Discrete Quantitative Nodal Theorem

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Abstract

We prove a theorem that can be thought of as a common generalization of the Discrete Nodal Theorem and (one direction of) Cheeger's Inequality for graphs. A special case of this result will assert that if the second and third eigenvalues of the Laplacian are at least ε apart, then the subgraphs induced by the positive and negative supports of the eigenvector belonging to λ_2 are not only connected, but edge-expanders (in a weighted sense, with expansion depending on ε).

Mathematics Subject Classifications: 05C50, 05C40

1 Introduction

In the theory of Riemannian manifolds, two basic theorems connect the geometry of the manifold to the spectrum of the Laplace operator on the manifold: Courant's Nodal Theorem and Cheeger's Inequality. Both of these have analogues in graph theory.

It is a basic simple fact that the graph is connected if and only if the smallest eigenvalue of its (combinatorial) Laplacian (which is always 0) has multiplicity one. Discrete Cheeger inequalities (Alon and Milman [2], Alon [1], Dodziuk and Kendall [6], Jerrum and Sinclair [12]) give a quantitative version of this: Roughly speaking, a graph is an expander if and only if the second smallest eigenvalue of its Laplacian is bounded away from zero.

The simplest version of the Discrete Nodal Theorem asserts that if x is an eigenvector of the Laplacian of a connected graph G belonging to the second smallest eigenvalue, and this eigenvalue has multiplicity one, then the positive and negative supports of x induce connected subgraphs (Fiedler [9]). If the second smallest eigenvalue has higher multiplicity, there are exceptions (a simple example is the 3-star), but they can be characterized [10, 11].

The Discrete Nodal Theorem was extended to higher eigenvectors by Fiedler [9], Colin de Verdière [4], Davies, Gladwell, Leytold and Stadler [7], and Duval and Reiner [8]; to embedded graphs by Lin, Lippner, Mangoubi and Yau [13]; see also Bıyıkoğlu, Leydold and Stadler [3]. To motivate our results, let us quote a simple version. A *nodal domain* of a vector $v \in \mathbb{R}^V$ is a connected component of the subgraph induced by its positive support, or a connected component of the subgraph induced by its negative support.

Theorem 1. *Let G be a connected graph, let $\lambda_1 = 0 \leqslant \lambda_2 \leqslant \lambda_3 \leqslant \ldots \leqslant \lambda_n$ be the eigenvalues of its Laplacian, and assume that $\lambda_k < \lambda_{k+1}$ for some $k \geqslant 2$. Let y be an eigenvector belonging to λ_k. Then the number of nodal domains of y is at most k.*

There are conditions other than $\lambda_k < \lambda_{k+1}$ to guarantee that the number of nodal domains is at most k, for example, that y has minimal support among all eigenvectors belonging to λ_k.

In this note we prove a theorem that can be thought of as a common generalization of the Discrete Nodal Theorem and (one direction of) Cheeger's Inequality for graphs. A special case of our results will assert that if the second and third eigenvalues of the Laplacian are at least ε apart, then the subgraphs induced by the positive and negative supports of the eigenvector belonging to λ_2 are not only connected, but edge-expanders (in a weighted sense, with an expansion rate depending on ε).

2   The main result

Let $(w_i : i \in V)$ be a weighting of the nodes of the graph $G = (V, E)$ with nonnegative weights. For $S \subseteq V$, set $w(S) = \sum_{i \in S} w_i$, and $\nabla(S) = \{ij \in E : i \in S, j \in V \setminus S\}$. If $w(S) > 0$, we define the *edge-expansion* of S as

$$\Psi_w(S) = \Psi_{G,w}(S) = \frac{1}{w(S)} \sum_{ij \in \nabla(S)} \sqrt{w_i w_j}\,.$$

We say that G is a *c-expander with respect to w* ($c > 0$), if $\Psi_w(S) \geqslant c$ for every subset $S \subseteq V$ with $0 < w(S) < w(V)/2$.

To generalize this notion to multiway cuts, it is easier to formulate the contrapositive. We say that (G, w) is *(k, c)-partitionable*, if V has a partition $V = S_1 \cup \cdots \cup S_k$ into sets with $w(S_i) > 0$ such that $\Psi_w(S_i) < c$ for all $1 \leqslant i \leqslant k$. It is easy to check that if $k > 2$, then merging two classes in such a partition, the new class $S_i \cup S_j$ satisfies $\Psi_w(S_i \cup S_j) < c$. Hence every (k, c)-partitionable weighted graph is $(k - 1, c)$-partitionable as well.

For a vector $x \in \mathbb{R}^V$, we denote its positive and negative support by $\mathrm{supp}_+(x) = \{i \in V : x_i > 0\}$ and $\mathrm{supp}_-(x) = \{i \in V : x_i < 0\}$, and by G_x^+ and G_x^-, the subgraphs of G induced by $\mathrm{supp}_+(x)$ and $\mathrm{supp}_-(x)$ respectively.

