On the algebraic connectivity of some caterpillars: A sharp upper bound and a total ordering

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ABSTRACT

A caterpillar is a tree in which the removal of all pendant vertices makes it a path. Let $d \geq 3$ and $n > 2(d - 1)$ be given. Let $p = [p_1, p_2, \ldots, p_{d-1}]$ with $p_1 \geq 1, p_2 \geq 1, \ldots, p_{d-1} \geq 1$. Let $C(p)$ be the caterpillar obtained from the stars $S_{p_1}, S_{p_2}, \ldots, S_{p_{d-1}}$ and the path $P_{d-1}$ by identifying the root of $S_{p_i}$ with the $i$-vertex of $P_{d-1}$. Let

$$C = \{C(p) : p_1 + p_2 + \cdots + p_{d-1} = n - d + 1\}.$$ 

We prove that the algebraic connectivity of $C(p) \in C$ is bounded above by

$$\frac{1}{2} \left( 4 + \sigma - \sqrt{\sigma^2 + 4\sigma + 8} \right), \quad \sigma = 2 \cos \left( \frac{(d - 2)\pi}{d - 1} \right).$$

Moreover, we prove that if $d$ is even then $C(\bar{p})$,

$$\bar{p} = \left[ 1, \ldots, 1, \bar{p}_{\frac{d}{2}}, 1, \ldots, 1 \right], \quad \bar{p}_{\frac{d}{2}} = n - 2d + 3,$$

is the unique caterpillar in $C$ attaining the upper bound and that if $d$ is odd then the upper bound cannot be achieved. Finally, for $1 \leq k \leq \left\lfloor \frac{d-1}{2} \right\rfloor$, we give a total ordering by algebraic connectivity on

$$C_k = \{C(1, \ldots, 1, p_k, 1, \ldots, 1, p_{d-k}, 1, \ldots, 1) : p_k \leq p_{d-k} \}.$$
1. Introduction

Let $G = (V, E)$ be a simple undirected graph on $n$ vertices. The Laplacian matrix of $G$ is the matrix $L(G) = D(G) - A(G)$ where $A(G)$ is the adjacency matrix and $D(G)$ is the diagonal matrix of vertex degrees. It is well known that $L(G)$ is a positive semidefinite matrix and that $(0, e)$ is an eigenpair of $L(G)$ where $e$ is the all ones vector. In [1], some of the many results known for Laplacian matrices are given. Fiedler [2] proved that $G$ is a connected graph if and only if the second smallest Laplacian eigenvalue is positive. This eigenvalue is called the algebraic connectivity of $G$ and it is denoted by $a(G)$. In [3], a survey on old and new results on the algebraic connectivity of graphs is given.

A tree is a connected acyclic graph. Let $P_n$ be a path on $n$ vertices and $S_p$ be a star on $(p + 1)$ vertices. Let $S(a, b, d)$ be a tree with $n$ vertices and diameter $d$ obtained from the path $P_{d-1}$ and the stars $S_a$ and $S_b$ by identifying the pendant vertices in $P_{d-1}$ with the roots of the stars. We may consider $a \leq b$. Observe that $b = n - a - (d - 1)$.

The problem of ordering trees by algebraic connectivity is an active area of research. This problem has been totally solved by Grone and Merris in [4] for trees of diameter $d = 3$. They prove that the algebraic connectivity of $S(a, b, 3)$, $b = n - a - 2$, is the unique Laplacian eigenvalue less than 1 and it is a strictly decreasing function for $1 \leq a \leq \frac{1}{2}(n - 2)$. Important contributions to the problem for trees of order $n$ and diameter $d = 4$ are due to Zhang [5]. Yuan et al. [6] introduce six classes of trees with $n$ vertices and determine the ordering of those trees by this spectral invariant. Shao et al. [7] determine the first four trees of order $n \geq 9$ with the smallest algebraic connectivity. In this same year, Zhang and Liu [8] found the largest twelve values of algebraic connectivity of trees in a set of trees on $2k + 1$ vertices with nearly perfect matching. A total ordering by algebraic connectivity on

$$\left\{ S(a, b, d) : 1 \leq a \leq \frac{1}{2}(n - d + 1), \ b = n - a - (d - 1) \right\},$$

due to Fallat and Kirkland [9], is implicitly given in the proof of Theorem 3.2 in which they prove that among all trees of $n$ vertices and diameter $d$, the minimum algebraic connectivities is attained by the tree $S(\left\lfloor \frac{n - d + 1}{2} \right\rfloor, \left\lfloor \frac{n - d + 1}{2} \right\rfloor, d)$. In fact, the total ordering in $S(a, b, d)$ can be explicitly stated as follows.

**Theorem 1.** The algebraic connectivity of $S(a, b, d)$, $b = n - a - (d - 1)$, is a strictly decreasing function for $1 \leq a \leq \frac{1}{2}(n - (d - 1))$.

A caterpillar is a tree in which the removal of all pendant vertices makes it a path. We observe that the caterpillars are the trees having minimal algebraic connectivity among all trees with a given degree sequence [10].

Let $d \geq 3$ and $n > 2(d - 1)$. Let $p = [p_1, p_2, \ldots, p_{d-1}]$ where $p_1 \geq 1, p_2 \geq 1, \ldots, p_{d-1} \geq 1$.

Throughout this paper $C(p)$ is the caterpillar obtained from the stars $S_{p_1}, S_{p_2}, \ldots, S_{p_{d-1}}$ and the path $P_{d-1}$ by identifying the root of $S_{p_i}$ with the $i$-vertex of $P_{d-1}$. Let

$$C = \{ C(p) : p_1 + p_2 + \cdots + p_{d-1} = n - d + 1 \}.$$

We prove that if $C(p) \in C$ then

$$\frac{a(C(p))}{2} \leq \frac{1}{2} \left( 4 + \sigma - \sqrt{\sigma^2 + 4\sigma + 8} \right), \quad \sigma = 2 \cos \left( \frac{(d - 2)\pi}{d - 1} \right).$$

Moreover, we prove that if $d$ is even then $C(p)$,

$$\bar{p} = [1, \ldots, 1, \bar{p}_{d-1}, 1, \ldots, 1], \quad \bar{p}_{d-1} = n - 2d + 3,$$

is the unique caterpillar in $C$ for which the equality holds and that if $d$ is odd then the equality cannot be achieved. Finally, we give a total ordering by algebraic connectivity on the subclasses
\[ C_1 = \{ C(p_1, 1, \ldots, 1, p_{d-1}) \in C : p_1 \leq p_{d-1} \}, \]
\[ C_{d-1} = \left\{ C \left( 1, \ldots, 1, p_{d-1}, p_{d+1}, 1, \ldots, 1 \right) \in C : \frac{p_{d-1} + 1}{2} \leq p_{d+1} \right\}, \]

whenever \( d \) is odd, and for \( 1 < k < \left\lfloor \frac{d-1}{2} \right\rfloor \) on
\[ C_k = \{ C(1, \ldots, 1, p_k, 1, \ldots, 1, p_{d-k}, 1, \ldots, 1) \in C : p_k \leq p_{d-k} \} . \]

2. Preliminaries

A generalized Bethe tree is a rooted tree in which vertices at the same distance from the root have the same degree. In [11], we characterize completely the Laplacian eigenvalues of the tree \( P_m[B_i] \) obtained from the path \( P_m \) and \( m \) generalized Bethe trees \( B_1, B_2, \ldots, B_m \) by identifying the root of \( B_i \) with the \( i \)th vertex of \( P_m \). This is the case for the caterpillar \( C(p) \) in which the path is \( P_{d-1} \) and the \( (d - 1) \)-generalized Bethe trees are the stars \( S_{p_i}(1 \leq i \leq d - 1) \).

