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Extremal graphs for α-index

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Abstract. Let $N(G)$ be the number of vertices of the graph G. Let $P_l(B_i)$ be the tree obtained of the path P_l and the trees $B_1, B_2, ..., B_l$ by identifying the root vertex of B_i with the i-th vertex of P_l. Let $\mathcal{V}_n^m = \{P_l(B_i) : N(P_l(B_i)) = n; N(B_i) \geq 2; l \geq m\}$. In this paper, we determine the tree that has the largest α-index among all the trees in $\mathcal{V}_n^m$.
Keywords: Caterpillar, diameter, distance, index, tree.
MSC2010: 05C50, 05C76, 15A18, 05C12, 05C75.

Grafos extremales para α-índice

Resumen. Sea $N(G)$ el número de vértices del grafo G. Sean $P_l(B_i)$ los árboles obtenidos del camino P_l y los árboles $B_1, B_2, ..., B_l$, identificando el vértice raíz de B_i con el i-th vértice de P_l. Sea $\mathcal{V}_n^m = \{P_l(B_i) : N(P_l(B_i)) = n; N(B_i) \geq 2; l \geq m\}$. En este artículo determinamos el árbol que tiene el α-índice más grande entre todos los árboles en $\mathcal{V}_n^m$.
Palabras clave: Oruga, diámetro, distancia, índice, árbol.

1. Introduction

Let G be a simple undirected graph with vertex set $V(G)$ and edge set $E(G)$. The degree of a vertex $v \in V(G)$ is $d(v)$ or simply d_v. We denote by $N(G)$ the number of vertices of the graph G. A graph G is bipartite if there exists a partitioning of $V(G)$ into disjoint, nonempty sets V_1 and V_2 such that the end vertices of each edge in G are in distinct sets V_1, V_2. In this case V_1, V_2 are referred as a bipartition of G. A graph G is a complete bipartite graph if G is bipartite with bipartition V_1 and V_2, where each vertex in V_1 is connected to all the vertices in V_2. If G is a complete bipartite graph and $N(V_1) = p$ and $N(V_2) = q$, the graph G is written as $K_{p,q}$. The Laplacian matrix of G is the $n \times n$ matrix $L(G) = D(G) - A(G)$, where $A(G)$ and $D(G)$ are the matrices adjacency and diagonal of vertex degrees of G [7], [8], and [11], respectively. It is well known that $L(G)$ is a positive semi-definite matrix and that $(0, e)$ is an eigenpair of $L(G)$ where e is the

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all ones vector. The matrix $Q(G) = A(G) + D(G)$ is called the signless Laplacian matrix of G (see [4], [5], and [6]). The eigenvalues of $A(G)$, $L(G)$ and $Q(G)$ are called the eigenvalues, Laplacian eigenvalues and signless Laplacian eigenvalues of G, respectively. The matrices $Q(G)$ and $L(G)$ are positive semidefinite, (see [20]). The spectra of $L(G)$ and $Q(G)$ coincide if and only if G is a bipartite graph, (see [2], [4], [7], and [8]). The largest eigenvalue μ_1 of $L(G)$ is the Laplacian index of G, the largest eigenvalue $q_1(G)$ of $Q(G)$ is known as the signless Laplacian index of G and the largest eigenvalue $\lambda_1(G)$ of $A(G)$ is the adjacency index or index of G [3].

In [12], it was proposed to study the family of matrices $A_\alpha(G)$ defined for any real number $\alpha \in [0,1]$ as

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

Since $A_0(G) = A(G)$ and $2A_{1/2}(G) = Q(G)$, the matrices $A_\alpha(G)$ can underpin a unified theory of $A(G)$ and $Q(G)$. In this paper, the eigenvalues of the matrices $A_\alpha(G)$ are called the α-eigenvalues of G. We write $\rho_\alpha(G)$ for the spectral radii of the matrices $A_\alpha(G)$ and are called the α-indices of G. The α-eigenvalue set of G is called α-spectrum of G. The spectrum of a matrix M will be denoted by $Sp(M)$.

Let $[l]$ denote the set $\{1,2,...l\}$. Given a rooted graph, define the level of a vertex to be equal to its distance to the root vertex increased by one. A generalized Bethe tree is a rooted tree in which vertices at the same level have the same degree. Throughout this paper $\{B_i : i \in [l]\}$ is a set of generalized Bethe trees. Let P_l be a path of l vertices. In this paper, we study the tree $P_l\{B_i : i \in [l]\}$ obtained from P_l and $B_1, B_2, ..., B_l$, by identifying the root vertex of B_i with the i-th vertex of P_l where each B_i has order greater than or equal to 2. For brevity, we write $P_l(B_i)$ instead of $P_l\{B_i : i \in [l]\}$. Let

$$\mathcal{V}_n^m = \{P_l(B_i) : N(P_l(B_i)) = n; N(B_i) \geq 2; l \geq m\}.$$

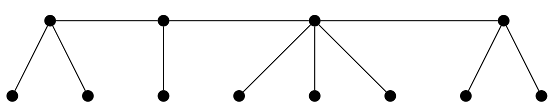

Figure 1. The complete caterpillar $P_4(K_{1,2}, K_{1,1}, K_{1,3}, K_{1,2})$.

In a graph, a vertex of degree at least 2 is called an internal vertex, a vertex of degree 1 is a pendant vertex and any vertex adjacent to a pendant vertex is a quasi-pendant vertex. We recall that a caterpillar is a tree in which the removal of all pendant vertices and incident edges results in a path. We define a complete caterpillar as a caterpillar in which each internal vertex is a quasi-pendant vertex.

A complete caterpillar $P_l(K_{1,p_i})$ is a graph obtained from the path P_l and the stars $K_{1,p_1}, ..., K_{1,p_l}$ by identifying the root of K_{1,p_i} with the i-th vertex of P_l where $p_i \geq 1$ for all $i \in [l]$ (see Fig. 1 for an example). Let $q \in [l]$. Let A_q be the complete caterpillar $P_l(K_{1,p_i})$, where $p_q = n - 2l + 1$ and $p_i = 1$ for all $i \neq q$.

Let $\mathcal{T}_{n,d}$ be the class of all trees on n vertices and diameter d. Let P_m be a path on m vertices and $K_{1,p}$ be a star on $p+1$ vertices.

