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ON THE REVERSE DISTANCE SPECTRAL RADIUS OF GRAPHS*

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Abstract: For a connected graph G with vertex set $V(G)$, the reverse distance matrix of G is defined as the matrix whose (u,v)-entry is $d - d_G(u,v)$ if $u \neq v$, and 0 otherwise for $u, v \in V(G)$, where d is the diameter and $d_G(u,v)$ is the distance between u and v in G. The reverse distance spectral radius of G is the largest eigenvalue of the reverse distance matrix of G. We determine the unique trees that minimize (maximize, respectively) the reverse distance spectral radius. We also identify the unique trees for which the complements minimize the reverse distance spectral radius and the unique n-vertex trees for which the complements achieve the i-th largest reverse distance spectral radius for all $i = 1, \dots, \lfloor \frac{n-2}{2} \rfloor$.

Key words: *reverse distance spectral radius, reverse distance matrix, distance matrix, extremal graph*

Mathematics Subject Classification: *05C50, 05C12, 15A42*

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1 Introduction

Throughout the graphs are simple and undirected. Let $G = (V(G), E(G))$ be a connected graph on n vertices with vertex set $V(G)$ and edge set $E(G)$. The *distance* between vertices u, v in G, denoted by $d_G(u,v)$, is the length of a shortest path between them in G. The *distance matrix* of G is defined as the $n \times n$ matrix $D(G) = (d_G(u,v))_{u,v \in V(G)}$. The spectral properties of the distance matrix received much attention, for which early work dated back to Graham and Pollack [7], Graham and Lovász [8] and Edelberg et al. [5] and recent results may be found in the survey by Aouchiche and Hansen [1].

The *diameter* $d(G)$ of a connected graph G is the greatest distance between any vertex pairs of G. The *reverse distance matrix* or *reverse Wiener matrix* [3, 17] of G is defined as the $n \times n$ matrix $\Lambda(G) = (r_G(u,v))_{u,v \in V(G)}$, where

$$r_G(u,v) = \begin{cases} d(G) - d_G(u,v) & \text{if } u \neq v, \\ 0 & \text{if } u = v. \end{cases}$$

Let J_n and I_n be the all one matrix and the identity matrix of order n, respectively. Then $\Lambda(G) = d(G)(J_n - I_n) - D(G)$. This matrix was proposed in [3] and it has been used as a source of molecular descriptors in chemical graph theory and in chemoinformatics [11, 14].

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A matrix is nonnegative if all its entries are nonnegative. For a square nonnegative matrix B, its spectral radius is the maximum modulus of its eigenvalues, denoted by $\rho(B)$. By the well known Perron-Frobenius theorem, $\rho(B)$ is an eigenvalue of B, see [12].

For a connected graph G, the eigenvalues of $\Lambda(G)$ are called the *reverse distance eigenvalues* of G. Note that the reverse distance matrix of a connected graph is symmetric and nonnegative. The reverse distance eigenvalues of G are all real, and the spectral radius of $\Lambda(G)$ is the largest reverse distance eigenvalue of G, denoted by $\rho(G)$, which we call the *reverse distance spectral radius* of G. This parameter is found to be a structural descriptor producing fair quantitative structure-property relationship models [10]. Bounds for the reverse distance spectral radius were given in [16, 17]. Compared with the much studied reverse Wiener index derived from the reverse distance matrix (see [15]), very little is known about the reverse distance spectral radius of graphs. Here we study the extremal properties of the reverse distance spectral radius.

Let $\mathbb{G}(n)$ be a class of connected graphs of order n. It is interesting to consider the problem to determine

$$\min\{\rho(G) : G \in \mathbb{G}(n)\} \text{ and } \max\{\rho(G) : G \in \mathbb{G}(n)\}$$

and characterize those graphs in $\mathbb{G}(n)$ that achieve the above minimum and maximum. In this paper, we determine the unique trees that minimize and maximize the reverse distance spectral radius, respectively. We also determine the unique trees that for which the complements minimize the reverse distance spectral radius, and the unique n-vertex trees for which the complements achieve the i-th largest reverse distance spectral radius for all $i = 1, \ldots, \lfloor \frac{n-2}{2} \rfloor$.

2 Preliminaries

Let K_n, S_n and P_n be the complete graph, the star and the path on n vertices, respectively. Let C_n be the cycle on $n \geq 3$ vertices.

As noted in [16], for a connected graph G on $n \geq 2$ vertices, $\Lambda(G)$ is irreducible if and only if G is not complete. For completeness, we include a proof here.

Lemma 2.1. *Let G be a connected graph with at least 2 vertices. Then $\Lambda(G)$ is irreducible if and only if G is not a complete graph.*

Proof. If G is a complete graph, then $\Lambda(G) = 0$, and so it is reducible.

