On the $\alpha$-spectral radius of unicyclic and bicyclic graphs with a fixed diameter

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Abstract
The $\alpha$-spectral radius of a connected graph $G$ is the spectral radius of $A_\alpha$-matrix of $G$. In this paper, we discuss the methods for comparing $\alpha$-spectral radius of graphs. As applications, we characterize the graphs with the maximal $\alpha$-spectral radius among all unicyclic and bicyclic graphs of order $n$ with diameter $d$, respectively. Finally, we determine the unique graph with maximal signless Laplacian spectral radius among bicyclic graphs of order $n$ with diameter $d$. From our conclusion, it is known that the result of Pai and Liu in (Ars Combin 249–265, 2017) is wrong.

Keywords Unicyclic graph · Bicyclic graph · Diameter · Alpha-spectral radius

Mathematics Subject Classification 05C35 · 05C50

1 Introduction

All graphs considered in this article are finite, undirected and simple. Let $G = (V(G), E(G))$ be a graph with $n$ vertices and $m$ edges (so $n = |V(G)|$ is its order and $m = |E(G)|$ is its size). Let $G$ be a graph with adjacency matrix $A(G)$ and $D(G)$ be the diagonal matrix of its vertex degrees. In Nikiforov (2017) the matrix $A_\alpha(G)$ has been defined for any real $\alpha \in [0, 1]$ as

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

which has recently attracted more and more researchers’ attention. One reason for this is that the $\alpha$-spectrum seems to be more informative than other commonly used graph matrices.
Note that $A_0(G) = A(G)$ and $2A_{1/2}(G) = Q(G)$, where $Q(G) = D(G) + A(G)$. Thus, the family $A_\alpha(G)$ extends both $A(G)$ and $Q(G)$.

For square matrix $A$, let $\phi(A, x) = \det(xI - A)$ denote the characteristic polynomial of $A$ and $\rho(A)$ be the spectral radius of $A$. We write $\phi_\alpha(G) = \phi(A_\alpha(G), x)$ and $\rho_\alpha(G) = \rho(A_\alpha(G))$, where $\rho_\alpha(G)$ is called the $\alpha$-spectral radius of $G$.

The study of the largest $\alpha$-eigenvalue remains an attractive topic for researchers. In particular, the extremal values of the $\alpha$-spectral radius for various classes of graphs, and corresponding extremal graphs, have been investigated.

Let $G$ be a connected graph with $n$ vertices and $m$ edges. If $m = n + c - 1$, then $G$ is called a $c$-cyclic graph. Specially, if $c = 0$, 1, or 2, then $G$ is called a tree, an unicyclic graph, a bicyclic graph. Let $G$ be a $c$-cyclic graph. The base of $G$, denoted by $\tilde{G}$, is the (unique) minimal $c$-cyclic subgraph of $G$. It is easy to see that $\tilde{G}$ can be obtained from $G$ by consecutively deleting pendant edges.

Let $N_G(v)$ denote the neighbor set of vertex $v$ in $G$, then $d_G(v) = |N_G(v)|$ is called the degree of $v$ of $G$. If there is no confusion, we write $N_G(v)$ as $N(v)$, and $d_G(v) = d(v) = d_v$.

The diameter of $G$, denoted $\text{diam}(G)$, is the maximal distance between any two vertices in the graph.

It is an interesting problem concerning graphs with maximal or minimal spectral radii over a given class of graphs. As early as 1985, Brualdi and Hoffman (1985) investigated the maximal spectral radius of the adjacency matrix of a graph in the set of all graphs with a given number of vertices and edges. Their work was followed by other people, in the connected graph case as well as in the general case. In Hansen and Stevanović (2008), Hansen et al. determined graphs with the largest spectral radius among all the graphs on $n$ vertices with given diameter $d$ or radius $r$. Several types of special graphs with diameter $d$ were also discussed. For example, the spectral radii and signless Laplacian spectral radii of trees, unicyclic graphs, bicyclic graphs and tricyclic graphs on $n$ vertices with fixed diameter were discussed in Guo (2007); Guo et al. (2005); Pai and Liu (2017); Liu et al. (2007); He and Li (2012); Geng and Li (2011). Nikiforov (2018) determined the graph with the largest $\alpha$-spectral radius among all graphs with $n$ vertices and diameter at least $d$.

In this paper, motivated by the above results, we will determine the extremal graph with maximal $\alpha$-spectral radius among all unicyclic or bicyclic graphs with $n$ vertices and diameter $d$, respectively.

2 Notations and preliminaries

Let $G$ be a connected graph with $V(G) = \{v_1, \ldots, v_n\}$. A column vector $x = (x_{v_1}, \ldots, x_{v_n})^T \in \mathbb{R}^n$ can be considered as a function defined on $V(G)$ which maps vertex $v_i$ to $x_{v_i}$, i.e., $x(v_i) = x_{v_i}$ for $i = 1, \ldots, n$. Then, $\sum_{[u, v] \in E(G)} \rho_\alpha(G) x = \alpha (x_u^2 + x_v^2) + 2(1 - \alpha) x_u x_v$.

If $G$ is connected then $A_\alpha(G)$ is irreducible, and by the Perron–Frobenius theory of non-negative matrices, $\rho_\alpha(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\rho_\alpha(G)$. We shall refer to such an eigenvector as the $\alpha$-Perron
vector of $G$. If $x$ is the $\alpha$-Perron vector of $G$, then for each $u \in V(G)$,
\[ \rho_{\alpha}(G)x_u = \alpha d(u)x_u + (1 - \alpha) \sum_{[u,v] \in E(G)} x_v. \]

For a unit column vector $x \in \mathbb{R}^n$ with at least one nonnegative entry, by Rayleigh quotient’s principle, we have $\rho_{\alpha}(G) \geq x^T A_{\alpha}(G)x$ with equality if and only if $x$ is the $\alpha$-Perron vector of $G$.

**Definition 2.1** Belardo et al. (2010) For any $n \times n$ matrix $A = (a_{ij})$, the Coates digraph associated to $A$, denoted by $G_A$, is a weighted digraph defined as follows:

- the vertex set of $G_A$ is equal to $\{1, 2, \ldots, n\}$, where the $i$th vertex corresponds to the $i$th row (or equivalently, to the $i$th column) of $A$;
- the arc set of $G_A$ consists of all arcs of the form $uv$ with weight $a_{uv} (1 \leq u, v \leq n)$; for $u = v$ the corresponding arc is a loop. If the weight of some arc is zero, then it is ignored.

For a Coates graph $G = G_A$, we call the matrix $A$, denoted by $A(G)$, the weighted adjacency matrix of $G$. Let $U$ be a vertex subset of graph $G$ and $G_\alpha$ be the Coates graph with respect to matrix $A_\alpha(G)$. We write $\psi_\alpha(G, U) = \phi(G_\alpha - U, x)$. The spectral radius of $A(G_\alpha - U)$ is denoted by $\rho(G_\alpha - U)$.

In the following lemma, we will list some results on nonnegative matrices, which follow directly from Perron–Frobenius theorem (see Berman and Plemmons (1994)).

**Lemma 2.1** Nikiforov (2017); Berman and Plemmons (1994); Shan et al. (2021) Let $A$ and $B$ be two nonnegative matrices.

(i). If $A \geq B$ and $A \neq B$, then the following holds:
\[ \phi(B, x) \geq \phi(A, x) \text{ for } x \geq \rho(A), \]
eq \rho(A)

especially, when $A$ is irreducible, the inequality is strict.

(ii). If there exists a principal submatrix $M$ of $A$ such that $B \leq M$, then $\rho(B) \leq \rho(A)$ and the inequality is strict when $A$ is irreducible.

**Proposition 2.1** Nikiforov and Rojo (2018) Let $\alpha \in [0, 1)$ and $G$ be a graph with $\rho_{\alpha}(G) > 2$. Take $P = u_1u_2 \ldots u_r (r \geq 2)$ be a pendant path in $G$ with root $u_1$ and $x$ be the $\alpha$-Perron vector of $G$. Then $x(u_i) > x(u_j)$ for $1 \leq i < j \leq r$.

**Lemma 2.2** Nikiforov and Rojo (2018) Let $G$ be a connected graph with $\alpha \in [0, 1)$. For $u, v \in V(G)$, suppose $N \subseteq N(v) \setminus (N(u) \cup \{u\})$. Let $G' = G - \{vw : w \in N\} + \{uw : w \in N\}$. If $N \neq \emptyset$ and $x = (x_1, \ldots, x_n)^T$ is the $\alpha$-Perron vector of $G$ such that $x_u \geq x_v$, then $\rho_\alpha(G') > \rho_\alpha(G)$.

By Lemma 2.2, we can easily obtain the following results.

**Lemma 2.3** Xue et al. (2018) Let $\alpha \in [0, 1)$, and $G$ be a connected graph and $e = uv$ be a cut-edge of $G$. Let $G'$ be the graph obtained from $G$ by deleting the edge $uv$, identifying $u$ with $v$, and adding a pendant edge to $u(= v)$. Then, $\rho_\alpha(G') > \rho_\alpha(G)$.

