

The spread of unicyclic graphs with given size of maximum matchings

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Abstract

The spread $s(G)$ of a graph G is defined as $s(G) = \max_{i,j} |\lambda_i - \lambda_j|$, where the maximum is taken over all pairs of eigenvalues of G . Let $U(n, k)$ denote the set of all unicyclic graphs on n vertices with a maximum matching of cardinality k , and $U^*(n, k)$ the set of triangle-free graphs in $U(n, k)$. In this paper, we determine the graphs with the largest and second largest spectral radius in $U^*(n, k)$, and the graph with the largest spread in $U(n, k)$.

KEY WORDS: spread, unicyclic graph, characteristic polynomial, eigenvalue

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1 Introduction

All graphs $G = (V, E)$ considered here are finite, undirected and simple. Let G be a graph with n vertices and $A(G)$ the adjacency matrix of G . The characteristic polynomial of $A(G)$ is $\phi(G, \lambda) = \det(\lambda I - A(G))$. The roots $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$ ($\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$) of $\phi(G, \lambda) = 0$ are called the eigenvalues of G . Since $A(G)$ is symmetric, all the eigenvalues of G are real.

The spread $s(G)$ of a graph G is defined as $s(G) = \max_{i,j} |\lambda_i - \lambda_j|$, where the maximum is taken over all pairs of eigenvalues of G . The spread of G is also defined as $s(G) = \lambda_1 - \lambda_n$, where λ_1, λ_n are the largest and least eigenvalues of $A(G)$, respectively. There have been some studies on

the spread of an arbitrary matrix and a graph (see [6, 12, 11, 9]).

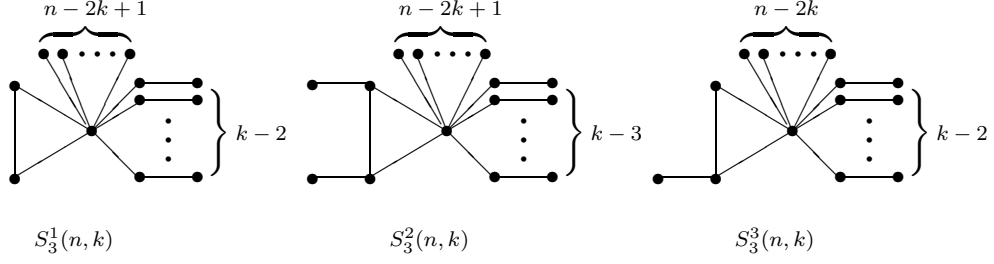


Fig. 1

Let $U(n, k)$ denote the set of all unicyclic graphs on n vertices with a maximum matching of cardinality k , and $U^*(n, k)$ the set of triangle-free graphs in $U(n, k)$. For a unicyclic graph G , let $C(G)$ denote the unique cycle of G and $g(G)$ the length of $C(G)$.

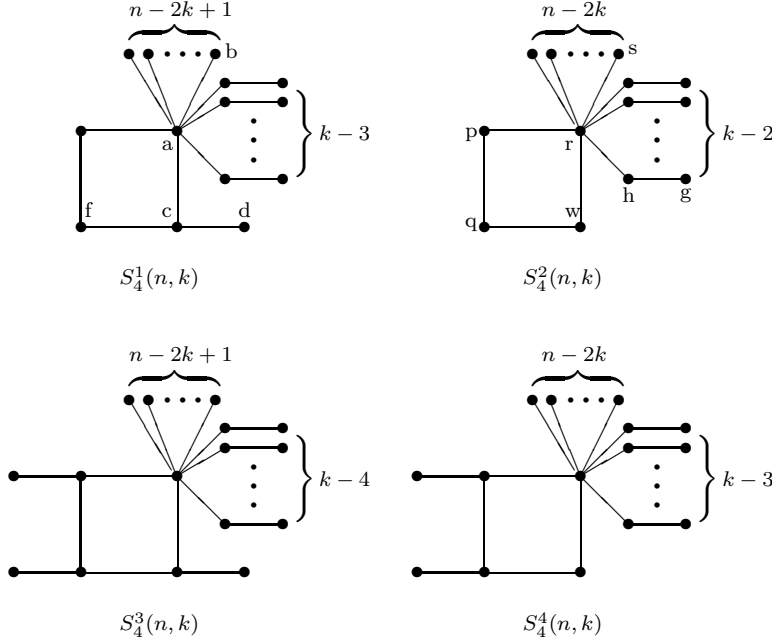


Fig. 2

Let $S_3^1(n, k)$ denote the graph on n vertices obtained from C_3 by attaching $n - 2k + 1$ pendant edges and $k - 2$ paths of length 2 to a vertex of C_3 , and $S_3^2(n, k)$ the graph on n vertices obtained from C_3 by attaching $n - 2k + 1$ pendant edges and $k - 3$ paths of length 2 to a vertex of C_3 , and one pendant edge to each of the other two vertices of C_3 . Let $S_3^3(n, k)$ denote the graph on n vertices obtained from C_3 by attaching $n - 2k$ pendant edges and $k - 2$ paths of length 2 to a vertex of C_3 , and one pendant edge to one of the other two vertices of C_3 (see Fig. 1).

