

ON THE DISTANCE SPECTRAL RADIUS OF UNICYCLIC GRAPHS WITH PERFECT MATCHINGS*

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Abstract. For a connected graph, the distance spectral radius is the largest eigenvalue of its distance matrix. Let U_{2k}^1 be the graph obtained from C_3 by attaching a path of length $n - 3$ at one vertex. Let U_{2k}^2 be the graph obtained from C_3 by attaching a pendant edge together with $k - 2$ paths of length 2 at the same vertex. In this paper, it is proved that U_{2k}^1 (resp., U_{2k}^2) is the unique graph with the maximum (resp., minimum) distance spectral radius among all unicyclic graphs with perfect matchings on $2k(k \geq 5)$ vertices.

Key words. Distance spectral radius, Unicyclic graph, Perfect matching.

AMS subject classifications. 05C50, 15A18.

1. Introduction. Let G be a connected graph with vertex set $\{v_1, v_2, \dots, v_n\}$. The distance between the vertices v_i and v_j is the length of a shortest path between them, and is denoted by $d_G(v_i, v_j)$, or $d(v_i, v_j)$. The *distance matrix* $D = D(G)$ of G is defined so that its (i, j) -entry is equal to $d_G(v_i, v_j)$. The largest eigenvalue of $D(G)$ is called the *distance spectral radius*, and is denoted by $\rho(G)$.

Balaban et al. [1] proposed the use of $\rho(G)$ as a molecular descriptor, while in [4] it was successfully used to infer the extent of branching and model boiling points of alkanes. Therefore, the study concerning the maximum (minimum) distance spectral radius of a given class of graphs is of great interest and significance. Recently, the maximum (minimum) distance spectral radius of a given class of graphs has been studied extensively. For example, Subhi and Powers [8] determined the graph with maximum distance spectral radius among all trees on n vertices; Stevanović and Ilić [9] determined the graph with maximum distance spectral radius among all trees with fixed maximum degree Δ ; Ilić [5] characterized the graph with minimum distance spectral radius among trees with given matching number; Bose et al. [2] studied the graphs with minimum (maximum) distance spectral radius among all graphs of order n with r pendent vertices; Zhang and Godsil [11] determined the graph with minimum distance spectral radius among all graphs of order n with k cut

*Received by the editors on August 23, 2013. Accepted for publication on August 11, 2014.
Handling Editor: Ravi Bapat.

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vertices (resp., k cut edges); Yu et al. [10] determined the unique graph with minimum (maximum) distance spectral radius among unicyclic graphs on n vertices; Milan Nath and Somnath Paul [7] determined the unique graph with minimum distance spectral radius among all connected bipartite graphs of order n with a given matching number (resp., with a given vertex connectivity).

A *unicyclic* graph is a connected graph in which the number of edges equals the number of vertices. A *rooted* graph has one of its vertex, called the root, distinguished from the others. We use the following notation to represent a unicyclic graph: $G = U(C_l; T_1, T_2, \dots, T_l)$, where C_l is the unique cycle in G with $V(C_l) = \{v_1, v_2, \dots, v_l\}$ such that v_i is adjacent to $v_{i+1} \pmod{l}$ for $1 \leq i \leq l$. For each i , let T_i be the rooted tree with root v_i (see Fig. 1). If $|V(T_i)| = 1$, we say T_i is a trivial tree. Let $\mathcal{U}(2k)$ denote the set of all unicyclic graphs on $2k$ vertices with perfect matchings. Let U_{2k}^1 be the graph obtained from C_3 by attaching a path of length $n - 3$ at a vertex. Let U_{2k}^2 be the graph obtained from C_3 by attaching a pendant edge together with $k - 2$ paths of length 2 at the same vertex.

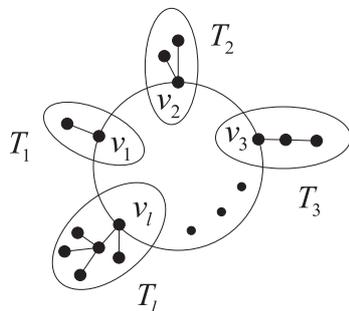


Fig. 1. Graph $U(C_l; T_1, T_2, \dots, T_l)$.

In this paper, we mainly consider the distance spectral radius of unicyclic graphs on $2k$ ($k \geq 3$) vertices with perfect matchings, and prove that U_{2k}^1 (resp., U_{2k}^2) is the unique graph with the maximum (resp., minimum) distance spectral radius among all unicyclic graphs with perfect matchings on $2k$ ($k \geq 5$) vertices.

2. Preliminaries. We first give some lemmas which we will use in the main results.

LEMMA 2.1. [9] *Let w be a vertex of the nontrivial connected graph G and for positive integers p and q , let $G_{p,q}$ denote the graph obtained from G by adding pendent paths $P = wv_1v_2 \dots v_p$ and $Q = wu_1u_2 \dots u_q$ of length p and q , respectively, at w . If $p \geq q \geq 1$, then $\rho(G_{p,q}) < \rho(G_{p+1,q-1})$.*

LEMMA 2.2. [11] *Let u and v be two adjacent vertices of a connected graph G and for positive integers k and l , let $G_{k,l}$ denote the graph obtained from G by adding paths of length k at u and length l at v . If $k > l \geq 1$, then $\rho(G_{k,l}) < \rho(G_{k+1,l-1})$; if $k = l \geq 1$, then $\rho(G_{k,l}) < \rho(G_{k+1,l-1})$ or $\rho(G_{k,l}) < \rho(G_{k-1,l+1})$.*

LEMMA 2.3. [3] $\rho(C_n) = \frac{n^2}{4}$, if n is even; $\rho(C_n) = \frac{n^2-1}{4}$, if n is odd.

LEMMA 2.4. [6] *Let $A = (a_{ij})$ be an $n \times n$ nonnegative matrix. Then*

$$\min_{1 \leq i \leq n} \sum_{1 \leq j \leq n} a_{ij} \leq \rho(A) \leq \max_{1 \leq i \leq n} \sum_{1 \leq j \leq n} a_{ij}.$$

LEMMA 2.5. *If $n \geq 10$ and n is even, then $\rho(U_n^2) < \rho(C_n)$.*

Proof. By Lemma 2.4, we get

$$\rho(U_n^2) \leq \max_{1 \leq i \leq n} \sum_{1 \leq j \leq n} d_{ij} = \frac{7n}{2} - 9.$$

By Lemma 2.3, we have

$$\rho(C_n) = \frac{n^2}{4}.$$

If $n = 10$, by matlab, we get $\rho(U_{10}^2) = 21.0245 < \rho(C_{10}) = 25$.