Suppose that $\Lambda(G)$ is reducible. Then there is a nonempty $V_1 \subset V(G)$ such that $d(G) - d_G(u,v) = r_G(u,v) = 0$ for any $u \in V_1$ and any $v \in V(G) \setminus V_1$. That is, $d(G) = d_G(u,v)$ for any $u \in V_1$ and any $v \in V(G) \setminus V_1$. As G is connected, there is an edge join some vertex, say u_0, in V_1 and some vertex, say v_0, in $V(G) \setminus V_1$. So $d(G) = d_G(u_0, v_0) = 1$. That is, G is a complete graph. □

The adjacency matrix of a graph G, denoted by $A(G)$, is the matrix $(a_{uv})_{u,v \in V(G)}$, where $a_{uv} = 1$ if u and v are adjacent and 0 otherwise. The largest eigenvalue of $A(G)$ is denoted by $\mu(G)$, which is known as the index or the spectral radius of G. It is well known that $\mu(G)$ is less than or equal to the maximum degree of G.

We may restate Corollary 2.2 in [12, p. 38] as follows:

Lemma 2.2. *Let B and C be $n \times n$ nonnegative matrices, where B is irreducible, $B - C$ is nonnegative and $B \neq C$. Then $\rho(B) > \rho(C)$.*

For an $n \times n$ nonnegative matrix M, it is known that $\mu(M) \le \max\{r_i : i = 1, \dots, n\}$ with equality when M is irreducible if and only if $r_1 = \dots = r_n$, where r_i is the i-th row sum of M for $i = 1, \dots, n$, see [12].

Let G be a noncomplete connected graph with $V(G) = \{v_1, \dots, v_n\}$. A real column vector $x = (x_{v_1}, \dots, x_{v_n})^\top$ can be considered as a function defined on $V(G)$ that maps vertex v_i to x_{v_i}, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \dots, n$. Then

$$x^\top \Lambda(G) x = \sum_{\{u,v\} \subseteq V(G)} 2(d(G) - d_G(u,v)) x_u x_v.$$

As $\Lambda(G)$ is a nonnegative irreducible matrix by Lemma 2.1, we have by the well known Perron-Frobenius theorem that $\rho(G)$ is simple and positive, and there is a unique positive unit eigenvector corresponding to $\rho(G)$, which we call the Λ-*vector* of G. If x is the Λ-vector of G, then we have the Λ-*eigenequation* of G for any vertex $u \in V(G)$,

$$\rho(G) x_u = \sum_{v \in V(G) \setminus \{u\}} (d(G) - d_G(u,v)) x_v.$$

If $y \in \mathbb{R}^n$ is a unit column vector and y contains at least one positive entry, then we have by Rayleigh's principle that

$$\rho(G) \ge y^\top \Lambda(G) y,$$

where the equality holds if and only if y is the Λ-vector of G.

Lemma 2.3. *Suppose that G is a connected noncomplete graph. Let u and v be two distinct vertices of G, and σ be an automorphism of G satisfying $\sigma(u) = v$. Then for the Λ-Perron vector x of G, $x_u = x_v$.*

Proof. Obviously, $\rho(G) = x^\top \Lambda(G) x$ since x is the Λ-Perron vector of G. Let P be the permutation matrix corresponding to the automorphism σ of G, i.e., the (u,v)-entry of P is 1 if and only if $\sigma(u) = v$ for $u, v \in V(G)$. Then $\Lambda(G) = P\Lambda(G)P^\top$. As $x^\top \Lambda(G) x = x^\top P \Lambda(G) P^\top x$, we have $\rho(G) = (P^\top x)^\top \Lambda(G) P^\top x$. Note that $P^\top x$ is also unite and positive. So $P^\top x$ is also the Λ-vector of G. Therefore $P^\top x = x$. Hence, if $\sigma(u) = v$, then $x_u = x_v$. $\square$

Let G be a graph. For a vertex $u \in V(G)$, the set of the vertices adjacent to u in G is denoted by $N_G(u)$, the degree of u in G is denoted by $\deg_G(u)$, i.e., $\deg_G(u) = |N_G(u)|$. Let $G - u$ be the subgraph of G obtained by deleting u and all edges incident to u. For $\emptyset \ne S \subset V(G)$, $G[S]$ denotes the subgraph of G induced by S. For a graph G, $\overline{G}$ denotes the complement of G. If $E_1 \subseteq E(\overline{G})$, then $G + E_1 = (V(G), E(G) \cup E_1)$, and if $E_1 \subseteq E(G)$, then $G - E_1 = (V(G), E(G) \setminus E_1)$. If $E_1 = \{uv\}$, then we write $G + uv$ or $G - uv$ for $G + E_1$ or $G - E_1$.

A *diametral path* in a connected graph G is any shortest path between vertices u and v such that $d_G(u,v)$ is equal to the diameter of G. A *caterpillar* is a tree in which the removal of each vertex of degree one outside a diametral path (if any exists) yields a path.

