

Schur reduction of trees and extremal entries of the Fiedler vector

H. Gernandt* J. P. Pade†

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Abstract

We study the eigenvectors of Laplacian matrices of trees. The Laplacian matrix is reduced to a tridiagonal matrix using the Schur complement. This preserves the eigenvectors and allows us to provide formulas for the ratio of eigenvector entries. We also obtain bounds on the ratio of eigenvector entries along a path in terms of the eigenvalue and Perron values. The results are then applied to the Fiedler vector. Here we locate the extremal entries of the Fiedler vector and study classes of graphs such that the extremal entries can be found at the end points of the longest path.

1 Introduction

For a simple undirected unweighted graph G with vertices $V(G) = \{v_1, \dots, v_n\}$ and edges $E(G)$ the *graph Laplacian* is given by $L(G) := D - A \in \mathbb{R}^{n \times n}$ where D is a diagonal matrix containing the degrees of the vertices and A is the adjacency matrix of the graph.

Since the seminal papers [18, 19] by M. Fiedler in the 1970s, the analysis of graph Laplacians has attracted a great deal of attention [21, 10, 39, 22, 12, 30]. It is well known that $L(G)$ is positive semi-definite with eigenvalues $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$.

A particular focus lies on the problem of establishing a connection between algebraic properties of the graph Laplacian and the topology of the underlying graph. For example, if G is connected then $\lambda_1 = 0$ is a simple eigenvalue. Many eigenvalue bounds have been established in dependence of the graph topology for the other eigenvalues [10] and especially for the smallest non-zero eigenvalue λ_2 , the so-called *algebraic connectivity* usually denoted by $a(G)$, see [1] for an overview. If $a(G)$ is a simple eigenvalue then the associated eigenvector is called *Fiedler vector* in honour to M. Fiedler [18].

However, apart from the original results from M. Fiedler, very few is known about the Fiedler vector and its connection to topological properties of the underlying graph, see [8, 28, 38]. Not only is a deeper knowledge of this relation of a theoretical interest, it is also of great importance for many applications. In networks of diffusively coupled elements it was shown that the dynamical impact of connecting two nodes through an additional edge is closely related to the corresponding entries in the Fiedler vector [34, 33]. Furthermore, the Fiedler vector plays a central role in random walks on graphs, and applications to community detection [27, 16].

In the above applications, the extremal values of the Fiedler vector are of special interest. For instance, in networks of diffusively coupled elements, they correspond to the nodes which have the greatest impact on the dynamics when connected through an additional edge.

*Institute of Mathematics, TU Ilmenau, Weimarer Straße 25, 98693 Ilmenau, Germany (hannes.gernandt@tu-ilmenau.de).

†Institute of Mathematics, Humboldt-University of Berlin, Unter den Linden 6, 10099 Berlin, Germany

In 1974 it was hypothesized by J. Rauch that for a somewhat generic choice of initial conditions, the extremal values of the solution to the heat equation are attained at the boundary of the considered domain [5]. This hypothesis turned out not to be true for certain domains [9]. Later on, it was found that the discrete analogue of this hypothesis plays an important role in medical imaging processing [11, 36]. In [11] it was hypothesized for trees that the extremal values of the Fiedler vector are attained at the two vertices which are connected by the longest path in the tree, or in other words, at the most distant vertices. It was only shown for a path though. And it was in 2013 that a counter-example among trees was found: the Fiedler rose [17, 26], see also [2]. Since then, to our knowledge no progress has been made in verifying the hypothesis for a nontrivial class of trees.

In this article, we investigate the structure of eigenvectors of trees. Here we use a graph reduction technique based on Schur complements which is similar to the well known Kron reduction [14, 37, 38]. However, our technique preserves the eigenvectors after reduction. This allows us to obtain formulas for the ratios of eigenvector entries. We also provide upper and lower bounds for the ratios of the eigenvector entries along paths in the tree and we prove the hypothesis for a class of trees.

The article is structured as follows. In Section 2, we recall basic notions from graph theory and linear algebra. The Schur reduction is introduced in Section 3 and its properties are studied. In Section 4 we provide formulas for the entries of Laplacian eigenvectors in terms of the Schur complement. In Section 5 we apply our results to the Fiedler vector. First, it is shown that the extremal entries of the Fiedler vector are located at the pendant vertices of the tree. Later on, we give conditions to find those pendant vertices where the extremal entries are located. Furthermore, we study generalizations of caterpillar trees, where we can show that the extremal entries of the Fiedler vector are located at the endpoints of the longest path. In this context, we also discuss the Fiedler rose from [17, 26]. Later in Section 6, we obtain bounds on the ratios of eigenvector entries along paths that depend only on the eigenvalues. Finally, in Section 7 we identify local extrema of the Fiedler vector in an even larger class of trees.

2 Notations and Preliminaries

In this section, we recall some notions from graph theory and linear algebra that we will use throughout the article.

For a graph G we denote by $V(G)$ and $E(G)$ its *set of vertices* and *edges*, respectively. Each edge $e \in E(G)$ connects two vertices, say $v, w \in V(G)$ and we also write vw instead of e . In this case, we say that v and w are *adjacent* and that e is *incident* with v and w .

The *degree* of a vertex v , i.e. the number of incident edges, is denoted by $\deg_G(v)$. A vertex $v \in V(G)$ with $\deg_G(v) = 1$ is called *pendant vertex*.

Let G be a connected graph. The *distance* $d(v, w)$ between two vertices $v, w \in V(G)$ is the number of edges in the shortest path between v and w . The *diameter* of G is then given by

$$d(G) := \max_{v, w \in V(G)} d(v, w).$$

The *path* with n vertices is denoted by P_n . We also study *star graphs*, i.e. trees T with diameter $d(T) = 2$, which we denote by S_n , where n is the number of vertices. The unique vertex in S_n with $n \geq 3$ which is not a pendant vertex is called *center* of S_n .

We recall some definitions from linear algebra. For this sake, we consider a matrix $M \in \mathbb{R}^{n \times n}$. We denote by $\sigma(M)$ the *spectrum*, i.e. the set of eigenvalues, of M . Furthermore, $\|M\| := \sup_{\|x\|=1} \|Mx\|$ is the *spectral norm*. If M is symmetric, then $\|M\|$ equals the eigenvalue with maximum modulus, i.e. the *spectral radius* $\rho(M)$. Recall that the row sum norm is given by $\|M\|_\infty := \max_{1 \leq i \leq n} \sum_{j=1}^n |m_{ij}|$ with $M = (m_{ij})_{i,j=1}^n \in \mathbb{R}^{n \times n}$. For a symmetric

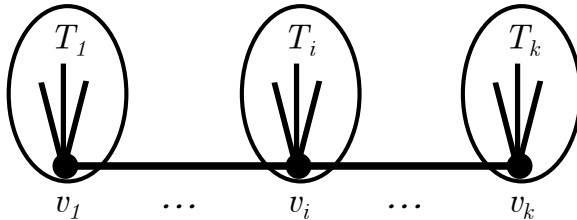


Figure 1: In a tree T we select a path $v_1 \dots v_k$. Then for each v_i on this path there is a unique maximal tree T_i with $V(T_i) \cap \{v_1, \dots, v_k\} = \{v_i\}$. Since T is a tree, there are no edges between T_i and T_j for $i \neq j$.

matrix M with nonnegative eigenvalues, we denote by $\lambda_{\min}(M)$ the smallest element in $\sigma(M)$ and if M is invertible we have $\lambda_{\min}(M) = \|M^{-1}\|^{-1}$.

Recall that for a block matrix $\mathcal{A} = \begin{pmatrix} A & B \\ B^\top & C \end{pmatrix} \in \mathbb{R}^{n \times n}$ with $C \in \mathbb{R}^{r \times r}$ invertible, the *Schur complement* with respect to the lower diagonal block C is given by

$$(\mathcal{A}/C) := A - BC^{-1}B^\top.$$

In the following we study the spectral properties of the *graph Laplacian* $L(G) = D - A$ where $D = \text{diag}(\deg_T(v_i))_{i=1}^n$ is the diagonal matrix of vertex degrees and $A = (a_{ij})_{i,j=1}^n$ is the adjacency matrix given by

$$a_{ij} = \begin{cases} 1, & \text{if } e = v_i v_j \in E(G), \\ 0, & \text{if } e = v_i v_j \notin E(G). \end{cases}$$

Since there is a natural labelling of the entries of the eigenvectors $(x_i)_{i=1}^n$ using the vertex set $V(G)$, we will also write x_{v_i} instead of x_i .

The associated *reduced Laplacian* $L_{v_i}(G) \in \mathbb{R}^{(n-1) \times (n-1)}$ is obtained by deleting the i -th row and the i -th column of $L(G)$.

It is a regular matrix which is also known under the names of grounded Laplacian matrix [29, 35, 40] and Dirichlet Laplacian matrix [6]. By the matrix-tree-theorem [31], $\det(L_{v_i}(G))$ is the number of spanning trees of G , so $\det(L_{v_i}(G)) > 0$, i.e. $L_{v_i}(T_i)$ is invertible. We also consider the *doubly reduced Laplacian* $L_{v_i, v_j}(G) \in \mathbb{R}^{(n-2) \times (n-2)}$ which is the matrix obtained from $L(G)$ by deleting simultaneously the rows and columns with index i and j .

Finally, we denote by \mathbb{N} the set of natural numbers including zero.

3 Schur reduction of trees

In this section, we present a reduction technique for the graph Laplacian that is based on the Schur complement.

Let $v_1 v_2 \dots v_k$ be a path in an arbitrary tree T . Then to each vertex v_i there is an associated unique maximal tree T_i attached to it with $V(T_i) \cap \{v_1, \dots, v_k\} = \{v_i\}$ (see Figure 1) such that there are no edges between T_i and T_j for all $i \neq j$ except for $v_i v_{i+1}$. We say that T_i is associated with v_i .

Therefore, after a suitable relabelling of vertices, the graph Laplacian of T can be written

with the reduced Laplacians $L_{v_i}(T_i)$ in the form

$$L(T) = \begin{bmatrix} \deg_T(v_1) & -1 & & & & & f_1^\top \\ -1 & \ddots & \ddots & & & & \ddots \\ & \ddots & \ddots & -1 & & & \\ f_1 & & -1 & \deg_T(v_k) & & & f_k^\top \\ & & & & L_{v_1}(T_1) & & \\ & & & & & \ddots & \\ & & & & & & L_{v_k}(T_k) \end{bmatrix} \quad (1)$$

where $f_i \in \mathbb{R}^{|V(T_k)|-1}$ is a vector with entries -1 if v_i and the vertex in T_i corresponding to the entry are adjacent or 0 if v_i is not adjacent with the corresponding vertex, i.e.

$$L(T_i) = \begin{bmatrix} L_{v_i}(T_i) & f_i \\ f_i^\top & \deg_T(v_i) \end{bmatrix}.$$

Note that for $\mathcal{A} = L(G)$ with a suitable reduced Laplacian $C = L_{v_i}(G)$ the Schur complement (\mathcal{A}/C) is also called a Kron reduction of the graph G , see [14].

