

The Second Largest Eigenvalue of a Tree*

A. Neumaier

Institut für Angewandte Mathematik
Universität Freiburg, West Germany

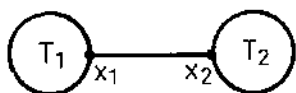
Submitted by N. Biggs

ABSTRACT

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

1. INTRODUCTION

Suppose that T is a tree, and λ 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) λ ? 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 λ 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 $\lambda_2(T) \leq \lambda$. Then either T contains a vertex x such that $\lambda_1(T - \{x\}) \leq \lambda$; or T is a λ -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 λ_1 denotes the largest eigenvalue.) Also, we find an upper bound $\lambda_2(T)$

*This work was done while the author was at the Technische Hogeschool Eindhoven with grant No. B-61-99 of the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

$\leq \sqrt{(n-3)/2}$ 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 $\lambda_2(T) \leq 2$. 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 $\lambda_2(T) \leq 2$ is needed. This was found tractable for trees and led to the present results. Applications to reflection groups will be reported elsewhere.

2. EIGENVALUES

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

$$\lambda_1(T) > \lambda_2(T) \geq \dots \geq \lambda_n(T)$$

($n =$ 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*

$$\lambda_{i+1}(T) \leq \lambda_i(T \setminus \{x\}) \leq \lambda_i(T) \quad (\text{IP})$$

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

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

$$\sum_{y \sim x} e_y = \lambda e_x \quad (1)$$

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

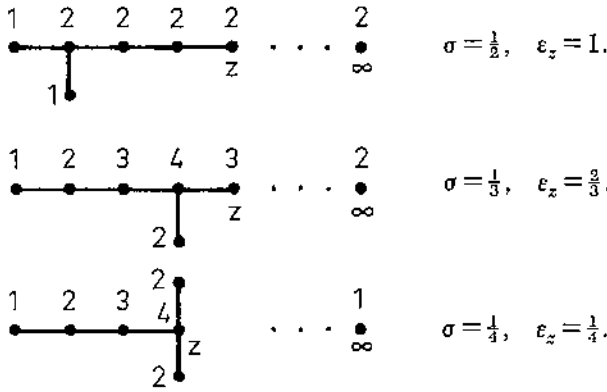
λ -eigenvector with respect to a vertex $z \in T$ if $e_z = 1$, and (1) holds for all $x \in T \setminus \{z\}$; in this case the number

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

is called a λ -exitvalue of T with respect to z . If the λ -exitvalue ε is zero, then λ is an eigenvalue of T , and e a corresponding eigenvector; if ε is nonzero, then it can be thought of as the entry of e at a hypothetical further vertex ∞ 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 “ λ ” from expressions like “ λ -eigenvector” or “ λ -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 σ times the label of vertex x .



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

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

the exitvalue satisfies

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

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

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

with side condition

$$\delta_z^T e = 1. \quad (4a)$$

Case 1: $\lambda I - A$ is nonsingular. Then (4) implies $e = \varepsilon(\lambda I - A)^{-1} \delta_z$ ($\delta_z^T e = \varepsilon(\lambda I - A)^{-1} \delta_z^T \delta_z$), 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 ε and e are unique, and in fact these expressions satisfy (4), (4a). Moreover, (3) holds.

Case 2: $\lambda I - A$ is singular. Then λ is an eigenvalue of T . Let e be a corresponding eigenvector. If $e_z = 0$, then e is also a λ -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 λ -eigenvector, then $e' - e$ is a λ -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 λ is an eigenvalue of T but not of $T \setminus \{z\}$, then λ is a simple eigenvalue, $\varepsilon_{T,z}(\lambda) = 0$, and the partial λ -eigenvector with respect to $z \in T$ is the unique λ -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 λ 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 λ is not an eigenvalue of $T \setminus \{z\}$. If $e(z)$ and ε_z denote the partial eigenvector and the exitvalue with*

respect to z , then:

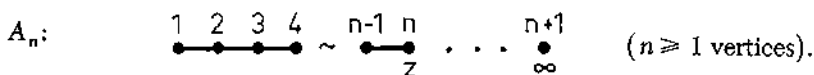
- (i) $\lambda_1(T) < \lambda$ iff $e(z) > 0, \epsilon_z > 0$.
- (ii) $\lambda_1(T) = \lambda$ iff $e(z) > 0, \epsilon_z = 0$.
- (iii) $\lambda_1(T - \{z\}) < \lambda < \lambda_1(T)$ iff $e(z) > 0, \epsilon_z < 0$.

