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

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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 $1_S$ its characteristic vector, that is $(1_S)_i = 1$ if $i \in S$ and 0 otherwise.
- Let $\text{vol}_S = \sum_{i \in S} d_i$ be the volume of $S$ (recall that $d_i$ is the degree of node $i$). Note: $\text{vol}_S = d^T 1_S$.
- Let $e_{\text{in}}(S) = 1^T_S A 1_S$ and $e_{\text{out}}(S) = 1^T_S A (1 - 1_S) = \text{vol}_S - e_{\text{in}}(S)$. 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 $v$,

$$
\begin{align*}
G : & \quad 4 \quad 1 \\
& \quad 2 \quad 3 \\
\end{align*}
\quad v = \begin{pmatrix} 1 \\ -2 \\ 0 \\ 0.1 \end{pmatrix} \quad \leadsto \quad G(S) : \quad 4 \quad 1 \\
& \quad 3
\end{align*}
$$

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

1 See e.g., [6, §5.7].
2 Graph partitioning problems

Proof. Proceed by contradiction. Assume that \( S = S_1 \cup S_2 \) with \( S_1 \cap S_2 = \emptyset \), 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 \( Av = \lambda v \) leads to

\[
A_{11}v_1 + A_{13}v_3 = \lambda_2 v_1 \\
A_{22}v_2 + A_{23}v_3 = \lambda_2 v_2.
\]

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

\[
y_i^TA_{ii}v_i + y_i^TA_{3i}v_3 = \lambda_2 y_i^Tv_i, \quad i = 1, 2.
\]

Since \( y_i^Tv_i > 0 \) we get \( \rho(A_{ii}) > \lambda_2 \) for \( i = 1, 2 \). Hence, the submatrix \( \begin{pmatrix} A_{11} & O \\ O & A_{22} \end{pmatrix} \) has 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 \( \lambda_i \) with \( i \geq 2 \). The result is that, if \( Av = \lambda v \) 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 \( S \cap \bar{S} = \emptyset \). The pair \( \{S, \bar{S}\} \) is a cut in \( G \).

For any \( S \subseteq V \) consider the number

\[
H(S) = e_{out}(S)/|S|,
\]

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 partitioning problems, a useful merit function of the graph cut \( \{S, \bar{S}\} \) (which is easily generalized to more than two sets) is the following:

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

As an exercise, you may fill in the blanks in the previous equality.\(^2\)

\(^2\) Note: \( e_{out}(S) = e_{out}(\bar{S}) \).
One of the main graph partitioning problems consists in computing

\[ h_G = \min_{S \subseteq V} h(S, \bar{S}) \]  

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 \( D = \text{Diag}(d_1, \ldots, d_n) \). 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

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

where the sum runs over the set of edges, every edge being counted only once. Thus, \( L \) is positive semidefinite; the vector \( 1 \) is in the kernel of \( L \), that is \( L1 = 0 \); and the dimension of \( \ker L \) is 1 if and only if \( G \) is connected.

**Exercise 2.1.** Prove (2). Deduce from it that the dimension of \( \ker L \) is equal to the number of connected components of \( G \).

*Hint: let \( S \) be the nodes in a connected component of \( G \) and consider \( v = 1_S \) in (2).*

For any given \( S \subseteq V \) we have

\[ 1_S^T L 1_S = 1_S^T D 1_S - 1_S^T A 1_S = \text{vol} S - e_{\text{in}}(S) = e_{\text{out}}(S). \]

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

\[ v_i = \begin{cases} |S|/n & i \in S \\ -|S|/n & i \notin S \end{cases} \]

You can easily verify the following equalities:

\[ 1^Tv = 0, \quad v^Tv = \frac{|S||\bar{S}|}{n}, \quad v^T L v = e_{\text{out}}(S), \quad h(S, \bar{S}) = \frac{e_{\text{out}}(S)}{v^Tv}. \]  

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

**Theorem 2.2.** Let \( G \) be connected, and let \( 0 = \lambda_1 < \lambda_2 \leq \ldots \lambda_n \) be the eigenvalues of \( L \). Then, \( h_G \leq \lambda_2 \).

**Proof.** Owing to the variational characterization of the eigenvalues of a symmetric matrix,\(^3\) we have exactly

\[ \lambda_2 = \min_{v : 1^Tv = 0} \frac{v^T L v}{v^Tv}. \]

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 \( \lambda_2 \), 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 \( \lambda_2 \) must be large.

\(^3\) See e.g., [6, §5.6].
2.2 The spectral cut

The nodal domains of an eigenvector associated to \( \lambda_2 \) 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 \( f \) be an eigenvector associated to \( \lambda_2 \) and let \( S = \{ i : f_i \geq 0 \} \). Then \( G(S) \) is connected.

**Proof.** By choosing a sufficiently large positive constant \( \alpha \), 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 \( \alpha > \lambda_2 > \ldots \geq \lambda_n \). 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 \( e_{out}(S) \) 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 vol \( S/\text{vol } V \)
- the probability that \( j \in T \) is 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

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

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!)

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

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

\[
1_S^T M 1_S = 1_S^T A 1_S - \frac{(d^T 1_S)^2}{\text{vol } V} = e_{in}(S) - \frac{(\text{vol } S)^2}{\text{vol } V} = Q(S).
\]
Note: $M1 = 0$, 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,

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

**Proof.** Noting that $e(S,T)$ is the number of edges connecting $S$ and $T$, straightforward computations prove that the left hand side of (4) is exactly $|1_T^TM1_T|$. Introduce the vectors $v = 1_S - (|S|/n)1$ and $w = 1_T - (|T|/n)1$. We have

$$1_T^Tv = 0, \quad \|v\|^2_2 = v^TMv = \frac{|S||S|}{n},$$

and analogous formulas for $w$. Finally, using $M1 = 0$ we have

$$|1_T^TM1_T| = |v^TMw| \leq \|v\|_2 \|w\|_2 \|M\|_2 \leq \sqrt{\frac{|S||S||T||T|}{n}} \|M\|_2.$$  

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 $\frac{n}{2} \rho(M)$, 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

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

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

$$m_G = \max_{v: 1^Tv = 0} \frac{v^TMv}{v^Tv}.$$  

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

**Remark 3.3.** The equation $M1 = 0$ 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 $Mv = m_Gv$, $1^Tv = 0$ and then set $S = \{i : v_i \leq 0\}$ [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 $G$.

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\(^4\) 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 (⋆) are requested for the final evaluation.

1. (⋆) 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 $d_i + d_j < \sqrt{\text{vol} \, V}$ then the set $S = \{i, j\}$ is a module.

4. Let $i$ and $j$ two distinct nodes in a undirected graph $G$. Let $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ 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.

References


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