# The Second Largest Eigenvalue of a Tree*

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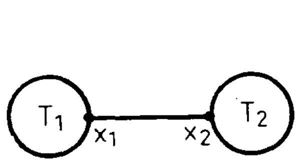
ABSTRACT

Denote by $\lambda_2(T)$ the second largest eigenvalue of a tree $T$. An easy algorithm is given to decide whether $\lambda_2(T) \leqslant \lambda$ for a given number $\lambda$, and a structure theorem for trees with $\lambda_2(T) \leqslant \lambda$ is proved. Also, it is shown that a tree $T$ with $n$ vertices has $\lambda_2(T) \leqslant [(n-3)/2]^{1/2}$; this bound is best possible for odd $n$.

## 1. INTRODUCTION

Suppose that $T$ is a tree, and $\lambda$ is a nonnegative real number. In this paper we investigate the question: When is the second largest eigenvalue $\lambda_2(T)$ of $T$ smaller than (or equal to) $\lambda$? As basic tool we use the concepts of partial eigenvectors and exitvalues. A partial eigenvector satisfies the eigenvector equation at all vertices but one; the difference at this vertex is given by the exitvalue. The distribution of zeros and signs in the partial eigenvector and the exitvalue is shown to determine the location of $\lambda$ within the spectrum of $T$. Among other things, we derive from this the following structure theorem (cf. Theorem 4.3 below): Let $T$ be a tree with $\lambda_2(T) \leqslant \lambda$. Then either $T$ contains a vertex $x$ such that $\lambda_1(T-(x\}) \leqslant \lambda$; or $T$ is a $\lambda$-twin, i.e., $T$ has the shape




with subtrees $T_1$ and $T_2$ satisfying $\lambda_1(T_i - \{x_i\}) < \lambda < \lambda_1(T_i)$ for $i = 1,2$. (Here $\lambda_1$ denotes the largest eigenvalue.) Also, we find an upper bound $\lambda_2(T)$

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$\leqslant \sqrt{(n-3)/2}$ on the second largest eigenvalue of a tree with $n$ vertices, and we determine completely the (infinitely many) trees achieving the bound.

The motivation for the problem considered stems from hyperbolic geometry: The bilinear form associated with a reflection group with Dynkin diagram $T$ is spherical, affine, or hyperbolic iff $\lambda_2(T) \leqslant 2$. The spherical and affine reflection groups are well known, and Koszul [7] determined the Dynkin diagrams for the minimal hyperbolic reflection groups.

To attack the problem of constructing and classifying other hyperbolic reflection groups, a simple decision algorithm for $\lambda_2(T) \leqslant 2$ is needed. This was found tractable for trees and led to the present results. Applications to reflection groups will be reported elsewhere.

## 2. EXITVALUES

In this section, $T$ is a connected graph (undirected, without loops or multiple edges). We denote by $A$ the adjacency matrix of $T$, i.e. the matrix $A = (a_{xy})_{x,y \in T}$ indexed by the vertices of $T$, such that $a_{xy} = 1$ if $xy$ is an edge, and $a_{xy} = 0$ otherwise. The characteristic polynomial of $T$ is denoted by $P_T(\lambda) = \det(\lambda I - A)$. We denote the eigenvalues of $A$, in decreasing order, by

$$\lambda_1(T) > \lambda_2(T) \geqslant \cdots \geqslant \lambda_n(T)$$

($n$ = number of vertices of $T$) and call them the eigenvalues of $T$ (similarly for eigenvectors). The eigenvalues of the subgraph $T \setminus \{x\}$ obtained by deleting the vertex $x \in T$ and the edges containing $x$ are related to the eigenvalues of $T$ by the *interlacing property*

$$\lambda_{i+1}(T) \leqslant \lambda_i(T - \{x\}) \leqslant \lambda_i(T) \tag{IP}$$

for $i = 1, \ldots, n-1$ (see [2] for a proof).

Let the term $\lambda$-eigenvalue denote an eigenvector of $T$ whose corresponding eigenvalue is $\lambda$. So $e$ is a $\lambda$-eigenvector (and $\lambda$ is an eigenvalue) iff $e$ is nonzero and satisfies the relation

$$\sum_{y \sim x} e_y = \lambda e_x \tag{1}$$

for all $x \in T$; here $\sim$ means "adjacent." We call a vector $e$ a *partial*

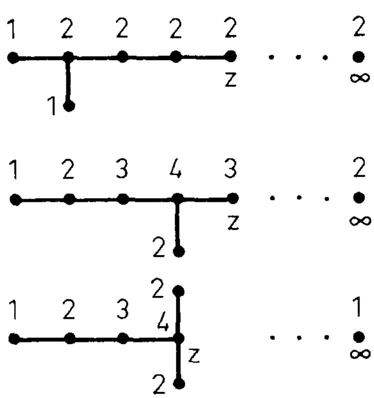
$\lambda$-*eigenvector* with respect to a vertex $z \in T$ if $e_z = 1$, and (1) holds for all $x \in T \setminus \{z\}$; in this case the number

$$\varepsilon_{T,z}(\lambda) = \lambda - \sum_{y \sim z} e_y \tag{2}$$

is called a $\lambda$-*exitvalue* of $T$ with respect to $z$. If the $\lambda$-exitvalue $\varepsilon$ is zero, then $\lambda$ is an eigenvalue of $T$, and $e$ a corresponding eigenvector; if $\varepsilon$ is nonzero, then it can be thought of as the entry of $e$ at a hypothetical further vertex $\infty$ adjacent with $z$. For a tree, the equations (1) can be solved recursively by assigning to some end vertex $x$ the number $e_x = 1$; in this way, one usually gets a multiple of a partial eigenvector.

REMARK. If no confusion is possible, we delete the prefix "$\lambda$-" from expressions like "$\lambda$-eigenvector" or "$\lambda$-exitvalue."