Let $D_{n,a}$ be a double star obtained by adding an edge between the centers of S_{a+1} and S_{n-a-1}, where $1 \le a \le \lfloor \frac{n-2}{2} \rfloor$.

Lemma 2.4. *For integers n and a with $n \ge 4$ and $1 \le a \le \lfloor \frac{n-2}{2} \rfloor$, the following statements are true.*

(i) *$\rho(D_{n,a})$ is the largest root of $f_{n,a}(t) = 0$, where*

$$\begin{aligned} f_{n,a}(t) = {} & t^4 - (n-4)t^3 - (6n - an + a^2 + 2a - 9)t^2 \\ & - (9n - 10an + 10a^2 + 20a - 10)t - 4n + 21an - 21a^2 - 42a + 4. \end{aligned}$$

(ii) *If* $a \geq 2$*, then* $\rho(D_{n,a-1}) > \rho(D_{n,a})$.

Proof. Let $u_1u_2u_3u_4$ be a path of length 3 in $D_{n,a}$, where u_2 is of degree $a+1$. Let x be the Λ-vector of $D_{n,a}$ and let $\rho_{n,a} = \rho(D_{n,a})$. By Lemma 2.3, the entry of x corresponding to each vertex of $N_{D_{n,a}}(u_2) \setminus \{u_3\}$ ($N_{D_{n,a}}(u_3) \setminus \{u_2\}$, respectively) is the same. Then by the Λ-eigenequations of $D_{n,a}$ for u_1, u_2, u_3 and u_4, we have

$$\begin{pmatrix} \rho_{n,a} - (a-1) & -2 & -1 & 0 \\ -2a & \rho_{n,a} & -2 & -(n-a-2) \\ -a & -2 & \rho_{n,a} & -2(n-a-2) \\ 0 & -1 & -2 & \rho_{n,a} - (n-a-3) \end{pmatrix} \begin{pmatrix} x_{u_1} \\ x_{u_2} \\ x_{u_3} \\ x_{u_4} \end{pmatrix} = 0.$$

As $x \neq 0$, the above system of homogeneous linear equations in the variables $x_{u_1}, x_{u_2}, x_{u_3}, x_{u_4}$ has a nontrivial solution. So the determinant of its coefficient matrix is zero. By direct calculation, the determinant is equal to $f_{n,a}(\rho_{n,a})$. Thus $\rho_{n,a}$ is the largest root of $f_{n,a}(t) = 0$. This proves Item (i).

For $a \geq 2$,we have

$$f_{n,a-1}(t) - f_{n,a}(t) = -(n-2a-1)(t+7)(t+3).$$

So $f_{n,a-1}(\rho_{n,a}) = f_{n,a-1}(\rho_{n,a}) - f_{n,a}(\rho_{n,a}) < 0$. Together with the fact that $f_{n,a-1}(t) \geq 0$ for $t \geq \rho_{n,a-1}$, it implies that $\rho_{n,a-1} > \rho_{n,a}$. This proves Item (ii). $\square$

For a tree T, if it is not a star, then $\overline{T}$ is connected, and if $d(T) \geq 3$, then $d\left(\overline{T}\right) \leq 3$.

Lemma 2.5. *For integers* n *and* a *with* $n \geq 4$ *and* $1 \leq a \leq \lfloor \frac{n-2}{2} \rfloor$*, the following statements are true.*

(i) $\rho\left(\overline{D_{n,a}}\right)$ *is the largest root of* $h_{n,a}(t) = 0$*, where*

$$\begin{aligned} h_{n,a}(t) = {} & t^4 - (2n-8)t^3 - (9n-22)t^2 + (4an - 10n - 4a^2 - 8a + 20)t \\ & + 9an - 9a^2 - 18a. \end{aligned}$$

(ii) *If* $a \geq 2$*, then* $\rho\left(\overline{D_{n,a-1}}\right) > \rho\left(\overline{D_{n,a}}\right)$.

(iii) $\rho\left(\overline{D_{n,\lfloor (n-2)/2 \rfloor}}\right) > n$.

Proof. Obviously, $d\left(\overline{D_{n,a}}\right) = 3$. Let $u_1u_2u_3u_4$ be a path of length 3 in $D_{n,a}$, where u_2 is of degree $a+1$. Let x be the Λ-vector of $\overline{D_{n,a}}$ and let $\mu_{n,a} = \rho\left(\overline{D_{n,a}}\right)$. By Lemma 2.3, the entry of x corresponding to each vertex of $N_{\overline{D_{n,a}}}(u_2) \setminus \{u_3\}$ ($N_{\overline{D_{n,a}}}(u_3) \setminus \{u_2\}$, respectively) is the same. Then by the Λ-eigenequations of $\overline{D_{n,a}}$ for u_1, u_2, u_3 and u_4, we have

$$\begin{pmatrix} \mu_{n,a} - 2(a-1) & -1 & -2 & -2(n-a-2) \\ -a & \mu_{n,a} & 0 & -2(n-a-2) \\ -2a & 0 & \mu_{n,a} & -(n-a-2) \\ -2a & -2 & -1 & \mu_{n,a} - 2(n-a-3) \end{pmatrix} \begin{pmatrix} x_{u_1} \\ x_{u_2} \\ x_{u_3} \\ x_{u_4} \end{pmatrix} = 0.$$