Example 1. The following caterpillar is obtained from the path \( P_6 \) and the stars \( S_2, S_1, S_2, S_5, S_3 \) and \( S_1 \) by identifying the root of each star with the corresponding vertex of \( P_6 \):

Thus we may apply the results in [11] to characterize the eigenvalues of the caterpillar \( C(p) \), in particular its algebraic connectivity. Let
\[ A(x) = \begin{bmatrix} 1 & \sqrt{x} \\ \sqrt{x} & x + 1 \end{bmatrix}, \]
\[ B(x) = \begin{bmatrix} 1 & \sqrt{x} \\ \sqrt{x} & x + 2 \end{bmatrix} \]
and
\[ E = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \]

Applying Theorem 4 of [11] to \( C(p) \), one can obtain the following theorem:

Theorem 2. The algebraic connectivity of \( C(p) \) is the smallest positive eigenvalue of the \( 2(d - 1) \times 2(d - 1) \) positive semidefinite matrix
\[ Z_{2(d-1)}(p) = \begin{bmatrix} A(p_1) & E & E & \cdots & E \\ E & B(p_2) & E & \cdots & E \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ E & \cdots & \cdots & \cdots & B(p_{d-2}) \\ E & \cdots & \cdots & \cdots & A(p_{d-1}) \end{bmatrix}. \]
Example 2. For the caterpillar in Example 1, we have \( \mathbf{p} = [2 \ 1 \ 2 \ 5 \ 3 \ 1] \) and then, from Theorem 2, its algebraic connectivity is the smallest positive eigenvalue of the \( 12 \times 12 \) matrix \( Z_{12}(\mathbf{p}) \) composed by the codiagonal blocks \( E \) and by following the diagonal blocks

\[
A(2) = \begin{bmatrix}
1 & \sqrt{2} \\
\sqrt{2} & 3
\end{bmatrix}, \quad B(1) = \begin{bmatrix}
1 & 1 \\
1 & 3
\end{bmatrix}, \quad B(2) = \begin{bmatrix}
1 & \sqrt{2} \\
\sqrt{2} & 4
\end{bmatrix}, \\
B(5) = \begin{bmatrix}
1 & \sqrt{5} \\
\sqrt{5} & 7
\end{bmatrix}, \quad B(3) = \begin{bmatrix}
1 & \sqrt{3} \\
\sqrt{3} & 5
\end{bmatrix}, \quad A(1) = \begin{bmatrix}
1 & 1 \\
1 & 2
\end{bmatrix}.
\]

The following lemma will play a special role in this paper. Let \( |A| \) be the determinant of a matrix \( A \) and let \( \widetilde{A} \) be the submatrix obtained from a matrix \( A \) by deleting its last row and its last column.

Lemma 1 ([12, Lemma 2.2]). For \( i = 1, 2, \ldots, m \), let \( B_i \) be a matrix of order \( k_i \times k_i \) and \( \mu_{ij} \) be arbitrary scalars and \( E_{ij} \) be the \( k_i \times k_j \) matrix with \( E_{ij}(i, j) = 1 \) and 0 elsewhere. Then

\[
\begin{vmatrix}
B_1 \mu_{1,2} E_{1,2} & \cdots & \mu_{1,m-1} E_{1,m-1} & \mu_{1,m} E_{1,m} \\
\mu_{2,1} E_{1,2} & B_2 & \cdots & \cdots & \mu_{2,m} E_{2,m} \\
\mu_{3,1} E_{1,3} & \cdots & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\mu_{m,1} E_{1,m} & \mu_{m,2} E_{2,m} & \cdots & \mu_{m,m-1} E_{m-1,m} & B_m
\end{vmatrix} = \begin{vmatrix}
|B_1| & \mu_{1,2} \widetilde{B}_2 & \cdots & \mu_{1,m-1} \widetilde{B}_{m-1} & \mu_{1,m} \widetilde{B}_m \\
\mu_{2,1} \widetilde{B}_1 & |B_2| & \cdots & \cdots & \mu_{2,m} \widetilde{B}_m \\
\mu_{3,1} \widetilde{B}_1 & \mu_{3,2} \widetilde{B}_2 & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\mu_{m,1} \widetilde{B}_1 & \mu_{m,2} \widetilde{B}_2 & \cdots & \mu_{m,m-1} \widetilde{B}_{m-1} & |B_m|
\end{vmatrix}.
\]

Next we derive explicit formulas for the eigenvalues of matrices that will appear in this paper. We define the \( 2m \times 2m \) matrices

\[
Z_{2m} = \begin{bmatrix}
A(1) & E \\
E & B(1) & E \\
\vdots & \vdots & \vdots \\
E & B(1) & E \\
E & A(1) & E
\end{bmatrix} = Z_{2m}(\mathbf{e}), \\
Y_{2m} = \begin{bmatrix}
B(1) & E \\
E & B(1) & E \\
\vdots & \vdots & \vdots \\
E & B(1) & E \\
E & E & B(1)
\end{bmatrix} = Y_{2m}(\mathbf{e}).
\]
\[ X_{2m} = \begin{bmatrix} \begin{array}{cccc} A(1) & E \\
E & B(1) & & \\
& & \ddots & \\
& & & B(1) \\
& & & E \\
& & & B(1) \end{array} \end{bmatrix} = X_{2m}(e) \]

and
\[ W_{2m} = \begin{bmatrix} \begin{array}{cccc} B(1) & E \\
E & B(1) & & \\
& & \ddots & \\
& & & B(1) \\
& & & E \\
& & & E \end{array} \end{bmatrix} = W_{2m}(e). \]

Throughout this paper, \( I \) is the identity matrix of the appropriate order and \( f \) is the function
\[ f(x) = \frac{1}{2} \left( 4 + x - \sqrt{x^2 + 4x + 8} \right). \]

One can easily prove that \( f \) is a strictly increasing function. This fact will be repeatedly used in this paper.