EXAMPLE. The following diagrams represent some partial eigenvectors and exitvalues for $\lambda = 2$. The reader can easily check the relations (1) and (2) for the vector $e$ whose $x$-entry is $\sigma$ times the label of vertex $x$.




$\sigma = \frac{1}{2}, \quad \varepsilon_z = 1.$

$\sigma = \frac{1}{3}, \quad \varepsilon_z = \frac{2}{3}.$

$\sigma = \frac{1}{4}, \quad \varepsilon_z = \frac{1}{4}.$

For an explanation of the fact that all entries are positive see Theorem 2.4.

THEOREM 2.1. *Suppose that the real number $\lambda$ is not an eigenvalue of $T - \{z\}$. Then, with respect to $z$, there is a unique partial $\lambda$-eigenvector, and* *the exitvalue satisfies*

$$\varepsilon_{T,z}(\lambda) = \frac{P_T(\lambda)}{P_{T\setminus\{z\}}(\lambda)}. \tag{3}$$

*Proof.* Denote by $\delta_z = (\delta_{xz})_{x\in T}$ the $z$th column of the identity matrix $I$, i.e., $\delta_z$ is the characteristic vector of $z$. Then $e$ is a partial $\lambda$-eigenvector and $\varepsilon$ the corresponding exitvalue iff $e$ is a solution of the homogeneous equation

$$(\lambda I - A - \varepsilon\delta_z\delta_z^T)e = 0, \tag{4}$$

with side condition

$$\delta_z^T e = 1. \tag{4a}$$

*Case 1*: $\lambda I - A$ *is nonsingular.* Then (4) implies $e = \varepsilon(\lambda I - A)^{-1}\delta_z(\delta_z^T e) = \varepsilon(\lambda I - A)^{-1}\delta_z$, and (4a) implies that $\varepsilon^{-1} = \delta_z^T(\lambda I - A)^{-1}\delta_z = P_{T\setminus\{z\}}(\lambda)/P_T(\lambda)$, by Cramer's rule. Hence $\varepsilon$ and $e$ are unique, and in fact these expressions satisfy (4), (4a). Moreover, (3) holds.

*Case 2*: $\lambda I - A$ *is singular.* Then $\lambda$ is an eigenvalue of $T$. Let $e$ be a corresponding eigenvector. If $e_z = 0$, then $e$ is also a $\lambda$-eigenvector of $T\setminus\{z\}$, contradiction. Hence we may normalize $e$ so that $e_z = 1$; then $e$ is a partial eigenvector with exitvalue $\varepsilon = 0$, and (3) holds. If $e'$ is another partial $\lambda$-eigenvector, then $e' - e$ is a $\lambda$-eigenvector of $T\setminus\{z\}$ whence $e' = e$. ■

Since the eigenvalues of $T\setminus\{z\}$ interlace the eigenvalues of $T$, (3) implies the following useful results.

COROLLARY 2.2. *If $\lambda$ is an eigenvalue of $T$ but not of $T\setminus\{z\}$, then $\lambda$ is a simple eigenvalue, $\varepsilon_{T,z}(\lambda) = 0$, and the partial $\lambda$-eigenvector with respect to $z \in T$ is the unique $\lambda$-eigenvector $e$ with $e_z = 1$.*

COROLLARY 2.3. *Between two consecutive eigenvalues of $T\setminus\{z\}$, and in the two infinite intervals remaining, $\varepsilon_{T,z}(\lambda)$ is an increasing function of $\lambda$ and assumes every value once.*

Partial eigenvectors and exitvalues can be used for the location of eigenvalues of $T$. The main tool is the following:

THEOREM 2.4. *Suppose that the real number $\lambda$ is not an eigenvalue of $T\setminus\{z\}$. If $e(z)$ and $\varepsilon_z$ denote the partial eigenvector and the exitvalue with* *respect to z, then*:

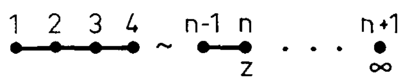
(i) $\lambda_1(T) < \lambda$ *iff* $e(z) > 0$, $\varepsilon_z > 0$.
(ii) $\lambda_1(T) = \lambda$ *iff* $e(z) > 0$, $\varepsilon_z = 0$.
(iii) $\lambda_1(T - \{z\}) < \lambda < \lambda_1(T)$ *iff* $e(z) > 0$, $\varepsilon_z < 0$.

REMARK. Motivated by Theorem 2.4(iii), we call a graph $T$ *λ-critical* at $z$ if $\lambda_1(T \setminus \{z\}) < \lambda < \lambda_1(T)$.

*Proof.* By (3), $\varepsilon_z = 0$ if $\lambda_1(T) = \lambda$, so the statements follow from Corollary 2.3 if we can show that $e(z) > 0$ iff $\lambda_1(T - \{z\}) < \lambda$.

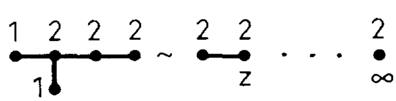
Now (4) holds with $\varepsilon = \varepsilon_z$, $e = e(z)$; hence for $B = A + \varepsilon\delta_z\delta_z^T$, we have $Be = \lambda e$, and for any $s$, $B + sI$ has the eigenvalue $\lambda + s$ and corresponding eigenvector $e$. But for large $s$, $B + sI$ is an irreducible nonnegative matrix. Hence the Frobenius-Perron theory (see e.g. [1]) shows that $e$ is positive iff $\lambda$ is the largest eigenvalue of $B$. But the proof of Theorem 2.1 shows that $tI - B$ is singular iff $\varepsilon = \varepsilon_{T,z}(t)$. Hence the eigenvalues of B are the solutions of $\varepsilon_{T,z}(t) = \varepsilon = \varepsilon_{T,z}(\lambda)$. So, by Corollary 2.3, $\lambda$ is the largest eigenvalue of $B$ iff $\lambda > \lambda_1(T \setminus \{z\})$. ■