In [19] the authors prove that the tree in $\mathcal{T}_{n,d}$ having the largest index is the caterpillar $P_{d,n-d}$ obtained from P_{d+1} on the vertices $1, 2, ..., d+1$ and the star $K_{1,n-d-1}$ identifying the root of $K_{1,n-d-1}$ with the vertex $\lceil \frac{d+1}{2} \rceil$ of P_{d+1}. In [10], for $3 \leq d \leq n-4$, the first

$\lfloor \frac{d}{2} \rfloor + 1$ indices of trees in $\mathcal{T}_{n,d}$ are determined. In [9], for $3 \le d \le n-3$, the first Laplacian spectral radii of trees in $\mathcal{T}_{n,d}$ are characterized. In [14] the authors present 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 [23], the authors gives three edge graft transformations on A_α-spectral radius. As applications, we determine the unique graph with maximum A_α-spectral radius among all connected graphs with diameter d, and determine the unique graph with minimum A_α-spectral radius among all connected graphs with given clique number. In [13] the authors gives several results about the A_α-matrices of trees. In particular, it is shown that if T_Δ is a tree of maximal degree Δ, then the spectral radius of $A_\alpha(T_\Delta)$ satisfies the tight inequality

$$\rho(A(T_\Delta)) < \alpha\Delta + 2(1-\alpha)\sqrt{\Delta - 1}.$$

The complete caterpillars were initially studied in [17] and [18]. In particular, in [17] the authors determine the unique complete caterpillars that minimize and maximize the algebraic connectivity (second smallest Laplacian eigenvalue) among all complete caterpillars on n vertices and diameter $m+1$. Below we summarize the result corresponding to the caterpillar attaining the largest algebraic connectivity.

Theorem 1.1 ([17] Theorems 3.3 and 3.6.). *Among all caterpillars on n vertices and diameter $m+1$, the largest algebraic connectivity is attained by the caterpillar $A_{\lfloor \frac{m+1}{2} \rfloor}$.*

Theorem 1.2 (Abreu, Lenes, Rojo [1]). *Let $\alpha = 0, 1/2$. Let G be a complete caterpillars on n vertices and diameter $m+1$. Then,*

$$\rho_\alpha(G) \le \rho_\alpha(A_{\lfloor \frac{m+1}{2} \rfloor}),$$

with equality if, and only if, $G \cong A_{\lfloor \frac{m+1}{2} \rfloor}$.

Numerical experiments suggest us that $A_{\lfloor \frac{m+1}{2} \rfloor}$ is also the tree attaining the largest α-index in the class $\mathcal{V}_n^m$. In this paper we prove that this conjecture is true; we come up with a bound for the whole family $A_\alpha(G)$, which implies the result of Abreu, Lenes, and Rojo. This is organized as follows. In Section 2, we introduce trees obtained of the path P_l and the trees $B_1, B_2, ..., B_l$ by identifying the root vertex of B_i with the i-th vertex of P_l and give a reduction procedure for calculating their α-spectra, thereby extending the main results of [15]. In the Section 3, we determine the graph that maximize the α-index in $\mathcal{V}_n^m$. We finish the section maximizing the α-index among all the unicyclic connected graphs on n vertices.

2. The α-eigenvalues of $P_l(B_i)$

Given a generalized Bethe tree B_i with k_i levels and an integer $j \in [k_i]$, we write n_{i,k_i-j+1} for the number of vertices at level j and d_{i,k_i-j+1} for their degree. In particular, $d_{i,1} = 1$ and $n_{i,k_i} = 1$. Further, for any $j \in [k_i - 1]$, let $m_{i,j} = n_{i,j}/n_{i,j+1}$. Then, for any $j \in [k_i - 2]$, we see that

$$n_{i,j} = (d_{i,j+1} - 1)n_{i,j+1},$$

and, in particular,

$$n_{i,k_i} = d_{i,k_i} = m_{i,k_i-1}.$$

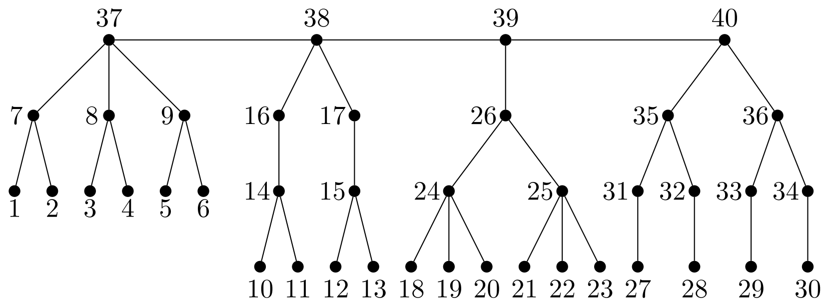

Figure 2. Labelling the tree $P_4(B_i)$.

For $i \in [l]$, it is worth pointing out that $m_{i,1}, ..., m_{i,k_i-1}$ are always positive integers, and that $n_{i,1} \geq n_{i,2} \geq \cdots \geq n_{i,k_i}$. We label the vertices of $P_l(B_i)$ as in [15]. (See figure 2).
Recall that the Kronecker product $C \otimes E$ of two matrices $C = (c_{i,j})$ and $E = (e_{i,j})$ of sizes $m \times m$ and $n \times n$, is an $mn \times mn$ matrix defined as $C \otimes E = (c_{i,j}E)$.
Two basic properties of $C \otimes E$ are the identities

$$(C \otimes E)^T = C^T \otimes E^T$$

and

$$(C \otimes E)(F \otimes H) = (CF \otimes EH),$$

which hold for any matrices of appropriate sizes.
We write I_l for the identity matrix of order l and $\mathbf{j}_l$ for the column l-vector of ones. For $i \in [l]$, let $s_i = \sum_{j=1}^{k_i-2} n_{i,j}$ and D_i be the matrix of order $s_i \times l$ defined by

$$D_i(p,q) = \begin{cases} 1, & \text{if } q = i \text{ and } s_i + 1 \leq p \leq s_i + n_{i,k_i-1}, \\ 0, & \text{elsewhere.} \end{cases}$$

