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Discrete Nodal Domain Theorems

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Abstract

We give a detailed proof for two discrete analogues of Courant's Nodal Domain Theorem.

1 Introduction

Courant's famous Nodal Domain Theorem for elliptic operators on Riemannian manifolds (see e.g. [1]) states

If $f_k$ is an eigenfunction belonging to the $k$-th eigenvalue (written in increasing order and counting multiplicities) of an elliptic operator, then $f_k$ has at most $k$ nodal domains.

When considering the analogous problem for graphs, M. Fiedler [4, 5] noticed that the second Laplacian eigenvalue is closely related to connectivity properties of the graph, and showed that $f_2$ always has exactly two nodal domains. It

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is interesting to note that his approach can be extended to show that \( f_k \) has no more than \( 2(k - 1) \) nodal domains, \( k \geq 2 \) [7]. Various discrete versions of the Nodal Domain theorem have been discussed in the literature [2, 6, 8, 3], however sometimes with ambiguous statements and incomplete or flawed proofs. The purpose of this contribution is not to establish new theorems but to summarize the published results in a single theorem and to present a detailed, elementary proof.

2 Preliminaries

Consider a simple, undirected, loop-free graph \( \Gamma \) with finite vertex set \( V \) and edge set \( E \). We write \( N := |V| \) and \( x \sim y \) if \( \{x, y\} \in E \). We introduce a weight function \( b \) on the edges of \( \Gamma \), conveniently defined as \( b : V \times V \rightarrow \mathbb{R} \) such that \( b(x, y) = b(y, x) > 0 \) if \( \{x, y\} \in E \) and \( b(x, y) = 0 \) otherwise, and a potential \( v : V \rightarrow \mathbb{R} \). We will consider the Schrödinger operator

\[
\mathcal{H} f(x) := \sum_{y \sim x} b(x, y) [f(x) - f(y)] + v(x)f(x).
\]

We shall assume that \( \Gamma \) is connected throughout this contribution.

The Perron-Frobenius theorem implies that the first eigenvalue \( \lambda_1 \) of \( \mathcal{H} \) is non-degenerate and the corresponding eigenfunction \( f_1 \) is positive (or negative) everywhere. Let

\[
\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_{k-1} \leq \lambda_k \leq \lambda_{k+1} \leq \cdots \leq \lambda_N
\]

be the list of eigenvalues of \( \mathcal{H} \) arranged in non-decreasing order and repeated according to multiplicity. Given \( k \) let \( \overline{k} \) and \( \underline{k} \) be the largest and smallest number \( h \) for which \( \lambda_h = \lambda_k \), respectively. Let \( f_k \) be any eigenfunction associated with the eigenvalue \( \lambda_k \). Without loss of generality we may assume that \( \{f_i\} \) is a complete orthonormal set of eigenfunctions satisfying \( \mathcal{H} f_i = \lambda_i f_i \). Since \( \mathcal{H} \) is a real operator, we can take all eigenfunctions to be real.

In the continuous setting one defines the nodal set of a continuous function \( f \) as the preimage \( f^{-1}(0) \). The nodal domains are the connected components of the complement of \( f^{-1}(0) \). In the discrete case this definition does not make sense since a function \( f \) can change sign without having zeroes. Instead we use the following

**Definition 1** \( D \) is a weak nodal domain of a function \( f : V \rightarrow \mathbb{R} \) if it is a maximal subset of \( V \) subject to the two conditions

(i) \( D \) is connected (as an induced subgraph of \( \Gamma \));
(ii) if \( x, y \in D \) then \( f(x)f(y) \geq 0 \).

\( D \) is a strong nodal domain if (\( \text{ii} \)) is replaced by

(\( \text{ii} \')) if \( x, y \in D \) then \( f(x)f(y) > 0 \).

In this contribution we are only interested in nodal domains of eigenfunctions \( f_k \) of the Schrödinger operator \( \mathcal{H} \). In the following, the term “nodal domain” will always refer to this case.

The following properties of weak nodal domains are elementary:

(a) Every point \( x \in V \) lies in some weak nodal domain \( D \).
(b) If \( D \) is a weak nodal domain then it contains at least one point \( x \in V \) with \( f_k(x) \neq 0 \) and \( f_k \) has the same sign on all non-zero points in \( D \). Thus each weak nodal domain can be called either “positive” or “negative”.
(c) If two weak nodal domains \( D \) and \( D' \) have non-empty intersection then \( f_k|_{D \cap D'} = 0 \) and \( D, D' \) have opposite sign.

Note that (a) need not hold for strong nodal domains, and (c) is replaced by: The intersection of two distinct strong nodal domains is empty.

3 Weak and Strong Nodal Domain Theorem

The main result of this contribution is

**Theorem 2 (Nodal Domain Theorem)** The eigenfunction \( f_k \) has at most \( k \) weak nodal domains and at most \( k' \) strong nodal domains.

