

ON GRAFT TRANSFORMATIONS DECREASING DISTANCE SPECTRAL RADIUS OF GRAPHS

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Abstract. The distance spectral radius of a connected graph is the largest eigenvalue of its distance matrix. In this paper, we give several less restricted graft transformations that decrease the distance spectral radius, and determine the unique graph with minimum distance spectral radius among homeomorphically irreducible unicyclic graphs on $n \geq 6$ vertices, and the unique tree with minimum distance spectral radius among trees on n vertices with given number of vertices of degree two, respectively.

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1. INTRODUCTION

We consider simple, finite, undirected and connected graphs. For $u \in V(G)$, let $N_G(u)$ be the set of neighbors of u in G . The degree of a vertex u in G , denoted by $\deg_G(u)$, is the number of edges incident to u in G .

A *homeomorphically irreducible tree* is a tree with no vertex of degree two [6]. A *homeomorphically irreducible unicyclic graph* is a unicyclic graph with no vertex of degree two.

Let G be a connected graph on n vertices. For $u, v \in V(G)$, the *distance* between u and v in G , denoted by $d_G(u, v)$, is the length of a shortest path connecting them in G . In particular, $d_G(u, u) = 0$. The *distance spectrum* of G is the spectrum of the *distance matrix* of G , defined as the n by n symmetric matrix $D(G) = (d_G(u, v))_{u, v \in V(G)}$. The *distance spectral radius* of G , denoted by $\rho(G)$, is the largest distance eigenvalue of G . Graham and Pollack [5] studied the distance spectrum for the first time due to its connection to a data communication problem. Now the distance spectrum has been studied extensively, see the survey [1]. Particularly, the distance spectral radius has received much attention. Graphs with minimum and/or maximum distance spectral radius have been determined for some classes of graphs, see, *e.g.*, [2, 7, 11–15]. Yu *et al.* [16] determined the graphs with minimum and maximum distance spectral radius among unicyclic graphs. Lin and Zhou [8] determined the trees with maximum distance spectral radius among trees on n vertices with given number of vertices of degree two.

To determine the structure of the graphs with minimum or maximum distance spectral radius in some class of graphs, we usually suppose the graph does not have the structure and perform surgery to obtain a graph for

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which the distance spectral radius is decreased or increased. Such surgery is known as *graft transformation(s)* in the literature, see, *e.g.*, [3, 4, 9, 14, 16].

In this paper, we propose some graft transformations in a more elaborate way. We propose some graft transformations with less restricted conditions that decrease the distance spectral radius, and as applications, we identify the unique graphs that minimize the distance spectral radius among homeomorphically irreducible unicyclic graphs on $n \geq 6$ vertices, and among trees on n vertices with given number of vertices of degree two, respectively.

2. PRELIMINARIES

Let G be a connected graph with $V(G) = \{v_1, \dots, v_n\}$. Since $D(G)$ is irreducible, by Perron–Frobenius theorem, $\rho(G)$ is simple and there is a unique unit positive eigenvector corresponding to $\rho(G)$, which is called the *distance Perron vector* of G , denoted by $x(G)$. If $y = (y_{v_1}, \dots, y_{v_n})^\top \in \mathbb{R}^n$ is unit and has at least one nonnegative entry, then by Rayleigh's principle, we have $\rho(G) \geq y^T D(G)y$ with equality if and only if $y = x(G)$. If $x = x(G)$, then for each $u \in V(G)$, we have $\rho(G)x_u = \sum_{v \in V(G)} d_G(u, v)x_v$, which is called the *distance eigenequation* of G at u .

Let $N \subseteq (N_G(u) \setminus N_G(v)) \setminus \{v\}$. Let $G' = G - uw + vw$ for $w \in N$. We say that G' is obtained from G by moving edge uw at u from u to v .

For a connected graph G with $V_1 \subseteq V(G)$, let $\sigma_G(V_1)$ be the sum of the entries of the distance Perron vector of G corresponding to the vertices in V_1 . Furthermore, if all the vertices of V_1 induce a connected subgraph H of G , then we write $\sigma_G(H)$ instead of $\sigma_G(V_1)$.

A *component* of a graph is a maximal connected subgraph, and a *cut edge* is an edge of a graph whose removal increases the number of components of the graph.

For a connected graph G , let $s(G)$ be the minimum row sum of $D(G)$. In [17], $\frac{s(G)}{n}$ is called the mean vertex deviation of G , where $n = |V(G)|$. It is known that $\rho(G) \geq s(G)$, see Theorem 1.1 in page 24 of [10].

