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The A_α-spectral Radius of Bicyclic Graphs with Given Degree Sequences

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Abstract. Let $A(G)$ and $D(G)$ be the adjacency matrix and the degree matrix of G, respectively. For any real $\alpha \in [0,1]$, Nikiforov defined the matrix $A_\alpha(G)$ as

$$A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G).$$

In this paper, we generalize some previous results about the $A_{1/2}$-spectral radius of bicyclic graphs with a given degree sequence. Furthermore, we characterize all extremal bicyclic graphs which have the largest A_α-spectral radius in the set of all bicyclic graphs with prescribed degree sequences.

1. Introduction

Throughout this paper, all graphs considered are simple connected and undirected. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Denote by $|V(G)| = n$ and $|E(G)| = m$ the order and the size of graph G, respectively. A connected graph is a *k-cyclic graph* if $k = m - n + 1$. Let $A(G)$ and $D(G)$ be respectively the *adjacency matrix* and the *diagonal matrix* of vertex degrees of G. We write $d_G(v)$, i.e., $d(v)$, for the degree of the vertex v in G, and $N_G(v)$ for the neighbor set of the vertex v in G. For any real $\alpha \in [0,1]$, Nikiforov [11] defined the matrix $A_\alpha(G)$ as

$$A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G).$$

It is clear that $A_0(G) = A(G)$, $A_1(G) = D(G)$ and $2A_{1/2}(G) = Q(G)$, where $Q(G)$ is the *signless Laplacian matrix*. Moreover, $L(G) = (A_\alpha(G) - A_\beta(G))/(\alpha - \beta)$ if $\alpha \neq \beta$ for any $\alpha, \beta \in [0,1]$, where $L(G)$ is the *Laplacian matrix*. The largest eigenvalue of $A_\alpha(G)$ is called the *$A_\alpha(G)$-spectral radius* (or *A_α-spectral radius* if there is no confusion) of G, and denote by $\rho(A_\alpha(G))$. As usual, T_n, P_n and C_n ($n \geq 3$) always represent the *tree*, *path* and *cycle*, respectively. We call a path $P_{k+1} = v_0v_1 \cdots v_{k-1}v_k$ is an *internal path* of G if $d(v_0) \geq 3$,

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$d(v_k) \geq 3$ and $d(v_i) = 2$ where $i = 1, 2, \ldots, k-1$. For a graph G, if $V'(G) \subseteq V(G)$ and $V'(G) \neq \emptyset$, then we denote by $G[V']$ the subgraph of G induced by V'. Let uv be a cut edge of G, if one component of $G - uv$ is a tree T (suppose $u \in V(T)$), then the induced subgraph $G[V(T) \cup \{v\}]$ is called a *hanging tree* on vertex v. For all other graph theoretic notations and terminologies not defined here, we refer the readers to [2].

Next, we introduce three kinds of bicyclic graphs. Let $\infty(n_1, n_2)$ denote the graph obtained from two cycles C_{n_1} and C_{n_2} ($n_1, n_2 \geq 3$) by identifying a vertex of C_{n_1} and C_{n_2}. The θ-graph is a 2-connected simple graph consisting of 3 internally disjoint paths between a pair of vertices of degree 3. Let $\theta(p, q, r)$ denote the θ-graph with order $n = p+q+r-4$, which is obtained from three vertex-disjoint paths P_p, P_q and P_r by identifying the three initial (resp. terminal) vertices of them, where $p, q, r \geq 2$ and at most one of p, q, r equals 2. Denote by $F(C_{n_1}, C_{n_2}, P_{p_1}, \ldots, P_{p_{d_1-4}})$ the graph obtained from $\infty(n_1, n_2)$ and $d_1 - 4$ paths by identifying the maximum degree vertex of $\infty(n_1, n_2)$ with one end vertex of each path of $d_1 - 4$ paths, where $d_1 \geq 5$.

A non-increasing sequence of nonnegative integers $\pi = (d_1, d_2, \ldots, d_n)$ is called *graphic* if there exists a simple graph G with order n having π as its vertex degree sequence. For a given graphic degree sequence π, let

$$\mathscr{G}_\pi = \{G \mid G \text{ is a connected graph with } \pi \text{ as its degree sequence}\}.$$

Note that $\mathscr{G}_\pi$ may be an empty set for some degree sequence π. Here we only consider that $\mathscr{G}_\pi$ is non-empty.

In order to explore the extent to which the summands of $A(G)$ and $D(G)$ determines the properties of $Q(G)$, Nikiforov [11] in 2017 proposed to study the convex combinations A_α-matrix of $A(G)$ and $D(G)$, and claimed in [12] that the matrices $A_\alpha(G)$ can underpin a unified theory of $A(G)$ and $Q(G)$. In recent years, the research of A_α-matrix is an intriguing topic in spectral graph theory, the reader may be referred to [5–10, 12–16] and the references therein.

Up until now, the problem concerning graphs with maximal A_α-spectral radius on graph perturbation of a given class of graphs has attracted the attention of several scholars. The unique graph with maximum A_α-spectral radius among all connected graphs with diameter d is determined by Xue et al. in [16]. The extremal graph with maximal A_α-spectral radius with fixed order and cut vertices, and the extremal tree with the maximal A_α-spectral radius with fixed order and matching number are characterized by Lin et al. in [7]. The extremal graphs with largest A_α-spectral radius with fixed vertex or edge connectivity are depicted by Wang in [15]. Most recently, the extremal graphs with maximum A_α-spectral radius among all graphs with given size (resp. clique number, chromatic number) where $1/2 \leq \alpha \leq 1$ are explored by Li and Qin in [6].