Let $G$ be a graph. Assume that $e_1 = uv, e_2 = wy, e'_1 = uw, e'_2 = vy$ and $e_1, e_2 \in E(G), e'_1, e'_2 \notin E(G)$. Take $G' = G - \{e_1, e_2\} + \{e'_1, e'_2\}$. We say that $G'$ is obtained from $G$ by 2-switching operation $e_1 \xrightarrow{v} (\overline{w}) e_2$. 

\[ v \]
Lemma 2.4 Guo and Zhou (2020) Let $G, G'$ be the graphs defined as above and $x$ be the $\alpha$-Perron vector of $G$ for $\alpha \in [0, 1)$. If $x_u \geq x_v$ and $x_w \geq x_v$, then $\rho_\alpha(G') \geq \rho_\alpha(G)$. Furthermore, if one of the two inequalities is strict, then $\rho_\alpha(G') > \rho_\alpha(G)$.

An internal path of $G$ is a path $P$ (or cycle) with vertices $v_1, v_2, \ldots, v_k$ (or $v_1 = v_k$) such that $d(v_1) \geq 3$, $d(v_k) \geq 3$ and $d(v_2) = \cdots = d(v_{k-1}) = 2$.

Lemma 2.5 (Li et al. 2019, Lemma 1.1) Let $G$ be a connected graph with $\omega$ be some edge on an internal path of $G$. Let $A_{G}$ be any symmetric square matrix of order $n$, and let $G_{uv}$ be any symmetric square matrix of order $n$, and let $G_{uv}$ denote the graph obtained from $G$ by subdividing of edge uv into edges uw and uv. Then $\rho_\alpha(G_{uv}) < \rho_\alpha(G)$.

Let $u, v$ be two vertices of connected graph $G$ with degree at least 2. Take $G_{u,v}(k, l)$ be the graph obtained from $G$ by attaching the pendant paths $P_k$ to $u$ and $P_l$ to $v$, respectively.

Lemma 2.6 Guo and Zhou (2020) Let $G_{u,v}(k, l)$ be as defined above. If $k - l \geq 2$ and $(u, v) \in E(G)$, then $\rho_\alpha(G_{u,v}(k - 1, l + 1)) > \rho_\alpha(G_{u,v}(k, l))$ for $\alpha \in [0, 1)$.

In Belardo et al. (2010), Francesco Belardo et al. present a Schwenk-like formula for symmetric matrices.

Theorem 2.1 Belardo et al. (2010) Let $A = (a_{ij})$ be any symmetric square matrix of order $n$, and let $G (= G_A)$ be its Coates digraph with $V(G) = \{1, 2, \ldots, n\}$. If $\nu$ is a fixed vertex of $G$ then

$$\phi(G) = (x - a_{\nu \nu}) \phi(G - \nu) - \sum_{u \neq \nu} a_{\nu u}^2 \phi(G - u - \nu) - 2 \sum_{C \in C_v(G)} \omega_C(\nu) \phi(G - V(C)),$$

where $C_v(G)$ is the set of all undirected cycles of $G$ of length $\geq 3$ passing through $\nu$ and $\omega_C(\nu) = \prod_{(i, j) \in E(C)} a_{ij}$.

Given two disjoint rooted graphs $G$ and $H$ with roots $u$ and $v$, respectively, then the coalescence of $G$ and $H$ is the graph $G(u, v)H$ obtained by identifying the roots $u$ and $v$. The coalescence of rooted graphs can be naturally extended to weighted digraphs (including weighted graphs).

Lemma 2.7 Belardo et al. (2010) Let $G(u, v)H$ be the coalescence of two rooted weighted digraphs (possibly with loops) $G$ and $H$ whose roots are $u$ and $v$, respectively. Then

$$\phi(G(u, v)H) = \phi(G)\phi(H - \nu) + \phi(G - u)\phi(H) - x\phi(G - u)\phi(H - \nu).$$

Given three disjoint rooted Coates (di)graphs $G_1, G_2$ and $H$, $u_i$ is the root vertex of $G_i$ for $i = 1, 2$ and $v_1, v_2$ are two vertices of $H$. The rooted product of $H$ and $G_1, G_2$ with respect to $(u_1, u_2)$ and $(v_1, v_2)$, denoted by $H(G_1, G_2)$, the Coates (di)graphs obtained from $G_1, G_2$ and $H$ by coalescing $u_i$ and $v_i$ into new vertices $w_i$ for $i = 1, 2$.

Repeatedly using Lemma 2.7, we have the following result.

Lemma 2.8 Let $G, H_i$ be connected graphs with $u, v \in V(G), w_i \in V(H_i)$ for $i = 1, 2$. Let $H = G(H_1, H_2)$ be rooted product of $G$ and $(H_1, H_2)$ with respect to $(u, v)$ and $(w_1, w_2)$, respectively, then

$$\phi_\alpha(H) = g g'_1 g_2' + g_u(g_1 - x g'_1) g_2' + g_v(g_2 - x g'_2) g_1' + g_{uv}(g_1 - x g'_1)(g_2 - x g'_2).$$

where $g = \phi_\alpha(G), g_u = \psi_\alpha(G, u), g_v = \psi_\alpha(G, v), g_{uv} = \psi_\alpha(G, \{u, v\}), g_1 = \phi_\alpha(H_1), g_1' = \psi_\alpha(H_1, w_1), g_2 = \phi_\alpha(H_2)$ and $g_2' = \psi_\alpha(H_2, w_2)$.
By Lemma 2.8, we can easily get the following lemma.

**Lemma 2.9** Let $G, H_1, H_2$ be connected graphs with $u \in V(G), \{u_i, v_i\} \subseteq V(H_i)$ for $i = 1, 2$. Take $G_i = H_i(G, G)$ be rooted product of $H_i$ and $(G, G)$ with respect to vertex sequences $(u_i, v_i)$ and $(u, u)$ for $i = 1, 2$. Let

$$DF_1(x) = \phi_\alpha(H_1) - \phi_\alpha(H_2),$$

$$DF_2(x) = \psi_\alpha(H_1, u_1) + \psi_\alpha(H_1, v_1) - \psi_\alpha(H_2, u_2) - \psi_\alpha(H_2, v_2),$$

$$DF_3(x) = \psi_\alpha(H_1, \{u_1, v_1\}) - \psi_\alpha(H_2, \{u_1, v_1\}).$$

Then,

$$\phi_\alpha(G_1) - \phi_\alpha(G_2) = DF_1(x)\psi_\alpha(G, u)^2 + DF_2(x)(\phi_\alpha(G) - x\psi_\alpha(G, u))\psi_\alpha(G, u)$$

$$+ DF_3(x)(\phi_\alpha(G) - x\psi_\alpha(G, u))^2.$$ 

### 3 Techniques for comparing the $\alpha$-spectral radii of graphs

In the following, we list some necessary lemmas which will be used in order to prove the main result of this article.

**Lemma 3.1** Let $G, H$ be connected graphs and $u \in V(G), v_1, v_2 \in V(H)$. For $i = 1, 2$, take $G_i = G(u, v_i)H$ and when $x \geq \rho(H_\alpha - v_1)$, if $\psi_\alpha(H, v_2) > \psi_\alpha(H, v_1)$ then $\rho_\alpha(G_1) < \rho_\alpha(G_2)$.

**Proof** By Lemma 2.7, for $i = 1, 2$, we have

$$\phi_\alpha(G_i, x) = \psi_\alpha(G, x)\phi_\alpha(H, x) + (\phi_\alpha(G, x) - x\psi_\alpha(G, u))\psi_\alpha(H, v_i).$$

Thus,

$$\phi_\alpha(G_2, x) - \phi_\alpha(G_1, x) = (\phi_\alpha(G, x) - x\psi_\alpha(G, u))(\psi_\alpha(H, v_2) - \psi_\alpha(H, v_1)). \quad (1)$$

By (i) of Lemma 2.1, we have $\phi_\alpha(G, x) - x\psi_\alpha(G, u) < 0$ for all $x \geq \rho_\alpha(G)$. By (ii) of Lemma 2.1, we have $\rho_\alpha(G_2) > \max\{\rho_\alpha(G), \rho(H_\alpha - v_1)\}$. From $\psi_\alpha(H, v_2) > \psi_\alpha(H, v_1)$ for $x \geq \rho(H_\alpha - v_1)$ and Formula (1), we have $\phi_\alpha(G_2, x) < \phi_\alpha(G_1, x)$ for $x \geq \rho_\alpha(G_2)$. Then $\rho_\alpha(G_1) < \rho_\alpha(G_2)$ hold. 

