

The spread of unicyclic graphs with given size of maximum matchings

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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 [9,11,12]).

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

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in $U(n, k)$. For a unicyclic graph G , let $C(G)$ denote the unique cycle of G and $g(G)$ the length of $C(G)$.

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 figure 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 figure 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

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

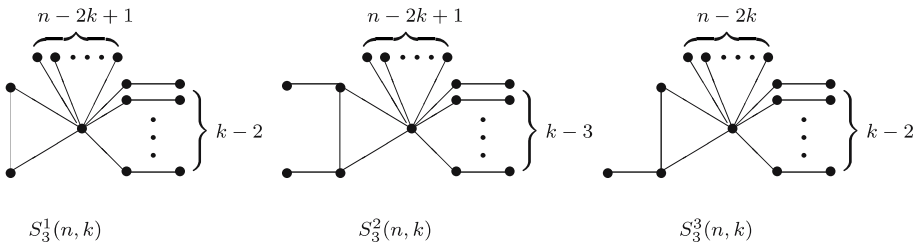


Figure 1. Graphs $S_3^1(n, k), S_3^2(n, k)$ and $S_3^3(n, k)$.

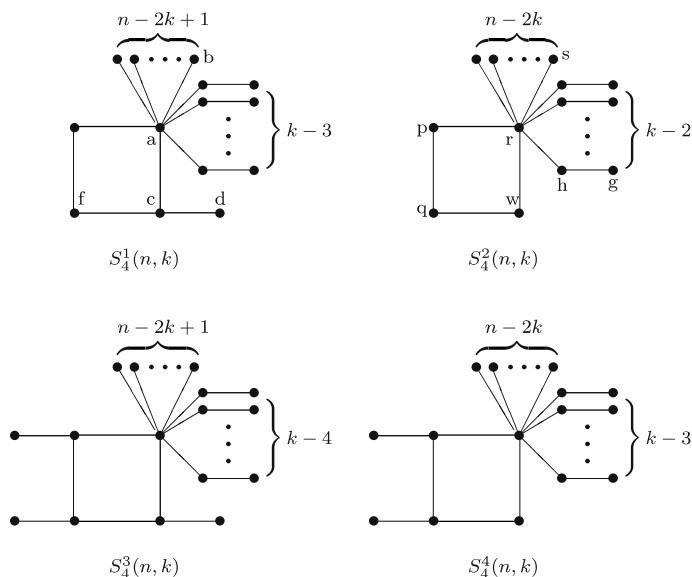


Figure 2. Graphs $S_4^i(n, k)$ for $i = 1, 2, 3, 4$.

Lemma 2 [10, 13]. 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 lemmas 4 and 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 figure 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.

By lemmas 3 and 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 edge, and other vertices of C_4 are attached by at most one pendant edge. Thus G^* must be a graph of figure 2.

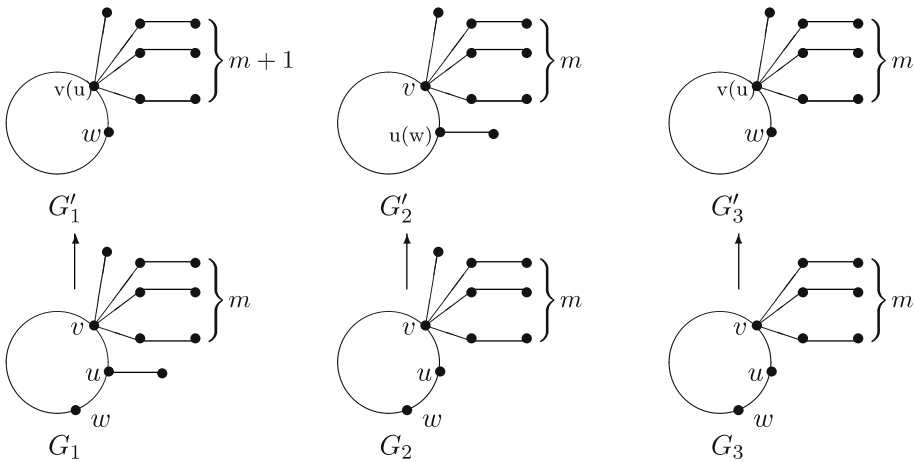


Figure 3. Graphs G_i and G'_i for $i = 1, 2, 3$.