In particular, with the degree sequence given in advance, Zhang [17] investigated all extremal trees with the largest Laplacian spectral radius in the set of all trees with a given degree sequence. Moreover, Zhang [18] also surveyed the unicyclic graphs that have the largest $A_{1/2}$-spectral radius (i.e., Q-spectral radius) for the prescribed degree sequence. In addition, Huang et al. [4] determined all extremal connected bicyclic graphs with the largest $A_{1/2}$-spectral radius in the set of all connected bicyclic graphs with prescribed degree sequences. To generalize these results, Li et al. [5] proposed the following problem.

Problem 1.1. [5] Let $0 \le \alpha < 1$ and π be a given graphic degree sequence, and

$$\mathscr{G}_\pi = \{G \mid G \text{ is connected with } \pi \text{ as its degree sequence}\}.$$

Characterize all extremal graphs such that their A_α-spectral radius reach the largest value in $\mathscr{G}_\pi$.

And then, they characterized respectively the extremal tree with the maximum A_α-spectral radius in $\mathscr{G}_\pi$ for a given tree degree sequence and the extremal unicyclic graph with the largest A_α-spectral radius in $\mathscr{G}_\pi$ for a given unicycilc degree sequence. Motivated by the above results, we continue this line of research by the next natural step, i.e., by considering the following problem.

Problem 1.2. For a given bicyclic graphic degree sequence π, let $\alpha \in [0,1)$ and

$$\mathscr{B}_\pi = \{B \in \mathscr{G}_\pi \mid B \text{ is a bicyclic graph with degree sequence } \pi\}.$$

Characterize all extremal bicyclic graphs which attain the maximal A_α-spectral radius in $\mathscr{B}_\pi$.

In this paper, we generalize some previous extremal results about the $A_{1/2}$-spectral radius among bicyclic graphs with a given degree sequence in [4]. Furthermore, we characterize all extremal bicyclic graphs which have the largest A_α-spectral radius in the set of all bicyclic graphs with the prescribed degree sequence, which gives a complete answer to Problem 1.2. The main result of this paper is as follows.

Theorem 1.3. *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a given non-increasing bicyclic degree sequence. Then B_π^* is a unique bicyclic graph with the largest A_α-spectral radius in $\mathscr{B}_\pi$, where B_π^* is shown in Section 3 and $\alpha \in [0,1)$.*

2. Preliminaries

In order to show our main result, we are about to introduce some definitions, propositions, lemmas and corollaries for later use.

Let G be a graph with a root v. We denote by $h(u) = \mathrm{dis}(u,v)$ the distance between $u \in V(G)$ and v. Besides, $h(u)$ is called the height of u.

Definition 2.1. [18, Definition 2.1] Let $G = (V(G), E(G))$ be a graph with a root $v_r \in V(G)$. A well-ordering $\prec$ of the vertices is called a bread-first-search ordering (BFS-ordering for short) if the following conditions hold for all vertices $u, v \in V(G)$:

(1) $u \prec v$ implies $h(u) \leq h(v)$.

(2) $u \prec v$ implies $d(u) \geq d(v)$.

(3) suppose $uv \in E(G)$, $xy \in E(G)$, $uy \notin E(G)$, $xv \notin E(G)$ with $h(u) = h(x) = h(v) - 1 = h(y) - 1$. If $u \prec x$, then $v \prec y$.

Proposition 2.2. (see [1, p. 11] or [3]) *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a non-increasing sequence. Then π is graphic if and only if $\sum_{i=1}^{n} d_i$ is even and*

$$\sum_{i=1}^{k} d_i \leq k(k-1) + \sum_{i=k+1}^{n} \min\{k, d_i\}, \tag{2.1}$$

where $1 \leq k \leq n$.

From Proposition 2.2, Huang et al. in [4] obtained the following proposition.

Proposition 2.3. [4, Proposition 3.2] *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a positive non-increasing integer sequence with even sum and $n \geq 4$. If π is a bicyclic graph sequence, then $\sum_{i=1}^{n} d_i = 2n + 2$ and (2.1) holds.*

Lemma 2.4. [11, Proposition 14] *For $\alpha \in [0, 1)$, let G be a graph and $\mathbf{X}$ be a non-negative eigenvector to $\rho(A_\alpha(G))$.*

(1) *If G is connected, then $\mathbf{X}$ is positive and is unique up to scaling.*

(2) *If G is not connected and U is the set of vertices with positive entries in $\mathbf{X}$, then the subgraph induced by U is a union of components H of G with $\rho(A_\alpha(H)) = \rho(A_\alpha(G))$.*

(3) *If G is connected and μ is an eigenvalue of $A_\alpha(G)$ with a nonnegative eigenvector, then $\mu = \rho(A_\alpha(G))$.*

(4) *If G is connected and H is a proper subgraph of G, then $\rho(A_\alpha(G)) > \rho(A_\alpha(H))$.*

Lemma 2.5. [5, Lemma 2.3] *Let $G \in \mathscr{G}_\pi$ be a connected graph with $\alpha \in [0, 1)$. Let $\mathbf{X}$ be a unit eigenvector of $A_\alpha(G)$ corresponding to $\rho(A_\alpha(G))$. Assume that $v_1u_1, v_2u_2 \in E(G)$ and $v_1v_2, u_1u_2 \notin E(G)$. Let G' be a new graph obtained from G by deleting edges v_1u_1, v_2u_2 and adding edges v_1v_2, u_1u_2. If $x_{v_1} \geq x_{u_2}$ and $x_{v_2} \geq x_{u_1}$, then $\rho(A_\alpha(G')) \geq \rho(A_\alpha(G))$. Furthermore, if one of the two inequalities is strict, then $\rho(A_\alpha(G')) > \rho(A_\alpha(G))$.*

