Applications to network analysis: Graph partitioning and community detection Lecture notes

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Lecture notes for the third part of the course "Nonnegative and spectral matrix theory with applications to network analysis", held within the Rome-Moscow school on Matrix Methods and Applied Linear Algebra, August–September 2014. The author is partially supported by Istituto Nazionale di Alta Matematica. This document is intended for internal circulation only.

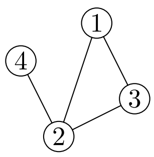
1 Nodal domains

In what follows, the graph $G = (V, E)$ is assumed to be undirected (so that A_G is symmetric). Hereafter, the following notations will be used in correspondence with an arbitrary set $S \subseteq V$:

- Denote by $|S|$ its cardinality (that is, the number of its elements), by $\bar{S}$ its complement (that is, $\bar{S} = V \setminus S$) and by $\mathbf{1}_S$ its characteristic vector, that is $(\mathbf{1}_S)_i = 1$ if $i \in S$ and 0 otherwise.
- Let $\operatorname{vol} S = \sum_{i \in S} d_i$ be the *volume* of S (recall that d_i is the degree of node i). Note: $\operatorname{vol} S = d^T \mathbf{1}_S$.
- Let $e_{\text{in}}(S) = \mathbf{1}_S^T A \mathbf{1}_S$ and $e_{\text{out}}(S) = \mathbf{1}_S^T A(\mathbf{1} - \mathbf{1}_S) = \operatorname{vol} S - e_{\text{in}}(S)$. Note: $e_{\text{out}}(S)$ is the number of edges joining S with $\bar{S}$ while $e_{\text{in}}(S)$ is twice the number of edges whose endpoints are both in S.
- The *subgraph induced by S* is the graph $G(S)$ whose adjacency matrix is $[A]_{i,j \in S}$.

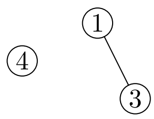
Let $0 \neq v \in \mathbb{R}^n$ and consider the set $S = \{i : v_i \geq 0\}$. The subgraph $G(S)$ may result in a collection of subgraphs which are disconnected one from the other. These components are called *nodal domains* of v. For example, for the following graph G and vector v,

G :



$$v = \begin{pmatrix} 1 \\ -2 \\ 0 \\ 0.1 \end{pmatrix} \quad \rightsquigarrow$$

$G(S)$:



the resulting nodal domains are the subgraphs $G(\{1,3\})$ and $G(\{4\})$.

Let $A = A_G$. A Perron vector v has positive entries, so that v has only nodal domain which is G itself. Obviously, we cannot say the same about other eigenvectors (why?). The goal of this section is to show something interesting about the nodal domains of eigenvectors associated to non-dominant eigenvalues of A [3]. Before going further, a basic fact in matrix theory must be recalled:

Lemma 1.1. [1] *Let $M \in \mathbb{R}^{p \times p}$ be a symmetric matrix, and let $N \in \mathbb{R}^{q \times q}$ be one of its principal submatrices. Let $\lambda_1(M) \geq \lambda_2(M) \geq \ldots \geq \lambda_p(M)$ and $\lambda_1(M) \geq \lambda_2(M) \geq \ldots \geq \lambda_q(N)$ denote the eigenvalues of M and N counted with their multiplicity, respectively. Then, $\lambda_i(M) \geq \lambda_i(N)$ for $i = 1, \ldots, q$.*

Theorem 1.2. *Let $A \geq O$ be irreducible and symmetric. Let $\rho(A) = \lambda_1 > \lambda_2 \geq \ldots \geq \lambda_n$ be its eigenvalues, let v be an eigenvector associated to λ_2, and let $S = \{i \in V : v \geq 0\}$. Then $G(S)$ is connected.*

[1] See e.g., [6, §5.7].

PROOF. Proceed by contradiction. Assume that $S = S_1 \cup S_2$ with $S_1 \cap S_2 = \varnothing$, both $G(S_1)$ and $G(S_2)$ are connected but there is no edge joining V_1 with V_2.