We now investigate the Schur complement with respect to the lower diagonal block $\text{diag}(L_{v_i}(T_i) - \lambda)_{i=1}^k$, which is given for $\lambda \notin \sigma(L_{v_i}(T_i))$ for all $i = 1, \dots, k$ by

$$S_{T_1, \dots, T_k}(\lambda) := ((L(T) - \lambda) / \text{diag}(L_{v_i}(T_i) - \lambda)_{i=1}^k) = \begin{pmatrix} s_{T_1}(\lambda) & -1 & & & \\ -1 & \ddots & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & & -1 & s_{T_k}(\lambda) \end{pmatrix} \quad (2)$$

where for $\lambda \notin \sigma(L_{v_i}(T_i))$ the function $s_{T_i}(\lambda)$ is given by

$$\begin{aligned} s_{T_i}(\lambda) &:= \deg_T(v_i) - \lambda - f_{T_i}(\lambda), \\ f_{T_i}(\lambda) &:= f_i^\top (L_{v_i}(T_i) - \lambda)^{-1} f_i. \end{aligned} \quad (3)$$

In the theorem below, we relate the eigenvectors of $L(T)$ and $S_{T_1, \dots, T_k}(\lambda)$. This will enable us to compare and estimate entries of the Fiedler vector of $L(G)$ in the subsequent sections.

Theorem 1. *Let T be a tree with $L(T)$ of the form (1) and let $\lambda \notin \sigma(L_{v_i}(T_i))$ for all $i = 1, \dots, k$ then the following holds.*

- (a) $\lambda \in \sigma(L(T))$ if and only if $\ker S_{T_1, \dots, T_k}(\lambda) \neq \{0\}$.
- (b) $(x_1, \dots, x_k, y_1^\top, \dots, y_k^\top)^\top \in \ker(L(T) - \lambda)$ if and only if $(x_1, \dots, x_k)^\top \in \ker S_{T_1, \dots, T_k}(\lambda)$ and

$$y_i = -(L_{v_i}(T_i) - \lambda)^{-1} f_i x_i, \quad i = 1, \dots, k. \quad (4)$$

- (c) We have $\dim \ker S_{T_1, \dots, T_k}(\lambda) \leq 1$, hence $(x_1, \dots, x_k)^\top$ in (b) is unique up to scaling and $\dim \ker(L(T) - \lambda) \leq 1$. Furthermore, every eigenvector for $\lambda \in \sigma(L(T))$ satisfies $x_1 \neq 0, x_k \neq 0$.

Proof. We abbreviate

$$A := \begin{pmatrix} \deg_T(v_1) - \lambda & -1 & & & \\ & -1 & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & \deg_T(v_k) - \lambda \end{pmatrix}, \quad B := \text{diag}(f_i^\top)_{i=1}^k, \quad C := \text{diag}(L_{v_i}(T_i))_{i=1}^k.$$

The Aitken block-diagonalization formula (cf. [3, 41]) gives us

$$L(T) - \lambda = \begin{bmatrix} A - \lambda & B \\ B^\top & C - \lambda \end{bmatrix} = \begin{bmatrix} I & B(C - \lambda)^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} S_{T_1, \dots, T_k}(\lambda) & 0 \\ 0 & C - \lambda \end{bmatrix} \begin{bmatrix} I & 0 \\ (C - \lambda)^{-1} B^\top & I \end{bmatrix}.$$

From this equation it is easy to see that (a) and (b) hold.

Clearly we have $\text{rk } S_{T_1, \dots, T_k}(\lambda) \geq k - 1$, as the first $k - 1$ columns of $S_{T_1, \dots, T_k}(\lambda)$ are linearly independent. Hence from the dimension formula we have

$$\dim \ker S_{T_1, \dots, T_k}(\lambda) = k - \text{rk } S_{T_1, \dots, T_k}(\lambda) \leq 1.$$

It remains to show that $x_1 \neq 0$ and $x_k \neq 0$ for an eigenvector $(x_1, \dots, x_k, y_1^\top, \dots, y_k^\top)^\top \in \ker L(T) - \lambda$. Assume that $x_1 = 0$ then we obtain from the equation $S_{T_1, \dots, T_k}(\lambda)x = 0$ that $x_i = 0$ for all $i = 1, \dots, k$ and hence from (4) we see that $y_i = 0$ for all $i = 1, \dots, k$ which is a contradiction. For $x_k = 0$ we can repeat the arguments from above. \square

The Schur reduction can also be applied to weighted trees, i.e. when each edge has a positive weight. It can also be applied if the attached graphs T_i are arbitrary connected graphs.

We prove some basic properties of the functions f_{T_i} .

Proposition 2. *Let T be a tree decomposed as in Figure 1. Consider the tree T_i and assume that T_i is partitioned into subgraphs $T_{i,1}, \dots, T_{i,l}$ as in Figure 2 that have only v_i as a joint vertex. Then $\sigma(L_{v_i}(T_i)) = \bigcup_{i=1}^l \sigma(L_{v_i}(T_{i,l}))$ and the following holds.*

- (a) $f_{T_i}(\lambda) = \sum_{j=1}^l f_{T_{i,j}}(\lambda)$ for all $\lambda \notin \sigma(L_{v_i}(T_i))$.
- (b) $f_{T_i}^{(k)}(\lambda) > f_{T_i}^{(k)}(0) > 0$ for all $\lambda \in (0, \lambda_{\min}(L_{v_i}(T_i)))$ and $k \in \mathbb{N}$.
- (c) We have $f_{T_i}(0) = \deg_{T_i}(v_i)$ and for all $k \in \mathbb{N} \setminus \{0\}$

$$\|L_{v_i}(T_i)\|^{-(k-1)} \leq \frac{f_{T_i}^{(k)}(0)}{k!(|V(T_i)| - 1)} \leq \|L_{v_i}(T_i)^{-1}\|^{k-1}.$$

In particular, for $k = 1$, we have $f'_{T_i}(0) = |V(T_i)| - 1$.

- (d) For all $\lambda \in (0, \lambda_{\min}(L_{v_i}(T_i)))$ we have

$$\frac{\lambda(|V(T_i)| - 1)}{1 - \|L_{v_i}(T_i)\|^{-1}\lambda} \leq f_{T_i}(\lambda) - \deg_{T_i}(v_i) \leq \frac{\lambda(|V(T_i)| - 1)}{1 - \|L_{v_i}(T_i)^{-1}\|\lambda}.$$

- (e) Let S_i be a subtree of T_i with $v_i \in V(S_i)$ that can be obtained from removing step by step pendant vertices. Then we have $\lambda_{\min}(L_{v_i}(T_i)) \leq \lambda_{\min}(L_{v_i}(S_i))$, $f_{S_i}^{(k)}(0) \leq f_{T_i}^{(k)}(0)$ for all $k \in \mathbb{N}$ and

$$f_{S_i}(\lambda) \leq f_{T_i}(\lambda), \quad \lambda \in (0, \lambda_{\min}(L_{v_i}(T_i))).$$

If in addition $S_i \neq T_i$, then all of the above inequalities are strict.

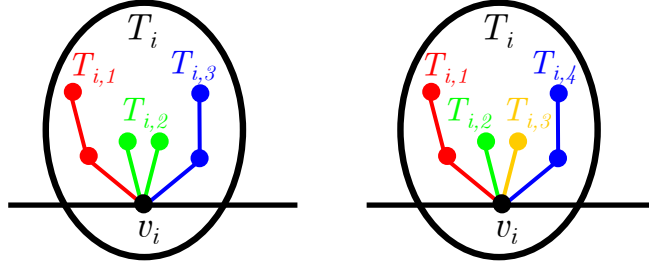


Figure 2: The figure illustrates the situation in Proposition 2. We see two possible partitions of the tree T_i into subtrees $T_{i,j}$.

Proof. After a relabelling of vertices we have

$$L_{v_i}(T_i) = \text{diag}(L_{v_i}(T_{i,1}), \dots, L_{v_i}(T_{i,l}))$$

and therefore $\sigma(L_{v_i}(T_i)) = \bigcup_{i=1}^l \sigma(L_{v_i}(T_{i,l}))$ holds. We decompose the vector

$$f_i = (f_{i,1}^\top, \dots, f_{i,l}^\top)^\top$$

where $f_{i,j} \in \mathbb{R}^{|V(T_{i,j})|-1}$ is a vector that is zero except for one entry -1 corresponding to the vertex that is the unique neighbor of v_i in $T_{i,j}$. Thus, we see that

$$\begin{aligned} f_{T_i}(\lambda) &= f_i^\top (L_{v_i}(T_i) - \lambda)^{-1} f_i \\ &= f_i^\top \text{diag}((L_{v_i}(T_{i,1}) - \lambda)^{-1}, \dots, (L_{v_i}(T_{i,l}) - \lambda)^{-1}) f_i \\ &= \sum_{j=1}^l f_{i,j}^\top (L_{v_i}(T_{i,j}) - \lambda)^{-1} f_{i,j} \\ &= \sum_{j=1}^l f_{T_{i,j}}(\lambda) \end{aligned} \quad (5)$$

which proves (a). The function f_{T_i} is analytic on $[0, \lambda_{\min}(L_{v_i}(T_i))]$ with derivatives given by

$$f_{T_i}^{(k)}(\lambda) = k! f_i^\top (L_{v_i}(T_i) - \lambda)^{-(k+1)} f_i, \quad k \geq 1. \quad (6)$$

From the choice of $\lambda \in (0, \lambda_{\min}(L_{v_i}(T_i)))$ and the Weyl bound [24, Theorem 4.3.1] implies that $L_{v_i}(T_i) - \lambda$ is positive definite and hence also $(L_{v_i}(T_i) - \lambda)^{-(k+1)}$ is positive definite for all $k \geq 1$. Thus, the right hand side in (6) is positive, as $f_i \neq 0$. This implies that $f_{T_i}^{(k)}$ is strictly monotonically increasing on $[0, \lambda_{\min}(L_{v_i}(T_i))]$, which proves (b).

