ALGEBRAIC CONNECTIVITY FOR SUBCLASSES OF CATERPILLARS

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A caterpillar is a tree in which the removal of all pendent vertices make it a path. In this paper, we consider two classes of caterpillars. We present an ordering of caterpillars by algebraic connectivity in one of them and find one that maximizes the algebraic connectivity in the other class.

1. PRELIMINARIES

Ordering of subclasses of trees by algebraic connectivity is a very active area of research. Let $\mathcal{G} = (V, E)$ be a simple undirected graph on n vertices. The Laplacian matrix of $\mathcal{G}$ is the $n \times n$ matrix $L(\mathcal{G}) = D(\mathcal{G}) - A(\mathcal{G})$ where $A(\mathcal{G})$ is the adjacency matrix and $D(\mathcal{G})$ is the diagonal matrix of vertex degrees. It is well known that $L(\mathcal{G})$ is a positive semidefinite matrix and that $(0, \mathbf{e})$ is an eigenpair of $L(\mathcal{G})$ where $\mathbf{e}$ is the all ones vector. Let us denote the eigenvalues of $L(\mathcal{G})$ by

$$0 = \lambda_n(\mathcal{G}) \leq \lambda_{n-1}(\mathcal{G}) \leq \cdots \leq \lambda_2(\mathcal{G}) \leq \lambda_1(\mathcal{G}).$$

In [**7**], some of the many results known for Laplacian matrices are given. FIEDLER [**3**] proved that $\mathcal{G}$ is a connected graph if and only if $\lambda_{n-1}(\mathcal{G}) > 0$. This eigenvalue is called the algebraic connectivity of $\mathcal{G}$ and it is denoted by $a(\mathcal{G})$. In [**1**], a survey on old and new results on the algebraic connectivity of graphs is given.

We recall that a tree is a connected acyclic graph. Let $\mathcal{P}_n$ be a path and $\mathcal{S}_n$ be a star both of them with n vertices. A caterpillar is a tree in which the removal of all pendent vertices makes it a path.

Let n and $d \geq 3$ fixed positive integers. Let p and q natural numbers such that $n = p+q+d-1$. For given p and q, let $\mathcal{S}_{n,d}(p, q)$ be the tree with n vertices and

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diameter d obtained from the path $\mathcal{P}_{d-1}$ and two stars on $p+1$ and $q+1$ vertices, $\mathcal{S}_{p+1}$ and $\mathcal{S}_{q+1}$, by identifying the pendent vertices in $\mathcal{P}_{d-1}$ with the centers of the stars. It's easy to see that $\mathcal{S}_{n,d}(p,q)$ is a caterpillar with n vertices and diameter d.

Ordering subclasses of trees by algebraic connectivity is extensively studied problem. The first paper about this appeared in 1990 and it is due to GRONE and MERRIS [5]. Since any tree of order n and diameter 3 can be expressed in the form of the caterpillar $\mathcal{S}_{n,3}(p,q)$ with $p \leq q$ and $1 \leq p \leq \frac{1}{2}(n-2)$, the following theorem solves the problem of ordering in the subclass of trees of order n and diameter 3.

Theorem 1. [5] *For fixed $n \geq 3$, the algebraic connectivity of $\mathcal{S}_{n,3}(p,q)$, $q = n-p-2$, is the unique Laplacian eigenvalue less than 1 and it is a strictly decreasing function for $1 \leq p \leq 1/2(n-2)$.*

Important contributions to the problem for trees of order n and diameter $d = 4$ are due to X-D ZHANG in [14]. YUAN et al. in [12] introduce six classes of trees with n vertices and determine the ordering of those trees by this spectral invariant. SHAO et al. in [10] determine the first four trees of order $n \geq 9$ with the smallest algebraic connectivity. In this same year, ZHANG and LIU in [15] find the largest twelve values of algebraic connectivity of trees in a set of trees on $2k+1$ vertices with nearly perfect matching. However, one of the most important ordering of trees is implicitly given by FALLAT and KIRKLAND in [2]. There, they exhibit the unique tree on n vertices and diameter d that minimizes the algebraic connectivity over all such trees.

Theorem 2. [2] *Among all trees on n vertices and diameter d, for each natural numbers p and q such that $n = p + q + d - 1$, the minimum algebraic connectivity is attained by $\mathcal{S}_{n,d}\left(\left\lfloor \dfrac{p+q}{2} \right\rfloor, \left\lceil \dfrac{p+q}{2} \right\rceil\right)$.*

Let $\mathbf{p} = [p_1, p_2, \ldots, p_{d-1}]$ such that $p_i \geq 1, 1 \leq i \leq d-1$, and $\sum\limits_{i=1}^{d-1} p_i = n - d + 1$. We denote $C(\mathbf{p})$ as the caterpillar obtained from the stars $\mathcal{S}_{p_1+1}, \mathcal{S}_{p_2+1}, \ldots, \mathcal{S}_{p_{d-1}+1}$ and the path $\mathcal{P}_{d-1}$ by identifying the center of $\mathcal{S}_{p_i+1}$ with the $i-$vertex of $\mathcal{P}_{d-1}$. From now on, let $\mathcal{S}_{n,d}$ and $\mathcal{C}_{n,d}$ the following subclasses of caterpillars with n and diameter d:

$$\mathcal{S}_{n,d} = \left\{ \mathcal{S}_{n,d}(p,q) : 1 \leq p \leq \frac{1}{2}(n-d+1), q = n-p-d+1 \right\}$$

and, for $n > 2(d-1)$,

$$\mathcal{C}_{n,d} = \left\{ C(p_1, p_2, \ldots, p_{d-1}) : p_i \geq 1, 1 \leq i \leq d-1, \sum_{i=1}^{d-1} p_i = n-d+1 \right\}.$$

We determine relationships between the values of the algebraic connectivity for trees in the classes above. For this, we organize the paper as follows: in Section 2, we present the basic results about Laplacian eigenvalues of generalized Bethe

trees that will be used to determine the algebraic connectivity of caterpillars in $\mathcal{S}_{n,d}$. In the next section, we give the ordering in that class (see Theorem 4). In Section 4, we prove that P_4 is the caterpillar with maximum algebraic connectivity among all caterpillars with n vertices and diameter d, when we take n and d as variables. Finally, in Section 5, we search for caterpillars with maximum algebraic connectivity in $C_{n,d}$. When the diameter is even, we completely solve the problem and, for the odd case, we only suggest a caterpillar that satisfies this property.