Let $S_4^1(n, k)$ denote the graph on n vertices obtained from C_4 by attaching $n - 2k + 1$ pendant edges and $k - 3$ paths of length 2 to one vertex of

C_4 , and one pendant edge to the adjacent vertex of C_4 . Let $S_4^2(n, k)$ denote the graph on n vertices obtained from C_4 by attaching $n - 2k$ pendant edges and $k - 2$ paths of length 2 to one vertex of C_4 . Let $S_4^3(n, k)$ denote the graph obtained from $S_4^1(n - 3, k)$ by attaching three pendant edges to the three vertices of degree 2 in C_4 . Let $S_4^4(n, k)$ denote the graph obtained from $S_4^1(n - 1, k)$ by attaching one pendant edge to the vertex f (see Fig. 2).

In this paper, we show that $S_4^1(n, k), S_4^2(n, k) (n \geq 2k)$ are the graphs with the largest and second largest spectral radius in $U^*(n, k)$ respectively, and $S_3^1(n, k)$ is the graph with the largest spread in $U(n, k)$.

2 Graphs with the largest and second largest spectral radius in $U^*(n, k)$

Lemma 1 [2] *Let uv be an edge of G , then*

$$\phi(G, \lambda) = \phi(G - uv, \lambda) - \phi(G - u - v, \lambda) - 2 \sum_{C \in \mathcal{C}(uv)} \phi(G - C, \lambda),$$

where $\mathcal{C}(uv)$ is the set of cycles that containing uv ; In particular, if uv is a pendant edge with the pendant vertex v , then

$$\phi(G, \lambda) = \lambda \phi(G - v, \lambda) - \phi(G - u - v, \lambda).$$

Lemma 2 [10] *Let G_1 and G_2 be two graphs. If $\phi(G_1, \lambda) < \phi(G_2, \lambda)$ for all $\lambda \geq \lambda_1(G_2)$, then $\lambda(G_1) > \lambda_1(G_2)$.*

Lemma 3 [10] *Let G be a connected graph, and let G' be a proper spanning subgraph of G . Then*

$$\phi(G', \lambda) > \phi(G, \lambda) \quad \text{for all } \lambda \geq \lambda_1(G).$$

Furthermore, we have $\lambda_1(G) > \lambda_1(G')$.

Unicyclic graphs are also viewed as planting some trees at vertices of the unique cycle of G . So, we can view the vertices $r_i (i = 1, \dots, g)$ of $C_g(G)$ as roots, and T_i as planting tree at $r_i (r_i \in T_i)$.

Let $G \in U^*(2k, k)$. If $v \in V(T_i)$ is a vertex furthest from the root r_i , and the distance is less than 2, then v is a pendant vertex. Let u be the vertex adjacent to v . Then $d(u) = 2$. Otherwise, G has no perfect matching. We define a transformation (F): Deleting the other edge that incident to u and adding an edge $r_i u$. Carry out transformation (F) to T_i repeatedly, we can obtain the graph G' such that only some paths of length 2 and at most one edge are attached to r_i .

Lemma 4 [1] Let $G \in U^*(2k, k)$, G' be the graph as above. Then $G' \in U^*(2k, k)$ and

$$\phi(G, \lambda) > \phi(G', \lambda) \quad \text{for all } \lambda \geq \lambda_1(G).$$

In particular, $\lambda_1(G') > \lambda_1(G)$

If we apply transform (F) to all planting trees T_i ($i = 1, 2, \dots, g(G)$) of G repeatedly, we can finally obtain a graph G'' such that for any vertex w of $C(G'')$, there are only some paths of length 2 and at most one pendant vertex that are attached to w .

Lemma 5 [7] Let u and v be two vertices in a non-trivial connected graph G , and suppose that s paths of length 2 are attached to G at u , and t paths of length 2 are attached to G at v to form a graph $G_{s,t}$. Then either

$$\lambda_1(G_{s+i,t-i}) > \lambda_1(G_{s,t}) \quad (1 \leq i \leq t) \quad \text{or}$$

$$\lambda_1(G_{s-i,t+i}) > \lambda_1(G_{s,t}) \quad (1 \leq i \leq s).$$

Apply Lemma 4, 5, we can get a graph H in $U(2k, k)$ such that all paths of length 2 are attached to one vertex of $C(H)$, other vertices are pendant ones, and just one of those is joining to one vertex of $C(H)$.

Lemma 6 [1] Let G_i, G'_i ($i = 1, 2, 3$) be the graphs shown in Fig.3. Then

$$\phi(G_i, \lambda) > \phi(G'_i, \lambda) \quad \text{for all } \lambda \geq \lambda(G_i)$$

In particular, we have $\lambda_1(G_i) < \lambda_1(G'_i)$ for $i = 1, 2, 3$, respectively.

