KYUNGPOOK Math. J. 54(2014), 425-441
http://dx.doi.org/10.5666/KMJ.2014.54.3.425

The Spectral Radii of Graphs with Prescribed Degree Sequence

Jianxi Li*
School of Mathematics and Statistics, Minnan Normal University, Zhangzhou, Fujian, P. R. China
Center for Discrete Mathematics, Fuzhou University, Fuzhou, Fujian, P. R. China
e-mail : ptjxli@hotmail.com

Wai Chee Shiu
Department of Mathematics, Hong Kong Baptist University, Kowloon Tong, Hong Kong, P. R. China
e-mail : wcshiu@hkbu.edu.hk

Abstract. In this paper, we first present the properties of the graph which maximize the spectral radius among all graphs with prescribed degree sequence. Using these results, we provide a somewhat simpler method to determine the unicyclic graph with maximum spectral radius among all unicyclic graphs with a given degree sequence. Moreover, we determine the bicyclic graph which has maximum spectral radius among all bicyclic graphs with a given degree sequence.

1. Introduction

Let G be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Its order is $|V(G)|$, denoted by n, and its size is $|E(G)|$, denoted by m. For $v \in V(G)$, let $N_G(v)$ (or $N(v)$ for short) be the set of all neighbors of v in G and let $d(v) = |N(v)|$ be the degree of v. We use $G - e$ and $G + e$ to denote the graphs obtained by deleting the edge e from G and by adding the edge e to G, respectively. For any nonempty subset W of $V(G)$, the subgraph of G induced by W is denoted by $G[W]$. The distance of u and v (in G) is the length of the shortest path between u and v, denoted by $d(u, v)$. For all other notions and definitions, not given here, see, for example, [1], or [4] (for graph spectra). For the basic notions and terminology on the spectral graph theory the readers are referred to [4].

Let $A(G)$ be the adjacency matrix of G. Its eigenvalues are called the eigenvalues

* Corresponding Author.
Received July 3, 2012; accepted March 14, 2013.
2010 Mathematics Subject Classification: 05C50.
Key words and phrases: pectral radius, degree sequence, unicyclic graph, bicyclic graph.

(or the spectrum) of G. They are real because $A(G)$ is symmetric. The eigenvalues of $A(G)$ are usually denoted by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The largest eigenvalue λ_1 is also called the *spectral radius* of G, denoted by ρ. The following description of the spectral radius ρ of G, is well known (see, for example, [5, p.49]):

$$\rho = \sup_{\|\mathbf{x}\|=1} \mathbf{x}^T A(G)\mathbf{x} \quad (\mathbf{x} \in \mathbb{R}^n) \tag{1.1}$$

We note here that the maximum is attained in (1.1) if and only if $\mathbf{x}$ is an eigenvector (for the largest eigenvalue) of $A(G)$. When G is connected, then $A(G)$ is irreducible and by the Perron-Frobenius Theorem (see e.g. [9]) the spectral radius ρ of G is simple and there is a unique positive unit eigenvector $\mathbf{x} = (x_v,\ v \in V(G))$, where x_v is also called the *ρ-weight* of the vertex v (with respect to $\mathbf{x}$). We refer to such an eigenvector as the *Perron vector* of G. Then we have the following set of equations, known in general as eigenvalue equations:

$$\rho x_v = \sum_{u \in N(v)} x_u \quad \text{for } v \in V(G). \tag{1.2}$$

A nonincreasing sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$ of nonnegative integers is called a *degree sequence* (or *graphic*) if there exists a graph G of order n for which $d_0, d_1, \ldots, d_{n-1}$ are the degrees of its vertices.

Given a degree sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$, let $\mathcal{G}_n^\pi$ be the set of all connected graphs of order n with this degree sequence. For any $G \in \mathcal{G}_n^\pi$, we have $\sum_{i=0}^{n-1} d_i = 2m$, and $k = m - n + 1$ is the number of independent cycles. Usually, such a graph G can be referred to as a k-cyclic graph (for example, a tree is a connected acyclic graph (so $k = 0$), a unicyclic graph is a connected graph containing exactly one cycle (so $k = 1$) and a bicyclic graph is a connected graph containing two independent cycles (so $k = 2$)). For any k-cyclic graph G, the *Perron-core* of G is the set of vertices $\{v_0, v_1, \ldots, v_{t-1}\}$ $(t \leq n)$ having the largest degree such that the graph constructed on such vertices is a k-cyclic graph. The remaining vertices of G form the *Perron-periphery*. Clearly the number of elements in the Perron-core depends on k, the number of independent cycles. So the vertices in the Perron-periphery lie on some hanging trees attached to the vertices of the Perron-core.

The Brualdi-Solheid problem (BSP for short) put forward the determination of graphs maximizing the spectral radius in a given set $\mathcal{S}$ of graphs. The BSP for $\mathcal{S} = \mathcal{G}_n^\pi$ has not been solved in general. The BSP for $\mathcal{G}_n^\pi$ if restricted on trees has been solved in [2]. Recently, Belardo *et al.* [3] solved the BSP for $\mathcal{G}_n^\pi$ if restricted on unicyclic graphs, and make the following general conjecture.

Conjecture 1.1. Let $G_{\max}^\pi$ be the graph which has maximum spectral radius among all graphs in $\mathcal{G}_n^\pi$. Then $G_{\max}^\pi$ is the unique graph consisting of a k-cyclic Perron-core and the vertices of the Perron-periphery are inserted in spiral like disposition (for a formal definition of spiral like disposition see [2]) with respect to the Perron-core.

The rest of this paper is organized as follows. In section 2, we present some useful lemmas. In section 3, we first introduce some properties of the graphs which maximize the spectral radii among all graphs in $\mathcal{G}_n^\pi$. Then using these results, we give a somewhat simpler method to determine the unicyclic graph which has maximum spectral radius among all unicyclic graphs with prescribed degree sequence. Moreover, we determine the bicyclic graph which has maximum spectral radius among all bicyclic graphs with prescribed degree sequence, which confirms Conjecture 1.1 with $k = 2$.

2. Preliminaries

Generally, it is natural to expect that ρ changes when G is perturbed, and we can ask whether ρ increases or decreases in such situations. The following two results are the part of standard folklore of graph perturbations. Their proofs appear in several literatures (see, for example, [5]). The first one is about the perturbation known as the (simultaneous) rotations (see Lemma 2.1), the second one is about the local switching (see Lemma 2.2). Recall that the local switching preserve the degree sequence and they play the crucial role in the next section.

Lemma 2.1.([5]) Let u and v be two vertices of a connected graph G (of order n) and let $N(u)\backslash N(v) = \{v_1, v_2, \ldots, v_s\}$ $(s \geq 1)$. Let G' be the graph obtained from G by deleting the edges $uv_i (1 \leq i \leq s)$, and then adding the edges vv_i $(1 \leq i \leq s)$. If $x_v \geq x_u$, then $\rho(G') > \rho(G)$.

