Fiedler Vector Method

Project for Linear algebra and its Applications

Sagnik Dutta   Nilava Metya   Sagnik Mukherjee

CHENNAI MATHEMATICAL INSTITUTE

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Statement

Given a (finite simple connected) graph $G = (V, E)$, partition $V = V_1 \sqcup V_2$ such that the number of "cut" edges is minimized, while keeping $|V_1| \simeq |V_2|$.

Terminology and definitions

To every finite undirected graph $G = (V, E)$, we can associate the following matrices:

- *Adjacency matrix* A of size $|V| \times |V|$. $A_{i,j} = \mathbf{1}_{\{i,j\} \in E}$.
- *Degree matrix* D of size $|V| \times |V|$. $D_{i,j} = \delta_i^j \cdot \deg(i)$.
- *Incidence matrix* H of size $|V| \times |E|$. $H_{v,e} = \begin{cases} 1 & \text{if } v \text{ adjacent to edge } e \\ 0 & \text{else} \end{cases}$.
- *Laplacian* $\mathcal{L}$ of size $|V| \times |V|$. $L = D - A$.

Elementary results

$\mathcal{L}$ has real eigenvalues.

$\mathcal{L}$ is real symmetric. ■

Fact: $\mathcal{L} = HH^t$.

$\mathcal{L}$ is positive semidefinite.

$\mathcal{L}\boldsymbol{v} = \lambda\boldsymbol{v}$, then $\lambda \|\boldsymbol{v}\|^2 = \langle \mathcal{L}\boldsymbol{v}, \boldsymbol{v} \rangle = \boldsymbol{v}^t H H^t \boldsymbol{v} = \|H^t \boldsymbol{v}\|^2$. ■

$\mathcal{L}$ has only nonnegative eigenvalues. We note that the eigenvalue 0 is always achieved. Indeed, $\mathcal{L}(1, \cdots, 1) = (0, \cdots, 0)$.

Modelling a partition

Recall that a partition of graph $G = (V, E)$ is a partition of $V = V_1 \sqcup V_2$. For a partition $P = (V_1, V_2)$, define its cut $\mathfrak{C}(P)$ to be the number of edges in E with at least one endpoint in each V_i.

Think of a partition as assigning ± 1 to each vertex, with the agreement that vertex i lies in V_1 when it's assigned $+1$, and it's in V_2 otherwise. Say vertex i is assigned x_i, which gives a vector $\boldsymbol{x} = (x_1, \cdots, x_n)$.

What is the cut value for the aforesaid assignment?

The cut value of partition $P = (V_1, V_2)$ is $\mathfrak{C}(P) = \sum_{\substack{\{i,j\}\in E \\ x_i \neq x_j}} 1$. Some clever manipulation gives

$$\begin{aligned} 4 \cdot \mathfrak{C}(P) = 4 \sum_{\substack{\{i,j\}\in E \\ x_i \neq x_j}} 1 &= \sum_{\substack{\{i,j\}\in E \\ x_i \neq x_j}} (\pm 2)^2 + \sum_{\substack{\{i,j\}\in E \\ x_i = x_j}} 0^2 \\ &= \sum_{\substack{\{i,j\}\in E \\ x_i \neq x_j}} (x_i - x_j)^2 + \sum_{\substack{\{i,j\}\in E \\ x_i = x_j}} (x_i - x_j)^2 \\ &= \sum_{\{i,j\}\in E} (x_i - x_j)^2 \end{aligned}$$

What does $|V_1| \simeq |V_2|$ mean?

If V_1 and V_2 were to have the same number of vertices, it simply means that equal number of verticles are assigned $+1$ and -1. This is to say that $\sum x_i = 0$.

Conversely $\sum x_i = 0$ (where each $x_i \in \{\pm 1\}$) means that same number of vertices are assigned ± 1 each. That simply means $|V_1| = |V_2|$.