Corollary 2.6. *Let B be a graph with the largest A_α-spectral radius in $\mathscr{B}_\pi$ and $\mathbf{X}$ be a unit eigenvector of $A_\alpha(B)$ corresponding to $\rho(A_\alpha(B))$. Assume that $v_1u_1, v_2u_2 \in E(B)$ and $v_1v_2, u_1u_2 \notin E(B)$. Let $B' = B - v_1u_1 - v_2u_2 + v_1v_2 + u_1u_2$. If B' is connected, then $B' \in \mathscr{B}_\pi$. Moreover, the following assertions hold in $\mathbf{X}$.*

(1) *If $x_{v_1} > x_{u_2}$, then $x_{v_2} < x_{u_1}$.*

(2) *If $x_{v_1} = x_{u_2}$, then $x_{v_2} = x_{u_1}$.*

Proof. Recall that a connected graph G is a bicyclic graph if $|E(G)| = |V(G)| + 1$. It is easy to see that $|V(B)| = |V(B')|$, $|E(B)| = |E(B')|$ and $|E(B)| = |V(B)| + 1$, which implies $|E(B')| = |V(B')| + 1$. Clearly, the degree sequence of B' is also π. Thus, if B' is a connected graph, B' is a bicyclic graph and $B' \in \mathscr{B}_\pi$. Let $\mathbf{X}$ be a unit eigenvector corresponding to $\rho(A_\alpha(B))$. Suppose $x_{v_2} \geq x_{u_1}$ in item (1), combining with $x_{v_1} > x_{u_2}$, one can deduce that $\rho(A_\alpha(B')) > \rho(A_\alpha(B))$ by Lemma 2.5, a contradiction.

Assume that $x_{v_2} \neq x_{u_1}$ in item (2). Then $x_{v_2} > x_{u_1}$ or $x_{v_2} < x_{u_1}$ holds. Without loss of generality, suppose $x_{v_2} > x_{u_1}$. Combining with $x_{v_1} = x_{u_2}$, we have $\rho(A_\alpha(B')) > \rho(A_\alpha(B))$ by Lemma 2.5, a contradiction. Thus, the conclusion of (2) holds. □

Lemma 2.7. [5, Lemma 2.5] *Let $G \in \mathscr{G}_\pi$ be a connected graph with $\alpha \in [0, 1)$ and $V(G) = \{v_0, v_1, \ldots, v_{n-1}\}$. Let $\rho(A_\alpha(G)) = \max\{\rho(A_\alpha(H)) \mid H \in \mathscr{G}_\pi\}$ and $\mathbf{X}$ be a unit eigenvector of $A_\alpha(G)$ corresponding to $\rho(A_\alpha(G))$. Then the following assertions hold.*

(1) *If $x_{v_i} \geq x_{v_j}$, then $d_G(v_i) \geq d_G(v_j)$.*

(2) *If $x_{v_i} = x_{v_j}$, then $d_G(v_i) = d_G(v_j)$.*

In Lemma 2.7 above, $i < j$ is redundant in assertion (1). So we omit it here.

Corollary 2.8. *Under the assumption above, if $d_G(u) > d_G(v)$, then $x_u > x_v$, where $u, v \in V(G)$.*

Proof. Assume that $x_v \geq x_u$, it follows from Lemma 2.7 that $d_G(v) \geq d_G(u)$, a contradiction. □

Lemma 2.9. [5, Lemma 1.1] *Let G be a connected graph with $\alpha \in [0, 1)$ and uv be an edge on an internal path of G. If G_{uv} is obtained from G by subdivision of edge uv into edges uw and wv, then $\rho(A_\alpha(G_{uv})) < \rho(A_\alpha(G))$.*

Let w be a vertex of connected graph G, and let $G(k, s)$ denote the graph obtained from $G \cup P_k \cup P_s$ by adding an edge between w and one of end vertices of P_k and P_s, respectively.

Lemma 2.10. [16, Theorem 2.6] *Let $G(k,s)$ be the graph defined above with $k \geq s+2$. If $0 \leq \alpha < 1$ and $\rho(A_\alpha(G(k,s))) \geq 2$, then*

$$\rho(A_\alpha(G(k,s))) < \rho(A_\alpha(G(k-1,s+1))).$$

Lemma 2.11. *Let B be a bicyclic graph with pendant vertices that has the largest A_α-spectral radius in $\mathscr{B}_\pi$, and $\mathbf{X}$ be a unit eigenvector of $A_\alpha(B)$ corresponding to $\rho(A_\alpha(G))$. Let $P = w_0w_1 \cdots w_kw_{k+1}$ ($k \geq 0$) be a hanging path with $d(w_0) \geq 2$ and $d(w_{k+1}) = 1$ in B, and $v_1v_2 \in E(B)$ be an edge of a cycle. If v_1w_j, v_1w_t and $v_2w_t \notin E(B)$ for $0 \leq j \leq k$ and $j < t \leq k+1$, then*

$$x_{v_2} > x_{w_j} > x_{w_{k+1}}.$$

Moreover, let T be a hanging tree on a vertex v and $v_1v_2 \in E(B)$ (where $v_1, v_2 \neq v$) be an edge of a cycle. If $v_1v \notin E(B)$, then $x_{v_2} > x_v$.

Proof. Since $d(w_j) \geq 2 > 1 = d(w_{k+1})$ ($0 \leq j \leq k$), it follows from Corollary 2.8 that $x_{w_j} > x_{w_{k+1}}$. Next, we need to show $x_{v_2} > x_{w_j}$.

