On the $\alpha$-index of graphs with pendent paths

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Abstract

Let $G$ be a graph with adjacency matrix $A(G)$ and let $D(G)$ be the diagonal matrix of the degrees of $G$. For every real $\alpha \in [0, 1]$, write $A_\alpha(G)$ for the matrix

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

This paper presents some extremal results about the spectral radius $\rho_\alpha(G)$ of $A_\alpha(G)$ that generalize previous results about $\rho_0(G)$ and $\rho_{1/2}(G)$.

In particular, write $B_{p,q,r}$ the graph obtained from a complete graph $K_p$ by deleting an edge and attaching paths $P_q$ and $P_r$ to its ends. It is shown that if $\alpha \in (0, 1)$ and $G$ is a graph of order $n$ and diameter at least $k$, then

$$\rho_\alpha(G) \leq \rho_\alpha(B_{n-k+2,\lfloor k/2 \rfloor,\lceil k/2 \rceil}),$$

with equality holding if and only if $G = B_{n-k+2,\lfloor k/2 \rfloor,\lceil k/2 \rceil}$. This result generalizes results of Hansen and Stevanović [5], and Liu and Lu [7].

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1 Introduction

Let $G$ be a graph with adjacency matrix $A(G)$, and let $D(G)$ be the diagonal matrix of its vertex degrees. In [9] the matrix $A_\alpha(G)$ has been defined for any real $\alpha \in [0, 1]$ as

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

Write $Q(G)$ for the signless Laplacian $A(G) + D(G)$ of $G$ and note that $A_0(G) = A(G)$ and $2A_{1/2}(G) = Q(G)$; thus, the family $A_\alpha(G)$ extends both $A(G)$ and $Q(G)$.

Write $\rho_\alpha(G)$ for the spectral radius of $A_\alpha(G)$ and call $\rho_\alpha(G)$ the $\alpha$-index of $G$. In the spirit of the general problem of Brualdi and Solheid [1], one can ask how large or how small can be

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the $\alpha$-index of graphs with some specific properties. For example: how large $\rho_\alpha(G)$ can be if $G$ is graph of order $n$ and diameter at least $k$? In fact, for $\alpha = 0$ this question has been answered by Hansen and Stevanović in [5].

Denote by $B_{p,q,r}$ the graph obtained from a complete graph $K_p$ by deleting an edge and attaching paths $P_q$ and $P_r$ to its ends\(^1\) (see Fig. 1 for an example). With this definition, Hansen and Stevanović’s result reads as:

**Theorem 1 (Hansen, Stevanović [5])** Let $G$ be a graph of order $n$ with $\text{diam}(G) \geq k$. If $k = 1$, then $\rho_0(G) = \rho_0(K_n)$. If $k \geq 2$, then

$$\rho_0(G) \leq \rho_0(B_{n-k+2,\lfloor k/2\rfloor,\lceil k/2\rceil}),$$

with equality holding if and only if $G = B_{n-k+2,\lfloor k/2\rfloor,\lceil k/2\rceil}$.

More recently, Liu and Lu [7] proved the same result for the spectral radius of $Q(G)$, that is, for $\alpha = 1/2$:

**Theorem 2 (Liu, Lu [7])** Let $G$ be a graph of order $n$ with $\text{diam}(G) \geq k$. If $k = 1$, then $\rho_{1/2}(G) = \rho_{1/2}(K_n)$. If $k \geq 2$, then

$$\rho_{1/2}(G) \leq \rho_{1/2}(B_{n-k+2,\lfloor k/2\rfloor,\lceil k/2\rceil}),$$

with equality if and only if $G = B_{n-k+2,\lfloor k/2\rfloor,\lceil k/2\rceil}$.

One of the main goals of this paper is to extend the above theorems for all $\alpha \in [0,1)$:

**Theorem 3** Let $\alpha \in [0,1)$ and $G$ be a graph of order $n$ with $\text{diam}(G) \geq k$. If $k = 1$, then $\rho_\alpha(G) = \rho_\alpha(K_n)$. If $k \geq 2$, then

$$\rho_\alpha(G) \leq \rho_\alpha(B_{n-k+2,\lfloor k/2\rfloor,\lceil k/2\rceil}),$$

with equality if and only if $G = B_{n-k+2,\lfloor k/2\rfloor,\lceil k/2\rceil}$.

A related extremal result is about connected graphs with given clique number. Denote by $PK_{p,q}$ the graph obtained by joining an end-vertex of the path $P_p$ to a vertex of the complete graph $K_q$. In [13], Stevanović and Hansen proved the following theorem:

\(^1\)Hansen and Stevanović call these graphs *bugs*. Recently, using some advanced techniques, the spectrum of $B_{p,q,r}$ has been calculated in [11].
Theorem 4 If $G$ is a connected graph of order $n$ with clique number $\omega \geq 2$, then

$$\rho_0(G) \geq \rho_0(PK_{n-\omega,\omega}),$$

with equality if and only if $G = PK_{n-\omega,\omega}$.

A different (and more involved) proof of Theorem 4 was given in [15] by Zhang, Huang, and Guo, who, in fact, determined the largest four values of $\rho_0(G)$.

We generalize Theorem 4 for any $\alpha \in [0,1)$:

Theorem 5 Let $\alpha \in [0,1)$. If $G$ is a connected graph of order $n$ with clique number $\omega \geq 2$, then

$$\rho_\alpha(G) \geq \rho_\alpha(PK_{n-\omega,\omega}),$$

with equality if and only if $G = PK_{n-\omega,\omega}$.

The rest of the paper is organized as follows. In Section 3 we study the distribution of the entries of Perron vectors of the $\alpha$-index along pendent paths in graphs. These results are used in Section 4 and in Section 5 to carry out the proofs of Theorem 3 and Theorem 5. In the last Section 6 we raise some open problems inspired by results of Li and Feng [6], whose solution could provide new tools in the study of the $\alpha$-index.

2 Notation and preliminaries

Given a graph $G$ and a vertex $u \in V(G)$, we write $\Gamma_G(u)$ for the set of neighbors of $u$ and set $d_G(u) := |\Gamma_G(u)|$. As usually, $P_n$ and $K_n$ denote the path and the complete graph of order $n$, and $K_n - e$ stands for $K_n$ with an edge removed.