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

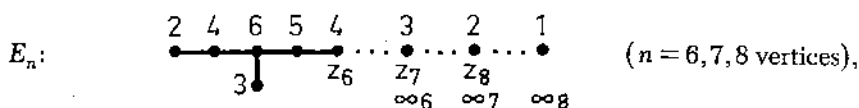
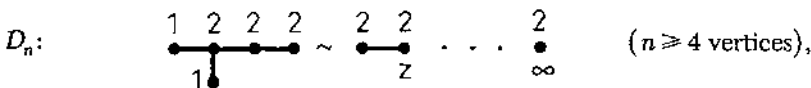
Proof. By (3), $\epsilon_z = 0$ if $\lambda_1(T) = \lambda$, so the statements follow from Corollary 2.3 if we can show that $e(z) > 0$ iff $\lambda_1(T - \{z\}) < \lambda$.

Now (4) holds with $\epsilon = \epsilon_z, e = e(z)$; hence for $B = A + \epsilon \delta_z \delta_z^T$, 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 λ is the largest eigenvalue of B . But the proof of Theorem 2.1 shows that $U - B$ is singular iff $\epsilon = \epsilon_{T,z}(\epsilon)$. Hence the eigenvalues of B are the solutions of $\epsilon_{T,z}(\epsilon) = \epsilon = \epsilon_{T,z}(\lambda)$. So, by Corollary 2.3, λ 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 $\epsilon_z > 0$ for some vertex z . If T is a chain, then (up to a scaling factor) $e(z)$ and ϵ_z are given by

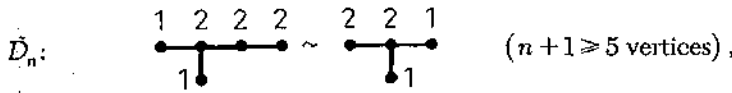


Similarly, we have

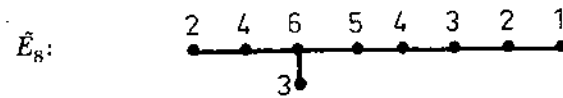
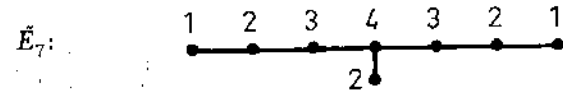
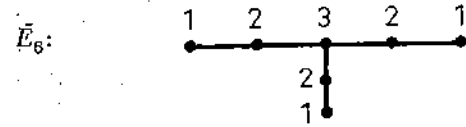


Hence these graphs have $\lambda_1(T) < 2$. Now the minimal trees not of type A_n ,

D_n or E_6, E_7, E_8 are

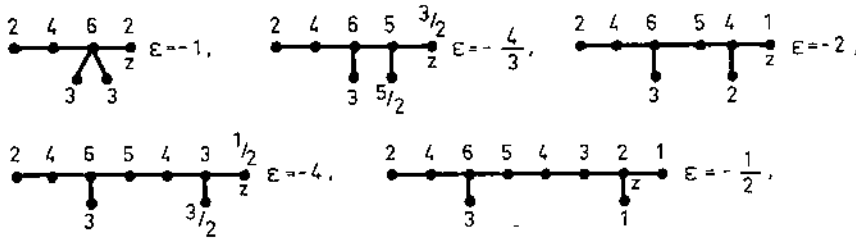


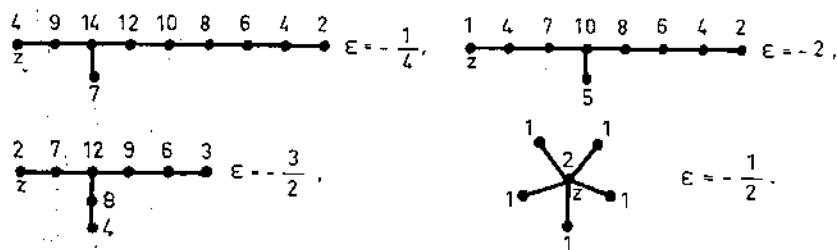
and



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.