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 figure 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 $S_4^1(2k, k) - fc \cong S_4^2(2k, k) - pq$. 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 $\lambda_1(S_4^2(2k, k)) > \lambda_1(S_4^3(2k, k)) > \lambda_1(S_4^4(2k, k))$. □

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 exists 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

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

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

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

If there is no pendant vertex adjacent 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 adjacent to v , then $P_4 \cup 2P_1 \cup (k - 4)P_2$ is a subgraph of $G - v - v_1$. For $\lambda > \lambda_1(G)$,

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

Similarly, the result follows. □

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

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

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. □

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

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

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 figure 4. Since, $P_3 \cup (n - 2k - 1)K_1 \cup (k - 2)K_2$ is a subgraph of $G'' - r - z$

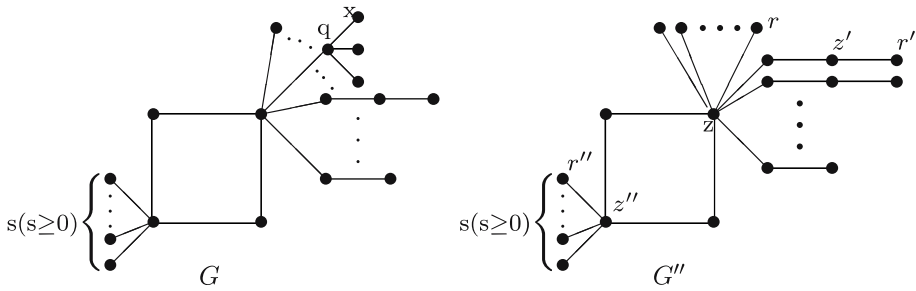


Figure 4. Graphs G and G'' .

(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.

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 figure 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. □

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 figure 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 $\lambda_n(G - e) \leq \lambda_n(G)$.

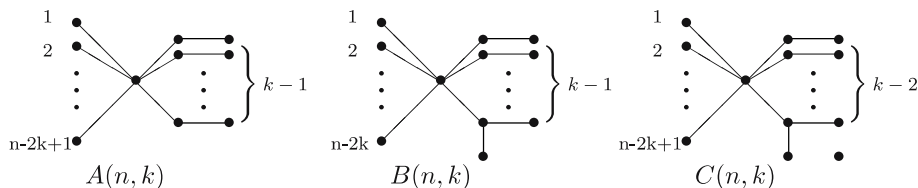


Figure 5. Graphs $A(n, k), B(n, k)$, and $C(n, k)$.

Proof. Let $X = (x_1, x_2, x_3, \dots, x_n)^T$ be the unity eigenvector of $\lambda_n(G)$, where $C_3(G) = v_1v_2v_3$ and x_1, x_2, x_3 correspond to $v_1v_2v_3$, respectively. Then there exist i, j ($1 \leq i < j \leq 3$) such that $x_ix_j \geq 0$. Otherwise, $x_1x_2 < 0, x_2x_3 < 0, x_3x_1 < 0$, which is impossible. By Rayleigh quotient, we have

$$\begin{aligned} \lambda_n(G - v_iv_j) &\leq X^T A(G - v_iv_j)X = X^T A(G)X - 2x_ix_j \\ &= \lambda_n(G) - 2x_ix_j \leq \lambda_n(G). \end{aligned}$$