**Lemma 3.2** Let $G$ and $H$ be two graphs, $w \in V(H)$ and $u_1, u_2 \in V(G)$ such that $N_G(u_1) \setminus \{u_2\} \subseteq N_G(u_2) \setminus \{u_1\}$. Take $H_1 = G(u_1, w)H$ and $H_2 = G(u_2, w)H$, then we have $\rho_\alpha(H_2) > \rho_\alpha(H_1)$.

**Proof** Let $C^*[u_1]$ be the set of all cycles containing $u_1$ in $G$ with $u_2 \notin V(C)$ and $C^*[u_2]$ be the set of all cycles containing $u_2$ in $G$ with $u_1 \notin V(C)$. Take $N_1 = N_G(u_1) \setminus \{u_2\}$ and $N_2 = N_G(u_2) \setminus \{u_1\}$. From $N_1 \subset N_2$, we know that $d(u_2) > d(u_1)$ and there exists an injective mapping $\Phi$ from $C^*[u_1]$ to $C^*[u_2]$ such that $V(C) \cup \{u_2\} = V(\Phi(C)) \cup \{u_1\}$ for any $C \in C^*[u_1]$.

Applying Theorem 2.1 to $A_\alpha(G)(u_1)$ and $A_\alpha(G)(u_2)$, respectively, we have

$$\psi_\alpha(G, u_1) = (x - \alpha d(u_2))\psi_\alpha(G, \{u_1, u_2\}) - (1 - \alpha)^2 \sum_{w \in N_2} \psi_\alpha(G, \{u_1, u_2, w\})$$

$$- 2 \sum_{Z \in C^*[u_2]} (1 - \alpha)^{|Z|} \psi_\alpha(G, V(Z) \cup \{u_1\}), \quad (2)$$

where $|Z|$ denotes the number of vertices in the cycle $Z$. This completes the proof.
\[ \psi_\alpha(G, u_2) = (x - \alpha d(u_1))\psi_\alpha(G, \{u_1, u_2\}) - (1 - \alpha)^2 \sum_{w \in N_1} \psi_\alpha(G, \{u_1, u_2, w\}) \]

\[ -2 \sum_{Z \in C^*[u_1]} (1 - \alpha)^{|Z|} \psi_\alpha(G, V(Z) \cup \{u_2\}). \tag{3} \]

Let \( DN = N_2 \setminus N_1 \) and \( DC = C^*[u_2] \setminus C^*[u_1] \). From Formulae (2) and (3), we have

\[ df(x) = \psi_\alpha(G, u_2) - \psi_\alpha(G, u_1) \]

\[ = \alpha(d(u_2) - d(u_1))\psi_\alpha(G, \{u_1, u_2\}) + (1 - \alpha)^2 \sum_{w \in DN} \psi_\alpha(G, \{u_1, u_2, w\}) \]

\[ + 2 \sum_{Z \in DC} (1 - \alpha)^{|Z|} \psi_\alpha(G, V(Z) \cup \{u_1\}). \]

Since \( A(G_\alpha - \{u_1, u_2\}), A(G_\alpha - \{u_1, u_2, w\}), A(G_\alpha - V(Z) \cup \{u_1\}) \) are principal submatrices of \( A(G_\alpha - u_1) \), the spectral radius of these submatrices are not more than \( \rho(G_\alpha - u_1) \) according to (ii) of Lemma 2.1. Hence, when \( x > \rho(G_\alpha - u_1) \), \( \psi_\alpha(G, \{u_1, u_2\}) > 0 \), \( \psi_\alpha(G, \{u_1, u_2, w\}) > 0 \) and \( \psi_\alpha(G, V(Z) \cup \{u_1\}) > 0 \). Therefore, \( \psi_\alpha(G, u_2) - \psi_\alpha(G, u_1) > 0 \) for \( x > \rho(G_\alpha - u_1) \). By Lemma 3.1, we have \( \rho_\alpha(H_2) > \rho_\alpha(H_1) \). \( \square \)

Knowing the symmetries of a graph \( G \) can be quite useful to find the spectral radius of the graph \( G \). Thus, we say that \( u \) and \( v \) are equivalent in \( G \), if there exists an automorphism \( \tau \) of \( G \) such that \( \tau(u) = v \).

Lemma 3.3 Let \( H_1, H_2 \) and \( G \) be three graphs, \( w_1 \in V(H_1), w_2 \in V(H_2) \) and \( u, v \in V(G) \) such that \( u \) and \( v \) be equivalent vertices in \( G \). Let \( H = G(H_1, H_2) \) be rooted graph of \( (H_1, H_2) \) and \( G \) with respect to vertex sequences \( (w_1, w_2) \) and \( (u, v) \), respectively, then

\[ \psi_\alpha(H, u) - \psi_\alpha(H, v) = g_3(F_1'F_2' - F_1F_2'), \]

where \( F_1 = \phi_\alpha(H_1), F_1' = \psi_\alpha(H_1, w_1), F_2 = \phi_\alpha(H_2), F_2' = \psi_\alpha(H_2, w_2) \) and \( g_3 = \psi_\alpha(G, \{u, v\}) \).

Proof Let \( g = \phi_\alpha(G), g_1 = \psi_\alpha(G, u), g_2 = \psi_\alpha(G, v) \), then by Lemma 2.7, we have

\[ \psi_\alpha(H, u) = \psi_\alpha(H_1, w_1)(\psi_\alpha(G, u)\psi_\alpha(H_2, w_2) + \psi_\alpha(G, \{u, v\})\phi_\alpha(H_2)) \]

\[ - x \psi_\alpha(G, \{u, v\})\psi_\alpha(H_2, w_2)) = F_1'(g_2F_2' + g_3F_2 - xg_3F_2'). \]

Similarly, we have

\[ \psi_\alpha(H, v) = g_1F_1'F_2' + g_3F_1F_2' - xg_3F_1F_2'. \]

Since \( u \) and \( v \) are equivalent vertices in \( G \), we have \( g_1 = g_2 \). Thus,

\[ \psi_\alpha(H, u) - \psi_\alpha(H, v) = g_3(F_1'F_2' - F_1F_2'). \]

\( \square \)

Let \( u \) be the pendant vertex of path \( P_1 \). In the sequel, we always denote \( f_{t-1}(x) = \psi_\alpha(P_t, u) \). If there is no confusion, we write \( f_{t-1}(x) \) as \( f_{t-1} \). It is easy to see that \( f_0(x) = 1, f_1(x) = x - \alpha \) and

\[ \phi_\alpha(P_1) = f_1(x) + \alpha f_{t-1}(x), \]

\[ f_t(x) = (x - 2\alpha)f_{t-1}(x) - (1 - \alpha)^2 f_{t-2}(x). \tag{4} \]
Then for \( l - k = p \geq 0 \), we have
\[
\phi_\alpha(P_{k+1}) f_i(x) - \phi_\alpha(P_{l+1}) f_k(x) = \frac{\phi_\alpha(P_{k+1}) f_k(x)}{\phi_\alpha(P_{l+1}) f_i(x)} = \left| \frac{f_{k+1}(x)}{f_i(x)} \right| ^2 \frac{f_k(x)}{f_{l+1}(x)} = \ldots \\
= (1 - \alpha)^{2k}((x - \alpha)f_p(x) - f_{p+1}(x)) \\
= (1 - \alpha)^{2k}(\alpha f_p(x) + (1 - \alpha)^2 f_{p-1}(x)) \quad (\text{for } p \geq 1).
\]

So, we have the following conclusion:

\textbf{Lemma 3.4} Suppose \( l, k \) are positive numbers with \( l \geq k \). Then, for \( x \geq 2 \),
\[
\phi_\alpha(P_{k+1}) f_i(x) - \phi_\alpha(P_{l+1}) f_k(x) = f_{k+1}(x)f_i(x) - f_k(x)f_{l+1}(x) \geq 0,
\]
and the equality holds if and only if \( l = k \).

\textbf{Lemma 3.5} Let \( u \) and \( v \) be two equivalent vertices of a connected graph \( G \), \( w \) be a vertex of a connected graph \( W \) and \( H = G_{u,v}(k, l) \). Take \( H_1 = H(u, w)W \) and \( H_2 = H(v, w)W \), if \( l - k \geq 1 \), then \( \rho_\alpha(H_2) > \rho_\alpha(H_1) \).

\textbf{Proof} By Lemma 3.3 and Formula (5), we have
\[
\psi_\alpha(H, v) - \psi_\alpha(H, u) = \psi_\alpha(G, \{u, v\})\left( \phi_\alpha(P_{k+1}) f_i(x) - f_k(x)\phi_\alpha(P_{l+1}) \right) \\
= \psi_\alpha(G, \{u, v\})\left( f_{k+1}(x)f_i(x) - f_k(x)f_{l+1}(x) \right).
\]

When \( l - k \geq 1 \), by Lemma 3.4, we have \( f_{k+1}(x)f_i(x) - f_k(x)f_{l+1}(x) > 0 \) for \( x \geq 2 \). Since \( \rho(H_\alpha - u) > \rho(G_\alpha - \{u, v\}) \), we have
\[
\psi_\alpha(H, v) - \psi_\alpha(H, u) > 0 \quad \text{for } x > \rho(H_\alpha - u).
\]

By Lemma 3.1, we have \( \rho_\alpha(H_2) > \rho_\alpha(H_1) \). \( \square \)

By Lemma 3.5, we can easily get the following corollary.