For an $n \times n$ symmetric matrix $A = [a_{i,j}]$ and a vector $x := (x_1, \ldots, x_n)$, we write $\langle Ax, x \rangle$ for the quadratic form of $A$, i.e.,

$$\langle Ax, x \rangle = \sum_{i,j} a_{i,j} x_i x_j.$$

In our proofs, we frequently use the following lemma that generalizes results known for the adjacency matrix and the signless Laplacian of graphs.

Lemma 6 Let $\alpha \in [0,1)$ and let $G$ be a graph of order $n$. Suppose that $u, v \in V(G)$ and $S \subset V(G)$ satisfy $u, v \notin S$ and for every $w \in S$, $\{u, w\} \in E(G)$ and $\{v, w\} \notin E(G)$. Let $H$ be the graph obtained by deleting the edges $\{u, w\}$ and adding the edges $\{v, w\}$ for all $w \in S$. If $S$ is nonempty and there is a positive eigenvector $(x_1, \ldots, x_n)$ to $\rho_\alpha(G)$ such that $x_v \geq x_u$, then

$$\rho_\alpha(H) > \rho_\alpha(G).$$
Thus, write crucial equation $\rho$ of the entries of an eigenvector to multiple pendent paths, which may share roots; e.g., the graph that the other root of ($P_\alpha$) investigate their Graphs with pendent paths arise often in spectral extremal graph theory; thus it is worth to

Let $3$ Graphs with pendent paths

Calculating the quadratic forms $\langle A_\alpha (H) x, x \rangle$ and $\langle A_\alpha (G) x, x \rangle$, we see that

$$\rho_\alpha (H) - \rho_\alpha (G) \geq \langle A_\alpha (H) x, x \rangle - \langle A_\alpha (G) x, x \rangle$$

$$= \alpha \left( \langle D (H) x, x \rangle - \langle D (G) x, x \rangle \right) + (1 - \alpha) \left( \langle A (H) x, x \rangle - \langle A (G) x, x \rangle \right)$$

$$= -\alpha |\| \mathbf{x} \|^2 + \alpha x_v^2 + 2(1-\alpha) \sum_{w \in S} x_w (-x_u + x_v)$$

$$= (x_v - x_u) \sum_{w \in S} (ax_v + ax_u + 2(1-\alpha) x_w) \geq 0.$$  

However, the equality $\rho_\alpha (H) = \rho_\alpha (G)$ is not possible, for otherwise $x$ is a positive eigenvector to $\rho_\alpha (H)$, leading to the contradictory equations

$$\rho_\alpha (G) x_v = \alpha d_G (v) x_v^2 + (1 - \alpha) \sum_{i \in \Gamma_G (v)} x_i$$

$$\rho_\alpha (H) x_v = \alpha d_H (v) x_v^2 + (1 - \alpha) \sum_{i \in \Gamma_H (v)} x_i > \alpha d_G (v) x_v^2 + (1 - \alpha) \sum_{i \in \Gamma_G (v)} x_i.$$  

$\square$

3 Graphs with pendent paths

Let $G$ be a connected graph containing a path $P$ as a subgraph. We say that $P$ is a pendent path if one of its ends is a cut vertex of $G$; call this vertex the root of $P$. Note that a graph can have multiple pendent paths, which may share roots; e.g., the graph $B_{p,q,r}$ has two pendent paths. Graphs with pendent paths arise often in spectral extremal graph theory; thus it is worth to investigate their $\alpha$-index in some generality.

For any vertex $u$ of a connected graph $G$, let $G_{p,q} (u)$ be the graph obtained by attaching the paths $P_p$ and $P_q$ to $u$. Similarly, for any two vertices $u$ and $v$ of a connected graph $G$, let $G_{p,q} (u,v)$ be the graph obtained by attaching the paths $P_p$ to $u$ and $P_q$ to $v$.

Let $\alpha \in [0,1)$. If $G$ is a graph with a pendent path $P$ and $\rho_\alpha (G) = \rho \geq 2$, then the distribution of the entries of an eigenvector to $\rho$ along $P$ is well determined. To prove this fact, we use the crucial equation

$$x^2 - \frac{\rho - 2\alpha}{1 - \alpha} x + 1 = 0.$$  

Thus, write $\gamma$ for the root of (1)

$$\gamma := \frac{1}{2} \left( \frac{\rho - 2\alpha}{1 - \alpha} + \sqrt{\left( \frac{\rho - 2\alpha}{1 - \alpha} \right)^2 - 4} \right),$$  

and note that $\gamma$ is real since $\rho \geq 2$; moreover, $\gamma \geq 1$, with strict inequality if $\rho > 2$. Note also that the other root of (1) is equal to $\gamma^{-1}$.

Our first statement shows that the entries of an eigenvector to $\rho_\alpha (G)$ decay exponentially along pendent paths in $G$.  

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Proposition 7 Let \( \alpha \in [0, 1) \), and let \( G \) be a graph with \( \rho := \rho_\alpha (G) \geq 2 \). Let \( P = (u_1, \ldots, u_{r+1}) \) be a pendant path in \( G \) with root \( u_1 \). Let \( x_1, \ldots, x_{r+1} \) be the entries of a positive unit eigenvector to \( \rho_\alpha (G) \) corresponding to \( u_1, \ldots, u_{r+1} \). If \( \gamma \) is defined by (2), then, for every \( i = 1, \ldots, r \), we have

\[
x_i > \gamma x_{i+1}.
\] (3)

Proof The eigenequation of \( A_\alpha (G) \) for \( x_{r+1} \) is

\[
\rho x_{r+1} = \alpha x_{r+1} + (1 - \alpha) x_r,
\]
yielding in turn

\[
x_r = \frac{\rho - \alpha}{1 - \alpha} x_{r+1} > \frac{1}{2} \left( \frac{\rho - 2\alpha}{1 - \alpha} + \sqrt{\left( \frac{\rho - 2\alpha}{1 - \alpha} \right)^2 - 4} \right) x_{r+1} = \gamma x_{r+1}.
\]

