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Spectral properties of a class of unicyclic graphs

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Abstract

The eigenvalues of G are denoted by $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$, where n is the order of G. In particular, $\lambda_1(G)$ is called the spectral radius of G, $\lambda_n(G)$ is the least eigenvalue of G, and the spread of G is defined to be the difference between $\lambda_1(G)$ and $\lambda_n(G)$. Let $\mathbb{U}(n)$ be the set of n-vertex unicyclic graphs, each of whose vertices on the unique cycle is of degree at least three. We characterize the graphs with the kth maximum spectral radius among graphs in $\mathbb{U}(n)$ for $k = 1$ if $n \geq 6$, $k = 2$ if $n \geq 8$, and $k = 3, 4, 5$ if $n \geq 10$, and the graph with minimum least eigenvalue (maximum spread, respectively) among graphs in $\mathbb{U}(n)$ for $n \geq 6$.

MSC: 05C50; 15A42

Keywords: spectral radius; least eigenvalue; spread; unicyclic graphs

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $\mathbf{A}(G)$ be the adjacency matrix of G. The characteristic polynomial of G is the characteristic polynomial of $\mathbf{A}(G)$, denoted by $\phi(G, x)$. The eigenvalues of G, denoted by $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$, are the eigenvalues of $\mathbf{A}(G)$, arranged in a non-increasing order, where n is the order of G.

In particular, $\lambda_1(G)$ is called the spectral radius of G, and we usually use $\lambda_n(G)$ to represent the least eigenvalue of G. The spread of G, denoted by $s(G)$, is the difference between the largest and the least eigenvalues, i.e., $s(G) = \lambda_1(G) - \lambda_n(G)$.

By the Perron-Frobenius theorem [1], for a connected graph G, corresponding to $\lambda_1(G)$, there is a unit eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ with all positive entries, known as the principal eigenvector of G. For a connected graph G, it is well known that [1]

$$\lambda_1(G) \geq -\lambda_n(G)$$

with equality if and only if G is bipartite.

A unicyclic graph is a connected graph with a unique cycle. The spectral radius of unicyclic graphs has been studied extensively these years. Guo [2] determined the graphs with the first ten maximum spectral radii among all the n-vertex unicyclic graphs for $n \geq 17$. Belardo *et al.* [3] determined the maximum spectral radius of unicyclic graphs with given girth. Yu and Tian [4] gave the first two spectral radii of unicyclic graphs with a given matching number. More results on the spectral radius of unicyclic graphs can be found in [5–7].

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The least eigenvalue of graphs is a relatively new topic in spectral graph theory. Fan *et al.* [8] characterized the graph with minimum least eigenvalue (the graph with maximum spread, respectively) among all the *n*-vertex unicyclic graphs for $n \geq 4$. Zhai *et al.* [9] determined the minimum least eigenvalue of unicyclic graphs with given diameter. Du [10] presented the first six minimum least eigenvalues of unicyclic graphs. This paper will continue the research of the spectral properties of unicyclic graphs, such as spectral radius, the least eigenvalue, and the spread.

A unicyclic graph is called fully loaded if every vertex on its unique cycle has degree at least three. Let $\mathbb{U}(n)$ be the set of *n*-vertex fully loaded unicyclic graphs, where $n \geq 6$. In this paper, we characterize the graphs with the *k*th maximum spectral radius among graphs in $\mathbb{U}(n)$ for $k = 1$ if $n \geq 6$, $k = 2$ if $n \geq 8$, and $k = 3, 4, 5$ if $n \geq 10$, and the graph with minimum least eigenvalue (maximum spread, respectively) among graphs in $\mathbb{U}(n)$ for $n \geq 6$.

2 Preliminaries

We use standard notation from spectral graph theory [1].

Let **x** be a unit eigenvector of G corresponding to $\lambda_1(G)$ or $\lambda_n(G)$. We say x_v is the element of **x** corresponding to $v \in V(G)$.

Lemma 1 ([3, 11]) *Let G be a connected graph, $rs \in E(G)$ and $rt \notin E(G)$. Let G' be the graph obtained from G by deleting the edge rs and adding the edge rt. Let **x** and **x**' be, respectively, the principal eigenvectors of G and G'. If $x_t \geq x_s$, then $\lambda_1(G') > \lambda_1(G)$ and $x'_t > x'_s$.*

For $u \in V(G)$, let $d_G(u)$ be the degree of u in G. A pendent vertex is a vertex of degree one.

Lemma 2 ([12]) *Let G be a connected graph with $uv \in E(G)$ and $d_G(u), d_G(v) \geq 2$. Suppose that u and v have no common neighbor. Let G' be the graph obtained from G by deleting the edge uv and identifying u and v, which is denoted by w, and attaching a pendent vertex to w. Then $\lambda_1(G') > \lambda_1(G)$.*

For a vertex subset V' of G, let $G - V'$ denote the graph formed from G by deleting all the vertices in V' and their incident edges. In particular, we write $G - u$ for $G - \{u\}$.

Lemma 3 ([1]) *Let v be a vertex of a graph G different from a cycle, and let $\varphi(v)$ be the set of the cycles containing v. Then*

$$\phi(G, x) = x \cdot \phi(G - v, x) - \sum_{vw \in E(G)} \phi(G - v - w, x) - 2 \sum_{Z \in \varphi(v)} \phi(G - V(Z), x).$$

In particular, if v is a pendent vertex of G with unique neighbor u, then

$$\phi(G, x) = x \cdot \phi(G - v, x) - \phi(G - v - u, x),$$

where $\phi(G - v - u, x) = 1$ if $G = P_2$.