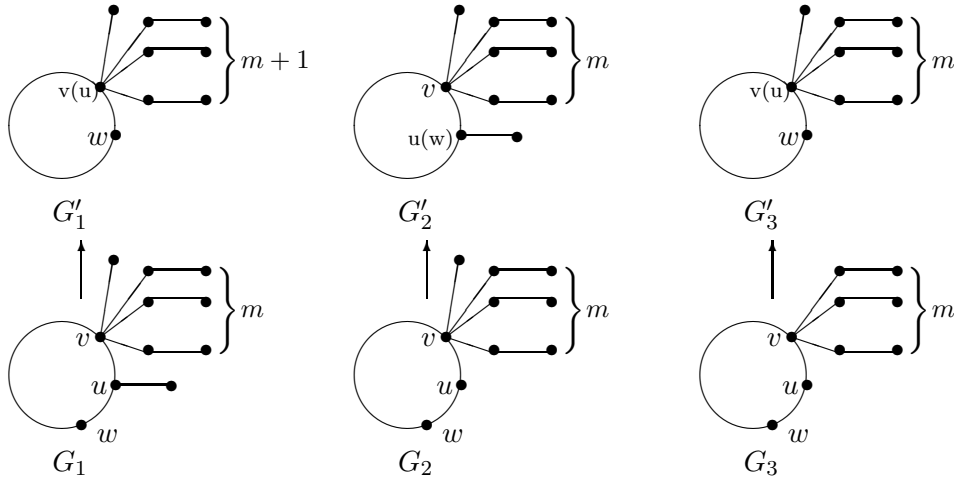


Fig.3

By Lemmas 3, 4, by a series of transforms, we can obtain a graph $G^* \in U^*(2k, k)$ such that $g(G^*) = 4$, a vertex of C_4 is attached by some paths of length 2 and at most one pendant vertex, and other vertices of C_4 are attached by at most one pendant vertex. Thus G^* must be a graph of Fig.2.

Lemma 7

$$\begin{aligned}\phi(S_4^1(2k, k), \lambda) &< \phi(S_4^2(2k, k), \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^2(2k, k)) \\ \phi(S_4^2(2k, k), \lambda) &< \phi(S_4^3(2k, k), \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^3(2k, k)) \\ \phi(S_4^3(2k, k), \lambda) &< \phi(S_4^4(2k, k), \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^4(2k, k)).\end{aligned}$$

In particular, $\lambda_1(S_4^1(2k, k)) > \lambda_1(S_4^2(2k, k)) > \lambda_1(S_4^3(2k, k)) > \lambda_1(S_4^4(2k, k))$.

Proof. Let $e = fc, e' = pq$ as shown in Fig.2. Delete e, e' from $S_4^1(2k, k), S_4^2(2k, k)$, respectively. By Lemma 1, we have

$$\begin{aligned}\phi(S_4^1(2k, k), \lambda) &= \phi(S_4^1(2k, k) - fc, \lambda) - \phi(S_4^1(2k, k) - f - c, \lambda) \\ &\quad - 2\phi(2K_1 \cup (k-3)K_2, \lambda) \\ \phi(S_4^2(2k, k), \lambda) &= \phi(S_4^2(2k, k) - pq, \lambda) - \phi(S_4^2(2k, k) - p - q, \lambda) \\ &\quad - 2\phi((k-2)K_2, \lambda)\end{aligned}$$

Obviously, $\phi(S_4^1(2k, k), \lambda) < \phi(S_4^2(2k, k), \lambda)$ for all $\lambda \geq \lambda_1(S_4^2(2k, k))$, since $S_4^1(2k, k) - f - c, 2K_1 \cup (k-3)K_2$ are subgraphs of $S_4^2(2k, k) - p - q, (k-2)K_2$ respectively, and $S_4^1(2k, k) - fc = S_4^2(2k, k) - pq$. By Lemma 2, we have $\lambda(S_4^1(2k, k)) > \lambda_1(S_4^2(2k, k))$.

Similarly, we can obtain

$$\begin{aligned}\phi(S_4^2(2k, k), \lambda) &< \phi(S_4^3(2k, k), \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^3(2k, k)) \\ \phi(S_4^3(2k, k), \lambda) &< \phi(S_4^4(2k, k), \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^4(2k, k)).\end{aligned}$$

Furthermore, we have $\lambda_1(S_4^2(2k, k)) > \lambda_1(S_4^3(2k, k)) > \lambda_1(S_4^4(2k, k))$. \square

In order to describe our results better, we first give the following lemma.

Lemma 8 *Let $G \in U^*(2k, k), G \not\cong S_4^1(2k, k), S_4^2(2k, k), v \in V(C(G))$. If there exist a path $P = vv_1v_2$ of length 2 attached to v and $G - v_1 - v_2 \not\cong S_4^1(2k-2, k-1)$, then*

$$\phi(G, \lambda) > \phi(S_4^2(2k, k), \lambda) \quad \text{for all } \lambda \geq \lambda_1(S_4^2(2k, k)).$$

Proof. By induction on k . By Lemma 1, we have

$$\begin{aligned}\phi(G, \lambda) &= \phi(G - vv_1, \lambda) - \phi(G - v - v_1, \lambda) \\ \phi(S_4^2(2k, k), \lambda) &= (\lambda^2 - 1)\phi(S_4^2(2k-2, k-1), \lambda) - \phi(P_3 \cup P_1 \cup (k-3)P_2, \lambda)\end{aligned}$$

Let $G - vv_1 = G' \cup v_1v_2$. Then $G' \in U^*(2(k-1), k-1)$, and $\phi(G, \lambda) = (\lambda^2 - 1)\phi(G', \lambda)$. By induction hypothesis, we have

$$(\lambda^2 - 1)\phi(S_4^2(2(k-1), k-1)) \leq (\lambda^2 - 1)\phi(G', \lambda), \quad \text{for } \lambda \geq \lambda_1(S_4^2(2k, k)).$$

If there is no pendant vertex attached to v , then $P_3 \cup P_1 \cup (k-3)P_2$ is subgraph of $G - v - v_1$. Using the result above and Lemmas 2 and 3, we can obtain the result.