EXAMPLE. We determine all connected graphs $T$ with largest eigenvalue $< 2$. Since a circuit is regular of valency 2, it has eigenvalue 2 and cannot be an induced subgraph of $T$. Hence $T$ is a tree. By Theorem 2.4(i), we have to find all trees with partial 2-eigenvector $e(z) > 0$ and 2-exitvalue $\varepsilon_z > 0$ for some vertex $z$. If $T$ is a chain, then (up to a scaling factor) $e(z)$ and $\varepsilon_z$ are given by

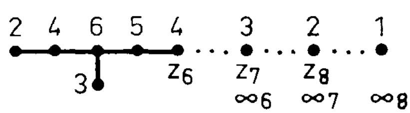
$A_n$: 

($n \geq 1$ vertices).

Similarly, we have

$D_n$: 

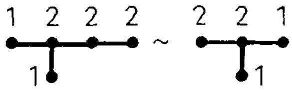
($n \geq 4$ vertices),

$E_n$: 

($n = 6, 7, 8$ vertices),

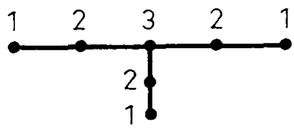
Hence these graphs have $\lambda_1(T) < 2$. Now the minimal trees not of type $A_n$,

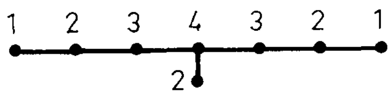
$D_n$ or $E_6$, $E_7$, $E_8$ are

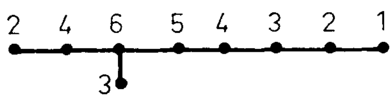
$\tilde{D}_n$: 

$(n+1 \geq 5$ vertices$)$,

and

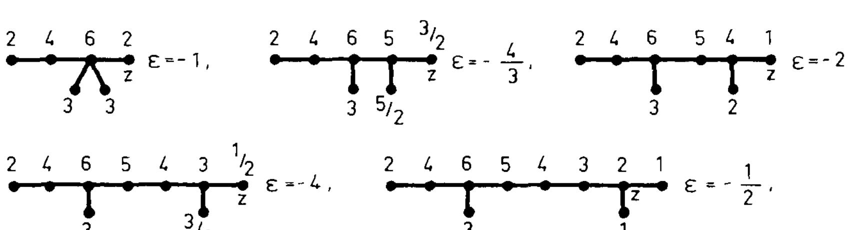
$\tilde{E}_6$: 

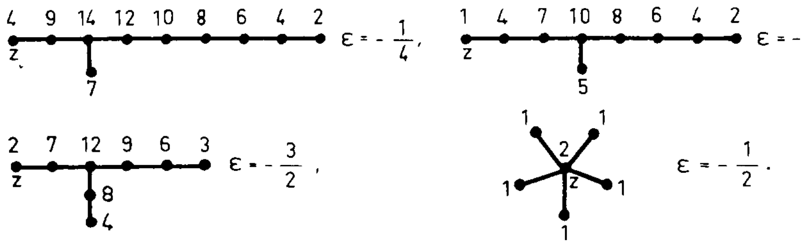

$\tilde{E}_7$: 


$\tilde{E}_8$: 


The vectors given are eigenvectors, and the exitvalue at any vertex is zero. Hence $A_n$, $D_n$, $E_6$, $E_7$, $E_8$ are the only trees with largest eigenvalue $<2$. In fact $\tilde{D}_n$, $\tilde{E}_6$, $\tilde{E}_7$, and $\tilde{E}_8$ are the only trees with largest eigenvalue 2 (among the nontrees, only the circuits $\tilde{A}_n$ occur). The results are all classical.

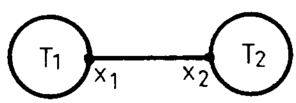
Example. In his lectures on hyperbolic coxeter groups, Koszul [7] determined all minimal Dynkin diagrams with $\lambda_1 > 2$ (Theorems 18-1 and 18-2). We reproduce here those diagrams which are trees without multiple edges. We also give the 2-exitvalue and a multiple of the partial 2-eigenvector with respect to a suitable vector indicated by $z$. This is sufficient to check that $\lambda_1 > 2$. Minimality and completeness are easily deduced from the previous example.






**Remark.** We shall call a graph $T$ *Euclidean* if $\lambda_1 \leq 2$, and *hyperbolic* if $\lambda_2 \leq 2 < \lambda_1$. We call $T$ *spherical* if $\lambda_1 < 2$, *affine* or *affine Euclidean* if $\lambda_1 = 2$, and *affine hyperbolic* if $\lambda_2 = 2$.

Now we consider graphs of shape




which we abbreviate by $(T_1, x_1, x_2, T_2)$. Thus the symbol means that $T_1$ and $T_2$ are graphs with disjoint vertex sets, $x_1 \in T_1$, $x_2 \in T_2$, and $(T_1, x_1, x_2, T_2)$ is the graph obtained from the disjoint union of $T_1$ and $T_2$ by adding the single edge $x_1 x_2$. In Section 4 we shall need a special case: We call $(T_1, x_1, x_2, T_2)$ a $\lambda$-*twin* if, for $i = 1, 2$, $T_i$ is $\lambda$-critical at $x_i$.