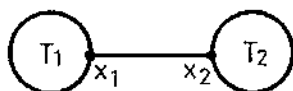
EXAMPLE. In his lectures on hyperbolic coxeter groups, Koszul [7] determined all minimal Dynkin diagrams with $\lambda_1 > 2$ (Theorems 18-1 and 18-2). We reproduce here those diagrams which are trees without multiple edges. We also give the 2-exitvalue and a multiple of the partial 2-eigenvector with 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_1x_2 . In Section 4 we shall need a special case: We call (T_1, x_1, x_2, T_2) a λ -*twin* if, for $i = 1, 2$, T_i is λ -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 λ -twin. For $i = 1, 2$, denote by ε_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 λ -critical at x_i , we have $P_i(t) := P_{T_i \setminus \{x_i\}}(t) > 0$ for all $t \geq \lambda$. In particular, the exitvalues $\varepsilon_i(t) := \varepsilon_{T_i, x_i}(t)$ are defined. Now by Theorem 2.1 and Proposition 2.5,

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

Put $\lambda_1 = \lambda_1(T)$, $\lambda_2 = \lambda_2(T)$, and denote by λ_3 the largest eigenvalue of T strictly smaller than λ_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 λ -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 λ 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 ε_i the partial eigenvector and the exitvalue of T_i with respect to x_i . Then λ is an eigenvalue of T iff $\varepsilon_1\varepsilon_2 = 1$; in this case, every λ -eigenvector has the form*

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

in particular, λ is a simple eigenvalue of T .

Proof. Suppose that λ is an eigenvalue of T , and e a λ -eigenvector. The numbers $s_i = e_{x_i}$ are nonzero, since otherwise $T_i \setminus \{x_i\}$ would have an eigenvalue λ 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 $x \in T$ λ -essential if

there is a λ -eigenvector e with $e_x \neq 0$, λ -special if it is not essential, but adjacent with some essential point, and λ -inessential otherwise. Call a tree T λ -primitive if λ is an eigenvalue of T and all vertices are λ -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_1x_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 λ -primitive iff T , but no extremal subtree of T , has eigenvalue λ .*

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

Conversely, if T contains extremal subtrees with eigenvalue λ , 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, λ 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 λ -eigenvector of T_1 . Hence by (I), $e_{x_2} = 0$. Since this holds for every λ -eigenvector e , x_2 is not λ -essential, and so T is not λ -primitive. ■

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

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

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

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

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

(iii) If x is a special vertex, then λ 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 λ of T for which there is some λ -eigenvector e with $e_x \neq 0$ (see Theorem 5.2 of [5], and its proof). Hence λ is an $(f-1)$ -fold eigenvalue of $T \setminus \{x\}$ iff x is λ -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 λ as an f -fold eigenvalue. But if x is special, then one extra relation $\sum_{y \sim x} e_y = 0$ has to be satisfied. So the eigenspace of $T \setminus \{x\}$ for λ must have one dimension more, i.e., λ 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 λ , $f \geq 1$. Denote by E the forest induced on the essential vertices. Then every component of E has λ 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 λ -primitive, and by Corollary 3.3, has λ 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 $\lambda_2(T) \leq \lambda$. Let us call a tree T λ -trivial if there is a vertex $x \in T$ such that $\lambda_1(T - \{x\}) \leq \lambda$ — equivalently, if all components of $T \setminus \{x\}$ are trees with largest eigenvalue $\leq \lambda$. Because the eigenvalues of $T \setminus \{x\}$ interlace those of T , a λ -trivial tree has $\lambda_2(T) \leq \lambda$. It is easy to find sufficient conditions for λ -triviality:

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

Proof. Let T_0 be an extremal subtree of T with eigenvalue λ , 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 λ ; the other eigenvalues are $\leq \lambda_2(T) \leq \lambda$. Hence T is λ -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 λ_2 -trivial.*

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

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

Proof. Suppose that T is not λ -trivial. By Proposition 4.1, T contains no extremal subtree with eigenvalue λ . 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 , $\lambda_1(T_1 \setminus \{x_1\}) \leq \lambda$, and hence $< \lambda$; so T_1 is critical at x_1 .

