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

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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 $(0, e)$ is an eigenpair of $L(G)$ where $e$ 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 $T_{n,d}$ 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 $T_{n,d}$ 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 $T_{n,d}$ 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 $T_{n,d}$ 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 $p = \left[ \begin{array}{c} p_1 & \ldots & p_{d-1} \end{array} \right]$.

Let $C_{n,d}$ be the class of all complete caterpillars on $n$ vertices and diameter $d$. A caterpillar $C(p)$ in $C_{n,d}$ 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 $p_1 \geq 1, p_2 \geq 1, ..., p_{d-1} \geq 1$ and $p_1 + \ldots + p_{d-1} = n - d + 1$. A special subclass of $C_{n,d}$ is $A_{n,d} = \{ A_1, A_2, \ldots, A_{d-2}, A_{d-1} \}$ where $A_k = C(p) \in C_{n,d}$ 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 \( C_{n,d} \) the largest algebraic connectivity is attained by the caterpillar \( A_{\left\lceil \frac{d}{2} \right\rceil} \).

Numerical experiments suggest us that \( A_{\left\lceil \frac{d}{2} \right\rceil} \) is also the caterpillar attaining the largest Laplacian index in the class \( C_{n,d} \). In this paper, we prove that this conjecture is true. Moreover, we prove that \( A_{\left\lceil \frac{d}{2} \right\rceil} \) also attains the largest adjacency index in \( C_{n,d} \). To get these results, we first prove that the caterpillars in \( C_{n,d} \) attaining the mentioned largest indices lie in \( A_{n,d} \) 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 \( C(p) \in C_{n,d} \). Let \( C(p) \in C_{n,d} \) with \( p = [p_1, p_2, \ldots, p_{d-1}] \). Then
\[
d(x_1) = p_1 + 1, \quad d(p_2) = p_2 + 2, \ldots, d(x_{d-2}) = p_{d-2} + 2, \quad d(p_{d-1}) = p_{d-1} + 1.
\]

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

$$T_u = T - v_1v_2 - \cdots - vv_s + uv_1 + uv_2 + \cdots + uv_t$$

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

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

Proof. Let $\#S$ be the cardinality of a set $S$. Let $d \geq 3$. Let $C(p) \in \mathcal{C}_{n,d}$ with $p = [p_1 \ p_2 \ \cdots \ p_{d-1}]$.

If $C(p) \in \mathcal{A}_{n,d}$ then there is nothing to prove. Let $C(p) \in \mathcal{C}_{n,d} - \mathcal{A}_{n,d}$. 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 $S(u) = \{u_1, u_2, \ldots, u_{p_i-1}, u_{p_j}\}$ and $S(v) = \{v_1, v_2, \ldots, v_{p_j-1}, v_{p_j}\}$ be the sets of pendant vertices adjacent to $u$ and $v$, respectively. Let

$$T_u = C(p) - v_1v_2 - \cdots - vv_{p_j-1} + uv_1 + uv_2 + \cdots + uv_{p_j-1}$$

and

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

Then $T_u = C(q) \in \mathcal{C}_{n,d}$ where $q = p$ except for $q_i = p_i + p_j - 1$ and $q_j = 1$ and $T_v = C(r) \in \mathcal{C}_{n,d}$ where $r = p$ except for $r_i = 1$ and $r_j = p_j + p_i - 1$. By Lemma 1, $\mu_1(T_u) > \mu_1(C(p))$ or $\mu_1(T_v) > \mu_1(C(p))$.

Suppose $\mu_1(T_u) > \mu_1(C(p))$. Let $S_1 = \{1 \leq i \leq d - 1 : q_i > 1\}$. By the definition of $T_u$, $\#S_1 = \#S - 1$. Suppose now $\mu_1(T_v) > \mu_1(C(p))$. 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 $A_k = C(\tilde{p}) \in \mathcal{A}_{n,d}$ where $\tilde{p}_i = 1$ for all $i \neq k$ and $\tilde{p}_k = n - 2d + 3$ such that $\mu_1(A_k) > \mu_1(C(p))$. □

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 $T = C(p_1, p_2) \in C_{n,3}$. By Theorem 2, there exists $C_1 = C(p_1 + p_2 - 1, 1) = C(n - 3, 1) \in C_{n,3}$ such that $\mu_1(C_1) \geq \mu_1(C)$ or there exists $C_2 = C(1, p_1 + p_2 - 1) = C(1, n - 3) \in C_{n,3}$ such that $\mu_1(C_2) \geq \mu_1(C)$. Since $C_1$ and $C_2$ are isomorphic caterpillars, the result follows. \hfill \Box

From Theorem 2, it follows that among the caterpillars in $C_{n,d}$ the largest Laplacian index is attained by a caterpillar in the subclass $A_{n,d}$. Next, we order the caterpillars in $A_{n,d}$ 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 $C(p)$ 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 $C(p)$ 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

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

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 $M(p)$ is singular, $\rho(M(p)) > 1$ and $\rho(M(p))$ is the Laplacian index of $C(p)$. 