Lemma 2.2.([5]) Let G (of order n) be a connected graph with u_1v_1, $u_2v_2 \in E(G)$ and u_1u_2, $v_1v_2 \notin E(G)$. Let G' be the graph obtained from G by the local switching, that consists of the deletion of edges u_1v_1 and u_2v_2, followed by the addition of edges u_1u_2 and v_1v_2 (see Fig. 1). If $(x_{u_1} - x_{v_2})(x_{u_2} - x_{v_1}) \geq 0$, then $\rho(G') \geq \rho(G)$, and the equality holds if and only if $x_{u_1} = x_{v_2}$ and $x_{u_2} = x_{v_1}$.

To state the next result (due to Hoffman and Smith), we need more definitions. An *internal path* in a graph, denoted by $v_1v_2 \cdots v_r$ is a path joining vertices v_1 and v_r which are both of degree greater than two (not necessarily distinct), while all other vertices (i.e., $v_2, \ldots, v_{r-1}$) are of degree equal to 2. We denote by C_n and W_n the cycle and the double-snake (the tree of order n having two vertices of degree three which are at distance $n - 5$).

Lemma 2.3.([8]) Let G' be the graph obtained from a graph G, which is neither C_n nor W_n, by inserting a vertex of degree two in an edge e. Then we have

(1) if e does not lie on an internal path, then $\rho(G') > \rho(G)$;

(2) if e lie on an internal path, then $\rho(G') < \rho(G)$.

If $G = C_n$ (resp. W_n) and $G' = C_{n+1}$ (resp. W_{n+1}), then $\rho(G') = \rho(G) = 2$.

Lemma 2.4.([8]) Let $G(k, l)$ be a graph obtained from a connected graph G by adding at a fixed vertex v two hanging paths whose lengths are k and l $(k \geq l \geq 1)$.

Then

$$\rho(G(k,l)) > \rho(G(k+1,l-1)).$$

3. Graphs with Maximum Spectral Radii

We introduce an ordering of the vertices $v_0, v_1, \ldots, v_{n-1}$ of a graph $G \in \mathcal{G}_n^\pi$ by means of breadth-first-search. Select a vertex $v_0 \in V(G)$ and start with vertex v_0 in layer 0 as root; all neighbors of v_0 belong to layer 1. Now we continue by recursion to construct all other layers, i.e., all neighbors of vertices in layer i, which are not in layers i or $i-1$, build up layer $i+1$. Note that all vertices in layer i have distance i from root v_0. We call this distance the *height* $h(v) = d(v, v_0)$ of a vertex v.

Note that one can draw these layers on circles, respectively. Thus such an ordering is also called *spiral like ordering*.

For the description of graphs which have maximum spectral radii, we need the following notion.

Definition 3.1. Let $G = (V, E)$ be a graph with root v_0. An ordering $\prec$ of the vertices is called a *breadth-first-search ordering* (BFS-ordering for short) if the following hold for all vertices v_i, $v_j \in V$ $(i \neq j)$:

(1) $v_i \prec v_j$ implies $h(v_i) \leq h(v_j)$

(2) $v_i \prec v_j$ implies $d(v_i) \geq d(v_j)$

(3) Let $v_iv_j \in E$, $v_lv_k \in E$, $v_iv_k \notin E$, $v_jv_l \notin E$ with $h(v_i) = h(v_l) = h(v_j) - 1 = h(v_k) - 1$. If $v_i \prec v_l$, then $v_j \prec v_k$.

We call a connected graph which has a BFS-ordering for its vertices a BFS-graph.

Let $G^\pi_{\max}$ be the graph which has maximum spectral radius among all graphs in $\mathcal{G}_n^\pi$. Let $\mathbf{x} = (x_{v_0}, x_{v_1}, \ldots, x_{v_{n-1}})$ $(x_{v_0} \geq x_{v_1} \geq \cdots \geq x_{v_{n-1}})$ be the Perron vector of $G^\pi_{\max}$.

The following result due to Biyukoğlu and Leydold [2], which provide a structural characterization for $G^\pi_{\max}$.

Lemma 3.2.([2]) There exists an ordering $\prec$ of $V(G^\pi_{\max})$ which is consistent with its Perron vector $\mathbf{x}$ in such a way that $x_{v_i} \geq x_{v_j}$ implies that $v_i \prec v_j$. Moreover, such an ordering $\prec$ of $V(G^\pi_{\max})$ satisfies the conditions (1) and (2) in Definition 3.1.

In fact the ordering $\prec$ of $V(G^\pi_{\max})$ in Lemma 3.2 also satisfies the condition (3) in Definition 3.1. Otherwise, by Lemma 3.2, there exists an ordering $\prec$ of $V(G^\pi_{\max})$ such that $v_0 \prec v_1 \prec \cdots \prec v_{n-1}$ (i.e., $x_{v_0} \geq x_{v_1} \geq \cdots \geq x_{v_{n-1}}$) implies that $h(v_0) \leq h(v_1) \leq \cdots \leq h(v_{n-1})$ and $d(v_0) \geq d(v_1) \geq \cdots \geq d(v_{n-1})$. Furthermore, if $v_iv_j \in E$, $v_lv_k \in E$, $v_iv_k \notin E$, $v_jv_l \notin E$ with $h(v_i) = h(v_l) = h(v_j) - 1 = h(v_k) - 1$. Suppose that $v_i \prec v_l$ and $v_j \succ v_k$, i.e., $x_{v_i} \geq x_{v_l}$ and $x_{v_j} < x_{v_k}$. Let

$$G' = G^\pi_{\max} - \{v_iv_j,\, v_lv_k\} + \{v_iv_k,\, v_lv_j\}.$$

Clearly, $G' \in \mathcal{G}_n^\pi$. Hence, Lemma 2.2 implies that $\rho(G^\pi_{\max}) < \rho(G')$. This is a contradiction.

Hence, we summary the above result as follows.

Theorem 3.3. *$G^\pi_{\max}$ is a BFS-graph. Moreover, $G^\pi_{\max}$ has a BFS-ordering of its vertices $v_0 \prec v_1 \prec \cdots \prec v_{n-1}$, which consists with the Perron vector $\mathbf{x}$ in such a way that $x_{v_0} \geq x_{v_1} \geq \cdots \geq x_{v_{n-1}}$.*

Let $\mathbf{x} = (x_{v_0}, x_{v_1}, \ldots, x_{v_{n-1}})$ $(x_{v_0} \geq x_{v_1} \geq \cdots \geq x_{v_{n-1}})$ be the Perron vector of $G^\pi_{\max}$. In fact, Theorem implies that there exists a well-ordering $V(G^\pi_{\max}) = \{v_0, v_1, \ldots, v_{n-1}\}$ of $G^\pi_{\max}$ with root v_0 such that

$$v_0 \prec v_1 \prec \cdots \prec v_{n-1} \text{ (i.e., } x_{v_0} \geq x_{v_1} \geq \cdots \geq x_{v_{n-1}})$$

implies that

$$h(v_0) \leq h(v_1) \leq \cdots \leq h(v_{n-1}) \text{ and } d(v_0) \geq d(v_1) \geq \cdots \geq d(v_{n-1}).$$

Let $V_i = \{v \in V(G^\pi_{\max}), h(v) = i\}$ for $i = 0, 1, \ldots, h(v_{n-1}) = p$. Hence we may relabel the vertices of $G^\pi_{\max}$ in such a way that $V_i = \{v_{i,1}, \ldots, v_{i,s_i}\}$ with $x_{v_{i,1}} \geq x_{v_{i,2}} \geq \cdots \geq x_{v_{i,s_i}}$ and $x_{v_{i,j}} \geq x_{v_{i+1,k}}$ for $i = 0, 1, \ldots, p-1$ and $1 \leq j \leq s_i$, $1 \leq k \leq s_{i+1}$ (Following, if a graph is a BFS-graph, we may keep this labeling and notation). Clearly, $V(G^\pi_{\max}) = V_1 \cup V_2 \cup \cdots \cup V_p$, $|V_1| = s_1 = d_0$ and $|V_i| = s_i$ for $2 \leq i \leq p$. Following, we give an example to explain this concept.

