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The largest Laplacian and adjacency indices of complete caterpillars of fixed diameter

Nair Abreu *
Universidade Federal do Ro de Janeiro, Brasil
Eber Lenes †
Universidad del Sinú, Colombia
and
Oscar Rojo ‡
Universidad Católica del Norte, Chile
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Abstract

A complete caterpillar is a caterpillar in which each internal vertex is a quasi-pendent vertex. In this paper, in the class of all complete caterpillars on n vertices and diameter d, the caterpillar attaining the largest Laplacian index is determined. In addition, it is proved that this caterpillar also attains the largest adjacency index.

Keywords : *Caterpillar, Laplacian matrix, Laplacian index, adjacency matrix, index, spectral radius.*

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1. Introduction

Let G be a simple undirected graph on n vertices. Let $D(G)$ be the diagonal matrix whose $(i,i)-$entry is the degree of the $i-th$ vertex of G and let $A(G)$ be the adjacency matrix of G. The matrix $L(G) = D(G) - A(G)$ is the Laplacian matrix of G. $L(G)$ is a positive semidefinite matrix and $(0,\mathbf{e})$ is an eigenpair of $L(G)$ where $\mathbf{e}$ is the all ones vector. The eigenvalues of $A(G)$ are called the eigenvalues of G while the eigenvalues of $L(G)$ are called the Laplacian eigenvalues of G. The largest eigenvalue $\mu_1(G)$ of $L(G)$ is known as the Laplacian index of G and the largest eigenvalue $\lambda_1(G)$ of $A(G)$ is the adjacency index or index of G [1].

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.

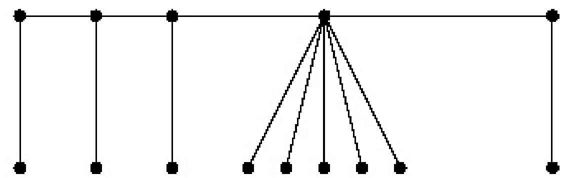
In [9] the authors prove that the tree in $\mathcal{T}_{n,d}$ having the largest index is the caterpillar $P_{d,n-d}$ obtained from P_{d+1} on the vertices $1,2,...,d+1$ and the star $K_{1,n-d-1}$ identifying the root of $K_{1,n-d-1}$ with the vertex $\left\lceil \frac{d+1}{2} \right\rceil$ of P_{d+1}. In [2], for $3 \leq d \leq n-4$, the first $\left\lfloor \frac{d}{2} \right\rfloor + 1$ indices of trees in $\mathcal{T}_{n,d}$ are determined. In [3], for $3 \leq d \leq n-3$, the first $\left\lfloor \frac{d}{2} \right\rfloor + 1$ Laplacian spectral radii of trees in $\mathcal{T}_{n,d}$ are characterized.

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.

Let $d \geq 3,\ n > 2(d-1)$ and $\mathbf{p} = \begin{bmatrix} p_1 & \ldots & \ldots & p_{d-1} \end{bmatrix}$.

Let $\mathcal{C}_{n,d}$ be the class of all complete caterpillars on n vertices and diameter d. A caterpillar $C(\mathbf{p})$ in $\mathcal{C}_{n,d}$ is obtained from the path P_{d-1} and the stars $K_{1,p_1}, K_{1,p_2}, ..., K_{1,p_{d-1}}$ by identifying the root of K_{1,p_i} with the $i-th$ vertex of P_{d-1} where $p_1 \geq 1, p_2 \geq 1, \ldots, p_{d-1} \geq 1$ and $p_1 + \ldots + p_{d-1} = n-d+1$. A special subclass of $\mathcal{C}_{n,d}$ is $\mathcal{A}_{n,d} = \{A_1, A_2, \ldots, A_{d-2}, A_{d-1}\}$ where $A_k = C(\mathbf{p}) \in \mathcal{C}_{n,d}$ with $p_i = 1$ for $i \neq k$ and $p_k = n-2d+3$.

Example 1. *$A_4 = C(\ 1\ \ 1\ \ 1\ \ 5\ \ 1\ )$ is the caterpillar*



of 14 *vertices and diameter* 6.

The complete caterpillars were initially studied in [5] and [6]. In particular, in [6] 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 d. Below we summarize the result corresponding to the caterpillar attaining the largest algebraic connectivity.