As each entry of x is not zero, the above homogeneous linear system in the variables $x_{u_1}, x_{u_2}, x_{u_3}, x_{u_4}$ has a nontrivial solution. So the determinant of its coefficient matrix is zero. By direct calculation, the determinant is equal to $h_{n,a}(\mu_{n,a})$. Thus $\mu_{n,a}$ is the largest root of $h_{n,a}(t) = 0$. This proves Item (i).

For $a \geq 2$, we have

$$h_{n,a-1}(t) - h_{n,a}(t) = -(n-2a-1)(4t+9).$$

So $h_{n,a-1}(\mu_{n,a}) = h_{n,a-1}(\mu_{n,a}) - h_{n,a}(\mu_{n,a}) < 0$. Together with the fact that $h_{n,a-1}(t) \geq 0$ for $t \geq \mu_{n,a-1}$, it implies that $\mu_{n,a-1} > \mu_{n,a}$. This proves Item (ii).

As

$$\begin{aligned} h_{n,\lfloor (n-2)/2 \rfloor}(n) &= \begin{cases} -\frac{(2n^2-3n-18)(2n^2+3n+2)}{4} & \text{if } n \text{ is even} \\ -\frac{(20n^4-201n^2-272n-123)}{20} & \text{if } n \text{ is odd} \end{cases} \\ &< 0, \end{aligned}$$

we have $\rho\left(\overline{D_{n,\lfloor (n-2)/2 \rfloor}}\right) > n$. This proves Item (iii). □

3 Main results

If G is a connected graph on n vertices that is not complete, then, by Lemma 2.1, $\Lambda(G)$ is irreducible. We have by Lemma 2.2 that $\rho(G) > \rho(K_n) = 0$ as $\Lambda(K_n)$ is an zero matrix. That is, for a connected graph G of order n, $\rho(G) \geq 0$ with equality if and only if G is the complete graph.

Theorem 3.1. *Let G be a connected graph of order n with diameter at least two. Then $\rho(G) \geq \mu(G)$ with equality if and only if the diameter of G is two.*

Proof. Denote by d the diameter of G. Then $d \geq 2$. By Lemma 2.1, $\Lambda(G)$ is irreducible. Note that the (u, v)-entry of $\Lambda(G) - A(G)$ is

$$\begin{cases} d-2 & \text{if } u \neq v \text{ and } uv \in E(G) \\ d - d_G(u,v) & \text{if } u \neq v \text{ and } uv \notin E(G) \\ 0 & \text{if } u = v \end{cases}$$

for $u, v \in V(G)$. So $\Lambda(G) - A(G)$ is nonnegative and it is the zero matrix if and only if $d = 2$. Thus, by Lemma 2.2, we have $\rho(G) \geq \mu(G)$ with equality if and only if $d = 2$. □

Let G be a connected graph of order n with diameter at least two. Then by [6, Corollary 2.9] and the remarks following [6, Corollary 2.6], we have $\rho(G) = \mu(G) \geq \sqrt{n-1}$ with equality if and only if G is isomorphic to S_n or one of the Moore graphs of diameter two: C_5, the Petersen graph, the Hoffman-Singleton graph, and the putative 57-regular graphs on 3250 nodes.

In what follows we determine the trees that minimize and maximize the reverse distance spectral radius over all trees of fixed order.

Let G be a connected graph with $u \in V(G)$. The *eccentricity* of u in G, denoted by $e_G(u)$ is the maximum distance from u to any other vertex in G. A *center* of a tree is a vertex with minimum eccentricity.

Lemma 3.2. *Let T be a tree of order n with diameter $d \geq 4$. Then there is a tree T' with diameter $d-2$ such that $\rho(T') < \rho(T)$.*

Proof. Let u be a center of T, and let $N_T(u) = \{u_1, \dots, u_s\}$, where $s = \deg_T(u)$. For $1 \le i \le s$, let T_i be the component of $T - u$ containing u_i, and let $V_i = V(T_i) \setminus \{u_i\}$ and $N_i = N_G(u_i) \setminus \{u\}$, where $i = 1, \dots, s$. As $d \ge 4$, there are two nonempty sets among the sets $N_1, \dots, N_s$. It is evident that $N_i \subseteq V_i$ for $i = 1, \dots, s$. Let

$$T' = T - \cup_{i=1}^s \{u_i w : w \in N_i\} + \{uw : w \in \cup_{i=1}^s N_i\}.$$