□

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 $n \geq 18; \lambda_n(S_3^1(n, k)) < \lambda_n(S_4^2(n, k))$ ($k = 2$), 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

$$g(-\sqrt{n - k + \frac{6}{5}}) = -\frac{1}{5}(4k - m - \frac{1}{5} - 10\sqrt{k + m + \frac{6}{5}}) < 0$$

$$(m \leq k \quad k \geq 24, m \leq k - 1 \quad k \geq 22, m \leq k - 2 \quad k \geq 22,$$

$$m \leq k - 3 \quad k \geq 20, m \leq k - 4 \quad k \geq 19, m \leq k - 5 \quad k \geq 17,$$

$$m \leq k - 6 \quad k \geq 16, m \leq k - 7 \quad k \geq 13, m \leq k - 8 \quad k \geq 8)$$

$$f(n - k + \frac{6}{5}) = \frac{1}{5}[(k + 6m - \frac{44}{5})(5k + 5m - 9) - 195] > 0$$

$$(m \geq 0 \quad k \geq 13, m \geq 1 \quad k \geq 8, m \geq 20 \quad k \geq 5, m \geq 3 \quad k \geq 3).$$

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

$$g(-\sqrt{n - k + \frac{2}{3}}) = -\frac{1}{3}(\sqrt{k + m + \frac{2}{3}} - 3)^2 - k + 3 + \frac{1}{3} < 0(k \geq 4, k = 3 \quad m \geq 1)$$

$$f(n - k + \frac{2}{3}) = \frac{1}{3}(k + m + \frac{2}{3})[(3k + 3m - 7)$$

$$(-k + 2m - \frac{20}{3}) - 75] + m + 1 > 0$$

$$(m \geq k + 1 \quad k \geq 7, m \geq k + 2 \quad k \geq 6, m \geq k + 3 \quad k \geq 4,$$

$$m \geq k + 5 \quad k \geq 3).$$

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 $m \geq 8$,

$$g(2 + m + \frac{1}{2}) = -\frac{1}{2}(\sqrt{2 + m + \frac{1}{2}} - 2)^2 + \frac{1}{2} < 0$$

$$\lambda_n(S_4^2(n, 2)) = -\sqrt{\frac{(m + 4) + \sqrt{m^2 + 16}}{2}} > -\sqrt{m + \frac{5}{2}}.$$