Theorem 1. *[6], Theorems 3.3 and 3.6. Among all caterpillars in $\mathcal{C}_{n,d}$ the largest algebraic connectivity is attained by the caterpillar $A_{\lfloor \frac{d}{2} \rfloor}$.*

Numerical experiments suggest us that $A_{\lfloor \frac{d}{2} \rfloor}$ is also the caterpillar attaining the largest Laplacian index in the class $\mathcal{C}_{n,d}$. In this paper, we prove that this conjecture is true. Moreover, we prove that $A_{\lfloor \frac{d}{2} \rfloor}$ also attains the largest adjacency index in $\mathcal{C}_{n,d}$. To get these results, we first prove that the caterpillars in $\mathcal{C}_{n,d}$ attaining the mentioned largest indices lie in $\mathcal{A}_{n,d}$ and then we order the caterpillars in this subclass by their Laplacian indices as well as by their adjacency indices.

2. The largest Laplacian index among all complete caterpillars

Let $x_1, x_2, ..., x_{d-1}$ be the vertices of the path P_{d-1} of the caterpillars $C(\mathbf{p}) \in \mathcal{C}_{n,d}$. Let $C(\mathbf{p}) \in C_{n,d}$ with $\mathbf{p} = [p_1, p_2, \ldots, p_{d-1}]$. Then

$$d(x_1) = p_1 + 1,\ d(p_2) = p_2 + 2, \ldots, d(x_{d-2}) = p_{d-2} + 2,\ d(p_{d-1}) = p_{d-1} + 1.$$

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

Lemma 1. *[3] Let u, v be two vertices of a tree T. For $1 \leq s \leq d(v)$, let $v_1, v_2, \ldots, v_s$ be some vertices in $N_T(v) - (N_T(u) \cup \{u\})$. For $1 \leq t \leq d(u)$, let $u_1, u_2, \ldots, u_t$ be some vertices in $N_T(u) - (N_T(v) \cup \{v\})$. Let*

$$T_u = T - vv_1 - vv_2 - \cdots - vv_s + uv_1 + uv_2 + \cdots + uv_s$$

and

$$T_v = T - uu_1 - uu_2 - \cdots - uu_t + vu_1 + vu_2 + \cdots + vu_t.$$

If both T_u and T_v are trees, then we have either $\mu_1(T_u) > \mu_1(T)$ or $\mu_1(T_v) > \mu_1(T)$.

We recall that $C(\mathbf{p}) = A_k \in \mathcal{A}_{n,d}$ if and only if $p_i = 1$ for $i \neq k$ and $p_k = n - 2d + 3$.

Theorem 2. Let $d \geq 3$. Let $C(\mathbf{p}) \in \mathcal{C}_{n,d}$. Then there exists a caterpillar $A_k \in \mathcal{A}_{n,d}$ such that $\mu_1(C(\mathbf{p})) \leq \mu_1(A_k)$ for some $1 \leq k \leq d-1$.

Proof. Let $\#S$ be the cardinality of a set S. Let $d \geq 3$. Let $C(\mathbf{p}) \in \mathcal{C}_{n,d}$ with $\mathbf{p} = \begin{bmatrix} p_1 & p_2 & \ldots & \ldots & p_{d-1} \end{bmatrix}$.

If $C(\mathbf{p}) \in \mathcal{A}_{n,d}$ then there is nothing to prove. Let $C(\mathbf{p}) \in \mathcal{C}_{n,d} - \mathcal{A}_{n,d}$. Let $S = \{1 \leq i \leq d-1 \ : p_i > 1\}$. Then $\#S \geq 2$. Let $i, j \in S$ with $i < j$. Let $u = x_i$ and $v = x_j$. Let $S(u) = \{u_1, u_2, \ldots, u_{p_i-1}, u_{p_i}\}$ and $S(v) = \left\{v_1, v_2, \ldots, v_{p_j-1}, v_{p_j}\right\}$ be the sets of pendant vertices adjacent to u and v, respectively. Let

$$T_u = C(\mathbf{p}) - vv_1 - vv_2 - \cdots - vv_{p_j-1} + uv_1 + uv_2 + \cdots + uv_{p_j-1}$$

and

$$T_v = C(\mathbf{p}) - uu_1 - uu_2 - \cdots - uu_{p_i-1} + vu_1 + vu_2 + \cdots + vu_{p_i-1}.$$

