ELSEVIER

Linear Algebra and its Applications 336 (2001) 51–60

LINEAR ALGEBRA AND ITS APPLICATIONS

www.elsevier.com/locate/laa

# Discrete nodal domain theorems

E. Brian Davies [a,*], Graham M.L. Gladwell [b], Josef Leydold [c,1], Peter F. Stadler [d,e,2]

[a] *Department of Mathematics, King's College, Strand, London WC2R 2LS, UK*
[b] *Department of Civil Engineering, University of Waterloo, Waterloo, Ont., Canada N2L 3G1*
[c] *Department for Applied Statistics and Data Processing, University of Economics and Business Administration, Augasse 2-6, A-1090 Wien, Austria*
[d] *Institute for Theoretical Chemistry and Molecular Structural Biology, University of Vienna, Währingerstrasse 17, A-1090 Vienna, Austria*
[e] *The Santa Fe Institute, 1399 Hyde Park Rd, Santa Fe, NM 87501, USA*

Received 25 September 2000; accepted 19 February 2001

Submitted by N.J. Higham

**Abstract**

We prove two discrete analogues of Courant's Nodal Domain Theorem. © 2001 Elsevier Science Inc. All rights reserved.

*Keywords:* Nodal domain; Sign graph; Graph Laplacian; Eigenfunctions

## 1. Introduction

Courant [5, Chapter 6, Section 6] stated a general theorem about the nodes of an eigenfunction: *Given the self-adjoint second order* (*elliptic*) *differential equation* $L[u] + \lambda\rho u = 0$ ($\rho > 0$) *for a domain G with arbitrary homogeneous boundary conditions*; *if its eigenfunctions are ordered according to increasing eigenvalues*,

* Corresponding author. Tel.: +44-020-7848-2698; fax: +44-020-7848-2017.

*E-mail addresses:* e.brian.davies@kcl.ac.uk (E.B. Davies), ggladwell@uwaterloo.ca (G.M.L. Gladwell), josef.leydold@statistik.wu-wien.ac.at (J. Leydold), studla@tbi.univie.ac.at, stadler@santafe.edu (P.F. Stadler).

URL: http://www.mth.kcl.ac.uk/staff/eb_davies.html (E.B. Davies), http://statistik.wu-wien.ac.at/staff/leydold (J. Leydold), http://www.tbi.univie.ac.at/~studla, (P.F. Stadler).

1 Tel.: +43-1-31336-4695; fax: +43-1-31336-738.

2 Tel.: +43-1-4277-52737; fax: +43-1-4277-52793.


PII: S 0 0 2 4 - 3 7 9 5 ( 0 1 ) 0 0 3 1 3 - 5

*then the nodes of the* nth *eigenfunction* $u_n$ *divide the domain into no more than n subdomains. No assumptions are made about the number of independent variables.*

The subdomains of which Courant writes have since become known as *nodal domains*, see e.g. [1]. Many other authors refer to nodal domains as well, meaning domains *bounded* by nodes, not domains on which the eigenfunctions vanish. The nodal sets themselves are known to be of zero Lebesgue measure and of dimension $m-1$ [2,14]. This terminology is now well-established in the PDE literature, but is inappropriate for graphs. A discrete eigenvector on a graph is defined only on the vertex set $V$ of a graph $\Gamma$. Thus, contrary to the situation on a manifold, it may change from positive to negative without passing through zero. The discrete analogue of a "nodal domain" is a connected set of vertices, i.e., a connected subgraph of $\Gamma$, on which the eigenvector has the same, strict or loose, sign. Now such a set of vertices is not "bounded" by "nodes"; it is merely "bounded" by vertices of the opposite loose sign. An appropriate name for such an entity would thus appear to be *sign* graph, rather than *nodal* graph.