For the proof of the assertion (c) we use (5) for $\lambda = 0$ and $l = \deg_{T_i}(v_i)$. Let the indices k and l of $L_{v_i}(T_{i,j})^{-1}$ correspond to the vertices $v, w \in V(T_i)$, respectively. Since T_i is a tree there are unique paths P_{v,v_i} and P_{w,v_i} in T_i from v_i to v and w , respectively. Then it was shown in [25, Proposition 1] that the entry of $L_{v_i}(T_{i,j})^{-1}$ with index (k, l) equals $|E(P_{v,v_i}) \cap E(P_{w,v_i})|$, i.e. the number of joint edges of both paths. We consider the diagonal entry that arises from $v = w = v_i^{(j)}$, where $v_i^{(j)}$ is the unique neighbor for v_i in $T_{i,j}$. Then $P_{v,v_i} = P_{w,v_i}$ is a path of length one and this gives us

$$f_{i,j}^\top L_{v_i}(T_{i,j})^{-1} f_{i,j} = 1.$$

Using this together with (5), we see that the first equality in (c) holds. The characterization of the entries of $L_{v_i}(T_i)^{-1}$ from [25, Proposition 1] yields

$$f_i^\top L_{v_i}(T_i)^{-2} f_i = (L_{v_i}(T_i)^{-1} f_i)^\top L_{v_i}(T_i)^{-1} f_i = \|(1, \dots, 1)^\top\|^2 = |V(T_i)| - 1. \quad (7)$$

The Cauchy-Bunjakowski inequality applied to (6) gives with (7)

$$f_{T_i}^{(k)}(\lambda) = k! f_i^\top (L_{v_i}(T_i) - \lambda)^{-(k+1)} f_i \leq k! \|L_{v_i}^{-1}\|^{(k-1)} \|L_{v_i}(T_i) f_i\|^2 = k! \|L_{v_i}^{-1}\|^{(k-1)} (|V(T_i)| - 1).$$

This is the upper bound in (c). The proof of the lower bound in (c) is similar using $\lambda_{\min}(L_{v_i}^{(k-1)})$ and that $\lambda_{\min}(L_{v_i}^{-1}) = \|L_{v_i}\|^{-1}$ holds.

For the proof of (d) we use (6) and obtain from a Taylor expansion of f_{T_i} at $\lambda = 0$

$$\begin{aligned} f_{T_i}(\lambda) &= \deg_{T_i}(v_i) + \sum_{k=2}^{\infty} \frac{f_{T_i}^{(k)}(0) \lambda^k}{k!} \\ &\leq \deg_{T_i}(v_i) + \sum_{k=1}^{\infty} (|V(T_i)| - 1) \|L_{v_i}(T_i)^{-1}\|^{k-1} \lambda^k \\ &\leq \deg_{T_i}(v_i) + (|V(T_i)| - 1) \lambda \sum_{k=0}^{\infty} \|L_{v_i}(T_i)^{-1}\|^k \lambda^k \\ &= \deg_{T_i}(v_i) + \frac{(|V(T_i)| - 1) \lambda}{1 - \lambda \|L_{v_i}(T_i)^{-1}\|}. \end{aligned}$$

This proves the upper bound in (d). The lower bound can be obtained similarly, by using the lower bound for $f_{T_i}^{(k)}(0)$ from (c).

We continue with the proof of (e). Since S_i can be obtained from T_i by removing pendant vertices, the matrix $L_{v_i}(S_i)$ can be obtained from $L_{v_i}(T_i)$ after applying negative rank one perturbations in combination with deletion of rows and columns with the same index. Therefore, we see from Weyl's interlacing inequality [24, Corollary 4.3.9] and Cauchy's interlacing inequality [24, Theorem 4.3.17] that $\lambda_{\min}(L_{v_i}(T_i)) \leq \lambda_{\min}(L_{v_i}(S_i))$. From the subgraph condition and the choice of v_i in S we have the following inequality for the entries of the reduced Laplacians

$$0 < (L_{v_i}(S_i)^{-1})_{k,l} \leq (L_{v_i}(T_i)^{-1})_{k,l} \quad (8)$$

for all $k, l = 1, \dots, |V(S_i)| - 1$ where we assume that the entries of the matrices are sorted in such a way that the corresponding vertices of S_i in T_i have the same index. From this it is easy to see that $f_{S_i}^{(k)}(0) \leq f_{T_i}^{(k)}(0)$ for all $k \in \mathbb{N}$. From the Taylor expansion of f_{T_i} and f_{S_i} at 0 we see that $f_{S_i}(\lambda) \leq f_{T_i}(\lambda)$. Let S_i be a proper subtree of T_i then the matrix $L_{v_i}(S_i)$ is a proper submatrix of $L_{v_i}(T_i)$ and the strictness of the inequalities follows from the positivity of the entries in (8). \square

The bound in (d) holds with equality if T_i is a star graph with center vertex v_i , because T_i can be decomposed into $T_{i,j}$ with $j = 1, \dots, \deg_{T_i}(v_i)$ which are graphs that consist of two vertices and one edge between them.

Note that the value $\lambda_{\min}(L_v(T))^{-1}$ equals $\|L_v(T)^{-1}\|$ which is known as the *Perron value* in the literature, see [25]. In the lemma below, we provide some upper and lower bounds for $\lambda_{\min}(L_{v_i}(T_i))$, and hence, for the Perron value, see also [4, Theorem 4.2].

Lemma 3. *Let T be a tree and let v be a vertex in T and consider for each pendant vertex w the path $v_1 = v \dots v_{d(v,w)+1} = w$ and let T_i be the tree associated with v_i then we have*

$$\max_{\deg_T(w)=1} \sqrt{\sum_{i=0}^{d(v,w)} i^2 |V(T_{i+1})|} \leq \lambda_{\min}(L_v(T))^{-1} = \|L_v(T)^{-1}\| \leq \max_{\deg_T(w)=1} \sum_{i=0}^{d(v,w)} i |V(T_{i+1})|.$$

Proof. Using the spectral radius we find $\rho(L_v(T)^{-1}) \leq \|L_v(T)^{-1}\|_{\infty}$ and hence

$$\lambda_{\min}(L_v(T)) = \|L_v(T)^{-1}\|^{-1} = \rho(L_v(T)^{-1})^{-1} \geq \|L_v(T)^{-1}\|_{\infty}^{-1}.$$

Now the upper bound is a simple consequence of the formula for the entries of $L_v(T)^{-1}$ from [25, Proposition 1]. It is easy to see that the maximum over the row sums is attained at rows that correspond to a pendant vertex w . The lower bound follows from the trivial estimate $\|L_v(T)^{-1}\| \geq \|L_v(T)^{-1}e_i\|$ where e_i is a canonical unit vector and taking the maximum over those unit vectors whose index corresponds to the pendant vertices in T . \square

The bounds above hold with equality for T given by $V(T) = \{v, w\}$ and $E(T) = \{vw\}$.

4 On the ratio of Laplacian eigenvector entries

In this section we use the Schur reduction in order to compare two eigenvector entries. In the following, we assume that a path $v_1 \dots v_k$ is given in T with associated trees T_i (see Figure 1).

First we consider the case $k = 2$ and $k = 3$, i.e. we study the eigenvector entries at vertices with distance less than or equal to two. In this case the ratio of the entries can be described in terms of the functions s_{T_1} and s_{T_2} from (3).

Proposition 4. *Let T be given as in Figure 1 with $\lambda \in \sigma(L(T))$ and associated eigenvector $x = (x_1, \dots, x_n)^\top$.*

- (a) *Assume that $k = 2$ and $\lambda \notin \sigma(L_{v_1}(T_1)) \cup \sigma(L_{v_2}(T_2))$, then the entries x_1 and x_2 of the eigenvector x for λ at v_1 and v_2 , respectively, satisfy $x_1, x_2 \neq 0$ and*

$$\frac{x_2}{x_1} = s_{T_1}(\lambda) = s_{T_2}(\lambda)^{-1}. \quad (9)$$

- (b) *Assume that $k = 3$ and $\lambda \notin \sigma(L_{v_i}(T_i))$ for $i = 1, 2, 3$. Then the entries x_1 and x_3 of the eigenvector x for λ at v_1 and v_3 , respectively, satisfy $x_1, x_3 \neq 0$ and*

$$\frac{x_3}{x_1} = \frac{s_{T_1}(\lambda)}{s_{T_3}(\lambda)}.$$

Proof. According to Theorem 1, the eigenvector entries x_1 and x_2 are the solution of the equation

$$\begin{pmatrix} s_{T_1}(\lambda) & -1 \\ -1 & s_{T_2}(\lambda) \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0. \quad (10)$$

Now the formula (9) immediately follows from (10).

We continue with the proof of (b). Applying the Schur reduction to the trees T_1 , T_2 and T_3 leads to the following system of equations

$$\begin{pmatrix} s_{T_2}(\lambda) & -1 & -1 \\ -1 & s_{T_1}(\lambda) & 0 \\ -1 & 0 & s_{T_3}(\lambda) \end{pmatrix} \begin{pmatrix} x_2 \\ x_1 \\ x_3 \end{pmatrix} = 0. \quad (11)$$

Again, we have from Theorem 1 that $x_1, x_3 \neq 0$ and solving the second and third component of the equation (11) for x_1 we see that (b) holds. \square

In the remainder of this section we consider the case that $k \geq 3$ and we assume that v_1 is a pendant vertex, i.e. $V(T_1) = \{v_1\}$. This allows us to compare the values of the eigenvectors at pendant vertices. We denote the subgraph that contains the path $v_1 \dots v_k$ and the trees T_1, \dots, T_{k-1} by \hat{T} .

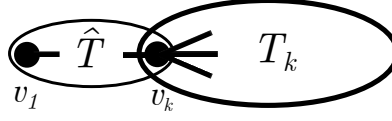


Figure 3: To compare the eigenvector entries at v_1 and v_k , we consider the subgraph \hat{T} that contains the path $v_1 \dots v_k$ and the associated trees T_1, \dots, T_{k-1} as in Figure 1.

Let $L_{v,w}(T)$ be the doubly reduced Laplacian, i.e. the matrix that is obtained by deleting the row and the column corresponding to the vertices v and w , then we can write $L(T)$ as

$$L(T) = \begin{bmatrix} L_{v_1, v_k}(\hat{T}) & -e_1 & -e_{k-2} & 0 \\ -e_1^\top & \deg(v_1) & 0 & 0 \\ -e_{k-2}^\top & 0 & \deg(v_k) & f_k^\top \\ 0 & 0 & f_k & L_{v_k}(T_k) \end{bmatrix}$$

where $e_1, e_{k-2} \in \mathbb{R}^{|\hat{T}|-2}$ are the canonical unit vectors and f_k is a vector with entries 0 and -1 describing the adjacency of v_k with vertices in T_k . Let x_1 and x_k be the entries of the eigenvector for $\lambda \in \sigma(L(T)) \setminus \sigma(L_{v_1, v_k}(\hat{T}))$. Then, we consider the kernel equations of the Schur complement $((L(T) - \lambda)/(L_{v_1, v_k}(\hat{T}) - \lambda))$ with $\deg(v_1) = 1$ leading to the equation

$$(1 - \lambda - e_1^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-1} e_1) x_1 - e_1^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-1} e_{k-2} x_k = 0.$$

We introduce the function $g_{v_1, v_k} : [0, \lambda_{\min}(L_{v_1, v_k}(\hat{T}))] \rightarrow \mathbb{R}$ given by

$$g_{v_1, v_k}(\lambda) := \frac{1 - \lambda - e_1^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-1} e_1}{e_{k-2}^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-1} e_1}, \quad (12)$$

then Theorem 1 implies for the eigenvector entries x_1 and x_k at v_1 and v_k , respectively,

$$g_{v_1, v_k}(\lambda) = \frac{x_k}{x_1}.$$

In the lemma below we state some properties of the function g_{v_1, v_k} .