We recall that the Kronecker product [13] of two matrices \( P = (p_{ij}) \) and \( Q = (q_{ij}) \) of sizes \( m \times m \) and \( n \times n \), respectively, is defined to be the \( (mn) \times (mn) \) matrix \( P \otimes Q = (p_{ij}Q) \). For matrices \( P, Q, R \) and \( S \) of appropriate sizes, we have
\[ (P \otimes Q) (R \otimes S) = (PR) \otimes QS. \] (1)

**Lemma 2.** The eigenvalues of \( Z_{2m} \) are
\[ \frac{1}{2} \left( 4 + \sigma_j \pm \sqrt{\sigma_j^2 + 4\sigma_j + 8} \right), \]
for \( j = 1, 2, \ldots, m \), where
\[ \sigma_j = 2 \cos \frac{(m + 1 - j) \pi}{m}. \]

In particular, the smallest positive eigenvalue of \( Z_{2m} \) is
\[ f(\sigma) = \frac{1}{2} \left( 4 + \sigma - \sqrt{\sigma^2 + 4\sigma + 8} \right), \]
\[ \sigma = \sigma_2 = 2 \cos \frac{(m - 1) \pi}{m}. \]

**Proof.** For brevity, we write \( A(1) = A \) and \( B(1) = B \). We have
\[ Z_{2m} = \begin{bmatrix} \begin{array}{cccc} B - E & E & E \\
E & B & E \\
& E & \ddots & \\
& & \ddots & E \\
& & & E \\
& & & B \end{array} \end{bmatrix}. \]

Then
\[ Z_{2m} = I_m \otimes B + T_m \otimes E, \]

where

\[
T_m = \begin{bmatrix}
-1 & 1 & & \\
1 & 0 & & \\
& & \ddots & \\
& & & 0 & 1 \\
& & & & 1 & -1
\end{bmatrix}.
\]

The eigenvalues of \( T_m \) in increasing order are

\[ \sigma_j = 2 \cos \left( \frac{m + 1 - j}{m} \pi \right), \quad 1 \leq j \leq m. \]

Let

\[
V = [v_1 \ v_2 \ \cdots \ v_{m-1} \ v_m]
\]

be a orthogonal matrix whose columns \( v_1, v_2, \ldots, v_m \) are eigenvectors corresponding to the eigenvalues \( \sigma_1, \sigma_2, \ldots, \sigma_m \). Using (1), we obtain

\[
(V \otimes I_m) Z_{2m} (V^T \otimes I_m) = (V \otimes I_m) (I_m \otimes B + T_m \otimes E) (V^T \otimes I_m) = I_m \otimes B + (V T_m V^T) \otimes E.
\]

Moreover

\[
(V T_m V^T) \otimes E = \begin{bmatrix}
\sigma_1 & & & \\
& \sigma_2 & & \\
& & \ddots & \\
& & & \sigma_m
\end{bmatrix} \otimes E
\]

\[
= \begin{bmatrix}
\sigma_1 E & & & \\
& \sigma_2 E & & \\
& & \ddots & \\
& & & \sigma_{m-1} E + \sigma_m E
\end{bmatrix}.
\]

Therefore

\[
(V \otimes I_m) Z_{2m} (V^T \otimes I_m) = \begin{bmatrix}
B + \sigma_1 E & & & \\
& B + \sigma_2 E & & \\
& & \ddots & \\
& & & B + \sigma_{m-1} E + \sigma_m E
\end{bmatrix}.
\]

Consequently

\[
\sigma(Z_{2m}) = \bigcup_{j=1}^m \sigma \left( \begin{bmatrix} 1 & 1 \\ 1 & 3 + \sigma_j \end{bmatrix} \right).
\]
Then the eigenvalues of $Z_{2m}$ are
\[ \frac{1}{2} \left( 4 + \sigma_j \pm \sqrt{\sigma_j^2 + 4\sigma_j + 8} \right) \]
for $j = 1, 2, \ldots, m$. Since $f(x) = \frac{1}{2} (4 + x - \sqrt{x^2 + 4x + 8})$ is strictly increasing and $f(\sigma_1) = f(-2) = 0$, the smallest positive eigenvalue of $Z_{2m}$ is
\[ f(\sigma_2) = \frac{1}{2} \left( 4 + \sigma_2 - \sqrt{\sigma_2^2 + 4\sigma_2 + 8} \right). \]
\[ \sigma_2 = 2 \cos \left( \frac{m - 1}{m} \pi \right). \]
The proof is complete. \( \square \)

Using the same technique, we now derive the eigenvalues of $Y_{2m}, X_{2m}$ and $W_{2m}$.

**Lemma 3.** The eigenvalues of $Y_{2m}$ are
\[ \frac{1}{2} \left( 4 + \rho_j \pm \sqrt{\rho_j^2 + 4\rho_j + 8} \right), \]
\[ \rho_j = 2 \cos \left( \frac{m + 1 - j}{m + 1} \pi \right) \]
for $j = 1, 2, \ldots, m$. In particular, its smallest eigenvalue is
\[ f(\rho) = \frac{1}{2} \left( 4 + \rho - \sqrt{\rho^2 + 4\rho + 8} \right), \]
\[ \rho = \rho_1 = 2 \cos \left( \frac{m\pi}{m + 1} \right). \]

**Proof.** Let $B(1) = B$. We have
\[ Y_{2m} = I_m \otimes B + R_m \otimes E, \]
where
\[
R_m = \begin{bmatrix}
0 & 1 \\
1 & 0 & \ddots \\
& \ddots & \ddots & \ddots \\
& & \ddots & 0 & 1 \\
& & & 1 & 0
\end{bmatrix}
\]
The eigenvalues of $R_m$ \cite{14} in increasing order are
\[ \rho_j = 2 \cos \left( \frac{m + 1 - j}{m + 1} \pi \right), \quad 1 \leq j \leq m. \]
As in the proof of Lemma 2, we obtain
\[ \sigma (Y_{2m}) = \bigcup_{j=1}^{m} \sigma \left( \begin{bmatrix}
1 & 1 \\
1 & 3 + \rho_j
\end{bmatrix} \right). \]
Thus the eigenvalues of $Y_{2m}$ are those given in (2). Since $f(x) = \frac{1}{2} (4 + x - \sqrt{x^2 + 4x + 8})$ is strictly increasing, the smallest eigenvalue of $Y_{2m}$ is obtained for $j = 1$ in (2). \( \square \)
Lemma 4. The eigenvalues of $X_{2m}$ and $W_{2m}$ are

$$\frac{1}{2} \left( 4 + \mu_j \pm \sqrt{\mu_j^2 + 4\mu_j + 8} \right),$$

$$\mu_j = 2 \cos \frac{2(m + 1 - j) \pi}{2m + 1}$$

for $j = 1, 2, \ldots, m$. In particular, its smallest eigenvalue is

$$f(\mu) = \frac{1}{2} \left( 4 + \mu - \sqrt{\mu^2 + 4\mu + 8} \right),$$

$$\mu = \mu_1 = 2 \cos \frac{2m\pi}{2m + 1}.$$

Proof. We observe that $X_{2m}$ and $W_{2m}$ are similar matrices. Let $A(1) = A$ and $B(1) = B$. We have

$$X_{2m} = \begin{bmatrix} B - E & E & E & \cdots & E \\ E & B & \cdots & & \cdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \cdots & & B & E & \cdots \\ E & \cdots & E & B & \cdots \end{bmatrix}.$$

Then

$$X_{2m} = I_m \otimes B + T_m \otimes E,$$

where

$$T_m = \begin{bmatrix} -1 & 1 & & & \\ 1 & 0 & \ddots & & \\ & \ddots & \ddots & \ddots & \vdots \\ \cdots & & 0 & 1 & \\ & & \cdots & 1 & 0 \end{bmatrix}.$$