Proceeding by induction, the eigenequation of \( A_\alpha (G) \) for \( x_i \), together with the induction assumption, gives

\[
\frac{\rho - 2\alpha}{1 - \alpha} x_i = x_{i+1} + x_{i-1} \leq \gamma^{-1} x_i + x_{i-1}
\]

\[
= \left( \frac{\rho - 2\alpha}{1 - \alpha} - \frac{1}{2} \left( \frac{\rho - 2\alpha}{1 - \alpha} - \sqrt{\left( \frac{\rho - 2\alpha}{1 - \alpha} \right)^2 - 4} \right) \right) x_i + x_{i-1}.
\]

Hence,

\[
x_{i-1} \geq \left( \frac{\rho - 2\alpha}{1 - \alpha} + \frac{1}{2} \left( \frac{\rho - 2\alpha}{1 - \alpha} - \sqrt{\left( \frac{\rho - 2\alpha}{1 - \alpha} \right)^2 - 4} \right) \right) x_i = \gamma x_i,
\]

completing the proof of Proposition 7. \( \square \)

Note the following simple, but useful consequence of Proposition 7:

Corollary 8 Given the hypotheses of Proposition 7, we have

\[
x_1 > \cdots > x_{r+1}.
\]

It turns out the inequality (3) is quite sharp. First, using linear recurrences, we obtain more precise information about \( x_1, \ldots, x_{r+1} \):

Lemma 9 With the hypotheses of Proposition 7, for every \( i = 1, \ldots, r+1 \), we have

\[
x_i = A \gamma^{r+2-i} + B \gamma^{i-r-2},
\] (4)

where \( (A, B) \) is the solution to the linear system

\[
X + Y = -\frac{\alpha}{1 - \alpha} x_{r+1},
\]

\[
X \gamma + Y \gamma^{-1} = x_{r+1}.
\] (5)
Proof Let \((A, B)\) be the (unique) solution to system (5). If \(r = 1\), then
\[
x_2 = A\gamma + B\gamma^{-1},
\]
and
\[
A\gamma^2 + B\gamma^{-2} = \frac{\rho - 2\alpha}{1 - \alpha} A\gamma - A + \frac{\rho - 2\alpha}{1 - \alpha} B\gamma^{-1} - B
\]
\[
= \frac{\rho - 2\alpha}{1 - \alpha} x_2 + \frac{\alpha}{1 - \alpha} x_2 = x_1,
\]
proving the assertion for \(r = 1\). If \(r > 1\), define the sequence \(z_0, \ldots, z_{r+1}\) by letting
\[
z_0 := -\frac{\alpha}{1 - \alpha} x_{r+1},
\]
and \(z_i := x_{r+2-i}\) for each \(i = 1, \ldots, r+1\). For \(i = 2, \ldots, r\) the eigenequations of \(A_\alpha (G)\) imply that
\[
\frac{\rho - 2\alpha}{1 - \alpha} x_i = x_{i+1} + x_{i-1}.
\]
Hence, \(z_1, \ldots, z_{r+1}\) satisfy the linear recurrence
\[
z_{i+1} = \frac{\rho - 2\alpha}{1 - \alpha} z_i - z_{i-1}.
\]
for \(i = 2, \ldots, r\). Note that the choice of \(z_0\) in equation (6) ensures that the above equality holds also for \(i = 1\). Hence, as known from the theory of linear recurrences, for \(i = 1, \ldots, r+1\), we have
\[
z_i = A\gamma^i + B\gamma^{-i},
\]
where \(A\) and \(B\) are determined by the conditions
\[
A\gamma^0 + B\gamma^0 = z_0 = -\frac{\alpha}{1 - \alpha} x_{r+1}
\]
\[
A\gamma + B\gamma^{-1} = z_1 = x_{r+1}.
\]
Clearly, \((A, B)\) is the solution to system (5). Returning back to \(x_i\), we obtain (4). \(\Box\)

Now, using Lemma 9, we give lower bounds which show that Proposition 7 is quite sharp:

Lemma 10 Given the hypotheses of Proposition 7, for every \(i = 1, \ldots, r\), we have
\[
\frac{x_i}{x_1} > \left(1 - \gamma^{-2}\right) \gamma^{-i+1},
\]
and
\[
\frac{x_{r+1}}{x_1} > \frac{(\gamma^2 - 1)(1 - \alpha)}{\gamma((1 - \alpha)(\gamma + \alpha)} \gamma^{-r}.
\]
Proof Let \((A, B)\) be the solution to system (5). Lemma 9 implies that

\[
\frac{x_i}{x_1} = \frac{A \gamma^{r+2-i} + B \gamma^{i-r-2}}{A \gamma^{r+1} + B \gamma^{-r-1}}
\]

for \(i = 1, \ldots, r + 1\). Solving system (5), we get

\[
A = \frac{\gamma - \alpha (\gamma - 1)}{(\gamma^2 - 1) (1 - \alpha)} x_{r+1},
\]

\[
B = -\frac{\gamma (\alpha (\gamma - 1) + 1)}{(\gamma^2 - 1) (1 - \alpha)} x_{r+1}.
\]

Hence \(A > 0, B < 0, \) and

\[
\frac{B}{A} = -\frac{\gamma (\alpha (\gamma - 1) + 1)}{\gamma - \alpha (\gamma - 1)} > -\frac{\gamma (1 (\gamma - 1) + 1)}{\gamma - 1 (\gamma - 1)} = -\gamma^2.
\]

Now, if \(1 \leq i \leq r\), we find that

\[
\frac{x_i}{x_1} = \frac{A \gamma^{r+2-i} + B \gamma^{i-r-2}}{A \gamma^{r+1} + B \gamma^{-r-1}} > \frac{A \gamma^{r+2-i} + B \gamma^{i-r-2}}{A \gamma^{r+1}} = \gamma^{i+1} + \frac{B}{A} \gamma^{-2r-3}
\]

\[
> \gamma^{-i+1} - \gamma^{-2r-1} = (1 - \gamma^{2i-2r-2}) \gamma^{-i+1} \geq (1 - \gamma^{-2}) \gamma^{-i+1},
\]

proving (7).