3. GRAFT TRANSFORMATIONS THAT DECREASE THE DISTANCE SPECTRAL RADIUS

Firstly, we give a result related to (the entries of) the distance Perron vector, which will be frequently used in the subsequent proofs.

Lemma 3.1. *Suppose that v, w be two non-adjacent neighbors of vertex u in a connected graph G . Let $x = x(G)$. Then $x_w + x_u - x_v > 0$.*

Proof. Let $V_1 = V(G) \setminus \{u, v, w\}$. For $z \in V_1$, one has $d_G(w, z) \geq 1$ and $d_G(u, z) - d_G(v, z) \geq -d_G(u, v) = -1$, so $d_G(w, z) + d_G(u, z) - d_G(v, z) \geq 0$. From the distance eigenequations of G at w , u and v , we have

$$\begin{aligned} \rho(G)x_w &= x_u + 2x_v + \sum_{z \in V_1} d_G(w, z)x_z, \\ \rho(G)x_u &= x_w + x_v + \sum_{z \in V_1} d_G(u, z)x_z, \\ \rho(G)x_v &= 2x_w + x_u + \sum_{z \in V_1} d_G(v, z)x_z. \end{aligned}$$

Thus

$$\begin{aligned} \rho(G)(x_w + x_u - x_v) &= -x_w + 3x_v + \sum_{z \in V_1} (d_G(w, z) + d_G(u, z) - d_G(v, z))x_z \\ &\geq -x_w + 3x_v, \end{aligned}$$

which implies $(\rho(G) + 1)(x_w + x_u - x_v) \geq x_u + 2x_v > 0$. So it follows that $x_w + x_u - x_v > 0$. \square

Now we turn our attention to some graft transformations that decrease the distance spectral radius.

Theorem 3.2. *Let G be a graph consisting of nontrivial connected graphs G_1 and G_2 sharing a unique vertex u such that $E(G) = E(G_1) \cup E(G_2)$. Suppose that u has neighbor v of degree at least two in G_2 satisfying that, for any $z \in V(G_2) \setminus \{u, v\}$, $d_G(u, z) \neq d_G(v, z)$. Let G' be the graph obtained from G by moving all the edges at v except uv from v to u . Then $\rho(G) > \rho(G')$.*

Proof. Let w be a neighbor of u in G_1 . Let $x = x(G')$. By Lemma 3.1, we have $x_w + x_u - x_v > 0$.

Let $S = \{z \in V(G_2) \setminus \{u, v\} : d_G(u, z) - d_G(v, z) = 1\}$. Let z be a neighbor of v in G_2 different from u . As $d_G(u, z) \neq d_G(v, z) = 1$ and $d_G(u, z) \leq d_G(v, z) + d_G(u, v) = 2$, one has $d_G(u, z) = 2$. So $z \in S$ and $S \neq \emptyset$.

Claim. $\frac{1}{2}x^\top(D(G) - D(G'))x \geq \sigma_{G'}(S)(\sigma_{G'}(G_1) - x_v)$.

Note first that, as we pass from G to G' , the distance between a vertex of S and a vertex of $V(G_1)$ is decreased by 1, and the distance between a vertex of S and v is increased by 1. So, to prove the claim, we need only to show that the distance between any other vertex pairs is decreased or remains unchanged.

It is evident that the distance between any two vertices in $V(G_1) \cup \{v\}$ remains unchanged as we pass from G to G' .

Suppose that $z_1, z_2 \in V(G_2) \setminus \{u, v\}$. Let P be a path from z_1 to z_2 with length $d_G(z_1, z_2)$ in G . If v lies outside P , then P is also a path connecting z_1 and z_2 in G' . Suppose that v lies on P . If u lies outside P , then the path obtained from P by replacing v with u is a path connecting z_1 and z_2 in G' . Otherwise, u lies on P . In this case, uv appears to be an edge on P . So the path obtained from P by deleting v is a path connecting z_1 and z_2 in G' . So the distance between any two vertices in $V(G_2) \setminus \{u, v\}$ is decreased or remains unchanged as we pass from G to G' .

Suppose that $z \in \bar{S} := (V(G_2) \setminus \{u, v\}) \setminus S$ (if $\bar{S} \neq \emptyset$). Then $d_G(u, z) - d_G(v, z) \neq 0, 1$. As $|d_G(u, z) - d_G(v, z)| \leq d_G(u, v) = 1$, one has $d_G(u, z) - d_G(v, z) = -1$. Let P be a path from u to z with length $d_G(u, z)$ in G . Then v lies outside P , so P is also a path from u to z in G' . Therefore, the distance between a vertex in \bar{S} and a vertex in $V(G_1) \cup \{v\}$ is decreased or remains unchanged as we pass from G to G' .