Then $T_u = C(\mathbf{q}) \in \mathcal{C}_{n,d}$ where $\mathbf{q} = \mathbf{p}$ except for $q_i = p_i + p_j - 1$ and $q_j = 1$ and $T_v = C(\mathbf{r}) \in \mathcal{C}_{n,d}$ where $\mathbf{r} = \mathbf{p}$ except for $r_i = 1$ and $r_j = p_j + p_i - 1$. By Lemma 1, $\mu_1(T_u) > \mu_1(C(\mathbf{p}))$ or $\mu_1(T_v) > \mu_1(C(\mathbf{p}))$. Suppose $\mu_1(T_u) > \mu_1(C(\mathbf{p}))$. Let $S_1 = \{1 \leq i \leq d-1 : q_i > 1\}$. By the definition of T_u, $\#S_1 = \#S - 1$. Suppose now $\mu_1(T_v) > \mu_1(C(\mathbf{p}))$. Let $S_2 = \{1 \leq i \leq d-1 : r_i > 1\}$. Also, by the definition of T_v, $\#S_2 = \#S - 1$. By a repeated application of the above argument, we finally arrive at a caterpillar $A_k = C(\widetilde{\mathbf{p}}) \in \mathcal{A}_{n,d}$ where $\widetilde{p}_i = 1$ for all $i \neq k$ and $\widetilde{p}_k = n - 2d + 3$ such that $\mu_1(A_k) > \mu_1(C(\mathbf{p}))$. $\square$

Corollary 1. *If $d = 3$ then $C(n-3, 1)$ has the largest Laplacian index among all trees on n vertices and diameter 3.*

Proof. Since any tree T on n vertices and diameter 3 is a complete caterpillar, we may take $T = C(p_1, p_2) \in \mathcal{C}_{n,3}$. By Theorem 2, there exists $C_1 = C(p_1 + p_2 - 1, 1) = C(n-3, 1) \in \mathcal{C}_{n,3}$ such that $\mu_1(C_1) \geq \mu_1(C)$ or there exists
$C_2 = C(1, p_1 + p_2 - 1) = C(1, n-3) \in \mathcal{C}_{n,3}$ such that $\mu_1(C_2) \geq \mu_1(C)$. Since C_1 and C_2 are isomorphic caterpillars, the result follows. □

From Theorem 2, it follows that among the caterpillars in $\mathcal{C}_{n,d}$ the largest Laplacian index is attained by a caterpillar in the subclass $\mathcal{A}_{n,d}$. Next, we order the caterpillars in $\mathcal{A}_{n,d}$ by their Laplacian indices.

A generalized Bethe tree is a rooted tree in which vertices at the same distance from the root have the same degree. In [7], we characterize the eigenvalues of the Laplacian and adjacency matrices of the tree $P_m\{B_i\}$ obtained from the path P_m and the generalized Bethe trees $B_1, B_2, ..., B_m$ obtained by identifying the root vertex of B_i with the $i-th$ vertex of P_m. This is the case for $C(\mathbf{p})$ in which the path is P_{d-1} and each star K_{1,p_i} is a generalized Bethe tree of 2 levels. From Theorem 2 in [7], we get

Theorem 3. The Laplacian eigenvalues of $C(\mathbf{p})$ are 1 with multiplicity $\sum_{i=1}^{d-1} p_i - (d-1)$ and the eigenvalues of the $(2d-2) \times (2d-2)$ irreducible nonnegative matrix

$$M(\mathbf{p}) = \begin{bmatrix} T(p_1) & E & & & \\ E & S(p_2) & E & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & S(p_{d-2}) & E \\ & & & E & T(p_{d-1}) \end{bmatrix}$$

where

$$T(x) = \begin{bmatrix} 1 & \sqrt{x} \\ \sqrt{x} & x+1 \end{bmatrix}, E = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, S(x) = T(x) + E.$$

Let $\rho(A)$ be the spectral radius of the matrix A.

Corollary 2. *The matrix $M(\mathbf{p})$ is singular, $\rho(M(\mathbf{p})) > 1$ and $\rho(M(\mathbf{p}))$ is the Laplacian index of $C(\mathbf{p})$.*

Proof. Since 0 is a Laplacian eigenvalue of any graph, an immediate consequence of Theorem 3 is that $M(\mathbf{p})$ is a singular matrix. Since $M(\mathbf{p})$ is a nonnegative irreducible matrix whose row sums are no constant, $\rho(M(\mathbf{p})) > 1$ [10]. From this fact and Theorem 3, $\rho(M(\mathbf{p}))$ is the Laplacian index of $C(\mathbf{p})$. □

Let $t(\lambda, x)$ and $s(\lambda, x)$ be the characteristic polynomials of the matrices $T(x)$ and $S(x)$ respectively. That is

$$t(\lambda, x) = \lambda^2 - (x+2)\lambda + 1$$

and

$$s(\lambda, x) = \lambda^2 - (x+3)\lambda + 2.$$

Then

$$s(\lambda, x) - t(\lambda, x) = 1 - \lambda.$$

Let us denote by $|A|$ the determinant of a square matrix A and by $\widetilde{B}$ the matrix obtained from a matrix B by deleting its last row and its last column. We recall Lemma 2.2 in [8].

