The spectral radius of unicyclic and bicyclic graphs with \( n \) vertices and \( k \) pendant vertices

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Abstract

In this paper, we determine graphs with the largest spectral radius among all the unicyclic and all the bicyclic graphs with \( n \) vertices and \( k \) pendant vertices, respectively.

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1. Introduction

The graphs in this paper are simple. Let \( G = (V, E) \) be a graph with \( n \) vertices and let \( A(G) \) be a \((0, 1)\)-adjacency matrix of \( G \). Since \( A(G) \) is symmetric, its eigenvalues are real. Without loss of generality, we can write them as \( \lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G) \) and call them the eigenvalues of \( G \). The characteristic polynomial of \( G \) is just \( \det(\lambda I - A(G)) \), denoted by \( P(G; \lambda) \). The largest eigenvalue \( \lambda_1(G) \) is called the spectral radius of \( G \), denoted by \( \rho(G) \). If \( G \) is connected, then \( A(G) \) is
irreducible and by the Perron–Frobenius theory of non-negative matrices, $\rho(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\rho(G)$. We shall refer to such an eigenvector as the Perron vector of $G$.

The investigation on the spectral radius of graphs is an important topic in the theory of graph spectra. For results on the spectral radius of graphs, one may refer to [1–16] and the references therein. Recently, the problem concerning graphs with maximal or minimal spectral radius of a given class of graphs has been studied extensively. The spectral radius of trees has been studied by many authors (see [2,5,6]). Xu [14] found the upper bound for spectral radii of trees on $n$ vertices with perfect matching and characterized the graph attained the upper bound. Berman and Zhang [1] studied the spectral radius of graphs with $n$ vertices and $k$ cut vertices. Liu et al. [11] studied the spectral radius of graphs with $n$ vertices and $k$ cut edges. Unicyclic graphs are connected graphs in which the number of edges equals the number of vertices and bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. The spectral radius of unicyclic graphs has also been studied by many authors (see [2,3,7,9,10]). Chang and Tian [3] determined graphs with the largest and the second largest spectral radius among all the unicyclic graphs on $n$ vertices with perfect matching. Chang et al. [4] determined graphs with the largest spectral radius among all the bicyclic graphs on $n$ vertices with perfect matching. Yu and Tian [15,16] determine, respectively, the graphs with the largest spectral radius among all the unicyclic graphs and all the bicyclic graphs on $n$ vertices with a maximum matching of cardinality $m$. A pendant vertex of $G$ is a vertex of degree 1. Very recently, Wu et al. [13] determine the graph with the largest spectral radius among all the trees with $n$ vertices and $k$ pendant vertices.

In this paper, we study the spectral radius of unicyclic and bicyclic graphs with $n$ vertices and $k$ pendant vertices. We determine graphs with the largest spectral radius among all the unicyclic graphs and all the bicyclic graphs with $n$ vertices and $k$ pendant vertices, respectively.

2. Preliminaries

Denote by $C_n$ and $P_n$ the cycle and the path, respectively, each on $n$ vertices. Let $G - x$ or $G - xy$ denote the graph that arises from $G$ by deleting the vertex $x \in V(G)$ or the edge $xy \in E(G)$. Similarly, $G + xy$ is a graph that arises from $G$ by adding an edge $xy \notin E(G)$, where $x, y \in V(G)$. We will use $\mathcal{U}_n(k)$ and $\mathcal{B}_n(k)$ to denote the sets of all unicyclic and bicyclic graphs with $n$ vertices and $k$ pendant vertices, respectively.

A unicyclic graph is either a cycle or a cycle with trees attached. Let $C_p$ and $C_q$ be two vertex-disjoint cycles. Suppose that $v_1$ is a vertex of $C_p$ and $v_l$ is a vertex of $C_q$. Joining $v_1$ and $v_l$ by a path $v_1v_2 \cdots v_l$ of length $l - 1$, where $l \geq 1$ and $l = 1$ means identifying $v_1$ with $v_l$, the resulting graph (Fig. 1), denoted by $B(p, l, q)$, is called an $\infty$-graph. Let $P_{l+1}$, $P_{p+1}$ and $P_{q+1}$ be three vertex-disjoint paths, where $l, p, q \geq 1$.
and at most one of them is 1. Identifying the three initial vertices and terminal vertices of them, respectively, the resulting graph (Fig. 2), denoted by $P(l, p, q)$, is called a $\theta$-graph. Obviously $B_n(k)$ consists of two types of graphs: one type, denoted by $B^+_n(k)$, are those graphs each of which is an $\infty$-graph with trees attached; the other type, denoted by $B^{++}_n(k)$, are those graphs each of which is a $\theta$-graph with trees attached. Then we have $B_n(k) = B^+_n(k) \cup B^{++}_n(k)$.