Now T is not λ -trivial; hence $T \setminus \{x_1\}$ has an eigenvalue $> \lambda$, and so $\lambda_1(T_2) > \lambda$. By construction, $\lambda_1(T_1) > \lambda \geq \lambda_2(T)$. 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 $\geq \lambda_2(T)$ of $T \setminus \{x_2\}$. By interlacing, the other eigenvalues of $T \setminus \{x_2\}$ are $\leq \lambda_2(T) \leq \lambda$. In particular, the eigenvalues of $T_2 \setminus \{x_2\}$ are $\leq \lambda$, 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 λ -twin cannot be λ -trivial, and that a tree can be written in at most one way as a λ -twin.

In Theorem 2.6, we showed how to decide whether a λ -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 λ -trivial trees. Note that $\lambda_2(T) < \lambda$ if this criterion fails.

THEOREM 4.4. *Let T be a λ -trivial tree, and $x \in T$ a vertex with $\lambda_1(T \setminus \{x\}) \leq \lambda$. Then $\lambda_2(T) = \lambda$ iff $f+1 \geq 2$ components of $T \setminus \{x\}$ have (largest) eigenvalue λ ; in this case, x is a special vertex of T , and λ 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 λ -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 λ ; 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 λ -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 λ -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 λ . Then $e_x \neq 0$, since otherwise e is a λ -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 $\lambda_1(T_1) <$

$\lambda, \lambda_1(T_2 \setminus \{x_2\}) < \lambda$. Denote by $e^{(i)}$ and ε_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 λ -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:

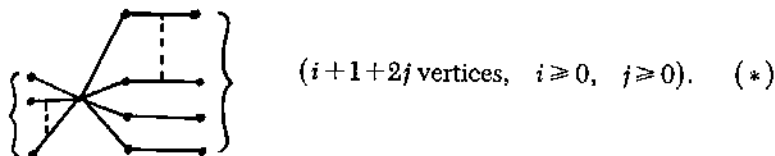
COROLLARY 4.4a. *Let e be an eigenvector for the second largest eigenvalue of a tree. If all entries of e are nonzero, then e has exactly one sign change.*

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

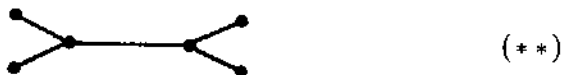
THEOREM 4.5 (Godsil). *Let e be an eigenvector for the eigenvalue $\lambda_i(T)$ of a tree. If all entries of e are nonzero, then e has exactly $i - 1$ sign changes.*

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 $\lambda_2 \leq 1$. 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



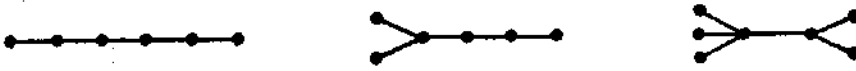
Also, if a tree T is 1-critical at x , then $T \setminus \{x\}$ is a coclique of size $s \geq 2$, say, and the exitvalue is $\varepsilon = 1 - s \leq -1$. Hence the only way to get a 1-twin with $\varepsilon_1 \varepsilon_2 \leq 1$ is to take $s_1 = s_2 = 2$; by Theorem 2.6, the only twin with $\lambda_2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



Hence we have:

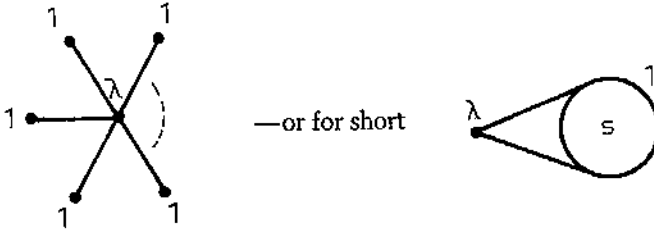
THEOREM 4.6. *A tree with $\lambda_2 \leq 1$ either is of shape (*), or is the graph (**).*