By a suitable permutation of rows and columns, we can assume that $v = (v_1, v_2, v_3)^T$ where $v_1 \geq 0$ and $v_2 \geq 0$ are the entries with indices in S_1 and S_2, respectively, and $v_3 < 0$ are the entries with indices in $\bar{S}$. Accordingly, the structure of A is

$$A = \begin{pmatrix} A_{11} & O & A_{13} \\ O & A_{22} & A_{23} \\ * & * & * \end{pmatrix}$$

where A_{11} and A_{22} are irreducible, and both A_{13} and A_{23} are nonzero (because A is irreducible). Then, equation $Av = \lambda_2 v$ leads to

$$\begin{aligned} A_{11}v_1 + A_{13}v_3 &= \lambda_2 v_1 \\ A_{22}v_2 + A_{23}v_3 &= \lambda_2 v_2. \end{aligned}$$

Let y_1 and y_2 be left Perron eigenvectors of A_{11} and A_{22}, respectively: $y_i^T A_{ii} = \rho(A_{ii}) y_i^T$. Then,

$$\underbrace{y_i^T A_{ii} v_i}_{=\rho(A_{ii}) y_i^T v_i} + \underbrace{y_i^T A_{i3} v_3}_{<0} = \lambda_2 y_i^T v_i, \qquad i = 1, 2.$$

Since $y_i^T v_i > 0$ we get $\rho(A_{ii}) > \lambda_2$ for $i = 1, 2$. Hence, the submatrix $\begin{pmatrix} A_{11} & O \\ O & A_{22} \end{pmatrix}$ hat at least 2 eigenvalues that are $> \lambda_2$. By Lemma 1.1 we deduce that also A has at least two eigenvalues $> \lambda_2$, thus contradicting the fact that $\rho(A)$ is simple. ■

Remarks:

- By applying Theorem 1.2 to $-v$ in place of v, you can deduce easily that also the set $\{i : v_i \leq 0\}$ induces a connected subgraph.
- The argument of the proof of Theorem 1.2 can be extended naturally to eigenvalues λ_i with $i \geq 2$. The result is that, if $Av = \lambda_i v$ and $S = \{i : v_i \geq 0\}$ then $G(S)$ is composed by no more than $i - 1$ connected components, see e.g., [3].

The subsequent sections outline two applicative contexts where nodal domains play an important role; see [5] for a reference.

2 Graph partitioning problems

A graph partitioning problem requires to partition the nodes of a given graph $G = (V, E)$ into pairwise disjoint sets (clusters) so that the number of edges running across different sets is minimized, in some sense.

Hereafter, I consider the special graph partitioning problem where we want to split V into two subsets S and $\bar{S}$, with $S \cup \bar{S} = V$ and $S \cap \bar{S} = \varnothing$. The pair $\{S, \bar{S}\}$ is a *cut* in G.

For any $S \subseteq V$ consider the number

$$H(S) = e_{\text{out}}(S)/|S|,$$

which is sometimes called the *conductance of* S. A set with high conductance has a relatively large amount of edges connecting it to its complement, with respect to the number of nodes. Conversely, a set having low conductance is a set that can be easily separated from the rest of the graph, by removing a quite small number of edges.

In the framework of graph partitoning preblems, a useful merit function of the graph cut $\{S, \bar{S}\}$ (which is easily generalized to more than two sets) is the following:

$$h(S, \bar{S}) = H(S) + H(\bar{S}) = \ldots = \frac{n}{|S||\bar{S}|} e_{\text{out}}(S).$$

As an exercise, you may fill in the blanks in the previous equality.[2]

[2] Note: $e_{\text{out}}(S) = e_{\text{out}}(\bar{S})$.

One of the main graph partitioning problems consists in computing

$$h_G = \min_{S\subseteq V} h(S,\bar{S}) \tag{1}$$

which is an important graph invariant. Indeed, a set attaining that minimum splits the graphs into two parts that are comparable in size and are connected by relatively few edges. The task of finding the set S which minimizes $h(S)$ is very hard. To help its solution, there exists an heuristic technique based on nodal domains that often goes very close to the true solution.