Lemma 4 ([11, 13]) *Let G be a connected non-trivial graph, and let H be a proper spanning subgraph of G. Then $\phi(H, x) > \phi(G, x)$ for $x \geq \lambda_1(G)$.*

Lemma 5 *Let G_0 be a connected graph with at least three vertices, where $u, v \in V(G_0)$, and let H_0 be a connected graph with $w \in V(H_0)$. Let G_1 (G_2, respectively) be the graph obtained from G_0 and H_0 by identifying u (v, respectively) with w. Let $\mathbf{y}$ ($\mathbf{y}'$, respectively) be a unit eigenvector of G_1 (G_2, respectively) corresponding to $\lambda_n(G_1)$ ($\lambda_n(G_2)$, respectively). Suppose that $|y_u| \leq |y_v|$.*

    (i) *[8] $\lambda_n(G_1) \geq \lambda_n(G_2)$ with equality if and only if $y_u = y_v$ and $\sum y_j = 0$, where the summation takes over all the neighbors of w in H_0.*

    (ii) *If $\lambda_n(G_1) > \lambda_n(G_2)$, then $|y'_u| < |y'_v|$.*

Proof We need only to prove (ii). If $|y'_u| \geq |y'_v|$, then by (i), $\lambda_n(G_1) \leq \lambda_n(G_2)$, which is a contradiction. □

By Lemma 5(i), we have the following.

Lemma 6 ([8]) *Let u be a vertex of a connected graph Q with at least two vertices. For integer $a \geq 1$, let G_1 be the graph obtained by attaching a star S_{a+1} at its center v to u of Q, and G_2 be the graph obtained by attaching $a + 1$ pendent vertices to u of Q. Then $\lambda_n(G_1) \geq \lambda_n(G_2)$.*

For an edge subset M of G, let $G - M$ denote the graph obtained from G by deleting the edges in M, and for an edge subset M^* of the complement of G, let $G + M^*$ denote the graph obtained from G by adding the edges in M^*.

3 Large spectral radius of graphs in $\mathbb{U}(n)$

In this section, we determine the first five maximum spectral radii of graphs in $\mathbb{U}(n)$.

Let $U_{n,m}$ be the unicyclic graph obtained from the cycle $C_m = v_1 v_2 \cdots v_m v_1$ by attaching $n - 2m + 1$ pendent vertices to v_1 and a pendent vertex to each of the other vertices on C_m. Obviously, $U_{n,m} \in \mathbb{U}(n)$.

Lemma 7 *Let $G \in \mathbb{U}(n)$ with unique cycle of length $m \geq 3$, where $n \geq 2m$. Then $\lambda_1(G) \leq \lambda_1(U_{n,m})$ with equality if and only if $G \cong U_{n,m}$.*

Proof Let G be a graph with maximum spectral radius satisfying the given condition. Let $C_m = v_1 v_2 \cdots v_m v_1$ be the unique cycle of G. By Lemma 2, the vertices of G outside C_m are all pendent vertices.

Suppose that $G \not\cong U_{n,m}$. Then we may choose two vertices, say v_i and v_j, on C_m such that $d_G(v_i), d_G(v_j) \geq 4$, where $1 \leq i < j \leq m$. Let $\mathbf{x}$ be the principal eigenvector of G. Suppose without loss of generality that $x_{v_i} \geq x_{v_j}$. Consider $G_1 = G - vv_j + vv_i$, where v is a neighbor of v_j outside C_m. Obviously, $G_1 \in \mathbb{U}(n)$ and its unique cycle is still of length m. By Lemma 1, $\lambda_1(G) < \lambda_1(G_1)$, which is a contradiction. Thus there is at most one vertex on C_m with degree at least four in G, *i.e.*, $G \cong U_{n,m}$. □

Lemma 8 *Let $G \in \mathbb{U}(n)$ with unique cycle of length $m \geq 4$, where $n \geq 2m$. Then $\lambda_1(G) \leq \lambda_1(U_{n,4})$ with equality if and only if $G \cong U_{n,4}$.*

Proof If $m \geq 5$, then applying Lemma 2 to $G = U_{n,m}$ by setting uv to be an edge on the cycle incident to the vertex of maximum degree, we have $\lambda_1(U_{n,m}) < \lambda_1(U_{n,m-1})$, and thus

$\lambda_1(U_{n,m}) < \lambda_1(U_{n,4})$. If $m = 4$, then by Lemma 7, $\lambda_1(G) \leq \lambda_1(U_{n,4})$ with equality if and only if $G \cong U_{n,4}$. □

Let $C_3(T_1, T_2, T_3)$ be the n-vertex unicyclic graph with the triangle $v_1 v_2 v_3 v_1$ such that the deletion of the three edges on the triangle would result in three vertex-disjoint trees T_1, T_2, T_3, where $v_i \in V(T_i)$ for $i = 1, 2, 3$.

Let $S_n(a, b, c) = C_3(T_1, T_2, T_3)$, where $|V(T_1)| = a - 1$, $|V(T_2)| = b - 1$, $|V(T_3)| = c - 1$, $a + b + c = n + 3$, $a \geq b \geq c \geq 2$, and T_1, T_2, T_3 are all stars with centers v_1, v_2, v_3, respectively. Obviously, $S_n(n - 3, 3, 3) \cong U_{n,3}$.

Lemma 9 *Among the graphs $S_n(a, b, c)$ with $a + b + c = n + 3$ and $a \geq b \geq c \geq 3$, $S_n(n - 3, 3, 3) \cong U_{n,3}$ for $n \geq 6$, $S_n(n - 4, 4, 3)$ for $n \geq 8$, and $S_n(n - 5, 5, 3)$ for $n \geq 10$ are, respectively, the unique graphs with the first, the second, and the third maximum spectral radii.*

Proof Let **x** be the principal eigenvector of $S_n(a, b, c)$.