Before introducing the formal definition of a sign graph, we formulate the discrete problem. Let $\mathbf{A} \in \mathbb{R}^{N\times N}$ be a real symmetric matrix with non-positive off-diagonal elements: if $i \neq j$, then $a_{ij} \leqslant 0$. $\mathbf{A}$ has eigenvalues $\lambda_i$, $i = 1, \ldots, N$, satisfying

$$\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_N. \tag{1}$$

With the matrix $\mathbf{A}$ we may associate a simple, undirected, loop-free graph $\Gamma$ with finite vertex set $V$ and edge set $E$. We denote the vertices by $P_i$, $i = 1, \ldots, N$. Vertices $P_i, P_j$ are *adjacent*, written $P_i \sim P_j$, or equivalently $\{P_i, P_j\} \in E$, iff $a_{ij} < 0$. It is well known that, under this association, the matrix $\mathbf{A}$ is irreducible iff the graph $\Gamma$ is connected. In this case the Perron–Frobenius theorem implies that $\lambda_1$ is non-degenerate, i.e., $\lambda_1 < \lambda_2$, and the first eigenvector can be chosen to be everywhere positive.

Matrices of this type naturally arise as discrete *Schrödinger operators*, e.g., in the *Hückel Molecular Orbital method* of Theoretical Organic Chemistry:

$$\mathscr{H} u_j = \sum_{P_i : P_i \sim P_j} a_{ij}\left[u_j - u_i\right] + a_{jj} u_j = [\mathbf{Au}]_j. \tag{2}$$

Here the diagonal terms play the role of the potential and the off-diagonal elements are binding energies between adjacent atoms.

We focus our attention on the $n$th eigenvalue of $\mathbf{A}$, and suppose that it has multiplicity $r$, so that

$$\lambda_{n-1} < \lambda_n = \lambda_{n+1} = \cdots = \lambda_{n+r-1} < \lambda_{n+r}. \tag{3}$$

We suppose $\mathbf{u}^{(n)} \equiv \mathbf{u} = \{u_1, u_2, \cdots, u_N\}$ is in the eigenspace of $\lambda_n$, so that

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{u} = \mathbf{0}. \tag{4}$$

The association $u_i \to P_i$ associates the real numbers $u_i$, $i = 1, \ldots, N$, with the vertices $P_i$ of $\Gamma$. The numbers $u_i$ will be positive, negative or zero. We introduce two definitions:

**Definition 1.** A *strong positive* (*negative*) *sign graph* $S$ is a maximal, connected subgraph of $\Gamma$, on vertices $P_i \in V$ with $u_i > 0$ ($u_i < 0$).

**Definition 2.** A *weak positive* (*negative*) *sign graph* $S$ is a maximal, connected subgraph of $\Gamma$, on vertices $P_i \in V$ with $u_i \geqslant 0$ ($u_i \leqslant 0$) and with at least one $P_i \in V$ having $u_i > 0$ ($u_i < 0$).

**Theorem 1.** *Any eigenvector corresponding to* $\lambda_n$ *has at most* $n + r - 1$ strong *sign graphs.*

**Theorem 2.** *If* $\Gamma$ *is connected, then any eigenvector corresponding to* $\lambda_n$ *has at most* $n$ weak *sign graphs.*

## 2. A review of previous research

The simplest non-trivial graph $\Gamma$ is a *path*, i.e., a tree with no branches. For a path, the matrix $\mathbf{A}$ is tridiagonal with negative off-diagonal. Research on the sign properties of the eigenvectors of a tridiagonal $\mathbf{A}$ goes back to the work of Gantmacher and Krein [11]. They show that the eigenvalues of $\mathbf{A}$ are all simple, and that the $n$th eigenvector has *exactly* $n$ strong sign graphs and *exactly* $n$ weak sign graphs. For a path one can simply count the number of changes in sign in the sequence $u_1, u_2, \ldots, u_N$. This special case shows that neither Theorem 1 nor Theorem 2 can be strengthened without additional assumptions.