From [2, Theorem 2.12] we have

**Proposition 2.5.** *The characteristic polynomial of $T = (T_1, x_1, x_2, T_2)$ is*

$$P_T(\lambda) = P_{T_1}(\lambda) P_{T_2}(\lambda) - P_{T_1 \setminus \{x_1\}}(\lambda) P_{T_2 \setminus \{x_2\}}(\lambda).$$

*As a consequence, we get the following theorem, whose importance will become clear in Section 4.*

**Theorem 2.6.** *Let $T = (T_1, x_1, x_2, T_2)$ be a $\lambda$-twin. For $i = 1, 2$, denote by $\varepsilon_i$ the (negative) exitvalue of $T_i$ with respect to $x_i$. Then*:

(i) $\lambda_2(T) < \lambda$ *iff* $\varepsilon_1 \varepsilon_2 < 1$.
(ii) $\lambda_2(T) = \lambda$ *iff* $\varepsilon_1 \varepsilon_2 = 1$.
(iii) $\lambda_2(T) > \lambda$ *iff* $\varepsilon_1 \varepsilon_2 > 1$.

*Proof.* Since $T_i$ is $\lambda$-critical at $x_i$, we have $P_i(t) := P_{T_i\setminus\{x_i\}}(t) > 0$ for all $t \geqslant \lambda$. In particular, the exitvalues $\varepsilon_i(t) := \varepsilon_{T_i, x_i}(t)$ are defined. Now by Theorem 2.1 and Proposition 2.5,

$$P_T(t) = [\varepsilon_1(t)\varepsilon_2(t) - 1] P_1(t) P_2(t). \tag{5}$$

Put $\lambda_1 = \lambda_1(T)$, $\lambda_2 = \lambda_2(T)$, and denote by $\lambda_3$ the largest eigenvalue of $T$ strictly smaller than $\lambda_2$. Then $P_T(t)$ is negative for $\lambda_2 < t < \lambda_1$, zero for $t = \lambda_2$, and positive for $\lambda_3 < t < \lambda_2$. On the other hand, $T_1$ and $T_2$ are $\lambda$-critical at $x_1$ and $x_2$, respectively, whence $T\setminus\{x_1\}$ has largest eigenvalue $> \lambda$, and $T\setminus\{x_1, x_2\}$ has largest eigenvalue $< \lambda$. So, by interlacing, $\lambda_3 < \lambda < \lambda_1$, and we get the result by putting $t = \lambda$ into (5). ∎

We also have some information on the eigenvectors of $(T_1, x_1, x_2, T_2)$, not necessarily a twin.

PROPOSITION 2.7. *Let $T = (T_1, x_1, x_2, T_2)$, and let the real number $\lambda$ be not an eigenvalue of $T_1\setminus\{x_1\}$ or $T_2\setminus\{x_2\}$. For $i = 1,2$, denote by $e^{(i)}$ and $\varepsilon_i$ the partial eigenvector and the exitvalue of $T_i$ with respect to $x_i$. Then $\lambda$ is an eigenvalue of $T$ iff $\varepsilon_1\varepsilon_2 = 1$; in this case, every $\lambda$-eigenvector has the form*

$$e = \begin{pmatrix} s_1 e^{(1)} \\ s_2 e^{(2)} \end{pmatrix}, \qquad s_2 = s_1\varepsilon_1, \quad s_1 = s_2\varepsilon_2; \tag{6}$$

*in particular, $\lambda$ is a simple eigenvalue of $T$.*

*Proof.* Suppose that $\lambda$ is an eigenvalue of $T$, and $e$ a $\lambda$-eigenvector. The numbers $s_i = e_{x_i}$ are nonzero, since otherwise $T_i\setminus\{x_i\}$ would have an eigenvalue $\lambda$ corresponding to the restriction of $e$ to $T_i\setminus\{x_i\}$. Hence we can write the restriction of $e$ to $T_i$ in the form $s_i\bar{e}^{(i)}$, and $\bar{e}^{(i)}$ is easily seen to be the (unique) partial eigenvector $e^{(i)}$ of $T_i$. Moreover, the relations (1) for $x = x_1$ and $x = x_2$ give $s_2 = s_1\varepsilon_1$, $s_1 = s_2\varepsilon_2$; in particular $\varepsilon_1\varepsilon_2 = 1$. Conversely, if $\varepsilon_1\varepsilon_2 = 1$, then (6) defines an eigenvector of $T$. ∎

## 3. SPECIAL VERTICES OF A TREE

From now on, $T$ is a tree. In this section we prove some results about the possible zero entries of an eigenvector of $T$. Call a vertex $x \in T$ $\lambda$-*essential* if there is a $\lambda$-eigenvector $e$ with $e_x \neq 0$, *$\lambda$-special* if it is not essential, but adjacent with some essential point, and *$\lambda$-inessential* otherwise. Call a tree $T$ *$\lambda$-primitive* if $\lambda$ is an eigenvalue of $T$ and all vertices are $\lambda$-essential.

A subtree $T_1$ of $T$ is called *extremal* if, for some vertex $x \in T$, $T_1$ is a component of $T \setminus \{x\}$; equivalently, if the graph $T_2 = T \setminus T_1$ (obtained by deleting the vertices of $T_1$) is nonempty and connected, hence also a tree. Note that in this case, $T_1$ and $T_2$ are connected by a unique edge $x_1 x_2$ with $x_1 \in T_1$, $x_2 \in T_2$, and $T = (T_1, x_1, x_2, T_2)$.

THEOREM 3.1. *A tree $T$ is $\lambda$-primitive iff $T$, but no extremal subtree of $T$, has eigenvalue $\lambda$.*

*Proof.* Let $T$ be a tree with eigenvalue $\lambda$, and let $e$ be a $\lambda$-eigenvector. If $e_x = 0$ for some $x \in T$, then the relations (1) show that each component of $T \setminus \{x\}$ which contains a vertex $y$ with $e_y \neq 0$ is an extremal subtree with eigenvalue $\lambda$. Hence if $T$ contains no extremal subtree with eigenvalue $\lambda$, then $T$ is $\lambda$-primitive.

