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EXTREMAL UNICYCLIC GRAPHS WITH MINIMAL DISTANCE SPECTRAL RADIUS[1]

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Abstract

The distance spectral radius $\rho(G)$ of a graph G is the largest eigenvalue of the distance matrix $D(G)$. Let $\mathscr{U}(n,m)$ be the class of unicyclic graphs of order n with given matching number m ($m \neq 3$). In this paper, we determine the extremal unicyclic graph which has minimal distance spectral radius in $\mathscr{U}(n,m) \setminus C_n$.

Keywords: distance matrix, distance spectral radius, unicyclic graph, matching.

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1. Introduction

Let $G = (V(G), E(G))$ be a connected simple graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$. Denote by $|E(G)|$ the size of G. A connected graph G is called a unicyclic graph if $|E(G)| = n$. For vertices $v_i, v_j \in V(G)$, the distance $d_G(v_i, v_j)$ is defined as the length of the shortest path between v_i and v_j in G. Let $D(G) = (d_{ij})_{v_i,v_j \in V(G)}$ be the distance matrix of G, where $d_{ij} = d_G(v_i, v_j)$. Since $D(G)$ is a symmetric real matrix, its eigenvalues are real.

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The maximum eigenvalue of $D(G)$ is called the distance spectral radius of G, denoted by $\rho(G)$.

As demonstrated by Consonni and Todeschini [5], the distance spectral radius is a useful molecular descriptor in QSPR modeling, for example, it was successfully used to infer the extent of branching and model boiling points of alkanes [6]. Therefore, the study of the distance spectral radius is of great interest and significance. An important direction is to determine the graphs with maximal or minimal distance spectral radius in a given class of graphs. In [13, 14], the authors provided the upper and lower bounds for $\rho(G)$ in terms of the number of vertices. Stevanović *et al.* [10] characterized the unique tree with fixed maximum degree that maximizes the distance spectral radius. In [7], Ilić attained the extremal tree with given matching number which minimizes the distance spectral radius. Yu *et al.* [11] obtained the extremal unicyclic graphs which have maximal and minimal distance spectral radius, respectively. For more details on distance spectral radius one may refer to [2, 3, 8, 12, 1, 9] and references therein.

Let $\mathscr{U}(n, m)$ be the class of unicyclic graphs of order n with given matching number m. In this paper, we will determine the extremal unicyclic graph which has minimal distance spectral radius in $\mathscr{U}(n, m)$.

In order to discuss our results, we first introduced some terminology and notation. For other undefined notation, we may refer to [4]. Denote by P_n and C_n the path and the cycle on n vertices, respectively. Let $N_G(v)$ be the neighbor set of the vertex v in G. Set $N_G[v] = N_G(v) \cup \{v\}$. The degree of v in G, denoted by $d_G(v)$, is equal to $|N_G(v)|$, i.e. the order of $N_G(v)$. Let $x = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})$ be the Perron eigenvector of $D(G)$ corresponding to the spectral radius $\rho(G)$, in which x_{v_i} corresponds to v_i.

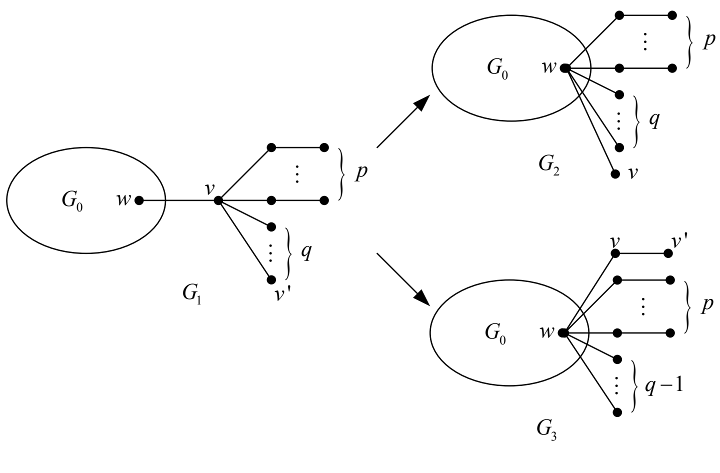

Figure 1. The graphs G_1, G_2, G_3.

2. The Transformations

Let G_0 be a nontrivial connected graph and wv its pendent edge, where $d_{G_0}(v) = 1$. Let G_1 be the graph obtained from G_0 by attaching p paths P_3 and q paths P_2 at v, where $p, q \geq 1$. Denote by G_2 the graph obtained from G_1 by removing p paths P_3 and q paths P_2 at v to w, and by G_3 the graph obtained from G_1 by removing p paths P_3 and $q-1$ paths P_2 at v to w, respectively (as shown in Figure 1).

Lemma 2.1. *Let G_0 be a unicyclic graph and G_i $(i = 1, 2, 3)$ be graphs as shown in Figure 1. Then $\rho(G_1) > \rho(G_i)$ for $i = 2, 3$.*

Proof. Let $V(G_1) = A \cup B \cup C \cup \{v\}$, where $A = \{v | v \in V(P_3 - v)$, P_3 is the pendent path attached at v in $G_1\}$, $B = \{v | v \in V(P_2 - v)$, P_2 is the pendent edge attached at v in $G_1\}$, $C = V(G_0)$. Let $A = A_1 \cup A_2$, where A_1 is the set of pendent vertices of G_1 in A and $A_2 = A - A_1$. Obviously, $V(G_1) = V(G_2)$.