Let $\beta = 1 - \alpha$, and assume that $P_l(B_i)$ is a tree labeled as described above. It is not hard to see that the matrix $A_\alpha(P_l(B_i))$ can be represented as a symmetric block tridiagonal matrix

$$\begin{bmatrix} X_1 & 0 & \cdots & 0 & \beta D_1 \\ 0 & X_2 & \ddots & & \beta D_2 \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & & 0 & X_l & \beta D_l \\ \beta D_1^T & \beta D_2^T & \cdots & \beta D_l^T & X_{l+1} \end{bmatrix},$$

where, for $i \in [l]$, the matrix X_i is the block tridiagonal matrix:

$$\begin{bmatrix} \gamma_{i,1} I_{n_{i,1}} & \beta I_{n_{i,2}} \otimes \mathbf{j}_{m_{i,1}} & & & \\ \beta I_{n_{i,2}} \otimes \mathbf{j}_{m_{i,1}}^T & \gamma_{i,2} I_{n_{i,2}} & \beta I_{n_{i,3}} \otimes \mathbf{j}_{m_{i,2}} & & \\ & \ddots & \ddots & \ddots & \\ & & & \gamma_{i,k_i-2} I_{n_{i,k_i-2}} & \beta I_{n_{i,k_i-2}} \otimes \mathbf{j}_{m_{i,k_i-2}} \\ & & \ddots & \beta I_{n_{i,k_i-1}} \otimes \mathbf{j}_{m_{i,k_i-2}}^T & \gamma_{i,k_i-1} I_{n_{i,k_i-1}} \end{bmatrix},$$

and

$$X_{l+1} = \begin{bmatrix} \gamma_{1,k_1}+\alpha & \beta & & & \\ \beta & \gamma_{2,k_2}+2\alpha & \beta & & \\ & \ddots & \ddots & \ddots & \\ & & \beta & \gamma_{l-1,k_l-1}+2\alpha & \beta \\ & & & \beta & \gamma_{l,k_l}+\alpha \end{bmatrix},$$

where

$$\gamma_{i,j} = \alpha d_{i,j}.$$

Let's define the polynomials $P_0(\lambda), P_1(\lambda), ..., P_l(\lambda)$ and $P_{i,j}(\lambda)$ for $i \in [l]$ and $j \in [k_i]$ as follows:

Definition 2.1. For $i \in [l]$ and $j \in [k_i]$, let

$$\gamma_{i,j} = \alpha d_{i,j}.$$

For $i \in [l]$, let

$$P_{i,0}(\lambda) = 1, P_{i,1}(\lambda) = \lambda - \alpha,$$

and for $i \in [l]$ and $j = 2, 3, ..., k_i - 1$, let

$$P_{i,j}(\lambda) = (\lambda - \gamma_{i,j})P_{i,j-1}(\lambda) - \beta^2 m_{i,j-1}P_{i,j-2}(\lambda). \tag{1}$$

Moreover, let

$$P_1(\lambda) = (\lambda - \gamma_{1,k_1} - \alpha)P_{1,k_1-1}(\lambda) - \beta^2 n_{1,k_1-1}P_{1,k_1-2}(\lambda),$$

$$P_l(\lambda) = (\lambda - \gamma_{l,k_l} - \alpha)P_{l,k_l-1}(\lambda) - \beta^2 n_{l,k_l-1}P_{l,k_l-2}(\lambda),$$

and

$$P_i(\lambda) = (\lambda - \gamma_{i,k_i} - 2\alpha)P_{i,k_i-1}(\lambda) - \beta^2 n_{i,k_i-1}P_{i,k_i-2}(\lambda), \tag{2}$$

for $i = 2, 3, ..., l-1$.

Theorem 2.2. *The characteristic polynomial $\phi(\lambda)$ of $A_\alpha(P_l(B_i))$ satisfies*

$$\phi(\lambda) = P(\lambda)\prod_{i=1}^{m}\prod_{j=1}^{k_i-1} P_{i,j}^{n_{i,j}-n_{i,j+1}}(\lambda), \tag{3}$$

where

$$P(\lambda) = \begin{vmatrix} P_1(\lambda) & -\beta P_{1,k_1-1}(\lambda) & & \\ -\beta P_{2,k_2-1}(\lambda) & \ddots & \ddots & \\ & \ddots & \ddots & -\beta P_{l-1,k_{l-1}-1}(\lambda) \\ & & -\beta P_{l,k_l-1}(\lambda) & P_l(\lambda) \end{vmatrix}.$$

Proof. Write $|A|$ for the determinant of a square matrix A. To prove 3, we shall reduce $\phi(\lambda) = |\lambda I - A_\alpha(P_l(B_i))|$ to the determinant of an upper triangular matrix. For a start, note that

$$\phi(\lambda)=\begin{vmatrix} X_1(\lambda) & 0 & \cdots & 0 & -\beta D_1 \\ 0 & X_2(\lambda) & \ddots & & -\beta D_2 \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & & 0 & X_l(\lambda) & -\beta D_l \\ -\beta D_1^T & -\beta D_2^T & \cdots & -\beta D_l^T & X_{l+1}(\lambda) \end{vmatrix},$$

where, for $i\in[l]$, the matrix $X_i(\lambda)$ given by,

$$\begin{bmatrix} P_{i,1}(\lambda)I_{n_{i,1}} & -\beta I_{n_{i,2}}\otimes \mathbf{j}_{m_{i,1}} & & & \\ -\beta I_{n_{i,2}}\otimes \mathbf{j}_{m_{i,1}}^T & (\lambda-\gamma_{i,2})I_{n_{i,2}} & -\beta I_{n_{i,3}}\otimes \mathbf{j}_{m_{i,2}} & & \\ & \ddots & \ddots & \ddots & -\beta I_{n_{i,k_i-1}}\otimes \mathbf{j}_{m_{i,k_i-2}} \\ & & & -\beta I_{n_{i,k_i-1}}\otimes \mathbf{j}_{m_{i,k_i-2}}^T & (\lambda-\gamma_{i,k_i-1})I_{n_{i,k_i-1}} \end{bmatrix},$$

and

$$X_{l+1}(\lambda)=\begin{bmatrix} \lambda-\gamma_{1,k_1}-\alpha & -\beta & & & \\ -\beta & \lambda-\gamma_{2,k_2}-2\alpha & -\beta & & \\ & \ddots & \ddots & \ddots & \\ & & & \lambda-\gamma_{l-1,k_l-1}-2\alpha & -\beta \\ & & & -\beta & \lambda-\gamma_{l,k_l}-\alpha \end{bmatrix}.$$

Let $\lambda\in\mathbb{R}$ be such that $P_{i,j}(\lambda)\neq 0$ for any $i\in[l]$ and $j\in[k_i-1]$; set $P_{i,j}=P_{i,j}(\lambda)$. For each $i\in[l]$ and for all $j\in[k_i-2]$, multiplying the j-th row of $X_i(\lambda)$ inserted in $\phi(\lambda)$ by $\frac{\beta P_{i,j-1}}{P_{i,j}}\otimes \mathbf{j}_{i,m_j}^T$ and add it to the next row. Since

$$\lambda-\gamma_{i,j+1}-\frac{\beta^2 m_{i,j}P_{i,j-1}}{P_{i,j}}=\frac{(\lambda-\gamma_{i,j+1})P_{i,j}-\beta^2 m_{i,j}P_{i,j-1}}{P_{i,j}}=\frac{P_{i,j+1}}{P_{i,j}},$$