$k$ paths $P_1, P_2, \ldots, P_k$ is said to have almost equal lengths if $|l_i - l_j| \leq 1$ for $1 \leq i, j \leq k$. Let $B^*_n(k)$ be the graph on $n$ vertices obtained from $B(3, 1, 3)$ by attaching $k$ paths of almost equal lengths at the vertex of degree 4. $B^{**}_n(k)$ be the graph on $n$ vertices obtained from $P(2, 1, 2)$ by attaching $k$ paths of almost equal lengths at one vertex of degree 3, and $B^{***}_n(k)$ be the graph on $n$ vertices obtained from $P(2, 1, 2)$ by attaching $k$ paths of almost equal lengths at one vertex of degree 2. We will show in the following that $B^*_n(k)$ and $B^{**}_n(k)$ are the graphs with maximal spectral radius in $B^+_n(k)$ and $B^{++}_n(k)$, respectively.

In order to complete the proofs of our main results, we need the following lemmas. For $v \in V(G)$, $d(v)$ denotes the degree of vertex $v$ and $N(v)$ denotes the set of all neighbors of vertex $v$ in $G$.

**Lemma 1** [11, 13]. Let $G$ be a connected graph and $\rho(G)$ be the spectral radius of $A(G)$. Let $u, v$ be two vertices of $G$ and $d(v)$ be the degree of vertex $v$. Suppose $v_1, v_2, \ldots, v_s \in N(v) \setminus N(u)(1 \leq s \leq d(v))$ and $x = (x_1, x_2, \ldots, x_n)$ is the Perron vector of $A(G)$, where $x_i$ corresponds to the vertex $v_i(1 \leq i \leq n)$. Let $G^*$ be the graph obtained from $G$ by deleting the edges $uv_i$ and adding the edges $uv_i(1 \leq i \leq s)$. If $x_u \geq x_v$, then $\rho(G) < \rho(G^*)$.

Let $G$ be a connected graph, and $uv \in E(G)$. The graph $G_{u,v}$ is obtained from $G$ by subdividing the edge $uv$, i.e., adding a new vertex $w$ and edges $uw, wv$ in $G - uv$. Hoffman and Smith define an internal path of $G$ as a walk $v_0v_1 \cdots v_s(s \geq 1)$ such that the vertices $v_0, v_1, \ldots, v_s$ are distinct, $d(v_0) > 2$, $d(v_s) > 2$, and $d(v_i) = 2$, whenever $0 < i < s$. And $s$ is called the length of the internal path. An internal path is closed if $v_0 = v_s$. They prove the following result.
Lemma 2 [8]. Let $uv$ be an edge of the connected graph $G$ on $n$ vertices.

(i) If $uv$ does not belong to an internal path of $G$, and $G \neq C_n$, then $\rho(G_{u,v}) > \rho(G)$;
(ii) If $uv$ belongs to an internal path of $G$, and $G = C_n$, then $\rho(G_{u,v}) < \rho(G)$.

Lemma 3 [7, 11]. Let $v$ be a vertex in a non-trivial connected graph $G$ and suppose that two paths of lengths $k, m (k \geq m \geq 1)$ are attached to $G$ by their end vertices at $v$ to form $G_{k,m}$. Then $\rho(G_{k,m}) > \rho(G_{k+1,m-1})$.

Lemma 4 [4]. Let $G$ be a connected graph, and $G'$ be a proper spanning subgraph of $G$. Then $P(G'; \lambda) > P(G; \lambda)$ for all $\lambda \geq \rho(G)$.

The following result is often used to calculate the characteristic polynomials of graphs.

Lemma 5 [3–5, 12]. Let $e = uv$ be an edge of $G$, and $C(e)$ be the set of all cycles containing $e$. The characteristic polynomial of $G$ satisfies

$$P(G; \lambda) = P(G - e; \lambda) - P(G - u - v; \lambda) - 2 \sum_{Z \in C(e)} P(G \setminus V(Z); \lambda),$$

where the summation extends over all $Z \in C(e)$.