If there exists a pendant vertex attached to v , then $P_4 \cup 2P_1 \cup (k-4)P_2$ is a subgraph of $G - v - v_1$. For $\lambda > \lambda_1(S_4^2(2k, k))$,

$$\begin{aligned} & \phi(P_3 \cup P_1 \cup (k-3)P_2, \lambda) - \phi(P_4 \cup 2P_1 \cup (k-4)P_2, \lambda) \\ &= \lambda^2(\lambda^2 - 2)(\lambda^2 - 1)^{k-3} - \lambda^2(\lambda^4 - 3\lambda^2 + 1)(\lambda^2 - 1)^{k-4} \\ &= \lambda^2(\lambda^2 - 1)^{k-4} > 0. \end{aligned}$$

Similarly, the result follows. \square

Lemma 9 *Let $G \in U^*(2k, k)$, and $G \not\cong S_4^1(2k, k)$ or $S_4^2(2k, k)$. Then*

$$\phi(S_4^2(2k, k), \lambda) < \phi(G, \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^2(2k, k)).$$

In particular, $\lambda_1(S_4^2(2k, k)) > \lambda_1(G)$.

Proof. It is trivial for $k = 2$. From the tables of [3, 4], we can obtain the result for $k = 3, 4$. Suppose now $k \geq 5$. If G is finally transformed into one of the graphs $S_4^2(2k, k)$, $S_4^3(2k, k)$ or $S_4^4(2k, k)$, then by Lemmas 5, 6, 7 and 8, the lemma holds. If G is transformed into $S_4^1(2k, k)$, let G' be transformed into $S_4^1(2k, k)$ at the last step, then $g(G') = 4$ or $g(G') = 5$.

If $g(G') = 5$, then G' satisfies the condition of Lemma 8. By Lemmas 5, 6 and 7, we can obtain the result.

If $g(G') = 4$, then either G' satisfies the condition of Lemma 8 or G' is the graph obtained from $S_4^1(8, 4)$ by attaching a path of length 2 to a vertex of planting subtree P_3 or a vertex of degree 3 in C_4 . we can obtain the result by simple computation and Lemmas 5, 6, 7 and 8. \square

Applying Lemmas 7 and 9, we can obtain

Lemma 10 *Let $G \in U^*(2k, k)$, and $G \not\cong S_4^1(2k, k)$, then*

$$\phi(S_4^1(2k, k), \lambda) < \phi(G, \lambda) \quad \text{for all } \lambda \geq \lambda(S_4^1(2k, k)).$$

In particular, $\lambda_1(S_4^1(2k, k)) > \lambda_1(G)$.

Lemma 11 [14] *Let $G \in U(n, k)$, $G \not\cong C_n$ ($n > 2k$). Then there is a maximal matching M and a pendant vertex v such that M does not meet v .*

Theorem 12 $S_4^1(n, k)$ is the graph with the maximal spectral radius in $U^*(n, k)$.

Proof. By induction on n . The result holds for $n = 2k$ by Lemma 7. Suppose that it is true for $n \leq m - 1$. Let $n = m$ ($m > 2k$). There exists a pendant edge e that does not belong to a maximal matching M of G . Let $e = wr$ with pendant vertex r . By Lemma 1, we have

$$\begin{aligned}\phi(S_4^1(n, k), \lambda) &= \lambda\phi(S_4^1(n-1, k), \lambda) - \phi(P_4 \cup (n-2k)K_1 \cup (k-3)K_2, \lambda) \\ \phi(G, \lambda) &= \lambda\phi(G-r, \lambda) - \phi(G-w-r, \lambda)\end{aligned}$$

where $G \in U^*(n, k)$, $G \not\cong S_4^1(n, k), S_4^2(n, k)$. By induction hypothesis, we have $\phi(S_4^1(n-1, k), \lambda) < \phi(G-r, \lambda)$ for $\lambda > \lambda_1(G-r)$.

It suffices to prove $\phi(P_4 \cup (n-2k)K_1 \cup (k-3)K_2, \lambda) > \phi(G-w-r, \lambda)$ for $\lambda > \lambda_1(G)$. Since any maximal matching M of G that misses r must meet w , otherwise $M \cup wr$ is a matching of G . $G-w-r$ has a maximal matching with value $k-1$.

Case 1: $P_4 \cup (n-2k)K_1 \cup (k-3)K_2$ is a subgraph of $G-w-r$. By Lemma 3, the result holds.

Case 2: $P_4 \cup (n-2k)K_1 \cup (k-3)K_2$ is not a subgraph of $G-w-r$. Let M' be an maximal matching of $G-w-r$. Let V' be the vertex set of M' , and $V'' = V(G-w-r) - V'$.

Claim 1. $G[V'']$ is empty. Otherwise, let $e_1 \in E(G[V''])$, then $M' \cup e_1$ is a matching of $G-w-r$ with cardinality k .

Claim 2. $G[V'] \setminus E(M')$ is empty.

Claim 3. $v \in V''$ is adjacent to at most one vertex of V' in $G-w-r$.

Claim 4. For any edge $e_2 = ij$ of M' , if i is adjacent to some vertices of V'' , then j must not be adjacent to any vertex of $G-w-r$ except for i .

Claim 5. $G-w-r$ contains no cycle.

Claim 6. $g(G) = 4$. If $g(G) \geq 5$, then $G-w-r$ can not satisfy the above claims.

So, the components of $G-w-r$ are isolated vertices, P_2 , or stars.

Let qx be an pendant edge of G with pendant vertex x . If q is not a vertex on the cycle, but q is adjacent to another pendant vertex in G , we can choose qx as deleting edge and x as deleting vertex. We know that $G-q-x$ contains a cycle. Then $P_4 \cup (n-2k)K_1 \cup (k-3)K_2$ must be a subgraph of $G-q-x$. Thus the result hold.