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

Appendix table

$n = 2k + m$	$\lambda_n(S_4^1(n, k))$	$\lambda_n(S_3^1(n, k))$
$k = 6 \quad m = 8 \ 7 \ 6 \ 5$	3.8256 3.6997 3.5705 3.4380	3.8570 3.7266 3.5917 3.4521
$k = 7 \quad m = 7 \ 6 \ 5 \ 4$	3.8347 3.7097 3.5815 3.4563	3.8662 3.7368 3.6032 3.4650
$\quad \quad m = 3$	3.3160	3.3217
$k = 8 \quad m = 8 \ 7 \ 6 \ 5$	4.0834 3.9649 3.8437 3.7195	4.1213 4.0000 3.8753 3.7468
$\quad \quad m = 4 \ 3 \ 2 \ 1$	3.5923 3.4623 3.3295 3.1940	3.6144 3.4777 3.3363 3.1901
$k = 9 \quad m = 9 \ 8 \ 7 \ 6 \ 5$	4.3187 4.2060 4.0909 3.9730 3.8525	4.3607 4.2462 4.1287 4.0082 3.8843
$\quad \quad m = 4 \ 3 \ 2 \ 1$	3.7292 3.6031 3.4742 3.3426	3.7568 3.6255 3.4901 3.3504
$k = 10 \quad m = 10 \ 9 \ 8 \ 7 \ 6$	4.7560 4.6529 4.5479 4.4407 4.3313	4.5871 4.4783 4.3669 4.2529 4.1361
$\quad \quad m = 5 \ 4 \ 3 \ 2$	4.2196 4.1055 3.9890 3.8694	4.6162 3.8931 3.7666 3.6364
$k = 11 \quad m = 11 \ 10 \ 9 \ 8 \ 7$	4.7560 4.6529 4.5479 4.4407 4.3313	4.8024 4.6985 4.5924 4.4840 4.3731
$\quad \quad m = 6 \ 5 \ 4 \ 3$	4.2196 4.1055 3.9890 3.8694	4.2597 4.1434 4.0242 3.9019
$k = 12 \quad m = 12 \ 11 \ 10 \ 9 \ 8$	4.9607 4.8616 4.7607 4.6580 4.5532	5.0083 5.9086 4.8071 4.7035 4.5977
$\quad \quad m = 7 \ 6 \ 5 \ 4$	4.4464 4.3375 4.2263 4.1128	4.4897 4.3793 4.2663 4.1507
$k = 13 \quad m = 15 \ 14 \ 13 \ 12$	5.1574 5.0619 4.9648 4.8660	5.2057 5.1099 5.0123 4.9130
$\quad \quad m = 11 \ 10 \ 9 \ 8$	4.7634 4.6630 4.5586 4.4522	4.8117 4.7084 4.6030 4.4954
$k = 14 \quad m = 14 \ 13 \ 12 \ 11$	5.3471 5.2548 5.1611 5.0658	5.3958 5.3033 5.2093 5.1137
$\quad \quad m = 10 \ 9 \ 8 \ 7$	4.9690 4.8704 4.7701 4.6679	5.0164 4.9173 4.8163 4.7133
$k = 15 \quad m = 15 \ 14 \ 13 \ 12$	5.5303 5.4410 5.3504 5.2583	5.5792 5.4898 5.3990 5.3067
$\quad \quad m = 11 \ 10 \ 9 \ 8$	5.1648 5.0697 4.9731 4.8748	5.2129 5.1175 5.0204 4.9216
$k = 16 \quad m = 16 \ 15 \ 14 \ 13$	5.7078 5.6211 5.5333 5.4442	5.7567 5.6700 5.5824 5.4929
$\quad \quad m = 12 \ 11 \ 10$	5.3337 5.2618 5.1685	5.4023 5.3102 5.2165
$k = 17 \quad m = 17 \ 16 \ 15 \ 14$	5.8799 5.7958 5.7105 5.6240	5.9288 5.8447 5.7594 5.6729
$\quad \quad m = 13 \ 12$	5.5363 5.4473	5.5851 5.4960
$k = 18 \quad m = 18 \ 17 \ 16 \ 15$	6.0472 5.9653 5.8824 5.7984	6.0960 6.0141 5.9312 5.8472
$\quad \quad m = 14 \ 13$	5.7132 5.6268	5.7620 5.6757
$k = 19 \quad m = 19 \ 18 \ 17 \ 16 \ 15$	6.2169 6.1303 6.0495 5.9677 5.8849	6.2586 6.1789 6.0982 6.0164 5.9337
$k = 20 \quad m = 20 \ 19 \ 18 \ 17 \ 16$	6.3688 6.2909 6.2122 6.1325 6.0517	6.4170 6.3393 6.2607 6.1810 6.1004
$k = 21 \quad m = 21 \ 20 \ 19 \ 18$	6.524 6.4476 6.3707 6.2930	6.5716 6.4957 6.4190 6.3413
$k = 22 \quad m = 22 \ 21 \ 20$	6.6750 6.6006 6.5255	6.7226 6.6484 6.5734
$k = 23 \quad m = 23$	6.8230	6.8703

Theorem 20. $S_3^1(n, k)$ ($n \geq 18, k \geq 2$) 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 $n \geq 18$.

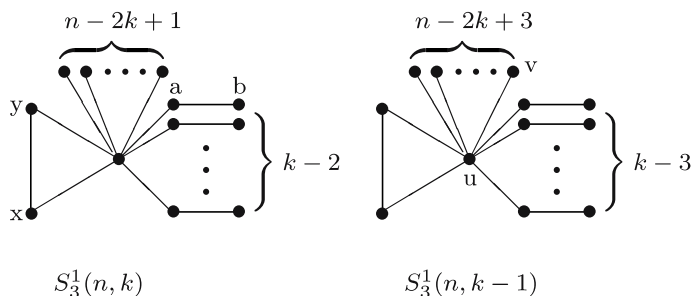


Figure 6. Graphs $S_3^1(n, k)$, $S_3^1(n, k - 1)$ and vertices a, b, u, v .

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

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 figure 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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