If $n \geq 12$ and n is even,

$$\rho(U_n^2) - \rho(C_n) \leq \left(\frac{7n}{2} - 9 \right) - \frac{n^2}{4} = -\frac{(n-7)^2 - 13}{4} < 0,$$

i.e., $\rho(U_n^2) < \rho(C_n)$.

So, in either case, we can get $\rho(U_n^2) < \rho(C_n)$, for $n \geq 10$ and n is even. \square

Let X be the Perron vector of G corresponding to $\rho(G)$. Suppose $T_i - \{v_i\} = \alpha K_2 \cup K_1$ and $T_{i+1} - \{v_{i+1}\} = \beta K_2 \cup \gamma K_1$ for some $1 \leq i \leq l$, where α and β are both nonnegative integers, $\gamma = 0$ or 1 . Using a symmetry, we can denote the coordinates of the Perron vector corresponding to the vertices in $V(T_i)$ and $V(T_{i+1})$ as shown in Fig. 2. Then, we have

LEMMA 2.6. (i) $c + d > b$; (ii) $h + d > c$; (iii) $a + b > c$; (iv) $c + d > h$; (v) $a + d > b$.

Proof. We first prove (i).

Let $S' = \alpha(a + b) + c + d$ and $S = \sum_{v_j \in V(G)} x_j$. Since

$$D(G)X = \rho(G)X,$$

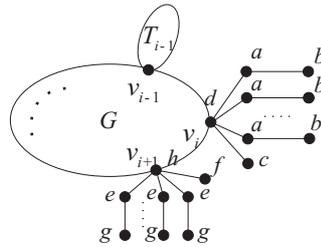


Fig. 2. Graph \$G\$.

we can easily get

$$(2.1) \quad \rho(G)x_i = \sum_{j=1}^{2k} d_{ij}x_j.$$

So, we have

$$\begin{aligned} \rho(G)c + \rho(G)d - \rho(G)b &\geq 2a + (\alpha + 4)b - 2c - d + (S - S' - x_{i-1} - h), \\ &\geq 2a + (\alpha + 4)b - 2c - d, \end{aligned}$$

i.e.,

$$(\rho(G) + 2)(c + d - b) \geq 2a + (\alpha + 2)b + d > 0,$$

which implies

$$c + d > b.$$

Similarly, we can prove (ii),(iii), (iv) and (v). \square

LEMMA 2.7. Let graphs \$G_1, G'_1, G_2, G'_2 \in \mathcal{U}(2k)\$ be as shown in Fig. 3, where \$p \ge 2\$ and \$q \ge 1\$. Then we have

$$(i) \rho(G_1) < \rho(G'_1); (ii) \rho(G_2) < \rho(G'_2).$$

Proof. We first prove (i).

Let \$X\$ be the Perron vector of \$G_1\$ corresponding to \$\rho(G_1)\$. Using a symmetry, we can denote the coordinates of the Perron vector corresponding to some vertices of \$G_1\$ as shown in Fig. 3. Let \$S = \sum_{v_i \in V(G_1)} x_i\$ and \$S' = S - p(a + b)\$, where \$p \ge 2\$. From

\$G_1\$ to \$G'_1\$, we have

$$\begin{aligned} \rho(G'_1) - \rho(G_1) &\geq X^T (D(G'_1) - D(G_1)) X \\ &= (p - 1)(a + b)(S' - a - b). \end{aligned}$$

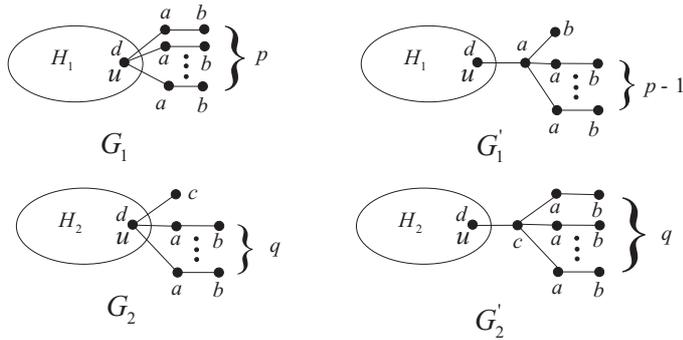


Fig. 3. Graphs G_1, G'_1, G_2, G'_2 .

In the following, we will prove $S' - a - b > 0$ into two cases.

If $H_1 = C_3$, let $C_3 = uvwu$. Then $S' = d + x_v + x_w$. By (2.1), we have

$$\rho(G_1)d + \rho(G_1)x_v + \rho(G_1)x_w - \rho(G_1)a - \rho(G_1)b = 4a + (p + 6)b - d - 3x_v - 3x_w,$$

i.e.,

$$(\rho(G_1) + 3)(S' - a - b) = 2d + a + (p + 3)b > 0.$$

So, we have $S' - a - b > 0$.

If $H_1 \neq C_3$, then $|V(H_1)| \geq 4$. There must exist some vertex $w \in V(H_1)$ such that $d_{H_1}(u, w) = 2$. Suppose $v \in N_{H_1}(u) \cap N_{H_1}(w)$. By (2.1), we have

$$\rho(G_1)S' - \rho(G_1)(a + b) \geq p(a + 2b) + 4a + 6b - 4S',$$

i.e., $(\rho(G_1) + 4)(S' - a - b) > p(a + 2b) + 2b > 0$, which implies $S' - a - b > 0$.

So, in either case, we can get $S' - a - b > 0$, which implies

$$\rho(G_1) < \rho(G'_1).$$

Similarly, we can prove (ii). \square

3. Main results.

THEOREM 3.1. U_{2k}^1 is the unique graph with the maximum distance spectral radius among all unicyclic graphs with perfect matchings on $2k$ ($k \geq 3$) vertices.

Proof. Choose $G \in \mathcal{U}(2k)$ such that $\rho(G)$ is as large as possible. Let $G = U(C_l; T_1, T_2, \dots, T_l)$ and $V(C_l) = \{v_1, v_2, \dots, v_l\}$. Let $X = (x_1, x_2, \dots, x_{2k})^T$ be the

Perron vector of G corresponding to $\rho(G)$, where x_i corresponds to the vertex v_i ($1 \leq i \leq 2k$).