Assume on the contrary that $x_{v_2} \leq x_{w_j}$. Clearly, we have $v_1v_2, w_jw_{j+1} \in E(B)$ and $v_1w_j, v_2w_{j+1} \notin E(B)$ due to v_1w_j, v_1w_t and $v_2w_t \notin E(B)$ for $0 \leq j \leq k$ and $j < t \leq k+1$. Let $G = B - v_1v_2 - w_jw_{j+1} + v_1w_j + v_2w_{j+1}$. Obviously, the degree sequence of G is π also. It is not difficult to see that G is connected with $|E(G)| = |V(G)| + 1$, and so, $G \in \mathscr{B}_\pi$. We claim that $x_{v_1} \leq x_{w_{j+1}}$ since if not, then $\rho(A_\alpha(G)) > \rho(A_\alpha(B))$ by Lemma 2.5, which contradicts the maximality of $\rho(A_\alpha(B))$.

When $j = k$, we get $x_{v_1} \leq x_{w_{k+1}}$. It follows from Lemma 2.7 that $2 \leq d(v_1) \leq d(w_{k+1}) = 1$, a contradiction.

When $0 \leq j \leq k-1$, if $j = k-1$, we let $G^{(1)} = B - v_1v_2 - w_{j+1}w_{j+2} + v_2w_{j+1} + v_1w_{j+2}$. As the same argument as G, one can get $G^{(1)} \in \mathscr{B}_\pi$, according to the maximality of $\rho(A_\alpha(B))$ and Corollary 2.6 we obtain $x_{v_2} \leq x_{w_{j+2}}$; otherwise, we construct another new graph $G^{(2)} = B - v_1v_2 - w_{j+2}w_{j+3} + v_1w_{j+2} + v_2w_{j+3}$ based on $G^{(1)}$. Clearly, $G^{(2)} \in \mathscr{B}_\pi$. Also by similar reasoning as above, one can get $x_{v_1} \leq x_{w_{j+3}}$. Then we repeat appropriately to construct $G^{(\ell)}$ until $j + \ell = k$, and therefore have

$$\min\{x_{v_1}, x_{v_2}\} \leq x_{w_{k+1}},$$

which implies $2 \leq \min\{d(v_1), d(v_2)\} \leq d(w_{k+1}) = 1$ by Lemma 2.7, a contradiction.

Furthermore, if T is a hanging tree on a vertex v and $v_1v \notin E(B)$, then there exists a path $P = vu_1 \cdots u_ku_{k+1}$ ($k \geq 0$) such that $d(u_{k+1}) = 1$. Using the same method as above, one can draw $x_{v_2} > x_v$.

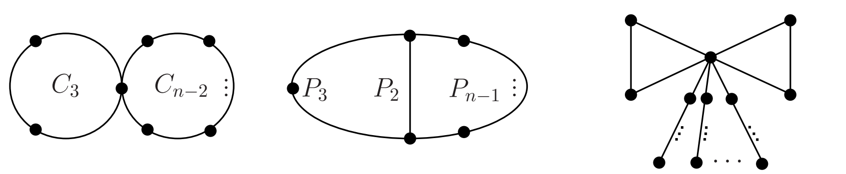
Summing up above, the proof completes. □

Lemma 2.12. *Let B be a bicyclic graph with pendant vertices that has the largest A_α-spectral radius in $\mathscr{B}_\pi$, and $\mathbf{X}$ be a unit eigenvector of $A_\alpha(B)$ corresponding to $\rho(A_\alpha(B))$. Then the vertex which has the largest component of $\mathbf{X}$ lies on a cycle.*

Proof. Without loss of generality, assume that v has the largest component of $\mathbf{X}$ but v doesn't lie on any cycle. We notice that B is a bicyclic graph, there must be a vertex u with $d(u) \geq 3$ which lies on some cycle. Because v has the largest component of $\mathbf{X}$, we have $x_v \geq x_u$. Further, by Lemma 2.7 it follows $d(v) \geq d(u) \geq 3$, which means that there exists a hanging tree on the vertex v. Then, one can find an edge w_1w_2 of a cycle such that $vw_1 \notin E(B)$. According to Lemma 2.11, we have $x_{w_2} > x_v$, which is a contradiction. Thus, the result follows. □

3. Main results

The breadth-first-search methods of tree and unicyclic graph have been introduced by Zhang [17, 18]. Let $\pi = (d_1, d_2, \ldots, d_n)$ $(n \geq 4)$ be a prescribed non-increasing bicyclic degree sequence. From Proposition 2.3 the degree sequence π was classified into four types by Huang et al. in [4], and then they introduced a special bicyclic graph B^*_π (see [4, p. 506]) for each type as follows:



$\infty(3, n-2)$ $\theta(3, 2, n-1)$ $F(C_3, C_3, P_{p_1}, \cdots, P_{p_{d_1-4}})$

Figure 3.1: Some related graphs.

(i) If $d_1 = 4$ and $d_i = 2$ for $2 \leq i \leq n$, then $B^*_\pi = \infty(3, n-2)$ (shown in Figure 3.1).

(ii) If $d_1 = d_2 = 3$ and $d_i = 2$ for $3 \leq i \leq n$, then $B^*_\pi = \theta(3, 2, n-1)$ (shown in Figure 3.1).

(iii) If $d_1 \geq 5$, $d_2 = 2$ and $d_n = 1$, then $B^*_\pi = F(C_3, C_3, P_{p_1}, \ldots, P_{p_{d_1-4}})$ where $|p_i - p_j| \leq 1$ for all $1 \leq i, j \leq d_1 - 4$ (shown in Figure 3.1).