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

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 $\tilde{B}$ 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

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

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 $M(p)$. 
Corollary 3. The characteristic polynomial of $M(p)$ is

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

From now on, let $a = n - 2d + 3$ and let $a_k$ 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, $A_k = C(a_k)$. Since the Laplacian index of $C(p) \in C_{n,d}$ is the spectral radius of $M(p)$, to find an order in $A_{n,d}$ by the Laplacian index is equivalent to order the matrices $M(a_1), M(a_2), \ldots, M(a_{d-1})$ 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 $M(a_k)$, that is,

$$\phi_k(\lambda) = |\lambda I - M(a_k)|.$$ 

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

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

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

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

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

Expanding along the first row, we obtain

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

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

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

Therefore

\begin{equation}
 r_k (\lambda) = \varphi_k (\lambda) + (1 - \lambda) r_{k-1} (\lambda).
\end{equation}

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 \( \phi_k (\lambda) = |\lambda I - M (a_k)| \) is \( t (\lambda, a_k) \) if \( k = 1 \) and \( s (\lambda, a_k) \) if \( k \neq 1 \). Since \( t (\lambda, a_k) = t (\lambda, 1) + (1 - a) \lambda \) and \( s (\lambda, a_k) = s (\lambda, 1) + (1 - a) \lambda \), by linearity on the \( k \)th column, we have

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

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

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

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Replacing in (2.3), we get

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

Thus

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

(2.4)

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

\[ r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \]

\[ = \left[ s(\lambda, 1) r_{k-1}(\lambda) - (\lambda - 1)^2 r_{k-2}(\lambda) \right] r_{d-k-2}(\lambda) \]

\[ - r_{k-1}(\lambda) \left[ s(\lambda, 1) r_{d-k-2}(\lambda) - (\lambda - 1)^2 r_{d-k-3}(\lambda) \right]. \]

Then

\[ r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \]

\[ = (\lambda - 1)^2 \left[ r_{k-1}(\lambda) r_{d-k-3}(\lambda) - r_{k-2}(\lambda) r_{d-k-2}(\lambda) \right]. \]

By a repeated application of this process, we conclude

\[ r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \]

\[ = (\lambda - 1)^{2(k-1)} \left[ r_1(\lambda) r_{d-2k-1}(\lambda) - r_{d-2k}(\lambda) \right]. \]

Therefore

\[ r_k(\lambda) r_{d-k-2}(\lambda) - r_{k-1}(\lambda) r_{d-k-1}(\lambda) \]

\[ = (\lambda - 1)^{2(k-1)} \left[ t(\lambda, 1) r_{d-2k-1}(\lambda) - s(\lambda, 1) r_{d-2k-1}(\lambda) + (\lambda - 1)^2 r_{d-2k-2}(\lambda) \right] \]

\[ = (\lambda - 1)^{2(k-1)} \left[ (\lambda - 1) r_{d-2k-1}(\lambda) + (\lambda - 1)^2 r_{d-2k-2}(\lambda) \right] \]

\[ = (\lambda - 1)^{2k-1} \left[ r_{d-2k-1}(\lambda) + (\lambda - 1) r_{d-2k-2}(\lambda) \right] \]

\[ = (\lambda - 1)^{2k-1} \varphi_{d-2k-1}(\lambda). \]
The last equality being a consequence of (2.2). Replacing in (2.4), we finally get
\[
\phi_k(\lambda) - \phi_{k+1}(\lambda) = (a - 1) \lambda (\lambda - 1)^{2k-1} \varphi_{d-2k-1}(\lambda).
\]

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 \( A_{n,d} \) by the Laplacian index.