Conversely, if $T$ contains extremal subtrees with eigenvalue $\lambda$, then let $T_1$ be minimal (with respect to inclusion) among these. Denote the tree $T \setminus T_1$ by $T_2$, so that $T = (T_1, x_1, x_2, T_2)$ for certain $x_1 \in T_1$, $x_2 \in T_2$. Since $T_1$ is minimal, $\lambda$ is not an eigenvalue of $T_1 \setminus \{x_1\}$. Now the restriction $e^{(1)}$ of $e$ to $T_1$ is a multiple of the partial eigenvector of $T_1$ with respect to $x_1$ (by Proposition 2.7), and by Corollary 2.2, $e^{(1)}$ is in fact a $\lambda$-eigenvector of $T_1$. Hence by (1), $e_{x_2} = 0$. Since this holds for every $\lambda$-eigenvector $e$, $x_2$ is not $\lambda$-essential, and so $T$ is not $\lambda$-primitive. ■

COROLLARY 3.2. *If $\lambda$ is a multiple eigenvalue of a tree $T$, then $T$ contains a $\lambda$-special point.*

*Proof.* For any $x \in T$, $T \setminus \{x\}$ still has $\lambda$ as an eigenvalue; hence some component of $T \setminus \{x\}$, which is an extremal tree, has $\lambda$ as an eigenvalue. By Theorem 3.1, $T$ is not primitive and hence contains a special point. ■

COROLLARY 3.3. *A $\lambda$-primitive tree has $\lambda$ as a simple eigenvalue, and the corresponding eigenvector has no zero entries.*

THEOREM 3.4. *Let $T$ be a tree with $f$-fold eigenvalue $\lambda$, $f \geqslant 1$. Then*:

(i) *If $x$ is an essential vertex then $\lambda$ is an $(f-1)$-fold eigenvalue of $T \setminus \{x\}$.*

(ii) *If $x$ is an inessential vertex, then $\lambda$ is an $f$-fold eigenvalue of $T \setminus \{x\}$.*

(iii) *If $x$ is a special vertex, then $\lambda$ is an $(f+1)$-fold eigenvalue of $T\setminus\{x\}$; moreover, $x$ is adjacent to at least two essential vertices.*

*Proof.* (i): In [5], it is shown that $P(T\setminus\{x\},t)/P(T,t)$, considered as a function in $t$, has simple poles just at those eigenvalues $\lambda$ of $T$ for which there is some $\lambda$-eigenvector $e$ with $e_x \neq 0$ (see Theorem 5.2 of [5], and its proof). Hence $\lambda$ is an $(f-1)$-fold eigenvalue of $T\setminus\{x\}$ iff $x$ is $\lambda$-essential.

(ii) and (iii): If $x$ is not essential, then an eigenvector $e$ of $T$ is also an eigenvector of $T\setminus\{x\}$. If $x$ is inessential, then the converse also holds, so $T\setminus\{x\}$ has $\lambda$ as an $f$-fold eigenvalue. But if $x$ is special, then one extra relation $\Sigma_{y\sim x}e_y=0$ has to be satisfied. So the eigenspace of $T\setminus\{x\}$ for $\lambda$ must have one dimension more, i.e., $\lambda$ is an $(f+1)$-fold eigenvalue of $T\setminus\{x\}$. If $x$ were only adjacent with one essential point $y$, then the relation would reduce to $e_y=0$, contradicting the fact that $y$ is essential. ■

COROLLARY 3.5. *Let $T$ be a tree with $f$-fold eigenvalue $\lambda$, $f\geq 1$. Denote by $E$ the forest induced on the essential vertices. Then every component of $E$ has $\lambda$ as a simple eigenvalue. Moreover, $f$ equals the number of components of $E$ minus the number of special vertices of $T$.*

*Proof.* For each $x\in E$, some eigenvector $e$ of $T$ has $e_x\neq 0$. Each such $e$ is also an eigenvector of $E$, and hence of the component of $E$ containing $x$. So every component of $E$ is $\lambda$-primitive, and by Corollary 3.3, has $\lambda$ as a simple eigenvalue. From this, and the preceding theorem, the second part follows. ■

EXAMPLE. Take $\lambda=0$. By Theorem 3.1, a 0-primitive tree consists of a single vertex, since every end vertex is an extremal subtree with eigenvalue $\lambda=0$. In particular, for an arbitrary tree, $E$ is a coclique. The 0-special vertices are closely related to *k-matchings* (sets of $k$ disjoint edges) of $T$. In fact, following some remarks by Godsil (private communication), we have

PROPOSITION 3.6. *Let $T$ be a tree with $n$ vertices, and let $k$ be the maximal size of a matching. Then:*

(i) *0 is an $(n-2k)$-fold eigenvalue of $T$.*
(ii) *No vertex is 0-inessential.*
(iii) *A vertex is 0-special iff it is common to all k-matchings.*
(iv) *An edge contains one or two 0-special vertices.*
(v) *There are exactly $k$ 0-special vertices, and every edge of a k-matching contains a unique 0-special vertex.*

*Proof.* (i) is well known; see e.g. Proposition 1.1 of [2].

If $x \in T$ is not common to all $k$-matchings then the maximal size of a matching of $T \setminus \{x\}$ is $k$, whence 0 is an $(n-1-2k)$-fold eigenvalue of $T \setminus \{x\}$ [apply (i) to $T \setminus \{x\}$]. Hence $x$ is 0-essential (Theorem 3.4). On the other hand, if $x \in T$ is common to all $k$-matchings, then the maximal size of a matching of $T \setminus \{x\}$ is $k-1$, 0 is an $(n+1-2k)$-fold eigenvalue of $T \setminus \{x\}$, and $x$ is 0-special. This proves (ii) and (iii). Since $E$, the set of 0-essential vertices, is a coclique, (iv) holds.