Now we complete the proof of the claim. As $\rho(G) \geq x^\top D(G)x$ and $\rho(G') = x^\top D(G')x$, one has $\rho(G) - \rho(G') \geq x^\top(D(G) - D(G'))x$. So, by the claim,

$$\begin{aligned} \frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2}x^\top(D(G) - D(G'))x \\ &\geq \sigma_{G'}(S)(\sigma_{G'}(G_1) - x_v) \\ &\geq \sigma_{G'}(S)(x_w + x_u - x_v) \\ &> 0, \end{aligned}$$

and thus $\rho(G) > \rho(G')$. □

In the following, we give some consequences of Theorem 3.2.

Corollary 3.3 ([14]). *Let G be a connected graph with a cut edge uv that is not a pendant edge. Let G' be the graph obtained from G by moving all edges at v except uv from v to u . Then $\rho(G) > \rho(G')$.*

Proof. Let G_1 be the component of $G - uv$ containing u and G_2 be the subgraph of G induced by $V(G) \setminus (V(G_1) \setminus \{u\})$. Note that $d_G(u, z) = d_G(v, z) + 1$ for any $z \in V(G_2) \setminus \{u, v\}$. So the result follows from Theorem 3.2. □

A chain in a graph G is a cycle C such that $G - E(C)$ has exactly $|V(C)|$ components. Length of the cycle C is the length of the chain. The following is Lemma 3.3 of [3].

Corollary 3.4. *Let G be a connected graph with a chain C of even length. Let uv be an edge on the chain C . Suppose that $\deg_G(u) \geq 3$. If $G' = G - \{vw : w \in N_G(v) \setminus \{u\}\} + \{uw : w \in N_G(v) \setminus \{u\}\}$, then $\rho(G) > \rho(G')$.*

Proof. Let G_1 be the component of $G - E(C)$ containing u , and G_2 be the subgraph of G induced by $V(G) \setminus (V(G_1) \setminus \{u\})$. Let $z \in V(G_2) \setminus \{u, v\}$. Note that $d_G(u, z) - d_G(v, z) = d_G(u, w) - d_G(v, w)$ for some w on C . If z lies on C , this is evident as $w = z$, otherwise, w is the vertex on C such that its distance to z is minimum among all the distances between vertices of C and z in G . As C is a chain, the shortest path connecting u (v , respectively) and w contains only vertices on C . As the length of C is even, there is a shortest path connecting u and w passing through v or a shortest path connecting v and w passing through u , implying that $|d_G(u, w) - d_G(v, w)| = 1$, so $d_G(u, z) \neq d_G(v, z)$. So the result follows from Theorem 3.2. \square

Corollary 3.5. *Let H be a graph consisting of two nontrivial connected graphs H_1 and H_2 sharing a unique vertex u such that $E(H) = E(H_1) \cup E(H_2)$. Suppose that uv_1, \dots, uv_k are pendant edges in H_1 , where $k \geq 1$ and that $N_{H_2}(u) = N_1 \cup N_2$, where $N_1, N_2 \neq \emptyset$ and $N_1 \cap N_2 = \emptyset$. Let*

$$G = H - \{uw : w \in N_1\} + \{v_k w : w \in N_1\}$$

or

$$G = H - \{uw : w \in N_2\} + \{v_k w : w \in N_2\}.$$

For any vertex $w \in V(H_2) \setminus \{u\}$, if all the paths from u to w with the length $d_H(u, w)$ pass only through vertices in N_1 or pass only through vertices in N_2 , then $\rho(G) > \rho(H)$.

Proof. Assume that $G = H - \{uw : w \in N_2\} + \{v_k w : w \in N_2\}$. Then H is obtainable from G by moving all the edges at v_k except uv_k from v_k to u . Let $G_1 = H_1 - v_k$ and let G_2 be the subgraph of G induced by $V(H_2) \cup \{v_k\}$. Suppose that $z \in V(G_2) \setminus \{u, v_k\}$, i.e., $z \in V(H_2) \setminus \{u\}$. Note that any shortest path from u to z in H_2 goes through only vertices in N_1 or N_2 . Correspondingly, any shortest path from u to z in G_2 goes through only vertices in N_1 , so $d_G(u, z) = d_G(v_k, z) - 1 < d_G(v_k, z)$, or any shortest path from u to z in G_2 goes through only vertices in N_2 , so $d_G(u, z) = d_G(v_k, z) + 1 > d_G(v_k, z)$. Now by Theorem 3.2, $\rho(G) > \rho(H)$. \square

If $k \geq 2$, then Corollary 3.5 becomes Theorem 2.4 of [16].