Lemma 5. *Let T be a tree decomposed into \hat{T} and T_k as in Figure 3 with $k \geq 3$ and $\deg_T(v_1) = 1$. Then g_{v_1, v_k} is strictly monotonically decreasing and*

$$g_{v_1, v_k}(0) = 1, \quad g'_{v_1, v_k}(0) = 1 - k - \sum_{i=1}^{k-2} i |V(T_{i+1})|.$$

Proof. For $\lambda \in \rho(L_{v_1, v_k}(\hat{T}))$ we introduce

$$g_1(\lambda) := 1 - \lambda - e_1^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-1} e_1, \quad g_2(\lambda) := e_{k-2}^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-1} e_1.$$

Since $L_{v_1, v_k}(\hat{T}) - \lambda$ is a matrix that has only positive diagonal entries and non-positive off-diagonal entries it follows from [20, Theorem 4.3] that $(L_{v_1, v_k}(\hat{T}) - \lambda)^{-1}$ has non-negative entries only. Hence, the derivatives of g_1 and g_2 satisfy for all $\lambda \in [0, \lambda_{\min}(L_{v_1, v_k}(\hat{T}))]$

$$g'_1(\lambda) = -1 - e_1^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-2} e_1 < 0, \quad g'_2(\lambda) = e_{k-2}^\top (L_{v_1, v_k}(\hat{T}) - \lambda)^{-2} e_1 \geq 0.$$

This implies that g_1 is strictly monotonically decreasing and that g_2 is strictly monotonically increasing on $[0, \lambda_{\min}(L_{v_1, v_k}(\hat{T}))]$. We will show in the second part of the proof that $g_2(0) =$

$\frac{1}{k-1} > 0$ which implies $g_2(\lambda) > 0$ for all $\lambda \in [0, \lambda_{\min}(L_{v_1, v_k}(\hat{T}))]$. Therefore the function g_{v_1, v_k} satisfies for all $0 \leq \lambda_1 < \lambda_2 < \lambda_{\min}(L_{v_1, v_k}(\hat{T}))$

$$g_{v_1, v_k}(\lambda_2) = \frac{g_1(\lambda_2)}{g_2(\lambda_2)} < \frac{g_1(\lambda_1)}{g_2(\lambda_2)} \leq \frac{g_1(\lambda_1)}{g_2(\lambda_1)} = g_{v_1, v_k}(\lambda_1)$$

and is therefore strictly monotonically decreasing on $(0, \lambda_{\min}(L_{v_1, v_k}(\hat{T}))$.

It remains to compute $g_{v_1, v_k}(0)$ and $g'_{v_1, v_k}(0)$. A short computation shows that

$$g'_{v_1, v_k}(0) = \frac{(-1 - e_1^\top L_{v_1, v_k}(\hat{T})^{-2} e_1) e_{k-2}^\top L_{v_1, v_k}(\hat{T})^{-1} e_1 - (1 - e_1^\top L_{v_1, v_k}(\hat{T})^{-1} e_1) e_{k-2}^\top L_{v_1, v_k}(\hat{T})^{-2} e_1}{(e_{k-2}^\top L_{v_1, v_k}(\hat{T})^{-1} e_1)^2}.$$

In the following we make a construction to apply the formula for the inverse of the reduced Laplacian from [25, Proposition 1].

We use that $L_{v_1, v_k}(\hat{T}) = L_{v_0}(\tilde{T})$ where \tilde{T} is the graph obtained from \hat{T} after merging v_1 and v_k to one vertex v_0 with degree 2. More precisely, we have $V(\tilde{T}) := (V(\hat{T}) \setminus \{v_1, v_k\}) \cup \{v_0\}$ and $E(\tilde{T}) := (E(\hat{T}) \setminus \{v_1 v_2, v_{k-1} v_k\}) \cup \{v_0 v_2, v_0 v_{k-1}\}$.

The graph $\tilde{T} - v_0 v_{k-1}$, where we delete the edge that connects v_0 with v_{k-1} , is a tree such that the formula from [25, Proposition 1] can be used. From the Sherman-Morrison-Woodbury formula, see e.g. [7], we conclude

$$L_{v_1, v_k}(\hat{T})^{-1} = L_{v_0}(\tilde{T})^{-1} = L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} - \frac{L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} e_{k-2} e_{k-2}^\top L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1}}{1 + e_{k-2}^\top L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} e_{k-2}}$$

and with [25, Proposition 1] we have

$$1 + e_{k-2}^\top L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} e_{k-2} = k - 1,$$

and hence, after a suitable permutation of the entries, it holds that

$$\begin{aligned} e_{k-2}^\top L_{v_1, v_k}(\hat{T})^{-1} &= \frac{1}{k-1} e_{k-2}^\top L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} \\ &= \frac{1}{k-1} \underbrace{(k-2, \dots, k-2, \dots)}_{\in \mathbb{R}^{1 \times |V(T_{k-1})|}} \underbrace{(1, \dots, 1)}_{\in \mathbb{R}^{1 \times |V(T_2)|}}, \\ L_{v_1, v_k}(\hat{T})^{-1} e_1 &= L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} e_1 - \frac{1}{k-1} L_{v_0}(\tilde{T} - v_0 v_{k-1})^{-1} e_{k-2} \\ &= \frac{1}{k-1} \left(\underbrace{(1, \dots, 1)}_{\in \mathbb{R}^{1 \times |V(T_{k-1})|}}, \dots, \underbrace{(k-2, \dots, k-2)}_{\in \mathbb{R}^{1 \times |V(T_2)|}} \right)^\top \end{aligned}$$

and hence

$$e_{k-2} L_{v_1, v_k}(\hat{T})^{-1} e_1 = \frac{1}{k-1}, \quad e_1^\top L_{v_1, v_k}(\hat{T})^{-1} e_1 = \frac{k-2}{k-1}.$$

This implies that for $\lambda = 0$ in (12) we have $g_{v_1, v_k}(0) = 1$.

Furthermore, we see that

$$\begin{aligned} g'_{v_1, v_k}(0) &= (k-1)(-1 - e_1^\top L_{v_1, v_k}(\hat{T})^{-2} e_{k-2} - e_1^\top L_{v_1, v_k}(\hat{T})^{-2} e_1) \\ &= (k-1)(-1 - e_1^\top L_{v_1, v_k}(\hat{T})^{-1} (L_{v_1, v_k}(\hat{T})^{-1} e_{k-2} + L_{v_1, v_k}(\hat{T})^{-1} e_1) \\ &= (k-1)(-1 - e_1^\top L_{v_1, v_k}(\hat{T})^{-1} (1, \dots, 1)^\top) \\ &= 1 - k - \sum_{i=1}^{k-2} i |V(T_{i+1})|. \end{aligned}$$

□

The corollary below is a consequence of Theorem 1 and Lemma 5. Here we compare the eigenvector entries at two pendant vertices.

Corollary 6. *Let T be a tree with pendant vertices w and w' and consider a vertex v with $w'v, wv \notin E(T)$ and let \hat{T} and \hat{T}' be the trees from Figure 3 for $w = v_1$ and $w' = v_1$ and $v = v_k$. Assume that $\lambda \in \sigma(L(T))$ with $\lambda < \min\{\lambda_{\min}(L_{w,v}(\hat{T})), \lambda_{\min}(L_{w',v}(\hat{T}'))\}$ then the entries x_w and $x_{w'}$ of the associated eigenvector satisfy*

$$g_{w,v}(\lambda)x_w = g_{w',v}(\lambda)x_{w'}.$$

Let λ be sufficiently small, then $x_v, x_w, x_{w'} \neq 0$ and $\frac{x_{w'}}{x_w} \geq 1$ if there exists an index $i_0 \geq 0$ with $g_{w,v}^{(i)}(0) = g_{w',v}^{(i)}(0)$ for all $i = 0, \dots, i_0$ and $g_{w,v}^{(i_0+1)}(0) > g_{w',v}^{(i_0+1)}(0)$.

We will see later that in the special case $\lambda = a(T)$, a large diameter of T_k implies that the value $a(T)$ is small (cf. (31)).

5 Extremal entries of the Fiedler vector

In this subsection, we consider the Fiedler vector, which is the eigenvector corresponding to the first nonzero eigenvalue $a(T)$ of $L(T)$. Here it is assumed that $a(T)$ is a simple eigenvalue of $L(T)$. Since T is connected, the vector $(1, \dots, 1)^\top$ is the, up to scaling, unique eigenvector for the eigenvalue 0. Since $L(T)$ is a symmetric matrix, the Fiedler vector is orthogonal to $(1, \dots, 1)^\top$ and hence, it contains both, positive and negative entries.

In the following, we will study the extremal entries. These entries were also studied in [26], where it was said that a graph has the *Fiedler extrema diameter* (FED) property, if the Fiedler vector has only two extrema that are located at the endpoints of the longest path.

In the lemma below, we show that the extremal entries of the Fiedler vector are located only at the pendant vertices, see also [26, Corollary 1].

Lemma 7. *Let T be a tree with a path $v_1 \dots v_k$ as in Figure 1 with diameter $d(T) \geq 2$ and Fiedler vector $x = (x_i)_{i=1}^n$, then the following holds.*

- (a) *The extremal entries of the Fiedler vector are located only at pendant vertices.*
- (b) *One of the following assertions holds:*
 - (i) *The entries of the Fiedler vector on the path $v_1 \dots v_k$ are monotonically decreasing or increasing.*
 - (ii) *We have $x_1, x_k \geq 0$ and there exists $x_{k'} \geq 0$ with $x_1 \geq x_2 \dots \geq x_{k'}$ and $x_{k'} \leq x_{k'+1} \leq \dots \leq x_k$.*
 - (iii) *We have $x_1, x_k \leq 0$ and there exists $x_{k'} \leq 0$ with $x_1 \leq x_2 \dots \leq x_{k'}$ and $x_{k'} \geq x_{k'+1} \geq \dots \geq x_k$.*

Proof. Let $(1, \dots, 1)^\top \in \mathbb{R}^n$ be the eigenvector corresponding to 0 and let $x = (x_1, \dots, x_n)^\top$ be the up to scaling unique eigenvector corresponding to $a(T)$. From [19, Corollary 2.3] we have that for any $\alpha \geq 0$ the induced subgraph T_α with vertices given by $V(T_\alpha) = \{v_i : x_i + \alpha \geq 0\}$ is connected. This implies that there is no negative local minimum of the vector on the entries x_2, \dots, x_{n-1} , i.e. $x_k \leq x_{k-1}$ and $x_k \leq x_{k+1}$ cannot hold for all $k = 2, \dots, n-1$. Repeating the arguments above with $-x$, we see that there is no positive local maximum of x on v_2, \dots, v_{n-1} .