Let x be the Perron vector of G_2. Using a symmetry, we can denote the coordinates of x corresponding to vertices in A_1 with b, in A_2 with a, and in B with c, respectively. By the Rayleigh quotient we have

$$\begin{aligned}
&\rho(G_1) - \rho(G_2) \geq x^T(D(G_1) - D(G_2))x \\
&= \textstyle\sum_{i \in V(G_1)} \sum_{j \in V(G_1)} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j \\
&= \textstyle\sum_{i \in C} \Big[\sum_{j \in C} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j + \sum_{j \in A} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j \\
&+ \textstyle\sum_{j \in B} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j + (d_{iv}(G_1) - d_{iv}(G_2)) x_i x_v \Big] \\
&+ \textstyle\sum_{i \in A} \Big[\sum_{j \in C} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j + \sum_{j \in A} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j \\
&+ \textstyle\sum_{j \in B} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j + (d_{iv}(G_1) - d_{iv}(G_2)) x_i x_v \Big] \\
&+ \textstyle\sum_{i \in B} \Big[\sum_{j \in C} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j + \sum_{j \in A} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j \\
&+ \textstyle\sum_{j \in B} (d_{ij}(G_1) - d_{ij}(G_2)) x_i x_j + (d_{iv}(G_1) - d_{iv}(G_2)) x_i x_v \Big] \\
&+ \textstyle\Big[\sum_{j \in C} (d_{vj}(G_1) - d_{vj}(G_2)) x_v x_j + \sum_{j \in A} (d_{vj}(G_1) - d_{vj}(G_2)) x_v x_j \\
&+ \textstyle\sum_{j \in B} (d_{vj}(G_1) - d_{vj}(G_2)) x_v x_j \Big] \\
&= 2 \left(\textstyle\sum_{i \in A} x_i + \sum_{i \in B} x_i \right) \left(\textstyle\sum_{j \in C} x_j - x_v \right).
\end{aligned}$$

By $D(G_2)x = \rho(G_2)x$, we have

$$\begin{aligned}
\rho(G_2)x_v &= \textstyle\sum_{i \in C} (d_{iw} + 1) x_i + 2pa + 3pb + 2qc, \\
\rho(G_2)x_w &= \textstyle\sum_{i \in C} d_{iw} x_i + pa + 2pb + (q+1)c,
\end{aligned}$$

since G_0 is a unicyclic graph and then $|V(G_0)| \geq 3$. Let $w', w'' \in V(G_0 - w)$.

Then

$$\rho(G_2)x_{w'} > \sum_{i\in C} d_{iw'}x_i + pa + 2pb + (q+1)c,$$
$$\rho(G_2)x_{w''} > \sum_{i\in C} d_{iw''}x_i + pa + 2pb + (q+1)c,$$

hence

$$\rho(G_2)(x_w + x_{w'} + x_{w''}) > \sum_{i\in C}(d_{iw}+1)x_i + 3pa + 6pb + 3(q+1)c > \rho x_v.$$

Note that $\sum_{j\in C} x_j \geq x_w + x_{w'} + x_{w''} > x_v$. Then $\rho(G_1) > \rho(G_2)$.

Similarly, let x be the Perron vector of G_3. By symmetry, we can set the coordinates of x corresponding to vertices in $A_1 \cup \{v'\}$ with b, in $A_2 \cup \{v\}$ with a, and in $B - v'$ with c, respectively. Then

$$\begin{aligned}\rho(G_1) - \rho(G_3) \geq & x^T(D(G_1) - D(G_3))x \\ = & \sum_{i\in V(G_1)} \sum_{j\in V(G_1)} (d_{ij}(G_1) - d_{ij}(G_2))x_i x_j \\ = & 2\left(\sum_{i\in A} x_i + \sum_{i\in B-v'} x_i\right)\left(\sum_{j\in C} x_j - x_v - x_{v'}\right) \\ = & 2\left(\sum_{i\in A} x_i + \sum_{i\in B-v'} x_i\right)\left(\sum_{j\in C} x_j - a - b\right).\end{aligned}$$

Obviously, if $\sum_{j\in C} x_j - a - b > 0$, then $\rho(G_1) > \rho(G_3)$.

Assume that $\sum_{j\in C} x_j - a - b \leq 0$. For a vertex $u \in C - w$, let $V_1 = \{v \in C | d_{G_0}(v,u) = d_{G_0}(v,w)\}, V_2 = \{v \in C | d_{G_0}(v,u) > d_{G_0}(v,w)\}, V_3 = \{v \in C | d_{G_0}(v,u) < d_{G_0}(v,w)\}$. Then $C = V_1 \cup V_2 \cup V_3$. From the eigenvalue equation $D(G_3)x = \rho(G_3)x$, we have

$$\rho(G_3)a = \sum_{i\in C}(d_{iw}+1)x_i + b + 2pa + 3pb + 2(q-1)c, \tag{2.1}$$

$$\rho(G_3)b = \sum_{i\in C}(d_{iw}+2)x_i + a + 3pa + 4pb + 3(q-1)c, \tag{2.2}$$

$$\rho(G_3)x_w = \sum_{i\in C} d_{iw}x_i + (p+1)a + 2(p+1)b + (q-1)c, \tag{2.3}$$

and

$$\begin{aligned}\rho(G_3)x_u = & \sum_{i\in V(G_0)} d_{iu}x_i + (d(u,w)+1)(p+1)a + (d(u,w)+2)(p+1)b \\ & + (q-1)(d(u,w)+1)c = \sum_{i\in V_1} d_{iu}x_i + \sum_{i\in V_2} d_{iu}x_i + \sum_{i\in V_3} d_{iu}x_i \\ & + (d_{uw}+1)(p+1)a + (d_{uw}+2)(p+1)b + (q-1)(d_{uw}+1)c \\ & > \sum_{i\in V_1} d_{iw}x_i + \sum_{i\in V_2} d_{iw}x_i + \sum_{i\in V_3} d_{iu}x_i + (d_{uw}+1)(p+1)a \\ & + (d_{uw}+2)(p+1)b + (q-1)(d_{uw}+1)c = \sum_{i\in V_1} d_{iw}x_i + \sum_{i\in V_2} d_{iw}x_i\end{aligned}$$

$$
\begin{aligned}
&+ \sum\nolimits_{i\in V_3}(d_{iu}+d_{uw})x_i - \sum\nolimits_{i\in V_3} d_{uw}x_i + (d_{uw}+1)(p+1)a \\
&+ (d_{uw}+2)(p+1)b + (q-1)(d_{uw}+1)c \geq \sum\nolimits_{i\in V_1} d_{iw}x_i + \sum\nolimits_{i\in V_2} d_{iw}x_i \\
&+ \sum\nolimits_{i\in V_3} d_{iw}x_i - \sum\nolimits_{i\in V_3} d_{uw}x_i + (d_{uw}+1)(p+1)a + (d_{uw}+2)(p+1)b \\
&+ (q-1)(d_{uw}+1)c > \sum\nolimits_{i\in C} d_{iw}x_i - d_{uw}\sum\nolimits_{i\in G_0} x_i + (d_{uw}+1)(p+1)a \\
&+ (d_{uw}+2)(p+1)b + (q-1)(d_{uw}+1)c \;\geq\; \sum\nolimits_{i\in C} d_{iw}x_i - d_{uw}(a+b) \\
&+ (d_{uw}+1)(p+1)a + (d_{uw}+2)(p+1)b + (q-1)(d_{uw}+1)c \\
&= \sum\nolimits_{i\in C} d_{iw}x_i + (a+b) + (1+d_{uw})pa + (2+d_{uw})pb + b \\
&+ (q-1)(d_{uw}+1)c.
\end{aligned}
$$