The *Laplacian* $\mathbf{L}$ of a graph $\Gamma$ has entries $\mathbf{L}_{ij} = -1$ iff $P_i \sim P_j$; the diagonal element $\mathbf{L}_{ii}$ equals the vertex degree of $P_i$ [3,15]. The associated quadratic form is

$$\mathscr{L} = \sum_{P_i \sim P_j} (u_i - u_j)^2 = \mathbf{u}^{\mathrm{T}}\mathbf{L}\mathbf{u}. \tag{5}$$

The Laplacian eigenvalues (eigenvectors) of $\Gamma$ are the eigenvalues (eigenvectors) of $\mathbf{L}$. Laplacian eigenvectors are of particular interest e.g. in the context of so-called fitness landscapes [13]. The first Laplacian eigenvalue is zero. Fiedler [7,8] noted that the second Laplacian eigenvalue is closely related to connectivity properties of the graph, and showed that if $\Gamma$ is connected, then the second Laplacian eigenvector has exactly two weak sign graphs. We can reinterpret the analysis in [9] to state that if $n \geqslant 2$, any eigenvector corresponding to $\lambda_n$ has at most $n - 1$ weak positive sign graphs and at most $n - 1$ weak negative sign graphs, so that $\mathbf{u}$ has at most $2(n-1)$ weak sign graphs in all.

Powers [16] extended Fiedler's analysis. He considered the *adjacency* matrix $\mathbf{A}$ of $\Gamma$, defined by $a_{ij} = 1$ if $P_i \sim P_j$, $a_{ij} = 0$ otherwise, including $a_{ii} = 0$, and labelled the eigenvalues in descending order, $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$. His results translate into equivalent ones for $-\mathbf{A}$, provided that the eigenvalues are reordered as in (1).

He sharpened Fiedler's upper bound $2(n-1)$ for the number of weak sign graphs. His bounds were specific to the adjacency matrix, and depended on the size of the eigenvalue.

Powers correctly stated and proved that an eigenvalue corresponding to $\lambda_n$ has at most $n+r-1$ strict sign graphs where $r$ is the multiplicity of $\lambda_n$, as in (3). This is Theorem 1, proved below. However he erroneously concluded that the bound could be reduced to $n+r-2$ if it is known that some edge of $\Gamma$ joins a vertex of a strictly positive sign graph to a vertex of a strictly negative sign graph, i.e., there exist $P_i$, $P_j$ such that $P_i \sim P_j$ and $u_i > 0, u_j < 0$.

Fig. 1 shows a counterexample which disproves this statement. The (negative) adjacency matrix has eigenvalues $-2, -1, -1, 0, 1, 1, 2$. One eigenvector corresponding to $\lambda_5 = 1$ is $\{0, 1, -1, -2, 2, 1, -1\}$, as shown. This eigenvector has six strong sign graphs while $n+r-2 = 5+2-2 = 5$; and yet there is a pair of $P_i \sim P_j$ such that $u_i > 0, u_j < 0$.

Variants of this error appear elsewhere. Thus Theorem 2.4 of Friedman [10] and Theorem 4.4 of Van der Holst [17] can be phrased as follows: *If an eigenvector* **u** *corresponding to* $\lambda_n$ *has* more *than n strong sign graphs*, *then there is* no *pair of adjacent vertices*, *i.e.*, $P_i \sim P_j$, *such that* $u_i > 0$, $u_j < 0$, *i.e.*, *there is no edge that joins any two strong sign graphs.* The example in Fig. 1 disproves this also: the eigenvector shown has $6 > n = 5$ strong sign graphs.

Duval and Reiner [6] tried to show that an eigenvector corresponding to $\lambda_n$ has no more than $n$ strong sign graphs. Friedman [10], however, had given the simple example of a star on $N$ vertices for which the second Laplacian eigenvalue has multiplicity $N-1$, and has an eigenvector with $N-1$ strong sign graphs but, as always, exactly two weak sign graphs. If therefore $N-1 > 2$, i.e., $N \geqslant 4$, then a second eigenvector has more than 2 strong sign graphs, falsifying Theorem 6 and Corollary 7 of [6]. When $N = 4$ the Laplacian eigenvalues are $\lambda_1 = 0, \lambda_2 = \lambda_3 = 1$, and $\lambda_4 = 3$. Fig. 2 shows a second Laplacian eigenvector which has 3 ($> 2$) strong sign graphs.