By choosing x_1 and x_k as pendant vertices, we see that the extremal values are attained at the pendant vertices. It remains to show that they are only attained at pendant vertices. Since $d(T) \geq 2$ we have from [12, p. 187] that

$$a(T) \leq 2 \left(1 - \cos \left(\frac{\pi}{d(T) + 1} \right) \right) < 1.$$

Let v_1 be a pendant vertex with neighbor v_2 then the eigenvector equation $(1-a(T))x_1 = x_2$. Since $a(T) < 1$, we have $x_1 > x_2 > 0$ or $x_1 < x_2 < 0$. Hence only the values at the pendant vertices are extremal. This finishes the proof of (i). Now (ii) and (iii) are a simple consequence of the previous arguments on the non-existence of local maxima and minima. \square

As a first application, we consider *caterpillar trees* which are trees that consist of one central path to which all other vertices have distance one. These graphs have been well investigated and find applications in chemistry and physics [23, 15]. Here the trees T_i in Figure 1 are star graphs S_{r_i} with $r_i \in \mathbb{N}$ and center v_i and we can further decompose T_i into the trees $T_{i,j}$ for $j = 1, \dots, \deg_{T_i}(v_i)$ which consist of one edge only. In this case $L_{v_i}(T_{i,j}) = 1$ and hence $\sigma(L_{v_i}(T_i)) = \{1\}$.

Corollary 8. *Let T be a caterpillar tree with $d(T) \geq 3$. Then, the extremal values of the Fiedler vector are attained at the pendant vertices in T_1 and in T_k .*

Proof. This is essentially a consequence of Lemma 7. But we have to exclude that $x_1 = x_2$ holds, i.e. we have strict monotonicity $x_1 > x_2 > 0$ or $x_1 < x_2 < 0$. To see this we use the Schur reduction with $\lambda = a(T) < 1 = \lambda_{\min}(L_{v_1}(T_1))$. Considering the kernel of $S_{T_1, \dots, T_k}(a(T))$, we see from (9) that

$$\frac{x_2}{x_1} = s_{T_1}(\lambda) = 1 + \deg_{T_1}(v_1) - \lambda - \frac{\deg_{T_1}(v_1)}{1 - \lambda}.$$

The assumption $x_1 = x_2$ and $\lambda = a(T)$ leads to

$$1 = 1 - a(T) - \frac{a(T) \deg_{T_1}(v_1)}{1 - a(T)}$$

and therefore $a(T) = 0$ or $a(T) = \deg_{T_1}(v_1) + 1 > 1$ which is not possible. Thus, we have shown that $x_1 \neq x_2$. A similar argument shows that $x_{k-1} \neq x_k$ holds and therefore the extremal entries are located at the pendant vertices in T_1 and T_k . \square

From Corollary 8 we see that the (FED) property only holds if we assume that the caterpillar tree also satisfies $|V(T_1)|, |V(T_k)| = 2$.

The theorem below provides properties of the entries of the Fiedler vector for graphs that, are slightly more general than caterpillar trees.

Theorem 9. *Let T be a tree which is decomposed into subtrees $T_{i,j}$ with $i = 1, \dots, k$ and $j = 1, \dots, \deg_{T_i}(v_i)$ then the following holds.*

- (a) *If $a(T) < \lambda_{\min}(L_{v_i}(T_{i,j}))$ for all $i = 1, \dots, k, j = 1, \dots, \deg_{T_i}(v_i)$ then $a(T)$ is a simple eigenvalue of $L(T)$.*
- (b) *Under the assumption of (a) assume additionally that $k \geq 3$ and that there exist pendant vertices $w_j \in V(T_j)$ with $j = 1, k$ such that*

$$0 < g_{w_j, v_j}(a(T)) \leq \min_{\substack{i \in \{1, \dots, k\} \setminus \{j\} \\ v \in V(T_i), \deg_{T_i}(v) = 1}} g_{v, v_i}(a(T)), \quad j = 1, k.$$

Then the values of the Fiedler vector at w_1 and w_k have a different sign and are extremal. If these vertices are unique, then the property (FED) holds.

- (c) Assume that there are pendant vertices $w, w' \in V(T_i)$ from some $i = 1, \dots, k$ with disjoint paths $w = v_1, \dots, v_{d(w,v)-1} = v$ and $w' = v'_1, \dots, v'_{d(w',v)-1} = v$ and such that

$$-d(w, v) - \sum_{i=1}^{d(w,v)-1} i|V(S_{i+1})| > -d(w', v) - \sum_{i=1}^{d(w',v)-1} i|V(S'_{i+1})|$$

holds, where S_i and S'_i are the trees associated with the path $w = v_1, \dots, w_{d(v_1,v)-1} = v$ and $w' = v'_1, \dots, w'_{d(v_1,v)-1} = v$, respectively. Then for k sufficiently large, the entries x, x' of the Fiedler vector in T_i at w, w' satisfy $\frac{x'}{x} \geq 1$.

Proof. Given that (A1) holds, then Theorem 1 implies that $a(T)$ is simple. The proof of (a) is similar to the proof of Proposition 10 and therefore omitted.

We continue with the proof of (b). Note that the assumption (A1) implies with Cauchy's interlacing inequality [24, Theorem 4.3.17] that $a(T) \leq \lambda_{\min}(L_{v_i,v}(T_{i,j}))$ for all $v \in V(T_{i,j})$.

We apply Lemma 7 (b). From the assumption in (a) and Theorem 1, we see that $x_1 \neq 0$. Without restriction, we assume that $x_1 > 0$ holds. This excludes case (iii) in Lemma 7. Assume further, that we are in case (ii) of this lemma. Then all entries of the Fiedler vector x_1, \dots, x_k are nonnegative since we assumed $g_{v,v_i}(a(T)) > 0$ for all $i = 1, \dots, k$ and all pendant vertices $v \in V(T_i)$. Therefore, again by Lemma 7 applied to T_i all vertices in T_i have nonnegative values of the Fiedler vector. This implies that all entries of the Fiedler vector are nonnegative, which is not possible, since $(1, \dots, 1)^T \in \mathbb{R}^n$ is orthogonal to x . Therefore case (ii) in Lemma 7 (b) cannot hold. As a consequence, we are in the case (i) in this lemma. Now we consider a path from the pendant vertex w_1 in T_1 to the pendant vertex w_k in T_k which must be either monotonic decreasing or increasing. The previous arguments imply that $x_k < 0$ and therefore the entries of the Fiedler vector on the selected path are decreasing. Hence the entries w_1 and w_k have a different sign. The assumption on w_1 implies that the value of the Fiedler vector at w_1 is extremal among all vertices in T_1 by Corollary 6. It remains to show that w_1 is then the remaining vertices in the trees T_2, \dots, T_k . Now one can show that $x_1 > x_2$, Since $d(T) \geq k \geq 3$ this can be shown in the same way as in the proof of Corollary 8 which proves the previous claim. Hence w_1 is maximal, since we assumed that $x_1 > 0$ and a repetition of the arguments from above proves that the value of the Fiedler vector at w_k is minimal.

For the proof of (c) we use the bound [12, p. 187]

$$a(T) \leq 2 - 2 \cos\left(\frac{\pi}{d(T) + 1}\right) \leq 2 - 2 \cos\left(\frac{\pi}{k}\right) \quad (13)$$

and hence $a(T) \rightarrow 0$ as $k \rightarrow \infty$. Therefore, for sufficiently large k , we see from Lemma 5 that the assumptions of Corollary 6 are fulfilled and thus, the assertion (c) follows. \square

As a special case, we assume that $T_{i,j} = S$ holds for all $i = 1, \dots, k$ and all $j = 1, \dots, \deg_{T_i}(v_i)$ and some graph S . In the graph S we select a pendant vertex $v_0 \in V(S)$ that is identified with v_i .

Corollary 10. *Let T be an S -caterpillar tree with a central path $v_1 \dots v_k$ and assume that $a(T) < \lambda_{\min}(L_{v_0}(S))$. Then there exists a Fiedler vector and the following holds:*

- (a) *The extremal entries of the Fiedler vector are located at the pendant vertices in the trees attached to v_1 and to v_k .*
- (b) *Assume that there is a unique vertex v in S that minimizes*

$$g'_{v,v_1}(0) = -d(v_1, v) - \sum_{i=1}^{d(v_1,v)-1} i|V(S_{i+1})| \quad (14)$$

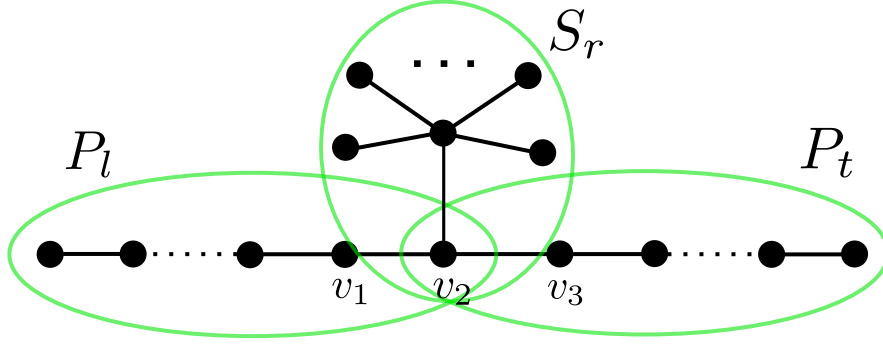


Figure 4: The Fiedler rose consisting of the paths P_l , P_t and a star graph S_r glued together at the vertex v_2 .

where S_i are the unique trees associated with the path $w_1 = v_1, \dots, w_{d(v_1, v)-1} = v$. Then the extremal entries of the Fiedler vector are attained at v in the trees attached to v_1 and v_k if k is sufficiently large.