Lemma 6. Let $v_0$ be a vertex of a tree $T$. $T$ is attached to $P(2, 1, 2)$ by $v_0$ at a vertex of degree 2 and 3, respectively, to form $G_2$ and $G_3$. Then $\rho(G_3) > \rho(G_2)$.

Proof. Let $G_1$ be $C_4$ with $T$ attached by $v_0$ at a vertex of $C_4$. By Lemma 5, we have

$$P(G_2; \lambda) = P(G_1; \lambda) - \lambda P(T; \lambda) - 2\lambda P(T - v_0; \lambda) - 2P(T; \lambda),$$
$$P(G_3; \lambda) = P(G_1; \lambda) - \lambda^2 P(T - v_0; \lambda) - 2\lambda P(T - v_0; \lambda) - 2\lambda P(T - v_0; \lambda).$$

By Lemma 4, $\lambda P(T - v_0; \lambda) - P(T; \lambda) > 0$ holds for $\lambda \geq \rho(T)$. Moreover it is well known that $\rho(G_2) > \rho(T)$. From the above arguments, we have

$$P(G_2; \lambda) - P(G_3; \lambda) = (\lambda + 2)(\lambda P(T - v_0; \lambda) - P(T; \lambda)) > 0$$
holds for $\lambda \geq \rho(G_2)$. It follows that $\rho(G_3) > \rho(G_2)$. This completes the proof. \qed
Let $G$ be a connected graph and $T$ be a tree such that $T$ is attached to a vertex $v$ of $G$. The vertex $v$ is called the root of $T$, or the root-vertex of $G$. Throughout this paper, we assume that $T$ does not include the root.

3. Main results

**Theorem 1.** Let $G$ be a graph in $\mathcal{B}_n^+(k), k \geq 1$. Then

\[ \rho(G) \leq \rho(B_n^+(k)), \]

and the equality holds if and only if $G = B_n^+(k)$.

**Proof.** Choose $G \in \mathcal{B}_n^+(k)$ such that the spectral radius of $G$ is as large as possible. Denote the vertex set of $G$ by \{v_1, v_2, \ldots, v_n\}, and the Perron vector of $G$ by $x = (x_1, x_2, \ldots, x_n)$, where $x_i$ corresponds to the vertex $v_i (1 \leq i \leq n)$.

We first prove that $G$ is an $\infty$-graph $B(p, 1, q)$ with one tree $T$ attached to the vertex of degree 4, denoted by $v_1$. Let $B(p, l, q)$ be the $\infty$-graph in $G$, and $v_1v_2 \cdots v_l$ be the path joining the cycles $C_p$ and $C_q$ in $B(p, l, q)$.

We claim that $l = 1$. Assume, on the contrary, that $l > 1$. Without loss of generality, we may assume that $x_1 \geq x_l$. Denote by $v_l + 1$ a neighbor of $v_l$ which belongs to $C_q$. Let $G^* = G - \{v_1z_1, \ldots, v_1z_t\} + \{v_1z_1, \ldots, v_1z_t\}$.

Then $G^* \in \mathcal{B}_n^+(k)$. By Lemma 1, we have $\rho(G^*) > \rho(G)$, a contradiction. Hence $l = 1$.

Assume that there exists a vertex $v_i$ of $B(p, 1, q)$ such that $v_i \neq v_1$ and there exist a tree $T$ attached to $v_i$. By symmetry, we may assume that $v_i$ is a vertex of $C_p$. Denote $N(v_i) = \{v_{i-1}, v_{i+1}, z_1, \ldots, z_s\}$, and $N(v_1) = \{v_{j-1}, v_{j+1}, w_1, \ldots, w_t\}$, where $v_{i-1}$, $v_{i+1}$, $v_{j-1}$, $v_{j+1}$ are vertices of $C_p$. Then $s \geq 1$ and $t \geq 2$. If $x_1 \geq x_i$, let

\[ G^* = G - \{v_1z_1, \ldots, v_1z_t\} + \{v_1z_1, \ldots, v_1z_t\}. \]

If $x_1 < x_i$, let

\[ G^* = G - \{v_1w_1, \ldots, v_1w_t\} + \{v_1w_1, \ldots, v_1w_t\}. \]

Then in either case $G^* \in \mathcal{B}_n^+(k)$. By Lemma 1, we have $\rho(G^*) > \rho(G)$, a contradiction. Hence $G$ has a unique attached tree.