Now $|V_1| \simeq |V_2|$ simply means we want $|\sum x_i|$ to be as small as possible. That is, $\sum x_i \simeq 0$.

GOAL

Find $\boldsymbol{x} \in \{\pm 1\}^n$ with $\sum x_i \simeq 0$ such that

$$\sum_{\{i,j\} \in E} (x_i - x_j)^2$$

is minimized.

Note that the condition of each x_i being ± 1 implies $\sum x_i^2 = n$. The converse is true if we ask each $x_i \in [-1, 1]$. So we are not giving up much.
Asking for only an approximate solution, we replace the condition $\sum x_i \simeq 0$ with $\sum x_i = 0$.

NEW (approximate) GOAL

Find $\boldsymbol{x} \in \mathbb{R}^n$ with $\sum x_i = 0$ such that

$$\sum_{\{i,j\} \in E} (x_i - x_j)^2$$

is minimized (subject to $\sum_i x_i^2 = 1$).

Bring in the matrices ⋯

Some clever manipulation:

$$\sum_{\{i,j\}\in E}(x_i - x_j)^2 = \sum_{\{i,j\}\in E}\left(x_i^2 + x_j^2 - 2x_ix_j\right) = \sum_i \underbrace{\deg(i)}_{d_i} x_i^2 - 2\sum_{\{i,j\}\in E} x_ix_j$$

$$= \boldsymbol{x}^t \begin{bmatrix} d_1 & & \\ & \ddots & \\ & & d_n \end{bmatrix} \boldsymbol{x} - \boldsymbol{x}^t A\boldsymbol{x} = \boldsymbol{x}^t(D - A)\boldsymbol{x} = \boldsymbol{x}^t \mathcal{L}\boldsymbol{x}$$

Illustration for =

$$\begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x & y \end{bmatrix} \begin{bmatrix} a_{11}x + a_{12}y \\ a_{21}x + a_{22}y \end{bmatrix} = a_{11}x^2 + (a_{12} + a_{21})xy + a_{22}y^2.$$

If the above matrix is symmetric, then the result is $a_{11}x^2 + \underline{2a_{12}}xy + a_{22}y^2$.

So our problem becomes $\cdots$

For what $\boldsymbol{x}$ is $\boldsymbol{x}^t \mathcal{L} \boldsymbol{x}$ minimized, subject to $\|\boldsymbol{x}\|^2 = n$ and $\langle \boldsymbol{x}, (1, \cdots, 1) \rangle = 0$.

An equivalent optimization problem is

Find the argument $\boldsymbol{x}$ for

$$\min_{\substack{\boldsymbol{x} \perp (1,\cdots,1) \\ \|\boldsymbol{x}\| \neq 0}} \frac{\boldsymbol{x}^t \mathcal{L} \boldsymbol{x}}{\|\boldsymbol{x}\|^2} = \min_{\substack{\boldsymbol{x} \perp (1,\cdots,1) \\ \|\boldsymbol{x}\| \neq 0}} R_{\mathcal{L}}(\boldsymbol{x}).$$

Recall from class

If $A_{n\times n}$ is a real symmetric positive semidefinite matrix with eigenvalues $0 \leq \lambda_1 \leq \cdots \leq \lambda_n$ with eigenbasis $(\boldsymbol{v}_1, \cdots, \boldsymbol{v}_n)$ (such that $A\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$) then

$$\min_{\substack{\boldsymbol{x}\perp\langle \boldsymbol{v}_1,\cdots,\boldsymbol{v}_k\rangle \\ \|\boldsymbol{x}\|\neq 0}} R_{\mathcal{L}}(\boldsymbol{x}) = \lambda_{k+1}.$$

Our interest is

In particular for $k = 1$

$$\min_{\substack{\boldsymbol{x} \perp (1, \cdots, 1) \\ \|\boldsymbol{x}\| \neq 0}} R_{\mathcal{L}}(\boldsymbol{x}) = \lambda_2$$

because 0 is always an eigenvalue of $\mathcal{L}$ corresponding to the eigenvector $(1, 1, \cdots, 1)$.