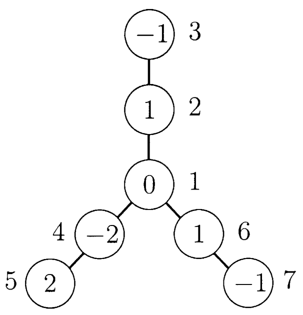


Fig. 1. The eigenvector corresponding to $\lambda_5$ has six strong sign graphs.

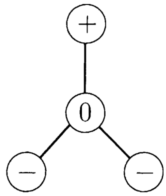


Fig. 2. This second eigenvector has three strong sign graphs.

Colin de Verdière [4] correctly stated that any eigenvector corresponding to $\lambda_n$ has at most $n$ weak sign graphs (Theorem 2), but his proof relies on unsubstantiated assertions. Friedman's [10] proof of Theorem 2 is incomplete also.

The present paper has a somewhat curious history. In March 2000, one of us, GMLG, submitted a manuscript to LAA containing proofs of Theorems 1 and 2 and pointing out the error in [6]. Soon after EBD, JL, and PFS independently submitted a joint manuscript to LAA which gave essentially the same proof of Theorem 1 and a substantially shorter proof of Theorem 2. The present contribution is an amalgamation of these two manuscripts.

## 3. Strong sign graphs

Let $\mathbf{A}$ be as in Section 1, let the eigenvalues be labelled as in (1) and (3), and suppose $\mathbf{u}$ is in the eigenspace of $\lambda_n$. We introduce the concept of *adjacency*.

**Definition 3.** Two different strong or weak sign graphs $S_1$, $S_2$ are said to be *adjacent* if there exist $P_1 \in S_1$, $P_2 \in S_2$ such that $P_1 \sim P_2$.

It follows from this definition that if two different sign graphs are adjacent, then they have opposite signs. For if they had the same sign then neither would be maximal. Suppose $\mathbf{u}$ has $m$ strong sign graphs $S_i$, $i = 1, \ldots, m$. Define $m$ vectors $\mathbf{w}_i$, $i = 1, \ldots, m$, such that

$$\mathbf{w}_i = \begin{cases} \mathbf{u} & \text{on } S_i, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

Explicitly, let $\mathbf{w}_i = \{w_{i,1}, w_{i,2}, \ldots, w_{i,N}\}$. Then $w_{i,j} = u_j$ if $P_j \in S_i$, $w_{i,j} = 0$ otherwise.

Thus

$$\mathbf{u} = \sum_{i=1}^{m} \mathbf{w}_i. \tag{7}$$

Now form

$$\mathbf{v} = \sum_{i=1}^{m} c_i \mathbf{w}_i. \tag{8}$$

Using straightforward algebra, we may verify Duval and Reiner's [6] useful.

**Lemma 1.**

$$\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda\mathbf{v}^{\mathrm{T}}\mathbf{v} = \sum_{i=1}^{m} c_i^2 \mathbf{w}_i^{\mathrm{T}}(\mathbf{A}\mathbf{u} - \lambda\mathbf{u}) - \frac{1}{2}\sum_{i,j=1}^{m}(c_i - c_j)^2 \mathbf{w}_i^{\mathrm{T}}\mathbf{A}\mathbf{w}_j.$$

This leads to:

**Theorem 1.** *Any eigenvector corresponding to* $\lambda_n$ *has at most* $n + r - 1$ *strong sign graphs.*

**Proof.** Since none of the $\mathbf{w}_i$ is identically zero and they are disjoint, their linear span has dimension $m$. It follows that there exist non-zero real coefficients $c_i$, $i = 1, \ldots, m$, such that $\mathbf{v}$ is non-zero and is orthogonal to the first $(m - 1)$ eigenvectors $\mathbf{u}^{(j)}$, $j = 1, \ldots, m - 1$ of $\mathbf{A}$, i.e.,

$$\mathbf{v}^{\mathrm{T}}\mathbf{u}^{(j)} = 0, \quad j = 1, 2, \ldots, m - 1. \tag{9}$$