Finally, denote by $e$ and $s$ the numbers of 0-essential and 0-special vertices, respectively. $E$ is an $e$-coclique; hence by (i) and Corollary 3.5, the multiplicity of 0 is $n-2k=e-s$. But $n=e+s$, whence $s=k$; i.e., $T$ contains $k$ 0-special vertices. On each edge of a $k$-matching there is at least one, and hence exactly one, of these vertices. ∎

## 4. THE SECOND LARGEST EIGENVALUE OF A TREE

Here we investigate the structure of trees with $\lambda_2(T) \leqslant \lambda$. Let us call a tree $T$ *$\lambda$-trivial* if there is a vertex $x \in T$ such that $\lambda_1(T-\{x\}) \leqslant \lambda$—equivalently, if all components of $T \setminus \{x\}$ are trees with largest eigenvalue $\leqslant \lambda$. Because the eigenvalues of $T \setminus \{x\}$ interlace those of $T$, a $\lambda$-trivial tree has $\lambda_2(T) \leqslant \lambda$. It is easy to find sufficient conditions for $\lambda$-triviality:

PROPOSITION 4.1. *If a tree $T$ with $\lambda_2(T) \leqslant \lambda$ contains extremal subtrees with eigenvalue $\lambda$, then $T$ is $\lambda$-trivial.*

*Proof.* Let $T_0$ be an extremal subtree of $T$ with eigenvalue $\lambda$, and let $x$ be the vertex such that $T_0$ is a component of $T \setminus \{x\}$. Since the eigenvalues of $T \setminus \{x\}$ interlace those of $T$, $T \setminus \{x\}$ has exactly one eigenvalue $> \lambda_2(T)$, which must be $\lambda$; the other eigenvalues are $\leqslant \lambda_2(T) \leqslant \lambda$. Hence $T$ is $\lambda$-trivial. ∎

Using Theorem 3.1 and Corollary 3.2, we immediately obtain

COROLLARY 4.2. *If $\lambda_2(T)$ is a multiple eigenvalue of a tree $T$, then $T$ is $\lambda_2$-trivial.*

We are now able to prove our main result. Together with Theorem 2.6, it characterizes all trees with $\lambda_2(T) \leqslant \lambda$.

THEOREM 4.3. *A tree $T$ with $\lambda_2(T) \leqslant \lambda$ is either $\lambda$-trivial or a $\lambda$-twin.*

*Proof.* Suppose that $T$ is not $\lambda$-trivial. By Proposition 4.1, $T$ contains no extremal subtree with eigenvalue $\lambda$. But there are extremal subtrees with largest eigenvalue $>\lambda$, since for all $x\in T$, $\lambda_1(T\setminus\{x\})>\lambda$. Let $T_1$ be an extremal subtree, minimal with respect to the property $\lambda_1(T_1)>\lambda$. With $T_2=T\setminus T_1$, $T$ can be written as $T=(T_1,x_1,x_2,T_2)$. By minimality of $T_1$, $\lambda_1(T_1\setminus\{x_1\})\leqslant\lambda$, and hence $<\lambda$; so $T_1$ is critical at $x_1$.

Now $T$ is not $\lambda$-trivial; hence $T\setminus\{x_1\}$ has an eigenvalue $>\lambda$, and so $\lambda_1(T_2)>\lambda$. By construction, $\lambda_1(T_1)>\lambda\geqslant\lambda_2(T)$. Since $T\setminus\{x_2\}$ is the disjoint union of $T_1$ and $T_2\setminus\{x_2\}$, $\lambda_1(T_1)$ is an eigenvalue $\geqslant\lambda_2(T)$ of $T\setminus\{x_2\}$. By interlacing, the other eigenvalues of $T\setminus\{x_2\}$ are $\leqslant\lambda_2(T)\leqslant\lambda$. In particular, the eigenvalues of $T_2\setminus\{x_2\}$ are $\leqslant\lambda$, and hence even $<\lambda$. Therefore $T_2$ is critical at $x_2$, and $T$ is a twin. ■

REMARK. It is easy to see that a $\lambda$-twin cannot be $\lambda$-trivial, and that a tree can be written in at most one way as a $\lambda$-twin.

In Theorem 2.6, we showed how to decide whether a $\lambda$-twin $T$ has $\lambda_2(T)<\lambda$ or $\lambda_2(T)=\lambda$; the next result complements this by a criterion for $\lambda_2(T)=\lambda$ for $\lambda$-trivial trees. Note that $\lambda_2(T)<\lambda$ if this criterion fails.

THEOREM 4.4. *Let $T$ be a $\lambda$-trivial tree, and $x\in T$ a vertex with $\lambda_1(T\setminus\{x\})\leqslant\lambda$. Then $\lambda_2(T)=\lambda$ iff $f+1\geqslant 2$ components of $T\setminus\{x\}$ have (largest) eigenvalue $\lambda$; in this case, $x$ is a special vertex of $T$, and $\lambda$ is an $f$-fold eigenvalue of $T$.*

*Proof.* A 0-trivial tree is a star, and the statement is obvious. Hence assume that $\lambda\neq 0$. Suppose that $\lambda_2(T)=\lambda$, and let $e$ be a $\lambda$-eigenvector of $T$. Denote by $T'$ the tree induced on the set consisting of $x$ and those components of $T\setminus\{x\}$ which have some nonzero entry in $e$. Suppose first that $T'\setminus\{x\}$ contains a component $T_0$ with largest eigenvalue $\lambda$; let $x_0$ be the vertex in $T_0$ adjacent to $x$. If $e_{x_0}=0$, then the restriction of $e$ to $T_0\setminus\{x_0\}$ is a $\lambda$-eigenvector of $T_0\setminus\{x_0\}$ (nonzero by construction of $T'$). But $\lambda_1(T_0\setminus\{x_0\})<\lambda_1(T_0)=\lambda$, contradiction. Hence $e_{x_0}\neq 0$, and $e$ can be normalized so that $e_{x_0}=1$. Then the restriction of $e$ to $T_0$ is a partial eigenvector of $T_0$, and by Theorem 2.2, it is an eigenvector. Therefore, the relations (1) for $x=x_0$ imply $e_x=0$. This holds for every $\lambda$-eigenvector $e$ of $T$; so $x$ is special. Now apply Theorem 3.4(iii) to get the desired result.