Suppose $M(G)$ is any perfect matching of G . If there exists some $1 \leq i \leq l$ such that $v_i v_{(i+1) \bmod l} \in M(G)$, we may assume $v_1 v_2 \in M(G)$. Then $v_2 v_3 \notin M(G)$ and $v_1 v_l \notin M(G)$. If $v_i v_{(i+1) \bmod l} \notin M(G)$ for any $1 \leq i \leq l$, then $v_2 v_3 \notin M(G)$ and $v_1 v_l \notin M(G)$. So, in either case, we can always assume $v_2 v_3 \notin M(G)$ and $v_1 v_l \notin M(G)$.

Claim 1. $l = 3$.

Otherwise, we may assume $l \geq 4$.

Case 1. $l = 4$.

If $\sum_{v_i \in V(T_4)} x_i \geq \sum_{v_i \in V(T_3)} x_i$, let

$$G' = G - \{v_1 v_4\} + \{v_1 v_3\}.$$

Then $G' \in \mathcal{U}(2k)$. From G to G' , the distances between $V(T_1)$ and $V(T_3)$ are decreased by 1; the distances between $V(T_1)$ and $V(T_4)$ are increased by 1; the distances between $V(T_2)$ and $V(T_1) \cup V(T_3) \cup V(T_4)$, $V(T_3)$ and $V(T_4)$ are unchanged. So, we have

$$\begin{aligned} \rho(G') - \rho(G) &\geq X^T (D(G') - D(G)) X \\ &= 2 \sum_{v_j \in V(T_1)} x_j \left(\sum_{v_i \in V(T_4)} x_i - \sum_{v_i \in V(T_3)} x_i \right) \\ &\geq 0. \end{aligned}$$

In the following, we will prove $\rho(G) \neq \rho(G')$.

If not, then X is also the Perron vector of G' corresponding to $\rho(G')$. According to (2.1), we have

$$\rho(G)x_4 = \sum_{v_j \in V(T_4)} d_{4j}x_j + \sum_{v_j \in V(T_1)} (d_{1j} + 1)x_j + \sum_{v_j \in V(T_2)} (d_{2j} + 2)x_j + \sum_{v_j \in V(T_3)} (d_{3j} + 1)x_j,$$

$$\rho(G')x_4 = \sum_{v_j \in V(T_4)} d_{4j}x_j + \sum_{v_j \in V(T_1)} (d_{1j} + 2)x_j + \sum_{v_j \in V(T_2)} (d_{2j} + 2)x_j + \sum_{v_j \in V(T_3)} (d_{3j} + 1)x_j.$$

Since $\rho(G) = \rho(G')$, from the above two equations, we get

$$\sum_{v_j \in V(T_1)} x_j = 0,$$

which contradicts to the fact that X is a Perron eigenvector.

So, we have $\rho(G') > \rho(G)$, which is a contradiction.

If $\sum_{v_i \in V(T_4)} x_i < \sum_{v_i \in V(T_3)} x_i$, let

$$G' = G - \{v_2v_3\} + \{v_2v_4\}.$$

Then $G' \in \mathcal{U}(2k)$. Similar to the above, we can also get a contradiction.

Case 2. $l \geq 5$.

If $\sum_{v_i \in V(T_3) \cup \dots \cup V(T_{\lfloor \frac{l}{2} \rfloor + 1})} x_i \geq \sum_{v_i \in V(T_{\lfloor \frac{l}{2} \rfloor + 2}) \cup \dots \cup V(T_l)} x_i$, let

$$G' = G - \{v_2v_3\} + \{v_2v_l\}.$$

Then $G' \in \mathcal{U}(2k)$. From G to G' , the distances between $V(T_1)$ and $V(T_3) \cup \dots \cup V(T_{\lfloor \frac{l}{2} \rfloor})$ are increased by at least 1; the distances between $V(T_2)$ and $V(T_3) \cup \dots \cup V(T_{\lfloor \frac{l}{2} \rfloor + 1})$ are increased by at least 1; the distances between $V(T_2)$ and $V(T_{\lfloor \frac{l}{2} \rfloor + 2}) \cup \dots \cup V(T_l)$ are decreased by 1; the distances between $V(T_i)$ ($3 \leq i \leq l-1$) and $V(T_j)$ ($i < j \leq l$) are unchanged or increased by at least 1. So, we have

$$\begin{aligned} \rho(G') - \rho(G) &\geq X^T (D(G') - D(G)) X \\ &> 2 \sum_{v_j \in V(T_2)} x_j \left(\sum_{v_i \in V(T_3) \cup \dots \cup V(T_{\lfloor \frac{l}{2} \rfloor + 1})} x_i - \sum_{v_i \in V(T_{\lfloor \frac{l}{2} \rfloor + 2}) \cup \dots \cup V(T_l)} x_i \right) \\ &\geq 0, \end{aligned}$$

i.e., $\rho(G') > \rho(G)$, which is a contradiction.

If $\sum_{v_i \in V(T_3) \cup \dots \cup V(T_{\lfloor \frac{l}{2} \rfloor + 1})} x_i < \sum_{v_i \in V(T_{\lfloor \frac{l}{2} \rfloor + 2}) \cup \dots \cup V(T_l)} x_i$, let

$$G' = G - \{v_1v_l\} + \{v_1v_3\}.$$

Then $G' \in \mathcal{U}(2k)$. Similar to the above, we can also get a contradiction.

Claim 2. $G = U_{2k}^1$.

Since $G = U(C_3; T_1, T_2, T_3)$, using Lemma 2.1 frequently, we can first get each T_i ($1 \leq i \leq 3$) is a path. Then using Lemma 2.2 at most twice, we can get $G = U_{2k}^1$. \square

THEOREM 3.2. H_2 (see Fig. 4) is the unique graph with the minimum distance spectral radius among all unicyclic graphs with perfect matchings on 6 vertices.

