A Discrete Nodal Domain Theorem for Trees

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Abstract

Let G be a connected graph with n vertices and let $x = (x_1, \ldots, x_n)$ be a real vector. A positive (negative) sign graph of the vector x is a maximal connected subgraph of G on vertices $x_i > 0$ ($x_i < 0$). For an eigenvalue of a generalized Laplacian of a tree: We characterize the maximal number of sign graphs of an eigenvector. We give an $O(n^2)$ time algorithm to find an eigenvector with maximum number of sign graphs and we show that finding an eigenvector with minimum number of sign graphs is an NP-complete problem.

Keywords: discrete nodal domain theorem; eigenvectors of a matrix with non-positive off-diagonal elements; tree; graph Laplacian;

1 Introduction

Let $G = (V, E)$ be a graph with vertex set $V = \{1, \ldots, n\}$ and let $x = (x_1, \ldots, x_n)$ be a real vector. We associate the real numbers x_i with the vertices i of G, for $i = 1, \ldots, n$. A *positive (negative) sign graph* S is a maximal connected subgraph of G on vertices $i \in V$ with $x_i > 0$ $(x_i < 0)$.

We denote by $\eta(x)$ the number of sign graphs of the vector x.

For example, let G be the path P_6 and consider the vector $x = (1, 2, -1, 0, -1, 3)$. The vector x has two positive sign graphs, two negative sign graphs, and hence $\eta(x) = 4$.

The number of sign graphs of a graph G is at most the number of vertices of the induced bipartite subgraph of G with maximal number of vertices. To find such an induced bipartite subgraph of G is a well known NP-complete problem (see, e.g., [4]).

On the other hand, if A is a generalized Laplacian of G with eigenvalues $\lambda_1 \leq \cdots \leq \lambda_n$, then any eigenvector corresponding to eigenvalue λ_k with multiplicity r has at most $k + r - 1$ sign graphs of G. This theorem is called the *discrete nodal domain theorem* and it is the discrete analogue of Courant's nodal domain theorem for elliptic operators on Riemanian manifolds. For a proof of the discrete nodal domain theorem and some historical remarks see

Davies et al. [1].

Let G be a simple, undirected, loop-free graph with n vertices. We call a symmetric real $n \times n$ matrix A a *generalized Laplacian* of G if $a_{uv} < 0$ when u and v are adjacent vertices of G and $a_{uv} = 0$ when u and v are distinct and not adjacent. There are no constraints on the diagonal entries of A. We say G is the *graph of* A and we say A is the *matrix of* G.

We focus our attention on the k-th eigenvalue of generalized Laplacian A, and suppose that it has multiplicity r, so that

$$\lambda_1 \leq \cdots \leq \lambda_{k-1} < \lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+r-1} < \lambda_{k+r} \leq \cdots \leq \lambda_n.$$

Throughout this paper we assume that the eigenvalues are numbered in non-decreasing order.

Theorem 1 (Discrete nodal domain [1]) *Let G be a connected graph and let A be generalized Laplacian of G then any eigenvector corresponding to the eigenvalue λ_k with multiplicity r has at most $k + r - 1$ sign graphs.*

In general, it is unknown, whether these upper bounds relating to the order of the eigenvalues are sharp for an arbitrary graph. Moreover, no method is known to construct an eigenvector to the eigenvalue λ_k with maximal or minimal number of the sign graphs. We look at the discrete nodal domain theorem for trees. We characterize for a tree: the maximal number of the sign graphs of an eigenvector corresponding to an eigenvalue λ_k. We give an $O(n^2)$ time algorithm to find an eigenvector with maximum number of the sign graphs, which corresponds to an eigenvalue λ_k. We show that to find an eigenvector of an eigenvalue λ_k, which has minimum number of the sign graphs, is NP-complete.

2 Nodal domain theorem for trees

We look at the discrete nodal domain theorem for trees. We begin with a special simple eigenvalue.

We say that y is a λ-*eigenvector* (of A) if $Ay = \lambda y$.