Finally,

$$
\begin{aligned}
\rho(G_3)x_u \;&\geq\; \textstyle\sum_{i\in C} d_{iw}x_i + \sum_{i\in C} x_i + (1+d_{uw})pa \\
&+\; (2+d_{uw})pb + b + (q-1)(d_{uw}+1)c.
\end{aligned} \tag{2.4}
$$

By (2.1) and (2.4), we have

$$
\rho(G_3)x_u > \sum\nolimits_{i\in C}(d_{iw}+1)x_i + b + 2pa + 3pb + 2(q-1)c = \rho(G_3)a,
$$

and by (2.2)–(2.4), we have

$$
\begin{aligned}
\rho(G_3)(x_u+x_w) &> 2\sum_{i\in C} d_{iw}x_i + \sum\nolimits_{i\in C} x_i + a + (2+d_{uw})pa + (4+d_{uw})pb \\
&+ (5+d_{uw})b + (2+d_{uw})(q-1)c \\
&> \sum\nolimits_{i\in C}(d_{iw}+2)x_i + a + 3pa + 4pb + 3(q-1)c = \rho(G_3)b.
\end{aligned}
$$

So $x_u > a, x_u + x_w > b$ for any $u \in C$. Then $\sum_{j\in C} x_j \geq x_{u'} + x_u + x_w > a + b$, a contradiction. This completes the proof. ∎

Lemma 2.2 [7]**.** *Let w be a vertex of the nontrivial connected graph G and for nonnegative integers p and q, let $G(p, q)$ denote the graph obtained from G by attaching pendant paths $P = wv_1v_2\cdots v_p$ and $Q = wu_1u_2\cdots u_q$. If $p \geq q \geq 1$, then $\rho(G(p+1, q-1)) > \rho(G(p, q))$.*

Lemma 2.3 [11]**.** *Suppose that a connected graph $G = G_p \cup G_0 \cup G'$ with $G_p \cap G_0 = G_p \cap G' = G_0 \cap G' = v_0$ and G_p consisting of pendant edges $v_0v_1, v_0v_2, \ldots, v_0v_k$ ($k \geq 3$). Let $S' = V(G')$. Suppose that $N_G(v_0) = N_1 \cup N_2$ satisfying that $N_1 \neq \emptyset, N_2 \neq \emptyset, N_1 \cap N_2 = \emptyset$. Let*

$$
H = G - \sum\nolimits_{v_i\in N_1} v_iv_0 - \sum\nolimits_{v_i\in N_2} v_iv_0 + \sum\nolimits_{v_i\in N_1} v_iv_{k-1} + \sum\nolimits_{v_i\in N_2} v_iv_k.
$$

For any vertex $v_j \in S' \setminus \{v_0\}$, if all the paths from v_0 to v_j with the length $d_G(v_0, v_j)$ pass only through N_1 or pass only through N_2, then $\rho(H) > \rho(G)$.

Lemma 2.4 [11]. *Suppose that a connected graph $G = G_p \cup G_0 \cup G'$ with $G_p \cap G_0 = G_p \cap G' = G_0 \cap G' = v_0$ and G_p consisting of pendant edges $v_0v_1, v_0v_2, \ldots, v_0v_k$ $(k \geq 2)$. Let $S' = V(G')$. Suppose that $N_G(v_0) = N_1 \cup N_2$ satisfying that $N_1 \neq \emptyset, N_2 \neq \emptyset, N_1 \cap N_2 = \emptyset$. Let*

$$H = G - \sum_{v_i \in N_1} v_i v_0 + \sum_{v_i \in N_1} v_i v_k$$

or

$$H = G - \sum_{v_i \in N_2} v_i v_0 + \sum_{v_i \in N_2} v_i v_k.$$

For any vertex $v_j \in S' \setminus \{v_0\}$, if all the paths from v_0 to v_j with the length $d_G(v_0, v_j)$ pass only through N_1 or pass only through N_2, then $\rho(H) > \rho(G)$.

Lemma 2.5. *Let C_g be an even cycle, let G be obtained from C_g by planting paths of length two to some vertices of C_g. For any edge $vv_0 \in E(C_g)$, if there exists at least one path of length two attached at v_0, then $\rho(G) > \rho(H)$, where $H = G - \sum_{v_i \in (N_G(v) - v_0)} v_i v + \sum_{v_i \in (N_G(v) - v_0)} v_i v_0$.*

Proof. Assume that $P^1 = v_0v^1w^1, P^2 = v_0v^2w^2, \ldots, P^p = v_0v^pw^p$ $(p \geq 1)$ are paths of length two, which are attached at v_0 in G. Let $S' = V(G) \setminus \{v^1, w^1, v^2, w^2, \ldots, v^p, w^p\}$ and $N_{C_g}(v_0) = \{v, w\}$. Let $S_1 = \{v_j | v_j \in S' \setminus \{v_0\}$, and any path from v_0 to v_j with the length $d_G(v_0, v_j)$ passes only through $v\}$, $S_2 = \{v_j | v_j \in S' \setminus \{v_0\}$, and any path from v_0 to v_j with the length $d_G(v_0, v_j)$ passes only through $w\}$, $S_3 = \{v_j | v_j \in S' \setminus \{v_0\}$, and there exist two different paths P_1, P_2 from v_0 to v_j with the same length $d_G(v_0, v_j)$, where P_1 passes through v, P_2 passes through $w\}$. Then $S' \setminus \{v_0\} = S_1 \cup S_2 \cup S_3$.