we obtain,

$$\phi(\lambda)=\begin{vmatrix} Y_1(\lambda) & 0 & \cdots & 0 & -\beta D_1 \\ 0 & Y_2(\lambda) & \ddots & & -\beta D_2 \\ \vdots & \ddots & \ddots & 0 & \vdots \\ 0 & & 0 & Y_l(\lambda) & -\beta D_l \\ 0 & 0 & \cdots & 0 & Y_{l+1}(\lambda) \end{vmatrix},$$

where, for $i\in[l]$, the matrix $Y_i(\lambda)$ is given by

$$\begin{bmatrix} P_{i,1}I_{n_{i,1}} & -\beta I_{n_{i,2}}\otimes \mathbf{j}_{m_{i,1}} & 0 & & \\ & \frac{P_{i,2}}{P_{i,1}}I_{n_{i,2}} & -\beta I_{n_{i,3}}\otimes \mathbf{j}_{m_{i,2}} & & \\ & & \ddots & \ddots & -\beta I_{n_{i,k_i-1}}\otimes \mathbf{j}_{m_{i,k_i-2}} \\ & & & & \frac{P_{i,k_i-1}}{P_{i,k_i-2}}I_{n_{i,k_i-1}} \end{bmatrix},$$

and

$$Y_{l+1}(\lambda)=\begin{bmatrix} \frac{P_1}{P_{1,k_1-1}} & -\beta & & & \\ -\beta & \frac{P_2}{P_{2,k_2-1}} & -\beta & & \\ & \ddots & \ddots & \ddots & \\ & & & \frac{P_{l-1}}{P_{l-1,k_{l-1}-1}} & -\beta \\ & & & -\beta & \frac{P_l}{P_{l,k_l-1}} \end{bmatrix}.$$

Thereby,

$$\begin{aligned}\phi(\lambda) &= \prod_{i=1}^{l+1}\left|Y_i(\lambda)\right| \\ &= \left|Y_{l+1}(\lambda)\right|\prod_{i=1}^{l} P_{i,1}^{n_{i,1}}\Big(\frac{P_{i,2}}{P_{i,1}}\Big)^{n_{i,2}}\Big(\frac{P_{i,3}}{P_{i,2}}\Big)^{n_{i,3}}\cdots\Big(\frac{P_{i,k_i-2}}{P_{i,k_i-3}}\Big)^{n_{i,k_i-2}}\Big(\frac{P_{i,k_i-1}}{P_{i,k_i-2}}\Big)^{n_{i,k_i-1}} \\ &= \left|Y_{l+1}(\lambda)\right|\prod_{i=1}^{l} P_{i,1}^{n_{i,1}-n_{i,2}}P_{i,2}^{n_{i,2}-n_{i,3}}\cdots P_{i,k_i-2}^{n_{i,k_i-2}-n_{i,k_i-1}}P_{i,k_i-1}^{n_{i,k_i-1}},\end{aligned}$$

where

$$\left|Y_{l+1}(\lambda)\right| =$$

$$\frac{1}{\prod_{i=1}^{l}P_{i,k_i-1}}\begin{vmatrix} P_1 & -\beta P_{1,k_1-1} & & & \\ -\beta P_{2,k_2-1} & P_2 & -\beta P_{2,k_2-1} & & \\ & \ddots & \ddots & \ddots & \\ & & -\beta P_{l-1,k_{l-1}-1} & P_{l-1} & -\beta P_{l-1,k_{l-1}-1} \\ & & & -\beta P_{l,k_l-1} & P_l \end{vmatrix}.$$

Hence

$$\left|\lambda I - A_\alpha(P_l(B_i))\right| = P(\lambda)\prod_{i=1}^{l}\prod_{j=1}^{n_{i,k_i-1}} P_{i,j}^{n_{i,j}-n_{i,j+1}}(\lambda).$$

Thus, the equality (3) is proved whenever $P_{i,j}(\lambda)\neq 0$ for any $i\in[l]$ and $j\in[k_i-1]$. Since for any $i\in[l]$ and $j\in[k_i-1]$ the polynomials $P_{i,j}(\lambda)$ have finitely many roots, the equality (3) is verified for infinitely many value of λ. The proof is complete. ☑

Definition 2.3. For $i\in[l]$ and $j\in[k_i-1]$, let $T_{i,j}$ be the $j\times j$ leading principal submatrix of the $k_i\times k_i$ symmetric tridiagonal matrix

$$T_i=\begin{bmatrix} \alpha d_{i,1} & \beta\sqrt{d_{i,2}-1} & & & \\ \beta\sqrt{d_{i,2}-1} & \alpha d_{i,2} & & & \\ & & \ddots & \beta\sqrt{d_{i,k_i-1}-1} & \\ & & \beta\sqrt{d_{i,k_i-1}-1} & \alpha d_{i,k_i-1} & \beta\sqrt{d_{i,k_i}} \\ & & & \beta\sqrt{d_{i,k_i}} & \gamma_{i,k_i}+\alpha c \end{bmatrix},$$

where $\beta=1-\alpha$, $c=2$ for $i\in[l-1]$ and $c=1$ for $i=1$ and $i=l$.

Since $d_s > 1$ for all $s = 2, ..., j$, each matrix T_j has nonzero codiagonal entries and it is known that its eigenvalues are simple. Using the well known three-term recursion formula for the characteristic polynomials of the leading principal submatrices of a symmetric tridiagonal matrix and the formulas (1) and (2), one can easily prove the following assertion:

Lemma 2.4. *Let $\alpha \in [0,1)$. Then*

$$\left|\lambda I - T_{i,j}\right| = P_{i,j}(\lambda)$$

and

$$\left|\lambda I - T_i\right| = P_i(\lambda),$$

for any $i \in [l]$ and $j \in [k_i - 1]$.

Let $\widetilde{A}$ be the matrix obtained from a matrix A by deleting its last row and last column. Moreover, for $i, j \in [r]$, let $E_{i,j}$ be the $k_i \times k_j$ matrix with $E_{i,j}(k_i, k_j) = 1$ and zeroes elsewhere. We recall the following Lemma.