To prove Lemma 11, we need a proposition:

3.1 Perron vectors of graphs with pendent paths

In this subsection, we prove a structural inequality about the Perron vectors of graphs with pendent paths.

Lemma 11 Let \(\alpha \in [0, 1)\) and \(H\) be a connected graph with \(\rho_\alpha (H) \geq 5/2\). Let \(u\) and \(v\) be vertices of \(H\). Attach a path \(P := \{u_1 = u, \ldots, u_p\}\) to \(u\) and a path \(Q := \{v_1 = v, \ldots, v_q\}\) to \(v\), and write \(G\) for the resulting graph. Let \(x\) be a positive unit eigenvector to \(\rho := \rho_\alpha (G)\); write \(x_1, \ldots, x_p\) for the \(x\)-entries of \(u_1, \ldots, u_p\) and \(y_1, \ldots, y_q\) for the \(x\)-entries of \(v_1, \ldots, v_q\). If \(p \geq q + 2\), then

\[
\frac{y_q}{x_{p-1}} \geq \frac{3y_1}{2x_1}
\]

To prove Lemma 11, we need a proposition:
Proposition 12  Let $\alpha \in [0, 1)$ and $\rho \geq 5/2$. If $\gamma$ is defined as in (2), then
\[
\gamma \geq \frac{2\rho - 1 - 3\alpha}{2 - 2\alpha}.
\]

Proof In view of (2), it is enough to prove that
\[
\sqrt{(\rho - 2\alpha)^2 - 4 (1 - \alpha)^2} - (\rho - 1 - \alpha) \geq 0.
\]
Indeed, we see that
\[
\sqrt{(\rho - 2\alpha)^2 - 4 (1 - \alpha)^2} - (\rho - 1 - \alpha) = \frac{2\rho (1 - \alpha) - a^2 + 6\alpha - 5}{\sqrt{(\rho - 2\alpha)^2 - 4 (1 - \alpha)^2} + (\rho - 1 - \alpha)} \\
\geq \frac{5 (1 - \alpha) - a + 6\alpha - 5}{\sqrt{(\rho - 2\alpha)^2 - 4 (1 - \alpha)^2} + (\rho - 1 - \alpha)} = 0,
\]
completing the proof of Proposition 12.

Proof of Lemma 11 To begin with, note that Proposition 7 implies that
\[
x_{p-1} < \gamma^{-p+2} x_1,
\]
and inequality (8) implies that
\[
y_q > \frac{(\gamma^2 - 1) (1 - \alpha)}{\gamma ((1 - \alpha) \gamma + a)} \gamma^{-q+1} y_1.
\]
Dividing (11) by (10), we see that
\[
\frac{y_q}{x_{p-1}} > \frac{(\gamma^2 - 1) (1 - \alpha)}{\gamma ((1 - \alpha) \gamma + a)} \gamma^{-q+1} \frac{y_1}{x_1} \geq \frac{(\gamma^2 - 1) (1 - \alpha) y_1}{(1 - \alpha) \gamma + a} \frac{1}{x_1}. \tag{12}
\]
Thus, to finish the proof it is enough to show that
\[
\frac{(\gamma^2 - 1) (1 - \alpha)}{(1 - \alpha) \gamma + a} \geq \frac{3}{2}.
\]
Assume for a contradiction that the above inequality fails, and recall that $\gamma$ is a root of the equation (1), implying in particular that
\[
(\gamma^2 - 1) (1 - \alpha) = (\rho - 2\alpha) \gamma - 2 (1 - \alpha).
\]
Hence, we get
\[
\frac{3}{2} > \frac{(\rho - 2\alpha) \gamma - 2 (1 - \alpha)}{(1 - \alpha) \gamma + a} \geq \frac{(5/2 - 2\alpha) \gamma - 2 + 2\alpha}{(1 - \alpha) \gamma + a}.
\]
yielding in turn
\[(3 - 3\alpha)\gamma + 3\alpha > (5 - 4\alpha)\gamma - 4 + 4\alpha,
\]
and further
\[\gamma < \frac{4 - \alpha}{2 - \alpha}.
\]
To get the desired contradiction, we invoke Proposition 12, which gives
\[\frac{4 - \alpha}{2 - \alpha} > \frac{4 - 3\alpha}{2 - 2\alpha}.
\]
and, after some algebra, this inequality reduces to
\[3\alpha^2 < 2\alpha^2,
\]
an apparent contradiction that completes the proof of Lemma 11.

\[\square
\]

4 Proof of Theorem 3

Our proof of Theorem 3 is based on two independent results: first, proving that if \(G\) has a maximal \(\alpha\)-index among all graphs of order \(n\) and diameter at least \(k\), then \(G\) is isomorphic to \(B_{n-k+2,p,k-p}\) for some \(p\), satisfying \(1 \leq p \leq k\); and second, proving that among all graphs \(B_{n-k+2,p,k-p}\) (1 \(\leq p \leq \lfloor k/2 \rfloor\), the maximal \(\alpha\)-index is attained when \(p = \lfloor k/2 \rfloor\). We start with establishing the second result, which is based on the following crucial lemma:

Lemma 13 Let \(\alpha \in [0, 1)\) and \(k \geq 4\). If \(p \geq q + 2\) and \(q \geq 1\), then
\[\rho_\alpha (B_{k,p,q}) < \rho_\alpha (B_{k,p-1,q+1}).
\]

To prove the lemma, we need a lower bound on the \(\alpha\)-index of the graph \(K_k - e\):

Proposition 14 If \(k \geq 4\), then
\[\rho_\alpha (K_k - e) \geq k - 3 + 2\alpha.
\]

Proof First, since the entries of an eigenvector to \(K_k - e\) take only two values, it is not hard to show that \(\rho_\alpha (K_k - e)\) is the larger root of the equation
\[X^2 - (k - 3 + k\alpha)X + (k - 2)((k + 1)\alpha - 2) = 0.
\]