(iv) If $d_1 \geq d_2 \geq 3$ and $d_n = 1$, then B^*_π was defined by the breadth-first-search method in the following: select a vertex v_{01} as a root and begin with v_{01} in the zeroth layer. Put $s_1 = d_1$ and select s_1 vertices $\{v_{11}, v_{12}, \ldots, v_{1,s_1}\}$ of the first layer such that they are adjacent to v_{01}, and v_{11} is adjacent to v_{12} and v_{13}. Thus $d(v_{01}) = d_1 = s_1$. For the second layer, put $d(v_{1i}) = d_{i+1}$ $(i = 1, 2, \ldots, s_1)$ and select $s_2 = \sum_{i=1}^{s_1} d(v_{1i}) - s_1 - 4$ vertices $\{v_{21}, v_{22}, \ldots, v_{2,s_2}\}$ of the second layer such that $d_{v_{11}} - 3$ vertices are adjacent to v_{11}, $d_{v_{12}} - 2$ (resp. $d_{v_{13}} - 2$) vertices are adjacent to v_{12} (resp. v_{13}), and $d_{v_{1i}} - 1$ vertices are adjacent to v_{1i} for $i = 4, 5, \ldots, s_1$. One can continue to construct all other layers by recursion, and assume that all vertices of the t-th $(t \geq 2)$ layer have been constructed and are denoted by $\{v_{t1}, v_{t2}, \ldots, v_{t,s_t}\}$. Now using the induction hypothesis, one can construct all the vertices of the $(t+1)$-th layer. Put $d(v_{ti}) = d_{i+1+\sum_{j=1}^{t-1} s_j}$ $(i = 1, 2, \ldots, s_t)$ and select $s_{t+1} = \sum_{i=1}^{s_t} d(v_{ti}) - s_t$ vertices $\{v_{t+1,1}, \ldots, v_{t+1,s_{t+1}}\}$ in the $(t+1)$-th layer such that $d(v_{ti}) - 1$ vertices are adjacent to v_{ti} for $i = 1, 2, \ldots, s_t$. In this way, one can obtain only one bicyclic graph B_π^* with degree sequence π, see Example 3.1 for instance.

Example 3.1. Let $\pi = \{5, 5, 3, 3, 1, 1, 1, 1, 1, 1\}$ be a given bicyclic degree sequence. Then by the construction (iv) above, B_π^* is the desired bicyclic graph with order 10 shown in Figure 3.2.

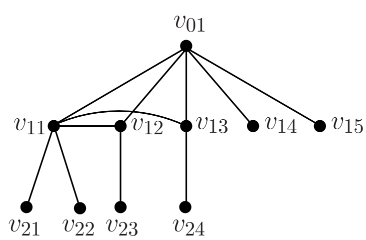


Figure 3.2: Graph B_π^*.

Lemma 3.2. [5, Theorem 2.6] *Let $G \in \mathscr{G}_\pi$ be a connected graph with $\alpha \in [0, 1)$. If $\rho(A_\alpha(G)) = \max\{\rho(A_\alpha(H)) \mid H \in \mathscr{G}_\pi\}$, then G has a BFS-ordering, and $u \prec v$ implies $x_u \geq x_v$.*

Let B be the bicyclic graph with the largest A_α-spectral radius in $\mathscr{B}_\pi$, and $\mathbf{X}$ be a unit eigenvector of $A_\alpha(B)$ corresponding to $\rho(A_\alpha(B))$ whose entries are labeled as x_{v_r} at vertex v_r. By Lemma 3.2, there exists a BFS-ordering of B, such that

$$v_1 \prec v_2 \prec v_3 \prec \cdots \prec v_{n-1} \prec v_n,$$
$$x_{v_1} \geq x_{v_2} \geq x_{v_3} \geq \cdots \geq x_{v_{n-1}} \geq x_{v_n},$$
$$d(v_1) \geq d(v_2) \geq d(v_3) \geq \cdots \geq d(v_{n-1}) \geq d(v_n)$$

and

$$h(v_1) \leq h(v_2) \leq h(v_3) \leq \cdots \leq h(v_{n-1}) \leq h(v_n).$$

Let $V_i = \{v \mid v \in V(G), h(v) = i\}$ for $i = 0, 1, \ldots, p$ $(= h(v_n))$. Hence, we can relabel the vertices of B in such a way that $V_i = \{v_{i1}, v_{i2}, \ldots, v_{is_i}\}$ with $x_{v_{i1}} \geq x_{v_{i2}} \geq \cdots \geq x_{v_{is_i}}$,

$x_{v_{ij}} \geq x_{v_{i+1,k}}$ and $d(v_{ij}) \geq d(v_{i+1,k})$ for $0 \leq i \leq p-1$, $1 \leq j \leq s_i$, and $1 \leq k \leq s_i$. To exactly, $s_1 = d(v_1) = d(v_{01}) = d_1$.

Lemma 3.3. *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a non-increasing bicyclic degree sequence with $d_1 = 4$ and $d_i = 2$ for $2 \leq i \leq n$. Then $B^*_\pi = \infty(3, n-2)$ is the only bicyclic graph which has the largest A_α-spectral radius in $\mathscr{B}_\pi$ (shown in Figure 3.1).*

Proof. Note that $d_{v_{01}} = 4$ and $d_{v_{ij}} = 2$ for $1 \leq i \leq p$, $1 \leq j \leq s_i$, that is, $\pi = (4, 2, 2, \ldots, 2)$. There must exist a bicyclic graph G such that $G \in \mathscr{B}_\pi$ by Proposition 2.3. Let B be a bicyclic graph that has the largest A_α-spectral radius in $\mathscr{B}_\pi$. Then, according to the composition of B we distinguish three cases below.

Case 1. If there exactly exists an edge $v_{1j}v_{1k} \in E(B)$ for $1 \leq j < k \leq 4$, then $B \cong \infty(3, n-2)$.