The eigenvalues of $T_m$ [14] in increasing order are

$$\mu_j = 2 \cos \frac{2(m + 1 - j) \pi}{2m + 1}, \quad 1 \leq j \leq m.$$

Again as in the proof of Lemma 2, we obtain

$$\sigma(X_{2m}) = \bigcup_{j=1}^{m} \sigma \left( \begin{bmatrix} 1 & 1 \\ 1 & 3 + \mu_j \end{bmatrix} \right).$$

Thus the eigenvalues of $X_{2m}$ are as in (3). Since $f(x) = \frac{1}{2} (4 + x - \sqrt{x^2 + 4x + 8})$ is strictly increasing, the smallest eigenvalue of $X_{2m}$ is obtained for $j = 1$ in (3). \hfill \Box

3. A sharp upper bound on the algebraic connectivity

In this Section, we derive an upper bound on the algebraic connectivity of the caterpillars in $C$. We recall the following lemma.
**Lemma 5** [15, Corollary 4.2]. Let \(v\) be a pendant vertex of the graph \(\tilde{G}\). Let \(G\) be the graph obtained from \(\tilde{G}\) by removing \(v\) and its edge. Then the eigenvalues of \(L(G)\) interlace the eigenvalues of \(L(\tilde{G})\).

From Lemma 5, it follows

**Corollary 1.** Let \(T\) be a subtree of the tree \(\tilde{T}\). Then
\[
a(\tilde{T}) \leq a(T).
\]

**Theorem 3.** If \(C(p) \in C\) then
\[
a(C(p)) \leq f(\sigma),
\]
\[
f(\sigma) = \frac{1}{2} \left( 4 + \sigma - \sqrt{\sigma^2 + 4\sigma + 8} \right),
\]
\[
\sigma = 2 \cos \left( \frac{(d-2)\pi}{d-1} \right).
\]

If \(d\) is even then
\[
a(C(\tilde{p})) = f(\sigma),
\]
where
\[
\tilde{p} = \left[ 1, \ldots, 1, \tilde{p}_{\frac{d}{2}}, 1, \ldots, 1 \right],
\]
\[
\tilde{p}_{\frac{d}{2}} = n - 2d + 3
\]
and \(C(\tilde{p})\) is the unique caterpillar in \(C\) attaining the upper bound. If \(d\) is odd then the upper bound cannot be achieved.

**Proof.** Let \(e = [1, 1, \ldots, 1]\) with \((d-1)\) entries. Since \(C(e)\) is a subtree of any \(C(p) \in C\), from Corollary 1
\[
a(C(p)) \leq a(C(e)).
\]
From Theorem 2, \(a(C(e))\) is the smallest positive eigenvalue of the matrix \(Z_{2(d-1)}\). Moreover, from Lemma 2
\[
a(C(e)) = f(\sigma) = \frac{1}{2} \left( 4 + \sigma - \sqrt{\sigma^2 + 4\sigma + 8} \right),
\]
\[
\sigma = 2 \cos \left( \frac{(d-2)\pi}{d-1} \right).
\]
From (6) and (7), the upper bound in (4) is immediate.

Next we prove that the upper bound in (4) is attained whenever \(d\) is even by the caterpillar \(C(\tilde{p})\) with \(\tilde{p}\) as in (5). Suppose \(d = 2s + 2\). Observe that \(C(\tilde{p}) \in C\). We claim that \(a(C(\tilde{p})) = a(C(e))\). From Theorem 2, \(a(C(\tilde{p}))\) and \(a(C(e))\) are the smallest positive eigenvalues of the matrices \(Z_{2(d-1)}(\tilde{p})\) and \(Z_{2(d-1)}\), respectively. These matrices have the forms
\[
Z_{2(d-1)}(\tilde{p}) = \begin{bmatrix} X_{d-2} & \left[ 0 \ E \right]^T & 0 \\ 0 & E & \left[ E \ 0 \right] \\ B(\tilde{p}_{s+1}) & \left[ E \ 0 \right]^T & W_{d-2} \end{bmatrix}
\]
and
\[
Z_{2(d-1)} = \begin{bmatrix} X_{d-2} & \left[ 0 \ E \right]^T & 0 \\ 0 & E & \left[ E \ 0 \right]^T \\ \left[ 0 \ E \right] & B(1) & \left[ E \ 0 \right] \end{bmatrix},
\]
where 0 is the zero matrix of appropriate order. Let \( U \) and \( V \) be the submatrices of \( Z_{2(p-1)}(\tilde{p}) \) and \( Z_{2(p-1)} \) obtained by deleting their \( d \) th rows and columns, respectively. Then

\[
U = V = \begin{bmatrix} X_{d-2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & W_{d-2} \end{bmatrix}.
\]

Since \( X_{d-2} \) and \( W_{d-2} \) are similar, the eigenvalues of \( U \) and \( V \) are 1 and the eigenvalues of \( X_{d-2} \) with multiplicity 2. An easy computation shows that \( \det X_{d-2} = 1 \). Thus at least one eigenvalue of \( X_{d-2} \) with multiplicity 2 is strictly less than 1. Moreover, by the Cauchy interlacing property for the eigenvalues of Hermitian matrices, the eigenvalues of \( U \) and \( V \) interlace the eigenvalues of \( Z_{2(d-1)}(\tilde{p}) \) and \( Z_{2(d-1)} \), respectively. These facts all together imply that the smallest positive eigenvalues of \( \tilde{p} = \begin{bmatrix} a & -p & -d & -p \\ -p & 1 & 0 & 0 \\ 0 & 0 & 1 & -d \\ -p & 0 & 0 & 1 \end{bmatrix} \) are equal to the smallest eigenvalue of \( X_{d-2} \). That is, \( a(C(\tilde{p})) = a(C(e)) \). We have proved that if \( d \) is even then the upper bound (4) is attained by \( C(\tilde{p}) \).

Finally, we prove that if \( d \) is even then \( C(\tilde{p}) \) is the unique caterpillar in \( C \) attaining the upper bound (4) and that if \( d \) is odd then this upper bound cannot be achieved. Suppose that \( a(C(\tilde{p})) = f(\sigma) \) for some \( C(\tilde{p}) \) in \( C \). For even \( d \), we assume that \( C(\tilde{p}) \) is not isomorphic to \( C(\tilde{p}) \). Since \( n > 2d - 2 \), at least one component \( p_i \) of \( \tilde{p} \) is strictly greater than 1. We may assume \( 1 \leq j \leq \frac{1}{2} \lfloor d - 1 \rfloor \). We have \( p_1 > 1 \) or \( p_1 = 1 \). We first consider \( p_1 > 1 \). In this case, let \( q = [2, 1, \ldots, 1] \) with \( (d - 1) \) entries. We have

\[
a(C(\tilde{p})) \leq a(C(q)) \leq a(C(e)) = f(\sigma) \).
\]