2. THE ALGEBRAIC CONNECTIVITY OF $\mathcal{S}_{n,d}\left(p,q\right)$

A *generalized Bethe tree* is a rooted tree in which vertices at the same level from the root have the same degree. We may consider $\mathcal{S}_{n,d}\left(p,q\right)$ as the union of two generalized Bethe trees with a common root v which is the root of $\mathcal{S}_{p+1}$. Let us illustrate this fact with the following example.

EXAMPLE 1. For instance, $\mathcal{S}_{10,4}\left(3,4\right)$ is the union of two generalized Bethe trees with vertex degree sequences, from the pendent vertices to the root v, given by $(1,3)$ and $\left(1,5,2,1\right),$ respectively.

In [**8**], we have characterized completely the Laplacian eigenvalues of a tree, including their multiplicities, given by the union of two generalized Bethe trees having a common root. Applying Theorem 2 from [8] to the tree $\mathcal{S}_{n,d}\left(p,q\right)$, we have the following lemma.

The degree of the common root v as a vertex of $\mathcal{S}_{10,4}\left(3,4\right)$ is $3+1=4.$

Lemma 1. *The eigenvalues of $\mathcal{S}_{n,d}\left(p,q\right)$ are 1, with multiplicity at least $p+q-2$, and the eigenvalues of the singular tridiagonal symmetric matrix $A\left(p\right)$ of order $\left(d+1\right):$*

$$
(1) \qquad A\left(p\right) =
\begin{bmatrix}
1 & \sqrt{p} & & & & & \\
\sqrt{p} & p+1 & 1 & & & & \\
& 1 & 2 & \ddots & & & \\
& & \ddots & \ddots & \ddots & & \\
& & & \ddots & 2 & 1 & \\
& & & & 1 & q+1 & \sqrt{q} \\
& & & & & \sqrt{q} & 1
\end{bmatrix}.
$$

In order to prove our first main result, we recall the following lemmas:

Lemma 2. [**3**] *If $\mathcal{T}$ is a tree of order n then $a\left(\mathcal{T}\right) \leq 1$ and the equality occurs if and only if $\mathcal{T}$ is the star graph $\mathcal{S}_n$.*

Lemma 3. [**4**] *Let A be an $m \times m$ symmetric tridiagonal matrix with nonzero codiagonal entries. Then the eigenvalues of any $\left(m-1\right) \times \left(m-1\right)$ principal sub-*

*matrix strictly interlace the eigenvalues of A. In particular, the eigenvalues of A
are simple.*

We are ready to characterize the algebraic connectivity of $\mathcal{S}_{n,d}(p,q)$.

Theorem 3. *The algebraic connectivity of $\mathcal{S}_{n,d}(p,q)$ is the smallest eigenvalue of
the positive definite tridiagonal matrix $B(p)$ of order d:*

(2)
$$
B(p) = \begin{bmatrix}
p+1 & \sqrt{p} & & & & & \\
\sqrt{p} & 2 & 1 & & & & \\
 & 1 & \ddots & \ddots & & & \\
 & & \ddots & \ddots & 1 & & \\
 & & & 1 & 2 & \sqrt{q} & \\
 & & & & \sqrt{q} & q+1
\end{bmatrix}.
$$

Proof. By Lemma 1 and Lemma 2, the algebraic connectivity of $\mathcal{S}_{n,d}(p,q)$ is the
smallest positive eigenvalue of the matrix $A(p)$ given in (1). This matrix has the
LL^T-decomposition
$$
A(p) = LL^T,
$$
where L is the lower bidiagonal matrix

$$
L = \begin{bmatrix}
1 & & & & & \\
\sqrt{p} & 1 & & & & \\
 & 1 & \ddots & & & \\
 & & \ddots & 1 & & \\
 & & & 1 & \sqrt{q} & \\
 & & & & 1 & 0
\end{bmatrix}
$$

of order $(d+1)$. Computing the product $L^T L$, we obtain

(3)
$$
L^T L = \widetilde{A}(p) = \begin{bmatrix}
p+1 & \sqrt{p} & & & & & 0 \\
\sqrt{p} & 2 & 1 & & & & \vdots \\
 & \ddots & \ddots & \ddots & & & \\
 & & \ddots & \ddots & 1 & & \\
 & & & 1 & 2 & \sqrt{q} & \vdots \\
 & & & & \sqrt{q} & q+1 & 0 \\
0 & \cdots & & & \cdots & 0 & 0
\end{bmatrix}.
$$

We recall the fact that if A and B are complex matrices, AB and BA have the same
nonzero eigenvalues [**13**], to conclude that $A(p) = LL^T$ and $\widetilde{A}(p) = L^T L$ have the
same nonzero eigenvalues. Therefore, the algebraic connectivity of $\mathcal{S}_{n,d}(p,q)$ is the

smallest eigenvalue of $\widetilde{A}(p)$. From (3), the nonzero eigenvalues of $\widetilde{A}(p)$ are the eigenvalues of the matrix $B(p)$ of order d given in (2). The proof is complete. $\square$

At this point, we introduce the following notations:

$\beta(\lambda, p)$ is the characteristic polynomial of the $d \times d$ matrix $B(p)$ defined in (2) and $\alpha_1(p) < \alpha_2(p) < \ldots < \alpha_d(p)$ are the eigenvalues of $B(p)$.