Theorem 2. *Let $\lambda_1 = 0 \leqslant \lambda_2 \leqslant \lambda_3 \leqslant \ldots \leqslant \lambda_n$ be the eigenvalues of the Laplacian L of a graph $G = (V, E)$. Let y be an eigenvector belonging to λ_k ($1 \leqslant k \leqslant n$), and set $w_i = y_i^2$ and $c = (\lambda_{k+1} - \lambda_k)/2$. Suppose that the weighted graph (G_y^+, w) is (a, c)-partitionable, and (G_y^-, w) is (b, c)-partitionable. Then $a + b \leqslant k$.*

Proof. Let us write $G^+ = G^+_y$, $V^+ = \mathrm{supp}_+(y)$ and $\Psi^+(S) = \Psi_{G^+,w}(S)$ for $S \subseteq V^+$, and define G^-, V^- and Ψ^- analogously. Note that $\Psi^+(S) = 0$ if S induces a connected component of G^+. Let $V^+ = V_1 \cup \cdots \cup V_a$ be a partition with $\Psi^+(V_i) < c$, and let $V^- = V_{a+1} \cup \cdots \cup V_{a+b}$ be an analogous partition. Let us assume (by way of contradiction) that $a + b \geqslant k + 1$; we may assume (by merging partition classes) that $a + b = k + 1$.

Let $M = L - \lambda_k I$, so that $My = 0$. Let $y^i \in \mathbb{R}^V$ denote the vector obtained from y by replacing all entries in $V \setminus V_i$ by 0. This vector is nonzero, because $|y^i|^2 = w(V_i) > 0$ by the definition of (k,c)-partitionable graphs. Furthermore, $y^i \geqslant 0$ for $1 \leqslant i \leqslant a$, $y^i \leqslant 0$ for $a + 1 \leqslant i \leqslant a + b$, and $y = y^1 + \cdots + y^{k+1}$. Let $z_i = |y^i|$, $\widehat{y}^i = (1/z_i)y^i$, and $z = (z_1, \ldots, z_{k+1})^\top$. Consider the $(k+1) \times (k+1)$ matrix B defined by

$$B_{ij} = \langle \widehat{y}^i, M\widehat{y}^j \rangle = \frac{1}{z_i z_j} \langle y^i, My^j \rangle,$$

and let $\mu_1 \leqslant \ldots \leqslant \mu_{k+1}$ be its eigenvalues. Note that for $i \leqslant a$, we have

$$\Psi^+(V_i) = \frac{1}{z_i^2} \sum_{u \in V_i} \sum_{v \in V_+ \setminus V_i} y_u y_v = -\frac{1}{z_i^2} \sum_{j \leqslant a, j \neq i} \langle y^i, My^j \rangle = -\frac{1}{z_i} \sum_{j \leqslant a, j \neq i} B_{ij} z_j. \qquad (1)$$

Analogous formula holds for $i > a$.

Let us start with some elementary properties of B. We have $\langle y^i, My^j \rangle \leqslant 0$ if $i \neq j$ and $1 \leqslant i, j \leqslant a$, which implies that $B_{ij} \leqslant 0$ in this case. Similarly $B_{ij} \leqslant 0$ if $i \neq j$ and $a + 1 \leqslant i, j \leqslant k + 1$, and $B_{ij} \geqslant 0$ if $i \leqslant a < j$, or the other way around. Furthermore, we have $Bz = 0$; indeed,

$$(Bz)_i = \sum_{j=1}^{k+1} \frac{1}{z_i} \langle y^i, My^j \rangle = \frac{1}{z_i} \langle y^i, My \rangle = 0.$$

Since the vectors $\widehat{y}^i$ ($i = 1, \ldots, k+1$) are mutually orthogonal unit vectors, the matrix B is a principal submatrix of M in an appropriate orthonormal basis. By the Interlacing Eigenvalues Theorem, we have

$$\lambda_i - \lambda_k \leqslant \mu_i \qquad (i = 1, \ldots, k+1). \qquad (2)$$

Let C be a symmetric $(k+1) \times (k+1)$ matrix, given by

$$C_{ij} = \begin{cases} B_{ij} & \text{if } i \neq j \text{ and either } i, j \leqslant a \text{ or } i, j \geqslant a + 1, \\ \Psi^+(V_i), & \text{if } i = j \leqslant a, \\ \Psi^-(V_i), & \text{if } i = j \geqslant a + 1, \\ 0, & \text{otherwise.} \end{cases}$$

Then for $1 \leqslant i \leqslant a$, using (1),

$$(Cz)_i = \Psi^+(V_i)z_i + \sum_{j \leqslant a, j \neq i} B_{ij} z_j = 0.$$

Similar computation works for $i > a$, to get $Cz = 0$.

Claim. *The matrices C and $C - B$ are positive semidefinite.*

Indeed, from our discussion of the signs of the entries of B, it follows that the off-diagonal entries of C and of $C - B$ are nonpositive. We also have $(C - B)z = Cz = Bz = 0$, which implies that their diagonal entries are nonnegative. Let $D = \mathrm{diag}(z)$, then the matrix DCD has nonnegative entries in the diagonal, nonpositive entries everywhere else, and every row-sum is 0. So this matrix is diagonally dominant, and hence positive semidefinite, which implies that C is positive semidefinite. For the matrix $C - B$ the conclusion follows similarly.