Thus \( a(C(q)) = f(\sigma) \). Applying Lemma 1 to \( \lambda I - Z_{2(d-1)}(q) \), we have

\[
|\lambda I - Z_{2(d-1)}(q)| = \begin{vmatrix} \lambda - A(2) & -E \\ -E & \lambda I - B(1) & -E \\ & \ddots & \ddots \\ & & \lambda I - B(1) & -E \\ & & & \lambda I - A(1) \end{vmatrix}
\]

Applying linearity on the first column

\[
|\lambda I - Z_{2(d-1)}(q)| = \begin{vmatrix} -\lambda & 1 - \lambda \\ 1 - \lambda & \lambda^2 - 4\lambda + 2 & 1 - \lambda \\ & \ddots & \ddots \\ & & \lambda^2 - 4\lambda + 2 & 1 - \lambda \\ & & & \lambda^2 - 3\lambda + 1 \end{vmatrix}
\]
\[ \lambda I - Z_{2(d-1)} - \lambda I - W_{2(d-2)} \]

Therefore
\[ |\lambda I - Z_{2(d-1)}(q)| - |\lambda I - Z_{2(d-1)}| = -\lambda |\lambda I - W_{2(d-2)}| \] (8)

From (8) for \( \lambda = a(C(q)) = f(\sigma) \), we have
\[ 0 = -f(\sigma) |f(\sigma)I - W_{2(d-2)}| \] (9)

From Lemma 4, the two smallest eigenvalues of \( W_{2(d-2)} \) are \( f(\mu_1) \) and \( f(\mu_2) \) with \( \mu_1 = 2 \cos \frac{2(d-2)\pi}{2d-3} \) and \( \mu_2 = 2 \cos \frac{2(d-3)\pi}{2d-3} \). One can easily verify \( f(\mu_1) < f(\sigma) < f(\mu_2) \). Hence \( |f(\sigma)I - W_{2(d-2)}| \neq 0 \) and thus (9) is a contradiction. We consider now \( p_1 = 1 \). Then \( p_j > 1 \) for some \( 2 \leq j \leq \frac{1}{2} (d-1) \). In this case, let \( q = [1, \ldots, 2, 1, \ldots, 1] \) with \( (d-1) \) entries in which \( q_j = 2 \). Then \( a(C(p)) < a(C(q)) \) \( \leq f(\sigma) \). Thus \( a(C(q)) = f(\sigma) \). Again, we use Lemma 1 to obtain the determinant of \( \lambda I - Z_{2(d-1)}(q) \) and then applying linearity on the jth column, we get
\[ |\lambda I - Z_{2(d-1)}(q)| - |\lambda I - Z_{2(d-1)}| = -\lambda |\lambda I - X_{2(j-1)}| \] (10)

From (10) for \( \lambda = f(\sigma) = a(C(q)) \), we have
\[ 0 = -f(\sigma) |f(\sigma)I - X_{2(j-1)}| |f(\sigma)I - W_{2(d-j-1)}| \]

This is a contradiction because \( |f(\sigma)I - X_{2(j-1)}| \neq 0 \) and \( |f(\sigma)I - W_{2(d-j-1)}| \neq 0 \). This completes the proof. \( \square \)

It is an open problem to find an explicit sharp upper bound for the algebraic connectivity of caterpillars in \( C \) whenever \( d \) is odd.

4. Total ordering on the subclasses \( C_k \)

In this section, we find a total ordering by algebraic connectivity on the subclasses \( C_k \). Since the \( 2(d-1) \times 2(d-1) \) matrices in Theorem 2 that define the corresponding algebraic connectivities have different forms, we study separately the subclasses \( C_1, C_{\frac{d-1}{2}} \) and \( C_k \) for \( 1 < k < \lceil \frac{d-1}{2} \rceil \).

4.1. Total ordering on \( C_1 \)

An immediate consequence of Theorem 2 is

**Lemma 6.** The algebraic connectivity of the caterpillar \( C(a, 1, \ldots, 1, b) \in C_1 \) is the smallest positive eigenvalue of \( 2(d-1) \times 2(d-1) \) matrix

\[
Z_{2(d-1)}(a, 1, \ldots, 1, b) =
\begin{bmatrix}
A(a) & E \\
E & B(1) \end{bmatrix}
\]

where \( 1 \leq a \leq \frac{1}{2} (n - 2d + 4) \) and \( b = n - 2d + 4 - a \).

**Theorem 4.** The algebraic connectivity of \( C(a, 1, \ldots, 1, b) \in C_1 \) is a strictly decreasing function for \( 1 \leq a \leq \frac{1}{2} (n - 2d + 4) \).
**Proof.** We have $b - a + 1 > 0$. We write $Z(a, b)$ instead of $Z_{2(d-1)}(a, 1, \ldots, 1, b)$ and $B(1) = B$. We look for the difference $|\lambda I - Z(a, b)| - |\lambda I - Z(a - 1, b + 1)|$.

We apply Lemma 1 to obtain

$$|\lambda I - Z(a, b)| = \begin{vmatrix} \lambda I - A(a) & -E \\ -E & \lambda I - B \\ \vdots \\ -E & \vdots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots & -E \\ -E & \ddots & \ddots & \ddots & \ddots & \lambda I - B \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & -E \\ -E & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \lambda I - B \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \lambda I - A(b) \end{vmatrix}$$

$$|\lambda I - A(a)| 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
= |\lambda I - B| 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
= |\lambda I - (a + 2)\lambda + 1| 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
- \lambda 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
0 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
= \lambda^2 - (a + 2)\lambda + 1 - \lambda^2 - 4\lambda + 2 
= \lambda^2 - 4\lambda + 2 - \lambda^2 - 4\lambda + 2 
= \lambda^2 - (b + 2)\lambda + 1 - \lambda^2 - (b + 2)\lambda + 1 
= d_1 + d_2.$$

Applying linearity on the first column

$$|\lambda I - Z(a, b)| 
\begin{vmatrix} \lambda^2 - (a + 1)\lambda + 1 \\ \lambda^2 - 4\lambda + 2 \\ \vdots \\ 1 - \lambda \end{vmatrix} 
= |\lambda I - B| 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
= |\lambda I - (b + 2)\lambda + 1| 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
- \lambda 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
0 
\begin{vmatrix} 1 - \lambda \\ 1 - \lambda \\ \vdots \\ 1 - \lambda \end{vmatrix} 
= \lambda^2 - (a + 2)\lambda + 1 - \lambda^2 - 4\lambda + 2 
= \lambda^2 - 4\lambda + 2 - \lambda^2 - 4\lambda + 2 
= \lambda^2 - (b + 2)\lambda + 1 - \lambda^2 - (b + 2)\lambda + 1 
= d_1 + d_2.$$

Applying linearity on the last column of $d_1$

$$|\lambda I - Z(a, b)|$$
Reversing the rows and the columns of the last determinant, we have

\[
\begin{vmatrix}
\lambda^2 - (a + 1)\lambda + 1 & 1 - \lambda \\
1 - \lambda & \lambda^2 - 4\lambda + 2 & \ddots & \\
& \ddots & \ddots & 1 - \lambda \\
& & \ddots & \lambda^2 - 4\lambda + 2 \\
& & & 1 - \lambda & \lambda^2 - (b + 3)\lambda + 1
\end{vmatrix}
\]