2.1 The Laplacian matrix

Let $D = \mathrm{Diag}(d_1,\dots,d_n)$. The matrix $L = D - A$ is called *Laplacian matrix of G.* This is one of the most useful matrices associated to a graph. The study of its spectral properties and applications has been pioneered by M. Fiedler, see e.g., [2].

For every $v \in \mathbb{R}^n$ we have

$$v^T L v = \sum_{ij\in E} (v_i - v_j)^2, \tag{2}$$

where the sum runs over the set of edges, every edge being counted only once. Thus, L is positive semidefinite; the vector $\mathbf{1}$ is in the kernel of L, that is $L\mathbf{1} = 0$; and the dimension of $\mathrm{ker}L$ is 1 if and only if G is connected.

Exercise 2.1. Prove (2). Deduce from it that the dimension of $\mathrm{ker}L$ is equal to the number of connected components of G.
Hint: let S be the nodes in a connected component of G and consider $v = \mathbf{1}_S$ in (2).

For any given $S \subseteq V$ we have

$$\mathbf{1}_S^T L\mathbf{1}_S = \mathbf{1}_S^T D\mathbf{1}_S - \mathbf{1}_S^T A\mathbf{1}_S = \mathrm{vol}\, S - e_{\mathrm{in}}(S) = e_{\mathrm{out}}(S).$$

Define $v \in \mathbb{R}^n$ as $v = \mathbf{1}_S - (|S|/n)\mathbf{1}$, that is

$$v_i = \begin{cases} |\bar{S}|/n & i \in S \\ -|S|/n & i \notin S. \end{cases}$$

You can easily verify the following equalities:

$$\mathbf{1}^T v = 0, \qquad v^T v = \frac{|S||\bar{S}|}{n}, \qquad v^T L v = e_{\mathrm{out}}(S), \qquad h(S,\bar{S}) = \frac{v^T L v}{v^T v}. \tag{3}$$

We obtain a nontrivial lower bound for the number h_G defined in (1):

Theorem 2.2. *Let G be connected, and let $0 = \lambda_1 < \lambda_2 \le \dots \lambda_n$ be the eigenvalues of L. Then, $h_G \le \lambda_2$.*

Proof. Owing to the variational characterization of the eigenvalues of a symmetric matrix,[3] we have exactly

$$\lambda_2 = \min_{v:\mathbf{1}^T v = 0} \frac{v^T L v}{v^T v}.$$

Moreover, by (3), all possible values of $h(S,\bar{S})$ are contained in the right hand side of the previous equality. ■

Hence, the eigenvalue λ_2, which is named the *algebraic connectivity of G* after [2], tells us how easy is to split the graph into two (roughly balanced) pieces. Indeed, if $\lambda_2 \approx 0$ then G can be easily disconnected (in particular, if $\lambda_2 = 0$ then G is already divided into at least two parts) while, if h_G is large then also λ_2 must be large.

[3] See e.g., [6, §5.6].

2.2 The spectral cut

The nodal domains of an eigenvector associated to λ_2 often provide good approximations to the cut $\{S, \bar{S}\}$ which optimizes $h(S, \bar{S})$. Their connectedness is considered in the following result:

Theorem 2.3. *Let G be a connected, undirected graph. Suppose that the Laplacian matrix L has eigenvalues $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$. Let f an eigenvector associated to λ_2 and let $S = \{i : f_i \geq 0\}$. Then $G(S)$ is connected.*

PROOF. By choosing a sufficiently large positive constant α, the matrix $M = \alpha I - L = \alpha I - D + A$ is nonnegative and irreducible. Moreover, any eigenvector of M is also an eigenvector of L, and conversely. Indeed, $Mv = \mu v \iff Lv = (\alpha - \mu)v$. In particular we see that the eigenvalues of M are the numbers $\alpha > \alpha - \lambda_2 \geq \ldots \geq \lambda_n$. The claim follows immediately from Theorem 1.2. ■

3 Community detection

The goal of a community detection problem is to reveal the presence of "communities", that is, groups of nodes that are tightly connected. Community detection is different from graph partitioning, under many respects. Indeed, a good division of a network into communities is not merely one in which there are few edges between communities; it is one in which edges between communities are fewer than expected. Indeed, according to the original idea of Newman and Girvan [4], a set $S \subset V$ can be recognized as a community only if the number $e_{\text{out}}(S)$ is smaller than the average value of that number, if edges are placed at random.