\textbf{Corollary 3.1} Let \( u \) and \( v \) be two vertices of a connected graph \( G \) such that \( N_G(u) \setminus \{v\} = N_G(v) \setminus \{u\} \), \( H_3 \) denotes the graph obtained from \( G_{u,v}(k, l) \) by identifying vertex \( u \) with the center of \( K_{1, s} \) and \( H_4 \) denotes the graph obtained from \( G_{u,v}(k, l) \) by identifying vertex \( v \) with the center of \( K_{1, s} \). If \( l - k \geq 1 \), then \( \rho_\alpha(H_4) > \rho_\alpha(H_3) \).

\section{The extremal graphs with the maximal \( \alpha \)-spectral radius among \( \mathcal{U}(n, d) \)}

Let \( \mathcal{G}_t(n, d) \) denote the set of all the \( n \)-vertex \( t \)-cyclic graphs with diameter \( d \). The sets \( \mathcal{G}_1(n, d) \) and \( \mathcal{G}_2(n, d) \) also are written as \( \mathcal{U}(n, d) \) and \( \mathcal{B}(n, d) \), respectively.

\textbf{Proposition 4.1} Let \( G \) be the graph with maximal \( \alpha \)-spectral radius among \( \mathcal{G}_t(n, d), \ (t > 0) \). Then \( G \) has the following properties:

(i) If \( e \) is an edge in some internal path of \( G \), then \( e \) must be in a \( C_3 \) of \( G \).
(ii) For any path \( P \) of length \( d \) in \( G \), \( V(P) \cap V(\bar{G}) \neq \emptyset \) always holds.
(iii). Let \( P \) be a path of length \( d \) in \( G \) and \( U = V(P) \setminus V(\hat{G}) \). When \( U \neq \emptyset \), take \( U' = V(G) \setminus (V(P) \cup V(\hat{G})) \). Then, there exists some vertex \( w \) in \( V(\hat{G}) \) such that \( G[U' \cup \{w\}] \) is a star \( S \) with center \( w \).

**Proof** (i). Assume \( e \) is an edge in some internal path of \( G \) and there exists no \( C_3 \) in \( G \) such that \( e \in E(C_3) \). Let \( G' \) be the graph obtained from \( G \) by contracting edge \( e \). By Lemma 2.5, we have \( \rho_{\alpha}(G) < \rho_{\alpha}(G') \). It is easy to see that \( 0 \leq \text{diam}(G) - \text{diam}(G') \leq 1 \). When \( \text{diam}(G) = \text{diam}(G') + 1 \), take \( G^* \) be a graph obtained from \( G' \) by attaching a pendant edge to one end vertex of some path of length \( d - 1 \) in \( G' \). When \( \text{diam}(G) = \text{diam}(G') \), suppose that \( u \in V(G') \) is not end vertex of any path of length \( d \) in \( G' \). Take \( G^* \) be a graph obtained from \( G' \) by attaching a pendant edge to vertex \( u \). We have \( G^* \in \mathcal{C}_1(n, d) \). By (ii) of Lemma 2.1, \( \rho_{\alpha}(G') < \rho_{\alpha}(G^*) \). So \( \rho_{\alpha}(G) < \rho_{\alpha}(G^*) \), a contradiction. Hence, \( e \) must be in a \( C_3 \) of \( G \).

(ii). Assume that \( P \) is path of length \( d \) in \( G \) such that \( V(P_{d+1}) \cap V(\hat{G}) = \emptyset \). Then \( P_{k} = u_1u_2 \ldots u_k \) \((k \geq 2)\) be the shortest path between \( P \) and \( \hat{G} \). Applying Lemma 2.3 to the edge \( u_1u_2 \), we get a graph \( G^* \in \mathcal{C}_1(n, d) \) such that \( \rho_{\alpha}(G) < \rho_{\alpha}(G^*) \), a contradiction. Hence, \( V(P_{d+1}) \cap V(\hat{G}) \neq \emptyset \).

(iii). Let \( G' = G[V(P) \cup V(\hat{G})] \) and \( G^* = G - E(G') \). Assume that there exist two connected components, denoted by \( T_1, T_2 \), with order greater than one of \( G^* \). By Lemma 2.3, \( T_1 \) and \( T_2 \) must be star graphs with center vertices, denoted by \( u, v \), in \( V(G') \). Take \( G_1 \) (or \( G_2 \)) be the graphs obtained from \( G \) by removing tree \( T_1 \) (or \( T_2 \)) from \( u \) to \( v \) (or \( v \) to \( u \)). By Lemma 2.2, we have \( \rho_{\alpha}(G) < \rho_{\alpha}(G_1) \) or \( \rho_{\alpha}(G) < \rho_{\alpha}(G_2) \), where \( G_1, G_2 \in \mathcal{C}_1(n, d) \), a contradiction. So there exists at most one connected component, denoted by \( T \), with order greater than one in \( G^* \). By Lemma 2.4 and (i) of Lemma 2.1, \( |V(T) \cap V(\hat{G})| = 1 \) holds. Then, \( T \) is the desired star graph \( S \).  

For \( G \in \mathcal{H}(n, d) \), we have \( n \geq 3 \) and \( 1 \leq d \leq n - 2 \). If \( d = 1 \), then \( G \cong C_3 \). Therefore, in the following, we assume that \( d \geq 2 \) and \( n \geq 4 \).

Suppose that \( V(C_3) = \{w_1, w_2, w_3\} \), We construct some unicyclic graphs obtained from \( C_3 \) as follows (see Fig. 1):

- \( \Delta_1(s; a, b) \): the graph obtained from \( C_3 \) by attaching \( s \) pendant edges, pendant path of length \( a \) and pendant path of length \( b \) to vertex \( w_2 \).
- \( \Delta_2(s; a, b) \): the graph obtained from \( C_3 \) by attaching \( s \) pendant edges and pendant path of length \( a \) to vertex \( w_2 \) and attaching pendant path of length \( b \) to vertex \( w_3 \), respectively.

Let \( \mathcal{A}_i(n, d) \) denote the set consisting of all graphs \( \Delta_i(s; a, b) \) with \( n \) vertices and diameter \( d \) for \( i = 1, 2 \). Take \( U_1^1(n, d) = \Delta_1(s; a, b) \in \mathcal{A}_1(n, d) \) if \( 0 \leq a - b \leq 1 \) and \( d = a + b \). Take \( U_2^1(n, d) = \Delta_2(s; a, b) \in \mathcal{A}_2(n, d) \) if \( 0 \leq a - b \leq 1 \) and \( d = a + b + 1 \).

The authors of Liu et al. (2007) and He and Li (2012) determined that \( U_2^2(n, d) \) is the unique graph with maximal adjacency spectral radius and signless Laplacian spectral radius, respectively, among \( \mathcal{A}(n, d) \).
be the bicyclic graph obtained by coalescence two copies of the cycle graph $C_n$ from two vertex-disjoint cycles $C_{n_1}$ and $C_{n_2}$.

**Lemma 4.1** For any graph $G \in \mathbf{\Delta}_1(n, d)$, with $d > 2$, there exists a graph $G' \in \mathbf{\Delta}_2(n, d)$ such that $\rho_{\alpha}(G) < \rho_{\alpha}(G')$.

**Proof** Since $G \in \mathbf{\Delta}_1(n, d)$, there exist $s$, $a$, and $b$ such that $G = \Delta_1(s; a, b)$ with $d = a + b$ and $|a - b| \leq 1$. Without loss of generality, we can assume that $b \geq 2$, since $d > 2$. Let $H_1$ be the pendant path of length $b - 1$ and $H_2$ the graph obtained from $C_2$ by attaching $s + 1$ pendant edges $w_2 z_i (i = 1, \ldots, s + 1)$ and pendant path of length $a$ to vertex $w_2$. Let $u$ be a pendant vertex of $H_1$, then $\Delta_1(s; a, b) = H_1(u, z_{s+1}) H_2$ and $G' = \Delta_2(s + 1; a, b - 1) = H_1(u, w_3) H_2 \in \mathbf{\Delta}_2(n, d)$. Clearly, $N_{H_2}(z_{s+1}) \subset N_{H_2}(w_3)$, then by Lemma 3.2, we have $\rho_{\alpha}(G) = \rho_{\alpha}(\Delta_1(s; a, b)) < \rho_{\alpha}(\Delta_2(s + 1; a, b - 1)) = \rho_{\alpha}(G')$. □

**Theorem 4.1** The graph $U_2^*(n, d)$ is the unique graph with the maximal $\alpha$-spectral radius among $\Psi(n, d)$.