Example 3.4. In Figure 2 the unique graph maximizing the spectral radius among all uncyclic graphs with degree sequence $(5^{(1)}, 4^{(2)}, 3^{(1)}, 2^{(2)}, 1^{(8)})$ is depicted. The exponent in the degree sequence denote the number of vertices in the graph having such a degree. On the left there is a original graph, and on the right there is its relabeled graph.

First, we show the following result.

Lemma 3.5. If $G^\pi_{\max}$ is not a regular graph, then $x_{v_{0,1}} > x_{v_{1,s_1}}$ and $x_{v_{1,1}} > \min\limits_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\}$.

Proof. Recall that for any graph G with maximum degree Δ, we have $\rho(G) \leq \Delta$, and the equality holds if and only of G is regular (see [4]). Thus $d_0 = d(v_{0,1}) > \rho(G^\pi_{\max})$, since $G^\pi_{\max}$ is not a regular graph. Hence, from (1.2), we have

$$d_0 x_{v_{0,1}} > \rho(G^\pi_{\max}) x_{v_{0,1}} = \sum_{i=1}^{s_1} x_{v_{1,i}} \geq d_0 x_{v_{1,s_1}}.$$

Therefore, $x_{v_{0,1}} > x_{v_{1,s_1}}$.

Let $x_{v_{2,t}} = \min\limits_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\}$. Suppose that $x_{v_{1,1}} = x_{v_{2,t}}$. Then $x_{v_{1,1}} = \cdots = x_{v_{1,s_1}} = x_{v_{2,t}}$. From (1.2), we have

$$\rho(G^{\pi}_{\max})x_{v_{0,1}} = \sum_{i=1}^{s_1} x_{v_{1,i}} = d(v_{0,1})x_{v_{1,1}} \tag{3.1}$$

and

$$\rho(G^{\pi}_{\max})x_{v_{1,1}} = x_{v_{0,1}} + (d(v_{1,1})-1)x_{v_{1,1}}, \text{ i.e., } (\rho(G^{\pi}_{\max}) - d(v_{1,1})+1)x_{v_{1,1}} = x_{v_{0,1}}. \tag{3.2}$$

Combining (3.1) and (3.2), we have

$$\rho(G^{\pi}_{\max})(\rho(G^{\pi}_{\max}) - d(v_{1,1})+1) = d(v_{0,1}). \tag{3.3}$$

On the other hand, we have

$$\rho(G^{\pi}_{\max})x_{v_{2,t}} = \sum_{uv_{2,t}\in E(G^{\pi}_{\max})} x_u \le d(v_{2,t})x_{v_{1,1}}, \text{ i.e., } \rho(G^{\pi}_{\max}) \le d(v_{2,t}) \le d(v_{1,1}).$$

Note that G is non-regular, hence $\rho(G^{\pi}_{\max}) < d(v_{0,1}) = d_0$. Then in view of (3.3), we have $d(v_{0,1}) \le \rho(G^{\pi}_{\max}) < d(v_{0,1})$, a contradiction. □

We define a partial ordering on degree sequences as follows: for two degree sequences $\pi = (d_0, d_1, \ldots, d_{n-1})$ $\pi' = (d'_0, d'_1, \ldots, d'_{n-1})$, we write $\pi \trianglelefteq \pi'$ if and only if $\sum_{i=0}^{n-1} d_i = \sum_{i=0}^{n-1} d'_i$ and $\sum_{i=0}^{k} d_i \le \sum_{i=0}^{k} d'_i$ for all $k = 0, \ldots, n-1$. Recall that the degree sequences are non-increasing. Such an ordering is also called a *majorization*. Biyukoğlu and Leydold [2] proved that

Lemma 3.6.([2]) Let π and π' be two distinct degree sequences with $\pi \trianglelefteq \pi'$. Let $G^{\pi}_{\max}$ and $G^{\pi'}_{\max}$ be two graphs with maximum spectral radii among all graphs in the sets $\mathcal{G}^{\pi}_n$ and $\mathcal{G}^{\pi'}_n$, respectively. Then $\rho(G^{\pi}_{\max}) < \rho(G^{\pi'}_{\max})$.

Belardo *et al.* [3] characterize the unicyclic graph with maximum spectral radius among all unicyclic graphs with prescribed degree sequence. Using above results, following, we will provide a somewhat simpler method to determine the unicyclic graph which has maximum spectral radius among all unicyclic graphs with prescribed degree sequence. Moreover, we also determine the bicyclic graph which has maximum spectral radius among all bicyclic graphs with prescribed degree sequence. It confirms Conjecture 1.1 with $k = 2$.

3.1. Unicyclic graphs

Given a non-increasing sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$ with $\sum_{i=0}^{n-1} d_i = 2n$, if there exists a unicyclic graph having π as its degree sequence, then π is called *unicyclic graphic*. Let $\mathcal{U}^{\pi}_n$ be the set of all unicyclic graphs of order n with degree sequence π. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be unicyclic graphic with $n \ge 3$. We construct a special unicyclic graph U^*_{π} as follows: If $d_0 = 2$, then let $U^*_{\pi} = C_n$. If $d_0 \ge 3$ and $d_1 = 2$, then let U^*_{π} be the unicyclic graph obtained by attaching $d_0 - 2$

paths of almost equal lengths to one vertex of C_3. If $d_1 \geq 3$, then let $d(v_i) = d_i$ for $0 \leq i \leq n-1$. Then let U_π^* be the unicyclic graph consisting of $C_3 = v_0v_1v_2v_0$ and the remaining vertices (i.e., $v_3, \ldots, v_{n-1}$) appear in spiral like disposition with respect to C_3 starting from v_3 that is adjacent to v_0.

Lemma 3.7. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be unicyclic graphic with $d_1 = 2$. Then U_π^* is the only unicyclic graph with maximum spectral radius among all graphs in $\mathcal{U}_n^\pi$.

Proof. Let G be a unicyclic graph with maximum spectral radius among all unicyclic graphs with degree sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$. If $d_0 = 2$, then G must be the cycle C_n and the assertion holds. Now assume that $d_0 \geq 3$. Since $d_1 = 2$, G must be the graph obtained from a cycle C_k and $d_0 - 2$ paths P_{n_i} by identifying one vertex of C_k and one end vertex of each P_{n_i} for $i = 1, 2, \ldots, d_0 - 2$. Clearly, $n = k + \sum_{i=1}^{d_0-2} n_i$. Lemma 2.3 implies that $k = 3$. Otherwise, we may contract an edge of C_k (which decreases the cycle length), and subdivide an edge of one path P_{n_i}. Clearly, the resulting graph $G' \in \mathcal{U}_n^\pi$. By Lemma 2.3, we have $\rho(G) < \rho(G')$. This is a contradiction. Moreover, Lemma 2.4 implies that $|n_i - n_j| \leq 1$ for all $1 \leq i, j \leq d_0 - 2$. Therefore, $G \cong U_\pi^*$. □

Lemma 3.8. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be unicyclic graphic with $d_1 \geq 3$. Then U_π^* is the only unicyclic graph with maximum spectral radius among all graphs in $\mathcal{U}_n^\pi$.