Lemma 2. *For $i = 1, 2, ..., r$, let B_i be a matrix of order $k_i \times k_i$ and $\mu_{i,j}$ be arbitrary scalars. Then*

$$\begin{vmatrix} B_1 & \mu_{1,2}E_{1,2} & \cdots & \mu_{1,r-1}E_{1,r-1} & \mu_{1,r}E_{1,r} \\ \mu_{2,1}E_{1,2}^T & B_2 & \cdots & \cdots & \mu_{2,r}E_{2,r} \\ \mu_{3,1}E_{1,3}^T & \mu_{3,2}E_{2,3}^T & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & B_{r-1} & \mu_{r-1,r}E_{r-1,r} \\ \mu_{r,1}E_{1,r}^T & \mu_{r,2}E_{2,r}^T & \cdots & \mu_{r,r-1}E_{r-1,r}^T & B_r \end{vmatrix}$$

$$= \begin{vmatrix} |B_1| & \mu_{1,2}\left|\widetilde{B_2}\right| & \cdots & \mu_{1,r-1}\left|\widetilde{B_{r-1}}\right| & \mu_{1,r}\left|\widetilde{B_r}\right| \\ \mu_{2,1}\left|\widetilde{B_1}\right| & |B_2| & \cdots & \cdots & \mu_{2,r}\left|\widetilde{B_r}\right| \\ \mu_{3,1}\left|\widetilde{B_1}\right| & \mu_{3,2}\left|\widetilde{B_2}\right| & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & |B_{r-1}| & \mu_{r-1,r}\left|\widetilde{B_r}\right| \\ \mu_{r,1}\left|\widetilde{B_1}\right| & \mu_{r,2}\left|\widetilde{B_2}\right| & \cdots & \mu_{r,r-1}\left|\widetilde{B_{r-1}}\right| & |B_r| \end{vmatrix}.$$

The notation $|A|_l$ 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 application of Lemma 2 to the characteristic polynomial of $M(\mathbf{p})$.

Corollary 3. *The characteristic polynomial of* $M(\mathbf{p})$ *is*

$$|\lambda I - M(\mathbf{p})| = \begin{vmatrix} t(\lambda,p_1) & 1-\lambda & & & \\ 1-\lambda & s(\lambda,p_2) & 1-\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,p_{d-2}) & 1-\lambda \\ & & & 1-\lambda & t(\lambda,p_{d-1}) \end{vmatrix}_{d-1}.$$

From now on, let $a = n-2d+3$ and let $\mathbf{a}_k$ be the $(d-1)-$dimensional vector in which the $k-th$ component is equal to a and all the other components are equal to 1. Using this notation, $A_k = C(\mathbf{a}_k)$. Since the Laplacian index of $C(\mathbf{p}) \in \mathcal{C}_{n,d}$ is the spectral radius of $M(\mathbf{p})$, to find an order in $\mathcal{A}_{n,d}$ by the Laplacian index is equivalent to order the matrices $M(\mathbf{a}_1), M(\mathbf{a}_2), \ldots, M(\mathbf{a}_{d-1})$ by their spectral radii. Since A_k and A_{d-k} are isomorphic, we may take $1 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor$. Let $\phi_k(\lambda)$ be the characteristic polynomial of $M(\mathbf{a}_k)$, that is,

$$\phi_k(\lambda) = |\lambda I - M(\mathbf{a}_k)|.$$

By Corollary 3, the $(k,k)-$ entry of $\phi_k(\lambda) = |\lambda I - M(\mathbf{a}_k)|$ is $t(\lambda,a)$ if $k=1$ and $s(\lambda,a)$ if $k \neq 1$.

Let $\mathbf{e}_l$ be the all ones column vector with l entries. Let $\varphi_l(\lambda) = |\lambda I - M(\mathbf{e}_l)|$. By application of Corollary 3, we have

$$\varphi_l(\lambda) = \begin{vmatrix} t(\lambda,1) & 1-\lambda & & & \\ 1-\lambda & s(\lambda,1) & 1-\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & 1-\lambda \\ & & & 1-\lambda & t(\lambda,1) \end{vmatrix}_{l}.$$

Let

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

and, for $2 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor$, let

$$r_k(\lambda) = \begin{vmatrix} s(\lambda,1) & 1-\lambda & & & \\ 1-\lambda & \ddots & 1-\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & 1-\lambda \\ & & & 1-\lambda & t(\lambda,1) \end{vmatrix}_{k}.$$

Expanding along the first row, we obtain

$$r_k(\lambda) = s(\lambda,1)\, r_{k-1}(\lambda) - (\lambda-1)^2\, r_{k-2}(\lambda). \tag{2.1}$$