By linearity on the first column

\[
\begin{vmatrix}
\lambda^2 - (a + 1)\lambda + 1 & 1 - \lambda \\
1 - \lambda & \lambda^2 - 4\lambda + 2 & \ddots & \\
& \ddots & \ddots & 1 - \lambda \\
& & \ddots & \lambda^2 - 4\lambda + 2 \\
& & & 1 - \lambda & \lambda^2 - (b + 2)\lambda + 1
\end{vmatrix}
\]
Hence
\[ |\lambda I - Z(a, b)| - |\lambda I - Z(a - 1, b + 1)| = \lambda^2 (b - a + 1) V(\lambda), \tag{11} \]

where
\[
V(\lambda) = \begin{vmatrix}
\lambda^2 - 4\lambda + 2 & 1 - \lambda & \\
1 - \lambda & \lambda^2 - 4\lambda + 2 & \ddots & \\
& \ddots & \ddots & 1 - \lambda \\
& & 1 - \lambda & \lambda^2 - 4\lambda + 2
\end{vmatrix}
= \det |\lambda I - Y_{2(d-3)}|.
\]

Then
\[
V(\lambda) = \prod_{j=1}^{2(d-3)} (\lambda - \gamma_j)
\]
in which \(\gamma_1 < \gamma_2 < \cdots < \gamma_{2(d-3)}\) are the eigenvalues of \(Y_{2(d-3)}\). Next we compare the smallest positive eigenvalue of \(Z_{2(d-1)}\) with the smallest eigenvalue of \(Y_{2(d-3)}\). By Lemmas 2 and 3, these eigenvalues are
\[
f(\sigma) = \frac{1}{2} \left(4 + \sigma - \sqrt{\sigma^2 + 4\sigma + 8}\right),
\sigma = 2 \cos \left(\frac{(d - 2)\pi}{d - 1}\right)
\]
and
\[
\gamma_1 = f(\rho) = \frac{1}{2} \left(4 + \rho - \sqrt{\rho^2 + 4\rho + 8}\right),
\rho = 2 \cos \left(\frac{(d - 3)\pi}{d - 2}\right).
\]

From the fact that \(f\) is a strictly increasing function, \(f(\sigma) < \gamma_1 = f(\rho)\). Therefore \(V(\lambda) > 0\) for all \(\lambda \in (0, f(\sigma))\). We apply this result in (11) to obtain
\[ |\lambda I - Z(a, b)| - |\lambda I - Z(a - 1, b + 1)| > 0 \tag{12} \]
for all \(\lambda \in (0, f(\sigma))\). Let
\[
\alpha_1 = 0 < \alpha_2 < \alpha_3 < \cdots < \alpha_{2(d-1)}
\]
and
\[
\beta_1 = 0 < \beta_2 < \beta_3 < \cdots < \beta_{2(d-1)}
\]
be the eigenvalues of \(Z(a, b)\) and \(Z(a - 1, b + 1)\), respectively. From Theorem 3 and Lemma 6, \(\beta_2 \in (0, f(\sigma))\). Then, from (12) for \(\lambda = \beta_2\)
\[ |\beta_2 I - Z(a, b)| > 0. \tag{13} \]
Moreover
\[ |\lambda I - Z(a, b)| = \lambda \prod_{j=2}^{2(d-1)} (\lambda - \alpha_j) \]
and
\[ |\lambda I - Z(a - 1, b + 1)| = \lambda \prod_{j=2}^{2(d-1)} (\lambda - \beta_j). \]
Suppose $\beta_2 \leq \alpha_2$. Then $\beta_2 \leq \alpha_j$ for $j = 2, 3, \ldots, 2(d - 1)$. Hence
\[
|\beta_2 I - Z(a, b)| - |\beta_2 I - Z(a - 1, b + 1)|
= |\beta_2 I - Z(a, b)| = \beta_2 \prod_{j=2}^{2(d-1)} (\beta_2 - \alpha_j) \leq 0.
\]
This inequality contradicts (13), and therefore $\beta_2 > \alpha_2$. □

From Theorem 4, it follows

**Corollary 2.** Among all trees in $C_1$ the maximum algebraic connectivity is attained by the caterpillar $C(1, 1, \ldots, 1, n - 2d + 3)$ and the minimum algebraic connectivity is attained by $C(\lceil \frac{n-2d+4}{2} \rceil, 1, \ldots, 1, \lceil \frac{n-2d+4}{2} \rceil)$.

4.2. Total ordering on $C_{\frac{d-1}{2}}$ for odd $d$

We search for a total ordering on
\[ C_{\frac{d-1}{2}} = \left\{ C \left(1, \ldots, 1, p_{\frac{d-1}{2}}, p_{\frac{d+1}{2}}, 1, \ldots, 1\right) \in C : p_{\frac{d-1}{2}} \leq p_{\frac{d+1}{2}} \right\}, \]
whenever $d$ is odd. Let $p_{\frac{d-1}{2}} = a$ and $p_{\frac{d+1}{2}} = b$. Thus a caterpillar in $C_{\frac{d-1}{2}}$ is of the form $C(1, \ldots, 1, a, b, 1, \ldots, 1)$ in which $a + b = n - 2d + 4$ and $a \leq b$. For brevity, we write $C(a, b)$ instead of $C(1, \ldots, 1, a, b, 1, \ldots, 1)$.

**Lemma 7.** For odd $d$, the algebraic connectivity of $C(a, b) \in C_{\frac{d-1}{2}}$ is the smallest positive eigenvalue of the $2(d - 1) \times 2(d - 1)$ positive semidefinite matrix
\[
R(a, b) = \begin{bmatrix}
X_{d-3} & F & 0 & 0 \\
F^T & B(a) & E & 0 \\
0 & E & B(b) & F^T \\
0 & 0 & F & X_{d-3}
\end{bmatrix},
\]
where $F$ is a matrix of order $(d - 3) \times 2$ with $F(d - 3, 2) = 1$ and zeros elsewhere.

**Proof.** From Theorem 2 the algebraic connectivity of $C(a, b) \in C_{\frac{d-1}{2}}$ is the smallest positive eigenvalue of the matrix
\[
U(a, b) = \begin{bmatrix}
X_{d-3} & F & 0 & 0 \\
F^T & B(a) & E & 0 \\
0 & E & B(b) & G^T \\
0 & 0 & G & W_{d-3}
\end{bmatrix},
\]
where $G$ is a matrix of order $(d - 3) \times 2$ with $G(2, 2) = 1$ and zeros elsewhere. Clearly, there is a permutation matrix $P$ such that $PW_{d-3}P^T = X_{d-3}$ and $PG = F$. Then
\[
\begin{bmatrix}
I & 0 & 0 & 0 \\
0 & I & 0 & 0 \\
0 & 0 & I & 0 \\
0 & 0 & 0 & P
\end{bmatrix}U(a, b)\begin{bmatrix}
I & 0 & 0 & 0 \\
0 & I & 0 & 0 \\
0 & 0 & I & 0 \\
0 & 0 & 0 & P^T
\end{bmatrix} = R(a, b). \quad □
\]

**Theorem 5.** For odd $d$, the algebraic connectivity of $C(1, \ldots, 1, a, b, 1, \ldots, 1) \in C_{\frac{d-1}{2}}$ is a strictly decreasing function for $1 \leq a \leq \frac{1}{2}(n - 2d + 4)$. 