Proof. Let G be a unicyclic graph with maximum spectral radius among all graphs in $\mathcal{U}_n^\pi$. Then Theorem 3.3 implies that G must be a BFS-graph. We keep the labeling of its vertices as defined below Theorem 3.3. It suffices to show that $v_{1,1}v_{1,2} \in E(G)$.

Since G is a unicyclic graph, there exists only one cycle C in G. Let $v_{r,q}$ be the smallest height among vertices in $V(C)$, i.e., $h(v_{r,q}) = r \leq h(u)$ for every $u \in V(C)$.

Suppose that $v_{1,1}v_{1,2} \notin E(G)$. Now we consider the following three cases:

Case 1. $v_{r,q} = v_{0,1}$.

Since G is a unicyclic graph, $|E(G[V_1])| \leq 1$.

(i) $|E(G[V_1])| = 1$.

Suppose that $v_{1,1}v_{1,i} \in E(G)$ $(i \geq 3)$. Since G is a unicyclic graph and $d(v_{1,2}) \geq d(v_{1,i}) \geq 2$, there exists a vertex $v_{2,t} \in V_2$ such that $v_{1,2}v_{2,t} \in E(G)$ but $v_{1,i}v_{2,t} \notin E(C)$. Let

$$G' = G - \{v_{1,1}v_{1,i},\, v_{1,2}v_{2,t}\} + \{v_{1,1}v_{1,2},\, v_{1,i}v_{2,t}\}.$$

Then $G' \in \mathcal{U}_n^\pi$. Moreover, Lemma 3.5 implies that $x_{v_{1,1}} > \min_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\} \geq x_{v_{2,t}}$. And $x_{v_{1,2}} \geq x_{v_{1,i}}$. Therefore, by Lemma 2.2 we have $\rho(G) < \rho(G')$. This is a contradiction.

Suppose that $v_{1,i}v_{1,j} \in E(G)$ $(j > i \geq 2)$. Since G is a unicyclic graph and $d(v_{1,1}) = d_1 \geq 3$, there exists a vertex $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(G)$ and

$x_{v_{2,t}} = \min_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\}$. Clearly, $v_{1,1}v_{1,i} \notin E(G)$ and $v_{1,j}v_{2,t} \notin E(G)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\ v_{1,i}v_{1,j}\} + \{v_{1,1}v_{1,i},\ v_{1,j}v_{2,t}\}.$$

Then $G' \in \mathfrak{U}_n^\pi$. Moreover, we claim that $x_{v_{1,1}} > x_{v_{1,j}}$ or $x_{v_{1,i}} > x_{v_{2,t}}$ (otherwise, $x_{v_{1,1}} = x_{v_{1,j}} = x_{v_{1,i}} = x_{v_{2,t}}$, by Lemma 3.5, it is impossible). Therefore, Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction too.

(ii) $|E(G[V_1])| = 0$.

In this case, there exist two vertices $v_{1,i} \in V_1$ $(i \geq 2)$ and $v_{2,j} \in V_2$ such that $v_{1,i}v_{2,j} \in E(C)$. Since G is a unicyclic graph and $d(v_{1,1}) = d_1 \geq 3$, there exists a vertex $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(G)$ but $v_{1,1}v_{2,t} \notin E(C)$. Clearly, $v_{1,i}v_{2,t} \notin E(G)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\ v_{1,i}v_{2,j}\} + \{v_{1,1}v_{1,i},\ v_{2,t}v_{2,j}\}.$$

Then $G' \in \mathfrak{U}_n^\pi$. Moreover, by Lemma 3.5, we have $x_{v_{1,1}} > \min_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\} \geq x_{v_{2,j}}$. Recall that $x_{v_{1,i}} \geq x_{v_{2,t}}$. Therefore, Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

Case 2. $v_{r,q} = v_{1,1}$.

There exists a vertex $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(C)$. Since G is a unicyclic graph and $d(v_{1,2}) \geq d(v_{2,t}) \geq 2$, there exists a vertex $v_{2,j} \in V_2$ such that $v_{1,2}v_{2,j} \in E(G)$ but $v_{1,2}v_{2,j} \notin E(C)$. Clearly, $v_{2,t}v_{2,j} \notin E(G)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\ v_{1,2}v_{2,j}\} + \{v_{1,1}v_{1,2},\ v_{2,t}v_{2,j}\}.$$

Then $G' \in \mathfrak{U}_n^\pi$. Similarly, we have $x_{v_{1,1}} > x_{v_{2,j}}$ and $x_{v_{1,2}} \geq x_{v_{2,t}}$. Hence, Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

Case 3. $v_{r,q} \neq v_{0,1},\ v_{1,1}$.

There exists $v_{r+1,t} \in V_{r+1}$ such that $v_{r,q}v_{r+1,t} \in E(C)$. Since G is a unicyclic graph, from the choice of $v_{r,q}$, it is clear that there is no edges in $G[V_i]$ for $0 \leq i \leq r$. Hence $|V_r| \geq d_0 \geq 3$. Since $d(v_{r+1,t}) \geq 2$, there must exist two vertices $v_{r,i} \in V_r$ and $v_{r+1,j} \in V_{r+1}$ such that $v_{r,i}v_{r+1,j} \in E(G)$ but $v_{r,i}v_{r+1,j} \notin E(C)$. Let

$$G^* = G - \{v_{r,q}v_{r+1,t},\ v_{r,i}v_{r+1,j}\} + \{v_{r,i}v_{r,q},\ v_{r+1,j}v_{r+1,t}\}.$$

Then $G^* \in \mathfrak{U}_n^\pi$. Since $x_{v_{r,q}} \geq x_{v_{r+1,j}}$ and $x_{v_{r,i}} \geq x_{v_{r+1,t}}$, Lemma 2.2 implies that $\rho(G) \leq \rho(G^*)$. Clearly, the smallest height of the cycle in G^* is less than r. By repeating the argument of Case 3 or Cases 1 and 2, it is easy to see that G is not a unicyclic graph with maximum spectral radius among all graphs in $\mathfrak{U}_n^\pi$. This is a contradiction.

From the above discussions, the proof is completed. □

Combining Lemmas 3.7 and 3.8, we have the following result.

Theorem 3.9. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be unicyclic graphic. Then U^*_π is the only unicyclic graph having maximum spectral radius among all graphs in $\mathcal{U}^\pi_n$.