Here comes an important question: How we quantify the expected number of edges between two arbitrary subsets of a random graph? One of the most convenient and widespread solutions to this problem is based on the following argument, which supposes that we know the degrees $d_1, \ldots, d_n$ of all nodes of G but not the way they are connected.

The total number of (undirected) edges in the graph is $\frac{1}{2}\text{vol}\, V$ (why?). Let S and T be two arbitrary disjoint subsets of V. Pick any of the edges in E, say ij. If edges are placed at random, then

- the probability that $i \in S$ is $\text{vol}\, S/\text{vol}\, V$
- the probability that $j \in T$ is $\text{vol}\, T/\text{vol}\, V$
- the probability that ij connects S and T is $2\,\text{vol}\, S\,\text{vol}\, T/(\text{vol}\, V)^2$.

But there are exactly $\frac{1}{2}\text{vol}\, V$ edges in G. Hence the average number of edges running between S and T can be estimated as $\text{vol}\, S\,\text{vol}\, T/\text{vol}\, V$. That estimate is not rigorous (because the argument allows the presence of multiple edges between two nodes) but is a good approximation of the exact value, in particular when G is sparse, that is $\text{vol}\, V \ll n^2$, as is often the case with complex networks found in real world.

3.1 The modularity matrix

Define the *modularity* of $S \subseteq V$ as

$$Q(S) = \frac{\text{vol}\, S\,\text{vol}\, \bar{S}}{\text{vol}\, V} - e_{\text{out}}(S).$$

This is the difference between the number of edges connecting S with its exterior and the expectation of that number if edges were placed at random. Hence, the inequality $Q(S) > 0$ may indicate that S is a "community" inside G, and we say that S is a *module*. On the other hand, if $Q(S) \leq 0$ then S is well connected with its exterior, and it is unlikely to be a "community".

Note that $Q(S) = Q(\bar{S})$. Moreover, we have the alternative formula (prove it!)

$$Q(S) = e_{\text{in}}(S) - \frac{(\text{vol}\, S)^2}{\text{vol}\, V}.$$

Introduce the *modularity matrix* $M = A - dd^T/\text{vol}\, V$. Then,

$$\mathbf{1}_S^T M \mathbf{1}_S = \mathbf{1}_S^T A \mathbf{1}_S - \frac{(d^T \mathbf{1}_S)^2}{\text{vol}\, V} = e_{\text{in}}(S) - \frac{(\text{vol}\, S)^2}{\text{vol}\, V} = Q(S).$$

Note: $M\mathbf{1} = 0$, whence $Q(V) = 0$. The following result tells us that if $\rho(M)$ is small then G "looks like a random graph."

Theorem 3.1. *Let S and T be any two disjoint subsets of V, and let $e(S,T)$ denote the number of edges joining S and T. Then,*

$$\left| e(S,T) - \frac{\operatorname{vol} S \operatorname{vol} V}{\operatorname{vol} V} \right| \leq \frac{\sqrt{|S||\bar{S}||T||\bar{T}|}}{n} \rho(M). \tag{4}$$