Let x be the Perron vector of $D(H)$. By symmetry, we can let $x_{v^1} = \cdots = x_{v^p} = a, x_{w^1} = \cdots = x_{w^p} = b$ and $x_v = c$. By the Rayleigh quotient we have

$$\begin{aligned}
\frac{1}{2}(\rho(G) - \rho(H)) \geq \frac{1}{2}x^T(D(G) - D(H))x = \frac{1}{2}\sum_{i \in V(G)} \sum_{j \in V(G)} (d_{ij}(G) \\
- d_{ij}(H))x_i x_j = (pa + pb + x_{v_0} - x_v)\left(\sum_{j \in S_1} x_j + \sum_{j \in S_3} x_j\right) \\
+ \sum_{j \in S_1} x_j \sum_{j \in S_2} x_j \\
> (pa + pb + x_{v_0} - x_v)\left(\sum_{j \in S_1} x_j + \sum_{j \in S_3} x_j\right) \\
\geq (a + b + x_{v_0} - x_v)\left(\sum_{j \in S_1} x_j + \sum_{j \in S_3} x_j\right).
\end{aligned}$$

From the eigenvalue equation $D(H)x = \rho(H)x$, we have

$$\begin{aligned}
\rho(H)a &= \sum_{v_i \in S'} (d_{v_i v_0} + 1)x_i + 2(p-1)a + 3(p-1)b + b, \\
\rho(H)b &= \sum_{v_i \in S'} (d_{v_i v_0} + 2)x_i + 3(p-1)a + 4(p-1)b + a, \\
\rho(H)x_{v_0} &= \sum_{v_i \in S'} d_{v_i v_0} x_i + pa + 2pb, \\
\rho(H)x_v &= \sum_{v_i \in S'} (d_{v_i v_0} + 1)x_i + 2pa + 3pb.
\end{aligned}$$

It is easy to see that

$$\begin{aligned}\rho(H)(a+b+x_{v_0}) &= \Big[\sum\nolimits_{v_i\in S'}(d_{v_iv_0}+1)x_i+2pa+3pb\Big]\\ &\quad+2\sum_{v_i\in S'}(d_{v_iv_0}+1)x_i+4ap-4a+6bp-6b\\ &> \rho(H)x_v,\end{aligned}$$

so $a+b+x_{v_0}>x_v$. Then $\rho(G)>\rho(H)$. ■

Lemma 2.6 [11]**.** *Suppose that G_1 is a connected graph with $V(G_1)=\{v_0,v_{k+1},v_{k+2},\dots,v_{n-1}\}$ $(n-k\geq 3)$. Graphs G of order n consists of the complete graph G_1 and pendant edges v_0v_1,$v_0v_2,\dots,v_0v_k$. Graph H of order n consists of G_1 and pendant stars S_{t_i} attached at each vertex v_i (v_i is the center of S_{t_i}) of the complete graph G_1, where stars can be trivial (with only one vertex). Then we have $\rho(H)>\rho(G)$.*

3. Properties of a Unicyclic Graph with Minimal Distance Spectral Radius in $\mathscr{U}(n,m)\setminus\{C_n\}$

Let G^* be the graph in $\mathscr{U}(n,m)\setminus\{C_n\}$ with minimal distance spectral radius, and $C_g=(u_1,u_2,\dots,u_g,u_1)$ be its unique cycle. Then it can be obtained from C_g by planting trees to some vertices of C_g.

Proposition 3.1. *All pendant paths in G^* have lengths one or two.*

Proof. If there exists a pendant path of length $p>2$ in G^*, then we can replace the path by two paths with lengths 2 and $p-2$. Denote the new graph by $\widetilde{G}$. Obviously, $\widetilde{G}\in\mathscr{U}(n,m)\setminus\{C_n\}$. By Lemma 2.2, it has smaller distance spectral radius than G^*, a contradiction. ■

Proposition 3.2. *All the planting trees in G^* must consist of paths with lengths 1 or 2.*

Proof. Otherwise, by Proposition 3.1, there are some pendant paths with lengths 2 or 1 attached at a vertex v, where $v\notin V(C_g)$ (as shown in Figure 1). Let w be the adjacent vertex of v which is nearest to C_g and let M be a matching with maximum cardinality in G^*. If $wv\notin M$, thenwe can apply transformation to get G_1. If $wv\in M$, then we can get G_2. In each case, the matching number is an invariant and by Lemma 2.1, we know that the new graph has smaller distance spectral radius than G^*, also a contradiction. ■

Proposition 3.3. *If C_g is the unique cycle in G^*, then $g=3$.*

Proof. Let $d(v_{i_0}) \geq 3, v_{i_0} \in \{v_1, v_2, \ldots, v_g\}$. Denote by T_{i_0} the nontrivial attaching tree to C_g rooted at vertex v_{i_0}. Suppose $g \geq 4$ is odd. Let

$$G' = G^* - \sum\nolimits_{v_i \in N_{G^*}(v_{i_0-1}) \setminus \{v_{i_0}\}} v_i v_{i_0-1} - \sum\nolimits_{v_i \in N_{G^*}(v_{i_0+1}) \setminus \{v_{i_0}\}} v_i v_{i_0+1}$$
$$+ \sum\nolimits_{v_i \in N_{G^*}(v_{i_0-1}) \setminus \{v_{i_0}\}} v_i v_{i_0} + \sum\nolimits_{v_i \in N_{G^*}(v_{i_0+1}) \setminus \{v_{i_0}\}} v_i v_{i_0}.$$

Note that for any vertex $v_t \in V(G^*) \setminus V(T_{i_0})$, all paths from v_{i_0} to v_t with length $d_{G'}(v_{i_0}, v_t)$ pass only through v_{i_0-2} or only through v_{i_0+2} in G'. By Lemma 2.3, we have $\rho(G') < \rho(G^*)$, it is a contradiction.

Assume $g \geq 4$ is even and there exists a pendant edge attached at a vertex of C_g, say v_{i_0}. Let

$$G' = G^* - \sum\nolimits_{v_i \in N_{G^*}(v_{i_0-1}) \setminus \{v_{i_0}\}} v_i v_{i_0-1} + \sum\nolimits_{v_i \in N_{G^*}(v_{i_0-1}) \setminus \{v_{i_0}\}} v_i v_{i_0}.$$

Note that for any vertex $v_t \in V(G^*) \setminus V(T_{i_0})$, all paths from v_{i_0} to v_t with the length $d_{G'}(v_{i_0}, v_t)$ pass only through v_{i_0-2} or only through v_{i_0+2} in G'. By Lemma 2.4, we have $\rho(G') < \rho(G^*)$, also a contradiction.