Let $\mathcal{U}_n$ be the set of all unicyclic graphs of order n, $\mathcal{U}_{n,k}$ be the set of all unicyclic graphs of order n with k pendent vertices and $\mathcal{U}^\pi_{n,k}$ be the set of all unicyclic graphs of order n with k pendent vertices and degree sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$. Thus $d_{n-k-1} > 1$ and $d_{n-k} = \cdots = d_{n-1} = 1$. Let $U^*_{\pi'}$ be the unicyclic graph with maximum spectral radius among all graphs in $\mathcal{U}^{\pi'}_{n,k}$, where $\pi' = (k+2, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{k})$. By Lemma 3.7. it is obvious that $U^*_{\pi'}$ is the unicyclic graph obtained from a triangle and k paths of almost equal lengths by identifying one vertex of the triangle and one end of each path of the k paths. It is easy to see that $\pi \trianglelefteq \pi'$ for each π, where π is the degree sequence of unicyclic graph of order n with k pendent vertices. So that by Lemma 3.6, the following result is obvious.

Theorem 3.10.([6]) Let $G \in \mathcal{U}_{n,k}$. Then $\rho(G) \leq \rho(U^*_{\pi'})$, and the equality holds if and only if $G \cong U^*_{\pi'}$, where $\pi' = (k+2, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{k})$.

Since U^* is the only unicyclic graph with degree sequence $\pi^* = (n-1, 2, 2, 1, \ldots, 1)$ and for each unicyclic graphic degree sequence π, we have $\pi \trianglelefteq \pi^*$. So that Lemma 3.6 implies that

Theorem 3.11.([6]) Let $G \in \mathcal{U}_n$. Then $\rho(G) \leq \rho(U^*)$, and the equality holds if and only if $G \cong U^*$.

3.2. Bicyclic graphs

To state the main results in this subsection, we need to define the following two kinds of bicyclic graphs.

Let $B(l, s, k)$ be the bicyclic graph obtained from two cycles C_l and C_k, by joining a path of length $s-1$ between them, where $l \geq k \geq 3$ and $s \geq 1$ (see Fig. 4).

Let $P(p, l, q)$ $(1 \leq l \leq \min\{p, q\})$ be the bicyclic graph obtained from the cycle C_{p+q}: $v_1 v_2 \cdots v_p v_{p+1} \cdots v_{p+q} v_1$ by connecting vertices v_1 and v_{p+1} with a new path $v_1 u_1 \cdots u_{l-1} v_{p+1}$ of length l (see Fig. 4).

Similarly, for a given non-increasing sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$ with $\sum_{i=1}^{n-1} d_i = 2(n+1)$, if there exists a bicyclic graph having π as its degree sequence, then π is called *bicyclic graphic*. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be bicyclic graphic with $n \geq 4$. We construct a special bicyclic graph B^*_π as follows: If $d_0 = 4$ and $d_1 = 2$, then let $B^*_\pi = B(n-2, 1, 3)$. If $d_0 \geq 5$ and $d_1 = 2$, then let B^*_π be the bicyclic graph obtained from $B(3, 1, 3)$ by attaching $d_0 - 4$ paths of almost equal lengths to the vertex of degree 4. If $d_0 = d_1 = 3$ and $d_2 = 2$, then let $B^*_\pi = P(n-2, 1, 2)$ (or $P(2, 1, n-2)$). If $d_0 = d_1 = d_2 = 3$, then let $d(v_i) = d_i$ for $0 \leq i \leq n-1$. Then let B^*_π be the bicyclic graph consisting of $P(2, 1, 2)$ (shown in Fig. 5.) and the remaining vertices (i.e., $v_4, \ldots, v_{n-1}$) appear in spiral like disposition with respect to $P(2, 1, 2)$ starting from v_4 that is adjacent to v_2. If $d_0 \geq 4$ and $d_1 \geq 3$, let $d(v_i) = d_i$ for $0 \le i \le n-1$. Then let B_π^* be the bicyclic graph consisting of $P(2,1,2)$ (shown in Fig. 5.) and the remaining vertices (i.e., $v_4, \ldots, v_{n-1}$) appear in spiral like disposition with respect to $P(2,1,2)$ starting from v_4 that is adjacent to v_0.

Lemma 3.12. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be bicyclic graphic with $d_1 = 2$. Then B_π^* is the only bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$.

Proof. Let G be a bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$. Theorem 3.3 implies that G is a BFS-graph. Suppose that $d_0 \ge 5$. Similar to the proof of Lemma 3.7, the assertion holds. Now assume that $d_0 = 4$. Then G must be $B(l,1,k)$ $(l+k = n+1)$. It suffices to prove that $k = 3$. Moreover, since G is a BFS-graph, keeping the labeling as mentioned above, we only need to show that $|E(G[V_1])| \ge 1$. Otherwise, there exists $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(G)$, and there exists an edge $v_{1,i}v_{2,j}$ $(2 \le i \le 4)$ such that $v_{1,i}v_{2,j}$ and $v_{1,1}v_{2,t}$ lie on the different cycles since $d(v_{0,1}) = d_0 = 4$. Now, let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,i}v_{2,j}\} + \{v_{1,1}v_{1,i},\, v_{2,t}v_{2,j}\}.$$

Then $G' \in \mathcal{B}_n^\pi$. From Lemma 3.5, we know that $x_{v_{1,1}} > x_{v_{2,t}} \ge x_{2,j}$ and $x_{v_{1,i}} \ge x_{v_{2,t}}$. Therefore, Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction. □

To deal with the case $d_1 \ge 3$, we need consider the following two subcases:

Subcase A: $d_0 = 3$. Since $d_0 \ge d_1 \ge \cdots \ge d_{n-1}$, $d_0 = d_1 = 3$ and $d_i \le 3$ $(3 \le i \le n-1)$.

Subcase B: $d_0 \ge 4$.

Such two cases will be solved in Lemmas 3.13 and 3.14, respectively.

Lemma 3.13. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be bicyclic graphic with $d_0 = d_1 = 3$. Then B_π^* is the only bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$.

Proof. Let G be a bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$. Theorem 3.3 implies that G is a BFS-graph.

Suppose that $d_2 = 2$. Then G must be either $B(l,2,k)$ or $P(p,1,q)$. If $G \cong B(l,2,k)$, then let

$$G' = G - \{v_{1,1}v_{2,1},\, v_{1,2}v_{2,3}\} + \{v_{1,1}v_{1,2},\, v_{2,1}v_{2,3}\}.$$

Clearly, $G' \in \mathcal{B}_n^\pi$ and $\rho(G) < \rho(G')$. Thus, $G \cong P(p,1,q)$. Similarly, we can show that $p = n-2$ or $q = n-2$. So that the assertion holds.

Suppose that $d_2 = 3$. By using the same argument as the proof of Theorem 3.14 below, the assertion holds. □

Theprem 3.14. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be bicyclic graphic with $d_0 \ge 4$ and $d_1 \ge 3$. Then B_π^* is the only bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$.

Proof. Let G be a bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$. Then Theorem 3.3 implies that G is a BFS-graph. Keeping the labeling of its vertices and notations as mentioned above, we only need to show that $v_{1,1}v_{1,2}, v_{1,1}v_{1,3} \in E(G)$.