Lemma 2.5 ([16]). *For $i, j \in [r]$, let C_i be a matrix of order $k_i \times k_i$ and $\mu_{i,j}$ be arbitrary scalars. Then,*

$$\begin{vmatrix} C_1 & \mu_{1,2}E_{1,2} & \cdots & \mu_{1,r-1}E_{1,r-1} & \mu_{1,r}E_{1,r} \\ \mu_{2,1}E_{1,2}^T & C_2 & \cdots & \cdots & \mu_{2,r}E_{2,r} \\ \mu_{3,1}E_{1,3}^T & \mu_{3,2}E_{2,3}^T & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & C_{r-1} & \mu_{r-1,r}E_{r-1,r}^T \\ \mu_{r,1}E_{1,r}^T & \mu_{r,2}E_{2,r}^T & \cdots & \mu_{r,r-1}E_{r-1,r}^T & C_r \end{vmatrix}$$

$$= \begin{vmatrix} \left|C_1\right| & \mu_{1,2}\left|\widetilde{C_2}\right| & \cdots & \mu_{1,r-1}\left|\widetilde{C_{r-1}}\right| & \mu_{1,r}\left|\widetilde{C_r}\right| \\ \mu_{2,1}\left|\widetilde{C_1}\right| & \left|C_2\right| & \cdots & \cdots & \mu_{2,r}\left|\widetilde{C_r}\right| \\ \mu_{3,1}\left|\widetilde{C_1}\right| & \mu_{3,2}\left|\widetilde{C_2}\right| & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \left|C_{r-1}\right| & \mu_{r-1,r}\left|\widetilde{C_r}\right| \\ \mu_{r,1}\left|\widetilde{C_1}\right| & \mu_{r,2}\left|\widetilde{C_2}\right| & \cdots & \mu_{r,r-1}\left|\widetilde{C_{r-1}}\right| & \left|C_r\right| \end{vmatrix}.$$

From now on, for $i \in [l-1]$, by F_i we denote the matrix of order $k_i \times k_{i+1}$ whose entries are 0, except for the entry $F_i(k_i, k_{i+1}) = 1$.

Lemma 2.6. *Let $r = \sum_{i=1}^{l} k_i$. Let $M(P_l(B_i))$ be the symmetric matrix of order $n \times n$ defined by*

$$\begin{bmatrix} T_1 & \beta F_1 & & \\ \beta F_1^T & T_2 & \ddots & \\ & \ddots & \ddots & \beta F_{l-1} \\ & & \beta F_{l-1}^T & T_l \end{bmatrix}.$$

Then,

$$\left|\lambda I - M(P_l(B_i))\right| = P(\lambda).$$

Proof. The characteristic polynomial of the matrix $M(P_l(B_i))$ is given by

$$\begin{vmatrix} \lambda I - T_1 & -\beta F_1 & & \\ -\beta F_1^T & \lambda I - T_2 & \ddots & \\ & \ddots & \ddots & -\beta F_{l-1} \\ & & -\beta F_{l-1}^T & \lambda I - T_l \end{vmatrix}.$$

From Lemma 2.5, we have that $\left|\lambda I - M(P_l(B_i))\right|$ is given by

$$\begin{vmatrix} |\lambda I - T_1| & -\beta\left|\widetilde{\lambda I - T_1}\right| & & & \\ -\beta\left|\widetilde{\lambda I - T_2}\right| & |\lambda I - T_2| & -\beta\left|\widetilde{\lambda I - T_2}\right| & & \\ & \ddots & \ddots & \ddots & \\ & & -\beta\left|\widetilde{\lambda I - T_{l-1}}\right| & |\lambda I - T_{l-1}| & -\beta\left|\widetilde{\lambda I - T_{l-1}}\right| \\ & & & -\beta\left|\widetilde{\lambda I - T_l}\right| & |\lambda I - T_l| \end{vmatrix}.$$

Since $\widetilde{\lambda I - T_i} = \lambda I - T_{i,k_i-1}$ for $i \in [l]$, by Lemma 2.4, the proof is complete. ☑

Theorem 2.2, Lemma 2.4, Lemma 2.6, and the interlacing property for the eigenvalues of hermitian matrices yield the following summary statement:

Theorem 2.7. *Let $\alpha \in [0,1)$. Then:*

1. *the α-spectrum of $P_l(B_i)$ is*

$$\Big[\bigcup_{i=1}^{l}\bigcup_{j=1}^{k_i-1} Sp(T_{i,j})\Big] \cup Sp(M(P_l(B_i)));$$

2. *the multiplicity of each eigenvalue of $T_{i,j}$ as an α-eigenvalue of $P_l(B_i)$ is $n_{i,j} - n_{i,j+1}$, if $i \in [l]$ and $j \in [k_i - 1]$, and is 1 if $i \in [l]$ and $j = k_i$;*
3. *$\rho_\alpha(P_l(B_i))$ is the largest eigenvalue of $M(P_l(B_i))$;*
4. *$\rho_\alpha(P_l(B_i)) > \alpha$.*

3. The α-index of graphs

In Theorem 2.7, we characterize the α-eigenvalues of the trees $P_l(B_i)$ obtained from path P_l and the generalized Bethe trees $B_1, B_2, ..., B_l$ obtained identifying the root vertex of B_i with the i-th vertex of P_l. This is the case for the caterpillars $P_l(K_{1,p_i})$ in which the path is P_l and each star K_{1,p_i} is a generalized Bethe tree of 2 levels. From Theorem 2.7, we get

Lemma 3.1. *Let $\alpha \in [0,1)$. Then:*

1. *the α-spectrum of $P_l(K_{1,p_i})$ is formed by α with multiplicity $\sum_{i=1}^{l} p_i - l$, and the eigenvalues of the $2l \times 2l$ irreducible nonnegative matrix*
$$M(P_l(K_{1,p_i})) = \begin{bmatrix} T(p_1) & \beta E & & & \\ \beta E & S(p_2) & \beta E & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & S(p_{l-1}) & \beta E \\ & & & \beta E & T(p_l) \end{bmatrix},$$
where
$$T(x) = \begin{bmatrix} \alpha & \beta\sqrt{x} \\ \beta\sqrt{x} & \alpha(x+1) \end{bmatrix}, E = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}; S(x) = T(x) + \alpha E,$$
2. *$\rho_\alpha(P_l(K_{1,p_i}))$ is the largest eigenvalue of $M(P_l(K_{1,p_i}))$;*
3. *$\rho_\alpha(P_l(K_{1,p_i})) > \alpha$.*

Let $t(\lambda, x)$ and $s(\lambda, x)$ be the characteristic polynomials of the matrices $T(x)$ and $S(x)$, respectively. That is,
$$t(\lambda, x) = \lambda^2 - \alpha(x+2)\lambda + \alpha^2(x+1) - \beta^2 x$$
and
$$s(\lambda, x) = \lambda^2 - \alpha(x+3)\lambda + \alpha^2(x+2) - \beta^2 x.$$
Then,
$$s(\lambda, x) - t(\lambda, x) = \alpha(\alpha - \lambda).$$
The notation $\left|A\right|_l$ will be used to denote the determinant of the matrix A of order $l \times l$. The next result is an immediate consequence of the Lemma 2.5.