Corollary 3.3 may be generalized as the following version.

Theorem 3.6. *Let G be the graph obtained from vertex disjoint nontrivial connected graphs G_1 and G_2 with $u \in V(G_1)$ and $v \in V(G_2)$ by adding a path $P_t = v_1 \dots v_t$ with $v_1 = u$ and $v_t = v$, where $t \geq 2$, $V(G_1) \cap V(P_t) = \{v_1\}$ and $V(G_2) \cap V(P_t) = \{v_t\}$. Let G' be the graph obtained from G by moving all the edges at v_t in $E(G_2)$ from v_t to v_1 . Then $\rho(G) > \rho(G')$.*

Proof. Let $x = x(G')$. Let $p = \lfloor \frac{t}{2} \rfloor$ and $p_1 = \lceil \frac{t}{2} \rceil$.

Let $\Gamma = \sum_{i=1}^p x_{v_i} + \sigma_{G'}(V(G_1) \setminus \{v_1\}) + \sigma_{G'}(V(G_2) \setminus \{v_t\}) - \sum_{i=p_1+1}^t x_{v_i}$.

From the distance eigenequations of G' at v_{p_1+1} and v_p , we have

$$\rho(G') (x_{v_{p_1+1}} - x_{v_p}) = (p_1 + 1 - p)\Gamma. \quad (3.1)$$

For $i = 1, \dots, p-1$, from the distance eigenequations of G' at v_{t+1-i} , v_i , $v_{t+1-(i+1)}$ and v_{i+1} , we have

$$\begin{aligned} & \rho(G') ((x_{v_{t+1-i}} - x_{v_i}) - (x_{v_{t+1-(i+1)}} - x_{v_{i+1}})) \\ &= \rho(G') (x_{v_{t+1-i}} - x_{v_i}) - \rho(G') (x_{v_{t+1-(i+1)}} - x_{v_{i+1}}) \\ &= 2 \left(\sum_{j=1}^i x_{v_j} + \sigma_{G'}(V(G_1) \setminus \{v_1\}) + \sigma_{G'}(V(G_2) \setminus \{v_t\}) - \sum_{j=t+1-i}^t x_{v_j} \right) \\ &= 2\Gamma - 2 \sum_{j=i+1}^p x_{v_j} + 2 \sum_{j=p_1+1}^{t-i} x_{v_j} \end{aligned}$$

$$= 2\Gamma + 2 \sum_{j=i+1}^p (x_{v_{t+1-j}} - x_{v_j}). \quad (3.2)$$

We claim that $x_{v_{t+1-i}} - x_{v_i}$ and Γ have common sign for $i = 1, \dots, p$ by induction on i . If $i = p$, then it follows from (3.1). Suppose that $1 \leq i \leq p-1$, and $x_{v_{t+1-j}} - x_{v_j}$ and Γ have common sign for $i+1 \leq j \leq p$. So $\sum_{j=i+1}^p (x_{v_{t+1-j}} - x_{v_j})$ and Γ have common sign. Thus, from (3.2), $(x_{v_{t+1-i}} - x_{v_i}) - (x_{v_{t+1-(i+1)}} - x_{v_{i+1}})$ and Γ have common sign. This, together with the induction assumption that $x_{v_{t+1-(i+1)}} - x_{v_{i+1}}$ and Γ have common sign, implies that $x_{v_{t+1-i}} - x_{v_i}$ and Γ have common sign.

Note that

$$\Gamma > \sum_{i=1}^p x_{v_i} - \sum_{i=p+1}^t x_{v_i} = - \sum_{i=1}^p (x_{v_{t+1-i}} - x_{v_i}).$$

This requires the above common sign to be $+$. Again, from (3.1) and (3.2), we have $x_{v_{t+1-i}} - x_{v_i} > x_{v_{t+1-(i+1)}} - x_{v_{i+1}} > 0$ for $i = 1, \dots, p-1$, *i.e.*, $0 < x_{v_{t+1-i}} - x_{v_i} < x_{v_{t+2-i}} - x_{v_{i-1}}$ for $i = 2, \dots, p$. It follows that for $i = 2, \dots, p$,

$$0 < x_{v_{t+1-i}} - x_{v_i} < x_{v_t} - x_{v_1}. \quad (3.3)$$

As $P_t = v_1 \dots v_t$ is a proper induced subgraph of G' and $d_{P_t}(v_i, v_j) = d_{G'}(v_i, v_j)$ for any $1 \leq i < j \leq t$, we have $s(G') > s(P_t)$. Note that $\rho(G') \geq s(G')$ ([10], Thm. 1.1 in p. 24) and $s(P_t) = \left\lfloor \frac{t^2}{4} \right\rfloor$ [17]. So

$$\rho(G') \geq s(G') > s(P_t) = \left\lfloor \frac{t^2}{4} \right\rfloor. \quad (3.4)$$