Next suppose that $T'\setminus\{x\}$ has no component with largest eigenvalue $\lambda$. Then $e_x\neq 0$, since otherwise $e$ is a $\lambda$-eigenvector of $T'\setminus\{x\}$, and $\lambda_1(T'\setminus\{x\})<\lambda$. Since $\lambda\neq 0$, some neighbor $x_1$ of $x$ must have $e_{x_1}\neq 0$ [by (1)]. Write $x_2=x$, write $T_1$ for the component of $T'\setminus\{x_2\}$ containing $x_1$, and $T_2$ for the component of $T'\setminus\{x_1\}$ containing $x_2$. Then $T'=(T_1,x_1,x_2,T_2)$, and $\lambda_1(T_1)<$

$\lambda$, $\lambda_1(T_2\backslash\{x_2\}) < \lambda$. Denote by $e^{(i)}$ and $\varepsilon_i$ the partial eigenvector and exitvalue of $T_i$ with respect to $x_i$. Then by Theorem 2.4, $e^{(1)} > 0$, $\varepsilon_1 > 0$, $e^{(2)} > 0$, and by Proposition 2.7, $e$ or $-e$ is positive on $T'$, hence nonnegative on $T$. But this implies (Perron-Frobenius) that $\lambda = \lambda_1(T) > \lambda_2(T)$, a contradiction.

The converse follows again from Theorem 3.4(iii). ■

The theorems just proved have an interesting corollary. Let $e$ be a $\lambda$-eigenvector of a tree $T$. We say that an edge $xy$ of $T$ is a *sign change* of $e$ if $e_x e_y < 0$. From our Theorems 4.3 and 4.4, and Theorems 2.4(iii) and 2.6(ii), we find:

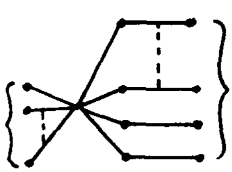
COROLLARY 4.4a. *Let e be an eigenvector for the second largest eigenvalue of a tree. If all entries of e are nonzero, then e has exactly one sign change.*

This is a special case of the following theorem [6]:

THEOREM 4.5 (Godsil). *Let e be an eigenvector for the eigenvalue* $\lambda_i(T)$ *of a tree. If all entries of e are nonzero, then e has exactly* $i-1$ *sign changes.*

Note that the special case $i=1$ (no sign change) of Theorem 4.5 is a consequence of Perron-Frobenius theory. Also, the case where $T$ is a path is a special case of a result of Gantmacher and Krein [4] on oscillation matrices (their Satz 6 in Kap. II, §5).

EXAMPLE. We determine the trees with $\lambda_2 \leqslant 1$. It is obvious that a tree with largest eigenvalue $<1$ is a single vertex, and a tree with largest eigenvalue $=1$ is a single edge. Hence the 1-trivial graphs are of the shape



$(i+1+2j$ vertices, $i \geqslant 0$, $j \geqslant 0)$. $(*)$

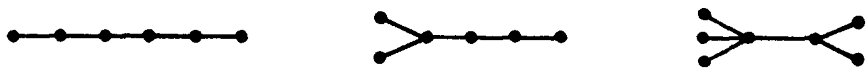
Also, if a tree $T$ is 1-critical at $x$, then $T\backslash\{x\}$ is a coclique of size $s \geqslant 2$, say, and the exitvalue is $\varepsilon = 1 - s \leqslant -1$. Hence the only way to get a 1-twin with $\varepsilon_1\varepsilon_2 \leqslant 1$ is to take $s_1 = s_2 = 2$; by Theorem 2.6, the only twin with $\lambda_2 \leqslant \lambda$ is

$(**)$

Hence we have:

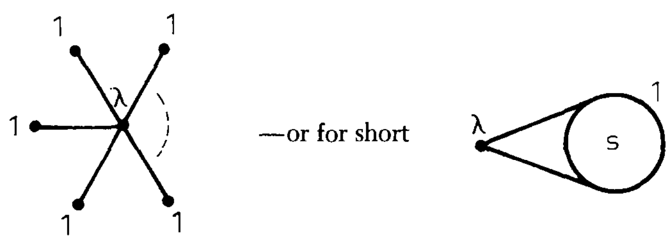
THEOREM 4.6. *A tree with $\lambda_2 \leqslant 1$ either is of shape* $(*)$, *or is the graph* $(**)$.

REMARK. A different proof can be given by forbidden subtrees. In fact, by the tables in [2], the second largest eigenvalues of the trees

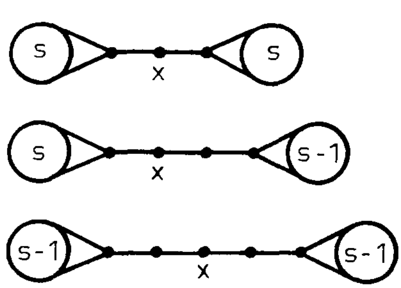


are $>1$, and the trees $(*)$, $(**)$ are the only trees with no such induced subtree.