If G contains no such construction, then G must be a graph G'' as shown in Fig.4. Since $P_3 \cup (n-2k-1)K_1 \cup (k-2)K_2$ is a subgraph of $G''-r-z$ (or $G''-r'-z'$ or $G''-r''-z''$), we can easily obtain that $\lambda_1(S_4^2(n, k)) > \lambda_1(G'')$

by induction.

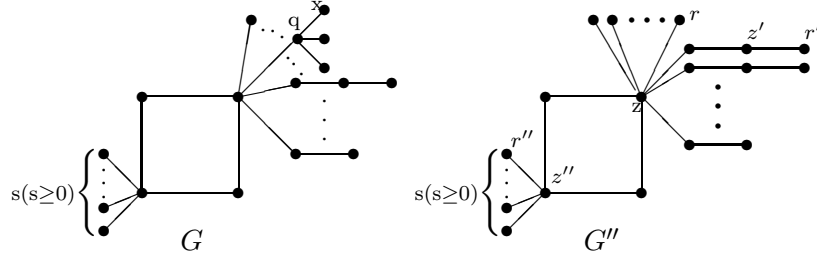


Fig. 4

In the following, we prove that $\lambda_1(S_4^1(n, k)) > \lambda_1(S_4^2(n, k))$.

Let c, d be vertices of $S_4^1(n, k)$ and g, h be vertices of $S_4^2(n, k)$ as shown in Fig.2. By Lemma 1, we have

$$\begin{aligned}\phi(S_4^1(n, k), \lambda) &= \lambda\phi(S_4^1(n, k) - d, \lambda) - \phi(S_4^1(n, k) - c - d, \lambda) \\ \phi(S_4^2(n, k), \lambda) &= \lambda\phi(S_4^2(n, k) - g, \lambda) - \phi(S_4^2(n, k) - h - g, \lambda).\end{aligned}$$

It is obvious that $S_4^1(n, k) - d \cong S_4^2(n, k) - g$, and that $S_4^1(n, k) - c - d$ is a subgraph of $S_4^2(n, k) - g - h$. By Lemmas 3 and 4, we can obtain the result. \square

Theorem 13 $S_4^2(n, k)$ is the graph with the second maximal spectral radius in $U^*(n, k)$.

Proof. By induction on n . Let v be the pendant vertex of G not met by a maximal matching M , u be its adjacent vertex. By Lemma 3, we have

$$\begin{aligned}\phi(S_4^2(n, k), \lambda) &= \lambda\phi(S_4^2(n-1, k), \lambda) - \phi((n-2k-1)K_1 \cup P_3 \cup (k-2)K_2, \lambda) \\ \phi(G, \lambda) &= \lambda\phi(G-v, \lambda) - \phi(G-u-v, \lambda)\end{aligned}$$

where $G \in U^*(n, k)$ and $G \not\cong S_4^1(n, k), S_4^2(n, k)$.

Case 1: $P_3 \cup (n-2k-1)K_1 \cup (k-2)K_2$ is a subgraph of $G-u-v$. By Lemma 3, the result holds.

Case 2: $P_3 \cup (n-2k-1)K_1 \cup (k-2)K_2$ is not a subgraph of $G-u-v$. M', V', V'' are defined as in Theorem 11. It is obvious that $E[V' : V'']$ and $E(G[V''])$ are empty. We also know that $E(G[V']) \setminus E(M)$ is not empty, otherwise we can not reconstruction G such that it contains a cycle. So, $P_4 \cup (n-2k)K_1 \cup (k-3)K_2$ is a subgraph of $G-u-v$.

By Lemma 3, for $\lambda > \lambda_1(G) > \lambda_1(G-u-v)$

$$\phi(P_4 \cup (n-2k)K_1 \cup (k-3)K_2, \lambda) > \phi(G-u-v, \lambda),$$

and since for $\lambda > \lambda_1(G)$

$$\begin{aligned} & \phi(P_3 \cup (n - 2k - 1)K_1 \cup (k - 2)K_2, \lambda) - \phi(P_4 \cup (n - 2k)K_1 \cup (k - 3)K_2, \lambda) \\ &= \lambda^{n-2k}(\lambda^2 - 2)(\lambda^2 - 1)^{k-2} - \lambda^{n-2k}(\lambda^4 - 3\lambda^2 + 1)(\lambda^2 - 1)^{k-3} \\ &= \lambda^{n-2k}(\lambda^2 - 1)^{k-3} > 0 \end{aligned}$$

combining the induction hypothesis and Lemmas 3 and 5, we can obtain the result. \square

3 The graph with maximal spread in $U(n, k)$

In order to describe our results, we need give some definitions and lemmas. Let $T(n, k)$ be the set of all trees on n vertices with a maximal matching of cardinality k . Let $A(n, k), B(n, k), C(n, k)$ be the trees as shown in Fig.5.

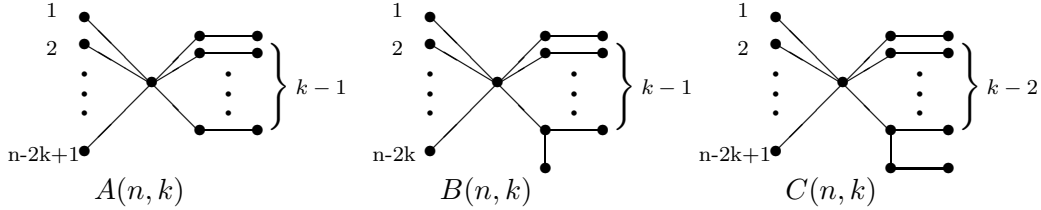


Fig. 5

Lemma 14 [8] $A(n, k), B(n, k)$ ($n > 2k$) are the graphs with the maximal and second maximal spectral radius in $T(n, k)$, respectively; $A(2k, k), C(2k, k)$ are the graphs with the maximal and second maximal spectral radius in $T(2k, k)$, respectively.