Next, we show that the largest eigenvalue of the matrix C satisfies

$$\lambda_{\max}(C) < 2c. \tag{3}$$

Indeed, let u be the eigenvector of C belonging to $\lambda_{\max}(C)$. We may assume that $u_1 = z_1 > 0$ and $|u_i| \leqslant z_i$ for all i. Then, using that $C_{1i} \leqslant 0$ for $i \neq 1$, we get

$$\lambda_{\max}(C)u_1 = \sum_i C_{1i}u_i \leqslant C_{11}u_1 - \sum_{i>1} C_{1i}z_i = 2C_{11}u_1 < 2cu_1.$$

This proves (3).

Positive semidefiniteness of $C - B$ implies that μ_{k+1}, the largest eigenvalue of B, is bounded above by $\lambda_{\max}(C)$. Hence by (2),

$$\lambda_{k+1} - \lambda_k \leqslant \mu_{k+1} \leqslant \lambda_{\max}(C) < 2c, \tag{4}$$

which contradicts the choice of c. $\qquad\square$

The case $k = 2$ is worth stating separately:

Corollary 3. *If y is an eigenvector belonging to λ_2, then both G_y^+ and G_y^- are $(\lambda_3 - \lambda_2)/2$-expanders with respect to the weights y_i^2.*

From our considerations, we can derive two other inequalities:

Corollary 4. *If y is an eigenvector belonging to λ_k, $a + b = k + 1$, $\{U_1, \ldots, U_a\}$ is a partition of $\mathrm{supp}_+(y)$ and $\{V_1, \ldots, V_b\}$ is a partition of $\mathrm{supp}_-(y)$ with $w(U_i), w(V_i) > 0$, then*

$$\lambda_{k+1} - \lambda_k \leqslant 2 \max \left\{ \Psi^+(U_1), \ldots, \Psi^+(U_a), \Psi^-(V_1), \ldots, \Psi^-(V_b) \right\}.$$

and

$$\lambda_{k+1} - \lambda_k \leqslant \sum_{i=1}^a \Psi^+(U_i) + \sum_{i=1}^b \Psi^-(V_i).$$

(The second inequality is stronger in those cases only when the expansions of the sets are very different)

Proof. The first inequality is an easy rephrasing of Theorem 2. To prove the second, it suffices to notice that the matrix C in the proof above is positive semidefinite. Hence its largest eigenvalue is bounded above by its trace. Since $C - B$ is positive semidefinite, it follows that

$$\mu_{a+b} \leqslant \text{tr}(C) = \sum_i C_{ii} = \sum_{i=1}^{a} \Psi^+(U_i) + \sum_{i=1}^{b} \Psi^-(V_i). \qquad \square$$

3   Examples

There is no easy converse to Corollary 3. The following example shows that even if $\lambda_2 = \lambda_3$, no separation property for the positive and negative supports of any eigenvector belonging to λ_2 follows.

Example 5. Let C_n denote the cycle of length n, with its nodes labeled $0, 1, \ldots, n-1$ in the natural order. Let C_n^k denote the graph obtained from C_n by connecting any two nodes at distance of at most k along the cycle. The eigenvalues of the adjacency matrix are $\mu_r = 2\sum_{h=1}^{k} \cos(hr\pi i/n)$, $r = 0, 1, \ldots n-1$. The smallest eigenvalue of the Laplacian is $\lambda_1 = 2 - \mu_0 = 0$, and it is not hard to see that the second smallest eigenvalues are $\lambda_2 = \lambda_3 = 2 - \mu_1 = 2 - \mu_{n-1}$. So the gap $\lambda_3 - \lambda_2 = 0$. For every eigenvector x belonging to λ_2, its positive support is induced by a half-cycle, which is easily seen to be a c-expander (even if weighted with the squared entries of the eigenvector) for $c = \Theta(k^2/n^2)$.

The assertion of the main theorem (or of its corollary) does not remain true without the weights, as the following example shows.

Example 6. Consider two isomorphic D-regular expanders G_1 and G_2 with p nodes. Connect two corresponding nodes a_1 and a_2 in G_1 and G_2 by a path P of length $q+1$, to get a connected graph G with $n = 2p + q$ nodes. We assume that $q, p \to \infty$ and $q = o(p)$. Let $\lambda_1 = 0 < \lambda_2 \leqslant \ldots \leqslant \lambda_n$ be its eigenvalues of its Laplacian, with unit length eigenvectors $v_1 = (1/\sqrt{n})\mathbb{1}, v_2, \ldots, v_n$.

It is not hard (but a little tedious) to see that this is a counterexample. Informally, the graph is "almost disconnected", and hence λ_2 is small (less than $2/p$). On the other hand, $\lambda_3 - \lambda_2$ will be of the same order as the eigenvalue gap of G_1, which is of constant magnitude. The positive support of v_2 will consist of G_1 and half of the path P, which is not an expander in the unweighted sense.

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