

Locating the extremal entries of the Fiedler vector for rose trees

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In this note we locate the extremal entries of the Fiedler vector for the class of rose trees, which consists of paths with a star graph attached to it. We derive directly from the eigenvector equation conditions to characterize in which cases the extremal values are located either at the end points of the path or on the pendant vertices of the star graph.

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Graph Laplacians and the Fiedler vector. In this note we consider undirected, unweighted graphs G with n vertices $V(G) = \{v_1, \dots, v_n\}$ and a set of edges $E(G)$ with elements of the form vw for two vertices $v, w \in V(G)$. We are interested in the graph Laplacian $L(G) := D - A$ where $D = \text{diag}(\deg(v_i))_{i=1}^n$ is a diagonal matrix containing the degrees of the edges, i.e. $\deg(v)$ is the number of edges that contain v . The adjacency matrix $A \in \mathbb{R}^{n \times n}$ is a zero-one-matrix with entry one at position (i, j) iff $v_i v_j \in E(G)$. It is well known that $L(G)$ is positive semi-definite with eigenvalues $0 = \lambda_1(G) \leq \dots \leq \lambda_n(G)$. Moreover, $\lambda_1(G)$ is a simple eigenvalue iff G is connected, i.e. there is a path between any two vertices. In this case $\lambda_2(G)$ is called the *algebraic connectivity* denoted by $a(G)$ and if the associated eigenspace is one-dimensional, the (up to scaling) unique eigenvector is called the *Fiedler vector*. Since $L(G)$ is a symmetric matrix the eigenvector $(1, \dots, 1)^T$ for the eigenvalue $\lambda_1(G) = 0$ is orthogonal to the Fiedler vector and therefore this vector contains positive and negative entries. In the remainder we study the location of the extremal entries of the Fiedler vector if the graph G is a tree, i.e. there is a unique path between any two vertices. For trees the vertices with $\deg(v) = 1$ are called *pendant vertices* and they will be of special interest in the following.

Location of the extremal entries. It is a well known result due to Fiedler [5] that the extremal entries of the Fiedler vector are located at the pendant vertices of the tree, see also [6, Lemma 8]. This result was recently extended to quantum graphs in [8]. If $a(G) = \lambda_2(G) < 1$ then one can see directly from the eigenvector equation $L(G)x = a(G)x$, $x \in \mathbb{R}^n$, that the absolute value at the pendant vertex v is strictly larger than the value at the unique vertex w with $vw \in E(G)$. However it remains unclear at which pendant vertices these entries are located.

It was conjectured that the extremal entries are located at the most distant vertices in the tree. A counter example to this conjecture are rose trees studied in [1, 3, 7]. A rose tree is given by two paths P_l and P_t with l and t vertices, respectively, and a star graph S_r with r vertices where we select a pendant vertex in each of the graphs and glue them together at a vertex v_B which satisfies then $\deg(v_B) = 3$. Roughly speaking, it was shown in [7] that for fixed l and t the number r can be made large enough, such that one extremal entry moves from the end point of the paths P_l or P_t to the pendant vertices of the star graph S_r .

Before we characterize the locations of the extremal entries for rose trees, we state the following auxiliary result.

Lemma 1 *Let G be a connected graph with Laplacian $L(G)$, eigenvalue $\lambda > 0$ and eigenvector $x = (x_i)_{i=1}^n$ then $\sum_{i=1}^n x_i = 0$ and the following holds.*

- (a) *Let P be a permutation matrix, i.e. $P^2 = I_n$ with $PL(G)P = L(G)$ then Px is also an eigenvector of $L(G)$ for λ .*
- (b) *Let $G = P_n$ be a path with n vertices v_1, \dots, v_n then $x_n = \frac{2}{\sqrt{4-\lambda}} \cos((n-1/2)\zeta)x_1$ with $\zeta = \arccos(1 - \lambda/2)$.*
- (c) *Let $G = S_{n-1}$ with center v_1 and pendant vertices v_2, \dots, v_{n-1} then $(1 - \lambda)x_2 = \dots = (1 - \lambda)x_r = x_1$.*

Proof. Since G is connected, $\lambda_1(G) = 0$ is a simple eigenvalue with eigenvector $(1, \dots, 1)^T$. The symmetry of $L(G)$ implies that x is orthogonal to this vector and therefore $\sum_{i=1}^n x_i = 0$. To prove (a), observe that $L(G)x = \lambda x$ implies $L(G)Px = PL(G)PPx = \lambda Px$. Therefore $Px \neq 0$ is also an eigenvector of λ . In particular if λ is simple then there exists $\alpha \neq 0$ with $Px = \alpha x$. The proof of (b) is based on deriving a linear second-order difference equation from the eigenvector equation and can be found e.g. in [6, Lemma 15] and (c) follows directly from the eigenvector equation $L(G)x = \lambda x$. \square

In the following we denote the entries at the pendant vertices in the rose tree by x_{P_l} , x_{P_t} and x_{S_r} . Below we state the main result on the location of extremal entries of rose trees and provide an elementary proof. For arbitrary trees one can characterize the extremal entries of the Fiedler vector using the Schur reduction method from [6], which is a technique to obtain a smaller (weighted) graph in such a way that the original eigenvector is preserved.

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Theorem 2 Let T be a rose tree with parameters l, t, r and $1 \leq l \leq t$ and $r \geq 2$ then the following holds for $\lambda = a(T)$.