As u is a center of T, it lies on any diametral path of T, so u is a center of T' and T' is a tree of order n with diameter $d-2$. As we pass from T to T', the distance between a vertex of V_i and a vertex of V_j with $1 \le i < j \le s$ is decreased by 2, the distance between a vertex of V_i with $1 \le i \le s$ and u is decreased by 1, the distance between a vertex of V_i with $1 \le i \le s$ and u_i is increased by 1, the distance between a vertex of V_i with $1 \le i \le s$ and u_j with $1 \le j \le s$ and $j \ne i$ is decreased by 1, and the distances between other vertex pairs remain unchanged. Correspondingly, we have

$$\begin{aligned}(\Lambda(T))_{w,z} - (\Lambda(T'))_{w,z} &= 2 - (d_T(w,z) - d_{T'}(w,z)) \\ &= \begin{cases} 0 & \text{if } w \in V_i, z \in V_j, 1 \le i < j \le s, \\ 1 & \text{if } w \in V_i, z = u, 1 \le i \le s, \\ 3 & \text{if } w \in V_i, z = u_i, 1 \le i \le s, \\ 1 & \text{if } w \in V_i, z = u_j, 1 \le i, j \le s, j \ne i, \\ 2 & \text{otherwise.} \end{cases}\end{aligned}$$

Therefore $\rho(T) > \rho(T')$ by Lemma 2.2. □

Theorem 3.3. *Let T be a tree of order n. Then $\rho(T) \ge \sqrt{n-1}$ with equality if and only if $T \cong S_n$.*

Proof. It is known that $\rho(S_n) = \mu(S_n) = \sqrt{n-1}$. The result is trivial if $n \le 3$. If $n = 4$, then $T \in \{S_n, P_n\}$, and by calculation, $\rho(S_n) = \sqrt{3} \approx 1.732 < 4.162 \approx \rho(P_n)$. So the result follows for $n = 4$.

Suppose that $n \ge 5$. Let T be the tree on n vertices that minimizes the reverse distance spectral radius. Let d be the diameter of T. Then by Lemma 3.2, $d = 2, 3$. Suppose that $d = 3$. Then $T \cong D_{n,a}$, where $1 \le a \le \left\lfloor \frac{n-2}{2} \right\rfloor$. By Lemma 2.4 (ii), $T \cong D_{n,\lfloor (n-2)/2 \rfloor}$. From the expression for $f_{n,\lfloor (n-2)/2 \rfloor}(t)$ given in Lemma 2.4 (i), we have

$$\begin{aligned} f_{n,\lfloor (n-2)/2 \rfloor}\left(\frac{n-1}{2}\right) &= \begin{cases} -(n+13)(n-1) & \text{if } n \text{ is odd} \\ -\frac{3}{16}(n+13)(5n-7) & \text{if } n \text{ is even} \end{cases} \\ &< 0. \end{aligned}$$

From this, together with the fact that $f_{n,\lfloor (n-2)/2 \rfloor}(\lambda) \ge 0$ for $\lambda \ge \rho\left(D_{n,\lfloor (n-2)/2 \rfloor}\right)$, we have $\rho(T) = \rho\left(D_{n,\lfloor (n-2)/2 \rfloor}\right) > \frac{n-1}{2} \ge \rho(S_n)$, a contradiction. Therefore $d = 2$, i.e., $T \cong S_n$. □

Next, we propose a local transformation on a connected graph that increases the reverse distance spectral radius.

Lemma 3.4. *Let G be a graph with three induced subgraphs G_1, G_2 and G_3 such that $|V(G_i)| \ge 2$ for $i = 1, 2, 3$, $V(G_i) \cap V(G_j) = \{u\}$ for $1 \le i < j \le 3$ and $\cup_{i=1}^3 V(G_i) = V(G)$, see Fig. 1. Suppose that v is the unique neighbor of u in G_3. Let $G' = G - \{uw : w \in N_{G_2}(u) \setminus \{v\}\} + \{vw : w \in N_{G_2}(u) \setminus \{v\}\}$. If $d(G') = d(G) + 1$, then $\rho(G) < \rho(G')$.*

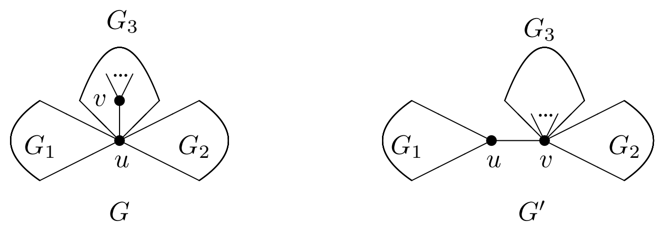

Fig. 1. The graphs G and G' in Lemma 3.4.