Hence, one gets
\[\rho_\alpha (K_k - e) = \frac{1}{2} \left( k - 3 + k\alpha + \sqrt{(k - 3 + k\alpha)^2 - 4(k - 2)((k + 1)\alpha - 2)} \right)
\[= \frac{1}{2} \left( k - 3 + k\alpha + \sqrt{k^2(1 - \alpha)^2 + 2(k - 4)(1 - \alpha) + 1} \right).
\]
Assume for a contradiction that (13) fails, implying that

\[ k - 3 + k\alpha + \sqrt{k^2 (1 - \alpha)^2 + 2 (k - 4) (1 - \alpha) + 1} < 2k - 6 + 4\alpha, \]

and therefore,

\[ \sqrt{k^2 (1 - \alpha)^2 + 2 (k - 4) (1 - \alpha) + 1} < (k - 4) (1 - \alpha) + 1. \]

Squaring both sides, we get

\[ k^2 (1 - \alpha)^2 + 2 (k - 4) (1 - \alpha) + 1 < (k - 4) (1 - \alpha)^2 + 2 (k - 4) (1 - \alpha) + 1, \]

which is an obvious contradiction. Proposition 14 is proved. \(\square\)

**Proof of Lemma 13** We adopt the setup of Lemma 11: Let \(u\) and \(v\) be the two nonadjacent vertices of \(B_{k,p,q}\); let \(P := \{u_1 = u, \ldots, u_p\}\) be the path attached to \(u\) and a \(Q := \{v_1 = v, \ldots, v_q\}\) be the path attached to \(v\). Let \(x\) be a positive unit eigenvector to \(\rho := \rho_\alpha (B_{k,p,q})\); write \(x_1, \ldots, x_p\) for the \(x\)-entries of \(u_1, \ldots, u_p\) and \(y_1, \ldots, y_q\) for the \(x\)-entries of \(v_1, \ldots, v_q\). For convenience, write \(H\) for the subgraph of \(B_{k,p,q}\) that is isomorphic to \(K_k - e\).

Note that by deleting the edge \(\{u_p, u_{p-1}\}\) and adding the edge \(\{u_p, v_q\}\), the graph \(B_{k,p,q}\) is transformed into \(B_{k,p-1,q+1}\). Now, calculating the quadratic forms \(\langle A_\alpha (B_{k,p-1,q+1}) x, x \rangle\) and \(\langle A_\alpha (B_{k,p,q}) x, x \rangle\), we see that

\[ \rho_\alpha (B_{k,p-1,q+1}) - \rho_\alpha (B_{k,p,q}) \geq \langle A_\alpha (B_{k,p-1,q+1}) x, x \rangle - \langle A_\alpha (B_{k,p,q}) x, x \rangle \]
\[ = -ax_p^2 + ay_q^2 + 2 (1 - \alpha) x_p (-x_{p-1} + y_q) \]
\[ = (ax_{p-1} + ay_q + 2 (1 - \alpha) x_p) (y_q - x_{p-1}). \]

To prove the theorem, it is enough to show that \(y_q / x_{p-1} \geq 1\), thus, this inequality is our goal to the end of the proof.

First, Lemma 11 gives

\[ \frac{y_q}{x_{p-1}} > \frac{3y_1}{2x_1^2} \quad (14) \]

thereby our task is reduced to showing that \(y_1 / x_1 \geq 2 / 3\). Further, the eigenequations of \(A_\alpha (G)\) for \(u\) and \(v\) give

\[ \rho x_1 = \alpha (k - 1) x_1 + (1 - \alpha) \sum_{i \in \Gamma_H(u) \setminus \{v\}} x_i + (1 - \alpha) x_2, \]
\[ \rho y_1 = \alpha (k - 1) y_1 + (1 - \alpha) \sum_{i \in \Gamma_H(v) \setminus \{u\}} x_i. \]

Since \(\sum_{i \in \Gamma_H(u) \setminus \{v\}} x_i = \sum_{i \in \Gamma_H(v) \setminus \{u\}} x_i\), writing \(S\) for \(\sum_{i \in \Gamma_H(u) \setminus \{v\}} x_i\), we see that

\[ (\rho - (k - 1) \alpha) x_1 = (1 - \alpha) S + (1 - \alpha) x_2 \]
\[ < (1 - \alpha) S + \gamma^{-1} (1 - \alpha) x_1, \]

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yielding in turn
\[
\left( \rho - (k - 1) \alpha - \gamma^{-1} (1 - \alpha) \right) x_1 < (1 - \alpha) S.
\]
Likewise, we get
\[
(\rho - (k - 1) \alpha) y_1 \geq (1 - \alpha) S.
\]
Dividing the last inequality by the previous one, we find that
\[
\frac{y_1}{x_1} > \frac{\rho - (k - 1) \alpha - \gamma^{-1} (1 - \alpha)}{\rho - (k - 1) \alpha} = 1 - \frac{1 - \alpha}{(\rho - (k - 1) \alpha) \gamma}.
\]
Hence, to show that \( y_1 / x_1 \geq 2/3 \), it is enough to prove the inequality
\[
1 - \alpha (\rho - (k - 1) \alpha) \gamma \leq \frac{1}{3}.
\]
Proposition 14 gives
\[
\frac{1 - \alpha}{(\rho - (k - 1) \alpha) \gamma} < \frac{1 - \alpha}{(k - 3 + 2\alpha - (k - 1) \alpha) \gamma} = \frac{1}{(k - 3) \gamma}.
\]
In particular, since \( \gamma \geq 2 \), the theorem is proved for \( k \geq 5 \). Moreover, if \( k = 4 \), Proposition 12 implies that \( \gamma \geq 3 \), as long as \( \alpha \geq 2/3 \); hence, the theorem is proved also for \( k = 4 \) and \( \alpha \geq 2/3 \).