Since $s(\lambda,x) = t(\lambda,x) + 1 - \lambda$, by linearity on the first column, we have

$$r_k(\lambda) = \begin{vmatrix} t(\lambda,1) & 1-\lambda & & & \\ 1-\lambda & s(\lambda,1) & 1-\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & 1-\lambda \\ & & & 1-\lambda & t(\lambda,1) \end{vmatrix}_k + (1-\lambda)\, r_{k-1}(\lambda).$$

Therefore

$$r_k(\lambda) = \varphi_k(\lambda) + (1-\lambda)\, r_{k-1}(\lambda). \tag{2.2}$$

Let $1 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor - 1$. We search for the difference $\phi_k(\lambda) - \phi_{k+1}(\lambda)$. We recall that $(k,k)-$ entry of $\phi_k(\lambda) = |\lambda I - M(\mathbf{a}_k)|$ is $t(\lambda,a)$ if $k=1$ and $s(\lambda,a)$ if $k \neq 1$. Since $t(\lambda,a) = t(\lambda,1) + (1-a)\lambda$ and $s(\lambda,a) = s(\lambda,1) + (1-a)\lambda$, by linearity on the $k-th$ column, we have

$$\phi_k(\lambda) = \begin{vmatrix} t(\lambda,1) & 1-\lambda & & & \\ 1-\lambda & s(\lambda,1) & 1-\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & 1-\lambda \\ & & & 1-\lambda & t(\lambda,1) \end{vmatrix}_{d-1} \tag{2.3}$$

$$+(1-a)\lambda \begin{vmatrix} r_{k-1}(\lambda) & 0 \\ 0 & r_{d-k-1}(\lambda) \end{vmatrix}.$$

The $(k+1,k+1)-$entry of the determinant of order $d-1$ on the second right hand of (2.3) is $s(\lambda,1)$ and since $s(\lambda,1) = s(\lambda,a) + (a-1)\lambda$, by linearity on the $(k+1)-th$ column, we obtain

$$\begin{vmatrix} t(\lambda,1) & 1-\lambda & & & \\ 1-\lambda & s(\lambda,1) & 1-\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & 1-\lambda \\ & & & 1-\lambda & t(\lambda,1) \end{vmatrix}_{d-1}$$

$$= \phi_{k+1}(\lambda) + (a-1)\lambda \begin{vmatrix} r_k(\lambda) & 0 \\ 0 & r_{d-k-2}(\lambda) \end{vmatrix}.$$

Replacing in (2.3), we get

$$\begin{aligned} & \phi_k(\lambda) - \phi_{k+1}(\lambda) \\ = \quad & (1-a)\lambda \begin{vmatrix} r_{k-1}(\lambda) & 0 \\ 0 & r_{d-k-1}(\lambda) \end{vmatrix} + (a-1)\lambda \begin{vmatrix} r_k(\lambda) & 0 \\ 0 & r_{d-k-2}(\lambda) \end{vmatrix}. \end{aligned}$$

Thus

$$\phi_k(\lambda) - \phi_{k+1}(\lambda) = (a-1)\lambda\left[r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda)\right]. \tag{2.4}$$

Applying the recurrence formula (2.1) to $r_k(\lambda)$ and $r_{d-k-1}(\lambda)$, we obtain

$$\begin{aligned} & r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \\ = \quad & \left[s(\lambda,1) r_{k-1}(\lambda) - (\lambda-1)^2 r_{k-2}(\lambda)\right] r_{d-k-2}(\lambda) \\ & - r_{k-1}(\lambda)\left[s(\lambda,1) r_{d-k-2}(\lambda) - (\lambda-1)^2 r_{d-k-3}(\lambda)\right]. \end{aligned}$$

Then

$$\begin{aligned} & r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \\ = \quad & (\lambda-1)^2\left[r_{k-1}(\lambda) r_{d-k-3}(\lambda) - r_{k-2}(\lambda) r_{d-k-2}(\lambda)\right]. \end{aligned}$$

By a repeated application of this process, we conclude

$$\begin{aligned} & r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \\ = \quad & (\lambda-1)^{2(k-1)}\left(r_1(\lambda) r_{d-2k-1}(\lambda) - r_{d-2k}(\lambda)\right). \end{aligned}$$

Therefore

$$\begin{aligned} & r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \\ = \quad & (\lambda-1)^{2(k-1)}\left[t(\lambda,1) r_{d-2k-1}(\lambda) - s(\lambda,1) r_{d-2k-1}(\lambda) + (\lambda-1)^2 r_{d-2k-2}(\lambda)\right] \\ = \quad & (\lambda-1)^{2(k-1)}\left[(\lambda-1) r_{d-2k-1}(\lambda) + (\lambda-1)^2 r_{d-2k-2}(\lambda)\right] \\ = \quad & (\lambda-1)^{2k-1}\left[r_{d-2k-1}(\lambda) + (\lambda-1) r_{d-2k-2}(\lambda)\right] \\ = \quad & (\lambda-1)^{2k-1}\varphi_{d-2k-1}(\lambda). \end{aligned}$$