Proof. Let $A_i = V(G_i) \setminus \{u\}$ for $i = 1, 2, 3$. As we pass from G to G', the distance between a vertex of A_2 and a vertex of A_3 is decreased by 1, the distance between a vertex of A_2 and a vertex of $A_1 \cup \{u\}$ is increased by 1, and the distances between other vertex pairs remain unchanged. As $d(G') = d(G) + 1$, we have

$$\begin{aligned}(\Lambda(G'))_{wz} - (\Lambda(G))_{wz} &= 1 - (d_{G'}(w,z) - d_G(w,z)) \\ &= \begin{cases} 2 & \text{if } w \in A_2, z \in A_3, \\ 0 & \text{if } w \in A_2, z \in A_1 \cup \{u\}, \\ 1 & \text{otherwise.} \end{cases}\end{aligned}$$

Therefore $\rho(G') > \rho(G)$ by Lemma 2.2. □

Corollary 3.5. *Let T be a caterpillar of order n with diameter $d \geq 3$. If $T \ncong P_n$, then there is a tree T' with diameter $d + 1$ such that $\rho(T') > \rho(T)$.*

Proof. Let $P = v_0 v_1 \dots v_d$ be a path of length d in T. Suppose that i with $1 \leq i \leq d - 1$ is the smallest index such that $\deg_T(v_i) \geq 3$. Let v_i' be a neighbor of v_i outside the path P. Construct a tree $T' = T - \{v_i w : w \in N_T(v_i) \setminus \{v_i', v_{i-1}\}\} + \{v_i' w : w \in N_T(v_i) \setminus \{v_i', v_{i-1}\}\}$. Obviously, the diameter of T' is $d + 1$. Then by Lemma 3.4, $\rho(T') > \rho(T)$. □

Theorem 3.6. *For integer $n \geq 5$, let T be a tree of order n. Then $\rho(T) \leq \rho(P_n)$ with equality if and only if $T \cong P_n$.*

Proof. Let T be the tree on n vertices with maximum reverse distance spectral radius. Let $P = u_0 u_1 \dots u_d$ be a diametral path of T, where $d \geq 3$. Assume that i with $1 \leq i \leq d - 1$ is the maximum number such that $\deg_T(u_i) \geq 3$. Let v be a neighbor of u_i outside P. Let $T' = T - \{u_i w : w \in N_T(u_i) \setminus \{u_{i-1}, v\}\} + \{vw : w \in N_T(u_i) \setminus \{u_{i-1}, v\}\}$. Note that $d(T') = d(T) + 1$. By Lemma 3.4, $\rho(T') > \rho(T)$, a contradiction. Thus the degree of u_i for each $1 \leq i \leq d - 1$ is 2. Therefore $T \cong P_n$. □

For integers n, i with $n \geq 3$ and $1 \leq i \leq \lfloor \frac{n}{2} \rfloor$, let $P_{n,i}$ be the tree obtained from a path $u_1 u_2 \dots u_{n-1}$ by adding a new edge incident to u_i. Obviously, $P_{n,1} = P_n$.

For integer $n \geq 5$, let T be a tree that maximizes the reverse distance spectral radius over all trees of order n that is not the path. By the same argument as in the proof of Theorem 3.6, T is a caterpillar. Let d be the diameter of T. Since $T \ncong P_n$, we have $d \leq n - 2$. By Lemma 3.4 or Corollary 3.5, we have $d = n - 2$, implying that $T \cong P_{n,i}$ for some i with $2 \leq i \leq \lceil \frac{n-1}{2} \rceil$. For $n = 6$, $\rho(P_{n,2}) \approx 10.0496$, $\rho(P_{n,3}) \approx 9.7374$; for $n = 7$, $\rho(P_{n,2}) \approx 15.3187$, $\rho(P_{n,3}) \approx 15.6637$; for $n = 8$, $\rho(P_{n,2}) \approx 22.9053$, $\rho(P_{n,3}) \approx 23.6338$, $\rho(P_{n,4}) \approx 23.8893$; for $n = 9$, $\rho(P_{n,2}) \approx 31.4756$, $\rho(P_{n,3}) \approx 32.3361$, $\rho(P_{n,4}) \approx 32.7955$. So, we conjecture that $P_{n,\lfloor n/2\rfloor}$ is the only tree with the second largest reverse distance spectral radius over all trees on $n \geq 5$ vertices.

Now we turn to consider the reverse distance spectral radius of the complement of a non-star tree.