In the remaining case \( (k = 4 \text{ and } \alpha < 2/3) \), using the bounds \( \rho \geq 5/2 \) and \( \gamma \geq 2 \), we see that
\[
\frac{1 - \alpha}{(\rho - (k - 1) \alpha) \gamma} \leq \frac{1 - \alpha}{(5/2 - 3\alpha) 2} = \frac{1 - \alpha}{5 - 6\alpha} < \frac{1}{3}.
\]
Theorem 13 is proved.
\[\square\]

**Corollary 15** If \( p \) and \( q + r \) are fixed, then
\[
\rho_\alpha(B_{p,q,r}) \leq \rho_\alpha(B_{p,\lfloor(q+r)/2\rfloor,\lceil(q+r)/2\rceil})
\]

**Proof of Theorem 3** The statement is clear if \( k = 1 \), for \( K_n \) is the only graph of order \( n \) and diameter 1. Suppose that \( k \geq 2 \), and let \( G \) be a graph with maximal \( \alpha \)-index among all graphs of order \( n \) and \( \text{diam}(G) \geq k \). This choice implies that \( G \) is edge-maximal, that is, no edge can be added to \( G \) without diminishing its diameter; in particular, \( \text{diam}(G) = k \). In the light of Corollary 15, we only need to show that \( G = B_{n-k+2,p,k-p} \) for some \( p \), satisfying \( 1 \leq p \leq k - 1 \).

Set for short \( \rho := \rho_\alpha(G) \). Let \( u,v \) be vertices of \( G \) at distance exactly \( k \), and for every \( i = 0, \ldots, k \), let \( V_i \) be the set of vertices at distance \( i \) from \( u \). Since \( G \) is edge-maximal, for every \( i = 0, \ldots, k - 1 \), the set \( V_i \cup V_{i+1} \) induces a complete graph. It is also clear that \( |V_0| = 1 \); moreover, it is not hard to see that \( |V_k| = 1 \). Indeed, assume for a contradiction that \( |V_k| \geq 2 \), and add all edges between \( V_{k-2} \) and \( V \setminus \{v\} \). These additional edges do not diminish the
distance between \( u \) and \( v \); hence \( G \) is not edge-maximal, contradicting its choice; therefore 
\[ |V_k| = 1. \]

Further, well-known bounds for \( \rho_a(G) \) show that
\[ \Delta(G) \geq \rho_a(G) > \rho_a(B_{n-k+2, k/2, [k/2]}) > \rho_a(K_{n-k+2 - \epsilon}) > \delta(K_{n-k+2 - \epsilon}) = n-k, \]
and so, \( \Delta(G) \geq n-k+1 \). Suppose that \( w \) is vertex of maximum degree in \( G \), and let say \( w \in V_i \). Clearly, \( 0 < i < k \), and in view of
\[ d(w) = |V_{i-1}| + |V_i| + |V_{i+1}| - 1, \]
we find that
\[ n-k+2 \leq |V_{i-1}| + |V_i| + |V_{i+1}| = n - \sum_{j<i-1} |V_j| - \sum_{j>i+1} |V_j| = n - (k+1-3) = n-k+2. \]

Hence, if \( j < i-1 \) or \( j > i+1 \), then \( |V_i| = 1 \); furthermore, \( |V_{i-1}| + |V_i| + |V_{i+1}| = n-k+2 \).

If \( |V_{i-1}| = |V_{i+1}| = 1 \), then obviously \( G = B_{n-k+2,0,k-0} \), so Theorem 3 is proved in this case. We shall show that all other cases lead to contradictions, by constructing a graph \( H \) of order \( n \) and \( \text{diam}(G) = k \) with \( \rho_a(H) > \rho \). Suppose that \( x := (x_1, \ldots, x_n) \) is a positive unit vector to \( \rho_a(G) \).

First, consider the case \( |V_{i-1}| = 1 \) and \( |V_{i+1}| \geq 2 \). If \( |V_i| = 1 \), the proof is completed, so we suppose that \( |V_i| \geq 2 \). Let \( V_{i-1} = \{a\}, V_{i+2} = \{b\} \), and suppose by symmetry that \( x_b \geq x_a \). Choose a vertex \( w \in V_i \), delete the edge \( \{w,a\} \), add the edge \( \{w,b\} \), and write \( H \) for the resulting graph. In other words, \( H \) is obtained by moving the vertex \( w \) from \( V_i \) into \( V_{i+1} \). By symmetry, \( x_{w'} = x_w \) for any \( w' \in V_i \); thus the choice of \( G \) implies that
\[ 0 \geq \rho_a(H) - \rho \geq \langle A_a(H)x,x \rangle - \langle A_a(G)x,x \rangle \]
\[ \geq (1-\alpha) (\langle A(H)x,x \rangle - \langle A(G)x,x \rangle) + \alpha (\langle D(H)x,x \rangle - \langle D(G)x,x \rangle). \]

On the other hand, it is not hard to see that
\[ \langle A(H)x,x \rangle - \langle A(G)x,x \rangle = 2x_w(x_b-x_a), \]
\[ \langle D(H)x,x \rangle - \langle D(G)x,x \rangle = x_b^2 - x_a^2. \]

Hence,
\[ 0 \geq (x_b - x_a) (2(1-\alpha) x_w + \alpha (x_b + x_a)) \geq 0, \]
implying that \( \rho_a(H) = \rho_a(G) \) and that \( x \) is an eigenvector to \( \rho_a(H) \). However, the neighborhood of \( a \) in \( H \) is a proper subset of the neighborhood of \( a \) in \( G \), so the eigenvalues for \( \rho_a(H) \) and \( \rho_a(G) \) for the vertex \( a \) are contradictory.

The same argument disposes also of the case \( |V_{i-1}| \geq 2 \) and \( |V_{i+1}| = 1 \); thus, to complete the proof, it remains to consider the case \( |V_{i-1}| \geq 2 \) and \( |V_{i+1}| \geq 2 \).