Case 2. If there exist two independent edges between v_{11}, v_{12}, v_{13} and v_{14} in B, say $v_{11}v_{12} \in E(B)$ and $v_{13}v_{14} \in E(B)$, then we consider two subcases in the following. When $|V(B)| = 5$, we have $B = \infty(3,3)$; when $|V(B)| \geq 6$, B is a disconnected graph which contains $\infty(3,3)$ as its a component. So we omit it because $\mathscr{B}_\pi$ is a set of connected bicyclic graphs with degree sequence π.

Case 3. If $v_{1j}v_{1k} \notin E(B)$ for all $1 \leq j < k \leq 4$, then combining with the degree sequence $\pi = (4, 2, 2, \ldots, 2)$, we can assume that there exist two cycles $C_1 = \{v_{01}, v_{11}, u_1, \ldots, u_{n_1}, v_{12}, v_{01}\}$ and $C_2 = \{v_{01}, v_{13}, w_1, \ldots, w_{n_2}, v_{14}, v_{01}\}$, and $|V(C_1) \cap V(C_2)| = v_{01}$, where $n_1, n_2 \geq 1$ and $n_1 + n_2 + 5 = n$. From Lemma 3.2 one can see that B has a BFS-ordering, this implies $x_{v_{11}} \geq x_{v_{13}} \geq x_{u_1} \geq x_{w_1}$, and so, $x_{v_{13}} \geq x_{u_1}$, $x_{v_{11}} \geq x_{v_{13}} \geq x_{w_1}$. Since $d(v_{01}) > d(v_{11})$, it follows from Corollary 2.8 that $x_{v_{01}} > x_{v_{11}}$, together with the maximality of $\rho(A_\alpha(B))$ and Corollary 2.6 one can obtain $x_{v_{13}} > x_{u_1}$. Furthermore, we notice that $v_{11}u_1, v_{13}w_1 \in E(B)$ but $v_{11}v_{13}, u_1w_1 \notin E(B)$. Let $B' = B - v_{11}u_1 - v_{13}w_1 + v_{11}v_{13} + u_1w_1$. It is clear that $B' \in \mathscr{B}_\pi$. Thus, it follows from Lemma 2.5 that $\rho(A_\alpha(B')) > \rho(A_\alpha(B))$, a contradiction.

Thus, the proof is completed. □

Lemma 3.4. *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a non-increasing bicyclic degree sequence with $d_1 = d_2 = 3$ and $d_i = 2$ for $3 \leq i \leq n$. Then $B^*_\pi = \theta(3, 2, n-1)$ is the only bicyclic graph that has the largest A_α-spectral radius in $\mathscr{B}_\pi$ (shown in Figure 3.1).*

Proof. Let B be a bicyclic graph that has the largest A_α-spectral radius in $\mathscr{B}_\pi$, where $\pi = (3, 3, 2, \ldots, 2)$, i.e., $d(v_{01}) = d(v_{11}) = 3$, $d(v_{12}) = d(v_{13}) = d(v_{ij}) = 2$ for $2 \leq i \leq p$ and $1 \leq j \leq s_i$. Then by Lemma 3.2, B has a BFS-ordering. In accordance with above, we discuss three cases as follows.

Case 1. If $v_{11}v_{12} \in E(B)$ or $v_{11}v_{13} \in E(B)$, then $B \cong \theta(3, 2, n-1)$.

Case 2. If $v_{11}v_{12} \in E(B)$ and $v_{11}v_{13} \in E(B)$, then we consider the following two situations. When $|V(B)| = 4$, we have $B = \theta(3,2,3)$; when $|V(B)| \geq 5$, the graph B is a disconnected graph containing $\theta(3,2,3)$ as its component. Since $\mathscr{B}_\pi$ is a set of connected bicyclic graphs with degree sequence π, we omit it.

Case 3. If $v_{11}v_{12}, v_{11}v_{13} \notin E(B)$, then we consider two subcases below.

Subcase 3.1. There exist two disjoint cycles C_1 and C_2 in B. Then C_1 and C_2 connect by precisely one edge since if not, there is a path P_k ($k \geq 3$) to connect C_1 and C_2. According to Lemma 2.12, we may suppose $v_{01} \in V(C_2)$ without loss of generality, and then, denote by $P_k = v_{01}v_{11} \cdots w$ where $w \in V(C_1)$ and $d(v_{01}) = d(w) = 3$. It is not difficult to find that $v_{11} \prec w$. So, from Lemma 3.2 we have $x_{v_{11}} \geq x_w$. On the other hand, because $d(v_{11}) = 2 < 3 = d(w)$, one can derive that $x_{v_{11}} < x_w$ by Corollary 2.8, a contradiction. Let $C_1 = \{v_{11}, u_1, \ldots, u_{l_1}, v_{11}\}$ ($l_1 \geq 2$) and $C_2 = \{v_{01}, v_{12}, w_1, \ldots, w_{l_2}, v_{13}, v_{01}\}$ ($l_2 \geq 1$). Since $d(v_{11}) > d(w_1)$, it follows from Corollary 2.8 that $x_{v_{11}} > x_{w_1}$. Also because $v_{12} \prec u_1$ we have $x_{v_{12}} \geq x_{u_1}$ by Lemma 3.2. Note that $v_{11}u_1, v_{12}w_1 \in E(B)$ and $v_{11}v_{12}, u_1w_1 \notin E(B)$. Let $B' = B - v_{11}u_1 - v_{12}w_1 + v_{11}v_{12} + u_1w_1$. Then we can deduce that $\rho(A_\alpha(B')) > \rho(A_\alpha(B))$, which contradicts the maximality of $\rho(A_\alpha(B))$.