Lemma 15 [5] Let $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$ ($\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$) be the eigenvalues of graph G . If G is connected, then

$$|\lambda_i(G)| \leq \lambda_1(G), \quad i = 1, 2, \dots, n.$$

If G is bipartite, then $\lambda_1(G) = -\lambda_n(G)$.

Lemma 16 [14] $S_3^1(n, k)$ is the graph with the largest spectral radius in $U(n, k)$ except for $n = 2k = 6$.

Lemma 17 Let $G \in U(n, k), g(G) = 3$. Then there exists an edge e of $E(C_3)$ such that $\lambda_n(G - e) \leq \lambda_n(G)$.

Proof. Let $X = (x_1, x_2, x_3, \dots, x_n)^T$ be the unity eigenvector of $\lambda_n(G)$, where $C_3(G) = v_1 v_2 v_3$ and x_1, x_2, x_3 correspond to $v_1 v_2 v_3$, respectively.

Then there exist i, j ($1 \leq i \leq j \leq 3$) such that $x_i x_j \geq 0$. Otherwise, $x_1 x_2 < 0, x_2 x_3 < 0, x_3 x_1 < 0$, which is impossible. By Rayleigh quotient, we have

$$\begin{aligned}\lambda_n(G - v_i v_j) &\leq X^T A(G - v_i v_j) X = X^T A(G) X - 2x_i x_j \\ &= \lambda_n(G) - 2x_i x_j \leq \lambda_n(G)\end{aligned}$$

□

Lemma 18 *Let $G \in U(n, k)$, $g(G) = 3$, and $G \not\cong S_3^1(n, k)$. Then $\lambda_n(S_4^1(n, k)) \leq \lambda_n(G)$ for $k \geq 3$; $\lambda_n(S_4^2(n, k)) \leq \lambda_n(G)$ for $k = 2$.*

Proof. By Lemma 4, we can obtain a tree G' from G by deleting an edge of C_3 such that $\lambda_n(G') \leq \lambda_n(G)$.

If $G' \in T(n, k)$, by Lemma 3 we have $\lambda_1(A(n, k)) \geq \lambda_1(G')$. Since $A(n, k)$ is a subgraph of $S_4^1(n, k)$, by Lemma 3 we have $\lambda_1(S_4^1(n, k)) \geq \lambda_1(A(n, k))$. Since $S_4^1(n, k), G'$ are all bipartite, by Lemma 15 we have

$$\lambda_n(S_4^1(n, k)) = -\lambda_1(S_4^1(n, k)) \leq -\lambda_1(A(n, k)) \leq -\lambda_1(G') = \lambda_n(G') \leq \lambda_n(G).$$

If $G' \in T(n, k-1)$, since $G \not\cong S_3^1(n, k)$ we know $G' \not\cong A(n, k-1)$. Since $B(n, k-1)$ is a subgraph of $S_4^1(n, k)$, similarly, we can obtain $\lambda_n(S_4^1(n, k)) \leq \lambda_n(G)$.

If $k = 2$, we can obtain that $\lambda_1(S_4^2(n, k)) > \lambda_1(B(n, k-1))$ easily. Similar to the above proof, we can obtain the result. □

Lemma 19 $\lambda_n(S_3^1(n, k)) < \lambda_n(S_4^1(n, k))$ ($k \geq 3$), for $n \geq 17$; $\lambda_n(S_3^1(n, k)) < \lambda_n(S_4^2(n, k))$ ($k = 2$), for $n \geq 12$.

Proof. By Lemma 3, we can get

$$\begin{aligned}\phi(S_3^1(n, k), \lambda) &= \lambda^{n-2k}(\lambda^2 - 1)^{k-2}[\lambda^4 - (n - k + 2)\lambda^2 - 2\lambda + (n - 2k + 1)] \\ \phi(S_4^2(n, k), \lambda) &= \lambda^{n-2k}(\lambda^2 - 1)^{k-3}[\lambda^6 - (n - k + 3)\lambda^4 + (3n - 4k)\lambda^2 - (2n - 4k)] \\ \phi(S_4^1(n, k), \lambda) &= \lambda^{n-2k}(\lambda^2 - 1)^{k-4}[\lambda^8 - (n - k + 4)\lambda^6 + (4n - 5k + 2)\lambda^4 \\ &\quad - (4n - 7k + 3)\lambda^2 + n - 2k + 1]\end{aligned}$$

Let

$$\begin{aligned}f(x) &= x^4 - (n - k + 4)x^3 + (4n - 5k + 2)x^2 - (4n - 7k + 3)x + n - 2k + 1 \\ h(\lambda) &= \lambda^6 - (n - k + 3)\lambda^4 + (3n - 4k)\lambda^2 - (2n - 4k) \\ g(\lambda) &= \lambda^4 - (n - k + 2)\lambda^2 - 2\lambda + (n - 2k + 1).\end{aligned}$$

We know that $f(0) = n - 2k + 1 > 0$, $f(\frac{3-\sqrt{5}}{2}) = -x^3 < 0$ ($x > 0$), $f(1) = k - 3 > 0$, $f(\frac{3+\sqrt{5}}{2}) = -x^3 < 0$ ($x > 0$), $g(-\sqrt{n - k + 2}) = 2\sqrt{n - k + 2} + (n - 2k + 1) > 0$. Let $n = 2k + m$ ($k \geq 3$).