Since G is a bicyclic graph, there exist two independent cycles, say C_1 and C_2, in G. Let $v_{r,q}$ be the smallest height among vertices in $V(C_1)$ or $V(C_2)$, i.e., $h(v_{r,q}) = r \le h(u)$ for any $u \in V(C_1 \cup C_2)$ (if there exist $v_{r,q_1} \in V(C_1)$ and $v_{r,q_2} \in V(C_2)$, then $q = \min\{q_1, q_2\}$). Now we consider the following three cases:

Case 1. $v_{r,q} = v_{0,1}$.

First, we claim that $|E(G[V_1])| \ge 1$.

Suppose not, i.e., $|E(G[V_1])| = 0$. Since $v_{0,1} \in V(C_1 \cup C_2)$, there exist $v_{1,i} \in V_1$ $(i \ge 2)$ and $v_{2,j} \in V_2$ such that $v_{1,i}v_{2,j} \in E(C_1 \cup C_2)$.

Suppose that there exists $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(G)$ but $v_{1,1}v_{2,t} \notin E(C_1 \cup C_2)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,i}v_{2,j}\} + \{v_{1,1}v_{1,i},\, v_{2,t}v_{2,j}\}.$$

Then $G' \in \mathcal{B}_n^\pi$. Moreover, recall that $x_{v_{1,1}} > x_{v_{2,j}}$ and $x_{v_{1,i}} \ge x_{v_{2,t}}$. Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

Suppose that for each $v_{2,k} \in N(v_{1,1})$, $v_{1,1}v_{2,k} \in E(C_1 \cup C_2)$. Since $d(v_{1,1}) = d_1 \ge 3$ and G is a bicyclic graph, there exist at least one edge $v_{1,1}v_{2,t}$ ($v_{2,t} \in N(v_{1,1})$) such that $v_{1,1}v_{2,t}$ and $v_{1,i}v_{2,j}$ are in the different independent cycles. Let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,i}v_{2,j}\} + \{v_{1,1}v_{1,i},\, v_{2,t}v_{2,j}\}.$$

Similarly, we have $G' \in \mathcal{B}_n^\pi$ and $\rho(G) < \rho(G')$. This is a contradiction too.

On the other hand, since G is a bicyclic graph, $|E(G[V_1])| \le 2$. Therefore, we only need to consider the following two subcases:

(a) $|E(G[V_1])| = 2$. It suffices to prove that $v_{1,1}v_{1,2},\, v_{1,1}v_{1,3} \in E(G)$.

Suppose that $v_{1,i}v_{1,j},\, v_{1,l}v_{1,k} \in E(G)$ $(j > i \ge 2,\ k > l \ge 2)$. Since $d(v_{1,1}) = d_1 \ge 3$, there exists $v_{2,t} \in V_2$ such that $x_{v_{2,t}} = \min\limits_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\}$ and $v_{1,1}v_{2,t} \in E(G)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,i}v_{1,j}\} + \{v_{1,1}v_{1,i},\, v_{1,j}v_{2,t}\}.$$

Similarly, we have $G' \in \mathcal{B}_n^\pi$ and $\rho(G) < \rho(G')$. This is a contradiction.

Suppose that $v_{1,1}v_{1,i},\, v_{1,l}v_{1,k} \in E(G)$ $(k > l \ge 2)$. Then there exists $v_{2,t} \in V_2$ such that $x_{v_{2,t}} = \min\limits_{v_{2,i} \in N(v_{1,1})} \{x_{v_{2,i}}\}$, $v_{1,1}v_{2,t} \in E(G)$ and $v_{1,k}v_{2,t} \notin E(G)$ since $d(v_{1,1}) = d_1 \ge 3$ and G is a bicyclic graph. Let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,l}v_{1,k}\} + \{v_{1,1}v_{1,l},\, v_{1,k}v_{2,t}\}.$$

Then $G' \in \mathcal{B}_n^\pi$. Moreover, we claim that $x_{v_{1,1}} > x_{v_{1,k}}$ or $x_{v_{1,l}} > x_{v_{2,t}}$ (Otherwise, $x_{v_{1,1}} = x_{v_{1,l}} = x_{v_{1,k}} = x_{v_{2,t}}$. By Lemma 3.5, it is impossible). Hence Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

Suppose that $v_{1,1}v_{1,i}$, $v_{1,1}v_{1,j} \in E(G)$ for $2 \le i < j \le s_1$. We claim that $i = 2$ and $j = 3$.

Suppose that, i.e., $i \ne 2$ or $j \ne 3$. If $i \ne 2$, since $d(v_{1,2}) \ge d(v_{1,i}) \ge 2$ and G is a bicyclic graph, there exists $v_{2,t} \in V_2$ such that $v_{1,2}v_{2,t} \in E(G)$ and $v_{1,i}v_{2,t} \notin E(G)$. Let

$$G' = G - \{v_{1,1}v_{1,i},\, v_{1,2}v_{2,t}\} + \{v_{1,1}v_{1,2},\, v_{1,i}v_{2,t}\}.$$

Then $G' \in \mathcal{B}_n^\pi$. Moreover, recall that $x_{v_{1,1}} > x_{v_{2,t}}$ and $x_{v_{1,2}} \ge x_{v_{1,i}}$. Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

Similarly, if $j \ne 3$, since $d(v_{1,3}) \ge d(v_{1,j}) \ge 2$, there exists $v_{2,t} \in V_2$ such that $v_{1,3}v_{2,t} \in E(G)$ and $v_{1,j}v_{2,t} \notin E(G)$. Let

$$G' = G - \{v_{1,1}v_{1,j},\, v_{1,3}v_{2,t}\} + \{v_{1,1}v_{1,3},\, v_{1,j}v_{2,t}\}.$$

Then $G' \in \mathcal{B}_n^\pi$ and $\rho(G) < \rho(G')$. This is a contradiction too.

(b) $|E(G[V_1])| = 1$.

First, similar to the proof of Case 1 (i) in Lemma 3.8, we claim that $v_{1,1}v_{1,2} \in E(G)$.

Hence, without loss of generality, we may assume that $C_1 = v_{0,1}v_{1,1}v_{1,2}v_{0,1}$. Let $v_{k,l}$ be the smallest height among vertices in $V(C_2)$, i.e., $h(v_{k,l}) = k \le h(v)$ for any $v \in V(C_2)$. Then there are four cases:

(1) $v_{k,l} = v_{0,1}$.
Since C_1 and C_2 are two independent cycles in G, there exist $v_{1,i} \in V_1$ $(i \ge 3)$ and $v_{2,j} \in V_2$ such that $v_{1,i}v_{2,j} \in E(C_2)$. On the other hand, since $d_0 = |V_1| \ge 4$, $d(v_{1,1}) = d_1 \ge 3$ and $d(v_{1,i}) \ge 2$ for $2 \le i \le |V_1|$, there exist $v_{1,s} \in V_1$ $(s \ne i)$ and $v_{2,t} \in V_2$ such that $v_{1,s}v_{2,t} \in E(G)$ but $v_{1,s}v_{2,t} \notin E(C_2)$. Let

$$G_1 = G - \{v_{1,i}v_{2,j},\, v_{1,s}v_{2,t}\} + \{v_{1,i}v_{1,s},\, v_{2,j}v_{2,t}\}.$$

Then $G_1 \in \mathcal{B}_n^\pi$. If $s = 1$, then similarly we claim that $x_{v_{1,s}} > x_{v_{2,j}}$ or $x_{v_{1,i}} > x_{v_{2,t}}$. Hence Lemma 2.2 implies that $\rho(G) < \rho(G_1)$ yielding a contradiction. If $s \ne 1$, since $x_{v_{1,s}} \ge x_{v_{2,j}}$ and $x_{v_{1,i}} \ge x_{v_{2,t}}$, Lemma 2.2 implies that $\rho(G) \le \rho(G_1)$. Moreover, since $v_{1,1}v_{1,2}$, $v_{1,i}v_{1,s} \in E(G_1)$, using the same argument as in Subcase (a) (on G_1), we can obtain a contradiction too.