We second prove that each vertex $v$ of $T$ has degree $d(v) \leq 2$, e.t., $G$ is an $\infty$-graph $B(p, 1, q)$ with $k$ paths attached to $v_1$. On the contrary, if there exists one vertex $v_i$ of $T$ such that $d(v_i) > 2$. Denote $N(v_i) = \{z_1, z_2, z_3, \ldots, z_l\}$, and $N(v_1) = \{w_1, w_2, w_3, w_4, \ldots, w_j\}$. Assume that $z_1, w_3$ belong to the path joining $v_1$ and $v_i$, and that $w_1, w_2$ belong to $C_p$. If $x_1 \geq x_i$, let

\[ G^* = G - \{v_1z_3, \ldots, v_1z_l\} + \{v_1z_3, \ldots, v_1z_l\}. \]
If $x_1 < x_1$, let
\[ G^* = G - [v_1w_1, v_1w_3, v_1w_4, v_1w_5] + [v_1w_1, v_1w_3, v_1w_4, v_1w_5]. \]
Then in either case $G^* \in \mathcal{B}_n^+(k)$. By Lemma 1, we have $\rho(G^*) > \rho(G)$, a contradiction. Hence $G$ is an infinite graph $B(p, 1, q)$ with $k$ paths attached to $v_1$.

Moreover, we claim that the $k$ paths attached to $v_1$ are almost equal lengths. Assume that $P_1, P_2, \ldots, P_k$ are the $k$ paths. We will prove that $|l_i - l_j| \leq 1$ for $1 \leq i, j \leq k$. If there exist two paths, say $P_i$ and $P_j$, such that $l_i - l_j \geq 2$. Denote $P_i = v_1u_1u_2 \cdots u_{l_i}$ and $P_j = v_1w_1w_2 \cdots w_{l_j}$. Let
\[ G^* = G - [u_{l_i-1}u_{l_i}] + [w_{l_j-1}w_{l_j}]. \]
Then $G^* \in \mathcal{B}_n^+(k)$. By Lemma 3, we have $\rho(G^*) > \rho(G)$, a contradiction.

Finally, we show that both $C_p$ and $C_q$ have length 3. Assume that $p \geq 4$. Let $C_p = v_1v_2 \cdots v_p v_1$ and let $P_m = v_1u_1u_2 \cdots u_m$ be a path attached to the infinite graph $B(p, 1, q)$, where $m \geq 1$. Obviously, $G \neq C_n, G \neq W_n, v_1v_2 \cdots v_p v_1$ is a closed internal path, and $v_1u_1u_2 \cdots u_m$ is not an internal path. Let
\[ G^* = G - [v_1w_2, v_3v_4, v_4v_3] + [v_2v_4, u_m v_3]. \]
Then $G^* \in \mathcal{B}_n^+(k)$. By Lemma 2, we have $\rho(G^*) > \rho(G)$, a contradiction. Hence $p = 3$. Similarly, we can verify that $q = 3$.

Combining above arguments, we have $G = B_n^*(k)$. This completes the proof. \(\square\)

**Theorem 2.** Let $G$ be a graph in $\mathcal{B}_n^+(k), k \geq 1$. Then
\[ \rho(G) \leq \rho(B_n^*(k)), \]
and the equality holds if and only if $G = B_n^*(k)$.

**Proof.** Choose $G \in \mathcal{B}_n^+(k)$ such that the spectral radius of $G$ is as large as possible. Denote the vertex set of $G$ by $\{v_1, v_2, \ldots, v_n\}$ and the Perron vector of $G$ by $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, where $x_i$ corresponds to the vertex $v_i (1 \leq i \leq n)$.

Using Lemma 1, similarly to the proof of Theorem 1 we can verify that $G$ is a $	heta$-graph $P(l, p, q)$ with $k$ paths of almost equal lengths attached to one vertex denoted by $v_1$. We will use $P_m = v_1u_1u_2 \cdots u_m$ to denote one of the $k$ paths.