Suppose that $a > b$. If $x_{v_1} < x_{v_2}$, then by Lemma 1,

$$\lambda_1(S_n(a, b, c)) < \lambda_1(S_n(a - 1, b + 1, c)) < \cdots < \lambda_1(S_n(b, a, c)),$$

which is a contradiction. If $x_{v_1} \geq x_{v_2}$, then by Lemma 1,

$$\lambda_1(S_n(a, b, c)) < \lambda_1(S_n(a + 1, b - 1, c)).$$

If $a = b$, then whether $x_{v_1} \geq x_{v_2}$ or $x_{v_1} < x_{v_2}$, we have by Lemma 1 that

$$\lambda_1(S_n(a, b, c)) < \lambda_1(S_n(a + 1, b - 1, c)).$$

Then

$$\lambda_1(S_n(a, b, c)) < \lambda_1(S_n(a + 1, b - 1, c))$$

for $b \geq 4$. This implies that among the graphs $S_n(a, b, 3)$ with $a + b + 3 = n + 3$ and $a \geq b \geq 3$, $S_n(n - 3, 3, 3) \cong U_{n,3}$ for $n \geq 6$, $S_n(n - 4, 4, 3)$ for $n \geq 8$, and $S_n(n - 5, 5, 3)$ for $n \geq 10$ are, respectively, the unique graphs with the first, the second, and the third maximum spectral radius.

If $c \geq 4$, then by similar arguments as above,

$$\lambda_1(S_n(a, b, c)) \leq \lambda_1(S_n(n - 5, 4, 4)) < \lambda_1(S_n(n - 5, 5, 3)).$$

Now the result follows. □

Let U_n^1 be the unicyclic graph obtained by attaching a path on two vertices to the vertex of degree $n - 5$ of $S_{n-2}(n - 5, 3, 3)$, where $n \geq 8$. Let U_n^2 be the unicyclic graph obtained by attaching a path on two vertices to the vertex of degree two of $S_{n-2}(n - 4, 3, 2)$, where $n \geq 7$. Let U_n^3 be the unicyclic graph obtained by attaching a path on two vertices to the vertex of degree $n - 6$ of $S_{n-2}(n - 6, 4, 3)$, where $n \geq 10$.

For $u, v \in V(G)$, let $d_G(u, v)$ be the distance from u to v in G.

Let P_n be the path on n vertices. Let $G \cup H$ be the vertex-disjoint union of graphs G and H.

Lemma 10 *Let $G = C_3(T_1, T_2, T_3)$ with $|V(T_1)| = a-1$, $|V(T_2)| = b-1$, $|V(T_3)| = 2$, $a+b = n$, $a \geq b$, $b = 3, 4$, and $n \geq 10$. Suppose that $G \not\cong S_n(a, b, c), U_n^1, U_n^2$. Then $\lambda_1(G) < \lambda_1(S_n(n-5, 5, 3))$.*

Proof First suppose that $b = 3$. Let $r = \max\{d_G(u, v_1) : u \in V(T_1)\}$. Obviously, $r \geq 2$ as $G \not\cong S_n(a, b, c)$.

If $r \geq 3$, then by Lemma 2, we may get a unicyclic graph with $r = 2$ with a larger spectral radius.

Suppose that $r = 2$.

If there are at least two non-pendent neighbors of v_1 outside the triangle in G, then by Lemma 2, we may get a unicyclic graph with exactly one non-pendent neighbor of v_1 outside the triangle with a larger spectral radius.

Suppose that there is exactly one non-pendent neighbor, say w, of v_1 outside the triangle of G. Let $d_G(v_1) = s$ and $d_G(w) = t$. Obviously, $s \geq 3$, and $t \geq 3$ as $G \not\cong U_n^1$. If $t = 3$, then G is the graph obtained by attaching a pendent vertex to the vertex of degree two in U_{n-1}^1, which is denoted by L_n. If $t = n-5$, then G is the graph obtained by attaching $n-6$ pendent vertices to a pendent vertex of $S_6(3, 3, 3)$, which is denoted by H_n.

Suppose that $4 \leq t \leq n - 6$. Let $\mathbf{x}$ be the principal eigenvector of G. If $x_w \geq x_{v_1}$, then by Lemma 1, $\lambda_1(G) < \lambda_1(H_n)$. If $x_w < x_{v_1}$, then by Lemma 1, $\lambda_1(G) < \lambda_1(L_n)$. Thus

$$\lambda_1(G) < \max\{\lambda_1(L_n), \lambda_1(H_n)\}.$$

Now we compare $\lambda_1(L_n)$ with $\lambda_1(H_n)$. Let $r_n(x) = \phi(L_n, x) - \phi(H_n, x)$. Applying Lemma 3 to $G = L_n$ by setting v to be a pendent neighbor of v_1,

$$\phi(L_n, x) = x \cdot \phi(L_{n-1}, x) - x^{n-9}\phi(P_3 \cup P_4, x),$$

and to $G = H_n$ by setting v to be a pendent vertex whose unique neighbor is of degree $n-5$,

$$\phi(H_n, x) = x \cdot \phi(H_{n-1}, x) - x^{n-7}\phi(S_5(3, 3, 2), x),$$

which implies that

$$\begin{aligned}
r_n(x) &= x \cdot r_{n-1}(x) + x^{n-7}\phi(S_5(3, 3, 2), x) - x^{n-9}\phi(P_3 \cup P_4, x) \\
&= x \cdot r_{n-1}(x) + x^{n-7}(x^5 - 5x^3 - 2x^2 + 3x) \\
&\quad - x^{n-9}(x^3 - 2x)(x^4 - 3x^2 + 1) \\
&= x \cdot r_{n-1}(x) + 2x^{n-8}(1 - 2x^2 - x^3).
\end{aligned}$$

Note that $r_8(x) = 0$ as $L_8 = H_8$, and it is easily seen that $1 - 2x^2 - x^3 < 0$ for $x > 1$, and thus $r_n(x) < 0$ (*i.e.*, $\phi(L_n, x) < \phi(H_n, x)$) for $x > 1$, which implies that $\lambda_1(L_n) > \lambda_1(H_n)$. Then

$$\lambda_1(G) \leq \lambda_1(L_n)$$

if $b = 3$.