Let \( V_{i-2} = \{a\}, c \in V_{i-1}, d \in V_{i+1}, \) and \( V_{i+2} = \{b\} \). Our first step is to show that
\[ x_c > x_a. \]  
(16)
Note that if \( i \geq 3 \), and \( V_{i-3} = \{ z \} \), then Proposition 7 gives \( x_z < x_a \). Hence, setting \( l := |V_{i-1}| \), the eigenfunction for the vertex \( a \) implies that

\[
\rho x_a < \alpha (l + 1) x_a + (1 - \alpha) x_a + (1 - \alpha) l x_c,
\]

yielding in turn

\[
x_c > \frac{\rho - 1 - \alpha l}{1 - \alpha} x_a = \left( \rho - 1 + \frac{\rho - 1 - l}{1 - \alpha} \right) x_a.
\]

Since

\[
\rho - 1 \geq n - k - 1 = |V_{i-1}| + |V_i| + |V_{i+1}| - 3 \geq |V_{i-1}| = l,
\]

inequality (16) is proved. By symmetry, we also see that \( x_d > x_b \). Suppose, again by symmetry, that \( x_b \geq x_a \), which yields \( x_a \leq x_b < x_d \). Choose a vertex \( w \in V_{i-1} \), delete the edge \( \{ w, a \} \), add the edges \( \{ w, s \} \) for all \( s \in V_{i+1} \), and write \( H \) for the resulting graph. In other words, \( H \) is obtained by moving the vertex \( w \) from \( V_{i-1} \) into \( V_i \). The choice of \( G \) implies that

\[
0 \geq \rho_a (H) - \rho \geq \langle A_a (H) \mathbf{x}, \mathbf{x} \rangle - \langle A_a (G) \mathbf{x}, \mathbf{x} \rangle \\
\geq (1 - \alpha) \left( \langle A (H) \mathbf{x}, \mathbf{x} \rangle - \langle A (G) \mathbf{x}, \mathbf{x} \rangle \right) + \alpha \left( \langle D (H) \mathbf{x}, \mathbf{x} \rangle - \langle D (G) \mathbf{x}, \mathbf{x} \rangle \right).
\]

On the other hand, it is not hard to see that

\[
\langle A (H) \mathbf{x}, \mathbf{x} \rangle - \langle A (G) \mathbf{x}, \mathbf{x} \rangle = 2 x_w |V_{i+1}| x_d - 2 x_w x_a > (x_d - x_a) x_w \\
\langle D (H) \mathbf{x}, \mathbf{x} \rangle - \langle D (G) \mathbf{x}, \mathbf{x} \rangle = |V_{i+1}| x_d^2 - x_a^2 > x_d^2 - x_a^2.
\]

Hence,

\[
0 \geq 2 (1 - \alpha) (x_d - x_a) x_w + \alpha \left( x_d^2 - x_a^2 \right) = (x_d - x_a) (2 (1 - \alpha) x_w + \alpha (x_d + x_a)) > 0.
\]

This contradiction completes the proof of Theorem 3. \( \square \)

## 5 Proof of Theorem 5

Our proof of Theorem can be broken into several distinct steps, which are formulated below as separate propositions in a slightly more general form.

**Proposition 16** Let \( \alpha \in [0, 1) \), let \( G \) be a connected graph with \( \rho_a (G) \geq 2 \), and let \( u \in V (G) \). If \( q \geq 1 \) and \( p \geq q \), then

\[
\rho_a (G_{p+q} (u)) \geq \rho_a (G_{p+q-1,1} (u))
\]

with equality if and only if \( q = 1 \).
Proof If $q = 1$, there is nothing to prove, so suppose that $q \geq 2$. Let $P_{p+q-1} = (v_1 = u, \ldots, v_{p+q-1})$ be the path attached to $u$, let $x$ be a positive eigenvector to $\rho = \rho_\alpha (G_{p+q-1,1}(u))$, and let $x_1, \ldots, x_{p+q-1}$ be the $x$-entries of $v_1, \ldots, v_{p+q-1}$. Delete the edge $\{v_{p+1}, v_p\}$ and add the edge $\{v_{p+1}, v_1\}$, thus obtaining the graph $G_{p,q}(u)$. Since Corollary 8 implies that $x_1 > x_p$, Lemma 6 implies that $\rho_\alpha (G_{p,q}(u)) > \rho_\alpha (G_{p+q-1,1}(u))$. □

Proposition 17 Let $\alpha \in [0,1)$, let $G$ be a connected graph with $\rho_\alpha (G) \geq 2$, and let $u \in V(G)$. It $G_u(T)$ is the graph obtained by identifying $u$ with a vertex of a tree $T$ of order $n$, then

$$\rho_\alpha (G_T(u)) \geq \rho_\alpha (G_{n,1}(u)).$$

with equality if and only if $G_T(u) = G_{n,1}(u)$.

We omit the proof of Proposition 17, which can be carried out along well-known lines, by applying Proposition 16 to recursively flatten $T$ until it becomes a path (see, e.g., [13] for more details.)

Proof of Theorem 5 Let $G$ be a graph with minimal $\alpha$-index among all connected graphs of order $n$ and clique number $\omega$. If $\omega = 2$, then $G$ must be a path, as the path it the graph with smallest $\alpha$-index among connected graphs of given order (see [10]). Thus, we suppose that $\omega \geq 3$ and let $H$ be a complete subgraph of $G$ of order $\omega$.

Further, $G$ should be edge-minimal, that is, the removal of any edge of $G$ either makes $G$ disconnected or its clique number diminishes. In particular, if $G'$ is the graph obtained by removing the edges of $H$, then the components of $G'$ are trees, and each component has exactly one vertex in common with $H$. It follows that $G$ is isomorphic to a complete graph of order $\omega$ with trees attached to some of its vertices. Moreover, Proposition 17 implies that each of those trees must be a pendant path. To complete the proof, we show that there is only one such path.

Let $S = V(H)$, let $u, v \in S$, and suppose that a path $P_p = (v_1 = v, \ldots, v_p)$ is attached to $v$ and $P_q = (u_1 = u, \ldots, u_q)$ is attached to $v$. Let $F$ be the graph obtained by deleting the edge $\{u_2, u_1\}$ and adding the edge $\{u_2, v_p\}$, that is, $F$ is obtained by removing $P_q$ and extending $P_p$ to $P_{p+q-1}$. To complete the proof, we need to show that $\rho_\alpha (G) > \rho_\alpha (F)$.