Theorem 2 *Let G be a tree and let A be a generalized Laplacian of G. If y is a λ_k-eigenvector without a vanishing coordinate, then y has exactly k sign graphs.*

The following lemma plays a important role in the proof of the theorem 2.

Lemma 1 (Fiedler [3]) *Let A be a generalized Laplacian of a tree. If y is a λ_k-eigenvector without a vanishing coordinate, then λ_k is simple and there are exactly $n-k$ (unordered) pairs (i,j), $i \neq j$, for which $a_{ij}y_iy_j < 0$.*

Proof of Theorem 2: By lemma 1, λ_k is simple and there are exactly $n-k$ edges ij, for which y_i and y_j have the same sign. Note that $a_{ij}y_iy_j < 0$ if and only if i and j are adjacent and y_i and y_j have the same sign. We divide V in three disjoint sets in the following way:

$P = \{i \in V \ : \ y_i > 0, \text{ there is an edge } ij \in E, \text{ s.t. } y_j > 0\}$,

$M = \{i \in V \ : \ y_i < 0, \text{ there is an edge } ij \in E, \text{ s.t. } y_j < 0\}$. C is the set of remaining vertices. The induced subgraphs $G[P]$ and $G[M]$ are forests. Let p and m are the number of components of $G[P]$ and $G[M]$, respectively. $G[P]$ and $G[M]$ have $|P|-p$ edges and $|M|-m$ edges, respectively. Since $\{P, M, C\}$ is a partition of V and using lemma 1, we see $|P| - p + |M| - m = n - k$. Now we show that $\eta(y) = k$. Let i and j be vertices of C. If y_i and y_j have the same sign, then i and j are not adjacent. Let $C_- = \{i \in C \ : \ y_i < 0\}$ and $C_+ = \{i \in C \ : \ y_i > 0\}$. By the definition of P and M, there exist no edges between C_- and M and no edges between C_+ and P, respectively. Consequently the number of sign graphs of y is equal to $|C| + p + m$. Thus

$$\eta(y) = |C| + p + m = n - |P| - |M| + |P| + |M| - n + k = k.$$

□

We remark that R. Roth [5] proved that the largest eigenvalue of the generalized Laplacian of a bipartite graph satisfies the condition of theorem 2.

Next we consider eigenvectors of trees with vanishing coordinates.

Let $G = (V, E)$ be a connected graph, and let A be a generalized Laplacian of G. Let Z be a subset of V, let $G_1, \ldots, G_m$ be the components of $G - Z$ and let $A_1, \ldots, A_m$ be generalized Laplacians of $G_1, \ldots, G_m$. We say $(A_1, \ldots, A_m, A_Z)$ is a *rearrangement of* A, if we rearrange the matrix A with permutation similarity operations in the following way:

$$A = \begin{pmatrix} A_1 & A_{12} & \cdots & A_{1Z} \\ \vdots & \ddots & \cdots & \vdots \\ A_{m1} & \cdots & A_m & A_{mZ} \\ A_{Z1} & \cdots & A_{Zm} & A_Z \end{pmatrix}$$

Theorem 3 *Let G be a tree with n vertices and let A be a generalized Laplacian of G. Let λ be an eigenvalue of A with multiplicity $r \geq 2$. Then there exists a rearrangement $(A_1, \ldots, A_m, A_Z)$ of A such that the following statements hold:*

(i) λ is a simple eigenvalue of $A_1, \ldots, A_m$.

The matrix A_j has a λ-eigenvector without vanishing coordinates, for $j = 1, \ldots, m$.

(ii) Let $k_1, \ldots, k_m$ be the positions of λ in the spectrum of $A_1, \ldots, A_m$ in non-decreasing order. Then the number of sign graphs of an eigenvector

of λ is at most $k_1 + \cdots + k_m$,

(iii) There exists an eigenvector of λ with $k_1 + \cdots + k_m$ sign graphs. Such an eigenvector can be found in $O(n^2)$ time.

For the proof of Theorem 3 we need the following two lemmas. We shall prove lemma 3 after the proof of Theorem 3.