The last equality being a consequence of (2.2). Replacing in (2.4), we finally get

$$\phi_k(\lambda) - \phi_{k+1}(\lambda) = (a-1)\,\lambda\,(\lambda-1)^{2k-1}\,\varphi_{d-2k-1}(\lambda)\,. \tag{2.5}$$

From the Perron-Frobenius Theory for nonnegative matrices [10], if A is a nonnegative irreducible matrix then A has a unique eigenvalue equal to its spectral radius $\rho(A)$ and $\rho(A)$ increases whenever any entry of A increases. Hence $\rho(B) < \rho(A)$ if B is a proper submatrix of a nonnegative irreducible matrix A.

The next theorem gives a total ordering in $\mathcal{A}_{n,d}$ by the Laplacian index.

Theorem 4. Let $d \geq 4$. Then

$$\mu_1(A_1) = \mu_1(A_{d-1}) < \mu_1(A_2) = \mu_1(A_{d-2}) < \ldots < \mu_1\left(A_{\lfloor \frac{d}{2} \rfloor}\right) =$$

$$\mu_1\left(A_{d-\lfloor \frac{d}{2} \rfloor}\right).$$

Proof. Since A_k and A_{d-k} are isomorphic caterpillars, we may take $1 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor$. Let $1 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor - 1$. From Corollary 2, $\rho(M(\mathbf{a}_k)) = \mu_1(A_k) > 1$. Moreover, from the fact that $M(\mathbf{a}_k)$ is a nonnegative irreducible matrix, $\mu_1(A_k)$ is a simple eigenvalue. The identity (2.5) involves the polynomials $\phi_k(\lambda)$ and $\phi_{k+1}(\lambda)$ of degrees $2d-2$ which are the characteristic polynomials of $M(\mathbf{a}_k)$ and $M(\mathbf{a}_{k+1})$, respectively. Let

$$\mu_1(A_k) = \alpha_1 > \alpha_2 \geq \ldots \geq \alpha_{2d-2} = 0$$

and

$$\mu_1(A_{k+1}) = \beta_1 > \beta_2 \geq \ldots \geq \beta_{2d-2} = 0$$

be the eigenvalues of $M(\mathbf{a}_k)$ and $M(\mathbf{a}_{k+1})$, respectively. Then (2.5) becomes

$$\lambda\Pi_{j=1}^{2d-3}(\lambda-\alpha_j) - \lambda\Pi_{j=1}^{2d-3}(\lambda-\beta_j) = (a-1)\,\lambda\,(\lambda-1)^{2k-1}\,\varphi_{d-2k-1}(\lambda)\,. \tag{2.6}$$

We recall that $\varphi_{d-2k-1}(\lambda)$ of degree $2d-4k-2$ is the characteristic polynomial of the matrix $M(\mathbf{e}_{d-2k-1})$ whose spectral radius is $\mu_1(C(\mathbf{e}_{d-2k-1}))$.

Since $M(\mathbf{e}_{d-2k-1})$ is a proper submatrix of $M(\mathbf{a}_k)$, $\mu_1(C(\mathbf{e}_{d-2k-1})) < \mu_1(A_k)$. Hence $\varphi_{d-2k-1}(\mu_1(A_k)) > 0$. We claim $\mu_1(A_k) < \mu_1(A_{k+1})$. Suppose that $\mu_1(A_k) \geq \mu_1(A_{k+1})$. Then $\mu_1(A_k) \geq \beta_j$ for all j. Taking $\lambda = \mu_1(A_k)$ in (2.6), we obtain

$$-\mu_1(A_k)\Pi_{j=1}^{2d-3}(\mu_1(A_k)-\beta_j) =$$

$$(a-1)\mu_1(A_k)(\mu_1(A_k)-1)^{2k-1}\varphi_{d-2k-1}(\mu_1(A_k))$$

which is a contradiction because

$$-\mu_1(A_k)\Pi_{j=1}^{2d-3}(\mu_1(A_k)-\beta_j) \leq 0$$

and

$$(a-1)\mu_1(A_k)(\mu_1(A_k)-1)^{2k-1}\varphi_{d-2k-1}(\mu_1(A_k)) > 0.$$

Therefore $\mu_1(A_k) < \mu_1(A_{k+1})$. This completes the proof. □

Theorem 5. Among all complete caterpillars on n vertices and diameter d the largest Laplacian index is attained by $A_{\lfloor \frac{d}{2} \rfloor}$.