If $v_1$ is a vertex of degree 3 of $P(l, p, q)$, we will show that $G = B_n^*(k)$. By the definition, we have that $l, p, q \geq 1$ and at most one of them is 1. We claim that one of them is 1 and the other two are 2. Assume, on the contrary, that $l \geq 3$. Put $P_l = v_1v_2 \cdots v_{l+1}$. Obviously, $G \neq C_n, G \neq W_n, v_1v_2 \cdots v_{l+1}$ is a closed internal path, and $v_1u_1u_2 \cdots u_m$ is not an internal path. Let
\[ G^* = G - [v_2v_3, v_3v_4, v_4v_3] + [v_2v_4, u_m v_3]. \]
Then $G^* \in \mathcal{B}_n^+(k)$. By Lemma 2, we have $\rho(G^*) > \rho(G)$, a contradiction. Hence $l \leq 2$. Similarly, we can verify that $p \leq 2, q \leq 2$, and that one and only one of $l, p$ and $q$ is 1. Thus $G = B_n^*(k)$.

If $v_1$ is a vertex of degree 2 of $P(l, p, q)$, we will get a contradiction. Denote by $u, v$ the two vertices of degree 3 of $P(l, p, q)$. By the definition, in $P(l, p, q)$
there exist three internal paths joining \( u \) and \( v \), the lengths of which are \( l, p \) and \( q \), respectively. We will use \( P_{l+1} \), \( P_{p+1} \) and \( P_{q+1} \) to denote them. Without loss of generality, we may assume that \( v_1 \) is a vertex of \( P_{l+1} \). Let \( v_1v_2 \cdots v_s \) be the unique internal path joining \( v_1 \) and \( u \), where \( v_s = u \). If \( s \geq 3 \), let \( G^* = G - \{v_1v_2, v_2v_3, \ldots, v_{s-1}v_s\} \).

Then \( G^* \in \mathcal{B}_{n+1}(k) \). By Lemma 2, we have \( \rho(G^*) > \rho(G) \), a contradiction. Hence \( s = 2 \), and so \( u \) and \( v_1 \) are adjacent. Similarly, we can verify that \( v_1 \) and \( v_2 \) are adjacent, and that one of \( p \) and \( q \) is 1 and the other is 2. Thus \( G = B_{n+2}(k) \). This contradicts the definition of \( G \) since by Lemma 5 we have \( \rho(B_{n+2}(k)) > \rho(B_{n+2}(k)) \).

From the above arguments, we have \( G = B_{n+2}(k) \). This completes the proof. \( \square \)

Combining Theorems 1 and 2, we have following.

**Theorem 3.** Let \( G \) be a graph in \( \mathcal{B}_n(k), k \geq 1 \). Then

\[
\rho(G) \leq \max(\rho(B^*_n(k)), \rho(B^{**}_n(k))).
\]

Let \( \Delta^k_n \) be a graph on \( n \) vertices obtained from \( C_3 \) by attaching \( k \) paths of almost equal lengths at one vertex. As far as maximal spectral radius is concerned we can prove the following Theorem 4.

**Theorem 4.** Let \( U \) be a unicyclic graph with \( n \) vertices and \( k \) pendant vertices. Then

\[
\rho(U) \leq \rho(\Delta^k_n),
\]

and the equality holds if and only if \( U = \Delta^k_n \).

The proof of Theorem 4 is similar to that of Theorem 1. From Theorem 1 and Lemma 3, we can prove the following.

**Theorem 5.** Let \( 1 \leq k < n - 3 \). Then \( \rho(\Delta^k_n) < \rho(\Delta^{k+1}_n) \).

**Proof.** Since \( k < n - 3 \), it follows that there exists a path \( P_l = v_1v_2 \cdots v_l \) attached to the root vertex \( v_1 \) of \( \Delta^k_n \) such that \( l \geq 3 \). Let

\[
U = \Delta^k_n - \{v_{l-1}v_l\} + \{v_1v_l\}.
\]

Then \( U \in \mathcal{B}_{n+1}(k) \). By Lemma 3, we have \( \rho(\Delta^k_n) < \rho(U) \). By Theorem 4, we have \( \rho(U) < \rho(\Delta^{k+1}_n) \). Hence \( \rho(\Delta^k_n) < \rho(\Delta^{k+1}_n) \). This completes the proof. \( \square \)

As an immediate consequence of Theorems 4 and 5, we have the following Corollary 1, which is the main result in \([9]\).

**Corollary 1.** Let \( U \) be a unicyclic graph on \( n \) vertices. Then

\[
\rho(U) \leq \rho(\Delta^{n-3}_n).
\]
References