**Proof.** The proof of the Nodal Domain Theorem is based upon deriving a contradiction from

- **Hypothesis W:** \( f_k \) has \( k' \) > \( k \) weak nodal domains, and
- **Hypothesis S:** \( f_k \) has \( k' \) > \( k' \) strong nodal domains,

respectively.

We call the domains \( D_1, D_2, \ldots, D_{k'} \) and define

\[
g_i(x) := \begin{cases} f_k(x) & \text{if } x \in D_i \\ 0 & \text{otherwise} \end{cases}
\]  

(3)

for \( 1 \leq i \leq k' \). None of the functions \( g_i \) is identically zero. Since they have disjoint supports their linear span has dimension \( k' \). It follows that there exist
constants $\alpha_i \in \mathbb{R}$ such that

$$g := \sum_{i=1}^{k'} \alpha_i g_i$$

is non-zero and satisfies $\langle g, f_j \rangle = 0$ for $i \leq j < k'$. Without loss of generality we can assume $\langle g, g \rangle = 1$, where $\langle \cdot, \cdot \rangle$ denotes the standard scalar product on $\mathbb{R}^N$. Therefore we have

$$\langle \mathcal{H} g, g \rangle \geq \lambda_{k'}.$$  

Under hypothesis W we know that

$$\lambda_{k'} \geq \lambda_k.$$  

Under hypothesis S we have

$$\lambda_{k'} > \lambda_k$$

since the last eigenvalue that is equal to $\lambda_k$ has index $\overline{k}$.

It will be convenient to introduce $S := \{ x \in V \mid f_k(x) \neq 0 \}$ and to define $\alpha : V \to \mathbb{R}$ by

$$\alpha(x) := \begin{cases} \alpha_i & \text{if } x \in S \cap D_i \text{ for some } i \\ 0 & \text{otherwise} \end{cases}$$

so that $g(x) = \alpha(x)f_k(x)$ for all $x \in V$.

**Lemma 1.** Assuming hypotheses W or S, we have $\langle \mathcal{H} g, g \rangle \leq \lambda_k$.

**Proof.** We have

$$g(x)\mathcal{H} g(x) = g(x) \sum_{y \sim x} b(x, y) \left[ g(x) - g(y) \right] + g^2(x)v(x)$$

$$= \alpha(x)f_k(x) \sum_{y \sim x} b(x, y) \left[ \alpha(x)f_k(x) - \alpha(y)f_k(y) \right] + \alpha^2(x)f_k^2(x)v(x)$$

$$= \alpha^2(x)f_k(x) \sum_{y \sim x} b(x, y) \left[ f_k(x) - f_k(y) \right] + \alpha^2(x)f_k^2(x)v(x)$$

$$+ \alpha(x)f_k(x) \sum_{y \sim x} b(x, y) \left[ \alpha(x) - \alpha(y) \right] f_k(y)$$

$$= \alpha^2(x)f_k(x)\mathcal{H} f_k(x) + \text{Rem}(x) = \alpha^2(x)\lambda_k f_k^2(x) + \text{Rem}(x)$$

$$= \lambda_k g^2(x) + \text{Rem}(x)$$

Summing over the vertex set yields

$$\langle \mathcal{H} g, g \rangle = \lambda_k + \text{Rem}$$

(10)
where
\[ \text{Rem} = \sum_{x \in V} \sum_{y \sim x} b(x, y) \alpha(x) [\alpha(x) - \alpha(y)] f_k(x) f_k(y) \]
\[ = -\frac{1}{2} \sum_{x, y \in V} b(x, y) [\alpha(x) - \alpha(y)]^2 f_k(x) f_k(y) \] (11)

by symmetrizing. A term of the remainder Rem vanishes if \( f_k(x) = 0 \) or \( f_k(y) = 0 \). If \( f_k(x)f_k(y) > 0 \) and \( x \sim y \), i.e. \( b(x, y) > 0 \), then \( x \) and \( y \) lie in the same nodal domain and thus \( \alpha(x) = \alpha(y) \), and the corresponding contribution to Rem vanishes as well. The only remaining terms are those for which \( f_k(x)f_k(y) < 0 \) and \( x \sim y \). So we see that \( \text{Rem} \leq 0 \).
Thus we have \( \langle \mathcal{H}g, g \rangle \leq \lambda_k \langle g, g \rangle = \lambda_k \).

Under hypothesis S, eqns. (5), (7), and Lemma 1 lead to the desired contradiction, proving the second part of the theorem.

Under hypothesis W, eqns. (5), (6), and Lemma 1 imply \( \langle g, \mathcal{H}g \rangle = \lambda_k \). Since \( g \) is by construction orthogonal to all eigenvectors \( f_j, j < k < k' \), a simple variational argument implies
\[ \mathcal{H}g = \lambda_k g. \] (12)

For the second step of the proof of the Weak Nodal Domain Theorem we exploit the fact that the remainder \( \text{Rem} = 0 \) as a consequence of eqn. (12). We proceed with a unique continuation result for the function \( \alpha \).