As we pass from G to G' , the distance between a vertex of $V(G_2) \setminus \{v_t\}$ and a vertex of $V(G_1) \setminus \{v_1\}$ is decreased by $t-1$, the distance between a vertex of $V(G_2) \setminus \{v_t\}$ and v_i for $i = 1, \dots, t$ is decreased by $t-2i+1$, and the distances between all other vertex pairs remain unchanged. Let $A = (t-1)\sigma_{G'}(V(G_1) \setminus \{v_1\}) + \sum_{i=1}^p (t-2i+1)(x_{v_i} - x_{v_{t+1-i}})$, *i.e.*,

$$A = (t-1)\sigma_{G'}(V(G_1) \setminus \{v_1\}) + \sum_{i=1}^t (t-2i+1)x_{v_i}.$$

So

$$\begin{aligned} \frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2}x^\top (D(G) - D(G'))x \\ &= \sigma_{G'}(V(G_2) \setminus \{v_t\}) \left((t-1)\sigma_{G'}(V(G_1) \setminus \{v_1\}) + \sum_{i=1}^t (t-2i+1)x_{v_i} \right) \\ &= \sigma_{G'}(V(G_2) \setminus \{v_t\}) \cdot A. \end{aligned} \quad (3.5)$$

Let G^* be the graph obtained from G by moving all the edges at v_1 in $E(G_1)$ from v_1 to v_t . Let $y = x(G^*)$. Let $B = (t-1)\sigma_{G^*}(V(G_2) \setminus \{v_t\}) + \sum_{i=1}^p (t-2i+1)(y_{v_{t+1-i}} - y_{v_i})$, *i.e.*,

$$B = (t-1)\sigma_{G^*}(V(G_2) \setminus \{v_t\}) - \sum_{i=1}^t (t-2i+1)y_{v_i}.$$

By the similar arguments as above, we have

$$\frac{1}{2}(\rho(G) - \rho(G^*)) \geq \frac{1}{2}y^\top (D(G) - D(G^*))y$$

$$\begin{aligned}
&= \sigma_{G^*}(V(G_1) \setminus \{v_1\}) \left((t-1)\sigma_{G^*}(V(G_2) \setminus \{v_t\}) - \sum_{i=1}^t (t-2i+1)y_{v_i} \right) \\
&= \sigma_{G'}(V(G_1) \setminus \{v_1\}) \cdot B.
\end{aligned} \tag{3.6}$$

It is evident that $\phi : V(G') \rightarrow V(G^*)$ defined by

$$\phi(w) = \begin{cases} w & \text{if } w \in V(G_1) \setminus \{u\} \text{ or } w \in V(G_2) \setminus \{v\}, \\ v_{t+1-i} & \text{if } w = v_i \text{ with } i = 1, \dots, t \end{cases}$$

is an isomorphism from G' to G^* . Let M be the permutation matrix associated to this isomorphism. That is, the nonzero entries of M are $M_{ww} = 1$ if $w \in V(G_1) \setminus \{u\}$ or $w \in V(G_2) \setminus \{v\}$, $M_{v_iv_{t+1-i}} = 1$ for $i = 1, \dots, t$. Then $M^T D(G') M = D(G^*)$. As $\rho(G') = x^\top D(G') x = (Mx)^\top D(G^*) Mx$, Mx is the distance Perron vector of G^* and so $y = Mx$ by the Perron–Frobenius theorem. That is, $y_w = x_w$ if $w \in V(G_1) \setminus \{u\}$ or $w \in V(G_2) \setminus \{v\}$, and $y_{v_i} = x_{v_{t+1-i}}$. Then $B = (t-1)\sigma_{G'}(V(G_2) \setminus \{v_t\}) + \sum_{i=1}^p (t-2i+1)(x_{v_i} - x_{v_{t+1-i}})$. From the distance eigenequations of G' at v_t and v_1 , we have

$$\begin{aligned}
\rho(G')(x_{v_t} - x_{v_1}) &= (t-1)(\sigma_{G'}(V(G_1) \setminus \{v_1\}) + \sigma_{G'}(V(G_2) \setminus \{v_t\})) \\
&\quad + \sum_{i=1}^p (t-2i+1)(x_{v_i} - x_{v_{t+1-i}}) \\
&= A + B - \sum_{i=1}^p (t-2i+1)(x_{v_i} - x_{v_{t+1-i}}) \\
&= A + B + \sum_{i=1}^p (t-2i+1)(x_{v_{t+1-i}} - x_{v_i}).
\end{aligned}$$