Without loss of generality we can take $\mathbf{v}^{\mathrm{T}}\mathbf{v} = 1$. Therefore, by the minimax theorem [5, Chapter 1, Section 4] we have

$$\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} \geqslant \lambda_m. \tag{10}$$

Now use Lemma 1 with $\lambda = \lambda_n$, $\mathbf{u} \equiv \mathbf{u}^{(n)}$. We find

$$\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda_n = -\frac{1}{2}\sum_{i,j=1}^{m}(c_i - c_j)^2 \mathbf{w}_i^{\mathrm{T}}\mathbf{A}\mathbf{w}_j. \tag{11}$$

A term $\mathbf{w}_i^{\mathrm{T}}\mathbf{A}\mathbf{w}_j$ is non-zero only if $\mathbf{w}_i$, $\mathbf{w}_j$ correspond to adjacent sign graphs; adjacent sign graphs have opposite signs; adjacent sign graphs are disjoint. This means that any non-zero product $\mathbf{w}_i^{\mathrm{T}}\mathbf{A}\mathbf{w}_j$ involves only negative, off-diagonal terms in $\mathbf{A}$; therefore

$$\mathbf{w}_i^{\mathrm{T}}\mathbf{A}\mathbf{w}_j = (+)(-)(-) = +. \tag{12}$$

Therefore, Eq. (11) gives

$$\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda_n \leqslant 0. \tag{13}$$

This combined with (10) states that $\lambda_m \leqslant \lambda_n$. Since $\lambda_n < \lambda_{n+r}$, we have $\lambda_m < \lambda_{n+r}$, and have $m < n + r$, i.e., $m \leqslant n + r - 1$. $\square$

**Discussion.** The logical negative form of Theorem 2.4 of [10] and Theorem 4.4 of [4], which we have already falsified by counterexample, is as follows: *If there is a pair of vertices* $P_i$, $P_j$ *such that* $u_i > 0$, $u_j < 0$ *and* $P_i \sim P_j$, *then* $\mathbf{u}$ *has no more than n strong sign graphs*, *i.e.*, $m \leqslant n$. We can deduce $m \leqslant n$ from (10) and (11) if we can show that the R.H.S. of (11) is strictly negative. For then (13) would be replaced by

$$\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda_n < 0, \tag{14}$$

so that $\lambda_m < \lambda_n$ and $m < n$. But to deduce (14) it is not enough that there is one term $\mathbf{w}_i^{\mathrm{T}}\mathbf{A}\mathbf{w}_j$ which is strictly positive, as suggested; we must also have $c_i \neq c_j$. That is why the purported theorem is false; we can deduce only (13).

## 4. Weak sign graphs

We first derive some preliminary results about zero vertices of $\mathbf{u}$.

(i) *A zero vertex of* $\mathbf{u}$ *is either adjacent only to other zero vertices*, *i.e.*, *it is an* interior *vertex of a zero graph*; *or is adjacent to vertices of* both *strict signs*: *it is a* boundary *vertex.* The vector $\mathbf{u}$ satisfies $\mathbf{A}\mathbf{u} = \lambda\mathbf{u}$, i.e.,

$$\sum_{j=1}^{N} a_{ij}u_j = \lambda u_i. \tag{15}$$

If $u_i = 0$, then $\sum_{j=1}^{N'} a_{ij}u_j = 0$, where the sum is taken over all $j$ with $j \neq i$. Since $a_{ij} = 0$ unless $P_i \sim P_j$, the sum may be taken over those $j$ for which $P_i \sim P_j$; for those $j$, $a_{ij} < 0$. Since all the coefficients in the restricted sum are strictly negative, either all $u_j$ for which $P_i \sim P_j$ are zero, or there is positive *and* a negative among them.

(ii) *Each zero vertex belongs to exactly one weak positive sign graph and exactly one weak negative sign graph.*
This follows directly from the definition of weak sign graphs.

(iii) *If two different weak sign graphs* $S_1, S_2$ *have a non-zero intersection*, *i.e.*, *they overlap*, *they must have opposite signs*. For otherwise neither would be maximal. If $S_1 \cap S_2 \neq 0$ and $P_i \in S_1 \cap S_2$, then $u_i = 0$.