If $g \geq 4$ is even and there exists no pendant edge attached at a vertex of C_g, then it must have at least one path of the length two attached at some vertex of C_g, say v_{i_0}, and we set $vv_{i_0} \in E(C_g)$. Let

$$H = G^* - \sum\nolimits_{v_i \in (N_G(v) - v_{i_0})} v_i v + \sum\nolimits_{v_i \in (N_G(v) - v_{i_0})} v_i v_{i_0}.$$

By Lemma 2.5, we have $\rho(H) < \rho(G^*)$, it is also a contradiction. Hence $g = 3$. ■

Proposition 3.4. *One of the vertices in $\{u_1, u_2, u_3\}$ must have an attached pendant edge.*

Proof. Otherwise, all the planting paths are lengths 2. Obviously, there is a matching M of maximum cardinality such that no edge from M is incident to u_1, and there exists at least one path of length 2 attached at u_1. We replace one path of length two attached at u_1 by two pendant edges. Denote the new graph by $\hat{G}$. Obviously, $\hat{G} \in \mathscr{U}(n, m) \setminus \{C_n\}$. By Lemma 2.2, it has smaller distance spectral radius than G^*, a contradiction. ■

Let $V(C_3) = \{u_1, u_2, u_3\}$. Denote by $U(p_1, q_1; p_2, q_2; p_3, q_3; m)$ the graph obtained from C_3 by planting p_i paths of length two and q_i paths of length one to u_i with matching number m, where integers $p_i, q_i \geq 0$ for $i = 1, 2, 3$ (as shown in Figure 2). Let

$$\begin{aligned}\mathscr{A}(n, m) \;&= \{U(p_1, q_1; p_2, q_2; p_3, q_3; m) | 3 \\ &+ \textstyle\sum_{i=1}^{3} (2p_i + q_i) = n, p_i, q_i \geq 0, i = 1, 2, 3\}.\end{aligned}$$

Remark 1. In order to find the graph G^* with minimal distance spectral radius in $\mathscr{U}(n, m) \setminus \{C_n\}$, by Propositions 3.1–3.4, we only need to consider the graphs in $\mathscr{A}(n, m)$.

4. The Unicyclic Graph with Minimal Distance Spectral Radius in $\mathscr{U}(n,m) \setminus \{C_n\}$

Let $p_1 = \max\{p_1, p_2, p_3\}$. From Lemmas 4.1–4.5, for simplicity, let $A = U(p_1, q_1; p_2, q_2; p_3, q_3; m)$, and in A, let V_1 be the set of vertices of all the pendant paths attaching at u_1. If $q_2 \geq 1$, then let V_3 be the set of vertices of all the pendant paths of length two and the first $q_2 - 1$ pendant edges attached at u_2, excluding u_2, Let $V_4 = \{u_2, v\}$ and $V_2 = V - (V_1 \cup V_3 \cup V_4)$. If $q_2 = 0$, let V_3 be the set of vertices of all the pendant paths of length two attaching at u_2 excluding u_2. Let $V_4 = \{u_2\}$ and $V_2 = V - (V_1 \cup V_3 \cup V_4)$ (as shown in Figure 2).

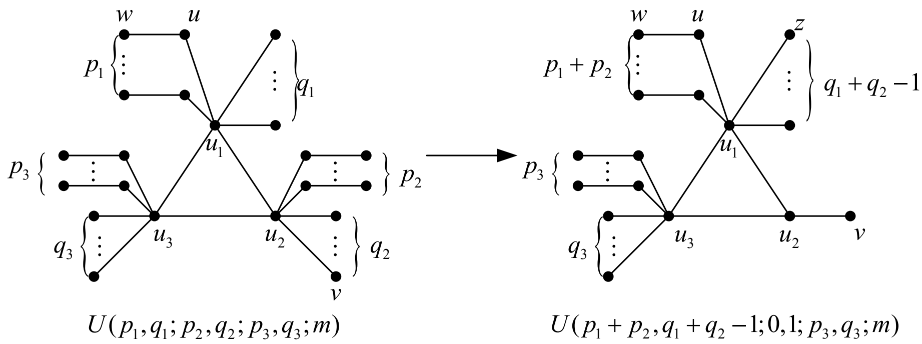

Figure 2. The graphs $U(p_1, q_1; p_2, q_2; p_3, q_3; m), U(p_1 + p_2, q_1 + q_2 - 1; 0, 1; p_3, q_3; m)$.

Lemma 4.1. *If* $p_1 = 1, q_1 \geq 1, q_2 \geq 0$, *then* $\rho(U(p_1, q_1; p_2, q_2; p_3, q_3; m)) > \rho(U(p_1 + p_2, q_1 + q_2 - 1; 0, 1; p_3, q_3; m))$.

Proof. If $q_2 \geq 1$, then set $B = U(p_1 + p_2, q_1 + q_2 - 1; 0, 1; p_3, q_3; m)$. If $q_2 = 0$, then set $B = U(p_1 + p_2, q_1; 0, 0; p_3, q_3; m)$. Let x be the Perron vector of $D(B)$.

Case 1. If $q_2 \geq 1$, then we have

$$\frac{1}{2}(\rho(A) - \rho(B)) \geq \frac{1}{2}x^T(D(A) - D(B))x = \sum\nolimits_{j\in V_3} x_j \left(\sum\nolimits_{i\in V_1} x_i - x_{u_2} - x_v\right).$$

By $D(H)x = \rho(H)x$ and the symmetry of x, we have

$$\begin{aligned}\rho(B)x_w &= x_u + 3(p_1 + p_2 - 1)x_u + 4(p_1 + p_2 - 1)x_w + 3(q_1 + q_2 - 1)x_z \\ &\quad + 2x_{u_1} + 3x_{u_2} + 4x_v + \sum\nolimits_{i\in V_2} d_{iw}x_i,\end{aligned}$$

$$\begin{aligned}\rho(B)x_u &= x_w + 2(p_1 + p_2 - 1)x_u + 3(p_1 + p_2 - 1)x_w + 2(q_1 + q_2 - 1)x_z \\ &\quad + x_{u_1} + 2x_{u_2} + 3x_v + \sum\nolimits_{i\in V_2} d_{iu}x_i,\end{aligned}$$

$$\rho(B)x_{u_1} = (p_1+p_2)x_u + 2(p_1+p_2)x_w + (q_1+q_2-1)x_z + x_{u_2} + 2x_v + \sum\nolimits_{i\in V_2} d_{iu_1}x_i,$$
$$\rho(B)x_z = 2(p_1+p_2)x_u + 3(p_1+p_2)x_w + 2(q_1+q_2-2)x_z + x_{u_1} + 2x_{u_2} + 3x_v + \sum\nolimits_{i\in V_2} d_{iz}x_i,$$
$$\rho(B)x_{u_2} = 2(p_1+p_2)x_u + 3(p_1+p_2)x_w + 2(q_1+q_2-1)x_z + x_{u_1} + x_v + \sum\nolimits_{i\in V_2} d_{iu_2}x_i,$$
$$\rho(B)x_v = 3(p_1+p_2)x_u + 4(p_1+p_2)x_w + 3(q_1+q_2-1)x_z + 2x_{u_1} + x_{u_2} + \sum\nolimits_{i\in V_2} d_{iv}x_i.$$