Lemma 2 (Fiedler [3]) *Each eigenvector corresponding to a multiple eigenvalue of a matrix of a tree has at least one vanishing coordinate.*

We remark that M. Fiedler proved the results of lemmas 1 and 2 for a more general matrix of a tree.

Lemma 3 *Let $x^1, \ldots, x^k$ be linearly independent vectors in $\mathbb{R}^n$ and $k < n$. If all linear combinations of $x^1, \ldots, x^k$ have a vanishing coordinate, then the vectors $x^1, \ldots, x^k$ have a common vanishing coordinate.*

Proof of Theorem 3: Let λ be an eigenvalue of A with multiplicity $r \geq 2$. Let $y^1, \ldots, y^r$ be linearly independent λ-eigenvectors. Let Z be the set of all common vanishing coordinates of $y^1, \ldots, y^r$. By lemmas 2 and 3, Z is not empty and the choice of $y^1, \ldots, y^r$ has no influence on Z. The graph $G - Z$ is a forest with components $T_1, \ldots, T_m$. Let $A_1, \ldots, A_m$ be generalized

Laplacians of $T_1, \dots, T_m$. According to the rearrangement $(A_1, \dots, A_m, A_Z)$ the matrix A has the following form:

$$A = \begin{pmatrix} A_1 & 0 & \cdots & 0 & A_{1Z} \\ 0 & A_2 & \cdots & 0 & A_{2Z} \\ 0 & \cdots & \ddots & 0 & \vdots \\ 0 & \cdots & 0 & A_m & A_{mZ} \\ A_{Z1} & \cdots & \cdots & A_{Zm} & A_Z \end{pmatrix}$$

(i) We write each eigenvector y of λ as $y = (y_{T_1}, \dots, y_{T_m}, 0, \dots, 0)$, where y_{T_j} denotes the coordinates of eigenvector y belonging to the tree T_j. By the definition of Z, the coordinates of eigenvector y belonging to Z are equal to zero. Thus the vector Ay has the following form:

$$Ay = (A_1 y_{T_1}, \dots, A_m y_{T_m}, *, \dots, *) = (\lambda y_{T_1}, \dots, \lambda y_{T_m}, 0, \dots, 0) = \lambda y$$

for each λ-eigenvector y. Therefore λ is an eigenvalue of the matrices $A_1, \dots, A_m$. Now we prove that λ is a simple eigenvalue of A_j and the matrix A_j has a λ-eigenvector without vanishing coordinates, for $j = 1, \dots, m$.

We show that the number of linearly independent vectors of $y^1_{T_j}, \dots, y^r_{T_j}$ is equal to one, for $j = 1, \dots, m$. Assume that there are linearly independent vectors $y^1_{T_j}, \dots, y^h_{T_j}$, $h \geq 2$. Then the vectors $y^1_{T_j}, \dots, y^h_{T_j}$ are linearly independent λ-eigenvectors of A_j. By lemmas 2 and 3, vectors $y^1_{T_j}, \dots, y^h_{T_j}$ have a common vanishing coordinate. Hence $y^1_{T_j}, \ldots, y^r_{T_j}$ have a common vanishing coordinate, a contradiction to the definition of Z.

We denote by b_j the only one linearly independent vector of $y^1_{T_j}, \ldots, y^r_{T_j}$, for $j = 1, \ldots, m$. The vector b_j is a λ-eigenvector of A_j, for $j = 1, \ldots, m$. The eigenvector b_j has no vanishing coordinate, for $j = 1, \ldots, m$. We suppose that b_j has a vanishing coordinate. Then $y^1_{T_j}, \ldots, y^r_{T_j}$ have a common vanishing coordinate, a contradiction to the definition of Z.

(ii) Let $k_1, \ldots, k_m$ be the positions of λ in the spectrum of $A_1, \ldots, A_m$ in non-decreasing order. The number of sign components of an eigenvector $y = (\beta_1 b_1, \ldots, \beta_l b_m, 0, \ldots, 0)$ is equal to the sum of the number of sign components of $\beta_1 b_1, \ldots, \beta_m b_m$. By theorem 2, $\eta(b_j) = k_j$, for $j = 1, \ldots, m$.
Therefore, $\eta(y) \leq k_1 + \cdots + k_m$.