If $0 \leq m \leq k$, then

$$\begin{aligned}
g(-\sqrt{n-k+\frac{6}{5}}) &= -\frac{1}{5}(4k-m-\frac{1}{5}-10\sqrt{k+m+\frac{6}{5}}) < 0 \\
(m \leq k \quad k \geq 24, m \leq k-1 \quad k \geq 22, m \leq k-2 \quad k \geq 22, \\
m \leq k-3 \quad k \geq 20, m \leq k-4 \quad k \geq 19, m \leq k-5 \quad k \geq 17, \\
m \leq k-6 \quad k \geq 16, m \leq k-7 \quad k \geq 13, m \leq k-8 \quad k \geq 8) \\
f(n-k+\frac{6}{5}) &= \frac{1}{5}[(k+6m-\frac{44}{5})(5k+5m-9)-195] > 0 \\
(m \geq 0 \quad k \geq 13, m \geq 1 \quad k \geq 8, m \geq 20 \quad k \geq 5, m \geq 3 \quad k \geq 3)
\end{aligned}$$

Combining the Appendix Table, We can obtain that $\lambda_n(S_3^1(n, k)) < \sqrt{n-k+\frac{6}{5}} < \lambda_n(S_4^1(n, k))$, ($n \geq 18$).

If $m \geq k+1$, then

$$\begin{aligned}
g(-\sqrt{n-k+\frac{2}{3}}) &= -\frac{1}{3}(\sqrt{k+m+\frac{2}{3}}-3)^2 - k + 3 + \frac{1}{3} < 0 \\
(k \geq 4, k = 3 \quad m \geq 1) \\
f(n-k+\frac{2}{3}) &= \frac{1}{3}(k+m+\frac{2}{3})[(3k+3m-7)(-k+2m-\frac{20}{3})-75] + m + 1 > 0 \\
(m \geq k+1 \quad k \geq 7, m \geq k+2 \quad k \geq 6, m \geq k+3 \quad k \geq 4, m \geq k+5 \quad k \geq 3).
\end{aligned}$$

Combining the Appendix Table, we can obtain that $\lambda_n(S_3^1(n, k)) < \sqrt{n-k+\frac{2}{3}} < \lambda_n(S_4^1(n, k))$, ($n \geq 18$).

If $k = 2$. $h(x) = x^6 - (m+5)x^4 + (3m+4)x^2 - 2m = (x^2-1)[x^4 - (m+4)x^2 + 2m]$. When $m \geq 8$,

$$\begin{aligned}
g(2+m+\frac{1}{2}) &= -\frac{1}{2}(\sqrt{2+m+\frac{1}{2}}-2)^2 + \frac{1}{2} < 0 \\
\lambda_n(S_4^2(n, 2)) &= -\sqrt{\frac{(m+4)+\sqrt{m^2+16}}{2}} > -\sqrt{m+\frac{5}{2}}.
\end{aligned}$$

Thus, we have $\lambda_n(S_3^1(n, 2)) < -\sqrt{m+\frac{5}{2}} < \lambda_n(S_4^2(n, 2))$. □

Theorem 20 $S_3^1(n, k)$ ($n \geq 18 \quad k \geq 2$) is the graph with the largest spread in $U(n, k)$.

Proof. Let $G \in U(n, k)$. If $g(G) = 3$, by Lemmas 16 and 18, we can obtain $s(S_3^1(n, k)) > s(G)$. If $g(G) \geq 4$, by Lemmas 12, 15, 16 and 19 we can obtain $s(S_3^1(n, k)) > s(S_4^1(n, k)) \geq s(G)$ for $k \geq 3$ and $s(S_3^1(n, k)) > s(S_4^2(n, k)) \geq s(G)$ for $k = 2$. □

Remark: Theorem 20 is still true except for a few graphs (see the Appendix Table) with $n \leq 17$, for example, $S_4^1(15, 5)$. For convenience, we just consider the case for $n \geq 18$.

Lemma 21 $s(S_3^1(n, k)) < s(S_3^1(n, k-1))$ ($n \geq 18 \quad k \geq 3$).

Proof. We first prove that $\lambda_1(S_3^1(n, k)) < \lambda_1(S_3^1(n, k - 1))$. We can delete the pendant vertices v, b of $S_3^1(n, k - 1), S_3^1(n, k)$ respectively (see Fig.6).

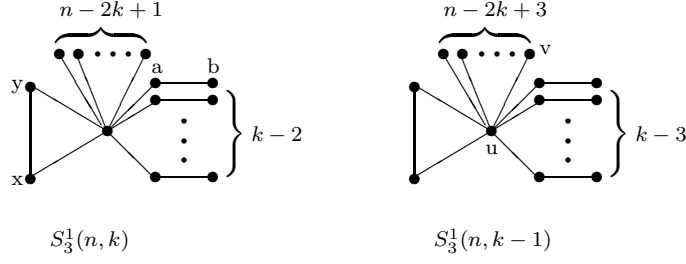


Fig. 6

Similar to the proof of Lemma 10, we can obtain the result. Since x, y are symmetrical, by Lemma 17 we have $\lambda_n(S_3^1(n, k) - xy) \leq \lambda_n(S_3^1(n, k))$. Since $\lambda_n(S_3^1(n, k) - xy)$ is a subgraph of $S_4^2(n, k - 1)$, then $\lambda_n(S_3^1(n, k) - xy) > \lambda_n(S_4^2(n, k - 1))$. By Lemmas 11 and 19, we have $\lambda_n(S_3^1(n, k - 1)) < \lambda_n(S_3^1(n, k))$. Thus $s(S_3^1(n, k)) < s(S_3^1(n, k - 1))$ ($k \geq 3$). \square

Using Theorem 20 and Lemma 21, it is not difficult to obtain the following theorem.