Note that $\sum_{i\in V_2} d_{iu}x_i = \sum_{i\in V_2} d_{iv}x_i, \sum_{i\in V_2} d_{iu_1}x_i = \sum_{i\in V_2} d_{iu_2}x_i$. Thus

$$\begin{aligned}\rho(B)(x_w + x_u + x_{u_1} + x_z - x_{u_2} - x_v) &= [3(p_1+p_2)-4]x_u + [5(p_1+p_2)-6]x_w \\ &\quad + [3(q_1+q_2)-5]x_z + x_{u_1} + 7x_{u_2} + 11x_v \\ &\quad + \sum\nolimits_{i\in V_2} d_{iz}x_i + \sum\nolimits_{i\in V_2} d_{iw}x_i \\ &> -x_u - x_w + x_z + x_{u_1} + 7x_{u_2} + 11x_v,\end{aligned}$$

since $p_1 = 1, q_1 \geq 1, q_2 \geq 1$. Furthermore,

$$\begin{aligned}\rho^2(B)(x_w + x_u + x_{u_1} + x_z - x_{u_2} - x_v) &> -\rho(B)x_u - \rho(B)x_w + \rho(B)x_z + \rho(B)x_{u_1} \\ &\quad + 7\rho(B)x_{u_2} + 11\rho(B)x_v \\ &= 44(p_1+p_2)x_u + 4x_u + 61(p_1+p_2)x_w \\ &\quad + 6x_w + 44(q_1+q_2-1)x_z + 4x_z \\ &\quad + 27x_{u_1} + 8x_{u_2} + 3x_v + 10\sum\nolimits_{i\in V_2} d_{iv}x_i \\ &\quad + 7\sum\nolimits_{i\in V_2} d_{iu_2}x_i - \sum\nolimits_{i\in V_2} x_i > 0.\end{aligned}$$

So $\sum_{i\in V_1} x_i - x_{u_2} - x_v \geq x_w + x_u + x_{u_1} + x_z - x_{u_2} - x_v > 0$. Then $\rho(A) > \rho(B)$.

Case 2. If $q_2 = 0$, then we have

$$\frac{1}{2}(\rho(A) - \rho(B)) \geq \frac{1}{2}x^T(D(A) - D(B))x = \sum\nolimits_{j\in V_3} x_j \left(\sum\nolimits_{i\in V_1} x_i - x_{u_2}\right).$$

By $D(H)x = \rho(H)x$ and the symmetry of x, we have

$$\rho(B)x_w = x_u + 3(p_1+p_2-1)x_u + 4(p_1+p_2-1)x_w + 3q_1x_z + 2x_{u_1} + 3x_{u_2} + \sum\nolimits_{i\in V_2} d_{iw}x_i,$$
$$\rho(B)x_u = x_w + 2(p_1+p_2-1)x_u + 3(p_1+p_2-1)x_w + 2q_1x_z + x_{u_1} + 2x_{u_2} + \sum\nolimits_{i\in V_2} d_{iu}x_i,$$

$$\rho(B)x_{u_1} = (p_1+p_2)x_u + 2(p_1+p_2)x_w + q_1x_z + x_{u_2} + \sum\nolimits_{i\in V_2} d_{iu_1}x_i,$$
$$\rho(B)x_{u_2} = 2(p_1+p_2)x_u + 3(p_1+p_2)x_w + 2q_1x_z + x_{u_1} + \sum\nolimits_{i\in V_2} d_{iu_2}x_i.$$

Note that $\sum_{i\in V_2} d_{iu_1}x_i = \sum_{i\in V_2} d_{iu_2}x_i$. Then

$$\rho(B)(x_w+x_u+x_{u_1}-x_{u_2}) = [4(p_1+p_2)-4]x_u + [6(p_1+p_2-6]x_w + 4q_1x_z + 2x_{u_1} + 6x_{u_2} + 14x_v + \sum\nolimits_{i\in V_2} d_{iw}x_i + \sum\nolimits_{i\in V_2} d_{iu}x_i > 0.$$

So $\sum_{i\in V_1} x_i - x_{u_2} \geq x_w + x_u + x_{u_1} - x_{u_2} > 0$. Then $\rho(A) > \rho(B)$. ■

Similarly to the proof of Case 2 in Lemma 4.1, we have the following lemma.

Lemma 4.2. *If $p_1 = 1, q_1 = q_2 = 0$, then $\rho(U(1,0;p_2,0;p_3,q_3;m)) > \rho(U(1+p_2,0;0,0;p_3,q_3;m))$.*

Lemma 4.3. *If $p_1 \geq 2$, then*
(i) *for $q_2 \geq 1$, $\rho(U(p_1,q_1;p_2,q_2;p_3,q_3;m)) > \rho(U(p_1+p_2,q_1+q_2-1;0,1;p_3,q_3;m))$,*
(ii) *for $q_2 = 0$, $\rho(U(p_1,q_1;p_2,0;p_3,q_3;m)) > \rho(U(p_1+p_2,q_1;0,0;p_3,q_3;m)) > \rho(U(p_1+p_2+p_3,q_1+q_3;0,0;0,0;m))$.*

Proof. If $q_2 \geq 1$, then set $B = U(p_1+p_2,q_1+q_2-1;0,1;p_3,q_3;m)$. If $q_2 = 0$, then set $B = U(p_1+p_2,q_1;0,0;p_3,q_3;m)$. Let x be the Perron vector of $D(B)$.