Suppose that $b = 4$. First suppose that $d_G(v_2) = 3$. Note that $G \not\cong U_n^2$, then by similar arguments as above, $\lambda_1(G) \leq \lambda_1(H)$, where H is the graph obtained by attaching a path on two vertices to the vertex of degree $n - 6$ in U_{n-2}^2. By Lemma 2, $\lambda_1(H) < \lambda_1(U_n^3)$. If $d_G(v_2) = 4$, then by similar arguments as above, $\lambda_1(G) \leq \lambda_1(U_n^3)$. Thus

$$\lambda_1(G) \leq \lambda_1\left(U_n^3\right)$$

if $b = 4$.

Now we have shown that

$$\lambda_1(G) \leq \max\left\{\lambda_1(L_n), \lambda_1\left(U_n^3\right)\right\}$$

for $b = 3$ or 4.

To determine $\max\{\lambda_1(L_n), \lambda_1(U_n^3)\}$, we compare $\lambda_1(U_n^3)$ with $\lambda_1(L_n)$. Let $T^{(1)}$ be the $(n-3)$-vertex tree obtained by attaching $n - 8$ pendent vertices to the center of the path on five vertices. Applying Lemma 3 to $G = U_n^3$ by setting v to be a pendent neighbor of v_2,

$$\phi\left(U_n^3, x\right) = x \cdot \phi\left(U_{n-1}^1, x\right) - x \cdot \phi\left(T^{(1)}, x\right),$$

and to $G = L_n$ by setting v to be a pendent vertex in T_1 of degree three,

$$\phi(L_n, x) = x \cdot \phi\left(U_{n-1}^1, x\right) - x \cdot \phi\left(S_{n-3}(n - 6, 3, 3), x\right).$$

Note that $T^{(1)}$ is a proper spanning subgraph of $S_{n-3}(n - 6, 3, 3)$, and thus by Lemma 4, $\phi(S_{n-3}(n - 6, 3, 3), x) < \phi(T^{(1)}, x)$ for $x \geq \lambda_1(S_{n-3}(n - 6, 3, 3))$, which implies that $\phi(U_n^3, x) < \phi(L_n, x)$ for $x \geq \lambda_1(S_{n-3}(n - 6, 3, 3))$, i.e., $\lambda_1(U_n^3) > \lambda_1(L_n)$. Thus

$$\lambda_1(G) \leq \lambda_1\left(U_n^3\right)$$

for $b = 3$ or 4.

Now we are left to compare $\lambda_1(U_n^3)$ with $\lambda_1(S_n(n - 5, 5, 3))$. Let $T^{(2)}$ be the $(n-4)$-vertex tree obtained by attaching $n - 7$ pendent vertices to an end vertex of the path on three vertices. Applying Lemma 3 to $G = U_n^3$ by setting v to be a pendent vertex whose unique neighbor is of degree two,

$$\phi\left(U_n^3, x\right) = x \cdot \phi\left(S_{n-1}(n - 5, 4, 3), x\right) - \phi\left(S_{n-2}(n - 6, 4, 3), x\right),$$

and to $G = S_n(n - 5, 5, 3)$ by setting v to be a pendent neighbor of v_2,

$$\phi\left(S_n(n - 5, 5, 3), x\right) = x \cdot \phi\left(S_{n-1}(n - 5, 4, 3), x\right) - x^2 \cdot \phi\left(T^{(2)}, x\right).$$

Note that $P_1 \cup P_1 \cup T^{(2)}$ is a proper spanning subgraph of $S_{n-2}(n - 6, 4, 3)$, and thus by Lemma 4, $\phi(S_{n-2}(n - 6, 4, 3), x) < x^2 \cdot \phi(T^{(2)}, x)$ for $x \geq \lambda_1(S_{n-2}(n - 6, 4, 3))$, which implies that $\phi(U_n^3, x) > \phi(S_n(n-5, 5, 3), x)$ for $x \geq \lambda_1(S_{n-2}(n-6, 4, 3))$, i.e., $\lambda_1(U_n^3) < \lambda_1(S_n(n-5, 5, 3))$.

Then the result follows. □

Lemma 11 *For* $n \geq 8$, $\lambda_1(U_n^2) < \lambda_1(U_n^1) < \lambda_1(S_n(n-4,4,3))$, *for* $n = 10$, $\lambda_1(U_n^2) < \lambda_1(U_n^1) < \lambda_1(S_n(n-5,5,3))$, *for* $n = 11$, $\lambda_1(U_n^2) < \lambda_1(S_n(n-5,5,3)) < \lambda_1(U_n^1)$, *and for* $n \geq 12$, $\lambda_1(S_n(n-5,5,3)) < \lambda_1(U_n^2) < \lambda_1(U_n^1)$.

Proof Let T be the $(n-3)$-vertex tree obtained by attaching $n-6$ pendent vertices to an end vertex of the path on three vertices.

Applying Lemma 3 to $G = U_n^1$ by setting v to be a pendent vertex whose unique neighbor is of degree two,

$$\phi(U_n^1, x) = x \cdot \phi(S_{n-1}(n-4,3,3), x) - \phi(S_{n-2}(n-5,3,3), x),$$

and to $G = S_n(n-4,4,3)$ by setting v to be a pendent neighbor of v_2,

$$\phi(S_n(n-4,4,3), x) = x \cdot \phi(S_{n-1}(n-4,3,3), x) - x \cdot \phi(T, x).$$

Note that $P_1 \cup T$ is a proper spanning graph of $S_{n-2}(n-5,3,3)$, and thus by Lemma 4,

$$x \cdot \phi(T, x) > \phi(S_{n-2}(n-5,3,3), x)$$

for $x \geq \lambda_1(S_{n-2}(n-5,3,3))$, which implies that

$$\phi(U_n^1, x) > \phi(S_n(n-4,4,3), x)$$

for $x \geq \lambda_1(S_{n-2}(n-5,3,3))$, i.e., $\lambda_1(U_n^1) < \lambda_1(S_n(n-4,4,3))$.

