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
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 $b : V \times V \to \mathbb{R}$ such that $b(x, y) = b(y, x) > 0$ if $\{x, y\} \in E$ and $b(x, y) = 0$ otherwise, and a potential $v : V \to \mathbb{R}$. We will consider the Schrödinger operator

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

(1)

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

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

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

(2)

be the list of eigenvalues of $H$ 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 $Hf_i = \lambda_if_i$. Since $H$ 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 $f : V \to \mathbb{R}$ 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 (ii) is replaced by

\((ii')\) 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 \(D, D'\) 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

$$g := \sum_{i=1}^{k'} \alpha_i g_i \quad (4)$$

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

$$\langle H g, g \rangle \geq \lambda_{k'} \quad (5)$$

Under hypothesis W we know that

$$\lambda_{k'} \geq \lambda_k \quad (6)$$

Under hypothesis S we have

$$\lambda_{k'} > \lambda_k \quad (7)$$

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

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

$$\alpha(x) := \begin{cases}
\alpha_i & \text{if } x \in S \cap D_i \text{ for some } i \\
0 & \text{otherwise}
\end{cases} \quad (8)$$

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

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

**Proof.** We have

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

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

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

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

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

$$= \lambda_kg^2(x) + \text{Rem}(x) \quad (9)$$

Summing over the vertex set yields

$$\langle H g, g \rangle = \lambda_k + \text{Rem} \quad (10)$$
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 \(\text{Rem}\) 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 \(\text{Rem}\) 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
\[
\langle Hg, g \rangle \leq \lambda_k \langle g, g \rangle = \lambda_k.
\]

\(\triangle\)

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 \(\langle g, Hg \rangle = \lambda_k\). Since \(g\) is by construction orthogonal to all eigenvectors \(f_j, j \leq k \neq k'\), a simple variational argument implies
\[
Hg = \lambda_k g.
\]

(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 equ.(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
\[
Hh = \lambda_k h \quad \text{and} \quad h|_{D_i} = 0.
\]

(13)

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

(14)

where \(B := \{y \in V | y \sim x \text{ and } y \notin D_i\}\). 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

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

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 \( \bigcup_i D_i \neq V \). 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 \( n - 1 \) leafs 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 [3] 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

$$f_5 = (2, -1 - \sqrt{5}, 0, (1 + \sqrt{5})/2, (1 + \sqrt{5})/2, -1, -1)$$  \hspace{1cm} (16)$$

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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