We now prove:

**Lemma 2.** *Suppose* $S_1, S_2$ *are adjacent weak sign graphs. There is a pair of vertices* $P_1, P_2$ *such that* $P_1 \in S_1$, *and* $P_2 \in S_2 \setminus S_1$ *and* $P_1 \sim P_2$.

**Proof.** Without loss of generality, assume that $S_1$ is weak positive and $S_2$ is weak negative. If $S_1, S_2$ are disjoint, then by the definition of adjacency, there exist $P_1 \in S_1$, $P_2 \in S_2$ such that $P_1 \sim P_2$; because $S_1, S_2$ are disjoint, $P_2 \in S_2 \setminus S_1$. Otherwise $S_1$, $S_2$ have a non-empty intersection $S_1 \cap S_2$. $S_1 \cap S_2$ is a strict subgraph of $\Gamma$ so that not all vertices $P_1 \in S_1 \cap S_2$ can be interior vertices in the sense of (i). Any boundary vertex $P_1$ will have the required property: for such a $P_1$, there will be a vertex $P_2$ such that $P_2 \sim P_1$, and $u_2 < 0$, i.e., $P_2 \in S_2 \setminus S_1$. $\square$

Now suppose that $\mathbf{u}$ has $m \geqslant n$ weak sign graphs $S_i$. We define $\mathbf{w}_i$, $i = 1, \ldots, m$, by (6), and we choose $c_i$, $i = 1, \ldots, m$, not all zero, to make $\mathbf{v}$ given by (8) orthogonal to the first $m - 1$ eigenvectors of $\mathbf{A}$. We prove a continuation result for the coefficients $c_i$, which is a discrete analogue of the unique continuation principle for eigenfunctions.

**Lemma 3.** *Suppose $m \geqslant n$, and two of the weak sign graphs $S_1$ and $S_2$ of* $\mathbf{u}$ *are adjacent. Without loss of generality we may suppose that $S_1$ is weak positive and $S_2$ weak negative. Then $c_2 = c_1$.*

**Proof.** The minimax theorem implies $\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda_m \geqslant 0$, and Lemma 1 implies $\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda_n \leqslant 0$, and

$$\sum_{i,j=1}^{m} (c_i - c_j)^2 \mathbf{w}_i^{\mathrm{T}} \mathbf{A}\mathbf{w}_j = 0. \tag{16}$$

Now use Lemma 2. If $S_1$, $S_2$ are disjoint, then there is a pair $P_1$, $P_2$ such that $P_1 \sim P_2$, $u_1 > 0$ and $u_2 < 0$, $a_{12} < 0$. Thus $\mathbf{w}_1^{\mathrm{T}}\mathbf{A}\mathbf{w}_2 \geqslant u_1 a_{12} u_2 > 0$, and (16) implies $c_1 = c_2$.

Otherwise $S_1$, $S_2$ overlap. Since $\mathbf{v}^{\mathrm{T}}\mathbf{A}\mathbf{v} - \lambda_n = 0$, $\mathbf{v}$, like $\mathbf{u}$, is in the eigenspace of $\lambda_n$, and therefore so is

$$\mathbf{z} = c_1\mathbf{u} - \mathbf{v} = \sum_{j=1}^{m} (c_1 - c_j)\mathbf{w}_j. \tag{17}$$

By definition $w_{j,i} = 0$ unless $P_i \in S_j$. Choose $P_1$, $P_2$ as in Lemma 2; $P_1 \in S_1 \cap S_2$ implies $w_{j,1} = 0$ for all $j$, so that $z_1 = 0$.