Then, by (3.3) and (3.4), we have

$$\begin{aligned}
A + B &= \rho(G')(x_{v_t} - x_{v_1}) - \sum_{i=1}^p (t-2i+1)(x_{v_{t+1-i}} - x_{v_i}) \\
&\geq \rho(G')(x_{v_t} - x_{v_1}) - \sum_{i=1}^p (t-2i+1)(x_{v_t} - x_{v_1}) \\
&= \left(\rho(G') - \sum_{i=1}^p (t-2i+1) \right) (x_{v_t} - x_{v_1}) \\
&= \left(\rho(G') - \left\lfloor \frac{t^2}{4} \right\rfloor \right) (x_{v_t} - x_{v_1}) \\
&> 0.
\end{aligned}$$

Thus $A > 0$ or $B > 0$. Now the result follows from (3.5) and (3.6). \square

Now we present the third graft transformation and consider its effect on the distance spectral radius.

Theorem 3.7. *Let G be a graph consisting of two nontrivial connected graphs G_1 and G_2 sharing a unique vertex u such that $E(G) = E(G_1) \cup E(G_2)$. Suppose that $N_{G_2}(u) = \{v_1, v_2\}$, $\deg_{G_2}(v_i) \geq 2$ for $i = 1, 2$, v_1 and v_2 are not adjacent, and for any $w \in V(G_2) \setminus \{u\}$, $d_{G_2}(v_1, w) \neq d_{G_2}(v_2, w)$. Let G' be the graph obtained from G by moving all the edges at v_i except uv_i from v_i to u for each $i = 1, 2$. Then $\rho(G) > \rho(G')$.*

Proof. For $i = 1, 2$, let $S_i = \{z \in V(G_2) \setminus \{v_i\} : d_{G_2}(u, z) - d_{G_2}(v_i, z) = 1\}$. As $\deg_{G_2}(v_i) \geq 2$, one has $S_i \neq \emptyset$ for $i = 1, 2$. As $d_{G_2}(v_1, w) \neq d_{G_2}(v_2, w)$ for any $w \in V(G_2) \setminus \{u\}$, one has $S_1 \cap S_2 = \emptyset$.

Choose $w \in N_{G_1}(u)$. Let $x = x(G')$, then by Lemma 3.1, we have $x_w + x_u - x_{v_i} > 0$ for $i = 1, 2$.

As we pass from G to G' , for $i = 1, 2$, the distance between a vertex of S_i and a vertex of $V(G_1)$ is decreased by 1, the distance between a vertex of S_i and v_i is increased by 1, and the distance between any other vertex pair is decreased or remains unchanged. So

$$\begin{aligned} \frac{1}{2}(\rho(G) - \rho(G')) &\geq \frac{1}{2}x^\top(D(G) - D(G'))x \\ &\geq \sum_{i=1}^2 \sigma_{G'}(S_i)(\sigma_{G'}(G_1) - x_{v_i}) \\ &\geq \sum_{i=1}^2 \sigma_{G'}(S_i)(x_w + x_u - x_{v_i}) \\ &> 0, \end{aligned}$$

and thus $\rho(G) > \rho(G')$. \square

The following is Lemma 3.4 of [3].

Corollary 3.8. *Let G be a connected graph with a chain C of odd length ℓ , where $\ell \geq 5$. Let uv_1 and uv_2 be two edges on the chain C . Suppose that $\deg_G(u) \geq 3$. If $G' = G - \{v_1w : w \in N_G(v_1) \setminus \{u\}\} - \{v_2w : w \in N_G(v_2) \setminus \{u\}\} + \{uw : w \in (N_G(v_1) \cup N_G(v_2)) \setminus \{u\}\}$, then $\rho(G) > \rho(G')$.*

Proof. Let G_1 be the component of $G - E(C)$ containing u , and G_2 be the subgraph of G induced by $V(G) \setminus (V(G_1) \setminus \{u\})$. Let $w \in V(G_2) \setminus \{u\}$. Denote by z the vertex on C such that its distance to w is minimum among all vertices of C . It is evident that $z = w$ if w lies on C . Then $d_G(v_1, w) - d_G(v_2, w) = d_G(v_1, z) - d_G(v_2, z)$. As C is a chain, the shortest path connecting v_1 (v_2 , respectively) and z contains only vertices on C . Let P (Q , respectively) be the shortest path connecting v_1 (v_2 , respectively) and z in G . If P and Q are edge disjoint, then $d_G(v_1, z) + d_G(v_2, z) = \ell - 2$, and as ℓ is odd, we have $d_G(v_1, z) \neq d_G(v_2, z)$. Otherwise, $|d_G(v_1, z) - d_G(v_2, z)| = d_G(v_1, v_2) = 2$, so $d_G(v_1, z) \neq d_G(v_2, z)$. In either case, $d_G(v_1, w) \neq d_G(v_2, w)$. So the result follows from Theorem 3.7. \square