So $\beta(\lambda, p) = (\lambda - \alpha_1(p))(\lambda - \alpha_2(p))\ldots(\lambda - \alpha_d(p))$.

From Theorem 3, $\alpha_1(p)$ is the algebraic connectivity of $\mathcal{S}_d(n, p, q)$ and from the fact that $B(p)$ is a positive definite matrix and also from Lemma 2, we have $0 < \alpha_1(p) < 1$.

Lemma 4. $[\mathbf{11}]$ *The characteristic polynomials of the $j \times j$ leading principal submatrices of the symmetric tridiagonal matrix Q_k of order $k \times k$,*

$$
Q_k = \begin{bmatrix}
a_1 & b_1 & & & & \\
b_1 & a_2 & b_2 & & & \\
& b_2 & \ddots & \ddots & & \\
& & \ddots & \ddots & \ddots & \\
& & & \ddots & a_{k-1} & b_{k-1} \\
& & & & b_{k-1} & a_k
\end{bmatrix},
$$

satisfy the three-term recursion formula

$$(4) \qquad Q_j(\lambda) = (\lambda - a_j)Q_{j-1}(\lambda) - b_{j-1}^2 Q_{j-2}(\lambda)$$

with

$$Q_0(\lambda) = 1 \ \text{and} \ Q_1(\lambda) = \lambda - a_1.$$

3. ORDERING OF TREES BY ALGEBRAIC CONNECTIVITY IN THE CLASS $\mathcal{S}_{n,d}$

The ordering given in the next theorem is embedded in the proof of Theorem 2 given by FALLAT and KIRKLAND [**2**]. However, we decided to include our proof here for two reasons. Firstly, to emphasize the ordering of trees in $\mathcal{S}_{n,d}$, and, secondly, because our arguments of proof are distinct that those used by the authors refereed above.

Theorem 4. *For given $n, d \geq 3$, the algebraic connectivity of $\mathcal{S}_{n,d}(p, q)$, $q = n - p - (d - 1)$, is a strictly decreasing function for $1 \leq p \leq \frac{1}{2}(n - (d - 1))$.*

Proof. Case $d = 3$: Then, $n = p + q + 2$. Although, in this case, GRONE and MERRIS have proved this result in [**5**], we prove it here by using Theorem 3. From

it, the algebraic connectivity of $\mathcal{S}_{n,3}(p,q)$ is the smallest eigenvalue $\alpha_1(p)$ of the 3×3 matrix

$$B(p) = \begin{bmatrix} p+1 & \sqrt{p} & \\ \sqrt{p} & 2 & \sqrt{q} \\ & \sqrt{q} & q+1 \end{bmatrix}.$$

It is easy to see that the eigenvalues of $\begin{bmatrix} p+1 & \sqrt{p} \\ \sqrt{p} & 2 \end{bmatrix}$ are 1 and $p+2$. By Lemma 3, these eigenvalues strictly interlace the eigenvalues of $B(p)$. Hence,

$$\alpha_1(p) < 1 < \alpha_2(p) < p+2 < \alpha_3(p).$$

It follows that $\alpha_1(p)$ is the unique Laplacian eigenvalue of $\mathcal{S}_{n,3}(p,q)$ in the interval $(0,1)$. Let $1 \leq p \leq \frac{1}{2}(n-4)$. Then, $p+1 \leq \frac{1}{2}(n-2)$ and $q-p-1 > n-4-2p \geq 0$. An easy computation shows that

$$\beta(\lambda, p) = \lambda^3 - (n+2)\lambda^2 + (pq + 2n + 1)\lambda - n.$$

So,

$$\beta(\lambda, p+1) - \beta(\lambda, p) = (q - p - 1)\lambda.$$

Since $\beta(\alpha_1(p), p) = 0$, $q - p - 1 > 0$ and $0 < \alpha_1(p) < 1$, we have

(5) $$\beta(\alpha_1(p), p+1) > 0.$$

It follows from this inequality that $\alpha_1(p) \neq \alpha_1(p+1)$. Suppose that $\alpha_1(p) < \alpha_1(p+1)$. Then,

$$\alpha_1(p) < \alpha_i(p+1), \quad i = 1, 2, 3.$$

Hence,

$$\beta(\alpha_1(p), p+1) = \prod_{i=1}^{3}(\alpha_1(p) - \alpha_i(p+1)) < 0,$$

which contradicts (5). Therefore, $\alpha_1(p) > \alpha_1(p+1)$. Thus, the proof for $d = 3$ is complete.

      Case $d = 4$: Then, $n = p + q + 3$. By Theorem 3, the algebraic connectivity of $\mathcal{S}_{n,4}(p,q)$ is the smallest eigenvalue $\alpha_1(p)$ of the 4×4 matrix

$$B(p) = \begin{bmatrix} p+1 & \sqrt{p} & & \\ \sqrt{p} & 2 & 1 & \\ & 1 & 2 & \sqrt{q} \\ & & \sqrt{q} & q+1 \end{bmatrix}.$$

One can easily get

(6) $$\beta(\lambda, p) = \lambda^4 - (n+3)\lambda^3 + (pq + 4n)\lambda^2 - (2pq + 4n - 2)\lambda + n.$$

Let $1 \leq p \leq \frac{1}{2}(n-5)$. Then, $p+1 \leq \frac{1}{2}(n-3)$ and $q-p-1 = n-p-3-p-1 > n-5-2p \geq 0$. Applying (6), we obtain

$$\beta(\lambda, p+1) - \beta(\lambda, p) = ((p+1)(q-1) - pq)\lambda^2 - 2((p+1)(q-1) - pq)\lambda.$$