Subcase 3.2. B has the form of $\theta(p,q,r)$. Using the similar argument as Subcase 3.1, one can find that the two vertices of degree 3 are adjacent. We may suppose that the two cycles are $C_1 = \{v_{01}, v_{11}, u_1, \ldots, u_{l_1}, v_{12}, v_{01}\}$ ($l_1 \geq 1$) and $C_2 = \{v_{01}, v_{11}, w_1, \ldots, w_{l_2}, v_{13}, v_{01}\}$ ($l_2 \geq 1$). As the same argument as above, we have $x_{v_{11}} > x_{w_{l_2}}$ and $x_{v_{13}} \geq x_{u_1}$. Let $B' = B - v_{11}u_1 - v_{13}w_{l_2} + v_{11}v_{13} + u_1w_{l_2}$. Then it follows from Lemma 2.5 that $\rho(A_\alpha(B')) > \rho(A_\alpha(B))$, which is a contradiction.

Summing up the above, the proof completes. □

Lemma 3.5. *Let $\pi = (d_1, d_2, \ldots, d_n)$ be a non-increasing bicyclic degree sequence with $d_1 \geq 5$, $d_2 = 2$ and $d_n = 1$. Then $B^*_\pi = F(C_3, C_3, P_{p_1}, \ldots, P_{p_{d_1-4}})$ is the only bicyclic graph that has the largest A_α-spectral radius in $\mathscr{B}_\pi$, where $|p_i - p_j| \leq 1$ for all $1 \leq i, j \leq d_1 - 4$ (shown in Figure 3.1).*

Proof. Let B be a bicyclic graph with order n that has the largest A_α-spectral radius in $\mathscr{B}_\pi$. Then combining the given degree sequence π with Proposition 2.3, B must have the form of $F(C_{n_1}, C_{n_2}, P_{p_1}, \ldots, P_{p_{d_1-4}})$. Thus, the following claims should be held.

Claim 1. $n_1 = n_2 = 3$.

Proof. We assume on the contrary that either $n_1 \geq 4$ or $n_2 \geq 4$ holds. Without loss of generality, suppose $n_1 \geq 4$. We construct a new graph G with order $n - 1$ from B by contracting an edge of C_{n_1}. Then conversely, one can obtain B from G by subdivision an edge of the resulting cycle C_{n_1-1}. So we have $\rho(A_\alpha(G)) > \rho(A_\alpha(B))$ by Lemma 2.9. And then, let G' be a graph with order n obtained from G by joining one ray (leg) on one of its pendent vertices. Clearly, $G' \in \mathscr{B}_\pi$. It follows from Lemma 2.4(4) that $\rho(A_\alpha(G')) > \rho(A_\alpha(G))$, which means $\rho(A_\alpha(G')) > \rho(A_\alpha(B))$, a contradiction. Hence, the claim holds. □

Claim 2. $|p_i - p_j| \leq 1$ *for* $1 \leq i, j \leq d_1 - 4$.

Proof. By contradiction, we may suppose that, without loss of generality, there exist two pendent paths P_{p_s}, P_{p_t} in B such that $p_s - p_t \geq 2$. Let B' denote the graph $F(C_{n_1}, C_{n_2}, P_{p_1}, \ldots, P_{p_{s-1}}, \ldots, P_{p_{t+1}}, \ldots, P_{p_{d_1-4}})$ obtained from $F(C_{n_1}, C_{n_2}, P_{p_1}, \ldots, P_{p_s}, \ldots, P_{p_t}, \ldots, P_{p_{d_1-4}})$ by deleting a pendent vertex of P_{p_s} and adding a pendent vertex of P_{p_t}. Then by Lemma 2.10, one can easily obtain that $\rho(A_\alpha(B')) > \rho(A_\alpha(B))$, a contradiction. □

From Claims 1 and 2, we complete the proof. □

Lemma 3.6. *Let* $\pi = (d_1, d_2, \ldots, d_n)$ *be a non-increasing bicyclic degree sequence with* $d_1 \geq d_2 \geq 3$ *and* $d_n = 1$. *Then* B^*_π *is the only bicyclic graph that has the largest* A_α*-spectral radius in* $\mathscr{B}_\pi$.

Proof. Let B be a bicyclic graph that has the largest A_α-spectral radius in $\mathscr{B}_\pi$. In accordance with Lemma 3.2, B has a BFS-ordering with root v_{01}, combining this with degree sequence π, one can see that $d(v_{01}) \geq d(v_{11}) \geq 3$ and $d(v_{12}) \geq d(v_{13}) \geq 2$. Let C_{n_1} and C_{n_2} denote the two cycles of B, which perhaps have some common vertices or connect by a unique path. If C_{n_1} and C_{n_2} are joined by a unique path, we denote the path by P_k for convenience. Without loss of generality, we may suppose that $v_{01} \in V(C_{n_1})$ by Lemma 2.12. To promote the proof, we need to prove the following claims.

Claim 1. $|V(C_{n_1}) \cap V(C_{n_2})| \geq 2$.

Proof. Assume that $|V(C_{n_1}) \cap V(C_{n_2})| \leq 1$, we distinct two cases to be considered here.

Case 1. $|V(C_{n_1}) \cap V(C_{n_2})| = 0$.

Subcase 1.1. There exists a hanging tree on v_{01}. Since $v_{01} \in V(C_{n_1})$, one can find an edge $w_1w_2 \in E(C_{n_2})$ $(w_1, w_2 \neq v_{01})$ such that $w_1v_{01} \notin E(B)$. Hence, it follows from Lemma 2.11 that $x_{w_2} > x_{v_{01}}$. In fact, from the BFS-ordering we know that $x_{v_{01}} > x_{w_2}$, a contradiction.