**Lemma 2.** If hypothesis W holds, \( \alpha_i \neq 0, x \in D_i, y \in D_j \setminus D_i, \) and \( \{x, y\} \in E \) then \( \alpha_j = \alpha_i \).

**Proof.** If \( x \in D_i, y \in D_j \setminus D_i, x \sim y, \) and \( f_k(x) \neq 0 \) then \( f_k(y) \neq 0 \) (otherwise \( y \in D_i \cap D_j \)), and hence \( f_k(x)f_k(y) < 0 \). From \( \text{Rem} = 0, f_k(x)f_k(y) < 0, \) and \( x \sim y \) we conclude that \( \alpha(x) = \alpha(y) \) and hence \( \alpha_i = \alpha(x) = \alpha(y) = \alpha_j. \)
Now assume that \( f_k(x) = 0 \). Define \( h := f_k - (1/\alpha_i)g \). Then
\[ \mathcal{H}h = \lambda_k h \quad \text{and} \quad h|_{D_i} = 0. \] (13)

We have
\[ 0 = \lambda_k h(x) = \mathcal{H}h(x) = \sum_{y \sim x} b(x, y) [h(x) - h(y)] + v(x)h(x) \]
\[ = -\sum_{y \in B} b(x, y)h(y) \] (14)

where \( B := \{y \in V \mid y \sim x \text{ and } y \notin D_i\} \). Note that \( B \neq \emptyset \) by the assumptions of the lemma. Suppose for definiteness that \( D_i \) is a positive nodal domain. Then \( y \in B \) satisfies \( f_k(y) < 0 \) since otherwise one would have to adjoin \( y \) to
Thus $B \cup \{x\}$ is a connected set on which $f_k \leq 0$. Therefore it is contained in the single (negative) nodal domain $D_j$. Therefore

$$0 = -\sum_{y \in B} b(x, y)h(y) = -\left(1 - \frac{\alpha_j}{\alpha_i}\right) \sum_{y \in B} b(x, y)f_k(y). \quad (15)$$

The terms in the sum are all negative, thus $\alpha_i = \alpha_j$. The same argument of course works when $D_i$ is a negative nodal domain. $\triangle$

We say that $D_i$ is adjacent to $D_j$ if there are $x \in D_i$ and $y \in D_j \setminus D_i$, $x \sim y$. Note that adjacent nodal domains must have opposite signs. Now consider a collection \{\(D_1, \ldots, D_l\)\} of nodal domains such that $\bigcup_i D_i \neq \emptyset$. Then there exists a nodal domain $D_j \neq D_i$, $i = 1, \ldots, l$, that is adjacent to some $D_i$, $i = 1, \ldots, l$, otherwise $\Gamma$ would not be connected.

Now we are in the position to prove the first part of the theorem. We assume hypothesis W and thus the conclusions of lemma 1 and lemma 2. Since $g \neq 0$ there exists an index $i$ for which $\alpha_i \neq 0$. If $D_j$ is a nodal domain adjacent to $D_i$ then lemma 2 implies $\alpha_j = \alpha_i$. Since the graph $\Gamma$ is connected by assumption, we conclude in a finite number of steps that $\alpha_j = \alpha_i$ for all $j$. Hence $g = \alpha_i f_k$. This, however, contradicts the fact that $\langle g, f_k \rangle = 0$. $\square$

4 Two Counter-Examples

Neither the Weak nor the Strong Nodal Domain theorem can be strengthened without additional assumptions. If $\Gamma$ is a path with $N$ vertices, then $f_k$ has always $k$ weak nodal domains. An example where $f_k$ has more than $k$ strong nodal domains is e.g. given by Friedman [6]: a star on $n$ nodes, i.e., a graph which is a tree with exactly one interior vertex, has a second eigenfunction with $n - 1$ strong nodal domains. For example, the star with 5 nodes has $\lambda_2 = \lambda_3 = \lambda_4 = 1$ and an eigenvector $f_2 = (0, 1, 1, -1, -1)$, where the first coordinate refers to the interior vertex. Since $f_2$ vanishes at the interior vertex each of the $n - 1$ leaves is a strong nodal domain. These eigenvectors of the stars may also serve as a counterexample to Theorem 6 and Corollary 7 of [3].

Theorems 2.4 of [6] and 4.4 of [8] can be rephrased as follows: If $f_k$ has more than $k$ strong nodal domains, then there is no pair of vertices such that $f_k(x) > 0$, $f_k(y) < 0$ and $x \sim y$, i.e., there is no edge that joins any two strong nodal domains. This statement is incorrect, as the following example shows.
This tree has eigenvalues $\lambda_5 = \lambda_6 = (3 + \sqrt{5})/2$ and a corresponding eigenvector

$$f_5 = (2, -1 - \sqrt{5}, 0, (1 + \sqrt{5})/2, (1 + \sqrt{5})/2, -1, -1)$$

from top to bottom. There are 5 weak and 6 strong nodal domains. Nevertheless, there are edges connecting strictly positive with strictly negative vertices.

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