\textbf{Proof.} Applying Lemma 1 to $|\lambda I - R(a, b)|$, we have

$$
|\lambda I - R(a, b)|
= \begin{vmatrix}
\lambda I - X_d & -F \\
-F^T & \lambda I - B(a) & -E \\
0 & -E & \lambda I - B(b) & -F^T \\
0 & 0 & -F & \lambda I - X_{d-3}
\end{vmatrix}
= |\lambda I - X_{d-3}| 
- \lambda
\begin{vmatrix}
|\lambda I - B(a)| & 1 - \lambda \\
0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{vmatrix}
= |\lambda I - X_{d-3}|
- \lambda
\begin{vmatrix}
\lambda^2 - (a + 3)\lambda + 2 & 1 - \lambda \\
0 & 1 - \lambda & \lambda^2 - (b + 3)\lambda + 2 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{vmatrix}
= |\lambda I - X_{d-3}|
+ d_1 + d_2.
$$

Applying linearity on the second column

$$
|\lambda I - R(a, b)|
= \begin{vmatrix}
|\lambda I - X_{d-3}|
& 1 - \lambda \\
|\lambda I - X_{d-3}| & \lambda^2 - (a + 2)\lambda + 2 & 1 - \lambda \\
0 & 1 - \lambda & \lambda^2 - (b + 3)\lambda + 2 & 1 - \lambda \\
0 & 0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{vmatrix}
= |\lambda I - X_{d-3}|
+ d_1 + d_2.
$$

Applying now linearity on the third column of $d_1$, we obtain

$$
|\lambda I - R(a, b)|
= \begin{vmatrix}
|\lambda I - X_{d-3}|
& 1 - \lambda \\
|\lambda I - X_{d-3}| & \lambda^2 - (a + 2)\lambda + 2 & 1 - \lambda \\
0 & 1 - \lambda & \lambda^2 - (b + 4)\lambda + 2 & 1 - \lambda \\
0 & 0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{vmatrix}
+ d_2.
$$

We observe that

$$
|\lambda I - R(a - 1, b + 1)|
= \begin{vmatrix}
|\lambda I - X_{d-3}|
& 1 - \lambda \\
|\lambda I - X_{d-3}| & \lambda^2 - (a + 2)\lambda + 2 & 1 - \lambda \\
0 & 1 - \lambda & \lambda^2 - (b + 4)\lambda + 2 & 1 - \lambda \\
0 & 0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{vmatrix}
= |\lambda I - R(a - 1, b + 1)|.
$$
Therefore

\[
|\lambda I - R(a, b)| - |\lambda I - R(a - 1, b + 1)| = |\lambda I - X_{d-3}| - |\lambda I - X_{d-3}|
\]

\[
= \left| \begin{array}{ccc}
|\lambda I - X_{d-3}| & 1 - \lambda & 0 \\
|\lambda I - X_{d-3}| & \lambda^2 - (a + 2)\lambda + 2 & 0 \\
0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{array} \right| 
\]

\[
= \left| \begin{array}{ccc}
|\lambda I - X_{d-3}| & 0 & 0 \\
|\lambda I - X_{d-3}| & -\lambda & 1 - \lambda \\
0 & 0 & |\lambda I - X_{d-3}|
\end{array} \right| 
\]

\[
= \lambda |\lambda I - X_{d-3}| \left| \begin{array}{ccc}
|\lambda I - X_{d-3}| & 1 - \lambda & 0 \\
|\lambda I - X_{d-3}| & \lambda^2 - (a + 2)\lambda + 2 & 0 \\
0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{array} \right| 
\]

\[
= \lambda \lambda |\lambda I - X_{d-3}| \left| \begin{array}{ccc}
|\lambda I - X_{d-3}| & 1 - \lambda & 0 \\
|\lambda I - X_{d-3}| & \lambda^2 - (a + 2)\lambda + 2 & 0 \\
0 & 1 - \lambda & |\lambda I - X_{d-3}|
\end{array} \right|
\]

\[
= \lambda^2 (b - a + 1).
\]

We have proved that

\[
|\lambda I - R(a, b)| - |\lambda I - R(a - 1, b + 1)| = \lambda^2 |\lambda I - X_{d-3}|^2 (b - a + 1)
\]

for all \( \lambda \). From Lemma 4, the smallest eigenvalue of \( X_{d-3} \) is

\[
f(\mu) = \frac{1}{2} \left( 4 + \mu - \sqrt{\mu^2 + 4\mu + 8} \right).
\]

\[
\mu = 2 \cos \left( \frac{(d - 3)\pi}{d - 2} \right).
\]

Then

\[
|\lambda I - R(a, b)| - |\lambda I - R(a - 1, b + 1)| > 0
\]

for all \( \lambda \in (0, f(\mu)) \). Let

\[
0 = \alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_{2(d-1)}
\]

and

\[
0 = \beta_1 < \beta_2 < \beta_3 < \cdots < \beta_{2(d-1)}
\]

be the eigenvalues of \( R(a, b) \) and \( R(a - 1, b + 1) \), respectively. We know that \( f(\sigma) = 2 \cos \left( \frac{(d - 2)\pi}{d - 1} \right) \) is an upper bound for the algebraic connectivity of the caterpillars in \( C \) and that \( f \) is a strictly increasing function. Then \( 0 < \beta_2 < f(\sigma) < f(\mu) \). Thus \( \beta_2 \in (0, f(\mu)) \). From (14) for \( \lambda = \beta_2 \), we have

\[
|\beta_2 I - R(a, b)| > 0.
\]

Moreover

\[
|\lambda I - R(a, b)| - |\lambda I - R(a - 1, b + 1)| = \lambda \prod_{i=2}^{2(d-1)} (\lambda - \alpha_i) - \lambda \prod_{i=2}^{2(d-1)} (\lambda - \beta_i).
\]

If \( \beta_2 \leq \alpha_2 \) then \( \beta_2 \leq \alpha_i \) for \( i = 2, 3, \ldots, 2(d-1) \) and thus
Corollary 3. For odd \(d\), among all trees in \(C_{\frac{d+1}{2}}\) the maximum algebraic connectivity is attained by the caterpillar \(C(1, \ldots, 1, p_{\frac{d+1}{2}}, 1, \ldots, 1)\) where \(p_{\frac{d+1}{2}} = n - 2d + 3\) and the minimum algebraic connectivity is attained by \(C(1, \ldots, 1, p_{\frac{d-1}{2}}, p_{\frac{d+1}{2}}, 1, \ldots, 1)\) where \(p_{\frac{d-1}{2}} = \lceil \frac{1}{2} (n - 2d + 4) \rceil \) and \(p_{\frac{d+1}{2}} = \lfloor \frac{1}{2} (n - 2d + 4) \rfloor \).