Lemma 3.7. *Suppose that ℓ is a positive integer and T_1 and T_2 are vertex disjoint nontrivial trees with $u_i \in V(T_i)$ for $i = 1, 2$. Denote by $F_{u_1,u_2;\ell}$ the tree obtained from T_1 and T_2 by connecting u_1 and u_2 with a path of length ℓ, and $H_{u_1,u_2;\ell}$ the tree obtained from T_1, T_2 and a path P of length ℓ with $V(P) \cap V(T_i) = \emptyset$ for $i = 1, 2$ by identifying u_1, u_2 and a terminal vertex of P, which is denoted by u_1, and the other terminal vertex is denoted by u_2, see Fig. 2. If $d(F_{u_1,u_2;\ell}) \geq 4$ and $d(H_{u_1,u_2;\ell}) \geq 3$, then $\rho\left(\overline{F_{u_1,u_2;\ell}}\right) < \rho\left(\overline{H_{u_1,u_2;\ell}}\right)$.*

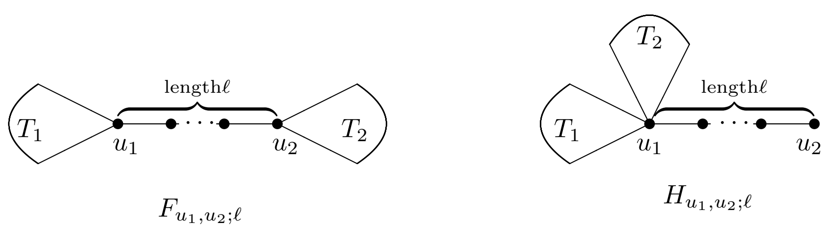

Fig. 2. The trees F and H in Lemma 3.7.

Proof. Let $F = F_{u_1,u_2;\ell}$ and $H = H_{u_1,u_2;\ell}$. Let x be the Λ-vector of $\overline{F}$. Suppose that $x_{u_1} \leq x_{u_2}$. Let $T = F - \{u_2 w : w \in N_{T_2}(u_2)\} + \{u_1 w : w \in N_{T_2}(u_2)\}$. Then $T \cong H$.

Suppose that $d(T) = 3$. Then T is a double star, and by Lemma 2.5 (iii), $|V(F)| < \rho\left(\overline{T}\right)$. As $d(F) \geq 4$, we have $d\left(\overline{F}\right) = 2$. Since $\rho\left(\overline{F}\right)$ is bounded above by the maximum row sum of $\Lambda(\overline{T})$, we have $\rho\left(\overline{F}\right) \leq |V(F)| - 2 < \rho\left(\overline{T}\right)$, as desired.

Suppose that $d(T) \geq 4$. Obviously, $d\left(\overline{F}\right) = d\left(\overline{T}\right) = 2$. It is easy to see that

$$\frac{1}{2}\left(\rho\left(\overline{T}\right) - \rho\left(\overline{F}\right)\right) \geq \frac{1}{2} x^\top \left(\Lambda\left(\overline{T}\right) - \Lambda\left(\overline{F}\right)\right) x = \sum_{w \in N_{T_2}(u_2)} x_w (x_{u_2} - x_{u_1}) \geq 0,$$

so $\rho\left(\overline{T}\right) \geq \rho\left(\overline{F}\right)$. If $\rho\left(\overline{T}\right) = \rho\left(\overline{F}\right)$, then $\rho\left(\overline{T}\right) = x^\top \Lambda\left(\overline{T}\right) x$, and thus x is also the Λ-Perron vector of $\overline{T}$. Then

$$0 = \rho\left(\overline{T}\right) x_{u_1} - \rho\left(\overline{F}\right) x_{u_1} = -\sum_{w \in N_{T_2}(u_2)} x_w < 0,$$

which is a contradiction. Therefore $\rho\left(\overline{F}\right) < \rho\left(\overline{T}\right) = \rho\left(\overline{H}\right)$. □

Let G be a nontrivial graph with a vertex u, and ℓ a positive integer. Let P be a path of length ℓ such that G and P are vertex disjoint. Denote by $G_u(\ell)$ the graph obtained from G by identifying u and a terminal vertex of P. In this case, we say that $G_u(\ell)$ is obtained from G by adding a hanging path of length ℓ at u. For integers $\ell, s \geq 1$, let $G_u(\ell, s) = (G_u(\ell))_u(s)$.

Corollary 3.8. *Let G be a nontrivial tree with $u \in V(G)$, and ℓ, s be positive integers. If $d(G_u(\ell, s)) \geq 3$, then $\rho\left(\overline{G_u(\ell + s)}\right) < \rho\left(\overline{G_u(\ell, s)}\right)$.*

Proof. We use the notations of Lemma 3.7. Let $T_1 = G$, $u_1 = u$, $T_2 = P_{s+1}$ with u_2 being a terminal vertex. Then $F_{u_1,u_2;\ell} \cong G_u(\ell + s)$, and $H_{u_1,u_2;\ell} \cong G_u(\ell, s)$. As $d(G_u(\ell, s)) \geq 3$, we have $d(G_u(\ell + s)) \geq 4$. The result follows from Lemma 3.7. □