Subcase 1.2. There exists a hanging tree on v_{11}. As the same arguments as above we can observe an edge w_1w_2 $(w_1, w_2 \neq v_{11})$ of a cycle such that $w_1v_{11} \notin E(B)$. Then by Lemma 2.11, $x_{w_2} > x_{v_{11}}$, which contradicts $x_{v_{11}} > x_{w_2}$.

Subcase 1.3. There doesn't exist a hanging tree on v_{01} and v_{11}. Combining $v_{01}v_{11} \in E(B)$ $(v_{01} \in V(C_{n_1}))$ with $|V(C_{n_1}) \cap V(C_{n_2})| = 0$, there must be $v_{01} \in V(C_{n_1}) \cap V(P_k)$ and $v_{11} \in V(C_{n_2}) \cap V(P_k)$. To exactly, $d(v_{01}) = d(v_{11}) = d(v_{12}) = 3$ and there exists a hanging tree on v_{12} since $d_n = 1$, and then, one can deduce $v_{12} \in V(C_{n_1})$. Meanwhile, there exists an edge $w_1w_2 \in E(C_{n_2})$ such that $w_1, w_2 \neq v_{12}$ and $w_1v_{12} \notin E(B)$, by Lemma 2.11, we obtain $x_{w_2} > x_{v_{12}}$, also a contradiction.

Case 2. $|V(C_{n_1}) \cap V(C_{n_2})| = 1$.

Let $\widehat{w}$ be the common vertex of C_{n_1} and C_{n_2}. If $\widehat{w} = v_{01}$, then $v_{01}v_{11} \in E(C_{n_i})$ for some i $(i = 1, 2)$ and there exists a hanging tree on v_{11} since $d(v_{11}) \geq 3$ and $d_n = 1$. We can find an edge w_1w_2 of a cycle such that $w_1, w_2 \neq v_{11}$ and $w_1v_{11} \notin E(B)$, it follows from Lemma 2.11 that $x_{w_2} > x_{v_{11}}$, a contradiction. Otherwise, $\widehat{w} \neq v_{01}$, by similar reasoning as above, it is also impossible. □

In accordance with Claim 1, one can deduce that B has a $\theta(p, q, r)$ as its induced subgraph. In this case, we assert that $d_{\theta(p,q,r)}(v_{01}) = d_{\theta(p,q,r)}(v_{11}) = 3$ since if not, we may suppose $d_{\theta(p,q,r)}(v_{01}) = 2$, then there exists a hanging tree on v_{01} in B since v_{01} is the maximum degree vertex. Take an edge w_1w_2 of a cycle such that $w_1, w_2 \neq v_{01}$ and $w_1v_{01} \notin E(B)$, by Lemma 2.11 it follows $x_{w_2} > x_{v_{01}}$, which leads to a contradiction.

Claim 2. $n_1 = n_2 = 3$.

Proof. Assume by a contradiction that either $n_1 \geq 4$ or $n_2 \geq 4$ holds. Without loss of generality, we may suppose that $n_1 \geq 4$ and $n_2 = 3$. Let $C_{n_1} = v_{01}v_{11}u_1u_2 \cdots u_lv_{12}(= u_{l+1})v_{01}$ and $C_{n_1} = v_{01}v_{11}v_{13}v_{01}$. Then we can conclude that if B contains hanging trees, then there is at least one vertex of v_{01}, v_{11} and v_{12} appending a hanging tree. Since if not, there exists a hanging tree on v_{13} (say). We take an edge $u_ru_{r+1} \in C_{n_1}$ such that $u_r, u_{r+1} \neq v_{13}$ and $u_{r+1}v_{13} \notin E(B)$, where $1 \leq r \leq l$. From Lemma 2.11 it follows that $x_{u_r} > x_{v_{13}}$. Since $v_{13} \prec u_r$, we derive that $x_{v_{13}} \geq x_{u_r}$, a contradiction. Thus, we may suppose that there exists a hanging tree on v_{11} without loss of generality. Then one can find an edge w_1w_2 of a cycle such that $w_1, w_2 \neq v_{11}$ and $w_1v_{11} \notin E(B)$. So, $x_{w_2} > x_{v_{11}}$ by Lemma 2.11, which leads to a contradiction. Consequently, the conclusion holds. □

From Claim 2, we know that B contains $\theta(2, 3, 3)$ as its induced subgraph, where $d_{\theta(2,3,3)}(v_{01}) = d_{\theta(2,3,3)}(v_{11}) = 3$.

Claim 3. $v_{12}, v_{13} \in \theta(2, 3, 3)$.

Proof. Suppose on the contrary that there is at least one vertex of v_{12} and v_{13}, say v_{13}, such that $v_{13} \notin \theta(2, 3, 3)$. Then there exists a hanging tree on v_{13} in B due to $d(v_{13}) \geq 2$. We can take an edge $v_{11}v_{1j}$ $(4 \leq j \leq d_1)$ in $E(\theta(2, 3, 3))$ such that $v_{11}v_{13} \notin E(B)$, then $x_{v_{1j}} > x_{v_{13}}$ by Lemma 2.11, which is not possible. □

According to Claim 3, we have $d_{\theta(2,3,3)}(v_{12}) = d_{\theta(2,3,3)}(v_{13}) = 2$, which means that $v_{11}v_{12}, v_{11}v_{13} \in E(\theta(2, 3, 3))$. Thus, combining with the BFS-ordering, we have that B must be isomorphic to B^*_π, as required. □

Proof of Theorem 1.3. Let B be a bicyclic graph that has the largest A_α-spectral radius in $\mathscr{B}_\pi$. Together with Lemmas 3.3, 3.4, 3.5 and 3.6, the proof therefore follows. $\square$

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