Proof. First, we need to verify that the assumptions of Theorem 9 (b) are fulfilled. The assumption on $a(T)$ implies by Theorem 1 that $x_1 \neq 0$. Without restriction, we can assume that $x_1 > 0$. We show that $g_{v, v_1}(a(T)) > 0$ holds for all pendant vertices v in S . Consider a path from $v \in V(T_1)$ to $v \in V(T_k)$ that contains v_1 . Then we apply Lemma 7 (b) to this selected path. Since we assumed $x_1 > 0$ the case (iii) is not possible. Assume that (ii) holds, then obviously $g_{v, v_1}(a(T)) > 0$, as $x_1 > 0$ and the value at $v \in V(T_1)$ is positive. Assume that (i) holds and that the entries are monotonically decreasing, then the value at $v \in V(T_1)$ is greater or equal to $x_1 > 0$ and again $g_{v, v_1}(a(T)) > 0$ follows. Consider now the case that the entries are monotonically increasing then $x_k \geq x_1 > 0$ and also the value at $v \in V(T_k)$ is positive. Therefore $g_{v, v_1}(a(T)) = g_{v, v_k}(a(T)) > 0$. shows that the assumptions of Theorem 9 (b) are satisfied. \square

Remark 11. Assume in Corollary 10 (b), that two pendant vertices v, w both minimize (14) and assume that $d(v, w) = 2$, then the eigenvector entries at v and w are the same and hence the extremal entries are located at these vertices. Otherwise, one has to compare higher order derivatives of g_{v, v_1} , to decide on which pendant vertices the extremal entry of the eigenvector is located.

Finally, we discuss the example of the Fiedler rose from [17, 26], where paths P_l , P_t and a star graph S_r are glued together at a pendant vertex (see Figure 4).

First, we represent the rose tree as in Figure 1. Without restriction, we can assume that $t \geq l$. Here we set $T_1 := P_{l-1}$, $T_2 := S_r$ and $V(T_i) := \{v_i\}$ for $3 \leq i \leq 2 + t - l$ and $T_{3+t-l} := P_{l-1}$. It is easy to see that

$$\lambda_{\min}(L_{v_1}(T_1)) = 2 - 2 \cos \left(\frac{\pi}{2l - 3} \right)$$

and hence

$$a(T) \leq 2 - 2 \cos \left(\frac{\pi}{t + l - 1} \right) < 2 - 2 \cos \left(\frac{\pi}{2l - 3} \right) \leq \lambda_{\min}(L_{v_1}(T_1)).$$

For fixed $r \geq 2$ we can always choose l large enough such that

$$a(T) < \lambda_{\min}(L_{v_2}(S_r))$$

and that the assumptions of Theorem 9 (b) are fulfilled. More precisely, we know from the upper bound in Lemma 3 that

$$\lambda_{\min}(L_{v_2}(S_r)) \geq \frac{1}{r}.$$

Together with the bound (13) for $a(T)$ we see that

$$1 - \frac{1}{2r} \leq \cos\left(\frac{\pi}{l+t-1}\right) \quad (15)$$

and this implies that the assumptions of Corollary 6 are fulfilled. Furthermore, let w_1 be a pendant vertex in T_1 then we will see later, from Lemma 14 that

$$g_{w_1, v_2}(\lambda) = \frac{2}{\sqrt{4-\lambda}} \cos\left((l-1/2) \arccos\left(1 - \frac{\lambda}{2}\right)\right)$$

and for a pendant vertex w_2 in T_2 one can find from (12) that

$$g_{w_2, v_2}(\lambda) = \lambda^2 - r\lambda + 1.$$

Assume now that $t > l$, then

$$g_{w_1, v_2}(a(T)) \geq g_{w_1, v_2}\left(2 - 2 \cos\left(\frac{\pi}{l+t-1}\right)\right) > 0$$

and from Theorem 9 (b) we see that

$$\frac{2}{\sqrt{4-a(T)}} \cos\left((l-3/2) \arccos\left(1 - \frac{a(T)}{2}\right)\right) < a(T)^2 - ra(T) + 1 \quad (16)$$

is a sufficient condition for that the extremal values of the Fiedler vector are located at the endpoints of the longest path in the Fiedler rose and (FED). Using the monotonicity of the functions g_{w_1, v_1} and g_{w_2, v_2} from Lemma 5 and the bounds (13) for $a(T)$ we see that the condition

$$\frac{\sqrt{2} \cos\left((l-3/2) \frac{\pi}{l+t-1}\right)}{\sqrt{1 + \cos\left(\frac{\pi}{l+t-1}\right)}} < \left(2 - 2 \cos\left(\frac{\pi}{l+t+r-1}\right)\right)^2 - r \left(2 - 2 \cos\left(\frac{\pi}{l+t+r-1}\right)\right) + 1 \quad (17)$$

is sufficient for (16) and this condition only depends on the parameters l, t and r . In summary, we have seen that for $t > l$ the conditions (15) and (17) are sufficient for (FED) to hold.

If T is a perfect rose tree, i.e. $t = l$ then we can conclude some more structural properties of the Fiedler vector and $a(T)$. We assume again that (15) holds and let l be so large that

$$g_{w_2, v_2}(a(T)) > g_{w_2, v_2}\left(2 - 2 \cos\left(\frac{\pi}{2l-1}\right)\right) > 0. \quad (18)$$

Assume that $a(T) < 2 - 2 \cos(\frac{\pi}{2l-1})$, then $g_{w_1, v_2}(a(T)) > 0$ and hence $x_{w_1}, x_{v_2} \neq 0$, say $x_{w_1}, x_{v_2} > 0$. This implies that all entries of the eigenvector on P_l are positive. Due to symmetry, also the Fiedler vector is also positive on the path P_t . Since $g_{w_2, v_2}(a(T)) > 0$ the Fiedler vector is nonnegative on S_r . This is a contradiction to the orthogonality to the eigenvector $(1, \dots, 1)^\top$.

Therefore, we have $a(T) = 2 - 2 \cos(\frac{\pi}{2l-1})$ which implies by Lemma 14 that $x_{v_2} = 0$. Hence, $x_{v_2} = g_{w_2, v_2}(a(T))x_{w_2} = 0$ and (18) imply that $x_{w_2} = 0$. Lemma 7 (b) implies that

the Fiedler vector is zero at all vertices of S_r . Furthermore, the extremal entries are located at v_1 and v_{2l-1} .

Let us now consider a rose tree with fixed l , but with sufficiently large $t > l$. In this setting, we assume that T_1 is decomposed into $T_{1,1} := P_l$, $T_{1,2} := S_r$ and set $T_2 := P_t$. We consider the rose tree for sufficiently large t , then we know from Corollary 6, where the extremal entries are located by looking at the derivatives

$$g'_{w_1, v_1}(0) = -\frac{l(l+1)}{2}, \quad g'_{w_2, v_1}(0) = -r.$$

If $r > \frac{l(l+1)}{2}$, then we have from Theorem 9 (c) that for sufficiently large t , the extremal entries of the Fiedler vector are located at $V(S_r) \setminus \{v_1\}$ and at the end of P_l .

On the other hand, if $r < \frac{l(l+1)}{2}$ then for sufficiently large t , the extremal values of the Fiedler vector are located at v and the end of the path P_l .

The Fiedler rose is a counter example to the conjecture that the extremal values of the Fiedler vector on trees are located at the end points of the longest path. In the following we apply this construction to arbitrary trees, to show that we can add a large star graph to a vertex on the longest path such that the extremal entries are located on this star graph. In particular, it is possible to move the extremal entries from the longest path to the pendant vertices of the star graph. The corollary below follows from Theorem 9 (c).

Corollary 12. *Let T be a tree with a path $v_1 \dots v_k$ and associated trees T_1, \dots, T_k and $k = d(T) + 1$. Then $d(T_i) \leq 2(i-1)$ for all $i \leq \lceil \frac{d(T)+1}{2} \rceil$. Assume that $k \geq 7$ and that $r \in \mathbb{N}$ satisfies*

$$-(r+1) < -3 - |V(T_2)| - 2|V(T_3)|.$$

Let $a(T)$ be sufficiently small with Fiedler vector $(x_i)_{i=1}^n$ with $x_1 > 0$. Then one can add S_r to T_4 , i.e. a pendant vertex of S_r is identified with v_4 . Let $v_S \in V(S_r)$ be a pendant vertex of the resulting graph then the entries of the Fiedler vector satisfy $\frac{x_{v_S}}{x_{v_1}} \geq 1$.

6 Bounds on the ratio of eigenvector entries along paths

In this section, we provide bounds on the ratios of Laplacian eigenvector entries that depend only on the eigenvalue, but not the resolvent of a reduced Laplacian.

The bounds are based on estimates for the entries of the kernel elements of the tridiagonal matrix $S_{T_1, \dots, T_k}(\lambda)$. Here we view this matrix as a perturbation of a tridiagonal Toeplitz matrix, where we allow only perturbations on the main diagonal.

Note that classical perturbation results for eigenvectors, like the Davis-Kahan theorem (cf. [13]) are not useful since the distance between the eigenvalues is small and also they do not provide good bounds for fixed entries.

First, we present the main result of this section. Assume that there exist $\underline{\zeta}_k, \bar{\zeta}_k \in (0, \frac{\pi}{2})$ such that

$$\begin{aligned} 2(1 - \cos(\bar{\zeta}_k)) &= \lambda + \min_{i=1, \dots, k} (f_{T_i}(\lambda) - \deg_T(v_i)), \\ 2(1 - \cos(\underline{\zeta}_k)) &= \lambda + \max_{i=1, \dots, k} (f_{T_i}(\lambda) - \deg_T(v_i)). \end{aligned} \tag{19}$$

Theorem 13. *Let $\lambda \notin \bigcup_{i=1}^{k-1} \sigma(L_{v_i}(T_i))$ be an eigenvalue of $L(T)$ such that (19) holds and let $x_1 > 0$. Then we have for all i with $0 < i < \min\{\frac{\pi}{2\underline{\zeta}_{k-1}} + 1/2, k\}$ that $x_i > 0$,*

$$\frac{\cos\left(\left(i + \frac{1}{2}\right)\underline{\zeta}_{k-1}\right)}{\cos\left(\left(i - \frac{1}{2}\right)\underline{\zeta}_{k-1}\right)} \leq \frac{x_{i+1}}{x_i} \leq \frac{\cos\left(\left(i + \frac{1}{2}\right)\bar{\zeta}_{k-1}\right)}{\cos\left(\left(i - \frac{1}{2}\right)\bar{\zeta}_{k-1}\right)}. \tag{20}$$

and

$$x_1 \frac{\cos\left(\left(i + \frac{1}{2}\right)\underline{\zeta}_{k-1}\right)}{\cos\left(\frac{1}{2}\underline{\zeta}_{k-1}\right)} \leq x_{i+1} \leq x_1 \frac{\cos\left(\left(i + \frac{1}{2}\right)\bar{\zeta}_{k-1}\right)}{\cos\left(\frac{1}{2}\bar{\zeta}_{k-1}\right)}. \quad (21)$$

Theorem 13 is a direct consequence of Theorem 15 below, where we bound the entries of kernel elements of the tridiagonal matrices of the form

$$A = \begin{pmatrix} 1 - \varepsilon_1 & -1 & & & \\ -1 & 2 - \varepsilon_2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 1 - \varepsilon_n \end{pmatrix} \in \mathbb{R}^{n \times n} \quad (22)$$

with $\varepsilon_1, \dots, \varepsilon_n \in [0, \infty)$. These matrices have the same structure as $S_{T_1, \dots, T_k}(\lambda)$ and hence the entries of the kernel elements of (22) are the entries of the eigenvectors of $L(T)$. If we delete the last column of A it is easy to see by induction that $\text{rk } A \geq n - 1$ and hence that $\dim \ker A \leq 1$.