(iii) Now we construct an eigenvector x of λ with $\eta(x) = k_1 + \cdots + k_m$ in following way: By the definition of b_j, the linearly independent eigenvectors $y^1, \ldots, y^r$ are $y^i = (\beta_{i1} b_1, \ldots, \beta_{im} b_m, 0, \ldots, 0)$, for $i = 1, \ldots, r$, where the coefficients $\beta_{i1}, \ldots, \beta_{im}$ are real numbers.

$x := y^1$;

for $i = 2, \ldots, r$ **do**

$x := x + \alpha_i y^i$,

choose α_i: $\alpha_i \neq 0$ and $\alpha_i \notin \{-\frac{x_j}{y^i_j} \ : \ y^i_j \neq 0\,,\ j = 1, \ldots, n\}$.

After this iteration we obtain $x = (\beta'_1 b_1, \ldots, \beta'_m b_m, 0, \ldots, 0)$. The coefficients $\beta'_1, \ldots, \beta'_m$ are nonzero numbers. Assume that there exists a $\beta_j = 0$. By the choice of α_i, then all $\beta_{1j}, \ldots, \beta_{rj}$ are equal to zero. This is a contradiction to the definition of Z.

Therefore, $\eta(x) = \eta(\beta_1 b_1) + \cdots + \eta(\beta_m b_m) = k_1 + \cdots + k_m$.

It is easy to see that we need $O(n^2)$ operations to find an eigenvector x with $\eta(x) = k_1 + \cdots + k_m$ from an arbitrary eigensystem of A.

$\square$

Corollary 1 *By theorem 3, if we replace the multiple eigenvalue λ by the simple eigenvalue λ with an eigenvector y, which has at least one vanishing coordinate, then the statements of theorem 3 also hold.*

Proof of Lemma 3: If $k = 1$, this is trivial. Let $k \geq 2$. Let y be a linear combination of $x^1, \ldots, x^{k-1}$. Let $Z_y = \{j \ : \ y_j = x_j^k = 0\}$. Without loss of generality let the first d coordinates of x^k be zero and all others elements of x^k be nonzero.

Claim 1: y and x^k have a common vanishing coordinate, i.e. Z_y is not empty. Suppose that y and x^k have no common vanishing coordinate. Then the first d elements of y are nonzero. Now we construct a new vector $t = y + \beta x^k$. We choose β in the following way: $\beta \neq 0$ and $\beta \neq \frac{-y_i}{x_i^k}$, for $i = d+1, \ldots, n$. Then t has no vanishing coordinate. This is a contradiction.

Claim 2: If u and y are linear combinations of $x^1, \ldots, x^{k-1}$, then $Z_u \cap Z_y \neq \emptyset$. Suppose that there exists u and y, such that $Z_u \cap Z_y = \emptyset$. By claim 1, Z_u and Z_y are not empty. Without loss of generality, the first d elements of u and y are look like: $u = (0, \ldots, 0, \pm, \ldots, \pm)$, $y = (\pm, \ldots, \pm, 0, \ldots, 0, \pm, \ldots, \pm)$. Now we construct a new vector $t = u + \beta y$. We choose β such that: $\beta \neq 0$ and $\beta \neq \frac{-u_i}{y_i}$, for $i = 1, \ldots, d$ and y_i are nonzero. Then t and x^k have no common zero coordinate. This is a contradiction to claim 1.

Now we define new vectors y^i in the following way:

$y^1 = x^1$, $y^i = y^{i-1} + \alpha_i x^i$, for $i = 2, \ldots, k-1$. We choose α_i such that: $\alpha_i \neq 0$ and $\alpha_i \neq -\frac{y_j^{i-1}}{x_j^i}$, for all x_j^i nonzero elements, for $j = 1, \ldots, d$.

Claim 3: Z_{y^i} is not empty and $Z_{y^i} = Z_{x^1} \cap \cdots \cap Z_{x^i}$, for $i = 1, \ldots, k-1$.