Since $\mathbf{z}$ is in the eigenspace of $\lambda_n$, we have

$$\lambda_n \mathbf{z} = \mathbf{A}\mathbf{z} = \sum_{j=1}^{m} (c_1 - c_j)\mathbf{A}\mathbf{w}_j \tag{18}$$

so that

$$\lambda_n z_1 = 0 = \sum_{j=2}^{m} (c_1 - c_j)(\mathbf{A}\mathbf{w}_j)_1 = \sum_{j=2}^{m} (c_1 - c_j) \sum_{i=2}^{N} a_{1i} w_{j,i}, \tag{19}$$

where we have used $w_{j,1} = 0$. The term $a_{1i}$, for $i \geqslant 2$, is zero unless $P_i \sim P_1$. Since $u_1 = 0$, all such $P_i$ are in $S_1$ or $S_2$. The sum in (19) is therefore over $j = 2$ only:

$$0 = (c_1 - c_2) \sum_{i=2}^{N} a_{1i} w_{2,i}. \tag{20}$$

Since $S_2$ is weak negative, $a_{1i} w_{2,i} \geqslant 0$ for $i = 1, \ldots, N$: each term in the sum is non-negative. Since $P_1 \sim P_2$ we have $a_{12} < 0$; since $P_2 \in S_2 \setminus S_1$, $w_{2,2} = u_2 < 0$, so that

$$\sum_{i=2}^{N} a_{1i} w_{2,i} \geqslant a_{12} u_2 > 0 \tag{21}$$

and hence $c_1 = c_2$. $\square$

This lemma states that if $m \geqslant n$, then two adjacent sign graphs appearing in $\mathbf{v}$ must appear with the same relative weights $c_1 = c_2$ as they did in $\mathbf{u}$.

We are now in a position to establish:

**Theorem 2.** *If $\Gamma$ is connected, any eigenvector corresponding to $\lambda_n$ has at most $n$ weak sign graphs.*

**Proof.** Suppose, if possible, that $\mathbf{u}$ has $m$ weak sign graphs $S_i$, $i = 1, \ldots, m$, and $m > n$. At least one of the coefficients $c_i$, say $c_1$, is nonzero. Since $n \geqslant 1$, we have $m \geqslant 2$. Since $\Gamma$ is connected, $S_1$ must be adjacent to at least one other sign graph, which we label $S_2$. Lemma 3 states that $c_2 = c_1$. If $m \geqslant 3$, one of $S_1$, $S_2$ must be adjacent to one of the remaining sign graphs $S_i$, $i = 3, \ldots, m$, say $S_3$, otherwise $\Gamma$ would not be connected. Therefore $c_3 = c_2 = c_1$ by Lemma 3. In $m - 1$ steps we conclude that $c_m = c_{m-1} = \cdots = c_1$. Hence $\mathbf{v} = c_1\mathbf{u}$. But $\mathbf{v}$ was constructed so that it was orthogonal to $\mathbf{u}^{(i)}$ for $i = 1, \ldots, m - 1$; if $m > n$, $\mathbf{v}$ is orthogonal to $\mathbf{u}^{(n)} = \mathbf{u}$ contradicting $\mathbf{v} = c_1\mathbf{u}$. Therefore $m \leqslant n$. $\square$

## 5. Concluding remarks

The proof of Theorem 1, on strong sign graphs, hinges on two fundamental results: Courant's minimax theorem, and Duval and Reiner's Lemma 1. Theorem 2, on weak sign graphs, used these two, the preliminary results (i)–(iii), and Lemmata 2 and 3. In finite element applications, one encounters not the standard eigenvalue problem (4), but the generalized problem

$$(\mathbf{K} - \lambda\mathbf{M})\mathbf{u} = \mathbf{0}, \tag{22}$$

where $\mathbf{K}$ is positive semi-definite and $\mathbf{M}$ is positive definite. Typically, the off-diagonal elements of $\mathbf{K}$ are non-positive, those of $\mathbf{M}$ are non-negative, and when $i \neq j$, $k_{ij} < 0, m_{ij} > 0$ iff $P_i \sim P_j$ [12].