4.3. Total ordering on \(C_k\) for \(1 < k < \lfloor \frac{d-1}{2} \rfloor \)
Here \(1 < k < \lfloor \frac{d-1}{2} \rfloor \). Since 
\(C_k = \{ C(1, \ldots, 1, p_k, 1, \ldots, 1, p_{d-k}, 1, \ldots, 1) \in C : p_k \leq p_{d-k} \} \),
a caterpillar in \(C_k\) is of the form \(C(1, \ldots, 1, a, 1, \ldots, 1, b, 1, \ldots, 1)\) in which \(a + b = n - 2d + 4\) and \(a \leq b\). We write \(C(a, b)\) instead of \(C(1, \ldots, 1, a, 1, \ldots, 1, b, 1, \ldots, 1)\).

Lemma 8. Let \(1 < k < \lfloor \frac{d-1}{2} \rfloor \). The algebraic connectivity of \(C(a, b) \in C_k\) is the smallest positive eigenvalue of the \(2(d-1) \times 2(d-1)\) positive semidefinite matrix 
\[
S(a, b) = \begin{bmatrix}
X_{2(k-1)} & F & G & H \\
F^T & B(a) & G & H^T \\
G^T & Y_{2(d-1-2k)} & B(b) & F \\
H & H^T & F & X_{2(k-1)}
\end{bmatrix},
\]
where \(F, G\) and \(H\) are matrices of order \(2k - 2 \times 2, 2 \times (2d - 2 - 4k)\) and \((2d - 2 - 4k) \times 2\), respectively, with zeros in all the entries except for \(F(2k - 2, 2) = 1, G(2, 2) = 1\) and \(H(2d - 2 - 4k, 2) = 1\).

Proof. We have \(1 < k < \lfloor \frac{d-1}{2} \rfloor \). Then \(d - 1 > 0\) and \(d - 1 - 2k > 0\). From Theorem 2 the algebraic connectivity of \(C(a, b) \in C_k\) is the smallest positive eigenvalue of the matrix 
\[
U(a, b) = \begin{bmatrix}
X_{2(k-1)} & F & G & H \\
F^T & B(a) & G & H^T \\
G^T & Y_{2(d-1-2k)} & B(b) & K \\
H & H^T & B(b) & W_{2(k-1)}
\end{bmatrix},
\]
where \(F, G, H, K\) are matrices of order \((2k - 2) \times 2, 2 \times (2d - 2 - 4k), (2d - 2 - 4k) \times 2\) and \(2 \times (2k - 2)\), respectively, with zeros in all the entries except for \(F(2k - 2, 2) = 1, G(2, 2) = 1, H(2d - 2 - 4k, 2) = 1\) and \(K(2, 2) = 1\). There is a permutation matrix \(P\) such that \(PW_{2(k-1)}P^T = X_{2(k-1)}\) and \(PK = F\). Then 
\[
\begin{bmatrix}
I & I & I & I \\
I & I & I & I \\
I & I & I & I \\
I & I & I & I
\end{bmatrix}
\begin{bmatrix}
U(a, b) \\
P
\end{bmatrix}
= S(a, b). \quad \square
**Theorem 6.** For $1 < k < \lfloor \frac{k-1}{2} \rfloor$, the algebraic connectivity of $C(1, \ldots, 1, a, 1, \ldots, 1, b, 1, \ldots, 1) \in C_k$ is a strictly decreasing function for $1 \leq a \leq \frac{1}{2}(n-2d+4)$.

**Proof.** We apply Lemma 1 to $|\lambda I - S(a, b)|$. Then, as in the proofs of Theorems 4 and 5, by repeated application of the fact that the determinant is multilinear, we get

$$|\lambda I - S(a, b)| - |\lambda I - S(a - 1, b + 1)| = \lambda^2 |\lambda I - X_{2(k-1)}|^2 |\lambda I - Y_{2(d-1-2k)}|(b - a + 1)$$

for all $\lambda$. From Lemma 4, the smallest eigenvalue of $X_{2(k-1)}$ is

$$f(\mu) = \frac{1}{2} \left( 4 + \mu - \sqrt{\mu^2 + 4\mu + 8} \right).$$

$$\mu = 2 \cos \frac{2(k-1)\pi}{2k-1}$$

and, from Lemma 3, the smallest eigenvalue of $Y_{2(d-1-2k)}$ is

$$f(\rho) = \frac{1}{2} \left( 4 + \rho - \sqrt{\rho^2 + 4\rho + 8} \right).$$

$$\rho = 2 \cos \frac{(d-1-2k)\pi}{d-2k}.$$

Let $m = \min\{f(\mu), f(\rho)\}$. We observe that $|\lambda I - Y_{2(d-1-2k)}|$ is a polynomial of even degree. Using this fact in (16),

$$|\lambda I - S(a, b)| - |\lambda I - S(a - 1, b + 1)| > 0$$

for all $\lambda \in (0, m)$. Let

$$0 = \alpha_1 < \alpha_2 \leq \alpha_3 < \cdots < \alpha_{2(d-1)}$$

and

$$0 = \beta_1 < \beta_2 \leq \beta_3 \leq \cdots \beta_{2(d-1)}$$

be the eigenvalues of $S(a, b)$ and $S(a - 1, b + 1)$, respectively. We know that $f(\sigma), \sigma = 2 \cos \frac{(d-2)\pi}{d-1}$, is an upper bound for the algebraic connectivity of the caterpillars in $C$ and that $f$ is strictly increasing. Hence

$$0 < \beta_2 < f(\sigma) < f(\mu).$$

Then $\beta_2 \in (0, m)$. From (17) for $\lambda = \beta_2$, we have

$$|\beta_2 I - S(a, b)| > 0.$$  

Moreover

$$|\lambda I - S(a, b)| - |\lambda I - S(a - 1, b + 1)| = \lambda \prod_{i=2}^{2(d-1)} (\lambda - \alpha_i) - \lambda \prod_{i=2}^{2(d-1)} (\lambda - \beta_i).$$

If $\beta_2 \leq \alpha_2$ then $\beta_2 \leq \alpha_i$ for $i = 2, 3, \ldots, 2(d-1)$ and thus

$$|\beta_2 I - S(a, b)| = \beta_2 \prod_{i=2}^{2(d-1)} (\beta_2 - \alpha_i) \leq 0.$$  

This is in contradiction with (15), and therefore $\alpha_2 < \beta_2$. The proof is complete. \(\square\)

From Theorem 6, it follows

**Corollary 4.** For $1 < k < \lfloor \frac{d-1}{2} \rfloor$, among all trees in $C_k$ the maximum algebraic connectivity is attained by the caterpillar $C(1, \ldots, 1, 1, \ldots, p_{d-k}, 1, \ldots, 1)$ where $p_{d-k} = n - 2d + 3$ and the minimum algebraic
connectivity is attained by $C(1, \ldots, 1, p_k, \ldots, p_{d-k}, 1, \ldots, 1)$ where $p_k = \lfloor \frac{1}{2} (n - 2d + 4) \rfloor$ and $p_{d-k} = \lceil \frac{1}{2} (n - 2d + 4) \rceil$.

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References