The matrix A can be viewed as a perturbation of the graph Laplacian $L(P_n)$ of the path with n vertices.

First, we investigate the case $\varepsilon_i = \varepsilon$ for some $\varepsilon \in [0, \infty)$. For $n \geq 3$ we consider the equation $Ax = 0$. Leaving out the n th component of this linear system of equations, we obtain

$$x_1 - x_2 = \varepsilon x_1, \quad -x_{i-1} + 2x_i - x_{i+1} = \varepsilon x_i, \quad 2 \leq i \leq n - 1. \quad (23)$$

Since we erased one equation, there is always a one dimensional solution space to the system (23) and an explicit solution is given in the lemma below, see also [26, Lemma 2] and [32, Remark 3.1].

Lemma 14. *Let $\varepsilon = 2(1 - \cos(\zeta))$ with $\zeta \in [0, \frac{\pi}{2})$. For fixed $x_1 \in \mathbb{R}$ the system (23) has the unique solution*

$$x_j = \frac{\sqrt{2} x_1}{\sqrt{1 + \cos(\zeta)}} \cos((j - 1/2)\zeta), \quad j = 2, \dots, n. \quad (24)$$

In particular, if $x_1 > 0$ then $x_1 > x_2 > \dots > x_k > 0$ for all $k < \frac{\pi}{2\zeta} + \frac{1}{2}$.

Proof. Expression (24) can easily be checked by plugging it into the equations (23). It remains to apply the addition theorem for cosine function. Assume now that $x_1 > 0$ then according to (24) we have $x_j > 0$ as long as $(j - 1/2)\zeta < \frac{\pi}{2}$. Solving this for j proves the proposition. \square

Now, we present the bounds for the entries of kernel elements of (22). We assume that there exist $\underline{\zeta}_k, \bar{\zeta}_k \in (0, \frac{\pi}{2})$ satisfying

$$\begin{aligned} \underline{\varepsilon}_k &:= 2(1 - \cos(\underline{\zeta}_k)) \geq \max_{i=1, \dots, k} \varepsilon_i, \\ \bar{\varepsilon}_k &:= 2(1 - \cos(\bar{\zeta}_k)) \leq \min_{i=1, \dots, k} \varepsilon_i. \end{aligned} \quad (25)$$

Theorem 15. *Let A be given by (22) with $A(x_1, \dots, x_k)^\top = 0$ and $x_1 > 0$ such that (25) holds for $\underline{\zeta}_{k-1}, \bar{\zeta}_{k-1} \in (0, \frac{\pi}{2})$. Then we have $x_1 > x_2 > \dots > x_i > 0$ for all $0 < i < \min\{\frac{\pi}{2\underline{\zeta}_{k-1}} + 1/2, k\}$ and*

$$\frac{\cos((i + 1/2)\underline{\zeta}_{k-1})}{\cos((i - 1/2)\underline{\zeta}_{k-1})} \leq \frac{x_{i+1}}{x_i} \leq \frac{\cos((i + 1/2)\bar{\zeta}_{k-1})}{\cos((i - 1/2)\bar{\zeta}_{k-1})}.$$

Proof. Define the sequence

$$\begin{aligned} F_1 &:= 1 - \varepsilon_1, \\ F_i &:= 2 - \varepsilon_i - F_{i-1}^{-1}, \quad i \geq 2 \end{aligned}$$

where the element F_i is only defined if $F_{i-1} \neq 0$. Then from the kernel equation for the matrix (22) it is easy to see that $F_1 = \frac{x_2}{x_1}$ and if $F_{i-1} = \frac{x_i}{x_{i-1}} \neq 0$ and it holds that

$$F_i = \frac{x_{i+1}}{x_i}.$$

Consider now an auxiliary sequence \underline{F}_i given by $\underline{F}_1 := 1 - \underline{\varepsilon}_{k-1}$ and for $i \geq 2$ by

$$\underline{F}_i := 2 - \underline{\varepsilon}_{k-1} - \underline{F}_{i-1}^{-1}$$

where again \underline{F}_i is only defined if $\underline{F}_{i-1} \neq 0$. Then we have

$$F_1 = 1 - \varepsilon_1 \geq 1 - \underline{\varepsilon}_{k-1} = \underline{F}_1$$

and it is easy to see by induction that for all $i \geq 2$ with $F_{i-1}, \underline{F}_{i-1} \neq 0$

$$F_i = 2 - \varepsilon_i - F_{i-1}^{-1} \geq 2 - \underline{\varepsilon}_{k-1} - \underline{F}_{i-1}^{-1} = \underline{F}_i. \quad (26)$$

In the following we choose \hat{x}_i such that $\hat{x}_1 = x_1$, $\hat{x}_2 = (1 - \mu)\hat{x}_1$ for some $\mu \in \mathbb{R}$ and

$$\underline{F}_i = \frac{\hat{x}_{i+1}}{\hat{x}_i}. \quad (27)$$

Plugging this into the definition of \underline{F}_i we obtain the a linear system of equations of the form (23)

$$\hat{x}_{i+1} = (2 - \underline{\varepsilon}_{k-1})\hat{x}_i - \hat{x}_{i-1}, \quad i \geq 2, \quad \hat{x}_2 = (1 - \underline{\varepsilon}_{k-1})\hat{x}_1. \quad (28)$$

Now one can apply Lemma 14 with $\varepsilon = \underline{\varepsilon}_{k-1} = 2(1 - \cos(\underline{\zeta}_k))$, to see that $\hat{x}_i > 0$ for the recursion given by (28) for all $i < \min \left\{ \frac{\pi}{2\underline{\zeta}_{k-1}} + 1/2, k \right\}$. Then the right hand side in (27) is greater than zero and therefore by (26), also $F_i > 0$ and hence $x_i > 0$ for all $i < \frac{\pi}{2\underline{\zeta}_{k-1}} + 1/2$. The explicit formula for \hat{x}_i from Lemma 14 in combination with (26) now leads to the lower bound.

The upper bound is obtained similarly by estimating ε_i from above

$$F_1 = 1 - \varepsilon_1 \leq 1 - \bar{\varepsilon}_{k-1} =: \bar{F}_1$$

where \bar{F}_i is for $i \geq 2$ given by

$$\bar{F}_i := 2 - \bar{\varepsilon}_{k-1} - \bar{F}_{i-1}^{-1}.$$

By induction we find for $i \geq 1$ as long as $F_{i-1} \geq 0$ that

$$F_i = 2 - \varepsilon_i - F_{i-1}^{-1} \leq 2 - \lambda - \bar{\varepsilon}_{k-1} - \bar{F}_{i-1}^{-1} = \bar{F}_i.$$

By the definition of \bar{F}_i , we see from Lemma 14 with $\varepsilon = \bar{\varepsilon}_{k-1}$ that the upper bound holds. \square

An obstacle of Theorem 13 is that one has to know the eigenvalue λ and the functions f_{T_i} . We introduce

$$\begin{aligned}\underline{\varepsilon}_k(\lambda) &:= \min_{i=1,\dots,k} \frac{|V(T_i)|\lambda - \|L_{v_i}(T_i)\|^{-1}\lambda^2}{1 - \|L_{v_i}(T_i)\|^{-1}\lambda}, \\ \bar{\varepsilon}_k(\lambda) &:= \max_{i=1,\dots,k} \frac{|V(T_i)|\lambda - \|L_{v_i}(T_i)\|^{-1}\lambda^2}{1 - \|L_{v_i}(T_i)\|^{-1}\lambda}.\end{aligned}\tag{29}$$

The corollary below follows from Theorem 13 and the bounds for f_{T_i} from Proposition 2 (d) applied to the right hand sides of (19). This implies that one can choose $\bar{\zeta}_k$ and $\underline{\zeta}_k$ in such a way that the bounds no longer depend on the functions f_{T_i} .

Corollary 16. *Let T be a tree with a path $v_1 \dots v_k$ and trees T_1, \dots, T_k as in Figure 1. Assume that $\lambda \in \sigma(L(T))$ satisfies*

$$\lambda < \min_{i=1,\dots,k-1} \lambda_{\min}(L_{v_i}(T_i))\tag{30}$$

and $0 \leq \underline{\varepsilon}_{k-1}(\lambda) \leq \bar{\varepsilon}_{k-1}(\lambda) \leq 2$.

Then λ is a simple eigenvalue with eigenvector x and the bounds on the ratios of entries of x , (20) and (21) hold with

$$\underline{\zeta}_{k-1} = \arccos\left(1 - \frac{1}{2}\bar{\varepsilon}_{k-1}(\lambda)\right), \quad \bar{\zeta}_{k-1} = \arccos\left(1 - \frac{1}{2}\underline{\varepsilon}_{k-1}(\lambda)\right).$$

Remark 17. *Assuming that $\lambda = a(T)$ one can use the bounds*

$$2 - 2 \cos\left(\frac{\pi}{n+1}\right) \leq a(T) \leq 2 - 2 \cos\left(\frac{\pi}{d(T)+1}\right)\tag{31}$$

from [12, p. 187] and [18], to see that the assumption (30) holds for sufficiently large diameters of T_k . Using the monotonicity of the right hand sides of (29) as a function of λ in combination with (31) one has expressions for $\bar{\zeta}_{k-1}$ and $\underline{\zeta}_{k-1}$ that also do not depend on $a(T)$.

Let T be a path then let T_i be given by $V(T_i) = \{v_i\}$ then $\underline{\varepsilon}_k(\lambda) = \bar{\varepsilon}_k(\lambda) = \lambda$ and the bounds in Theorem 13 and Corollary 16 hold with equality.

