the pendant vertices of T_i must be adjacent to v_i, the furthest vertex on its central path from v, for $i = 1, 2$. Thus for $G = T - V(T_1 \cup T_2) \cup \{v\}$, $T = G(l_1, r_1, 0, l_2, r_2, 0)$, where $l_i = d(v, v_i) + 1$ and $r_i = deg(v_i) - 1$ for $i = 1, 2$. By using Lemma 2.2, we can obtain a tree with the terminal distance spectral radius greater than ϱ_T, which is a contradiction with the choice of T. Hence T must be a caterpillar tree such that its pendant vertices are adjacent to the end vertices on its central path.

Thus $T = S^*(r, t, l)$ where $r + s$ is the number of pendant vertices of T and $l + 2$ is the diameter of T. If $r - s > 1$, from Lemma 3.1 we have $\varrho_T < \varrho_{S^*(r+1,t-1,l)}$, which is a contradiction with the choice of T. So $T = T^*_{n,k}$ and the theorem is proved. □

In what follows, the maximum terminal distance spectra radius of an n-vertex tree with k pendant vertices will be computed. For this purpose we assume that $\delta = 1$ if k is an even integer, and $\delta = 0$ otherwise.

Corollary 3.3.1. *Let T be an n-vertex tree with k pendant vertices. Then*

$$\varrho_T \leq k - 2 + \sqrt{\delta + \frac{k^2 - \delta}{4}(n - k + 1)}.$$

Proof. Let x be a positive eigenvector of $RD(T^*_{n,k})$ corresponding to $\varrho = \varrho_{T^*_{n,k}}$. By use of Lemma 2.1, x has two distinct components, so we denote by x_1 and x_2 these components of x. Put $\alpha = \lfloor \frac{k}{2} \rfloor$ and $\beta = \lceil \frac{k}{2} \rceil$. Thus the eigenvalue equations at x_1 and x_2 give the system

$$\varrho x_1 = 2(\alpha - 1)x_1 + \beta(n - k + 1)x_2,$$

$$\varrho x_2 = \alpha(n - k + 1)x_1 + 2(\beta - 1)x_2,$$

which, after eliminating x_1 and x_2, yields a quadratic equation in ϱ, whose positive solution is

$$k - 2 + \sqrt{\delta + \frac{k^2 - \delta}{4}(n - k + 1)};$$

by use of Theorem 3.3, $\varrho_T \leq \varrho_{T_{n,k}}$. Therefore the corollary is proved. □

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