Then,

(7) $$\beta(\lambda, p+1) - \beta(\lambda, p) = \lambda(\lambda-2)(q-p+1).$$

Since $\beta(\alpha_1(p), p) = 0$, $q-p+1 > 0$ and $0 < \alpha_1(p) < 1$, and from (7) we obtain

(8) $$\beta(\alpha_1(p), p+1) < 0.$$

It follows that $\alpha_1(p) \neq \alpha_1(p+1)$. Suppose that $\alpha_1(p) < \alpha_1(p+1)$. Then,

$$\alpha_1(p) < \alpha_i(p+1), \ \ i = 1, 2, 3, 4.$$

Hence,

$$\beta(\alpha_1(p), p+1) = \prod_{i=1}^{4}(\alpha_1(p) - \alpha_i(p+1)) > 0,$$

which contradicts (8). Therefore, $a(p) > a(p+1)$ and the proof of the case $d=4$ is complete.

Case $d \geq 5$: Let $1 \leq p \leq \frac{1}{2}(n-(d+1))$. Then, $p+1 \leq \frac{1}{2}(n-(d-1))$ and $q-p-1 > n-2p-(d+1) \geq 0$. The recursive formula (4) applied to $B(p)$ gives

$$\beta(\lambda, p) = (\lambda - (q+1))\gamma_{d-1}(\lambda, p) - q\gamma_{d-2}(\lambda, p),$$

where, for $j = d-1$ and $j = d-2$, $\gamma_j(\lambda, p)$ is the characteristic polinomial of the matrix

$$C_j(p) = \begin{bmatrix} p+1 & \sqrt{p} & & & & \\ \sqrt{p} & 2 & 1 & & & \\ & 1 & \ddots & \ddots & & \\ & & \ddots & \ddots & 1 & \\ & & & 1 & 2 \end{bmatrix}$$

of order $j \times j$. Similarly, the recursive formula (4) applied to the matrix $B(p+1)$ gives

$$\beta(\lambda, p+1) = (\lambda - q)\gamma_{d-1}(\lambda, p+1) - (q-1)\gamma_{d-2}(\lambda, p+1).$$

Then,

(9) $$\begin{aligned} \beta(\lambda, p+1) - \beta(\lambda, p) &= (\lambda - q)(\gamma_{d-1}(\lambda, p+1) - \gamma_{d-1}(\lambda, p)) \\ &\quad - q(\gamma_{d-2}(\lambda, p+1) - \gamma_{d-2}(\lambda, p)) + \gamma_{d-1}(\lambda, p) + \gamma_{d-2}(\lambda, p+1). \end{aligned}$$

At this point, we observe that $C_j(p)$ is similar to the $j \times j$ matrix

$$E_j(p) = \begin{bmatrix} 2 & 1 & & & \\ 1 & 2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 2 & \sqrt{p} \\ & & & \sqrt{p} & p+1 \end{bmatrix}.$$

Hence, the matrices $C_j(p)$ and $E_j(p)$ have the same characteristic polynomial. The recursive formula (4) applied to $E_{d-1}(p)$ and $E_{d-2}(p)$ gives

(10) $$\gamma_{d-1}(\lambda, p) = (\lambda - (p+1))\delta_{d-2}(\lambda) - p\delta_{d-3}(\lambda)$$

and

(11) $$\gamma_{d-2}(\lambda, p) = (\lambda - (p+1))\delta_{d-3}(\lambda) - p\delta_{d-4}(\lambda),$$

where, for $j = d-2$, $j = d-3$ and $j = d-4$, $\delta_j(\lambda)$ is the characteristic polynomial of the matrix

$$D_j = \begin{bmatrix} 2 & 1 & & & \\ 1 & 2 & 1 & & \\ & 1 & \ddots & \ddots & \\ & & \ddots & 2 & 1 \\ & & & 1 & 2 \end{bmatrix}$$

of order $j \times j$. Similarly,

(12) $$\gamma_{d-1}(\lambda, p+1) = (\lambda - (p+2))\delta_{d-2}(\lambda) - (p+1)\delta_{d-3}(\lambda)$$

and

(13) $$\gamma_{d-2}(\lambda, p+1) = (\lambda - (p+2))\delta_{d-3}(\lambda) - (p+1)\delta_{d-4}(\lambda).$$

From (10) and (12),

(14) $$\gamma_{d-1}(\lambda, p+1) - \gamma_{d-1}(\lambda, p) = -(\delta_{d-2}(\lambda) + \delta_{d-3}(\lambda)),$$

and, from (11) and (13),

(15) $$\gamma_{d-2}(\lambda, p+1) - \gamma_{d-2}(\lambda, p) = -(\delta_{d-3}(\lambda) + \delta_{d-4}(\lambda)).$$

Replacing (14) and (15) in (9), we have

$$\beta(\lambda, p+1) - \beta(\lambda, p) = -(\lambda - q)(\delta_{d-2}(\lambda) + \delta_{d-3}(\lambda)) + q(\delta_{d-3}(\lambda) + \delta_{d-4}(\lambda))$$
$$+\gamma_{d-1}(\lambda, p) + \gamma_{d-2}(\lambda, p+1).$$

Using now (10) and (13), we obtain

$$\beta\left(\lambda, p+1\right) - \beta\left(\lambda, p\right) = -\left(\lambda - q\right)\left(\delta_{d-2}\left(\lambda\right) + \delta_{d-3}\left(\lambda\right)\right) + q(\delta_{d-3}\left(\lambda\right) + \delta_{d-4}\left(\lambda\right))$$
$$+(\lambda - (p+1))\delta_{d-2}\left(\lambda\right) - p\delta_{d-3}\left(\lambda\right) + (\lambda - (p+2))\delta_{d-3}\left(\lambda\right)$$
$$- \left(p+1\right)\delta_{d-4}\left(\lambda\right).$$