Example 18. *Let us consider caterpillar trees and we assume that the central path is the unique longest path (see Figure 5). By Corollary 8 the extremal values of the Fiedler vector are attained at v_1 and v_k . Furthermore, each T_i is a star graph on $m_i + 1$ vertices while its central vertex v_i lies on the central path. It is easy to see that in this case $L_{v_i}(T_i) = I_{m_i}$ and each entry of f_i is one. Hence, we have $f_{T_i}(\lambda) = f_i^T (L_{v_i}(T_i) - \lambda I_{m_i})^{-1} f_i = \frac{m_i}{1-\lambda}$ and so*

$$f_{T_i}(\lambda) - \deg_{T_i}(v_i) = \frac{m_i}{1-\lambda} - m_i = \frac{\lambda}{1-\lambda} m_i.$$

If the caterpillar is nontrivial, i.e. not a simple path, we must have by the assumption that the central path is the unique longest path that $k \geq 3$. This implies $a(T) < 1$ and by the same assumption we have $\min_{i=1,\dots,\ell} m_i = 0$ for all $l \in \mathbb{N}$ with $l \leq k$. This yields the representations from Corollary 16

$$\begin{aligned}\min_{i=1,\dots,\ell} (f_{T_i}(\lambda) - \deg_{T_i}(v_i)) &= 0 \\ \max_{i=1,\dots,\ell} (f_{T_i}(\lambda) - \deg_{T_i}(v_i)) &\leq \frac{\lambda}{1-\lambda} \max_{i=1,\dots,\ell} m_i.\end{aligned}$$

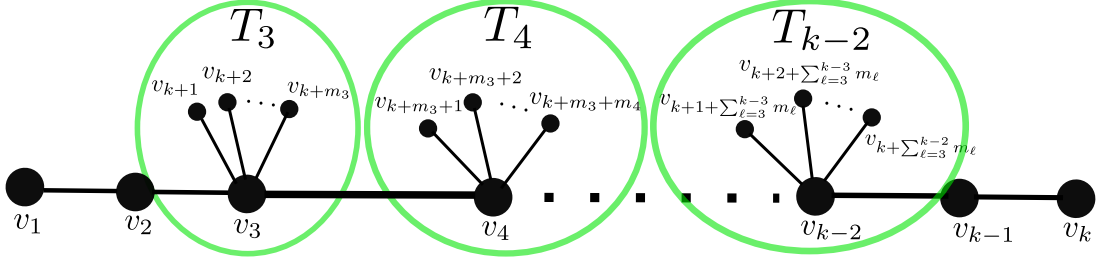


Figure 5: Caterpillar graphs with a central path being the unique longest path.

7 Local extrema of eigenvectors

For paths $v_1 \dots v_k$ in a tree T where v_1 is a pendant vertex, we have seen in Section 4 that the eigenvector entry $x_1 > 0$ at v_1 is larger than the value at v_2 for sufficiently small eigenvalues. Here we provide a condition for sufficiently small eigenvalues of $L(T)$ where one can check if v_1 is also extreme among all vertices in T_i for all $2 \leq i \leq k$.

We introduce the so-called L -configurations. The idea is to compare the entries of the eigenvector at the vertices v_i of the fixed path with the entries of the eigenvector at vertices in the attached trees T_i . We split up the tree T_i into $\deg_{T_i}(v_i)$ disjoint subtrees $T_{i,j}$. For a given path in T_i starting at v_i this path is in one tree $T_{i,j}$. Denote by $v_{i,j}^{(l)} = v_i, \dots, v_{i,j}^{(1)}$ the vertices on this path and to each vertex $v_{i,j}^{(m)}$ we consider the attached tree $T_{i,j}^{(m)}$ as in Figure 1. Then we apply the Schur reduction on the subpath $v_1 \dots v_{i-1}$ and on the subpath $v_{i,j}^{(1)} \dots v_{i,j}^{(l)}$.

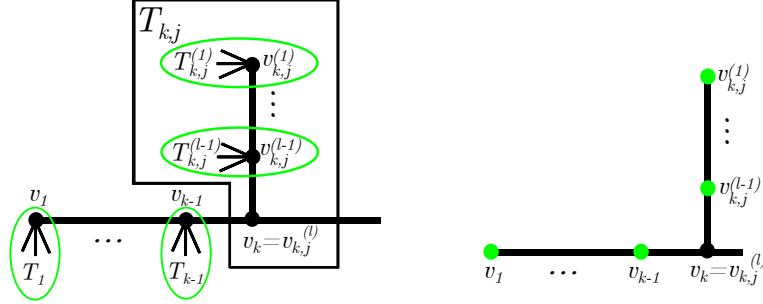


Figure 6: The figure shows an L -configuration, where we compare the entries of the eigenvector on the path $v_1 \dots v_{k-1}$ with the entries on the paths in $T_{k,j}$ for all $j = 1, \dots, \deg_{T_k}(v_k)$. The Schur reduction was applied only at the green colored vertices.

In the proposition below we show that under certain assumptions, the characteristic value at v_1 is maximal among all values at the green colored vertices in Figure 6.

Proposition 19. *Let λ be an eigenvalue of $L(T)$ with eigenvector entry $x_1 > 0$ such that (19) holds for some $\zeta_{k-1} \in (0, \frac{\pi}{2})$ with $k \leq \frac{\pi}{\zeta_{k-1}} + \frac{1}{2}$. Consider the setting in Figure 6 with vertices v_1, \dots, v_k of the lower path and vertices $v_{k,j}^{(1)}, \dots, v_{k,j}^{(l)} = v_k$ with $l \leq k$ on the vertical path at v_k . If for all $i = 1, \dots, l$ and $j = 1, \dots, \deg_{T_k}(v_k)$, $T_{k,j}^{(i)}$ can be obtained from T_i by removing pendant vertices*

then we have for all $i = 1, \dots, l$ that

$$x_1 \geq x_{k,j}^{(i)} \geq 0. \quad (32)$$

If $T_{k,j}^{(i)}$ is a proper subtree of T_i for some index i_0 then (32) is also strict for all $i_0 \leq i \leq l$. Furthermore, if $d(T_{k,j}) \leq k-1$ for all $j = 1, \dots, \deg_{T_k}(v_k)$ then (32) holds for all vertices of T_k .

Proof. We consider the following two sequences

$$F_1^|(\lambda) := s_{T_k^{(1)}}(\lambda), \quad F_i^|(\lambda) := s_{T_{k,j}^{(i)}}(\lambda) - F_{i-1}^|(\lambda)^{-1}, \quad i \geq 2$$

and

$$F_1^-(\lambda) := s_{T_1}(\lambda), \quad F_i^-(\lambda) := s_{T_i}(\lambda) - F_{i-1}^-(\lambda)^{-1}, \quad i \geq 2.$$

Since the kernel of the matrix (2) is the eigenvector at λ restricted to the path, it is easy to see from the equation $S_{T_1, \dots, T_k}(\lambda)x = 0$ and Theorem 13 that

$$F_i^-(\lambda) = \frac{x_{i+1}}{x_i} > 0, \quad F_i^|(\lambda) = \frac{x_{k,j}^{(i+1)}}{x_{k,j}^{(i)}} > 0. \quad (33)$$

The assumption that $T_{k,j}^{(1)}$ is a subtree of T_1 with Proposition 2 (e) implies that

$$0 < F_1^-(\lambda) \leq F_1^|(\lambda).$$

We estimate for $2 \leq i \leq l-1$ under the assumption that $F_{i-1}^-(\lambda) \leq F_{i-1}^|(\lambda)$ and with Proposition 2 (e)

$$\begin{aligned} 0 < F_i^-(\lambda) &= \deg(v_i) - \lambda - f_{T_i}(\lambda) - F_{i-1}^-(\lambda)^{-1} \\ &= \deg(v_i) - \deg_{T_i}(v_i) - \lambda - \sum_{m=1}^{\infty} \frac{f_{T_i}^{(m)}(0)\lambda^m}{m!} - F_{i-1}^-(\lambda)^{-1} \\ &\leq \deg(v_{k,j}^{(i)}) - \deg_{T_{k,j}^{(i)}}(v_{k,j}^{(i)}) - \lambda - \sum_{m=1}^{\infty} \frac{f_{T_{k,j}^{(i)}}^{(m)}(0)\lambda^m}{m!} - F_{i-1}^-(\lambda)^{-1} \\ &\leq \deg(v_k^{(i)}) - \lambda - f_{T_k^i}(\lambda) - F_{i-1}^|(\lambda)^{-1} \\ &= F_i^|(\lambda). \end{aligned}$$

Since both paths have a joint vertex at v_k , we have from the representation (33) that

$$\prod_{i=1}^{k-1} F_i^-(\lambda)x_1 = x_k = \prod_{i=1}^{l-1} F_i^|(\lambda)x_{k,j}^{(1)}$$

and since $0 < F_i(\lambda) < 1$,

$$\frac{x_1}{x_{k,j}^{(1)}} = \frac{\prod_{i=1}^{l-1} F_i^|(\lambda)}{\prod_{i=1}^{k-1} F_i^-(\lambda)} \geq \frac{\prod_{i=1}^{l-1} F_i^|(\lambda)}{\prod_{i=1}^{l-1} F_i^-(\lambda)} \geq 1.$$

Furthermore, $x_{k,j}^{(1)} \geq x_{k,j}^{(i)}$ for $i = 1, \dots, l$ implies (32). Assume that $d(T_{k,j}) \leq k-1$, then for all vertices $v \in V(T_{k,j})$ there exists a path $v = v_{k,j}^{(1)} \dots v_{k,j}^{(l)} = v_k$ and therefore (32) holds for all vertices of $T_{k,j}$. \square

8 Discussion

In this article, we have investigated the structure of Fiedler vectors of trees. One of our main tools is the Schur reduction introduced in Section 3. We remark that the reduction from equation (2) can be extended to graphs where the T_i are arbitrary graphs instead of trees. In both cases, applying the matrix-tree-theorem to a slightly modified graph, the resolvents in equation (3) can be computed combinatorically by counting spanning 2- and 3-forests. This enables one to relate the entries of the Fiedler vector to the graph topology in more detail and will be the topic of a future investigation.

Taylor expansion of ratios of Laplacian eigenvector entries then allows us to restrict the location of the extremal entries of the Fiedler vector. As an application we introduce caterpillar trees and a class of generalized caterpillars. We remark that not only can this approach be applied to other classes of trees, but due to the generality of Lemma 5, it can also be applied to other eigenvalues than the algebraic connectivity $a(T)$. Furthermore, we derive a sufficient criterion for the Fiedler rose to have the (FED) property and we show that the mechanism which destroys this property in the Fiedler rose can be generalized to a large class of trees T . More precisely, when gluing a star graph with sufficiently many leaves to T , one extremal entry of the Fiedler vector will lie on the star and therefore the (FED) property is not preserved.

Finally, we use the Schur reduction in order to bound ratios of eigenvector entries with applications to the Fiedler vector and introduce a large class of trees in which we can identify a local extremal value of a Laplacian eigenvector.

Although we have given partial answers for large classes of trees and identified other classes of trees for which the (FED) property holds true, it remains an open problem to identify the largest class of trees which possess the (FED) property.

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