By claim 1, Z_{y^i} is not empty. We prove the other argument with induction on i. For $i = 1$, $y^1 = x^1$. By claim 1, x^1 and x^k have a common zero coordinate. We suppose that the claim holds for $y^1, \ldots, y^{i-1}$. Now we show that it holds for $y^i = y^{i-1} + \alpha_i x^i$. We choose α_i as defined. By Claim 2, $Z_{y^{i-1}} \cap Z_{x^i} \neq \emptyset$. By the choice of α_i, $y^i_j = 0$ if and only if $j \in Z_{y^{i-1}}$ and $j \in Z_{x^i}$. It means that $j \in Z_{y^{i-1}} \cap Z_{x^i}$. By induction $Z_{y^{i-1}} = Z_{x^1} \cap \cdots \cap Z_{x^i - 1}$. Then $j \in Z_{x^1} \cap \cdots \cap Z_{x^i - 1} \cap Z^i_x$.

By claim 3, $Z_{y^{k-1}}$ is not empty and $Z_{y^{k-1}} = Z_{x^1} \cap \cdots \cap Z_{x^{k-1}}$. Therefore $x^1, \ldots, x^k$ have a common vanishing coordinate.

$\square$

3 Minimum number of sign graphs

In this section we show that the following problem is NP-complete.

MINIMUM NUMBER OF SIGN GRAPHS

Instance: An $n \times n$ matrix A, where A is a generalized Laplacian of a tree, an eigenvalue λ of A with multiplicity $r \geq 2$.

Question: Find an eigenvector y of λ such that the number of sign graphs of y is minimal.

Let A be a generalized Laplacian of a tree and λ is an eigenvalue of A with multiplicity $r \geq 2$. In theorem 3 we proved that linearly independent eigenvectors $y^1, \ldots, y^r$ of λ have common vanishing coordinates Z and $y^i = (\beta_{i1}b_1, \ldots, \beta_{im}b_m, 0, \ldots, 0)$, for $i = 1, \ldots, r$, where $b_1, \ldots, b_l$ are vectors without vanishing coordinates and $\beta_{i1}, \ldots, \beta_{im}$ are real numbers. m is the number of components of $G - Z$.

Let $B = (\beta_{ij})$, $i = 1, \ldots, m$, $j = 1, \ldots, r$. Then an eigenvector y of λ has the following form: $y = ((Bx)_1 b_1, \ldots, (Bx)_m b_m, 0, \ldots, 0)$, where $x = (x_1, \ldots, x_r)$ is a real vector. Let $k_1, \ldots, k_m$ are the number of sign components of $b_1, \ldots, b_m$. Now we define new variables $c_i(x)$, $i = 1, \ldots, m$ as follows:

$$c_i(x) = \begin{cases} 0, & \text{if} \quad (Bx)_i = 0, \\ 1, & \text{if} \quad (Bx)_i \neq 0. \end{cases}$$

Then $\eta(y) = k_1c_1(x) + \cdots + k_mc_m(x)$. Therefore MINIMUM NUMBER OF SIGN GRAPHS is equivalent to the following minimization problem:

$$\mathbf{min}\ k_1c_1(x) + \cdots + k_lc_l(x)$$

$$x = (x_1, \ldots, x_r) \text{ is a nonzero real vector.}$$

Consequently the decision problem of MINIMUM NUMBER OF SIGN GRAPHS is the following problem:

MIN(η)

Instance: An $(m \times r)$ matrix B with real entries, positive integers $k_1, \ldots, k_m$ and a positive integer s.

Question: Is there a nonzero rational vector $x = (x_1, \ldots, x_r)$, such that $k_1c_1(x) + \cdots + k_mc_m(x) \leq s$?