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

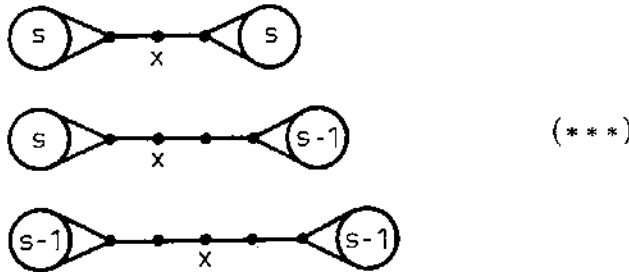


are > 1 , and the trees (*), (**) are the only trees with no such induced subtree.

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 $\lambda_2 \leq \sqrt{s}$. If $m \geq 2$, 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 λ_2). The trees (***) are extremal in the following sense:

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

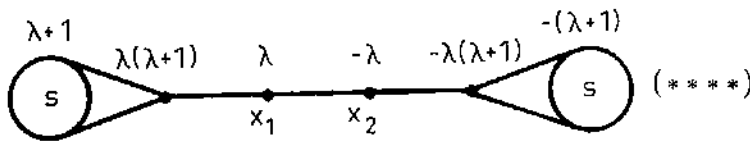
- (i) $\lambda_1(T) \leq \sqrt{n-1}$, with equality iff T is a star;
- (ii) $\lambda_2(T) \leq \sqrt{(n-3)}/2$, with equality iff T is one of the trees (***) .

Proof. (i): T is bipartite; hence with λ_1 , also $-\lambda_1$ is an eigenvalue of T . Therefore, $2\lambda_1^2 \leq \sum \lambda_i^2 = \text{tr } A^2 = 2 \times (\text{number of edges of } T) = 2(n-1)$, and so $\lambda_1 \leq \sqrt{n-1}$. If equality holds, then $\lambda_2 = \dots = \lambda_{n-1} = 0$, $\lambda_n = -\lambda_1$. 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 $\leq (n-1)/2$. For if $T \setminus \{x_1\}$ has a component T_0 of size $\geq n/2$, 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 $\leq (n-1)/2$, 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, $\lambda_2(T) \leq \lambda_1(T \setminus \{x\}) \leq \sqrt{(n-3)}/2$ 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 λ_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

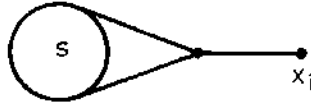


with $n = 2s + 4$ vertices; this can be verified for $n \leq 10$ by the tables in [2]. The second largest eigenvalue of (***) is the positive root λ of the

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 λ -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, \dots, z_s . Then the components of $T \setminus \{z\}$ can be labeled as T_1, \dots, T_s in such a way that $z_i \in T_i$ for $i = 1, \dots, s$. Let e_i and ε_i be the partial eigenvector and exitvalue of T_i with respect to z_i . If all ε_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 ε 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 ε_i becomes zero. But then T_i is an extremal subgraph with eigenvalue λ ; 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.

REFERENCES

1. A. Berman and R. J. Plemmons, *Nonnegative Matrices in the Mathematical Sciences*, Academic, New York, 1979.
2. D. M. Cvetcovic, M. Doob, and H. Sachs, *Spectra of Graphs*, Academic, New York, 1980.
3. M. Fiedler, Eigenvectors of acyclic matrices, *Czechoslovak Math. J.*, 25(100):607-618 (1975).
4. F. R. Gantmacher and M. G. Krein, *Oszillationsmatrizen, Oszillationskerne und kleine Schwingungen mechanischer Systeme*, Akademie Verlag, Berlin, 1960.
5. C. D. Godsil, Matchings and walks in graphs, *J. Graph Theory*, 5:285-297 (1981).
6. C. D. Godsil, Spectra of trees, in *Proceedings of the Conference on Convexity and Graph Theory (March 1981)*, to appear.
7. J. L. Koszul, Lectures on hyperbolic Coxeter groups, Dept. of Mathematics, Univ. of Notre Dame, 1967.
8. G. Maxwell, Hyperbolic trees, *J. Algebra* 54:46-49 (1978).

Received 9 June 1981