**Proof** Let $G$ be the graph with the maximal $\alpha$-spectral radius among $\Psi(n, d)$. By Proposition 4.1, we have $G \in \mathbf{\Delta}_1(n, d)$ or $G \in \mathbf{\Delta}_2(n, d)$. When $d = 1, 2$, we have $\mathbf{\Delta}_1(n, d) \cong \mathbf{\Delta}_2(n, d)$; when $d > 2$, according to Lemmas 2.6 and 4.1, we have $G \cong U_2^*(n, d)$. □

5 The extremal graphs with the maximal $\alpha$-spectral radius among $\mathcal{B}(n, d)$

It is known that there are two types of bases of bicyclic graphs, $\infty(n_1, n_2, n_3)$ is obtained from two vertex-disjoint cycles $C_{n_1}$ and $C_{n_2}$ by joining vertex $u$ of $C_{n_1}$ and vertex $v$ of $C_{n_2}$ by a path $P_{n_3}$ ($n_3 \geq 1$), $\theta(n_1, n_2, n_3)$ ($n_1 \geq n_2 \geq n_3$) is obtained from three pairwise internal disjoint paths of lengths $n_1$, $n_2$, $n_3$ from vertices $u$ to $v$ (see Fig. 2). The graphs $\infty(n_1, n_2, n_3)$ and $\theta(n_1, n_2, n_3)$ are referred to as $\infty$-graph and $\Theta$-graph, respectively.

Let

$$\mathcal{B}_1(n, d) = \{G | G \in \mathcal{B}(n, d) \text{ and } \hat{G} \text{ is } \infty \text{-graph}\},$$

$$\mathcal{B}_2(n, d) = \{G | G \in \mathcal{B}(n, d) \text{ and } \hat{G} \text{ is } \Theta \text{-graph}\}.$$

Let $\mathfrak{H}$ be the bicyclic graph obtained by coalescence two copies of the cycle graph $C_3$ with a common vertex. Suppose that $V(\mathfrak{H}) = \{w_0, w_1, w_2, w_3, w_4\}$ with $d(w_0) = 4$ and $\{(w_1, w_2), (w_3, w_4)\} \subset E(\mathfrak{H})$.

Let $\emptyset$ be the unique bicyclic graph of order 4 with $V(\emptyset) = \{w_1, w_2, w_3, w_4\}$ and $d(w_1) = d(w_3) = 2, d(w_2) = d(w_4) = 3$. We construct some bicyclic graphs obtained from $\emptyset$ as follows (see (a)–(e) of Fig. 3):
Fig. 3 $\Phi_i(s; a, b)$ for $i = 1, 2, 3, 4, 5$

- $\Phi_1(s; a, b)$: the graph obtained from $\Phi$ by attaching $s$ pendant edges and two pendant paths of lengths $a$ and $b$ to vertex $w_1$.
- $\Phi_2(s; a, b)$: the graph obtained from $\Phi$ by attaching $s$ pendant edges and two pendant paths of lengths $a$ and $b$ to vertex $w_2$.
- $\Phi_3(s; a, b)$: the graph obtained from $\Phi$ by attaching $s$ pendant edges and pendant path of length $a$ to vertex $w_2$ and attaching pendant path of length $b$ to $w_3$.
- $\Phi_4(s; a, b)$: the graph obtained from $\Phi$ by attaching $s$ pendant edges and pendant path of length $a$ to vertex $w_1$ and attaching pendant path of length $b$ to $w_3$.
- $\Phi_5(s; a, b)$: the graph obtained from $\Phi$ by attaching $s$ pendant edges to $w_2$ and attaching pendant paths of lengths $a$ and $b$ to vertex $w_1$ and $w_3$, respectively.

Let $\Phi_i(n, d)$ denote the set consisting of all graphs $\Phi_i(s; a, b)$ with $n$ vertices and diameter $d$ for $i = 1, \ldots, 5$. Take $\Phi(n, d) = \bigcup_{i=1}^{3} \Phi_i(n, d)$.

By Lemma 2.2, the following result can be deduced.

**Lemma 5.1** For any graph $G \in \mathcal{B}_1(n, d)$ with $\widehat{G} \cong \mathcal{X}$ there exists some graph $H \in \mathcal{B}_2(n, d)$ with $\widehat{H} \cong \Phi$ such that $\rho_\alpha(G) < \rho_\alpha(H)$.

**Proof** Suppose that $G \in \mathcal{B}_1(n, d)$ with $\widehat{G} = \mathcal{X}$ and $V(\mathcal{X}) = \{w_0, w_1, w_2, w_3, w_4\}$ with $d(w_0) = 4$ and $(\{w_1, w_2\}, \{w_3, w_4\}) \in E(\mathcal{X})$. Take $x$ be the $\alpha$-Perron vector of $G$. Wlog, suppose $x_{w_1} \geq x_{w_3}$. Let $H' = \widehat{G} - w_3w_4 + w_1w_4$. By Lemma 2.2, we have $\rho_\alpha(G) < \rho_\alpha(H')$. It is easy to see that $0 \leq \text{diam}(H') - \text{diam}(G) \leq 1$. If $\text{diam}(H') = d$, take $H = H'$. If $\text{diam}(H') = d + 1$, then $\text{diam}(H') \geq 4$. Therefore, there exist some non-pendant edge...
Lemma 5.2 The graph $B_3^*(n, d)$ is the unique graph with the maximal $\alpha$-spectral radius among $\mathcal{S}(n, d)$.

Proof (1). For fixed $s$, $a$ and $b$, take $G \cong \mathcal{S}$ with $V(G) = \{w_1, w_2, w_3, w_4\}$ and $d(w_1) = d(w_2) = 2, d(w_3) = d(w_4) = 3$ and $H$ be the graph obtained by attaching $s$ pendant edges and two pendant paths of lengths $a$ and $b$ to an isolated vertex $v$. Then $\mathcal{S}(s; a, b) = G(w_3, v)H$ and $\mathcal{S}(s; a, b) = G(w_2, v)H$. Since $N_G(w_3) \setminus \{w_2\} \subset N_G(w_2) \setminus \{w_3\}$, by Lemma 3.2, we have

$$\rho_\alpha(\mathcal{S}(s; a, b)) < \rho_\alpha(\mathcal{S}(s; a, b)).$$

(2). For fixed $s$, $a$ and $b$, let graph $G \cong \mathcal{S}(s; a, 1)$ and $H = P_b$ with pendant vertex $u$. Then $\mathcal{S}(s; a, b) \cong G(u_1, u)H$ and $\mathcal{S}(s + 1; a, b - 1) \cong G(w_4, u)H$. Clearly, when $b = 1$, $\mathcal{S}(s; a, 1) \cong \mathcal{S}(s + 1; a, 0)$. Since $N_G(u_1) \subset N_G(w_4)$, by Lemma 3.2, for $2 \leq b$, we have

$$\rho_\alpha(\mathcal{S}(s; a, b)) < \rho_\alpha(\mathcal{S}(s + 1; a, b - 1)).$$

If $\mathcal{S}(s; a, b) \in \mathcal{S}(n, d)$, then $\mathcal{S}(s + 1; a, b - 1)$ is also in $\mathcal{S}(n, d)$.

From above arguments in (1) and (2), we have that the graph with the maximal $\alpha$-spectral radius among $\mathcal{S}(n, d)$ must be in $\mathcal{S}(n, d)$. Then by Lemma 2.6 and Corollary 3.1, we have the graph $B_3^*(n, d)$ is the unique graph with the maximal $\alpha$-spectral radius among $\mathcal{S}(n, d)$. This completes the proof.

Lemma 5.3 When $d \geq 4$, for any $H_1 = \mathcal{S}(s; a, b) \in \mathcal{S}(n, d)$, there always exists some graph $H_2 \in \mathcal{S}(n, d)$ such that $\rho_\alpha(H_1) < \rho_\alpha(H_2)$.