Proof. There are 8 graphs in $\mathcal{U}(6)$ (see Fig. 4). By Lemma 2.1, we have

$$(3.1) \quad \rho(H_8) > \rho(H_5).$$

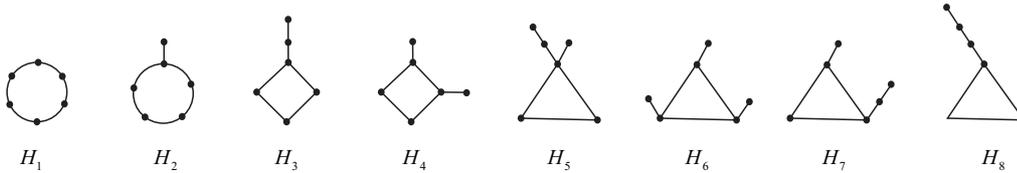


Fig. 4. Graphs H_1-H_8 .

By Lemma 2.2, we have

$$(3.2) \quad \rho(H_3) > \rho(H_4), \quad \rho(H_7) > \rho(H_6).$$

Combining (3.1), (3.2) and Table 3.1, we get $G = H_2$. \square

TABLE 3.1

G	H_1	H_2	H_4	H_5	H_6
$\rho(G)$	9.0000	8.8219	9.2606	9.3154	9.3852

THEOREM 3.3. G_9 (see Fig. 5) is the unique graph with the minimum distance spectral radius among all unicyclic graphs with perfect matchings on 8 vertices.

Proof. Choose $G \in \mathcal{U}(8)$ such that $\rho(G)$ is as small as possible. Let $G = U(C_l; T_1, T_2, \dots, T_l)$. Then, we get $l \leq 8$. By Lemma 2.1 and Lemma 2.7, we get $T_i - \{v_i\} = aK_1 \cup bK_2$ for $1 \leq i \leq l$, where $a = 0$ or 1. Since $|V(G)| = 8$, we have $G \in \{G_i | 1 \leq i \leq 18 \text{ and } i \text{ is an integer}\}$ (see Fig. 5).

By Lemma 2.2, we have

$$(3.3) \quad \rho(G_{11}) > \rho(G_{10}), \quad \rho(G_{15}) > \rho(G_{17}).$$

Combining (3.3) and Table 3.2, we get $G = G_9$. \square

TABLE 3.2

G	G_1	G_2	G_3	G_4	G_5	G_6	G_7	G_8
$\rho(G)$	16.0000	15.4245	16.4273	15.8882	15.3066	15.2065	15.7572	16.3222
G	G_9	G_{10}	G_{12}	G_{13}	G_{14}	G_{16}	G_{17}	G_{18}
$\rho(G)$	14.9363	15.5440	17.1619	16.1147	15.0744	17.2816	15.6487	16.1798

THEOREM 3.4. U_{2k}^2 is the unique graph with the minimum distance spectral radius among all unicyclic graphs with perfect matchings on $2k$ ($k \geq 5$) vertices.

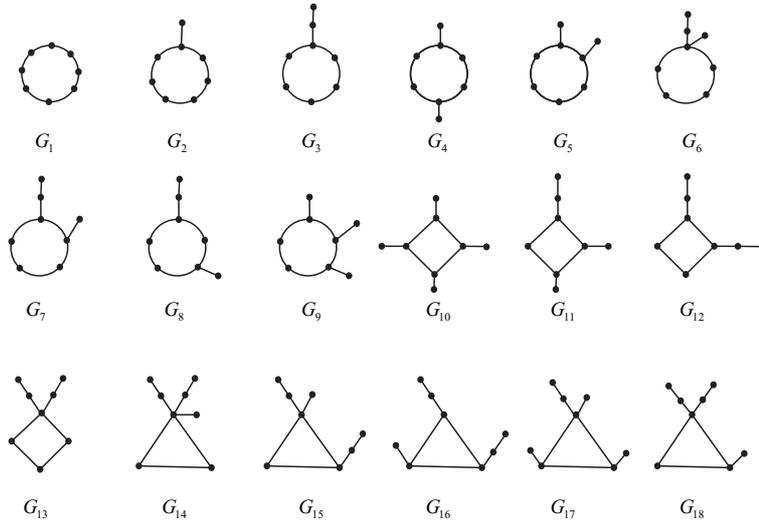


Fig. 5. Graphs G_1 – G_{18} .

Proof. Choose $G \in \mathcal{U}(2k)$ such that $\rho(G)$ is as small as possible. Let $G = U(C_l; T_1, T_2, \dots, T_l)$ and $C_l = v_1 v_2 \cdots v_l v_1$. By Lemma 2.1 and Lemma 2.7, we get $T_i - \{v_i\} = aK_1 \cup bK_2$ for $1 \leq i \leq l$, where $a = 0$ if $|V(T_i)|$ is odd, and $a = 1$ if $|V(T_i)|$ is even. In the following, we always assume $N_{T_i}(v_i) = \{v_j | v_j \in V(T_i) \text{ and } v_j \text{ is adjacent to } v_i\}$, $N'_{T_i}(v_i) = \{v_j | v_j \in N_{T_i}(v_i), d(v_j) = 2\}$ and $R_{T_i} = \{v_j | v_j \in N_{T_i}(v_i), d(v_j) = 1\} \cup \{v_i\}$. Then $|R_{T_i}| = 1$ or 2 . Suppose G' is the graph obtained from G by grafting some edges and $G' \in \mathcal{U}(2k)$. For some i , if T_i is still a rooted tree of G' , we still use T_i to denote the rooted tree with root v_i in G' ; if T_i is not a rooted tree of G' any more, but v_i is still a root, we always use T'_i to denote the rooted tree with root v_i in G' . Let $M(G)$ be any perfect matching of G .

Claim 1. $l \leq 4$.

Otherwise, we may assume $l \geq 5$.

Case 1. There exists some $1 \leq i \leq l$ such that $|V(T_i)| \geq 3$.

Without loss of generality, we may assume $|V(T_1)| \geq 3$.

Subcase 1.1. $v_{l-1}v_l \notin M(G)$ and $v_2v_3 \notin M(G)$.

Suppose $N'_{T_1}(v_1) = \{v_{11}, \dots, v_{1r}\}$ and $N'_{T_2}(v_2) = \{v_{21}, \dots, v_{2s}\}$.