Therefore,

$$\beta\left(\lambda, p+1\right) - \beta\left(\lambda, p\right) = \delta_{d-2}\left(\lambda\right)\left(-\lambda + q + \lambda - p - 1\right)$$
$$+\delta_{d-3}\left(\lambda\right)\left(-\lambda + q + q - p + \lambda - p - 2\right) + \delta_{d-4}\left(\lambda\right)\left(q - p - 1\right).$$

Then,

$$(16) \qquad \beta\left(\lambda, p+1\right) - \beta\left(\lambda, p\right) = \left(q - p - 1\right)\left(\delta_{d-2}\left(\lambda\right) + 2\delta_{d-3}\left(\lambda\right) + \delta_{d-4}\left(\lambda\right)\right).$$

We now apply the recursion formula (4) to D_{d-2} to see that

$$\delta_{d-2}\left(\lambda\right) = \left(\lambda - 2\right)\delta_{d-3}\left(\lambda\right) - \delta_{d-4}\left(\lambda\right).$$

Thus,

$$(17) \qquad\qquad \delta_{d-2}\left(\lambda\right) + 2\delta_{d-3}\left(\lambda\right) + \delta_{d-4}\left(\lambda\right) = \lambda\delta_{d-3}\left(\lambda\right).$$

From (16) and (17),

$$(18) \qquad\qquad \beta\left(\lambda, p+1\right) - \beta\left(\lambda, p\right) = \left(q - p - 1\right)\lambda\delta_{d-3}\left(\lambda\right).$$

We observe that D_{d-3} is a proper submatrix of $B\left(p\right)$. From Lemma 3, the smallest eigenvalue $\alpha_1\left(p\right)$ of $B\left(p\right)$ is strictly less than the smallest eigenvalue of D_{d-3}. Therefore,

$$\delta_{d-3}\left(\alpha_1\left(p\right)\right) < 0, \ \text{if } d \text{ is even}$$

or

$$\delta_{d-3}\left(\alpha_1\left(p\right)\right) > 0, \ \text{if } d \text{ is odd}.$$

By applying this result in (18), together with the facts $q - p - 1 > 0$, $\beta\left(\alpha_1\left(p\right), p\right) = 0$ and $0 < \alpha_1\left(p\right)$, we obtain

$$\beta\left(\alpha_1\left(p\right), p+1\right) < 0, \ \text{if } d \text{ is even}$$

or

$$\beta\left(\alpha_1\left(p\right), p+1\right) > 0, \ \text{if } d \text{ is odd}.$$

It follows that $\alpha_1\left(p\right) \neq \alpha_1\left(p+1\right)$. Suppose that $\alpha_1\left(p\right) < \alpha_1\left(p+1\right)$. Then,

$$\alpha_1\left(p\right) < \alpha_i\left(p+1\right), \ i = 1, 2, \ldots, d.$$

Therefore,

$$\beta\left(\alpha_1\left(p\right), p+1\right) = \prod_{i=1}^{d}\left(\alpha_1\left(p\right) - \alpha_i\left(p+1\right)\right) > 0, \ \text{if } d \text{ is even}$$

or

$$\beta\left(\alpha_1\left(p\right),p+1\right)=\prod_{i=1}^{d}\left(\alpha_1\left(p\right)-\alpha_i\left(p+1\right)\right)<0,\ \text{if } d \text{ is odd},$$

which is a contradiction. Consequently, $\alpha_1\left(p\right)>\alpha_1\left(p+1\right)$. The proof for case $d\geq 5$ is complete. $\qquad\square$

EXAMPLE 2. Let us consider the trees $\mathcal{T}_1$ and $\mathcal{T}_2$.

REMARK 1. We are ready to justify the inequality $a\left(\mathcal{T}_2\right)<a\left(\mathcal{T}_1\right)$ where $\mathcal{T}_1$ and $\mathcal{T}_2$ are the trees of Example 2.

Tree $\mathcal{T}_1$ Tree $\mathcal{T}_2$
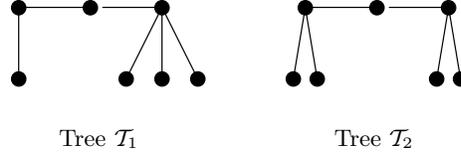
In fact, $\mathcal{T}_1=\mathcal{S}_{7,4}\left(1,3\right)$ and $\mathcal{T}_2=\mathcal{S}_{7,4}\left(2,2\right)$. We apply the case $d=4$ of Theorem 4 to obtain that $a\left(\mathcal{T}_2\right)<a\left(\mathcal{T}_1\right)$.

4. MAXIMIZING THE ALGEBRAIC CONNECTIVITY ON $\mathcal{C}_{n,d}$

From now on, $\mathbf{e}$ is the all ones vector of the appropriate order. We recall the following result.