Proof Let $H = \mathcal{S}(1; 0, 0) = \mathcal{S}(0, 0; a, b)$ and $G = K_{1, s}$ with $d_G(u) = s$. Then, $H_1 = \mathcal{S}(s; a, b) = H(w_1, u)G$ and $H_2 = \mathcal{S}(s; a, b) = H(w_2, u)G$. Take

$$h_1 = \psi_\alpha(H, \{w_1, w_2\}), h_2 = \psi_\alpha(H, \{w_1, w_2, w_3\}),$$

$$h_3 = \psi_\alpha(H, \{w_1, w_2, w_4\}), h_4 = \psi_\alpha(H, \{w_1, w_2, w_3, w_4\}),$$

and

$$h_5 = \begin{cases} \psi_\alpha(H, \{w_1, w_2, v_1\}) & \text{when } a \geq 1, \\ 0 & \text{otherwise}. \end{cases}$$

Applying Theorem 2.1 to $A(H_1 - w_1)$ and $A(H_1 - w_2)$, respectively, we have

$$\psi_\alpha(H, w_1) = (x - 3\alpha)h_1 - (1 - \alpha)^2(h_2 + h_3) - 2(1 - \alpha)^3h_4,$$

$$\psi_\alpha(H, w_2) = \begin{cases} (x - 3\alpha)h_1 - (1 - \alpha)^2(h_3 + h_5) & \text{when } a \geq 1, \\ (x - 2\alpha)h_1 - (1 - \alpha)^2h_3 & \text{otherwise}. \end{cases}$$
Then,
\[
\psi_a(H, w_2) - \psi_a(H, w_1) = \begin{cases} 
(1 - \alpha)^2(h_2 - h_5) + 2(1 - \alpha)^3h_4 & \text{when } a \geq 1, \\
\alpha h_1 + (1 - \alpha)^2h_2 + 2(1 - \alpha)^3h_4 & \text{otherwise}.
\end{cases}
\]

It is easy to see that when \(x > \rho(H_a - w_1), h_1, h_2, h_4\) are positive.

So, \(\psi_a(H, w_2) > \psi_a(H, w_1)\) for \(a = 0\).

Now consider the case for \(a \geq 1\). By direct calculation, we have
\[
h_2 = (x - 3\alpha)f_a(x)f_b(x), \quad h_4 = f_a(x)f_b(x),
\]
\[
h_5 = f_{a-1}(x)\psi_a(\Theta_4(0; 0, b), [w_1, w_2]) = f_{a-1}(x)(x - 3\alpha)f_{b+1}(x) - (\alpha(x - 3\alpha) + (1 - \alpha)^2)f_b(x)).
\]

Then, we have \(\psi_a(H, w_2) - \psi_a(H, w_1) = (1 - \alpha)^2f^* + 2(1 - \alpha)^3f_a(x)f_b(x),\) where
\[
f^* = (x - 3\alpha)f_a(x)f_b(x) - f_{a-1}(x)f_{b+1}(x) + (\alpha(x - 3\alpha) + (1 - \alpha)^2)f_b(x)f_{a-1}(x).
\]

When \(a \leq b + 1\), by Lemma 3.4, we have \(f_a(x)f_b(x) - f_{a-1}(x)f_{b+1}(x) \geq 0\) for \(x \geq 2\), and it is easy to see that when \(x > \rho(H_a - w_1), f_b(x), f_{a-1}(x)\) are positive. Then \(\psi_a(H, w_2) - \psi_a(H, w_1) > 0\) for \(x \geq \rho(H_a - w_1)\). Then by Lemma 3.1, we have \(\rho_a(\Theta_4(s; a, b)) < \rho_a(\Theta_5(s; a, b)). \Theta_5(s; a, b)\) is the desired graph for \(a \leq b + 1\).

When \(a \geq b + 2\), let \(x\) be the \(\alpha\)-Perron vector of \(H_1\) and \(v_0 = w_1, u_0 = w_3\), we distinguish the following cases.

**Case 1** \(x_{u_b} \geq x_{v_{a-1}}\).

Let \(H'_1 = H_1 - v_{a-1}v_a + u_bv_a = \Theta_4(s; a - 1, b + 1),\) by Lemma 2.2, we have \(\rho_a(\Theta_4(s; a - 1, b + 1)) \geq \rho_a(H'_1) = \rho_a(H_1) = \rho_a(\Theta_4(s; a, b)). \) Then, by this case and \(a \leq b + 1\), we have \(\rho_a(\Theta_4(s; a, b)) \leq \rho_a(B^*_4(n, d)) < \rho_a(B^*_5(n, d)). B^*_5(n, d)\) is the desired graph for this case.

**Case 2** \(x_{v_{a-1}} > x_{u_b}\).

**Subcase 5.1** \(x_{v_{a-i}} > x_{u_{b-i+1}}\) for \(1 < i \leq b\).

When \(i = b + 1\), we have \(x_{v_{a-b-1}} > x_{u_0}\), and by Proposition 2.1, we have \(x_{v_1} > x_{v_{a-b-1}} > x_{u_0}\), let \(H'_1 = H_1 - w_{a-b}u_b + w_a = \Theta_5(s; a - 1, b + 1)\), by Lemma 2.2, we have \(\rho_a(\Theta_5(s; a - 1, b + 1)) \geq \rho_a(H'_1) > \rho_a(H_1) = \rho_a(\Theta_4(s; a, b)) \Theta_5(s; a - 1, b + 1)\) is the desired graph for this subcase.

**Subcase 5.2** \(x_{v_{a-j+1}} > x_{u_{b-j+2}}\) and \(x_{v_{a-j}} \leq x_{u_{b-j+1}}\) for some \(1 < j \leq b\).

Let \(e_1 = v_{a-j+1}v_{a-j}, e_2 = u_{b-j+1}u_{b-j+2}\) and \(H'\) be the graph obtained from \(H\) by 2-switching operation \(e_1 \xrightarrow{v_{a-j}} e_2\). By Lemma 2.4, we have
\[
\rho_a(\Theta_4(s; a - 1, b + 1)) = \rho_a(H'_1) > \rho_a(H_1) = \rho_a(\Theta_4(s; a, b)).
\]

Then by this case and \(a \leq b + 1\), we have \(\rho_a(\Theta_4(s; a, b)) \leq \rho_a(B^*_4(n, d)) < \rho_a(B^*_5(n, d))\).

**Lemma 5.4** For \(a \geq b \geq 1\), then we have
\[
\rho_a(\Theta_5(s; a, b)) > \rho_a(\Theta_5(s; a + 1, b - 1)).
\]
**Proof** Let $x$ be the $\alpha$-Perron vector of $\phi_5(s; a + 1, b - 1)$ and $v_0 = w_1, u_0 = w_3$. Assume that $\rho_\alpha(\phi_5(s; a + 1, b - 1)) \geq \rho_\alpha(\phi_5(s; a, b))$. Then the following assertion holds:

**Assertion 1:** $x_{v_{a-i}} > x_{u_{b-i-1}}$ for all $i = 0, \ldots, b - 1$.

We prove the assertion by induction on $i$. If $x_{v_{a-1}} \geq x_{u_{b-1}}$, then for $H = \phi_5(s; a + 1, b - 1) - v_a v_{a+1} + u_{b-1}v_{a+1}$, we have $H \cong \phi_5(s; a, b)$, and thus by Lemma 2.2, we have $\rho_\alpha(\phi_5(s; a, b)) = \rho_\alpha(H) > \rho_\alpha(\phi_5(s; a + 1, b - 1))$, a contradiction. Thus, $x_{v_a} > x_{u_{b-1}}$.

The assertion holds for $i = 0$. If $b = 1$, then $i = 0$ and the claim follows. Suppose that $b \geq 2$, and $x_{v_{a-i}} > x_{u_{b-1}}$, where $0 \leq i \leq b - 2$. If $x_{u_{b-(i+1)}} \geq x_{v_{a-(i+1)}}$, let $e_1 = v_{a-(i+1)}v_{a-i}$, $e_2 = u_{b-(i+1)}u_{b-i-1}$ and $H'$ be the graph obtained from $\phi_5(s; a + 1, b - 1)$ by 2-switching operation $e_1 \leftrightarrow e_2$. We have $H' \cong \phi_5(s; a, b)$ and thus by Lemma 2.4, we have

$$\rho_\alpha(\phi_5(s; a, b)) = \rho_\alpha(H') > \rho_\alpha(\phi_5(s; a + 1, b - 1)),$$

which contradicts the assumption. Thus, $x_{v_{a-(i+1)}} > x_{u_{b-(i+1)}}$. So, Assertion 1 follows by induction.

By Assertion 1 for $i = b - 1$, we have $x_{v_{a-(b-1)}} > x_{u_{b-1}}$, and by Proposition 2.1, we have $x_{v_1} > x_{w_2}, x_{v_2} > x_{w_3},$ let $H_1 = \phi_5(s; a + 1, b - 1) - w_3 w_4 v_1 w_2 v_1 w_4$, we have $H_1 \cong \phi_4(s; b, a)$ and thus by Lemma 2.2, we have $\rho_\alpha(\phi_5(s; a + 1, b - 1)) < \rho_\alpha(H_1) = \rho_\alpha(\phi_4(s; b, a))$. For $b \leq a$, by Lemma 5.3, we have $\rho_\alpha(\phi_4(s; b, a)) < \rho_\alpha(\phi_5(s; a, b))$. Then $\rho_\alpha(\phi_5(s; a + 1, b - 1)) < \rho_\alpha(\phi_5(s; a, b))$, a contradiction. Thus, we have $\rho_\alpha(\phi_5(s; a, b)) > \rho_\alpha(\phi_5(s; a + 1, b - 1))$.

In the following, we will determine the graph with the maximal $\alpha$-spectral radius among $B(n, d)$.