Theorem 3.9. *For integer $n \geq 5$, let T be a non-star tree on n vertices for which the complement minimizes the reverse distance spectral radius. Then T is the path.*

Proof. Let d be the diameter of T. Obviously, $d \geq 3$. Suppose that $d = 3$. Then $T \cong D_{n,a}$ for some a with $1 \leq a \leq \lfloor \frac{n-2}{2} \rfloor$. So, by Lemma 2.5 (ii), $a = \lfloor \frac{n-2}{2} \rfloor$, i.e., $T \cong D_{n,\lfloor (n-2)/2 \rfloor}$. By Lemma 2.5 (iii), $\rho(\overline{T}) > n$. Let T_0 be any tree of order n with diameter at least 4. It is evident that the maximum degree of $\overline{T_0}$ is $n-2$. So $\rho(\overline{T_0}) = \mu(\overline{T_0}) \leq n-2 < n < \rho(\overline{T})$, a contradiction. It thus follows that $d \geq 4$.

Let u be a vertex of maximum degree in T. Suppose that $\deg_T(u) \geq 3$. Suppose that there is at least two vertices of degree at least 3 in T. Choose a vertex, say v of degree at least 3, such that $d_T(u, v)$ is as large as possible. It follows that there are two hanging paths P and Q at v. Let ℓ and s be the lengths of P and Q, respectively, where $\ell, s \geq 1$. Then $T \cong G_v(\ell, s)$, where $G = T[V(T) \setminus (V(P \cup Q) \setminus \{v\})]$. Evidently, $d(G_v(\ell, s)) \geq 4$. By Corollary 3.8, we have $\rho\left(\overline{G_v(\ell + s)}\right) < \rho\left(\overline{G_v(\ell, s)}\right) = \rho(\overline{T})$, a contradiction. Thus there is exactly one vertex of degree at least 3 in T. That is, T consists of $\deg_T(u)$ hanging paths at u. Let P' and Q' be two hanging paths at u, say of lengths ℓ' and s', respectively such that ℓ' is as long as possible. Then $T \cong G_u(\ell', s')$, where $G = T[V(T) \setminus (V(P' \cup Q') \setminus \{u\})]$. Note that $d(G_u(\ell', s')) \geq 4$. By Corollary 3.8, we have $\rho\left(\overline{G_u(\ell' + s')}\right) < \rho\left(\overline{G_u(\ell', s')}\right) = \rho(\overline{T})$, a contradiction. Thus $\deg_T(u) = 2$. Therefore $T \cong P_n$. □

Theorem 3.10. *For $n \geq 4$ and $k = 1, \ldots, \lfloor \frac{n-2}{2} \rfloor$, $D_{n,k}$ is the unique tree on n vertices for which the complement achieves the k-th largest reverse distance spectral radius.*

Proof. Let d be the diameter of T. Obviously, $d \geq 3$. If $d = 3$, then $T \cong D_{n,k}$, where $1 \leq k \leq \left\lfloor \frac{n-2}{2} \right\rfloor$. Suppose that $d \geq 4$. Then the diameter of $\overline{T}$ is two, so $\rho\left(\overline{T}\right) = \mu\left(\overline{T}\right) \leq n-2$ as the maximum degree of $\overline{T}$ is $n-2$. So, by Lemma 2.5 (iii), $\rho\left(\overline{T}\right) < \rho\left(\overline{D_{n,\lfloor (n-2)/2 \rfloor}}\right)$. Now the result follows from Lemma 2.5 (ii). □

4 Concluding remarks

In this article, we study the reverse distance spectral radius (i.e., the largest eigenvalue of the reverse distance matrix) of a connected graph, which is a molecular descriptor with applications [14]. Among others, we show that, over all n-vertex trees, the star is the unique one with the smallest reverse distance spectral radius, while the path is the unique one with the largest reverse distance spectral radius. So, the reverse distance spectral radius satisfies the most important requirement being a branching index [9] used to measure the structural branching of molecules [13].

As next step work, one may study the extremal problems over other classes of graphs or other reverse distance eigenvalues, and also the relationship between the reverse distance eigenvalues and other distance based graph invariants such as reverse Wiener index, proximity, and remoteness [17, 2].

There is a matrix called the complementary distance matrix in chemistry that is formed similarly as the reversed Wiener matrix, see, e.g. [11]. For a connected graph G, the *complementary distance matrix* $C(G)$ is an $n \times n$ matrix $(C(G))_{ij}$ such that $(C(G))_{ij} = d(G) + 1 - d_G(i, j)$ if $i \neq j$, and 0 otherwise. That is, $C(G) = \Lambda(G) + J_n - I_n$ with $n = |V(G)|$. Note that each non-diagonal entry of $C(G)$ is positive. By similar argument as above, quite similar results (on the extremal graphs) follow for the largest eigenvalue of the complementary distance matrix.

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