Lemma 3.2. *The characteristic polynomial of $M(P_l(K_{1,p_i}))$ is*
$$\begin{vmatrix} t(\lambda, p_1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda, p_2) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda, p_{l-1}) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda, p_l) \end{vmatrix}_l.$$

For $q \in [l]$, let A_q be the complete caterpillar $P_l(K_{1,p_i})$, where $p_q = n - 2l + 1$ and $p_i = 1$ for all $i \neq q$. We define
$$r_0(\lambda) = 1, r_1(\lambda) = t(\lambda, 1)$$
and, for $2 \leq q \leq \lfloor \frac{l+1}{2} \rfloor$, we define
$$r_q(\lambda) = \begin{vmatrix} s(\lambda, 1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda, 1) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda, 1) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda, 1) \end{vmatrix}_q.$$

Let $\phi_q(\lambda)$ be the characteristic polynomial of $M(A_q)$, then,

$$\phi_q(\lambda) = \left|\lambda I - M(A_q)\right|.$$

Lemma 3.3. *Let $\alpha \in [0,1)$. Then*

$$\phi_q(\lambda) - \phi_{q+1}(\lambda) = (a-1)(\alpha\lambda - 2\alpha + 1)(\beta(\lambda-\alpha))^{2q-1}[\alpha r_{m-2q}(\lambda) + \beta^2(\lambda-\alpha)r_{l-2q-1}(\lambda)]$$

for all $q \in \left[\lfloor \frac{l+1}{2} \rfloor - 1\right]$, where $l \geq 3$.

Proof. By Lemma 3.2, the (q,q)-entry of $\phi_q(\lambda) = \left|\lambda I - M(A_q)\right|$ is $t(\lambda,a)$ if $q = 1$ and $s(\lambda,a)$ if $q \neq 1$. Let $E_l \cong P_l(K_{1,p_i})$, where $p_i = 1$ for all $i \in [l]$. Let $\varphi_s(\lambda) = \left|\lambda I - M(E_s)\right|$. From Lemma 3.2, we have

$$\varphi_s(\lambda) = \begin{vmatrix} t(\lambda,1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda,1) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda,1) \end{vmatrix}_s .$$

Since

$$r_0(\lambda) = 1, r_1(\lambda) = t(\lambda,1)$$

and

$$r_q(\lambda) = \begin{vmatrix} s(\lambda,1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda,1) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda,1) \end{vmatrix}_q ,$$

for $q = 2, ..., \lfloor \frac{l+1}{2} \rfloor$; then, expanding along the first row, we obtain

$$r_q(\lambda) = s(\lambda,1)r_{q-1}(\lambda) - \beta^2(\lambda-\alpha)^2 r_{q-2}(\lambda). \tag{4}$$

Since $s(\lambda,x) = t(\lambda,x) + \alpha(\alpha-\lambda)$, by linearity on the first column, we have

$$r_q(\lambda) = \begin{vmatrix} t(\lambda,1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda,1) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda,1) \end{vmatrix}_q + \alpha(\alpha-\lambda)r_{q-1}(\lambda).$$

Then,

$$r_q(\lambda) = \varphi_q(\lambda) + \alpha(\alpha-\lambda)r_{q-1}(\lambda).$$

Let $q \in \left[\lfloor \frac{l+1}{2} \rfloor - 1\right]$. We search for the difference $\phi_q(\lambda) - \phi_{q+1}(\lambda)$. We recall that (q,q)-entry of $\phi_q(\lambda) = \left|\lambda I - M(A_q)\right|$ is $t(\lambda,a)$ if $q = 1$ and $s(\lambda,a)$ if $q \neq 1$. Since

$t(\lambda, a) = t(\lambda, 1) + (1-a)(\alpha\lambda - 2\alpha + 1)$ and $s(\lambda, a) = s(\lambda, 1) + (1-a)(\alpha\lambda - 2\alpha + 1)$, by linearity on the q-th column, we have

$$\phi_q(\lambda) = \begin{vmatrix} t(\lambda,1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda,1) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda,1) \end{vmatrix}_l + (1-a)(\alpha\lambda - 2\alpha + 1)\begin{vmatrix} r_{q-1}(\lambda) & 0 \\ 0 & r_{l-q}(\lambda) \end{vmatrix}. \tag{5}$$

The $(q+1, q+1)$-entry of the determinant of order l on the second right hand of (5) is $s(\lambda, 1)$, and since $s(\lambda, 1) = s(\lambda, a) + (a-1)(\lambda\alpha - 2\alpha + 1)$, by linearity on the $(q+1)$-th column, we obtain

$$\begin{vmatrix} t(\lambda,1) & \beta(\alpha-\lambda) & & & \\ \beta(\alpha-\lambda) & s(\lambda,1) & \beta(\alpha-\lambda) & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & \beta(\alpha-\lambda) \\ & & & \beta(\alpha-\lambda) & t(\lambda,1) \end{vmatrix}_l$$

$$= \phi_{q+1}(\lambda) + (1-a)(\alpha\lambda - 2\alpha + 1)\begin{vmatrix} r_q(\lambda) & 0 \\ 0 & r_{l-q-1}(\lambda) \end{vmatrix}.$$

Thereby,

$$\phi_q(\lambda) - \phi_{q+1}(\lambda) =$$
$$(1-a)(\alpha\lambda - 2\alpha + 1)\begin{vmatrix} r_{q-1}(\lambda) & 0 \\ 0 & r_{l-q}(\lambda) \end{vmatrix} + (a-1)(\alpha\lambda - 2\alpha + 1)\begin{vmatrix} r_q(\lambda) & 0 \\ 0 & r_{l-q-1}(\lambda) \end{vmatrix}.$$

Thus,

$$\phi_q(\lambda) - \phi_{q+1}(\lambda) = (a-1)(\alpha\lambda - 2\alpha + 1)[r_q(\lambda)r_{m-q-1}(\lambda) - r_{q-1}(\lambda)r_{m-q}(\lambda)].$$

Applying the recurrence formula (4) to $r_q(\lambda)$ and $r_{l-q}(\lambda)$, we obtain

$$\begin{aligned} r_q(\lambda)r_{l-q-1}(\lambda) - r_{q-1}(\lambda)r_{l-q}(\lambda) &= [s(\lambda,1)r_{q-1}(\lambda) - \beta^2(\lambda-\alpha)^2 r_{q-2}(\lambda)]r_{l-q-1}(\lambda) \\ &- r_{q-1}(\lambda)[s(\lambda,1)r_{l-q-1}(\lambda) - \beta^2(\lambda-\alpha)^2 r_{l-q-2}(\lambda)]. \end{aligned}$$