If l is even, let $G' = G - \{v_l v_{l-1}, v_l v_{11}, \dots, v_l v_{1r}\} + \{v_1 v_{l-1}, v_1 v_{11}, \dots, v_1 v_{1r}\}$. Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-1}; T'_1, T_2, \dots, T_{l-1})$. Let $X = (x_1, x_2, \dots, x_{2k})^T$ be the

Perron vector of G' corresponding to $\rho(G')$, where x_i corresponds to the vertex v_i ($1 \leq i \leq 2k$). For convenience, we can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_1)$ the same as $V(T_{i+1})$ in Fig. 2. Since $|V(T_1)| \geq 3$ and $\sum_{v_i \in R_{T_l}} x_i = e + g$ or f , from G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= 2 \sum_{v_i \in V(T_1)} x_i \sum_{v_j \in V(T_{\frac{l}{2}+1}) \cup \dots \cup V(T_{l-1})} x_j + 2 \sum_{v_i \in V(T_1) \cup \dots \cup V(T_{\frac{l}{2}})} x_i \sum_{v_j \in V(T_l) \setminus R_{T_l}} x_j \\ &\quad + 2 \sum_{v_i \in V(T_2)} x_i \sum_{v_j \in V(T_{\frac{l}{2}+2}) \cup \dots \cup V(T_{l-1})} x_j + 2 \sum_{v_i \in V(T_3)} x_i \sum_{v_j \in V(T_{\frac{l}{2}+3}) \cup \dots \cup V(T_{l-1})} x_j \\ &\quad + \dots + 2 \sum_{v_i \in V(T_{\frac{l}{2}-1})} x_i \sum_{v_j \in V(T_{l-1})} x_j \\ &\quad - 2 \sum_{v_i \in R_{T_l}} x_i \sum_{v_j \in V(T_{\frac{l}{2}+1}) \cup \dots \cup V(T_{l-1})} x_j - 2 \sum_{v_i \in R_{T_l}} x_i \sum_{v_j \in V(T_l) \setminus R_{T_l}} x_j \\ &> 2 \left(\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in R_{T_l}} x_i \right) \left(\sum_{v_j \in V(T_{\frac{l}{2}+1}) \cup \dots \cup V(T_{l-1}) \cup V(T_l) \setminus R_{T_l}} x_j \right) \\ &> 2[e + g + h - (e + g)] \left(\sum_{v_j \in V(T_{\frac{l}{2}+1}) \cup \dots \cup V(T_{l-1}) \cup V(T_l) \setminus R_{T_l}} x_j \right) \\ &> 0, \end{aligned}$$

which is a contradiction.

If l is odd, let

$$\begin{aligned} G' &= G - \{v_2v_3, v_2v_{21}, \dots, v_2v_{2s}\} - \{v_l v_{l-1}, v_l v_{l1}, \dots, v_l v_{lr}\} \\ &\quad + \{v_1v_3, v_1v_{21}, \dots, v_1v_{2s}\} + \{v_1v_{l-1}, v_1v_{l1}, \dots, v_1v_{lr}\}. \end{aligned}$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-2}; T'_1, T_3, \dots, T_{l-1})$. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &> 2 \left(\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in R_{T_2}} x_i \right) \left(\sum_{v_i \in V(T_3) \cup \dots \cup V(T_{\frac{l+1}{2}})} x_i + \sum_{v_i \in V(T_2) \setminus R_{T_2}} x_i \right) \\ &\quad + 2 \left(\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in R_{T_l}} x_i \right) \left(\sum_{v_i \in V(T_{\frac{l+1}{2}+1}) \cup \dots \cup V(T_{l-1})} x_i + \sum_{v_i \in V(T_l) \setminus R_{T_l}} x_i \right). \end{aligned}$$

Similar to the case that l is even, we can also get a contradiction.

Subcase 1.2. $v_{l-1}v_l \notin M(G)$ and $v_2v_3 \in M(G)$.

Suppose $N'_{T_1}(v_l) = \{v_{l1}, \dots, v_{lr}\}$ and $N'_{T_3}(v_3) = \{v_{31}, \dots, v_{3t}\}$. Let

$$G' = G - \{v_l v_{l-1}, v_l v_{l1}, \dots, v_l v_{lr}\} - \{v_3 v_4, v_3 v_{31}, \dots, v_3 v_{3t}\} \\ + \{v_1 v_{l-1}, v_1 v_{l1}, \dots, v_1 v_{lr}\} + \{v_2 v_4, v_2 v_{31}, \dots, v_2 v_{3t}\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-2}; T'_1, T'_2, T_4, \dots, T'_{l-1})$. From G' to G , we have

$$\rho(G) - \rho(G') \geq X^T (D(G) - D(G')) X \\ > 2 \left(\sum_{v_i \in V(T_1)} x_i + \sum_{v_i \in V(T_2)} x_i \right) \left(\sum_{v_i \in V(T_4) \cup \dots \cup V(T_{l-1})} x_i + \sum_{v_i \in (V(T_3) \setminus R_{T_3}) \cup (V(T_l) \setminus R_{T_l})} x_i \right) \\ (3.4) \quad - 2 \left(x_3 + \sum_{v_i \in R_{T_1}} x_i \right) \left(\sum_{v_i \in V(T_4) \cup \dots \cup V(T_{l-1})} x_i + \sum_{v_i \in (V(T_3) \setminus R_{T_3}) \cup (V(T_l) \setminus R_{T_l})} x_i \right).$$

We can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_1)$ and $V(T'_2)$ the same as $V(T_{i+1})$ and $V(T_i)$ in Fig. 2. Then, by Lemma 2.3 (ii), we have

$$\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in R_{T_1}} x_i + \sum_{v_i \in V(T_2)} x_i - x_3 \geq (e + g + h) - (e + g) + d - c \\ = h + d - c \\ (3.5) \quad > 0.$$

Combining (3.4) and (3.5), we get $\rho(G) > \rho(G')$, which is a contradiction.

Subcase 1.3. $v_{l-1}v_l \in M(G)$ and $v_2v_3 \in M(G)$.

If there exists some $i = 2, 3, l-1, l$ such that $|V(T_i)| \geq 3$, then dealing with this case the same as Subcase 1.1 and Subcase 1.2, respectively, we can get a contradiction.

Otherwise, $|V(T_2)| = |V(T_3)| = |V(T_{l-1})| = |V(T_l)| = 1$.

If $l = 5$, let

$$G' = G - \{v_3 v_4\} + \{v_1 v_3\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_3; T'_1, T_2, T_3)$. We can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_1)$ the same as $V(T_i)$ in Fig. 2. Using a symmetry, we can get $x_2 = x_3$. Since $|V(G)| \geq 10$, we have $|V(T_1)| \geq 6$. By

Lemma 2.3 (i), from G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= 2x_3 \sum_{v_i \in V(T_1)} x_i - 2x_2x_4 - 4x_3x_4 \\ &= 2x_3 \left(\sum_{v_i \in V(T_1)} x_i - 3x_4 \right) \\ &\geq 2x_3[2(a+b) + c + d - 3b] \\ &= 2x_3(2a + c + d - b) \\ &> 0, \end{aligned}$$

which is a contradiction.