Lemma 5. [**6**, Corollary 4.2] *Let v be a pendent vertex of the graph $\widetilde{\mathcal{G}}$. Let $\mathcal{G}$ be the graph obtained from $\widetilde{\mathcal{G}}$ by removing v and its edge. Then, the eigenvalues of $L\left(\mathcal{G}\right)$ interlace the eigenvalues of $L(\widetilde{\mathcal{G}})$.*

Corollary 1. *Let $\mathcal{T}$ be a subtree of the tree $\widetilde{\mathcal{T}}$. Then,*

$$(19)\qquad\qquad a(\widetilde{\mathcal{T}})\leq a\left(\mathcal{T}\right).$$

In particular, if $C\left(\mathbf{p}\right)\in\mathcal{C}_{n,d}$ and the order of $\mathbf{e}$ is $(d-1)$,

$$(20)\qquad\qquad a\left(C\left(\mathbf{p}\right)\right)\leq a\left(C\left(\mathbf{e}\right)\right).$$

Proof. From Lemma 5, it follows that the algebraic connectivity of a graph do not increase if a pendent vertex and its edge are added to the graph. From this fact and since we may construct $\widetilde{T}$ from T by successively adding in pendents vertices and edges, we conclude that $a(\widetilde{\mathcal{T}})\leq a\left(\mathcal{T}\right)$. Since $C(\mathbf{e})$ is a subtree of $C(\mathbf{p})$, (20) is an immediate consequence of (19). $\qquad\square$

Let $\mathcal{C}_n=\cup_{3\leq d\leq\lceil (n+1)/2\rceil}\mathcal{C}_{n,d}$ and $\mathcal{C}=\cup_{n\geq 4}\mathcal{C}_n$.

Corollary 2. *For every caterpillar $C(\mathbf{p})\in\mathcal{C}$, $a(C(\mathbf{p}))\leq a(\mathcal{P}_4)$.*

Proof. Since $d\geq 3$, the path $\mathcal{P}_4$ is a subtree of any caterpillar $C(\mathbf{p})\in\mathcal{C}$. From Corollary 1, the result is immediate. $\qquad\square$

Although the result given on Corollary 2 solves the problem of maximizing the algebraic connectivity on $\mathcal{C}$ in which n and d are variables, the problem to maximize the algebraic connectivity in $\mathcal{C}_{n,d}$, a subclass of $\mathcal{C}$ where n and $d \geq 3$ are fixed, is much difficult. Next we solve this problem for caterpillars of even diameter.

4.1 The case d even. If we find $C(\widetilde{\mathbf{p}})$ in $\mathcal{C}_{n,d}$ such that $a(C(\widetilde{\mathbf{p}})) = a(C(\mathbf{e}))$ then $C(\widetilde{\mathbf{p}})$ is the caterpillar in $\mathcal{C}_{n,d}$ with the greatest algebraic connectivity. We look for $C(\widetilde{\mathbf{p}})$.

In [9], one can find a complete characterization of the Laplacian eigenvalues of the tree $\mathcal{P}_m\{\mathcal{B}_i\}$ obtained from $\mathcal{P}_{d-1}$ and the generalized Bethe trees $\mathcal{B}_1, \mathcal{B}_2, \ldots, \mathcal{B}_{d-1}$ obtained by identifying the root vertex of $\mathcal{B}_i$ with the $i-th$ vertex of $\mathcal{P}_{d-1}$. In particular, the spectral radius and the algebraic connectivity are characterized. Before to recall these results, we introduce some notation.

For $i = 1, 2, \ldots, d-1$, let k_i be the number of levels of $\mathcal{B}_i$. For $j = 1, 2, 3, \ldots, k_i$, let d_{i,k_i-j+1} and n_{i,k_i-j+1} be the degree of the vertices and the number of them at the level j of $\mathcal{B}_i$. For $i = 1, 2, \ldots, d-1$, let

$$\Omega_i = \{j : 1 \leq j \leq n_{i,k_i-1} : n_{i,j} > n_{i,j+1}\}.$$

For $i = 1, 2, 3, \ldots, d-1$, let

$$(21) \quad T_i = \begin{bmatrix} d_{i,1} & \sqrt{d_{i,2}-1} & & & & \\ \sqrt{d_{i,2}-1} & d_{i,2} & & & & \\ & & \ddots & \sqrt{d_{i,k_i-1}-1} & & \\ & & \sqrt{d_{i,k_i-1}-1} & d_{i,k_i-1} & \sqrt{d_{i,k_i}} & \\ & & & \sqrt{d_{i,k_i}} & d_{i,k_i}+c \end{bmatrix}$$

of order $k_i \times k_i$, where $c = 2$ for $i = 2, 3, .., d-2$ and $c = 1$ for $i = 1$ and $i = d-1$. Moreover, for $i = 1, 2, \ldots, d-1$ and for $j = 1, 2, 3, \ldots, k_i - 1$, let $T_{i,j}$ be the $j \times j$ leading principal submatrix of T_i.

Let $r = \sum_{i=1}^{d-1} k_i$. Let G be the symmetric matrix of order $r \times r$ defined by

$$(22) \quad G = \begin{bmatrix} T_1 & E_1 & & & \\ E_1^T & T_2 & \ddots & & \\ & \ddots & \ddots & E_{(d-1)-1} & \\ & & E_{(d-1)-1}^T & T_{d-1} \end{bmatrix},$$

where E_i the matrix of order $k_i \times k_{i+1}$ whose entries are 0 except for the entry $E_i(k_i, k_{i+1}) = 1$.

We are ready to recall the main results of [9] concerning the Laplacian eigenvalues of $\mathcal{P}_{d-1}\{\mathcal{B}_i\}$.

Theorem 5. [9] (a) *The Laplacian spectrum of* $\mathcal{P}_{d-1}\{\mathcal{B}_i\}$ *is*

$$\sigma(L(\mathcal{P}_{d-1}\{\mathcal{B}_i\})) = \left(\cup_{i=1}^{d-1} \cup_{j\in\Omega_i} \sigma(T_{i,j})\right) \cup \sigma(G).$$

(b) *The multiplicity of each eigenvalue of the matrix $T_{i,j}$, as an eigenvalue of $L\left(P_{d-1}\left\{B_i\right\}\right)$, is at least $(n_{i,j} - n_{i,j+1})$ for $j \in \Omega_i$.*

(c) *The matrix G is singular.*

Theorem 6. [**9**] *The largest eigenvalue of the matrix G is the spectral radius of $L\left(\mathcal{P}_{d-1}\left\{\mathcal{B}_i\right\}\right).$*

Theorem 7. [**9**] *The smallest positive eigenvalue of the matrix G is the algebraic connectivity of $\mathcal{P}_{d-1}\left\{\mathcal{B}_i\right\}.$*

Clearly, each star $\mathcal{S}_{p_i+1}$ $(1 \leq i \leq d-1)$ is a generalized Bethe tree of 2 levels in which $d_{i,1} = 1,\ d_{i,2} = p_i,\ n_{i,1} = p_i,\ n_{i,2} = 1$.