(2)$v_{k,l} = v_{1,1}$.
There exists $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(C_2)$. Since $d(v_{0,1}) = d_0 \ge 4$ and $d(v_{1,i}) \ge d(v_{2,t}) \ge 2$, there exist $v_{1,i}$ $(i \ge 3)$ and $v_{2,j}$ such that $v_{1,i}v_{2,j} \in E(G)$ but $v_{1,i}v_{2,j} \notin E(C_2)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,i}v_{2,j}\} + \{v_{1,1}v_{1,i},\, v_{2,t}v_{2,j}\}.$$

Then $G' \in \mathcal{B}_n^\pi$. Moreover, recall that $x_{v_{1,1}} > x_{v_{2,j}}$ and $x_{v_{1,i}} \ge x_{v_{2,t}}$. Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

(3) $v_{k,l} = v_{1,2}$.
Similarly, there exist $v_{1,i}$ $(i \geq 3)$, $v_{2,j}$ and $v_{2,t}$ such that $v_{1,2}v_{2,t} \in E(C_2)$, $v_{1,i}v_{2,j} \in E(G)$ but $v_{1,i}v_{2,j} \notin E(C_2)$. Let

$$G_1 = G - \{v_{1,2}v_{2,t},\, v_{1,i}v_{2,j}\} + \{v_{1,2}v_{1,i},\, v_{2,t}v_{2,j}\}.$$

Clearly, $G_1 \in \mathcal{B}_n^\pi$ and $\rho(G) \leq \rho(G_1)$. Moreover, since $v_{1,1}v_{1,2}$, $v_{1,2}v_{1,i} \in E(G_1)$, using the same argument as in Subcase (a) (on G_1), we can obtain a contradiction too.

(4) $v_{k,l} \notin \{v_{0,1}, v_{1,1}, v_{1,2}\}$.
There exists $v_{k+1,t} \in V_{k+1}$ such that $v_{k,l}v_{k+1,t} \in E(C_2)$. Note that $|E(G[V_1])| = 1$ and $|E(G[V_i])| = 0$ for $2 \leq i \leq k$. Thus $|V_k| \geq d_0 - 1 \geq 3$. Then there exist $v_{k,i}$ $(i \neq l)$ and $v_{k+1,j}$ $(j \neq t)$ such that $v_{k,i}v_{k+1,j} \in E(G)$ but $v_{k,i}v_{k+1,j} \notin E(C_2)$. Let

$$G^* = G - \{v_{k,l}v_{k+1,t},\, v_{k,i}v_{k+1,j}\} + \{v_{k,l}v_{k,i},\, v_{k+1,t}v_{k+1,j}\}.$$

Then $G^* \in \mathcal{B}_n^\pi$. Moreover, since $x_{v_{k,l}} \geq x_{v_{k+1,j}}$ and $x_{v_{k,i}} \geq x_{v_{k+1,t}}$, Lemma 2.2 implies that $\rho(G) \leq \rho(G^*)$. Clearly, the smallest height of C_2 in G^* is less than k. Furthermore, by repeating the argument of (4), we will got a case referred to (1), (2) or (3). Thus G is not a bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$. This is a contradiction.

Case 2. $v_{r,q} = v_{1,1}$.

There exists $v_{2,t} \in V_2$ such that $v_{1,1}v_{2,t} \in E(C_1 \cup C_2)$. Since $d_0 \geq 4$ and $E(G[V_1]) = 0$, there exist $v_{1,i} \in V_1$ $(i \geq 2)$ and $v_{2,j} \in V_2$ such that $v_{1,i}v_{2,j} \in E(G)$ but $v_{1,i}v_{2,j} \notin E(C_1 \cup C_2)$. Let

$$G' = G - \{v_{1,1}v_{2,t},\, v_{1,i}v_{2,j}\} + \{v_{1,1}v_{1,i},\, v_{2,t}v_{2,j}\}.$$

Then $G' \in \mathcal{B}_n^\pi$. Moreover, recall that $x_{v_{1,1}} > x_{v_{2,j}}$ and $x_{v_{1,i}} \geq x_{v_{2,t}}$. Lemma 2.2 implies that $\rho(G) < \rho(G')$. This is a contradiction.

Case 3. $v_{r,q} \neq v_{0,1}, v_{1,1}$.

There exists $v_{r+1,t} \in V_{r+1}$ such that $v_{r,q}v_{r+1,t} \in E(C_1 \cup C_2)$. Recall that there is no edge in $G[V_i]$ for $0 \leq i \leq r$. Thus $|V_r| \geq d_0 \geq 4$. Then there exist $v_{r,i} \in V_r$ $(i \neq q)$ and $v_{r+1,j} \in V_{r+1}$ $(j \neq t)$ such that $v_{r,i}v_{r+1,j} \in E(G)$ but $v_{r,i}v_{r+1,j} \notin E(C_1 \cup C_2)$. Let

$$G^* = G - \{v_{r,q}v_{r+1,t},\, v_{r,i}v_{r+1,j}\} + \{v_{r,q}v_{r,i},\, v_{r+1,t}v_{r+1,j}\}.$$

Then $G^* \in \mathcal{B}_n^\pi$. Moreover, since $x_{v_{r,q}} \geq x_{v_{r+1,j}}$ and $x_{v_{r,i}} \geq x_{v_{r+1,t}}$, Lemma 2.2 implies that $\rho(G) \leq \rho(G^*)$. Clearly, the smallest height of the cycles in G^* is less than r. Furthermore, by repeating the argument of Case 3, or Cases 1 and 2. It is easy to know that G is not a bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}_n^\pi$. This is a contradiction.

From the above discussions, the proof is completed. □

Combining Lemmas 3.12, 3.13 and 3.14, we have the following result.

Theorem 3.15. Let $\pi = (d_0, d_1, \ldots, d_{n-1})$ be bicyclic graphic. Then B^*_π is the only bicyclic graph which has maximum spectral radius among all graphs in $\mathcal{B}^\pi_n$.

Let $\mathcal{B}_n$ be the set of all bicyclic graphs of order n, $\mathcal{B}_{n,k}$ be the set of all bicyclic graphs of order n with k pendent vertices and $\mathcal{B}^\pi_{n,k}$ be the set of all bicyclic graphs of order n with k pendent vertices and degree sequence $\pi = (d_0, d_1, \ldots, d_{n-1})$. Thus $d_{n-k-1} > 1$ and $d_{n-k} = \cdots = d_{n-1} = 1$. If $1 \le k \le n-5$, then it is easy to see that for each degree sequence π of bicyclic graph with k pendent vertices, we have $\pi \trianglelefteq \pi'$, where $\pi' = (k+4, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{k})$. Moreover, Lemma 3.12 implies that $B^*_{\pi'}$ is the bicyclic graph with maximum spectral radius among all graphs in $\mathcal{B}^{\pi'}_n$. If $k = n-4$, then there is only one bicyclic graph B^* with degree sequence $\pi^* = (n-1, 3, 2, 2, \underbrace{1, \ldots, 1}_{n-4})$. Hence, by Theorem 3.6, we have the following result.