Theorem 22 $S_3^1(n, 2)$ ($n \geq 18$) is the unique graph with the largest spread in the class of all unicyclic graphs with n vertices.

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• Appendix Table

$n = 2k + m$		$\lambda_n(S_4^1(n, k))$	$\lambda_n(S_3^1(n, k))$
$k = 6$	$m = 8\ 7\ 6\ 5$	3.8256 3.6997 3.5705 3.4380	3.8570 3.7266 3.5917 3.4521
$k = 7$	$m = 7\ 6\ 5\ 4$	3.8347 3.7097 3.5815 3.4563	3.8662 3.7368 3.6032 3.4650
	$m = 3$	3.3160	3.3217
$k = 8$	$m = 8\ 7\ 6\ 5$	4.0834 3.9649 3.8437 3.7195	4.1213 4.0000 3.8753 3.7468
	$m = 4\ 3\ 2\ 1$	3.5923 3.4623 3.3295 3.1940	3.6144 3.4777 3.3363 3.1901
$k = 9$	$m = 9\ 8\ 7\ 6\ 5$	4.3187 4.2060 4.0909 3.9730 3.8525	4.3607 4.2462 4.1287 4.0082 3.8843
	$m = 4\ 3\ 2\ 1$	3.7292 3.6031 3.4742 3.3426	3.7568 3.6255 3.4901 3.3504
$k = 10$	$m = 10\ 9\ 8\ 7\ 6$	4.7560 4.6529 4.5479 4.4407 4.3313	4.5871 4.4783 4.3669 4.2529 4.1361
	$m = 5\ 4\ 3\ 2$	4.2196 4.1055 3.9890 3.8694	4.6162 3.8931 3.7666 3.6364
$k = 11$	$m = 11\ 10\ 9\ 8\ 7$	4.7560 4.6529 4.5479 4.4407 4.3313	4.8024 4.6985 4.5924 4.4840 4.3731
	$m = 6\ 5\ 4\ 3$	4.2196 4.1055 3.9890 3.8694	4.2597 4.1434 4.0242 3.9019
$k = 12$	$m = 12\ 11\ 10\ 9\ 8$	4.9607 4.8616 4.7607 4.6580 4.5532	5.0083 5.9086 4.8071 4.7035 4.5977
	$m = 7\ 6\ 5\ 4$	4.4464 4.3375 4.2263 4.1128	4.4897 4.3793 4.2663 4.1507
$k = 13$	$m = 15\ 14\ 13\ 12$	5.1574 5.0619 4.9648 4.8660	5.2057 5.1099 5.0123 4.9130
	$m = 11\ 10\ 9\ 8$	4.7634 4.6630 4.5586 4.4522	4.8117 4.7084 4.6030 4.4954
$k = 14$	$m = 14\ 13\ 12\ 11$	5.3471 5.2548 5.1611 5.0658	5.3958 5.3033 5.2093 5.1137
	$m = 10\ 9\ 8\ 7$	4.9690 4.8704 4.7701 4.6679	5.0164 4.9173 4.8163 4.7133
$k = 15$	$m = 15\ 14\ 13\ 12$	5.5303 5.4410 5.3504 5.2583	5.5792 5.4898 5.3990 5.3067
	$m = 11\ 10\ 9\ 8$	5.1648 5.0697 4.9731 4.8748	5.2129 5.1175 5.0204 4.9216
$k = 16$	$m = 16\ 15\ 14\ 13$	5.7078 5.6211 5.5333 5.4442	5.7567 5.6700 5.8214 5.4929
	$m = 12\ 11\ 10$	5.3337 5.2618 5.1685	5.4023 5.3102 5.2165
$k = 17$	$m = 17\ 16\ 15\ 14$	5.8799 5.7958 5.7105 5.6240	5.9288 5.8447 5.7594 5.6729
	$m = 13\ 12$	5.5363 5.4473	5.5851 5.4960
$k = 18$	$m = 18\ 17\ 16\ 15$	6.0472 5.9653 5.8824 5.7984	6.0960 6.0141 5.9312 5.8472
	$m = 14\ 13$	5.7132 5.6268	5.7620 5.6757
$k = 19$	$m = 19\ 18\ 17\ 16\ 15$	6.2169 6.1303 6.0495 5.9677 5.8849	6.2586 6.1789 6.0982 6.0164 5.9337
$k = 20$	$m = 20\ 19\ 18\ 17\ 16$	6.3688 6.2909 6.2122 6.1325 6.0517	6.4170 6.3393 6.2607 6.1810 6.1004
$k = 21$	$m = 21\ 20\ 19\ 18$	6.524 6.4476 6.3707 6.2930	6.5716 6.4957 6.4190 6.3413
$k = 22$	$m = 22\ 21\ 20$	6.6750 6.6006 6.5255	6.7226 6.6484 6.5734
$k = 23$	$m = 23$	6.8230	6.8703