PROOF. Noting that $e(S,T) = \mathbf{1}_S^T A \mathbf{1}_T$, straightforward computations prove that the left hand side of (4) is exactly $|\mathbf{1}_S^T M \mathbf{1}_T|$. Introduce the vectors $v = \mathbf{1}_S - (|\bar{S}|/n)\mathbf{1}$ and $w = \mathbf{1}_T - (|\bar{T}|/n)\mathbf{1}$. We have

$$\mathbf{1}^T v = 0, \qquad \|v\|_2^2 = v^T v = \frac{|S||\bar{S}|}{n},$$

and analogous formulas for w. Finally, using $M\mathbf{1} = 0$ we have

$$|\mathbf{1}_S^T M \mathbf{1}_T| = |v^T M w| \leq \|v\|_2 \|w\|_2 \|M\|_2 \leq \frac{\sqrt{|S||\bar{S}||T||\bar{T}|}}{n} \|M\|_2.$$

To complete the proof it suffices to observe that $\|M\|_2 = \rho(M)$ since M is symmetric. ∎

Note that the right hand side of (4) is not larger than $\frac{n}{4}\rho(M)$, independently on S and T; but becomes a small multiple of $\rho(M)$ when both S and T are tiny.

3.2 The cut-modularity problem

In what follows, I will consider the simplest version of the community detection problem, where we look for a cut $\{S, \bar{S}\}$ which maximizes the merit function

$$q(S, \bar{S}) = \frac{Q(S)}{|S|} + \frac{Q(\bar{S})}{|\bar{S}|} = \ldots = Q(S) \frac{n}{|S||\bar{S}|}.$$

By arguing exactly as in Theorem 2.2 we can obtain the following result:

Theorem 3.2. *Let M be the modularity matrix of a connected graph, and let*

$$m_G = \max_{v : \mathbf{1}^T v = 0} \frac{v^T M v}{v^T v}. \tag{5}$$

Then, $\max_{S \subseteq V} q(S, \bar{S}) \leq m_G$.

Remark 3.3. *The equation $M\mathbf{1} = 0$ tells us that M has 0 as an eigenvalue; but that eigenvalue may not be simple. On the basis of the variational characterization of the eigenvalues of a symmetric matrix,[4] it is not difficult to conclude that the number m_G defined in (5) is the largest eigenvalue of M that remains after deflation of one zero eigenvalue from the spectrum of M.*

Analogously to the graph partitioning problem, the most popular and successful heuristic method to approximate the solution of the cut-modularity problem $\max_{S \subseteq V} q(S, \bar{S})$ is to compute an eigenvector v such that $Mv = m_G v$, $\mathbf{1}^T v = 0$ and then set $S = \{i : v_i \geq 0\}$ [5]. Actually, one can prove that[5]

- at least one subgraph among $G(S)$ and $G(\bar{S})$ is connected;
- there exist graphs such that only one among $G(S)$ and $G(\bar{S})$ is connected, while the other subgraph splits into any arbitrary number of nodal domains;
- there is a relationship between the number of positive eigenvalues of M and the number of distinct modules in G.

[4] See e.g., [6, §5.6].
[5] See the lecture by F. Tudisco "Spectral inequalities for the modularity of a graph". For a reference, see [1].

4 Exercises and problems

Exercises marked with a star ($\star$) are requested for the final evaluation.

1. ($\star$) Let G be a star graph with n nodes.
   - Compute the spectral decomposition of its modularity matrix M.
   - Compute the number m_G from (5).
   - Use the preceding results to prove that G has no modules.
2. Repeat the preceding exercise for a clique, that is the graph whose adjacency matrix is

$$A = \begin{pmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 1 \\ 1 & \cdots & 1 & 0 \end{pmatrix}.$$

3. Let i and j two distinct nodes in a loop-free graph G that are joined by an (undirected) edge, $i \sim j$. Let d_i and d_j be their respective degrees. Prove that if $d_i + d_j < \sqrt{\operatorname{vol} V}$ then the set $S = \{i, j\}$ is a module.
4. Let i and j two distinct nodes in a undirected graph G. Let $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$ be the eigenvalues of the Laplacian matrix. Prove that $\lambda_2 \leq \frac{1}{2}(d_i + d_j) + \delta \leq \lambda_n$ where $\delta = 1$ if $i \sim j$ and $\delta = 0$ otherwise.

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`Last update: September 17, 2014`