By Lemma 3, we have

$$\phi(U_n^1, x) = x^{n-8}[x^8 - nx^6 - 2x^5 + (4n-17)x^4 + 2x^3 - (4n-24)x^2 + n - 7],$$
$$\phi(U_n^2, x) = x^{n-6}[x^6 - nx^4 - 2x^3 + (4n-17)x^2 + 2x - 3n + 17],$$
$$\phi(S_n(n-5,5,3), x) = x^{n-6}[x^6 - nx^4 - 2x^3 + (5n-28)x^2 - 3n + 21],$$

and thus

$$\phi(U_n^1, x) - \phi(U_n^2, x) = -x^{n-8}(n-7)(x+1)(x-1),$$
$$\phi(U_n^2, x) - \phi(S_n(n-5,5,3), x) = x^{n-6}(n-7)f(x),$$

where

$$f(x) = (11 - n)x^2 + 2x - 4.$$

Obviously, $\phi(U_n^1, x) < \phi(U_n^2, x)$ for $x > 1$, i.e., $\lambda_1(U_n^1) > \lambda_1(U_n^2)$.

Note that $\lambda_1(G) > 2$ if G is a unicyclic graph different from a cycle. If $n = 10$, then

$$f(x) = x^2 + 2x - 4 > 0$$

for $x > 2$. If $n = 11$, then

$$f(x) = 2x - 4 > 0$$

for $x > 2$. If $n \geq 12$, then

$$f(x) = (11 - n)x^2 + 2x - 4$$

$$< (11 - n)2^2 + 2 \cdot 2 - 4 = 4(11 - n) < 0.$$

Thus $f(x) > 0$ for $x > 2$ if $n = 10, 11$ and $f(x) < 0$ for $x > 2$ if $n \geq 12$, which implies that $\lambda_1(U_n^2) < \lambda_1(S_n(n - 5, 5, 3))$ for $n = 10, 11$ and $\lambda_1(U_n^2) > \lambda_1(S_n(n - 5, 5, 3))$ for $n \geq 12$.

By direct calculation, we have $\lambda_1(U_n^1) < \lambda_1(S_n(n - 5, 5, 3))$ for $n = 10$ and $\lambda_1(U_n^1) > \lambda_1(S_n(n - 5, 5, 3))$ for $n = 11$.

The result follows easily.　　　　　　　　　　　　　　　　　　　　　　　　　　　□

Now we prove our main result in this section.

Theorem 1 *Among the graphs in* $\mathbb{U}(n)$,
  (i) $U_{n,3} \cong S_n(n - 3, 3, 3)$ *for* $n \geq 6$ *and* $S_n(n - 4, 4, 3)$ *for* $n \geq 8$ *are respectively the unique graphs with the first and the second maximum spectral radii;*
  (ii) $S_n(n - 5, 5, 3)$ *for* $n = 10$ *and* U_n^1 *for* $n \geq 11$ *are the unique graphs with the third maximum spectral radius;*
  (iii) $S_n(n - 5, 4, 4)$ *for* $n = 10$, $S_n(n - 5, 5, 3)$ *for* $n = 11$, *and* U_n^2 *for* $n \geq 12$ *are the unique graphs with the fourth maximum spectral radius;*
  (iv) U_n^1 *for* $n = 10$, U_n^2 *for* $n = 11$, *and* $S_n(n - 5, 5, 3)$ *for* $n \geq 12$ *are the unique graphs with the fifth maximum spectral radius,*

and the spectral radii of $U_{n,3} \cong S_n(n - 3, 3, 3)$, $S_n(n - 4, 4, 3)$, $S_n(n - 5, 5, 3)$, U_n^1 *and* U_n^2 *are, respectively, the largest roots of the equations on* x *as follows*:

$$x^6 - nx^4 - 2x^3 + (3n - 12)x^2 - n + 5 = 0,$$

$$x^6 - nx^4 - 2x^3 + (4n - 19)x^2 - 2n + 12 = 0,$$

$$x^6 - nx^4 - 2x^3 + (5n - 28)x^2 - 3n + 21 = 0,$$

$$x^8 - nx^6 - 2x^5 + (4n - 17)x^4 + 2x^3 - (4n - 24)x^2 + n - 7 = 0,$$

$$x^6 - nx^4 - 2x^3 + (4n - 17)x^2 + 2x - 3n + 17 = 0.$$

Proof Let $G \in \mathbb{U}(n)$ with unique cycle of length $m \geq 3$, where $n \geq 2m$.

If $m \geq 4$, then by Lemmas 8 and 2,

$$\lambda_1(G) \leq \lambda_1(U_{n,4}) < \lambda_1\big(S_n(n - 5, 5, 3)\big).$$

Suppose in the following that $m = 3$. Then $G \cong C_3(T_1, T_2, T_3)$, where $|V(T_1)| = a - 1$, $|V(T_2)| = b - 1$, $|V(T_3)| = c - 1$, $a + b + c = n + 3$, $a \geq b \geq c \geq 3$.

If $G \cong S_n(a, b, c)$, then by Lemma 9, $U_{n,3} \cong S_n(n - 3, 3, 3)$, $S_n(n - 4, 4, 3)$ and $S_n(n - 5, 5, 3)$ are, respectively, the unique graphs with the first, the second and the third maximum spectral radii.

Suppose that $G \not\cong S_n(a, b, c)$. If $c \geq 4$, then by Lemmas 2 and 9, $\lambda_1(G) < \lambda_1(S_n(n - 5, 5, 3))$. Suppose that $c = 3$. If $b = 3$ or 4 and $G \not\cong U_n^1, U_n^2$, then by Lemma 10, $\lambda_1(G) < \lambda_1(S_n(n - 5, 5, 3))$. If $b \geq 5$, then by Lemmas 2 and 9, $\lambda_1(G) < \lambda_1(S_n(n - 5, 5, 3))$. Thus

$$\lambda_1(G) < \lambda_1\big(S_n(n - 5, 5, 3)\big)$$

if $G \ncong S_n(n-3,3,3), S_n(n-4,4,3), S_n(n-5,5,3), U_n^1, U_n^2$ for $n \geq 10$.