Let $\rho = \rho_\alpha (F)$ and let $x$ be a positive eigenvector of $F$ to $\rho$. Write $x_1, \ldots, x_{p+q-1}$ for the entries of $x$ corresponding to $v_1, \ldots, v_p, u_2, \ldots, u_q$, and let $\gamma$ be defined by (2). Now, if $x_u \geq \gamma^{-1}x_p$, then Proposition 7 implies that $x_u \geq \gamma^{-1}x_1 > x_2 \geq x_p$, and so, Lemma 6 implies that $\rho_\alpha (G) > \rho_\alpha (F)$. Thus, we focus on showing that $x_u \geq \gamma^{-1}x_1$.

On the one hand, the eigenequation for $u$ is

$$\rho x_u = (\omega - 1)ax_u + (1 - \alpha)\sum_{i \in S \setminus \{u\}} x_i = (\omega \alpha - 1)x_u + (1 - \alpha)\sum_{i \in S} x_i,$$

and therefore,

$$(\rho + 1 - \omega \alpha)x_u = (1 - \alpha)\sum_{i \in S} x_i.$$
Likewise, for any $w \in S \setminus \{u, v\}$, the eigenequation for $w$ gives
\[(\rho + 1 - \omega \alpha) x_w \geq (1 - \alpha) \sum_{i \in S} x_i.\]

In particular, we see that $x_w \geq x_u$ for any $w \in S \setminus \{u, v\}$, since $\rho + 1 - \omega \alpha > \omega (1 - \alpha) > 0$.

Returning to the eigenequation for $u$, we find that
\[
\rho x_u = (\omega - 1) \alpha x_u + (1 - \alpha) \sum_{i \in S \setminus \{u\}} x_i \geq (\omega - 1) \alpha x_u + (1 - \alpha) \left( x_1 + (\omega - 2) x_u \right),
\]
yielding in turn
\[(\rho - \omega + 2 - \alpha) x_u \geq (1 - \alpha) x_1.\]
Assuming for a contradiction that $x_u < \gamma^{-1} x_1$, after some algebra, we get
\[
\frac{\rho - \omega + 2 - \alpha}{1 - \alpha} > \gamma = \frac{\rho - 2 \alpha}{2 (1 - \alpha)} + \frac{1}{2 (1 - \alpha)} \sqrt{(\rho - 2 \alpha)^2 - 4 (1 - \alpha)^2}
\]
and therefore,
\[
\rho - 2 \omega + 4 > \sqrt{(\rho - 2 \alpha)^2 - 4 (1 - \alpha)^2}. \quad (17)
\]
It is known that $\rho < \Delta (F) = \omega$, since $F$ is not a $\omega$-regular graph. Hence,
\[
\omega - 2 \omega + 4 > 0,
\]
a contradiction if $\omega \geq 4$. If $\omega = 3$, then (17) becomes
\[
\rho - 2 > \sqrt{(\rho - 2 \alpha)^2 - 4 (1 - \alpha)^2}.
\]

Squaring both sides of this inequality, we get
\[
\rho^2 - 4 \rho + 4 > \rho^2 - 4 \alpha \rho - 4 + 8 \alpha
\]
and so,
\[
8 (1 - \alpha) > 4 \rho (1 - \alpha).
\]
Therefore $\rho < 2$, an obvious contradiction, completing the proof of Theorem 5. $\square$

### 6 Some open problems

In this section we raise a few problems inspired by the results of Li and Feng [6], which have been presented in some detail in Section 6.2 of [3], and in Section 8.1 of [4].

**Conjecture 18** Let $\alpha \in [0, 1)$. If $G$ is a connected graph and $p \geq q + 2 \geq 3$, then
\[
\rho_\alpha \left( G_{p,q}(u) \right) < \rho_\alpha \left( G_{p,\frac{p+1}{2}}(u) \right).
\]
As shown by Li and Feng in [6], the above statement is true for \( \alpha = 0 \) (see also Theorem 8.1.20 in [4]). Moreover, Cvetković and Simić [2] showed that the statement is true for \( \alpha = 1/2 \) as well. However, none of these techniques applies directly for other \( \alpha \in [0, 1) \). Using edge rotation, we can show that the statement is true for any \( \alpha \in [0, 1) \) as long as \( \rho_\alpha (G_{p,q}(u)) \geq 9/4 \), but this constraint seems unnecessary strong.

Similar questions can be studied for pendent paths attached to different vertices of a connected graph \( G \).

**Conjecture 19** Let \( \alpha \in [0, 1) \). Let \( G \) be a connected graph, and let \( u \) and \( v \) be adjacent vertices of \( G \) of degree at least 2. If \( q \geq 1 \) and \( p \geq q + 2 \), then

\[
\rho_\alpha (G_{p,q}(u,v)) < \rho_\alpha (G_{p-1,q+1}(u,v)).
\]  

(18)

It has been shown by Li and Feng [6] that the above statement is true for \( \alpha = 0 \) (see also Theorem 8.1.22 in [4]). Again, their methods seem not immediately applicable to Conjecture 19.

Note that the requirement that the degree of \( u \) and \( v \) be at least 2 is important, for otherwise strict inequality may not always hold in (18); e.g., if \( G \) is an edge and \( u, v \) are its ends, then \( G_{3,1}(u,v) = G_{2,2}(u,v) = P_4 \). The requirement \( d_G(u) \geq 2 \) and \( d_G(v) \geq 2 \) has been omitted in Lemma 2.1 of [13] and in Lemma 4.3 of [12], which makes these statements technically incorrect, although their applications in [13] and in [12] are fine.

Further, Lemma 13 suggests that the requirement for \( u \) and \( v \) to be adjacent may not always be necessary, so we raise the following question:

**Question 20** For which connected graphs \( G \) the following statement is true:

Let \( \alpha \in [0, 1) \) and let \( u \) and \( v \) be non-adjacent vertices of \( G \) of degree at least 2. If \( q \geq 1 \) and \( p \geq q + 2 \), then

\[
\rho_\alpha (G_{p,q}(u,v)) < \rho_\alpha (G_{p-1,q+1}(u,v)).
\]

Little seems known about Question 20, even for \( \alpha = 0 \). It is not hard to find examples of trees showing that the opposite inequality may hold sometimes.

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