**Theorem 5.1** Let $G$ be the graph with the maximal $\alpha$-spectral radius among $B(n, d)$, then we have $G \cong B^*_5(n, d)$ or $G \cong B^*_5(n, d)$.

**Proof** By (i) of Proposition 4.1, we have $\hat{G} \in \{X, \phi\}$. And by Lemma 5.1, we have $\hat{G} = \phi$. Take $P$ be a path of $G$ with length $d$.

**Case 1** $|V(P) \cap V(\phi)| = 1$.

Applying Proposition 4.1 and Lemma 2.2, we can prove that $G \in \phi_1(n, d) \cup \phi_2(n, d)$. By Lemma 5.2, we have a graph $H \in \phi_3(n, d)$ such that $\rho_\alpha(H) > \rho_\alpha(G)$, a contradiction.

**Case 2** $|V(P) \cap V(\phi)| = 2$.

We have $|E(P) \cup E(\phi)| = 1$. $G \in \phi_3(n, d)$ can be deduced from the proof of (iii) of Proposition 4.1 and Lemma 2.2. By Lemma 5.2, we have $G \cong B^*_5(n, d)$.

**Case 3** $|V(P_{d+1}) \cap V(\phi)| = 3$.

Applying Proposition 4.1, we have $G \in \phi_1(n, d) \cup \phi_3(n, d)$. By Lemmas 5.3 and 5.4, we have further $G \cong B^*_5(n, d)$.

Combining Cases 1–3, we have $G \cong B^*_5(n, d)$ or $G \cong B^*_5(n, d)$. This completes the proof.

Take $n = 16, d = 9$ and $DR(\alpha) = \rho_\alpha(B^*_5(n, d)) - \rho_\alpha(B^*_5(n, d))$. By direct calculation, we obtain the value of $DR(\alpha)$ for $\alpha = 0.0, 0.1, \ldots, 0.8$.

From Table 1, it can be seen that the relative magnitudes of the $\alpha$-spectral radii of $B^*_5(n, d)$ and $B^*_5(n, d)$ depends upon the value of $\alpha$.

In Guo (2007), the graph $B^*_5(n, 3)$ and $B^*_5(n, d)$ are denoted by $P^6_4(3)$ and $P^+_d((d+2)/2)$, respectively. The following result is proved.
Theorem 5.2 (Guo (2007)) Let $H$ be the graph with the maximal adjacency spectral radius among $B(n, d)$, then $H \cong B_3^*(n, d)$ for $d = 3$ and $H \cong B_3^*(n, d)$ for $d \geq 4$.

In (Pai 2014, Theorem 5.1) and (Pai and Liu 2017, Theorem 3.1), the authors asserted that the above result also holds for signless Laplacian spectral radius. Unfortunately, this result is not correct. By numerical calculation, one can find that: For $n = 16$ and $d = 9$ and $\alpha = \frac{1}{2}$, $\rho_\alpha(B_3^*(16, 9)) \approx 4.6201$ and $\rho_\alpha(B_3^*(16, 9)) \approx 4.6171$. Since $\rho_Q(G) = 2\rho_{1/2}(G)$ for any graph $G$, we have $\rho_Q(B_3^*(n, d)) > \rho_Q(B_3^*(n, d))$, which does not agree with the assertion of Theorem 3.1 of Pai and Liu (2017).

In the following theorem, we determine the unique graph with the maximal $\alpha$-spectral radius among $B(n, d)$.

Theorem 5.3 Let $H$ be the graph with the maximal signless Laplacian spectral radius among $B(n, d)$, then $H \cong B_3^*(n, d)$ for $d \geq 3$.

Proof For $i = 1, 2, 3, 4$, take $G_i$ be graphs depicted in Fig. 4.

Let $H_i(a, b) = G_i(P_a, P_b)$ be the graph obtained from $G_i$ by attaching pendant paths $P_a$ and $P_b$ to $u_1$ and $v_1$, respectively. Then

\[
H_1(a, b) \cong \Phi_3(z; a, a - 1), \quad H_2(a, b) \cong \Phi_3(z + 1; a - 1, b - 1),
\]

\[
H_3(a, b) \cong \Phi_3(z; a, a), \quad H_4(a, b) \cong \Phi_3(z + 1; a - 1, b).
\]

Notice that $H_i(1, 1) = G_i$ for $i = 1, 2, 3, 4$. Take $a = b = l \geq 1$. We have for $d = 2l$ and $n = 2l + z + 3$, $H_1(a, b) \in \Phi_3(n, d)$, $H_2(a, b) \in \Phi_3(n, d)$ and for $d = 2l + 1$ and $n = 2l + z + 4$, $H_3(a, b) \in \Phi_3(n, d)$, $H_4(a, b) \in \Phi_3(n, d)$. By Lemmas 5.2 and 5.4, we know that

\[
B_3^*(n, d) = \begin{cases} 
  H_1(l, l), & \text{if } d = 2l; \\
  H_3(l, l), & \text{if } d = 2l + 1;
\end{cases}
\]

\[
B_3^*(n, d) = \begin{cases} 
  H_2(l, l), & \text{if } d = 2l; \\
  H_4(l, l), & \text{if } d = 2l + 1.
\end{cases}
\]

Since $K_{1, z+4}$ is a proper subgraph of $G_i$ for $i = 1, 2, 3, 4$, when $\alpha = \frac{1}{2}$, we have

\[
\rho_{1/2}(H_i(l, l)) > \rho_{1/2}(K_{1, z+4}) = \frac{z + 5}{2}.
\]

According to Theorem 5.1, to complete the proof, it suffices to show that

\[
\rho_{1/2}(\Phi_3(z; a, a)) > \rho_{1/2}(\Phi_3(z + 1; a - 1, b - 1)),
\]

\[
\rho_{1/2}(\Phi_3(z; a, a)) > \rho_{1/2}(\Phi_3(z + 1; a - 1, b)).
\]
\( \rho_1(B_3^*(n, d)) > \rho_1(B_3^*(n, d)) \) for \( d \geq 3 \).

Thus, it is sufficient to show that \( \phi_1(B_3^*(n, d)) < \phi_1(B_3^*(n, d)) \) for \( d \geq 3 \).

For \( l \geq 2 \), take \( dp_l(x) = \phi_\alpha(P_l) - x f_{l-1} \). By Lemma 2.9, for \( l \geq 2 \), we have

\[
DF(x) = \phi_\alpha(B_3^*(n, d)) - \phi_\alpha(B_3^*(n, d))
= DF_1(x) f_{l-1}^2(x) + DF_2(x) f_{l-1}(x) dp_l(x) + DF_3 dp_l(x)^2.
\]  

(6)

For \( i = 1, 2, 3, 4 \), denote \( F_{i1} = \phi_\alpha(G_i) \), \( F_{i2} = \psi_\alpha(G_i, u_i) \), \( F_{i3} = \psi_\alpha(G_i, v_1) \), \( F_{i4} = \psi_\alpha(G_i, \{u_1, v_1\}) \). Applying the technique of quotient matrix (see, e.g., Corollary 1 of Saravanan et al. (2021)), \( F_{ij} \) for \( i, j = 1, 2, 3, 4 \) can be obtained.

Take \( f_{ij} \) are polynomials which are listed in Appendix A. Then for \( 1 \leq j \leq 4 \), we have

\[
F_{1j} = (x - \frac{1}{2}) z^{-1} f_{1j}, \quad F_{2j} = (x - \frac{1}{2}) z^{-1} f_{2j}, \quad F_{3j} = (x - \frac{1}{2}) z^{-1} (x - 1) f_{3j}, \quad F_{4j} = (x - \frac{1}{2}) f_{4j}.
\]

**Case 1** \( d \equiv 0 \) (mod 2).

Setting \( d = 2l \), we have \( DF(x) = H_1(l, l) - H_2(l, l) \). Since \( G_1 \cong G_2 \), we have \( DF(x) = F_{11} - F_{21} = 0 \). According to Table 2, by directly calculation, we have

\[
DF_2(x) = \frac{1}{2} (x^2 - \frac{z+5}{2} x + 1) (x - \frac{1}{2})^z
\] and

\[
DF_3(x) = \frac{1}{4} (x^2 - \frac{z+5}{2} x + 1) (x - \frac{1}{2})^{z-1}.
\]

Then, by Formula (6), we have \( DF(x) = (2x - 1) f_{l-1}(x) + dp_l(x) \) \( dp_l(x) DF_3(x) \). Since \( \rho_1(H_2(l, l)) > \frac{z+5}{2} > \rho_\frac{z+5}{2} (P_l) (l \geq 2) \), we have \( f_l(x) > 0 (i \geq 2) \) when \( x \geq \rho_1(H_2(l, l)) \).

It is easy to see that

\[
(2x - 1) f_{l-1}(x) + dp_l(x) = (\frac{1}{2} f_{l-1}(x) + \phi_\frac{1}{2}(P_l)) > 0 \text{ when } x > 2.
\]

Since \( DF_3(x) > 0 \) and \( dp_l(x) < 0 \) when \( x > \frac{z+5}{2} \), we have

\( DF(x) = H_1(l, l) - H_2(l, l) \) < 0 when \( x \geq \rho_\frac{1}{2}(H_2(l, l)) \).