If $l = 6$, let

$$G' = G - \{v_3v_4, v_4v_5\} + \{v_1v_3, v_1v_4\}.$$

Then $G' \in \mathcal{U}(2k)$. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= 2 \sum_{v_i \in V(T_1)} x_i \left(x_3 + 2 \sum_{v_i \in V(T_4)} x_i \right) + 2x_3 \left(x_6 - \sum_{v_i \in V(T_4)} x_i - x_5 \right) - 4x_5 \sum_{v_i \in V(T_4)} x_i \\ &= 2x_3 \left(\sum_{v_i \in V(T_1)} x_i - x_5 + x_6 \right) + 2 \sum_{v_i \in V(T_4)} x_i \left(2 \sum_{v_i \in V(T_1)} x_i - x_3 - 2x_5 \right) \\ &> 0. \end{aligned}$$

If $l = 7$, $|V(T_4)| \geq 3$ or $|V(T_5)| \geq 3$, deal with the case the same as Subcase 1.2.

If $l = 7$, $|V(T_4)| = |V(T_5)| = 1$ and $|V(T_1)| = 4$, by matlab, we get $\rho(G) = 22.9526 > \rho(U_{10}^2) = 21.0245$, which is a contradiction.

If $l = 7$, $|V(T_4)| = |V(T_5)| = 1$ and $|V(T_1)| > 4$, let

$$G' = G - \{v_5v_6\} + \{v_1v_5\}.$$

Then $G' \in \mathcal{U}(2k)$. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= 2 \sum_{v_i \in V(T_1)} x_i x_4 + 4 \sum_{v_i \in V(T_1)} x_i x_5 + 2x_2x_5 - 2x_3x_6 - 4x_4x_6 - 4x_5x_6 \\ (3.6) \quad &> 2 \left(\sum_{v_i \in V(T_1)} x_i x_4 - x_3x_6 - 2x_4x_6 \right) + 4x_5 \left(\sum_{v_i \in V(T_1)} x_i - x_6 \right). \end{aligned}$$

Since v_3 and v_4 are symmetric in G' , we can assume $x_3 = x_4$. We can denote the coordinates of Perron vector X corresponding to vertices in $V(T_1)$ the same as $V(T_i)$ in Fig. 2. By Lemma 2.3 (i), we have

$$\begin{aligned}
 \sum_{v_i \in V(T_1)} x_i x_4 - x_3 x_6 - 2x_4 x_6 &= \left(\sum_{v_i \in V(T_1)} x_i - 3x_6 \right) x_4 \\
 &\geq (2(a+b) + c + d - 3b)x_4 \\
 &= (2a + c + d - b)x_4 \\
 &> 0,
 \end{aligned}
 \tag{3.7}$$

and

$$\sum_{v_i \in V(T_1)} x_i - x_6 > \sum_{v_i \in V(T_1)} x_i - 3x_6 > 0.
 \tag{3.8}$$

Combining (3.6), (3.7) and (3.8), we get $\rho(G) > \rho(G')$, which is a contradiction.

If $l = 7$ and $|V(T_4)| = |V(T_5)| = 2$, let

$$G' = G - \{v_3 v_4, v_4 v_5, v_5 v_6\} + \{v_1 v_4, v_1 v_5, v_1 v_6\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_3; T'_1, T_6, T_7)$. From G' to G , we have

$$\begin{aligned}
 \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\
 &= 2 \sum_{v_i \in V(T_1)} x_i \left(2 \sum_{v_i \in V(T_4)} x_i + 2 \sum_{v_i \in V(T_5)} x_i + x_6 \right) + 2x_2 \left(\sum_{v_i \in V(T_5)} x_i + x_6 \right) \\
 &\quad - 2x_3 \left(2 \sum_{v_i \in V(T_4)} x_i \sum_{v_i \in V(T_5)} x_i \right) \\
 &\quad + 2 \sum_{v_i \in V(T_4)} x_i \left(x_7 - \sum_{v_i \in V(T_5)} x_i \right) - 2 \sum_{v_i \in V(T_5)} x_i x_6 \\
 &> 4 \left(\sum_{v_i \in V(T_1)} x_i - x_3 \right) \sum_{v_i \in V(T_4)} x_i + 2x_6 \left(\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in V(T_5)} x_i \right) \\
 &\tag{3.9} + 2 \left(2 \sum_{v_i \in V(T_1)} x_i - x_3 - \sum_{v_i \in V(T_4)} x_i \right) \sum_{v_i \in V(T_5)} x_i.
 \end{aligned}$$

We can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_1)$ the same as $V(T_i)$ in Fig. 2. Since $|V(T_1)| \geq 3$, we have

$$\sum_{v_i \in V(T_1)} x_i - x_3 > a + b + d - b = a + d > 0.
 \tag{3.10}$$



Similarly, we can have

$$(3.11) \quad \begin{aligned} & \sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in V(T_5)} x_i > 0, \\ & 2 \sum_{v_i \in V(T_1)} x_i - x_3 - \sum_{v_i \in V(T_4)} x_i > 0. \end{aligned}$$

Combining (3.9), (3.10) and (3.11), we get $\rho(G) > \rho(G')$, which is a contradiction.

If $l \geq 8$, let

$$G' = G - \{v_3v_4, v_{l-2}v_{l-1}\} + \{v_2v_4, v_{l-2}v_l\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-2}; T_1, T_2', T_4, \dots, T_{l-2}, T_l')$. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') & \geq X^T (D(G) - D(G')) X \\ & > 2 \left(\sum_{v_i \in V(T_1)} x_i + x_2 + x_l - x_3 - x_{l-1} \right) \left(\sum_{v_i \in V(T_4) \cup \dots \cup V(T_{l-2})} x_i \right) \end{aligned}$$

Similarly to the case $l = 7$, we can also get a contradiction.

Case 2. For any $1 \leq i \leq l$, $|V(T_i)| = 2$.

If $l = 5$, by matlab, we get $\rho(G) = 21.7047 > \rho(U_{10}^2) = 21.0245$, which is a contradiction.