Theorem 3.16. Let $G \in \mathcal{B}_{n,k}$. Then $\rho(G) \le \rho(B^*_{\pi'})$ for $1 \le k \le n-5$, and the equality holds if and only if $G \cong B^*_{\pi'}$, where $\pi' = (k+4, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{k})$; and $\rho(G) = \rho(B^*)$ for $k = n-4$.

When $1 \le k \le n-6$. It is easy to check that $\pi' = (k+4, \underbrace{2, \ldots, 2}_{n-k-1}, \underbrace{1, \ldots, 1}_{k}) \trianglelefteq \pi'' = (k+5, \underbrace{2, \ldots, 2}_{n-k-2}, \underbrace{1, \ldots, 1}_{k+1})$. Then Theorem 3.6 implies that $\rho(B^*_{\pi'}) < \rho(B^*_{\pi''})$. Hence $\rho(B^*_{\pi'})$ is an increasing function for $1 \le k \le n-5$. Moreover, when $k = n-5$ there is only one bicyclic graph B^+ with degree sequence $(n-1, 2, 2, 2, 2, \underbrace{1, \ldots, 1}_{n-5})$. He *et al.* [7] proved that $\rho(B^+) < \rho(B^*)$. Then by Theorem 3.16, we have the following theorem.

Theorem 3.17.([7]) Let $G \in \mathcal{B}_n$. Then $\rho(G) \le \rho(B^*)$, and the equality holds if and only if $G \cong B^*$. Moreover, if $G \in \mathcal{B}_n$ and $G \ne B^*$, then $\rho(G) \le \rho(B^+)$, and the equality holds if and only if $G \cong B^+$.

Acknowledgments. The authors would like to thank the anonymous referees for their constructive corrections and valuable comments and the editor for his effort to improve readability of this paper. This work was supported by NSF of China (Nos. 11101358, 11471077, 61379021); NSF of Fujian (No. 2014J01020); China Postdoctoral Science Foundation(No. 2014M551831); General Research Fund of Hong Kong; Faculty Research Grant of Hong Kong Baptist University.

References

[1] J. Bondy, U. Murty, *Graph theory with applications*, New York, MacMillan, 1976.

[2] T. Biyukoğlu, J. Leydold,*Graphs with given degree sequence and maximal spectral radius*, Electron. J. Combin., **15**(2008), #R119.

[3] F. Belardo, E. M. Li Marzi, S. K. Simić, J. Wang, *On the spectral radius of unicyclic graphs with prescribed degree sequence*, Linear Algebra. Appl., **432**(2010), 2323-2334.

[4] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs: Theory and Applications*, 3rd ed., Johan Ambrosius Barth Verlag, Heidelberg, Leipzig, 1995.

[5] D. Cvetković, P. Rowlinson, S. Simić, *Eigenspaces of Graphs*, Cambridge University Press, 1997.

[6] S. Guo, *The spectral radius of unicyclic and bicyclic graphs with n vertices and k pendant vertices*, Linear Algebra Appl., **408**(2005), 78-85.

[7] X. He, Y. Liu, J. Shao, *On the spectral radii of bicyclic graphs*, J. Math. Res. Exposition., **27**(2007), 445-454.

[8] A. Hoffman, J. Smith, On the spectral radii of topologically equivalent graphs, in: M. Fiedler (Ed.), *Recent Advances in Graph Theory*, Academia Praha, 1975, pp.273-281.

[9] R. Horn, C. Johnson, *Matrix Analysis.* Reprinted with corrections. Cambridge University Press, 1990.

Figure 1: G and G' in Lemma 2.2

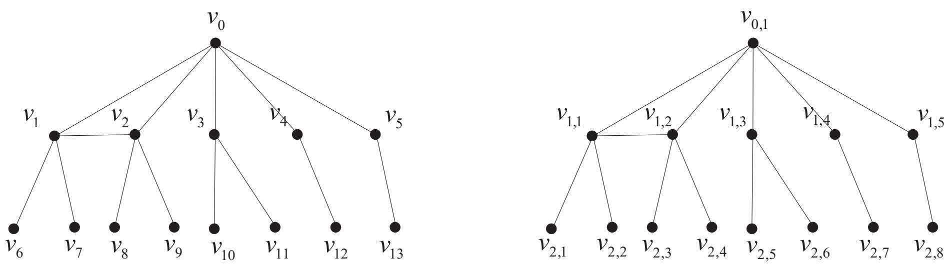

Figure 2: Original graph and its relabeled graph, where $V_1 = \{v_0\}$, $V_2 = \{v_1, v_2, v_3, v_4, v_5\}$ and $V_3 = \{v_6, v_7, v_8, v_9, v_{10}, v_{11}, v_{12}, v_{13}, v_{14}\}$

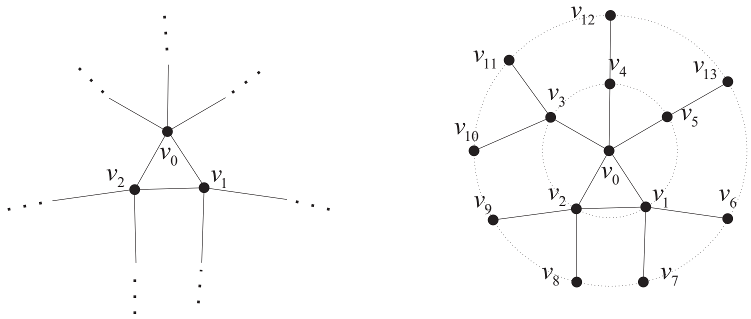

Figure 3: Spiral like disposition with respect to the cycle C (On the left) staring from v_3 that is adjacent to v_0

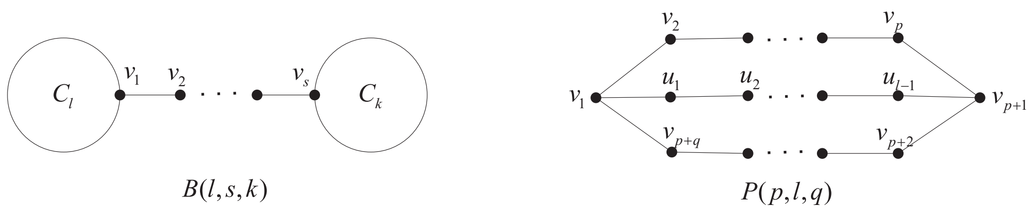

Figure 4: Bicyclic graphs $B(l,s,k)$ and $P(p,l,q)$.

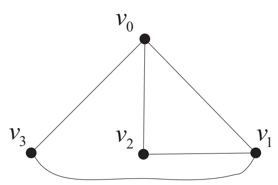

Figure 5: Bicyclic graph $P(2,1,2)$.