Since $\mathbf{M}$ is positive definite the minimax theorem holds for the ratio $\mathbf{v}^{\mathrm{T}}\mathbf{K}\mathbf{v}/\mathbf{v}^{\mathrm{T}}\mathbf{M}\mathbf{v}$. Duval and Reiner's Lemma 1 may also be generalized to read:

**Lemma 1′.**

$$\mathbf{v}^{\mathrm{T}}(\mathbf{K} - \lambda\mathbf{M})\mathbf{v} = \sum_{i=1}^{m} c_i^2\mathbf{w}_i^{\mathrm{T}}(\mathbf{K} - \lambda\mathbf{M})\mathbf{u} - \frac{1}{2}\sum_{i,j=1}^{m}(c_i - c_j)^2\mathbf{w}_i^{\mathrm{T}}(\mathbf{K} - \lambda\mathbf{M})\mathbf{w}_j.$$

*Since $\mathbf{K}$ is positive semi-definite and $\mathbf{M}$ positive definite, the eigenvalues are non-negative. This means that when $\mathbf{w}_i$, $\mathbf{w}_j$ correspond to adjacent sign graphs*

$$\mathbf{w}_i^{\mathrm{T}}(\mathbf{K} - \lambda\mathbf{M})\mathbf{w}_j = (+)\{(-) - (+)(+)\}(-) = (+). \tag{23}$$

All the arguments used to establish Theorems 1 and 2 proceed as before, with $\mathbf{A}$ replaced by $\mathbf{K} - \lambda\mathbf{M}$.

## Acknowledgments

This work was supported in part by the Austrian *Fonds zur Förderung der Wissenschaflichen Forschung*, Project No. P14094-MAT. The joint work of EBD, JL, and PFS was started in 1995 during EBD's visit at the *Erwin Schrödinger Institute for Mathematical Physics*.

## References

[1] I. Chavel, Eigenvalues in Riemannian Geometry, Academic Press, Orlando FL, 1984.
[2] S.Y. Cheng, Eigenfunctions and nodal sets, Comment. Math. Helvetica 51 (1976) 43–55.
[3] F.R.K. Chung, Spectral Graph Theory, CBMS, vol. 92, AMS, Providence RI, 1997.
[4] Y. Colin de Verdière, Multiplicités des valeurs propres laplaciens discrete at laplaciens continus, Rendi. Mat. 13 (1993) 433–460.
[5] R. Courant, D. Hilbert, Methods of Mathematical Physics, vol. 1, Interscience, New York, 1953.
[6] A.M. Duval, V. Reiner, Perron–Frobenius type results and discrete versions of nodal domain theorems, Linear Algebra Appl. 294 (1999) 259–268.
[7] M. Fiedler, Algebraic connectivity of graphs, Czechoslovak Math. J. 23 (1973) 298–305.
[8] M. Fiedler, Eigenvectors of acyclic matrices, Czechoslovak Math. J. 23 (1975) 607–618.
[9] M. Fiedler, A property of eigenvectors of non-negative symmetric matrices and its application to graph theory, Czechoslovak Math. J. 25 (1975) 619–633.
[10] J. Friedman, Some geometric aspects of graphs and their eigenfunctions, Duke Math. J. 69 (3) (1993) 487–525.
[11] F.R. Gantmacher, M.G. Krein, Oscillation Matrices and Kernels and Small Vibrations of Mechanical Systems. State Publishing House of Technical–Theoretical Literature, Moscow, Leningard, 1950. (English Translation by US Atomic Energy Commission, Washington, DC, 1961).
[12] G.M.L. Gladwell, H. Zhu, Courant's nodal-line theorem and its dicrete counterparts, Quart. J. Mech. Appl. Math. (2001) to appear.
[13] W. Hordijk, P.F. Stadler, Amplitude spectra of fitness landscapes, Adv. Complex Syst. 1 (1998) 39–66.
[14] F. John, Partial Differential Equations, Applied Mathematical Science, vol. 1, Springer, New York, 1981.
[15] B. Mohar, Some applications of Laplace eigenvalues of graphs. in: G. Hahn, G. Sabidussi (Eds.), Graph Symmetry: Algebraic Methods and Applications, NATO ASI Series C, vol. 497, Kluwer, Dordrecht, 1997, pp. 227–275.
[16] D.L. Powers, Graph partitioning by eigenvectors, Linear Algebra Appl. 101 (1988) 121–133.
[17] H. van der Holst, Topological and Spectral Graph Characterizations, Ph.D. Thesis, Universiteit van Amsterdam, 1996.