Corollary 3.9. *Let H be a graph consisting of two nontrivial connected graphs H_1 and H_2 sharing a unique vertex u such that $E(H) = E(H_1) \cup E(H_2)$. Suppose that uv_1, \dots, uv_k are pendant edges in H_1 , where $k \geq 2$ and that $N_{H_2}(u) = N_1 \cup N_2$, where $N_1, N_2 \neq \emptyset$ and $N_1 \cap N_2 = \emptyset$. Let*

$$G = H - \{uw : w \in N_{H_2}(u)\} + \{v_{k-1}w : w \in N_1\} + \{v_kw : w \in N_2\}.$$

For any vertex $w \in V(H_2) \setminus \{u\}$, if all the paths from u to w with length $d_G(u, w)$ pass only through N_1 or pass only through N_2 , then $\rho(G) > \rho(H)$.

Proof. Let $G_1 = H_1 - \{v_{k-1}, v_k\}$ and let G_2 be the subgraph of G induced by $V(H_2) \cup \{v_{k-1}, v_k\}$. Suppose that $z \in V(G_2) \setminus \{u\}$, i.e., $z \in (V(H_2) \setminus \{u\}) \cup \{v_{k-1}, v_k\}$. Note that any shortest path from u to z in H_2 goes through only vertices in N_1 or N_2 . Correspondingly, any shortest path from u to z in G_2 goes through only vertices in N_1 or N_2 . Consequently, $d_G(v_{k-1}, z) \neq d_G(v_k, z)$. Now by Theorem 3.7, $\rho(G) > \rho(H)$. \square

We remark that Corollary 3.9 and Theorem 3.7 are equivalent. If $k \geq 3$, then Corollary 3.9 is just Theorem 2.3 of [16].

4. GRAPHS MINIMIZING THE DISTANCE SPECTRAL RADIUS

First we determine the graphs that minimize the distance spectral radius among all homeomorphically irreducible unicyclic graphs on $n \geq 6$ vertices.

Lemma 4.1 ([9]). *For $k \geq 2$ and $1 \leq a_1 \leq a_2 - 2$, let G be a graph obtained from a connected graph G_0 with two vertices u_1 and u_2 such that $N_{G_0}(u_1) \setminus \{u_2\} \subseteq N_{G_0}(u_2) \setminus \{u_1\}$, by attaching a_i pendant vertices to u_i for each $i = 1, 2$. Let G' be the graph obtained from G by moving one pendant edge at u_2 from u_2 to u_1 . Then $\rho(G) < \rho(G')$.*

Let U_n be a unicyclic graph on n vertices obtained from a triangle K_3 with $V(K_3) = \{v_1, v_2, v_3\}$, by attaching a pendant vertex to v_i for $i = 1, 2$, respectively, and attaching $n - 5$ pendant vertices to v_3 .

Theorem 4.2. *Let G be a homeomorphically irreducible unicyclic graph on $n \geq 6$ vertices. Then $\rho(G) \geq \rho(U_n)$ with equality if and only if $G \cong U_n$.*

Proof. Let G be a homeomorphically irreducible unicyclic graph on n vertices that minimizes the distance spectral radius.

Let g be the girth of the unique cycle C of G . Let u be a vertex on C . Since G is a homeomorphically irreducible unicyclic graph, we have $\deg_G(u) \geq 3$. Let v_1, v_2 be two neighbors of u on C .

Suppose that $g \geq 4$. Suppose that g is even. Let G' be the graph obtained from G by moving all the edges at v_1 except uv_1 from v_1 to u . Note that G' is a homeomorphically irreducible unicyclic graph on n vertices. By Theorem 3.2 or Corollary 3.4, $\rho(G') < \rho(G)$, a contradiction. Thus g is odd. Let G'' be the graph obtained from G by moving all the edges at v_i except uv_i from v_i to u for each $i = 1, 2$. Obviously, G'' is a homeomorphically irreducible unicyclic graph on n vertices. By Theorem 3.7 or Corollary 3.8, we have $\rho(G'') < \rho(G)$, also a contradiction. It thus follows that $g = 3$.