Then,

$$r_q(\lambda)r_{l-q-1}(\lambda) - r_{q-1}(\lambda)r_{l-q}(\lambda) = \beta^2(\lambda-\alpha)^2[r_{q-1}(\lambda)r_{l-q-2}(\lambda) - r_{q-2}(\lambda)r_{l-q-1}(\lambda)].$$

By repeated applications of this process, we conclude that

$$r_q(\lambda)r_{l-q-1}(\lambda) - r_{q-1}(\lambda)r_{l-q}(\lambda) = [\beta(\lambda-\alpha)]^{2(q-1)}[r_1(\lambda)r_{l-2q}(\lambda) - r_{l-2q+1}(\lambda)].$$

Hence,

$$\begin{aligned} & r_q(\lambda)r_{l-q-1}(\lambda) - r_{q-1}(\lambda)r_{l-q}(\lambda) \\ = \ & [\beta(\lambda-\alpha)]^{2(q-1)}[t(\lambda,1)r_{l-2q}(\lambda) - s(\lambda,1)r_{l-2q}(\lambda) + \beta^2(\lambda-\alpha)^2 r_{l-2q-1}(\lambda)] \\ = \ & [\beta(\lambda-\alpha)]^{2(q-1)}[\alpha(\lambda-\alpha)r_{l-2q}(\lambda) + \beta^2(\lambda-\alpha)^2 r_{l-2q-1}(\lambda)] \\ = \ & [\beta(\lambda-\alpha)]^{2q-1}[\alpha r_{l-2q}(\lambda) + \beta^2(\lambda-\alpha) r_{l-2q-1}(\lambda)]. \end{aligned}$$

Thus,

$$\phi_q(\lambda) - \phi_{q+1}(\lambda) = (a-1)(\alpha\lambda - 2\alpha + 1)[\beta(\lambda-\alpha)]^{2q-1}[\alpha r_{l-2q}(\lambda) + \beta^2(\lambda-\alpha) r_{l-2q-1}(\lambda)].$$

☑

Let $\rho(A)$ be the spectral radius of the square matrix A. From Perron-Frobenius's Theory for nonnegative matrices [22], if A is a nonnegative irreducible matrix then A has a unique eigenvalue equal to its spectral radius and it increases whenever any entry of it increases. Hence, we have the next result.

Lemma 3.4 ([21]). *If A is a nonnegative irreducible matrix and B is any principal submatrix of A, then $\rho(B) < \rho(A)$.*

Let $\mathcal{C}_{n,l}$ be the class of all complete caterpillars on n vertices and diameter $l+1$. A special subclass of $\mathcal{C}_{n,l}$ is $\mathcal{A}_{n,l} = \{A_1, A_2, ..., A_l\}$, where $A_q \cong P_l(K_{1,p_i}) \in \mathcal{C}_{n,l}$, with $p_i = 1$ for $i \neq q$ and $p_q = n - 2l + 1$. Since A_q and A_{l-q+1} are isomorphic caterpillars for all $q \in \left[\lfloor \frac{l+1}{2} \rfloor\right]$, the next theorem gives a total ordering in $\mathcal{A}_{n,l}$ by the α-index.

Theorem 3.5. *Let $\alpha \in [0,1)$. Then*

$$\rho_\alpha(A_q) < \rho_\alpha(A_{q+1})$$

for all $q \in \left[\lfloor \frac{l+1}{2} \rfloor - 1\right]$, where $l \geq 3$.

Proof. Let $l \geq 3$. Let $q \in \left[\lfloor \frac{l+1}{2} \rfloor - 1\right]$. Let $\phi_q(\lambda)$ and $\phi_{q+1}(\lambda)$ be the characteristic polynomials of degrees $2l$ of the matrices $M(A_q)$ and $M(A_{q+1})$, respectively. The matrices $M(A_q)$ and $M(A_{q+1})$ are nonnegative irreducible matrices, then its spectral radii are simple eigenvalues.
Let

$$\rho_\alpha(A_q) = \mu_1 > \mu_2 \geq \cdots \geq \mu_{2l}$$

and

$$\rho_\alpha(A_{q+1}) = \gamma_1 > \gamma_2 \geq \cdots \geq \gamma_{2l}$$

be the eigenvalues of the matrices $M(A_q)$ and $M(A_{q+1})$, respectively.
By Lemma 3.3, we have

$$\begin{aligned} \phi_q(\lambda) - \phi_{q+1}(\lambda) &= \prod_{j=1}^{2l}(\lambda - \mu_j) - \prod_{j=1}^{2l}(\lambda - \gamma_j) \\ &= (a-1)(\alpha\lambda - 2\alpha + 1)(\beta(\lambda-\alpha))^{2q-1} \\ &\quad * [\alpha r_{l-2q}(\lambda) + \beta^2(\lambda-\alpha) r_{l-2q-1}(\lambda)]. \end{aligned} \tag{6}$$

We recall that $r_{l-2q}(\lambda)$ and $r_{l-2q-1}(\lambda)$ are the characteristic polynomials of the matrices $M(\widetilde{E_{l-2q+1}})$ and $M(\widetilde{E_{l-2q}})$ whose spectral radii are $\rho(M(\widetilde{E_{l-2q+1}}))$ and $\rho(M(\widetilde{E_{l-2q}}))$, respectively. The matrices $M(\widetilde{E_{l-2q+1}})$ and $M(\widetilde{E_{l-2q}})$ are principal submatrices of $M(A_q)$. By Lemma 3.4, $\rho(M(\widetilde{E_{l-2q+1}})) < \rho_\alpha(A_q)$ and $\rho(M(\widetilde{E_{l-2q}})) < \rho_\alpha(A_q)$.
Hence, $r_{l-2q}(\rho_\alpha(A_q)) > 0$ and $r_{l-2q-1}(\rho_\alpha(A_q)) > 0$. We claim that $\rho_\alpha(A_q) < \rho_\alpha(A_{q+1})$. Suppose $\rho_\alpha(A_q) \geq \rho_\alpha(A_{q+1})$. Then $\rho_\alpha(A_q) \geq \gamma_j$ for all j. Taking $\lambda = \rho_\alpha(A_q)$ in (6), we obtain

$$\begin{aligned} -\phi_{q+1}(\rho_\alpha(A_q)) &= -\prod_{j=1}^{2l}(\rho_\alpha(A_q) - \gamma_j) \\ &= (a-1)(\alpha\rho_\alpha(A_q) - 2\alpha + 1)(\beta(\rho_\alpha(A_q) - \alpha))^{2q-1} \\ &\quad * [\alpha r_{l-2q}(\rho_\alpha(A_q)) + \beta^2(\rho_\alpha(A_q) - \alpha) r_{l-2q-1}(\rho_\alpha(A_q))]. \end{aligned}$$

