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Paper

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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 Γ 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 Γ, 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*

$$\mathcal{H}f(x) := \sum_{y \sim x} b(x, y)\,[f(x) - f(y)] + v(x)f(x)\,. \tag{1}$$

We shall assume that Γ is connected throughout this contribution.

The Perron-Frobenius theorem implies that the first eigenvalue λ_1 of $\mathcal{H}$ is non-degenerate and the corresponding eigenfunction f_1 is positive (or negative) everywhere. Let

$$\lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_{k-1} \leq \lambda_k \leq \lambda_{k+1} \leq \cdots \leq \lambda_N \tag{2}$$

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 λ_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 $f : V \to \mathbb{R}$ if it is a maximal subset of V subject to the two conditions*

(i) D is connected (as an induced subgraph of Γ);

(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 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 $\underline{k}$ weak nodal domains and at most $\overline{k}$ strong nodal domains.*

Proof. The proof of the Nodal Domain Theorem is based upon deriving a contradiction from
Hypothesis W: *f_k has $k' > \underline{k}$ weak nodal domains*, and
Hypothesis S: *f_k has $k' > \overline{k}$ strong nodal domains*,
respectively.

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

$$g_i(x) := \begin{cases} f_k(x) & \text{if } x \in D_i \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

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

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

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 $\langle \, . \, , \, . \, \rangle$ denotes the standard scalar product on $\mathbb{R}^N$. Therefore we have

$$\langle \mathcal{H} g, g \rangle \geq \lambda_{k'} \, . \tag{5}$$

Under hypothesis W we know that

$$\lambda_{k'} \geq \lambda_k. \tag{6}$$

Under hypothesis S we have

$$\lambda_{k'} > \lambda_k \tag{7}$$

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

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

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

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

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

Proof. We have

$$\begin{aligned} g(x)\mathcal{H}g(x) &= g(x) \sum_{y \sim x} b(x,y)\,[g(x) - g(y)] + g^2(x) v(x) \\ &= \alpha(x) f_k(x) \sum_{y \sim x} b(x,y)\,[\alpha(x) f_k(x) - \alpha(y) f_k(y)] + \alpha^2(x) f_k^2(x) v(x) \\ &= \alpha^2(x) f_k(x) \sum_{y \sim x} b(x,y)\,[f_k(x) - f_k(y)] + \alpha^2(x) f_k^2(x) v(x) \\ &\qquad + \alpha(x) f_k(x) \sum_{y \sim x} b(x,y)\,[\alpha(x) - \alpha(y)]\, f_k(y) \\ &= \alpha^2(x) f_k(x) \mathcal{H} f_k(x) + \mathrm{Rem}(x) = \alpha^2(x) \lambda_k f_k^2(x) + \mathrm{Rem}(x) \\ &= \lambda_k g^2(x) + \mathrm{Rem}(x) \end{aligned} \tag{9}$$

Summing over the vertex set yields

$$\langle \mathcal{H} g, g \rangle = \lambda_k + \mathrm{Rem} \tag{10}$$

where

$$\begin{aligned}\mathrm{Rem} &= \sum_{x\in V}\sum_{y\sim x} b(x,y)\alpha(x)\left[\alpha(x)-\alpha(y)\right] f_k(x)f_k(y) \\ &= \frac{1}{2}\sum_{x,y\in V} b(x,y)\left[\alpha(x)-\alpha(y)\right]^2 f_k(x)f_k(y)\end{aligned} \tag{11}$$

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 Rem ≤ 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, $j < \underline{k} < k'$, a simple variational argument implies

$$\mathcal{H}g = \lambda_k g\,. \tag{12}$$

For the second step of the proof of the Weak Nodal Domain Theorem we exploit the fact that the remainder Rem $= 0$ as a consequence of equ.(12). We proceed with a unique continuation result for the function α.

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 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

$$\mathcal{H}h = \lambda_k h \qquad \text{and} \qquad h|_{D_i} = 0\,. \tag{13}$$

We have

$$\begin{aligned}0 = \lambda_k h(x) = \mathcal{H}h(x) &= \sum_{y\sim x} b(x,y)\left[h(x)-h(y)\right] + v(x)h(x) \\ &= -\sum_{y\in B} b(x,y)h(y)\end{aligned} \tag{14}$$

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

D_i. 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

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

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. △

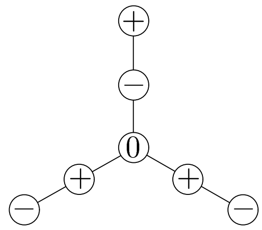
We say that D_i *is adjacent to* D_j if there are $x \in D_i$ and $y \in D_j \setminus D_i$, $x \sim y$. Note that adjacent nodal domains must have opposite signs. Now consider a collection $\{D_1, \dots, D_l\}$ of nodal domains such that $\bigcup_i D_i \neq V$. Then there exists a nodal domain $D_j \neq D_i$, $i = 1, \dots, l$, that is adjacent to some D_i, $i = 1, \dots, l$; otherwise Γ 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 Γ 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 $\langle g, f_k \rangle = 0$. □

4 Two Counter-Examples

Neither the Weak nor the Strong Nodal Domain theorem can be strengthened without additional assumptions. If Γ 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 [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

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

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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