**Theorem 4.** Let \( d \geq 4 \). Then
\[
\mu_1(A_1) = \mu_1(A_{d-1}) < \mu_1(A_2) = \mu_1(A_{d-2}) < \ldots < \mu_1\left(A_{\left\lfloor \frac{d}{2} \right\rfloor}\right) = \mu_1\left(A_{d-\left\lfloor \frac{d}{2} \right\rfloor}\right).
\]

**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, \( \rho(M(a_k)) = \mu_1(A_k) > 1 \). Moreover, from the fact that \( M(a_k) \) 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 \( M(a_k) \) and \( M(a_{k+1}) \), 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 \( M(a_k) \) and \( M(a_{k+1}) \), respectively. Then (2.5) becomes
\[
\lambda \Pi_{j=1}^{2d-3} (\lambda - \alpha_j) - \lambda \Pi_{j=1}^{2d-3} (\lambda - \beta_j) = (a - 1) \lambda (\lambda - 1)^{2k-1} \varphi_{d-2k-1}(\lambda).
\]
(2.6)

We recall that \( \varphi_{d-2k-1}(\lambda) \) of degree \( 2d - 4k - 2 \) is the characteristic polynomial of the matrix \( M(e_{d-2k-1}) \) whose spectral radius is \( \mu_1(C(e_{d-2k-1})) \).
Since \( M(e_{d-2k-1}) \) is a proper submatrix of \( M(a_k) \), \( \mu_1(C(e_{d-2k-1})) < \mu_1(A_k) \). 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. \( \square \)

**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. \( \square \)

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

\[
\mathbf{x} = [x_1 \ x_2 \ \ldots \ x_n]^T
\]

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
\[
\lambda_1 (G_u) - \lambda_1 (G) \geq x^T A(G_u)x - x^T A(G)x \\
= 2(x_u - x_v) \sum_{i=1}^{s} x_i \geq 0.
\]

Suppose that \( \lambda_1 (G_u) = \lambda_1 (G) \). Then, from the above inequality, we get
\[
x^T A(G_u)x = x^T A(G)x = \lambda_1 (G) = \lambda_1 (G_u).
\]

Since \( A(G_u) \) is a real symmetric matrix, from \( x^T A(G_u)x = \lambda_1 (G_u) \), we obtain
\[
A(G_u)x = \lambda_1 (G_u)x.
\]

It follows that
\[
\lambda_1 (G_u)x_v = \sum_{w \in N_G(v)} x_w.
\]

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

Subtracting (3.1) from (3.2), we obtain
\[
0 = \sum_{i=1}^{s} x_{v_i} > 0,
\]
which is a contradiction. Hence \( \lambda_1 (G_u) > \lambda_1 (G) \). \( \square \)

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
\[
G_u = G - vv_1 - vv_2 - \cdots - vv_s + uu_1 + uu_2 + \cdots + uu_t
\]
and
\[
G_v = G - uu_1 - uu_2 - \cdots - uu_t + vv_1 + vv_2 + \cdots + vv_s.
\]
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 \( C(p) \in \mathcal{C}_{n,d} \) with \( p = [p_1, \ldots, p_{d-1}] \). There exists a caterpillar \( A_k \in \mathcal{A}_{n,d} \) for some \( 1 \leq k \leq d - 1 \) such that \( \lambda_1(A_k) \geq \lambda_1(C(p)) \).

**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 \( C(p) \) 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

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

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 \( H(p) \) is the adjacency index of \( C(p) \).

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 \( H(p) \).
Corollary 6. The characteristic polynomial of $H(p)$ is

$$|\lambda I - H(p)|$$

$$= \begin{vmatrix} s(\lambda, p_1) & -\lambda & & & \\ -\lambda & s(\lambda, p_2) & -\lambda & & \\ & \ddots & \ddots & \ddots & \\ & & s(\lambda, p_{d-2}) & -\lambda & \\ & & & -\lambda & s(\lambda, p_{d-1}) \end{vmatrix}_{d-1}$$

We have $A_k = C(a_k)$. Since the adjacency index of $C(p) \in C_{n,d}$ is equal to the spectral radius of $H(p)$, to order the caterpillars in $A_{n,d}$ by their adjacency indices is equivalent to order the matrices $H(a_1), H(a_2), \ldots, H(a_{d-1})$ by their spectral radii. We may take $1 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor$.

Let

$$\phi_k(\lambda) = |\lambda I - H(a_k)|.$$  

Let

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

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

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

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 $1 \leq k \leq \left\lfloor \frac{d}{2} \right\rfloor - 1$.

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 $A_{n,d}$ by the adjacency index.
Theorem 8. Let \( d \geq 4 \). Then
\[
\lambda_1 (A_1) = \lambda_1 (A_{d-1}) < \lambda_1 (A_2) = \lambda_1 (A_{d-2}) < \ldots < \lambda_1 \left( A_{\left\lfloor \frac{d}{2} \right\rfloor} \right) = \lambda_1 \left( A_{d-\left\lfloor \frac{d}{2} \right\rfloor} \right).
\]

Proof. Similar to the proof of Theorem 4. \( \square \)

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

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

References


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