If $l = 6$, by matlab, we get $\rho(G) = 29.8114 > \rho(U_{12}^2) = 27.0578$, which is a contradiction.

If $l = 7$, by matlab, we get $\rho(G) = 37.9249 > \rho(U_{14}^2) = 33.1338$, which is a contradiction.

If $l = 8$, by matlab, we get $\rho(G) = 48.0000 > \rho(U_{16}^2) = 39.2346$, which is a contradiction.

If $l \geq 9$, let

$$G' = G - \{v_2v_3, v_3v_4, \dots, v_{l-2}v_{l-1}\} + \{v_1v_3, v_1v_4, \dots, v_1v_{l-1}\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_3; T_1', T_{l-1}, T_l)$. Since $\sum_{v_i \in V(T_2)} x_i = \dots = \sum_{v_i \in V(T_{l-2})} x_i$

and $\sum_{v_i \in V(T_{l-1})} x_i = \sum_{v_i \in V(T_l)} x_i$ in G' , from G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &> 2 \sum_{v_i \in V(T_1)} x_i \left(\sum_{v_i \in V(T_3)} x_i + \cdots + \sum_{v_i \in V(T_{l-1})} x_i \right) \\ &\quad + 2 \sum_{v_i \in V(T_2)} x_i \left(- \sum_{v_i \in V(T_3)} x_i + \sum_{v_i \in V(T_5)} x_i + \cdots + \sum_{v_i \in V(T_{l-1})} x_i \right) \\ &\quad + 2 \sum_{v_i \in V(T_3)} x_i \left(- \sum_{v_i \in V(T_4)} x_i + \sum_{v_i \in V(T_6)} x_i + \cdots + \sum_{v_i \in V(T_l)} x_i \right) \\ &\quad + \cdots + 2 \sum_{v_i \in V(T_{l-3})} x_i \left(- \sum_{v_i \in V(T_{l-2})} x_i + \sum_{v_i \in V(T_l)} x_i \right) \\ &\quad + 2 \sum_{v_i \in V(T_{l-2})} x_i \left(- \sum_{v_i \in V(T_{l-1})} x_i \right) \\ &> 0, \end{aligned}$$

which is a contradiction.

Case 3. For any $1 \leq i \leq l$, $|V(T_i)| \leq 2$, and there exists some $1 \leq j \leq l$ such that $|V(T_j)| = 1$.

For convenience, we may assume that $|V(T_1)| = 2$ and $|V(T_l)| = 1$.

Subcase 3.1. $|V(T_2)| = 1$.

Then $v_2v_3, v_{l-1}v_l \in M(G)$. Dealing with this case the same as Subcase 1.3.

Subcase 3.2. $|V(T_2)| = |V(T_3)| = 2$.

Then $v_{l-1}v_l \in M(G)$. Since $|V(G)| \geq 10$, we can get $l \geq 6$.

If $l = 6$, we get $\rho(G) = 22.3859 > \rho(U_{10}^2) = 21.0245$, which is a contradiction.

If $l = 7$ and $|V(T_4)| = 1$, we get $\rho(G) = 22.2365 > \rho(U_{10}^2) = 21.0245$, which is a contradiction.

If $l = 7$ and $|V(T_4)| = 2$, we get $\rho(G) = 30.0508 > \rho(U_{12}^2) = 27.0578$, which is a contradiction.

If $l \geq 8$ is odd, let

$$G' = G - \{v_2v_3, v_3v_4, v_{l-2}v_{l-1}\} + \{v_1v_3, v_1v_4, v_1v_{l-2}\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-4}; T'_1, T_4, \dots, T_{l-2})$. We can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_1)$ the same as $V(T_i)$ in Fig. 2. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &> 2 \left(\sum_{v_i \in V(T_1)} x_i - x_{l-1} \right) \left(\sum_{v_i \in V(T_4) \cup \dots \cup V(T_{l-2})} x_i \right) \\ &= (c + d - b) \left(\sum_{v_i \in V(T_4) \cup \dots \cup V(T_{l-2})} x_i \right) \\ &> 0. \end{aligned}$$

If $l \geq 8$ is even, let

$$G' = G - \{v_1v_l, v_3v_4, v_{l-2}v_{l-1}\} + \{v_2v_l, v_2v_4, v_{l-2}v_l\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-3}; T'_2, T_4, \dots, T_{l-2}, T'_l)$. We can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_2)$ and $V(T'_l)$ the same as $V(T_{i+1})$ and $V(T_i)$ in Fig. 2, respectively. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &> 2 \left(\sum_{v_i \in V(T_2)} x_i + x_l - x_{l-1} \right) \left(\sum_{v_i \in V(T_{\frac{l}{2}+1}) \cup \dots \cup V(T_{l-2})} x_i \right) \\ &= (h + f + d - c) \left(\sum_{v_i \in V(T_{\frac{l}{2}+1}) \cup \dots \cup V(T_{l-2})} x_i \right) \\ &> 0, \end{aligned}$$

which is a contradiction.

Subcase 3.3. $|V(T_2)| = 2, |V(T_3)| = 1$.

Then $v_3v_4, v_{l-1}v_l \in M(G)$. Since $|V(G)| \geq 10, |V(T_1)| = 2$ and $|V(T_l)| = 1$, we get $l \geq 7$.

If $l = 7$, we get $\rho(G) = 22.9172 > \rho(U_{10}^2) = 21.0245$, which is a contradiction.

If $l = 8$ and $|V(T_5)| = 1$, we get $\rho(G) = 23.3244 > \rho(U_{10}^2) = 21.0245$, which is a contradiction.

If $l = 8$ and $|V(T_5)| = 2$, we get $\rho(G) = 32.0000 > \rho(U_{12}^2) = 27.0578$, which is a contradiction.

If $l = 9$ and $|V(T_5)| = 1$ or $|V(T_7)| = 1$, we can deal with the case similarly to Subcase 1.3.

If $l = 9$ and $|V(T_5)| = 2$, $|V(T_7)| = 2$, we can deal with the case similarly to Subcase 3.2.