By Lemma 3.1, $\rho_\alpha(A_q) > \alpha$. Then $\alpha\rho_\alpha(A_q) - 2\alpha + 1 > 0$. Thus,

$$\begin{aligned} 0 &\geq -\prod_{j=1}^{2l}(\rho_\alpha(A_q) - \gamma_j) \\ &= (a-1)(\alpha\rho_\alpha(A_q) - 2\alpha + 1)(\beta(\rho_\alpha(A_q) - \alpha))^{2q-1} \\ &\quad * [\alpha r_{l-2q}(\rho_\alpha(A_q)) + \beta^2(\rho_\alpha(A_q) - \alpha) r_{l-2q-1}(\rho_\alpha(A_q))] \\ &> 0. \end{aligned}$$

which is a contradiction. The proof is complete. ☑

Lemma 3.6 ([?]). *Let A be a nonnegative symmetric matrix and x be a unit vector of $\mathbb{R}^n$. If $\rho(A) = x^T Ax$, then $Ax = \rho(A)x$.*

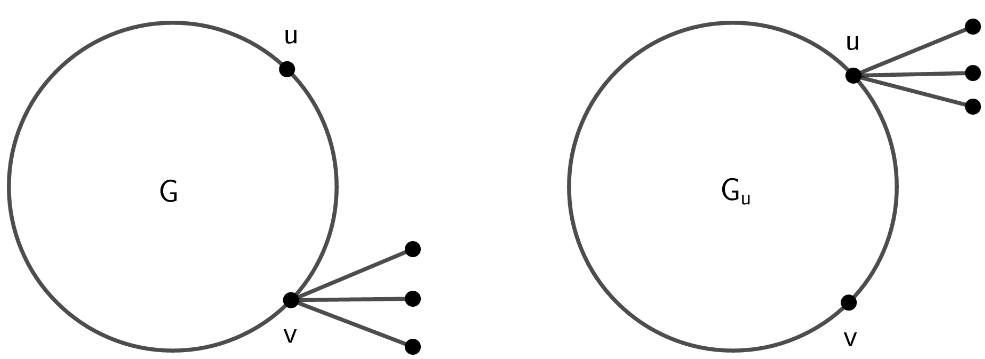

Figure 3. Graphs G and G_u with $s = 3$.

Let $N_G(v)$ be the vertex set adjacent to v in G.

Lemma 3.7 ([23]). *Let $\alpha \in [0, 1)$. Let G be a connected graph and $\rho_\alpha(G)$ be the α-index of G. Let u, v be two vertices of G. Suppose $v_1, v_2, ..., v_s$, are some vertices of $N_G(v) - (N_G(u) \cup \{u\})$ and $x = (x_1, x_2, ..., x_n)$ is the Perron's vector of $A_\alpha(G)$, where x_i corresponds to the vertex v_i for $i \in [s]$. Let*

$$G_u \cong G - vv_1 - \cdots - vv_s + uv_1 + \cdots + uv_s$$

(as shown in Fig. 3). If $x_u \geq x_v$, then $\rho_\alpha(G) < \rho_\alpha(G_u)$.

An immediate consequence of Lemma 3.7 is

Theorem 3.8. *Let $T \in \mathcal{V}_n^m$. Then*

$$\rho_\alpha(T) \leq \rho_\alpha(A_{\lfloor \frac{m+1}{2} \rfloor}), \tag{7}$$

where $A_{\lfloor \frac{m+1}{2} \rfloor} \in \mathcal{A}_{n,m}$. For $\alpha \in [0, 1)$, the bound (7) is attained if, and only if, $T \cong A_{\lfloor \frac{m+1}{2} \rfloor}$. For $\alpha = 1$, the bound (7) is attained if, and only if, $T \cong A_k$, where $k = 2, ..., \lfloor \frac{m+1}{2} \rfloor$ and $m \geq 3$ or $T \cong A_{\lfloor \frac{m+1}{2} \rfloor}$, where $m = 2$.

Proof. Let $\alpha \in [0, 1)$. Let $T \cong P_l(B_i) \in \mathcal{V}_n^m$. Let $x_1, x_2, ..., x_l$ be the vertices of the path P_l in the tree T. Let B_i be a tree with k_i levels for all $i \in [l]$. Suppose T has the largest α-index in $\mathcal{V}_n^m$.
Suppose $k_i > 2$ for some $2 \leq i \leq l - 1$. Let $u_1, ..., u_{s_i}$ be all the vertices in the second level of B_i; we can assume without loss of generality that u_{s_i} is an internal vertex. Let $w_1, ..., w_{r_i}$ be all the vertices of $N_G(u_{s_i}) - \{x_i\}$. Let

$$T_{x_i} \cong T - u_{s_i}w_1 - \cdots - u_{s_i}w_{r_i} + x_iw_1 + \cdots + x_iw_{r_i},$$

and

$$T_{u_{s_i}} \cong T - x_{i-1}x_i - x_{i+1}x_i - u_1x_i - \cdots - u_{s_i-1}x_i + x_{i-1}u_{s_i} + x_{i+1}u_{s_i} + u_1u_{s_i} + \cdots + u_{s_i-1}u_{s_i}.$$

By Lemma 3.7, $\rho_\alpha(T_{x_i}) > \rho_\alpha(T)$ or $\rho_\alpha(T_{u_{s_i}}) > \rho_\alpha(T)$. Moreover, $\rho_\alpha(T_{x_i}) \in \mathcal{V}_n^m$ and $\rho_\alpha(T_{u_{s_i}}) \in \mathcal{V}_n^m$, which is a contradiction. If $i = 1$ or $i = l$, we reason analogously. Then, $k_i = 2$ for all $i \in [l]$. This is,

$$T \cong P_l(K_{1,p_i}).$$

By reasoning analogously we can verify that

$$T \in \mathcal{A}_{n,m}.$$

Let $m \geq 3$. By Theorem 3.5,

$$\rho_\alpha(A_1) < \rho_\alpha(A_2) < \cdots < \rho_\alpha(A_{\lfloor \frac{m+1}{2} \rfloor}).$$

Then the largest α-index is attained by $A_{\lfloor \frac{m+1}{2} \rfloor}$. For $m = 2$ the result is immediate.
Let $\alpha = 1$; then $A_\alpha = D$, where D is the diagonal matrix of vertex degrees. Let $T \in \mathcal{V}_n^m$. Let $m = 3$; then the maximum degree of T is less than or equal to $n - 2l + 3$. Then, $\rho_\alpha(T) \leq n - 2l + 3 \leq \rho_\alpha(A_k)$ for all $k = 2, ..., \lfloor \frac{m+1}{2} \rfloor$. For $m = 2$ is result is immediate. ☑

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