Lemma 4 *The $(m \times r)$ matrix B of decision problem MIN(η) can be arbitrary large.*

Proof: The required example is constructed from the following result by I. Faria [2]. Let G be a graph and let the matrix $L = D - A$ be the Laplacian matrix of G, where A is the adjacency matrix of G and D is the diagonal matrix of vertex degrees of G. Let p be the number of vertices with degree one. Let q be the number of vertices, which are adjacent to a vertex with degree one. Then $\lambda = 1$ is an eigenvalue of L with multiplicity $r \geq p - q$. We consider a binary tree with n vertices and $n/2$ endvertices. Therefore $\lambda = 1$ is an eigenvalue of L with multiplicity $r \geq n/4$. It is straightforward to show that m is at least the number of endvertices. Thus $m \geq n/2$.

$\square$

Now we show that MIN(η) is NP-complete. For the proof we give another NP-complete problem. Let $x = (x_1 \ldots, x_n)$ be a real vector. We denote by *support*(x), the number of nonzero elements of x.

MINIMUM SUPPORT

Instance: An $(m \times r)$ matrix B with rational entries, a positive integer s.

Question: Is there a nonzero rational vector $x = (x_1, \ldots, x_r)$ such that *support*$(Bx) \leq s$?

Lemma 5 MINIMUM SUPPORT *is* NP-complete.

Theorem 4 *The decision problem* MIN(η) *is* NP-complete.

Proof: It is easy to see that MIN(η) is in NP. We reduce MINIMUM SUPPORT to MIN(η) in following way. We choose $k_1 = \cdots = k_m = 1$. The matrix B is the same matrix. We have the bound s. We assume that there is a vector x such that $c_1(x) + \cdots + c_m(x) \leq s$. By the definition of $c_1(x), \ldots, c_m(x)$, the inequality $c_1(x) + \cdots + c_m(x) \leq s$ holds if and only if $support(Bx) \leq s$. Therefore we have the solution of MINIMUM SUPPORT. Thus MIN(η) is NP-complete.

□

Proof of Lemma 5: It is easy to see that MINIMUM SUPPORT is in NP. The following problem is NP-complete:

ONE-IN-THREE

Instance: X a set with n elements and a subset T of $X \times X \times X$.

Question: Is there a subset Y of X, such that each triple $t = (t_1, t_2, t_3)$ in T has exactly one element in Y ?

ONE-IN-THREE is a variant of [LO4] in Garey and Johnson [4] page 259.

We reduce ONE-IN-THREE to MINIMUM SUPPORT in following way. For each element of X we give a variable x_i, for $i = 1, \ldots, n$. We add a new variable x_{n+1}. We introduce rows $x_i + x_{n+1}$ and $x_i - x_{n+1}$ in the matrix B, for $i = 1, \ldots, n$. For each triple $t = (t_i, t_j, t_k)$ in T we introduce the row $x_i + x_j + x_k + x_{n+1}$, $n+1$ times in B. We set the bound $s = n$. We assume that $support(Bx) \leq n$. Then each variable x_i is equal to x_{n+1} or $-x_{n+1}$, for $i = 1, \ldots, n$ and each expression $x_i + x_j + x_k + x_{n+1}$ is equal to zero. Otherwise $support(Bx) > n$. Now we put the variables $x_i = x_{n+1}$ in Y. It is easy to see that each triple $t = (t_1, t_2, t_3)$ in T has exactly one element in Y if and only if $x_i + x_j + x_k + x_{n+1}$ is equal to zero. Therefore we have the solution of ONE-IN-THREE. Thus MINIMUM SUPPORT is NP-complete.

□

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References

[1] E.B. Davies, G.M.L. Gladwell, J. Leydold, P.F. Stadler, Discrete nodal domain theorems, Linear Algebra Appl. 336:51-60 (2001).

[2] I. Faria, Permanental roots and the star degree of a graph, Linear Algebra Appl. 64:255-265 (1985).

[3] M. Fiedler, Eigenvectors of acyclic matrices, Czechoslovak Mathematical Journal, 25:607-618 (1975).

[4] M.R. Garey, D.S. Johnson, Computers and intractability. A guide to the theory of NP-completeness, W.H. Freeman and Company, San Francisco, 1979.

[5] R. Roth, On the eigenvectors belonging to the minimum eigenvalues of an essentially nonnegative symmetric matrix with bipartite graph, Linear Algebra Appl. 118:1-10 (1989).