Thus \( \rho_\frac{1}{2}(H_1(l, l)) \geq \rho_\frac{1}{2}(H_2(l, l)) \) follows for this case.

**Case 2** \( d \equiv 1 \) (mod 2).

Setting \( d = 2l + 1 \), we have \( DF(x) = H_3(l, l) - H_4(l, l) \).

According to Table 2, by directly calculation, we have

\[
DF_1(x) = -\frac{1}{4} x (x^2 - \frac{z+5}{2} x + 1) (x - \frac{1}{2})^{z+1},
\]

\[
DF_2(x) = -\frac{1}{2} (x^2 - \frac{z+5}{2} x + 1) (x^3 - 2x^2 + \frac{3}{2} x - \frac{1}{4} (x - \frac{1}{2})^{z-1},
\]

\[
DF_3(x) = -\frac{1}{2} (x^2 - \frac{z+5}{2} x + 1) (x - \frac{1}{2})^{z-1} (x - 1)^2.
\]

Take \( g(x) = -\frac{1}{8} (x^2 - \frac{z+5}{2} x + 1) (x - \frac{1}{2})^{z-1} \).

For \( \alpha = \frac{1}{2} \), since \( dp_1(x) = -\frac{1}{2} f_{l-1}(x) - \frac{1}{4} f_{l-2}(x) \), \( f_{l-1}(x) = (x - 1) f_{l-2}(x) - \frac{1}{4} f_{l-3}(x) \) for \( l \geq 3 \) and \( g(x) < 0 \), \( f_{l-2}(x) \) > \( f_{l-3}(x) \), \( 2x^3 - \frac{9}{4} x^2 + \frac{5}{2} x - \frac{1}{4} \geq \frac{3}{4} x^2 - \frac{9}{8} x + \frac{3}{8} \) hold when \( x > \frac{z+5}{2} \), by Formula (6), we have

\[
DF(x) = g(x) f_{l-1}(x) \left( 3(x - 1) (x - \frac{1}{2}) f_{l-1}(x) - (x^3 - 3x^2 + \frac{7}{2} x - \frac{5}{4}) f_{l-2}(x) \right)
+ \frac{1}{4} (x - 1)^2 f_{l-2}^2(x) g(x)
\]
\[ g(x)f_{i-1}(x)(3(x - 1)(x - \frac{1}{2})f_{i-1}(x) - (x^3 - 3x^2 + \frac{7}{2}x - \frac{5}{4})f_{i-2}(x)) = g(x)f_{i-1}(x)((2x^3 - \frac{9}{2}x^2 + \frac{5}{2}x - \frac{1}{4})f_{i-2}(x) - (\frac{3}{4}x^2 - \frac{9}{8}x + \frac{3}{8})f_{i-3}(x)) < 0 \]

holds, when \( x \geq \rho_{\frac{1}{2}}(H_2(l, l)) \) and \( l \geq 3 \).

When \( l = 2 \) and \( x > \frac{\alpha + \frac{5}{2}}{2} \), the following holds:

\[ 3(x - 1)(x - \frac{1}{2})f_{i-1}(x) - (x^3 - 3x^2 + \frac{7}{2}x - \frac{5}{4})f_{i-2}(x) = 2x^3 - 3x^2 + \frac{1}{4}x + \frac{1}{2} > 0. \]

Then \( DF(x) < 0 \) is also true when \( x \geq \rho_{\frac{1}{2}}(H_2(l, l)) \) and \( l = 2 \). Thus, \( \rho_{\frac{1}{2}}(H_3(l, l)) > \rho_{\frac{1}{2}}(H_4(l, l)) \) follows for this case. By Theorem 5.1, we have \( B^n_d(n, d) \) with the maximal signless Laplacian spectral radius among \( \mathcal{B}(n, d) \). This completes the proof. \( \square \)

Motivated by Theorems 5.1, 5.3 and results of numerical calculation, we conclude this paper with the following conjecture.

**Conjecture 5.1** When \( \frac{1}{2} < \alpha < 1 \), let \( G \) be the graph with the maximal \( \alpha \)-spectral radius among \( \mathcal{B}(n, d) \), then we have \( G \cong B^n_d(n, d) \).

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**Declarations**

**Conflict of interest** The authors declare that they have no conflict of interest.

**A The expressions of \( f_{ij} \) for \( i, j = 1, 2, 3, 4 \)**

| \( f_{11} \) | \( f_{12} \) | \( f_{13} \) | \( f_{14} \) | \( f_{22} \) | \( f_{23} \) | \( f_{24} \) | \( f_{31} \) | \( f_{32} \) | \( f_{33} \) | \( f_{34} \) | \( f_{41} \) | \( f_{42} \) | \( f_{43} \) | \( f_{44} \) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 9)x^2 + (z + 5)x - 1)(x - \frac{1}{2}) \) & \( (x^3 - \frac{1}{2}(z + 12)x^4 + (\frac{7}{2}z + 23)x^3 - (\frac{11}{2}z + 12)x^2 + (\frac{17}{2}z + \frac{5}{2})x - \frac{1}{8}) \) & \( (x^3 - \frac{1}{2}(z + 12)x^4 + (\frac{7}{2}z + 23)x^3 - (\frac{11}{2}z + 12)x^2 + (\frac{17}{2}z + \frac{5}{2})x - \frac{1}{8}) \) & \( (x^3 - \frac{1}{2}(z + 12)x^4 + (\frac{7}{2}z + 23)x^3 - (\frac{11}{2}z + 12)x^2 + (\frac{17}{2}z + \frac{5}{2})x - \frac{1}{8}) \) & \( (x^3 - \frac{1}{2}(z + 12)x^4 + (\frac{7}{2}z + 23)x^3 - (\frac{11}{2}z + 12)x^2 + (\frac{17}{2}z + \frac{5}{2})x - \frac{1}{8}) \) & \( (x^3 - \frac{1}{2}(z + 12)x^4 + (\frac{7}{2}z + 23)x^3 - (\frac{11}{2}z + 12)x^2 + (\frac{17}{2}z + \frac{5}{2})x - \frac{1}{8}) \) |}

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References

Belardo F, Li Marzi EM, Simić SK (2010) Combinatorial approach for computing the characteristic polynomial of a matrix. Linear Algebra and its Applications 433 (8) 1513–1523

Berman A, Plemmons RJ (1994) Nonnegative matrices in the mathematical sciences, Vol. 9 of Classics in Applied Mathematics

Brualdi RA, Hoffman AJ (1985) On the spectral radius of (0, 1)-matrices. Linear Algebra Appl 65:133–146

Geng X, Li S (2011) On the spectral radius of tricyclic graphs with a fixed diameter. Linear Multilinear Algebra 59(1):41–56

Guo SG (2007) On the spectral radius of bicyclic graphs with n vertices and diameter d. Linear Algebra Appl 422(1):119–132

Guo H, Zhou B (2020) On the α-spectral radius of graphs. Appl Anal Discrete Math 14:431–458

Guo SG, Xu GH, Chen YG (2005) The spectral radius of trees with n vertices and diameter d. Adv Math (China) 34(6):683–692

Hansen P, Stevanović D (2008) On bags and bugs. Discrete Appl Math 156(7):986–997

He S, Li S (2012) On the signless Laplacian index of unicyclic graphs with fixed diameter. Linear Algebra Appl 436(1):252–261

Li D, Chen Y, Meng J (2019) The $\alpha_A$-spectral radius of trees and unicyclic graphs with given degree sequence. Appl Math Comput 363:124622, 9

Liu H, Lu M, Tian F (2007) On the spectral radius of unicyclic graphs with fixed diameter. Linear Algebra Appl 420(2–3):449–457

Nikiforov V (2017) Merging the $A$- and $Q$-spectral theories. Appl Anal Discrete Math 11(1):81–107

Nikiforov V, Rojo O (2018) On the α-index of graphs with pendant paths. Linear Algebra Appl 550:87–104

Pai X (2014) On the laplacian coefficients and signless laplacian spectral radius of graphs (in Chinese). Phd thesis, Xidian University

Pai X, Liu S (2017) On the signless Laplacian spectral radius of bicyclic graphs with fixed diameter. Ars Combin 130:249–265

Saravanan M, Murugan SP, Arunkumar G (2021) A generalization of Fiedler’s lemma and the spectra of H-join of graphs. Linear Algebra Appl 625:20–43

Shan H, Wang F, He C (2021) Some α-spectral extremal results for some digraphs. Linear Multilinear Algebra. https://doi.org/10.1080/03081087.2021.1996523

Xue J, Lin H, Liu S, Shu J (2018) On the $A_\alpha$-spectral radius of a graph. Linear Algebra Appl 550:105–120

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