We apply the above results to $C\left(\mathbf{p}\right).$ The matrices T_i define in (21) become

$$T_1 = T\left(p_1\right) = \begin{bmatrix} 1 & \sqrt{p_1} \\ \sqrt{p_1} & p_1 + 1 \end{bmatrix},$$

$$T_i = S\left(p_i\right) = \begin{bmatrix} 1 & \sqrt{p_i} \\ \sqrt{p_i} & p_i + 2 \end{bmatrix} \quad (2 \leq i \leq (d-1) - 1),$$

$$T_{d-1} = T\left(p_{d-1}\right) = \begin{bmatrix} 1 & \sqrt{p_{d-1}} \\ \sqrt{p_{d-1}} & p_{d-1} + 1 \end{bmatrix}$$

and the matrices E_i become $E_1 = E_2 = \ldots = E_{(d-1)-1} = E = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$, where 0 denotes the zero matrix of the appropriate order.

Suppose $d = 2s + 2.$ Let $\mathbf{p} = [p_1, \ldots, p_s, p_{s+1}, p_s, \ldots, p_1].$

For the symmetric caterpillar $C\left(\mathbf{p}\right),$ the matrix G defined in (22) becomes

$$(23) \qquad G\left(\mathbf{p}\right) = \begin{bmatrix} U\left(p_1, \ldots, p_s\right) & \begin{bmatrix} 0 \\ E \end{bmatrix} & 0 \\ \begin{bmatrix} 0 & E \end{bmatrix} & \begin{bmatrix} 1 & \sqrt{p_{s+1}} \\ \sqrt{p_{s+1}} & p_{s+1} + 2 \end{bmatrix} & \begin{bmatrix} E & 0 \end{bmatrix} \\ 0 & \begin{bmatrix} E \\ 0 \end{bmatrix} & V\left(p_1, \ldots, p_s\right) \end{bmatrix},$$

where

$$U\left(p_1, \ldots, p_s\right) = \begin{bmatrix} T\left(p_1\right) & E & & & \\ E & S\left(p_2\right) & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & & E \\ & & & E & S\left(p_s\right) \end{bmatrix}$$

and

$$V\left(p_1, \ldots, p_s\right) = \begin{bmatrix} S\left(p_s\right) & E & & & & \\ E & S\left(p_{s-1}\right) & \ddots & & & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & & E \\ & & & & E & T\left(p_1\right) \end{bmatrix}.$$

Let J be the permutation matrix of order $2s$ in which the 2×2 blocks along the secondary diagonal is the identity matrix of order 2, that is,

$$J = \begin{bmatrix} & & & I_2 \\ & & I_2 & \\ & I_2 & & \\ I_2 & & & \end{bmatrix}.$$

For instance, if $d = 8$ then $s = 3$ and

$$J = \begin{bmatrix} & & & & & 1 \\ & & & & 1 & \\ & & & 1 & & \\ & & 1 & & & \\ & 1 & & & & \\ 1 & & & & & \end{bmatrix}.$$

We claim that the submatrices U and V in (23) are similar. In fact, $JUJ = V$. Therefore,

$$(24) \qquad G\left(\mathbf{p}\right) = \begin{bmatrix} U\left(p_1, \ldots, p_s\right) & \begin{bmatrix} 0 \\ E \end{bmatrix} & 0 \\ \begin{bmatrix} 0 & E \end{bmatrix} & \begin{bmatrix} \dfrac{1}{\sqrt{p_{s+1}}} & \sqrt{p_{s+1}} \\ \sqrt{p_{s+1}} & p_{s+1} + 2 \end{bmatrix} & \begin{bmatrix} E & 0 \end{bmatrix} \\ 0 & \begin{bmatrix} E \\ 0 \end{bmatrix} & JU\left(p_1, \ldots, p_s\right) J \end{bmatrix}.$$

Lemma 6. *Let $d = 2(s+1)$ and $\mathbf{p} = [p_1, \ldots, p_s, p_{s+1}, p_s, \ldots, p_1]$. The eigenvalues of $G\left(\mathbf{p}\right)$ are the eigenvalues of the positive semidefinite matrix*

$$G_1 = \begin{bmatrix} U\left(p_1, \ldots, p_s\right) & \begin{bmatrix} 0 \\ \sqrt{2}E \end{bmatrix} \\ \begin{bmatrix} 0 & \sqrt{2}E \end{bmatrix} & \begin{bmatrix} \dfrac{1}{\sqrt{p_{s+1}}} & \sqrt{p_{s+1}} \\ \sqrt{p_{s+1}} & p_{s+1} + 2 \end{bmatrix} \end{bmatrix}$$

and the eigenvalues of the positive definite matrix

$$G_2 = U\left(p_1, \ldots, p_s\right).$$

Proof. Easy computations show that $\det G_1 = 0$ and $\det G_2 = 1$. Let us consider the orthogonal matrix Q of order $(4s+2) \times (4s+2)$ defined as

$$
Q = \frac{1}{\sqrt{2}} \begin{bmatrix} I & 0 & J \\ 0 & \sqrt{2}I_2 & 0 \\ I & 0 & -J \end{bmatrix}.
$$