Suppose that G has an edge, say vw , outside C that is not a pendant edge. Evidently, vw is a cut edge of G . Let G^* be the graph obtained from G by moving all the edges at w except vw from w to v . It is obvious that G^* is a homeomorphically irreducible unicyclic graph on n vertices. By Theorem 3.2 or Corollary 3.3, $\rho(G^*) < \rho(G)$, a contradiction. Thus, every edge of G outside C is a pendant edge. That is, G is a unicyclic graph obtainable from a triangle K_3 with $V(K_3) = \{v_1, v_2, v_3\}$ by attaching a_i pendant vertices to v_i for $i = 1, 2, 3$, where $1 \leq a_1 \leq a_2 \leq a_3$.

If $n = 6, 7$, then $G \cong U_n$.

Suppose that $n \geq 8$ and $a_2 \geq 2$. Let \tilde{G} be the graph obtained from G by moving one pendant edge at v_2 from v_2 to v_3 . Obviously, \tilde{G} is a homeomorphically irreducible unicyclic graph on n vertices. By Lemma 4.1, $\rho(\tilde{G}) < \rho(G)$, a contradiction. So $a_2 = 1$. That is, $a_1 = a_2 = 1$ and $a_3 = n - 5$, i.e., $G \cong U_n$. \square

In the following, we determine the trees that minimize the distance spectral radius among all trees on n vertices with given number of vertices of degree two.

Let G be a connected graph with $v \in V(G)$. For $k, \ell \geq 0$, let $G(v, k, \ell)$ be the graph obtained from G by attaching two paths P_k and P_ℓ at one end vertices to v . The following lemma was established in [13], for which a simple argument was given in [15].

Lemma 4.3. *Let G be a connected graph with $v \in V(G)$. If $k \geq \ell \geq 1$, then $\rho(G(v, k, \ell)) < \rho(G(v, k+1, \ell-1))$.*

A tree is called starlike if it has exactly one vertex of degree at least three; this vertex is called the branching vertex. If the branch vertex has degree s , we call it an s -starlike tree. For an s -starlike tree T on n vertices with branching vertex u , each path connecting u and a pendant vertex is called a leg. Denote by a_1, \dots, a_s the lengths of the s legs of T . Then $a_1 + \dots + a_s = |E(T)| = n - 1$. Assume that $a_1 \geq \dots \geq a_s$. If $a_1 - a_s = 0, 1$, then the multiset $\{a_1, \dots, a_s\}$ composes of $\lfloor \frac{n-1}{s} \rfloor + 1$ with multiplicity r and $\lfloor \frac{n-1}{s} \rfloor$ with multiplicity $s - r$, where $r = n - 1 - s \lfloor \frac{n-1}{s} \rfloor$. In this case, we call it an s -starlike tree of almost equal leg lengths, denoted by $S_{n,s}$.

Let T be a tree on n vertices with t vertices of degree two. If $t = n - 2$, then $T \cong P_n$. Note that $t = n - 3$ is impossible, since T has at least two pendant vertices, and the remaining unique vertex has degree $2(n - 1) - 2(n - 3) - 1 \cdot 2 = 2$.

Theorem 4.4. *Let T be a tree on n vertices with t vertices of degree two, where $0 \leq t \leq n - 4$. Then $\rho(T) \geq \rho(S_{n,n-t-1})$ with equality if and only if $T \cong S_{n,n-t-1}$.*

Proof. Let T be a tree on n vertices with t vertices of degree two that minimizes the distance spectral radius. Since $0 \leq t \leq n - 4$, the maximum degree of T is at least three.

Suppose that there are at least two vertices of degree at least three in T . Then we choose two such vertices, say u and v , by requiring that the distance between them is as small as possible. Let P be the path connecting u and v . If u and v are not adjacent, then each vertex on P except u and v has degree two. Let w be the vertex adjacent to v on P ($w = u$ if u and v are adjacent). Let T' be the tree obtained from T by moving all the edges at v except wv from v to u . It is easily seen that T' possesses t vertices of degree two. By Theorem 3.6, $\rho(T') < \rho(T)$, a contradiction. Thus, T has exactly one vertex of degree at least three. That is, T is an s -starlike tree for some s . Assume a_1, \dots, a_s are the lengths of the legs, where $a_1 \geq \dots \geq a_s$. Then $\sum_{i=1}^s a_i = n - 1$ and $\sum_{i=1}^s (a_i - 1) = t$. So $s = n - t - 1$. By Lemma 4.3, $a_1 - a_{n-t-1} = 0, 1$. That is, T is an $(n - t - 1)$ -starlike tree of almost equal leg lengths, or $T \cong S_{n,n-t-1}$. \square

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