It follows from Lemma 11 that

$$\lambda_1(U_n^2) < \lambda_1(U_n^1) < \lambda_1(S_n(n-4,4,3))$$

for $n \geq 8$, and thus (i) follows.

Suppose that $G \ncong S_n(n-3,3,3), S_n(n-4,4,3)$.

Suppose that $n = 10$. If $m \geq 4$, then by Lemma 8 and direct calculation,

$$\lambda_1(G) \leq \lambda_1(U_{10,4}) < \lambda_1(U_{10}^1).$$

Suppose that $m = 3$. If $G \cong S_{10}(a,b,c)$, then $G \cong S_{10}(5,5,3)$ or $S_{10}(5,4,4)$. Suppose that $G \ncong S_{10}(a,b,c), U_{10}^1$. If $c \geq 4$, then by Lemmas 1 and 2, we may construct another graph still different from $S_{10}(a,b,c)$ and U_{10}^1 with a larger spectral radius. Suppose that $c = 3$. If $b = 3$ or 4 and $G \ncong U_{10}^2$, then similar to the proof of Lemma 10 and direct calculation,

$$\lambda_1(G) \leq \lambda_1(U_{10}^3) < \lambda_1(U_{10}^2) < \lambda_1(U_{10}^1).$$

If $b \geq 5$, then by Lemmas 1 and 2, we may construct another graph still different from $S_{10}(a,b,c)$ and U_{10}^1 with a larger spectral radius. So if $G \ncong S_{10}(a,b,c), U_{10}^1$, then

$$\lambda_1(G) < \lambda_1(U_{10}^1).$$

Now by direct calculation,

$$\lambda_1(U_{10}^1) < \lambda_1(S_{10}(5,4,4)) < \lambda_1(S_{10}(5,5,3)),$$

and thus the result for $n = 10$ follows.

Suppose that $n = 11$. If $m \geq 4$, then by Lemma 8 and direct calculation,

$$\lambda_1(G) \leq \lambda_1(U_{11,4}) < \lambda_1(U_{11}^2).$$

Suppose that $m = 3$. If $G \cong S_{11}(a,b,c)$, then $G \cong S_{11}(6,5,3), S_{11}(6,4,4)$, or $S_{11}(5,5,4)$. Suppose that $G \ncong S_{11}(a,b,c), U_{11}^1, U_{11}^2$. If $c \geq 4$, then by Lemmas 1 and 2, either $\lambda_1(G) < \lambda_1(U_{11}^2)$, or we may construct another graph still different from $S_{11}(a,b,c), U_{11}^1$ and U_{11}^2 with a larger spectral radius. Suppose that $c = 3$. If $b = 3$ or 4, then similar to the proof of Lemma 10 and direct calculation,

$$\lambda_1(G) \leq \lambda_1(U_{11}^3) < \lambda_1(U_{11}^2) < \lambda_1(U_{11}^1).$$

If $b \geq 5$, then by Lemmas 1 and 2, either $\lambda_1(G) < \lambda_1(U_{11}^2)$, or we may construct another graph still different from $S_{11}(a,b,c), U_{11}^1$ and U_{11}^2 with a larger spectral radius. So if $G \ncong S_{11}(a,b,c), U_{11}^1, U_{11}^2$, then

$$\lambda_1(G) < \lambda_1(U_{11}^2).$$

Now by direct calculation,

$$\lambda_1\big(S_{11}(5,5,4)\big) < \lambda_1\big(S_{11}(6,4,4)\big) < \lambda_1\big(U_{11}^2\big) < \lambda_1\big(S_{11}(6,5,3)\big) < \lambda_1\big(U_{11}^1\big),$$

and thus the result for $n = 11$ follows.

If $n \geq 12$, then the result follows from Lemma 11. □

4 The least eigenvalue of graphs in $\mathbb{U}(n)$

In this section, we determine the minimum least eigenvalue of graphs in $\mathbb{U}(n)$.

Lemma 12 *Let $G \in \mathbb{U}(n)$ with unique cycle of length m, where $n \geq 2m \geq 8$. Then $\lambda_n(G) \geq \lambda_n(U_{n,4})$ with equality if and only if $G \cong U_{n,4}$.*

Proof If $m \geq 4$, then by Lemma 8, the Perron-Frobenius theorem [1] and noting that $U_{n,4}$ is a bipartite graph, we have

$$-\lambda_n(G) \leq \lambda_1(G) \leq \lambda_1(U_{n,4}) = -\lambda_n(U_{n,4}),$$

and thus $\lambda_n(G) \geq \lambda_n(U_{n,4})$ with equality if and only if $G \cong U_{n,4}$. □

Lemma 13 *If $G \cong S_n(a,b,c)$ with $a + b + c = n + 3$ and $a \geq b \geq c \geq 3$, then $S_n(n-3,3,3) \cong U_{n,3}$ for $n \geq 6$ is the unique graph with minimum least eigenvalue.*

Proof Let $\mathbf{x}$ be a unit eigenvector of $S_n(a,b,c)$ corresponding to $\lambda_n(S_n(a,b,c)) = \lambda_n$.

Denote by u_1, u_2, u_3 a pendent neighbor of v_1, v_2, v_3 in $S_n(a,b,c)$, respectively. It is easily seen that

$$x_{u_1} = \frac{x_{v_1}}{\lambda_n}, \qquad x_{u_2} = \frac{x_{v_2}}{\lambda_n}, \qquad x_{u_3} = \frac{x_{v_3}}{\lambda_n}.$$

Suppose that $x_{u_2} = 0$ and $x_{v_1} = x_{v_2}$. Then $x_{v_1} = x_{v_2} = 0$. Since

$$\lambda_n x_{v_2} = (b-2)x_{u_2} + x_{v_1} + x_{v_3},$$

we have $x_{v_3} = 0$, and thus $x_{u_3} = 0$, *i.e.*, $\mathbf{x} = 0$, which is a contradiction. Then either $x_{u_2} \neq 0$ or $x_{v_1} \neq x_{v_2}$.