Proof. The case $d = 3$ is given in Corollary 1. If $d \geq 4$, the result follows from Theorem 2 and Theorem 4. □

3. The largest adjacency index among all complete caterpillars

In this section, we find the caterpillar having the largest adjacency index among all complete caterpillars on n vertices and diameter d.

Lemma 3. *Let u, v be two vertices of a connected graph G. For $1 \leq s \leq d(v)$, let $v_1, v_2, \ldots, v_s$ be some vertices in $N_G(v) - (N_G(u) \cup \{u\})$. Let*

$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \ldots & \ldots & x_n \end{bmatrix}^T$$

be the unit Perron vector of G corresponding to the adjacency index $\lambda_1(G)$. Let

$$G_u = G - vv_1 - \ldots - vv_s + uv_1 + \ldots + uv_s.$$

If $x_u \geq x_v$ then $\lambda_1(G_u) > \lambda_1(G)$.

Proof. By hypothesis, $x_u \geq x_v$. Then

$$\begin{aligned}\lambda_1(G_u) - \lambda_1(G) &\geq \mathbf{x}^T A(G_u)\mathbf{x} - \mathbf{x}^T A(G)\mathbf{x} \\ &= 2(x_u - x_v)\sum_{i=1}^{s} x_i \geq 0.\end{aligned}$$

Suppose that $\lambda_1(G_u) = \lambda_1(G)$. Then, from the above inequality, we get

$$\mathbf{x}^T A(G_u)\mathbf{x} = \mathbf{x}^T A(G)\mathbf{x} = \lambda_1(G) = \lambda_1(G_u).$$

Since $A(G_u)$ is a real symmetric matrix, from $\mathbf{x}^T A(G_u)\mathbf{x} = \lambda_1(G_u)$, we obtain

$$A(G_u)\mathbf{x} = \lambda_1(G_u)\mathbf{x}.$$

It follows that

$$\lambda_1(G_u)x_v = \sum_{w\in N_{G_u}(v)} x_w. \tag{3.1}$$

Moreover

$$\lambda_1(G)x_v = \sum_{w\in N_G(v)} x_w = \sum_{w\in N_{G_u}(v)} x_w + \sum_{i=1}^{s} x_{v_i}. \tag{3.2}$$

Subtracting (3.1) from (3.2), we obtain

$$0 = \sum_{i=1}^{s} x_{v_i} > 0,$$

which is a contradiction. Hence $\lambda_1(G_u) > \lambda_1(G)$. □

We comment that a version of Lemma 3 for the Laplacian index of a connected bipartite graph is given in [4].

An immediate consequence of Lemma 3 is

Lemma 4. *Let u, v be two vertices of a connected graph G. For $1 \leq s \leq d(v)$, let $v_1, v_2, \ldots, v_s$ be some vertices in $N_G(v) - (N_G(u) \cup \{u\})$. For $1 \leq t \leq d(u)$, let $u_1, u_2, \ldots, u_t$ be some vertices in $N_G(u) - (N_G(v) \cup \{v\})$. Let*

$$G_u = G - vv_1 - vv_2 - \cdots - vv_s + uv_1 + uv_2 + \cdots + uv_s$$

and

$$G_v = G - uu_1 - uu_2 - \cdots - uu_t + vu_1 + vu_2 + \cdots + vu_t.$$

Then $\lambda_1(G_u) > \lambda_1(G)$ or $\lambda_1(G_v) > \lambda_1(G)$.

By a repeated application of Lemma 4, using a similar argument to the proof of Theorem 2, we obtain

Theorem 6. Let $d \geq 3$. Let $C(\mathbf{p}) \in \mathcal{C}_{n,d}$ with $\mathbf{p} = [p_1, \ldots, p_{d-1}]$. There exists a caterpillar $A_k \in \mathcal{A}_{n,d}$ for some $1 \leq k \leq d-1$ such that $\lambda_1(A_k) \geq \lambda_1(C(\mathbf{p}))$.