Similarly to the proof of Case 1 in Lemma 4.1 for $q_2 \geq 1$, we have

$$\rho(B)(2x_w + 2x_u + x_{u_1} - x_{u_2} - x_v) > 6(p_1+p_2-1)x_u - 2x_u + 9(p_1+p_2-1)x_w - 3x_w > 0,$$

since $p_1 \geq 2, p_2 \geq 0$. So $\sum_{i\in V_1} x_i - x_{u_2} - x_v \geq 2x_w + 2x_u + x_{u_1} - x_{u_2} - x_v > 0$. Then $\rho(A) > \rho(B)$.

Similarly to the proof of Case 2 in Lemma 4.1 for $q_2 = 0$, we also have $\rho(A) > \rho(B)$. ■

Without loss of generality, let $q_1 \geq q_2 \geq q_3$ in the following.

Lemma 4.4. *If $p_1 = 0$, then*
(i) *for $q_3 \geq 1$, $\rho(U(0,q_1;0,q_2;0,q_3;3)) \geq \rho(U(0,q_1+q_2+q_3-2;0,1;0,1;3))$, and the equality holds if and only if $q_2 = q_3 = 1$;*
(ii) *for $q_3 = 0$, $\rho(U(0,q_1;0,q_2;0,0;2)) \geq \rho(U(0,q_1+q_2;0,0;0,0;2))$, and the equality holds if and only if $q_2 = 0$.*

Proof. Note that if $p_1 = 0$, then $p_2 = p_3 = 0$.

(i) If $q_3 \geq 1$, then $q_2 \geq 1$ and $m = 3$. Let $B = U(0, q_1 + q_2 - 1; 0, 1; 0, q_3; 3)$. Let x be the Perron vector of $D(B)$. Then $\frac{1}{2}(\rho(A) - \rho(B)) = \sum_{j \in V_3} x_j (\sum_{i \in V_1} x_i - \sum_{i \in V_4} x_i)$.

If $q_1 \geq 3$, then similarly to Lemma 4.1, we have $\rho(B)(3x_z + x_{u_1} - x_{u_2} - x_v) = 2(q_1 + q_2 - 4)x_z + 6x_{u_2} + 10x_v + 2\sum_{i \in V_2} d_{iz} x_i > 0$.

Then $\rho(A) > \rho(B)$. Repeatedly by this procedure, we can obtain our desirable result.

If $q_1 = 1$, then $q_2 = q_3 = 1$, and obviously, $U(0, q_1; 0, q_2; 0, q_3; 3) \cong U(0, 1; 0, 1; 0, 1; 3)$. If $q_1 = q_2 = 2$, by direct calculation, we have $\rho(U(0, 2; 0, 2; 0, 1; 3)) = 14.5394 > 14.2758 = \rho(U(0, 3; 0, 1; 0, 1; 3))$. This completes the proof of (i).

(ii) If $q_3 = 0$ and $q_2 = 0$, then obviously, $\rho(U(0, q_1; 0, q_2; 0, 0; 2)) = \rho(U(0, q_1 + q_2; 0, 0; 0, 0; 2))$. If $q_3 = 0$ and $q_2 \geq 1$, by Lemma 2.6, we have $\rho(U(0, q_1; 0, q_2; 0, 0; 2)) > \rho(U(0, q_1 + q_2; 0, 0; 0, 0; 2))$. ■

Remark 2. In fact, if $m = 2$, then we have

$$U(p_1, q_1; p_2, q_2; p_3, q_3; 2) \cong U(0, q_1; 0, q_2; 0, 0; 2).$$

By Lemma 4.4(ii), $\rho(U(p_1, q_1; p_2, q_2; p_3, q_3; 2)) \geq \rho(U(0, q_1 + q_2; 0, 0; 0, 0; 2))$.

Lemma 4.5. *If $p_1 = 1, q_1 = 0, q_2 \geq 1$, then*

(i) *for $p_2 = 1$, $\rho(U(1, 0; 1, q_2; p_3, q_3; m)) > \rho(U(0, 0; 2 + p_3, q_2 + q_3; 0, 0; m))$;*

(ii) *for $p_2 = 0, q_3 \geq 1$, $\rho(U(1, 0; 0, q_2; 0, q_3; 3)) \geq \rho(U(0, n - 5; 0, 1; 0, 1; 3))$;*

(iii) *for $p_2 = 0, q_3 = 0$, $\rho(U(1, 0; 0, q_2; 0, 0; 3)) \geq \rho(U(1, n - 5; 0, 0; 0, 0; 3))$.*

Proof. Since $p_1 = 1$, then $p_2 \leq 1, p_3 \leq 1$.

(i) If $p_2 = 1$, then take u_2 as u_1 in Lemmas 4.1 and 4.3, and by Lemmas 4.1 and 4.3, we know $\rho(U(1, 0; 1, q_2; p_3, q_3; m)) > \rho(U(0, 0; 2 + p_3, q_2 + q_3; 0, 0; m))$.

(ii) If $p_2 = 0, q_3 \geq 1$, then $p_3 = 0, m = 3$. By Lemma 2.2, we have $\rho(U(1, 0; 0, q_2; 0, q_3; 3)) > \rho(U(0, 2; 0, q_2; 0, q_3; 3))$. Furthermore, by Lemma 4.4(i), we have $\rho(U(0, 2; 0, q_2; 0, q_3; 3)) > \rho(U(0, n - 5; 0, 1; 0, 1; 3))$.

(iii) If $p_2 = 0, q_3 = 0$, then let $B = U(1, n - 5; 0, 0; 0, 0; 3)$. In A, let $V_1 = \{u, w, u_1\}, V_2 = \{u_3\}, V_3 = V(A) - V_1 - V_2 - V_4, V_4 = \{u_2\}$. Then

$$\begin{aligned}\frac{1}{2}(\rho(A) - \rho(B)) &\geq \sum_{j \in V_3} x_j \left(\sum_{i \in V_1} x_i - \sum_{i \in V_4} x_i\right) \\ &= (x_u + x_w + x_{u_1} - x_{u_2}) \sum_{j \in V_3} x_j.\end{aligned}$$