Suppose that $a > b$. If $|x_{v_1}| < |x_{v_2}|$, then by Lemma 5,

$$\lambda_n\big(S_n(a,b,c)\big) > \lambda_n\big(S_n(a-1,b+1,c)\big) > \cdots > \lambda_n\big(S_n(b,a,c)\big),$$

which is a contradiction. If $|x_{v_1}| \geq |x_{v_2}|$, then by Lemma 5(i) and noting that either $x_{u_2} \neq 0$ or $x_{v_1} \neq x_{v_2}$,

$$\lambda_n\big(S_n(a,b,c)\big) > \lambda_n\big(S_n(a+1,b-1,c)\big).$$

If $a = b$, then whether $|x_{v_1}| \geq |x_{v_2}|$ or $|x_{v_1}| < |x_{v_2}|$, by Lemma 5(i),

$$\lambda_n\big(S_n(a,b,c)\big) > \lambda_n\big(S_n(a+1,b-1,c)\big).$$

Then

$$\lambda_n\big(S_n(a,b,c)\big) > \lambda_n\big(S_n(a+1,b-1,c)\big)$$

for $b \geq 4$, and thus the result follows easily. □

Lemma 14 *Let* $G \cong C_3(T_1, T_2, T_3)$ *with* $a + b + c = n + 3$, $|V(T_1)| = a - 1$, $|V(T_2)| = b - 1$, $|V(T_3)| = c - 1$, $a \geq b \geq c \geq 3$, *and* $n \geq 7$. *Suppose that* $G \not\cong S_n(a,b,c)$. *Then* $\lambda_n(G) > \lambda_n(S_n(n-3,3,3))$.

Proof If $b \geq 4$ or $c \geq 4$, then by Lemmas 6 and 13,

$$\lambda_n(G) \geq \lambda_n\big(S_n(a,b,c)\big) > \lambda_n\big(S_n(n-3,3,3)\big).$$

Suppose that $b = c = 3$. Let $r = \max\{d_G(u,v_1) : u \in V(T_1)\}$. Obviously, $r \geq 2$ as $G \not\cong S_n(a,b,c)$.

If $r \geq 3$, then by Lemma 6, we may get a graph $G' \not\cong S_n(a,b,c)$ with $r = 2$ such that $\lambda_n(G) \geq \lambda_n(G')$.

Suppose that $r = 2$.

If there are at least two non-pendent neighbors of v_1 outside the triangle in G, then by Lemma 6, we may get a graph $G'' \not\cong S_n(a,b,c)$ with exactly one non-pendent neighbor of v_1 outside the triangle in G'' such that $\lambda_n(G) \geq \lambda_n(G'')$.

Suppose that there is exactly one non-pendent neighbor, say w, of v_1 outside the triangle in G. Denote by w_1 a pendent neighbor of w in G and by u a pendent neighbor of v_1 in G if existed.

Let **x** be a unit eigenvector of G corresponding to $\lambda_n(G) = \lambda_n$.

Suppose that $x_{w_1} = 0$ and $x_w = x_{v_1}$. Then $x_w = x_{v_1} = x_u = 0$. It is easily seen that

$$\lambda_n x_{v_1} = x_{v_2} + x_{v_3} = 0,$$

i.e., $x_{v_3} = -x_{v_2}$. On the other hand, note that

$$\lambda_n x_{v_2} = \frac{x_{v_2}}{\lambda_n} + x_{v_3} = \frac{x_{v_2}}{\lambda_n} - x_{v_2}.$$

If $x_{v_2} = 0$, then $x_{v_3} = 0$, which implies that **x** = 0, which is a contradiction. Suppose that $x_{v_2} \neq 0$. Then $\lambda_n = -\frac{1+\sqrt{5}}{2}$. Let H be the 5-vertex graph obtained by attaching a path on two vertices to a vertex of a triangle. Obviously, H is a subgraph of G, and thus by the interlacing theorem [1],

$$\lambda_n \leq \lambda_5(H) = -1.675 < -\frac{1+\sqrt{5}}{2} = \lambda_n,$$

which is a contradiction. Thus either $x_{w_1} \neq 0$ or $x_w \neq x_{v_1}$.

It follows from Lemma 5(i) that whether $|x_{v_1}| \geq |x_w|$ or $|x_{v_1}| < |x_w|$, we may get $\lambda_n(G) > \lambda_n(S_n(n-3,3,3))$. □

Let G be a unicyclic graph with at least ten vertices. It was shown in [6] that $\lambda_1(G) < \sqrt{n}$. Recall that [1] $-\lambda_n(G) \le \lambda_1(G)$, which implies that $\lambda_n(G) > -\sqrt{n}$. On the other hand, by the interlacing theorem [1],

$$\lambda_n(G) \le \lambda_3(P_3) = -\sqrt{2}.$$

Thus

$$-\sqrt{n} < \lambda_n(G) \le -\sqrt{2}.$$

Theorem 2 *Among the graphs in* $\mathbb{U}(n)$, $U_{n,4}$ *for* $n = 8, 9, 10$ *and* $U_{n,3} \cong S_n(n-3, 3, 3)$ *for* $n = 6, 7$ *and* $n \ge 11$ *are the unique graphs with minimum least eigenvalue, and the least eigenvalues of* $U_{n,3} \cong S_n(n-3, 3, 3)$ *and* $U_{n,4}$ *are, respectively, the smallest roots of the equations on* x *as follows*:

$$x^6 - nx^4 - 2x^3 + (3n-12)x^2 - n + 5 = 0,$$
$$x^8 - nx^6 + (5n-26)x^4 - (5n-32)x^2 + n - 7 = 0.$$

Proof Let $G \in \mathbb{U}(n)$, where $n \ge 6$. The case $n = 6$ is trivial. Suppose that $n \ge 7$.