EXAMPLE. A star with $n = s+1$ vertices,




—has largest eigenvalue $\sqrt{s} = \sqrt{n-1}$, since the indicated vector is a positive eigenvector for $\lambda = \sqrt{s}$. Hence a tree $T$ with a vertex $x$ such that $T \setminus \{x\}$ is a disjoint union of $m$ stars with $s+1$ vertices is $\sqrt{s}$-trivial; hence $\lambda_2 \leqslant \sqrt{s}$. If $m \geqslant 2$, then by Theorem 4.4, $\lambda_2 = \sqrt{s}$ is an $(m-1)$-fold eigenvalue of $T$. In particular, the three trees




$(***)$

have $n=2s+3$ vertices and $\lambda_2=\sqrt{s}=\sqrt{(n-3)/2}$ (in particular, there are trees with arbitrarily large $\lambda_2$). The trees $(***)$ are extremal in the following sense:

THEOREM 4.7. *Let T be a tree with n vertices. Then*

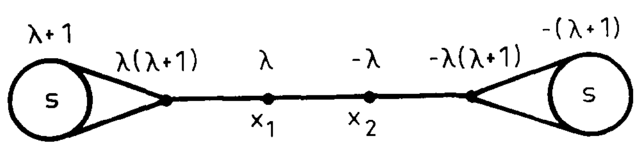
(i) $\lambda_1(T)\leqslant\sqrt{n-1}$, *with equality iff T is a star;*
(ii) $\lambda_2(T)\leqslant\sqrt{(n-3)/2}$, *with equality iff T is one of the trees* $(***)$.

*Proof.* (i): $T$ is bipartite; hence with $\lambda_1$, also $-\lambda_1$ is an eigenvalue of $T$. Therefore, $2\lambda_1^2\leqslant\Sigma\lambda_i^2=\operatorname{tr}A^2=2\times(\text{number of edges of }T)=2(n-1)$, and so $\lambda_1\leqslant\sqrt{n-1}$. If equality holds, then $\lambda_2=\cdots=\lambda_{n-1}=0$, $\lambda_n=-\lambda_1$. Hence $A$ has rank 2. Since $T$ is bipartite, this implies that $T$ is complete bipartite, and since $T$ is a tree, it must be a star.

(ii): There is a vertex $x\in T$ such that all components of $T\setminus\{x\}$ have size $\leqslant(n-1)/2$. For if $T\setminus\{x_1\}$ has a component $T_0$ of size $\geqslant n/2$, then the remaining components have size $<n/2-1$ together; thus if $x_2$ is the neighbor of $x_1$ in $T_0$ then in $T\setminus\{x_2\}$, the component of $x_1$ has size $<n/2$ and hence $\leqslant(n-1)/2$, and the other components of $T\setminus\{x_2\}$ are contained in $T_0\setminus\{x_2\}$ and hence have size less than the size of $T_0$. If we repeat this process, we obtain after a finite number of steps an $x$ with the required property.

Now, by interlacing, $\lambda_2(T)\leqslant\lambda_1(T\setminus\{x\})\leqslant\sqrt{(n-3)/2}$ by (i), and equality implies that some component $T_1$ of $T\setminus\{x\}$ has size $(n-1)/2$ and is a star. But then $T_1$ is an extremal subtree with eigenvalue $\sqrt{(n-3)/2}=\lambda_2$, and by Theorem 4.4, $T\setminus\{x\}$ has another component $T_2$ with eigenvalue $\lambda_2$, which again must be a star of size $(n-1)/2$. Now we already have all vertices, and the only ways of getting a tree are those shown in $(***)$. ■

REMARK. In particular, for a tree with an even number $n$ of vertices, $\lambda_2(T)<\sqrt{(n-3)/2}$. Probably the unique extremal trees in this case are

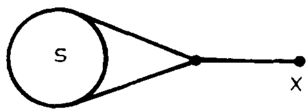



$(****)$

with $n=2s+4$ vertices; this can be verified for $n\leqslant10$ by the tables in [2]. The second largest eigenvalue of $(****)$ is the positive root $\lambda$ of the equation

$$\lambda^3 + \lambda^2 - (s+1)\lambda - s = 0,$$

as can be seen from the indicated eigenvector. Since $s = \lambda^2 - \lambda/(\lambda+1) < \lambda^2 < \lambda^2 + 1/(\lambda+1) = s+1$, it follows that




is $\lambda$-critical, and both exitvalues are $\varepsilon_1 = \varepsilon_2 = -1$. So we have a twin with $\varepsilon_1\varepsilon_2 = 1$ (cf. Proposition 2.7). (It is also seen that there is exactly one sign change.)

We end this section with explicit recursive formulas for the computation of partial eigenvectors and exitvalues of a tree. Let $T$ be a tree, and $z \in T$. Denote the neighbors of $z$ by $z_1, \ldots, z_s$. Then the components of $T \setminus \{z\}$ can be labeled as $T_1, \ldots, T_s$ in such a way that $z_i \in T_i$ for $i = 1, \ldots, s$. Let $e_i$ and $\varepsilon_i$ be the partial eigenvector and exitvalue of $T_i$ with respect to $z_i$. If all $\varepsilon_i$ are nonzero, then the partial eigenvector $e$ of $T$ has $e_z = 1$, and agrees on $T_i$ with $\varepsilon_i^{-1} e^{(i)}$ [by the relations (1)], and so is determined. Also, the exitvalue $\varepsilon$ of $T$ with respect to $z$ is given by the formula

$$\varepsilon = \lambda - \sum_i \varepsilon_i^{-1}.$$

These remarks can be used to find a partial eigenvector and/or an exitvalue recursively. The process breaks down if some $\varepsilon_i$ becomes zero. But then $T_i$ is an extremal subgraph with eigenvalue $\lambda$; so this breakdown cannot occur in the range $\lambda > \lambda_1(T \setminus \{z\})$.

Note that in actual computation it may be more convenient to compute a multiple of the partial eigenvector, and normalize at the end of the computation.

REMARK. After submission of the manuscript, I learnt that Godsil's Theorem 4.5 is a particular case of a theorem of Fiedler [3], and that a paper by Maxwell [8] contains the case $\lambda_2(T) \neq \lambda$ of my Theorem 4.3. I want to thank Jürgen Garloff and Barry Monson for calling my attention to these papers.

*I want to thank Chris Godsil for valuable suggestions which improved Section 3.*

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