One can easily check that

$$
QG(\mathbf{p})Q^T = \begin{bmatrix} U(p_1,\ldots,p_s) & \begin{bmatrix} 0 \\ \sqrt{2}E \end{bmatrix} & 0 \\ \begin{bmatrix} 0 & \sqrt{2}E \end{bmatrix} & \begin{bmatrix} 1 & \sqrt{p_{s+1}} \\ \sqrt{p_{s+1}} & p_{s+1}+2 \end{bmatrix} & 0 \\ 0 & 0 & U(p_1,\ldots,p_s) \end{bmatrix}.
$$

Then the matrix $G(\mathbf{p})$ in (24) is orthogonally similar to $\begin{bmatrix} G_1 & \\ & G_2 \end{bmatrix}$. $\qquad\square$

EXAMPLE 3. For the caterpillar we have $\mathbf{p} = \begin{bmatrix} 4 & 3 & 2 & 3 & 4 \end{bmatrix}$ and, from Lemma 6, the eigenvalues of $G(\mathbf{p})$ are the eigenvalues of the following matrices
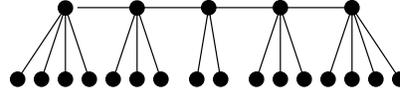
$$
G_1 = \begin{bmatrix} 1. & \sqrt{4} & 0 & 0 & 0 & 0 \\ \sqrt{4} & 5 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & \sqrt{3} & 0 & 0 \\ 0 & 1 & \sqrt{3} & 5 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 & 1 & \sqrt{2} \\ 0 & 0 & 0 & \sqrt{2} & \sqrt{2} & 4 \end{bmatrix} \quad \text{and } G_2 = \begin{bmatrix} 1 & \sqrt{4} & 0 & 0 \\ \sqrt{4} & 5 & 0 & 1 \\ 0 & 0 & 1 & \sqrt{3} \\ 0 & 1 & \sqrt{3} & 5 \end{bmatrix}.
$$

Theorem 8. *Let $d = 2(s+1)$ and $\mathbf{p} = [p_1,\ldots,p_s,p_{s+1},p_s,\ldots,p_1]$. The algebraic connectivity of the caterpillar $C(\mathbf{p})$ is the smallest eigenvalue of*

$$
U(p_1,\ldots,p_s) = \begin{bmatrix} T(p_1) & E & & \\ E & S(p_2) & \ddots & \\ & \ddots & \ddots & E \\ & & E & S(p_s) \end{bmatrix}.
$$

Proof. From Lemma 7, the smallest positive eigenvalue of $G(\mathbf{p})$ is the algebraic connectivity of the caterpillar $C(\mathbf{p})$. Then, we search for such smallest positive eigenvalue. From Lemma 6, the eigenvalues of $G(\mathbf{p})$ are the eigenvalues of the matrices G_1 and $G_2 = U(p_1,\ldots,p_s)$. We know that $\det G_1 = 0$ and $\det G_2 = 1$. So, the smallest eigenvalue of G_1 is 0 and the smallest eigenvalue of $G_2 = U(p_1,\ldots,p_s)$

is positive and strictly less than 1. Let G_{11} be the submatrix of G_1 obtained by deleting its last row and its last column. That is

$$G_{11} = \begin{bmatrix} G_2 & 0 \\ 0 & 1 \end{bmatrix}.$$

By the eigenvalue interlacing property for Hermitian matrices, the eigenvalues of $G_2 = U(p_1, \ldots, p_s)$ and the eigenvalue 1 interlace the eigenvalue of G_1. Therefore, the smallest eigenvalue of $U(p_1, \ldots, p_s)$ is the smallest positive eigenvalue of $G(\mathbf{p})$. This completes the proof. □

Corollary 3. *Let $d = 2(s+1)$ and $\widetilde{\mathbf{p}} = [p_1, p_2, \ldots, p_{d-1}]$ where $\widetilde{p}_i = 1$ for all $i \neq s+1$ and $\widetilde{p}_{s+1} = n - 2d + 3$. Then,*

$$a(C(\widetilde{\mathbf{p}})) = a(C(\mathbf{e})).$$

Proof. Follows straightforward from Theorem 8 and the fact that $U(p_1, \ldots, p_s)$ does not depend on p_{s+1}. □

Theorem 9. *Let $d = 2(s+1)$. Among the caterpillars in $\mathcal{C}_{n,d}$ the maximum algebraic connectivity is attained by the caterpillar $C(\widetilde{\mathbf{p}})$ defined in Corollary 3. That is $a(C(\mathbf{p})) \leq a(C(\widetilde{\mathbf{p}}))$, for all $C(\mathbf{p}) \in \mathcal{C}_{n,d}$.*

Proof. We begin observing that $C(\widetilde{\mathbf{p}}) \in \mathcal{C}_{n,d}$. Let $C(\mathbf{p}) \in \mathcal{C}_{n,d}$. From Corollary 1, $a(C(\mathbf{p})) \leq a(C(\mathbf{e}))$. If now we use Corollary 3, we can conclude that $a(C(\mathbf{p})) \leq a(C(\widetilde{\mathbf{p}}))$. □

4.2 The case d odd: a difficult problem. We have used AutoGraphiX and NewGraph systems to determine the algebraic connectivity of caterpillars in the family $\mathcal{C}_{n,d}$ for many different odd integer values of d. All the computations suggest that if $d = 2s+1$ and $\overline{\mathbf{p}} = [\overline{p}_1, \overline{p}_2, \ldots, \overline{p}_{d-1}]$, where $\overline{p}_i = 1$ for all $i \neq s+1$ and $\overline{p}_{s+1} = n - 2d + 3$, then the caterpillar $C(\overline{\mathbf{p}})$ has maximum algebraic connectivity among all caterpillars in $\mathcal{C}_{n,d}$.

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