If the unique cycle of G is of length at least four, then $n \ge 8$, and by Lemma 12, $\lambda_n(G) \ge \lambda_n(U_{n,4})$ with equality if and only if $G \cong U_{n,4}$.

If the unique cycle of G is of length three, then either $G \cong S_n(a, b, c)$, and thus by Lemma 13, $\lambda_n(G) \ge \lambda_n(S_n(n-3, 3, 3))$ with equality if and only if $G \cong S_n(n-3, 3, 3)$, or $G \not\cong S_n(a, b, c)$, and thus by Lemma 14, $\lambda_n(G) > \lambda_n(S_n(n-3, 3, 3))$.

Thus $S_n(n-3, 3, 3)$ is the unique graph with minimum least eigenvalue for $n = 7$, and

$$\lambda_n(G) \ge \min\{\lambda_n(U_{n,4}), \lambda_n(S_n(n-3, 3, 3))\}$$

for $n \ge 8$.

We are left to compare $\lambda_n(U_{n,4})$ and $\lambda_n(S_n(n-3, 3, 3))$ for $n \ge 8$. By direct calculation, we have $\lambda_n(U_{n,4}) < \lambda_n(S_n(n-3, 3, 3))$ for $n = 8, 9, 10$ and $\lambda_n(U_{n,4}) > \lambda_n(S_n(n-3, 3, 3))$ for $n = 11, 12, 13, 14, 15$. Suppose in the following that $n \ge 16$.

Let G_n be the n-vertex unicyclic graph obtained from $U_{n+1,4}$ by deleting the unique pendent neighbor of v_2.

By Lemma 1, $\lambda_1(G_n) > \lambda_1(U_{n,4})$. Note that both G_n and $U_{n,4}$ are bipartite graphs, and thus $\lambda_n(G_n) < \lambda_n(U_{n,4})$.

By Lemma 3,

$$\phi(S_n(n-3, 3, 3), x) = x^{n-6}f(x),$$
$$\phi(G_n, x) = x^{n-6}g(x),$$

where

$$f(x) = x^6 - nx^4 - 2x^3 + (3n-12)x^2 - n + 5,$$
$$g(x) = x^6 - nx^4 + (4n-19)x^2 - 2n + 11.$$

Obviously, $\lambda_n(S_n(n-3,3,3))$ and $\lambda_n(G_n)$ are, respectively, the smallest roots of $f(x) = 0$ and $g(x) = 0$.

It is easily seen that $f(x) = g(x) + h(x)$, where

$$h(x) = -2x^3 - (n-7)x^2 + n - 6.$$

Note that

$$h(0) = n - 6 > 0,$$
$$h(-\sqrt{2}) = -n + 8 + 4\sqrt{2} < 0,$$
$$h(-\sqrt{n}) = 2n^{3/2} - n^2 + 8n - 6 < 0,$$

and thus $h(x) < 0$ for $-\sqrt{n} < x \leq -\sqrt{2}$.

Let $r = \lambda_n(G_n)$. Note that $-\sqrt{n} < r \leq -\sqrt{2}$. It follows that $h(r) < 0$, and thus

$$f(r) = g(r) + h(r) = h(r) < 0,$$

which implies that $\lambda_n(S_n(n-3,3,3)) < \lambda_n(G_n)$.

Now we have $\lambda_n(S_n(n-3,3,3)) < \lambda_n(U_{n,4})$, and thus the result for $n \geq 8$ follows. $\qquad\square$

5 The maximum spread of graphs in $\mathbb{U}(n)$

Now we end this paper by determining the graph with maximum spread among graphs in $\mathbb{U}(n)$.

Theorem 3 *Among the graphs in $\mathbb{U}(n)$, where $n \geq 6$, $U_{n,4}$ for $n = 8$ and $U_{n,3}$ for $n \neq 8$ are the unique graphs with maximum spread.*

Proof By Theorems 1 and 2, the results for $n \neq 8, 9, 10$ follow.

Suppose in the following that $n = 8, 9, 10$.

If the unique cycle of G is of length at least four, then by Lemmas 8 and 12, $s(G) \leq s(U_{n,4})$ with equality if and only if $G \cong U_{n,4}$.

If the unique cycle of G is of length three, then by Theorem 1 and the proof of Theorem 2, $s(G) \leq s(U_{n,3})$ with equality if and only if $G \cong U_{n,3}$.

Then the results for $n = 8, 9, 10$ follow from direct calculations for $s(U_{n,3})$ and $s(U_{n,4})$.

$\qquad\square$

6 Results and discussion

In this paper, we mainly focus on the spectral properties of graphs in $\mathbb{U}(n)$, including the spectral radius, the least eigenvalue, and the spread. The main results obtained are as follows:

(i) the first five maximum spectral radii among graphs in $\mathbb{U}(n)$;

(ii) the minimum least eigenvalue among graphs in $\mathbb{U}(n)$;

(iii) the maximum spread among graphs in $\mathbb{U}(n)$.

7 Conclusions

The spectral radius, the least eigenvalue, and the spread are the most important spectral properties of graphs, which are also the corn of spectral graph theory. So the research for such graph-spectrum descriptors is of great importance and value.

As the simplest connected graphs, the trees and unicyclic graphs are always the focus of research in graph theory. The investigation of spectral properties of trees has a long history, and a large number of results have been established. In contrast, the research of spectral properties of unicyclic graphs is still inadequate.

In this paper, we focus on a type of unicyclic graphs, each of whose vertices on the unique cycle is of degree at least three, and establish some bounds for their spectral radii, least eigenvalues, and the spreads. In particular, we determine the first five maximum spectral radii, the minimum least eigenvalue, and the maximum spread, respectively.

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