If $l \geq 10$, Let

$$G' = G - \{v_4v_5, v_{l-2}v_{l-1}\} + \{v_2v_5, v_1v_{l-2}\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_{l-4}; T'_1, T'_2, T_5, \dots, T_{l-2})$. We can denote the coordinates of Perron vector X corresponding to vertices in $V(T'_1)$ and $V(T'_2)$ the same as $V(T_i)$ and $V(T_{i+1})$ in Fig. 2, respectively. By Lemma 2.3 (i), from G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &> 4 \left(\sum_{v_i \in V(T_1)} x_i + \sum_{v_i \in V(T_2)} x_i - x_4 - x_{l-1} \right) \left(\sum_{v_i \in V(T_5) \cup \dots \cup V(T_{l-2})} x_i \right) \\ &= 4(c + d + h + f - b - g) \left(\sum_{v_i \in V(T_5) \cup \dots \cup V(T_{l-2})} x_i \right) \\ &> 0, \end{aligned}$$

which is a contradiction.

Case 4. For any $1 \leq i \leq l$, $|V(T_i)| = 1$.

Then $G = C_n$. By Lemma 2.5, we have $\rho(G) > \rho(U_n^2)$, which is a contradiction.

Claim 2. $l = 3$.

Otherwise, we have $l = 4$. Let $G = U(C_4; T_1, T_2, T_3, T_4)$ and $C_4 = v_1v_2v_3v_4v_1$. Since $|V(G)| \geq 10$, there must exist some $1 \leq i \leq 4$ such that $|V(T_i)| \geq 3$. We may assume that $|V(T_1)| \geq 3$ and $|V(T_1)|$ has the same parity as $|V(T_2)|$.

Suppose $N_{T_2}'(v_2) = \{v_{21}, \dots, v_{2s}\}$. Let

$$G' = G - \{v_2v_{21}, \dots, v_2v_{2s}\} + \{v_1v_{21}, \dots, v_1v_{2s}\}.$$

Then $G' \in \mathcal{U}(2k)$ and $G' = U(C_3; T'_1, T_3, T_4)$. From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= 2 \sum_{v_i \in V(T_1)} x_i \sum_{v_j \in V(T_2) \setminus R_{T_2}} x_j + 2 \sum_{v_i \in V(T_1)} x_i \sum_{v_j \in V(T_3)} x_j \\ &\quad - 2 \sum_{v_i \in V(T_2) \setminus R_{T_2}} x_i \sum_{v_j \in R_{T_2}} x_j - 2 \sum_{v_i \in R_{T_2}} x_i \sum_{v_j \in V(T_3)} x_j \\ &= 2 \left(\sum_{v_i \in V(T_1)} x_i - \sum_{v_j \in R_{T_2}} x_j \right) \left(\sum_{v_j \in V(T_2) \setminus R_{T_2}} x_j + \sum_{v_j \in V(T_3)} x_j \right) \\ &> 0, \end{aligned}$$

which is a contradiction.

Claim 3. $G = U_{2k}^2$.

Otherwise, let $G = U(C_3; T_1, T_2, T_3)$. There must exist some $1 \leq i, j \leq 3$ such that $|V(T_i)|$ is even and $|V(T_j)| > 1$. We may assume $|V(T_1)|$ is even, $|V(T_2)| > 1$ and $|V(T_2)| \geq |V(T_3)|$.

If $|V(T_2)| = 2$, then we have $|V(T_3)| = 2$. Suppose $R_{T_3} \setminus \{v_3\} = \{v'_3\}$. Let

$$G' = G - \{v_2v_3\} + \{v_1v'_3\}.$$

Then $G' = U_{2k}^2$. Using a symmetry, we get $x_3 = x_{v'_3}$ in G' . From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= 2x_{v'_3} \sum_{v_i \in V(T_1)} x_i - 2x_3 \sum_{v_i \in V(T_2)} x_i \\ &= 2x_3 \left(\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in V(T_2)} x_i \right). \end{aligned}$$

Since $|V(G)| \geq 10$ and $|V(T_2)| = |V(T_3)| = 2$, we have $|V(T_1)| \geq 6$. So, we have $\sum_{v_i \in V(T_1)} x_i - \sum_{v_i \in V(T_2)} x_i > 0$. This implies $\rho(G) > \rho(G')$, which is a contradiction.

If $|V(T_2)| > 2$, we may assume $N'_{T_1}(v_1) = \{v_{11}, \dots, v_{1r}\}$, $R_{T_1} \setminus \{v_1\} = \{v'_1\}$ and $N'_{T_3}(v_3) = \{v_{31}, \dots, v_{3t}\}$. Let

$$\begin{aligned} G' &= G - \{v_1v_3, v_1v_{11}, \dots, v_1v_{1r}\} - \{v_3v_{31}, \dots, v_3v_{3t}\} \\ &\quad + \{v_2v'_1, v_2v_{11}, \dots, v_2v_{1r}\} + \{v_2v_{31}, \dots, v_2v_{3t}\}. \end{aligned}$$

Then $G' = U_{2k}^2$. Using a symmetry, we get $x_1 = x_{v'_1}$ in G' . From G' to G , we have

$$\begin{aligned} \rho(G) - \rho(G') &\geq X^T (D(G) - D(G')) X \\ &= -2x_1 \left(\sum_{v_i \in V(T_1) \setminus R_{T_1}} x_i + \sum_{v_i \in R_{T_3}} x_i \right) + 2x_{v'_1} \left(\sum_{v_i \in V(T_2)} + \sum_{v_i \in V(T_3) \setminus R_{T_3}} x_i \right) \\ &\quad + 2 \sum_{v_i \in V(T_2)} x_i \left(\sum_{v_i \in V(T_1) \setminus R_{T_1}} x_i + \sum_{v_i \in V(T_3) \setminus R_{T_3}} x_i \right) \\ &\quad + 2 \sum_{v_i \in V(T_3) \setminus R_{T_3}} x_i \left(\sum_{v_i \in V(T_1) \setminus R_{T_1}} x_i - \sum_{v_i \in R_{T_3}} x_i \right) \\ &> 2 \left(\sum_{v_i \in V(T_2)} x_i - x_1 \right) \sum_{v_i \in V(T_1) \setminus R_{T_1}} x_i + 2 \left(x_1 + \sum_{v_i \in V(T_3) \setminus R_{T_3}} x_i \right) \left(\sum_{v_i \in V(T_2)} x_i - \sum_{v_i \in R_{T_3}} x_i \right) \\ &> 0, \end{aligned}$$

which is a contradiction. \square

Acknowledgment. The author would like to thank the anonymous referees for their valuable comments and suggestions.

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