By $D(B)x = \rho(B)x$ and the symmetry of the components of x, we have

$$\begin{aligned}\rho(B)x_u &= x_w + x_{u_1} + 2q_2 x_z + 2x_{u_2} + 2x_{u_3}, \\ \rho(B)x_w &= x_u + 2x_{u_1} + 3q_2 x_z + 3x_{u_2} + 3x_{u_3}, \\ \rho(B)x_{u_1} &= x_u + 2x_w + q_2 x_z + x_{u_2} + x_{u_3}, \\ \rho(B)x_{u_2} &= 2x_u + 3x_w + 2q_2 x_z + x_{u_1} + x_{u_3},\end{aligned}$$

and $\rho(B)(x_u+x_w+x_{u_1}-x_{u_2}) = 2x_{u_1}+4q_2x_z+6x_{u_2}+3x_{u_3} > 0$. Then $\rho(A) > \rho(B)$. ■

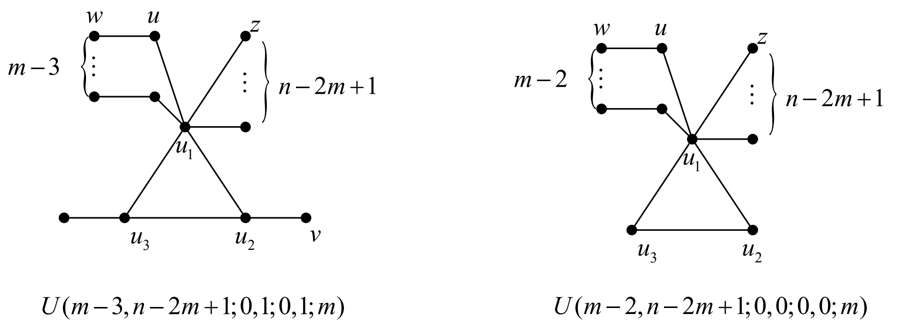

Figure 3. The graphs $U(m-3, n-2m+1; 0, 1; 0, 1; m)$ and $U(m-2, n-2m+1; 0, 0; 0, 0; m)$.

Remark 3. Using Lemmas 4.1–4.5, we have $G^* \in \{U(m-3, n-2m+1; 0, 1; 0, 1; m), U(m-2, n-2m+1; 0, 0; 0, 0; m)\}$.

Lemma 4.6. *If $m \geq 4$, then $\rho(U(m-3, n-2m+1; 0, 1; 0, 1; m)) > \rho(U(m-2, n-2m+1; 0, 0; 0, 0; m))$.*

Proof. Let x be the Perron vector of $U(m-2, n-2m+1; 0, 0; 0, 0; m)$ and $\rho = \rho(U(m-2, n-2m+1; 0, 0; 0, 0; m))$. By the symmetry of the components of x and the Rayleigh quotient, we have

$$\begin{aligned}&\tfrac{1}{2}(\rho(U(m-3, n-2m+1; 0, 1; 0, 1; m)) - \rho(U(m-2, n-2m+1; 0, 0; 0, 0; m)))\\ &= (m-1)x_u x_w + (m-3)x_u^2 + x_u x_{u_1} + (n-2m+1)x_u x_z - x_u x_{u_2} - 3x_{u_2} x_w\\ &\geq x_w(4x_u - 3x_{u_2}) + x_u(2x_u + x_{u_1} + x_z - x_{u_2}),\end{aligned}$$

since $m \geq 4, n \geq 2m$. By $D(U(m-2, n-2m+1; 0, 0; 0, 0; m))x = \rho x$, we have

$$\begin{aligned}\rho x_u &= x_{u_1} + 4x_{u_2} + 2(n-2m+1)x_z + 2(m-3)x_u + 3(m-3)x_w + x_w,\\ \rho x_w &= 2x_{u_1} + 6x_{u_2} + 3(n-2m+1)x_z + 3(m-3)x_u + x_u + 4(m-3)x_w,\\ \rho x_{u_1} &= 2x_{u_2} + (n-2m+1)x_z + (m-2)x_u + 2(m-2)x_w,\\ \rho x_z &= x_{u_1} + 4x_{u_2} + 2(n-2m)x_z + 2(m-2)x_u + 3(m-2)x_w,\\ \rho x_{u_2} &= x_{u_1} + x_{u_2} + 2(n-2m+1)x_z + 2(m-2)x_u + 3(m-2)x_w.\end{aligned}$$

Then

$$\begin{aligned}\rho(2x_u + x_{u_1} + x_z - x_{u_2}) &= 2x_{u_1} + 13x_{u_2} + [5(n-2m)+3]x_z\\ &\quad + (5m-14)x_u + (8m-20)x_w > 0,\\ \rho(\rho x_u + \rho x_w - x_{u_2}) &= 2x_{u_1} + 9x_{u_2} + 3(n-2m+1)x_z + (3m-10)x_u\\ &\quad + (4m-14)x_w > 0,\end{aligned}$$

$$\begin{aligned}
\rho(4x_u - 3x_{u_2}) &= x_{u_1} + 13x_{u_2} + 2(n-2m+1)x_z + 2(m-6)x_u \\
&\quad + 3(m-3)x_w - 5x_w \\
&> x_{u_1} + 13x_{u_2} + 2(n-2m+1)x_z - 4x_u - 2x_w \\
&> x_{u_1} + 13x_{u_2} + 2x_z - 4x_u - 2x_w, \\
\rho^2(4x_u - 3x_{u_2}) &> \rho x_{u_1} + 13\rho x_{u_2} + 2\rho x_z - 4\rho x_u - 2\rho x_w \\
&= 7x_{u_1} - 5x_{u_2} + [17(n-2m)+13]x_z \\
&\quad + (17m-22)x_u + (27m-38)x_w \\
&\geq 7x_{u_1} - 5x_{u_2} + 13x_z + 46x_u + 71x_w \\
&> 7x_{u_1} + 13x_z + 5(x_u + x_w - x_{u_2}) > 0,
\end{aligned}$$

hence $\rho(U(m-3, n-2m+1; 0,1; 0,1; m)) > \rho(U(m-2, n-2m+1; 0,0; 0,0; m)))$. ■

By Remarks 1–3 and Lemma 4.6, we finally conclude our main result.

Theorem 4.7. *Let G be a connected graph in $\mathscr{U}(n,m)$ $(m \neq 3)$ and $G \ncong C_n$. Then $\rho(G) \geq \rho(U(m-2, n-2m+1; 0,0; 0,0; m))$. The equality holds if and only if $G \cong U(m-2, n-2m+1; 0,0; 0,0; m)$.*

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