(a) $a(T)$ is a simple eigenvalue with $2 - 2 \cos(\frac{\pi}{l+t+r-1}) \leq a(T) \leq 2 - 2 \cos(\frac{\pi}{l+t-1})$.

(b) The entries x_{S_r}, x_{P_l} and x_{P_t} of the Fiedler vector are related by

$$(\lambda^2 - r\lambda + 1)x_{S_r} = \frac{2}{\sqrt{4 - \lambda}} \cos((l - 1/2)\zeta)x_{P_l} = \frac{2}{\sqrt{4 - \lambda}} \cos((t - 1/2)\zeta)x_{P_t}.$$

If $l < t$ then x_{P_l} and x_B are nonzero and have the same sign.

(c) If $r/2 - \sqrt{r^2/4 - 1} < 2 - 2 \cos(\frac{\pi}{2t-1})$ then the entries x_{P_l}, x_B, x_{P_t} are non-zero and have the same sign. Therefore the extremal entries are x_{S_r} and x_{P_t} .

(d) For l, r fixed and t sufficiently large there is one extremal entry x_{P_t} and a second extremal entry of opposite sign x_{S_r} , if $r > \frac{l(l+1)}{2}$, or x_{P_l} , if $r < \frac{l(l+1)}{2}$.

(e) If $1 - (2r)^{-1} \leq \cos(\frac{\pi}{l+t-1})$ and $\frac{\sqrt{2} \cos(\frac{(l-3/2)\pi}{l+t-1})}{\sqrt{1 + \cos(\frac{\pi}{l+t+r-1})}} < \left(2 - 2 \cos(\frac{\pi}{l+t+r-1})\right)^2 - r(2 - 2 \cos(\frac{\pi}{l+t+r-1})) + 1$ then the extremal entries are x_{P_l} and x_{P_t} .

Proof. The upper bound in (a) follows from [2, p. 187] and the lower bound can be found in [4]. The simplicity can be obtained from $a(T) < 1$ and that we can resolve the eigenvector equations hence there is up to scaling at most one solution of the eigenvector equation. We see by a direct calculation from the eigenvector equation $L(T)x = \lambda x$ and the previous Lemma 1 that

$$(r - 1 - \lambda)x_0 - (r - 1)x_{S_r} = (\lambda^2 - r\lambda + 1)x_{S_r} = x_B = \frac{\sqrt{2}}{\sqrt{1 + \cos(\zeta)}} \cos((l - 1/2)\zeta)x_{P_l} \tag{1}$$

where x_0 is the center of the star graph. If $l < t$ and $x_{P_l} > 0$ then the upper bound for $a(T)$ in (a) implies $x_l > 0$ which proves (b).

Next, we prove (c). For this we use the eigenvector equation $L(T)x = \lambda x$ at the row that corresponds to x_B and obtain

$$(3 - \lambda)x_B - x_{t-1} - x_{l-1} - x_0 = 0, \tag{2}$$

where x_0 is again the center of the star graph and x_{t-1} and x_{l-1} are the vertices on the paths connected to x_B . We assume that $\lambda < 2 - 2 \cos(\pi/(2t - 1))$ then we have $x_B \neq 0$ and we show that there is a positive solution to the above equation. One of these possible solutions is then $a(T)$. Since the Fiedler vector is unique up to scaling, we can assume without restriction that $x_B = 1$ and therefore we obtain with the formulas in (b) and Lemma 1 (b) in (2) that

$$3 - \lambda - \frac{\cos((t - 3/2)\zeta)}{\cos((t - 1/2)\zeta)} - \frac{\cos((l - 3/2)\zeta)}{\cos((l - 1/2)\zeta)} - \frac{1 - \lambda}{\lambda^2 - r\lambda + 1} = 0. \tag{3}$$

Recall that $\zeta = \arccos(1 - \lambda/2)$, hence $\lambda = 0$ is a solution to the above equation. Furthermore, we have poles for $\lambda \in \{r/2 \pm \sqrt{r^2/4 - 1}, 2 - 2 \cos(\pi/(2l - 1)), 2 - 2 \cos(\pi/(2t - 1))\}$.

Observe that there is no solution of (3) for $\lambda \in (0, r/2 - \sqrt{r^2/4 - 1})$ because then all eigenvector entries would be positive. This contradicts Lemma 1, where we have shown that the sum of all eigenvector entries is zero. Since the function tends to ∞ for $\lambda \downarrow r/2 - \sqrt{r^2/4 - 1}$ and to $-\infty$ for $\lambda \uparrow 2 - 2 \cos(\pi/(2t - 1))$ there is at least one solution $\lambda \neq 0$ in this interval. For all this solutions the corresponding eigenvector has the property that $x_{S_r} = \frac{1}{\lambda^2 - r\lambda + 1} < 0$ and $x_{P_t} > x_{P_l} > x_B > 0$. Hence the Fiedler vector also has this property.

We continue with the proof of (d). The upper bound for $a(T)$ in (a) implies that $a(T) \rightarrow 0$ as $t \rightarrow \infty$. The coefficients in (b) can be viewed as functions of λ and they have the same value at $\lambda = 0$. Therefore it remains to compare the derivatives of these functions, to decide which entry x_{S_r} or x_{P_l} is larger. Indeed we find the derivative of these functions at $\lambda = 0$ to be $-r$ and $-l(l + 1)/2$. This proves (d). For the proof of (e) we refer to [6, p. 111-112]. \square

Note that (a) and (c) for $l = t$, i.e. perfect rose trees, were already obtained in [7].

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