Corollary 4. *If $d = 3$ then $C(n-3, 1)$ has the largest adjacency index among all trees on n vertices and diameter 3.*

Proof. Clearly $A_1 = C(n-3,1)$ and $A_2 = C(1, n-3)$ are isomorphic caterpillars. Since any tree of diameter 3 is a complete caterpillar, from Theorem 6, $\lambda_1(A_1) = \lambda_1(A_2) \geq \lambda_1(T)$ for any tree T on n vertices and diameter 3. $\square$

Now, we order the caterpillars in $\mathcal{A}_{n,d}$ by their adjacency indices. From Theorem 6 in [7], we have

Theorem 7. The adjacency eigenvalues of $C(\mathbf{p})$ are 0 with multiplicity $\sum_{i=1}^{d-1} p_i - (d-1)$ and the eigenvalues of the $(2d-2) \times (2d-2)$ irreducible nonnegative matrix

$$H(\mathbf{p}) = \begin{bmatrix} S(p_1) & E & & & \\ E & S(p_2) & E & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & S(p_{d-2}) & E \\ & & & E & S(p_{d-1}) \end{bmatrix}$$

where

$$S(x) = \begin{bmatrix} 0 & \sqrt{x} \\ \sqrt{x} & 0 \end{bmatrix}, E = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

An immediate consequence of Theorem 3 is

Corollary 5. *The spectral radius of $H(\mathbf{p})$ is the adjacency index of $C(\mathbf{p})$.*

Let $s(\lambda, x)$ be the characteristic polynomial of $S(x)$. That is

$$s(\lambda, x) = \lambda^2 - x.$$

We now apply Lemma 2 to the matrix $H(\mathbf{p})$.

Corollary 6. *The characteristic polynomial of $H(\mathbf{p})$ is*

$$|\lambda I - H(\mathbf{p})| = \begin{vmatrix} s(\lambda,p_1) & -\lambda & & & \\ -\lambda & s(\lambda,p_2) & -\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,p_{d-2}) & -\lambda \\ & & & -\lambda & s(\lambda,p_{d-1}) \end{vmatrix}_{d-1}.$$

We have $A_k = C(\mathbf{a}_k)$. Since the adjacency index of $C(\mathbf{p}) \in \mathcal{C}_{n,d}$ is equal to the spectral radius of $H(\mathbf{p})$, to order the caterpillars in $\mathcal{A}_{n,d}$ by their adjacency indices is equivalent to order the matrices $H(\mathbf{a}_1), H(\mathbf{a}_2), \ldots, H(\mathbf{a}_{d-1})$ by their spectral radii. We may take $1 \le k \le \left\lfloor \frac{d}{2} \right\rfloor$.

Let

$$\phi_k(\lambda) = |\lambda I - H(\mathbf{a}_k)|.$$

Let

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

and, for $2 \le k \le \left\lfloor \frac{d}{2} \right\rfloor$, let

$$r_k(\lambda) = \begin{vmatrix} s(\lambda,1) & -\lambda & & & \\ -\lambda & \ddots & -\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & s(\lambda,1) & -\lambda \\ & & & -\lambda & s(\lambda,1) \end{vmatrix}_{k}.$$

Expanding along the first row, we have

$$r_k(\lambda) = s(\lambda,1)\, r_{k-1}(\lambda) - \lambda^2 r_{k-2}(\lambda).$$

Clearly $s(\lambda,a) = s(\lambda,1) + (1-a)$. Let $1 \le k \le \left\lfloor \frac{d}{2} \right\rfloor - 1$.

Applying the same techniques of Section 2, the difference $\phi_k(\lambda) - \phi_{k+1}(\lambda)$ becomes

$$\phi_k(\lambda) - \phi_{k+1}(\lambda) = (a-1)\,\lambda^{2k} r_{d-2k-2}(\lambda).$$

The next theorem gives a total ordering in $\mathcal{A}_{n,d}$ by the adjacency index.

Theorem 8. Let $d \geq 4$. Then

$$\lambda_1(A_1) = \lambda_1(A_{d-1}) < \lambda_1(A_2) = \lambda_1(A_{d-2}) < \ldots < \lambda_1\left(A_{\lfloor \frac{d}{2} \rfloor}\right) = \lambda_1\left(A_{d-\lfloor \frac{d}{2} \rfloor}\right).$$

Proof. Similar to the proof of Theorem 4. □

Theorem 9. Among all complete caterpillars on n vertices and diameter d the largest adjacency index is attained by $A_{\lfloor \frac{d}{2} \rfloor}$.

Proof. The case $d = 3$ is given in Corollary 4. If $d \geq 4$, the result follows from Theorem 6 and Theorem 8. □

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Nair Abreu
Production Engineering Program, PEP/COPPE
Universidade Federal do Rio de Janeiro
Rio de Janeiro,
Brazil
e-mail: nairabreunovoa@gmail.com

Eber Lenes
Departamento de Investigaciones
Universidad del Sinú. Elías Bechara Zainúm
Cartagena,
Colombia
e-mail:elenes@ucn.cl

and

O. Rojo
Department of Mathematics
Universidad Católica del Norte
Antofagasta,
Chile
e-mail : orojo@ucn.cl