Our algorithm

Initially we had asked that we'll take $i \in V_1$ if $x_i = +1$, and $i \in V_2$ if $x_i = -1$. But while arriving to our optimization problem, we were 'loose' about $x_i \in \{\pm 1\}$, we now our alrorithm becomes:

Look at the i^{th} component of a Fiedler vector. If it is < 0, put the i^{th} vertex in V_1, otherwise put it in V_2.

Theorem (Fiedler's theorem of connectivity of spectral graph partitions)

Let $G = (V, E)$ be a connected graph and let $\boldsymbol{x} = (x_1, \cdots, x_n)$ is the Fiedler vector for the Laplacian of this graph. Let $V_1 = \{i : x_i > 0\}$ and $V_2 = V \setminus V_1$. Let G_i be the subgraphs induced by V_i. Then G_i are both connected.

Suppose not . . .

(Re)label the vertices in a way such that $V_1 = \{1, \cdots, k\}, V_2 = \{k+1, \cdots, n\}$. For the sake of contradiction suppose G_1 has (at least) two connected components; say the vertices are $\{1, \cdots, t\}$ and $\{t+1, \cdots, k\}$. So the Laplacian looks like

$$\mathcal{L} = \begin{bmatrix} L_{11} & \mathbf{0} & L_{13} \\ \mathbf{0} & L_{22} & L_{23} \\ L_{13}^T & L_{23}^T & L_{33} \end{bmatrix}.$$

By nature of $\mathcal{L}$, the entries of L_{13}, L_{23} are nonpositive. Write the similar block form for

$$\boldsymbol{x} = \begin{bmatrix} (\boldsymbol{x}_1)_{t\times 1} \\ (\boldsymbol{x}_2)_{(k-t)\times 1} \\ (\boldsymbol{x}_3)_{(n-k)\times 1} \end{bmatrix}.$$

where components of $\boldsymbol{x}_1, \boldsymbol{x}_2$ are positive and those of $\boldsymbol{x}_3$ are negative.

We produce two eigenvalues of $\mathcal{L}$ which are less than λ_2. Contradiction!

$\mathcal{L}\boldsymbol{x} = \lambda_2 \boldsymbol{x} \implies L_{11}\boldsymbol{x}_1 + L_{13}\boldsymbol{x}_3 = \lambda_2 \boldsymbol{x}_1$
Fix any positive real $\varepsilon > 0$. Then $(\varepsilon I + L_{11})\boldsymbol{x}_1 + L_{13}\boldsymbol{x}_3 = (\varepsilon + \lambda_2)\boldsymbol{x}_1$.
Assume that $(\varepsilon I + L_{11})$ is invertible and its inverse Y is a positive matrix. Multiplying both sides of the above equation by Y, we get

$$\begin{aligned} \boldsymbol{x}_1 + Y L_{13}\boldsymbol{x}_3 &= (\varepsilon + \lambda_2) Y \boldsymbol{x}_1 \\ \implies \boldsymbol{x}_1^T \boldsymbol{x}_1 + \boldsymbol{x}_1^T Y L_{13}\boldsymbol{x}_3 &= (\varepsilon + \lambda_2)\boldsymbol{x}_1^T Y \boldsymbol{x}_1 \\ \implies (\varepsilon + \lambda_2)\frac{\boldsymbol{x}_1^T Y \boldsymbol{x}_1}{\boldsymbol{x}_1^T \boldsymbol{x}_1} &= 1 + \frac{\boldsymbol{x}_1^T Y L_{13}\boldsymbol{x}_3}{\boldsymbol{x}_1^T \boldsymbol{x}_1} > 1 \\ \implies (\varepsilon + \lambda_2)\lambda_t(Y) &= (\varepsilon + \lambda_2)\max_{v \neq 0}\frac{v^T Y v}{v^T v} > 1 \\ \implies \lambda_1(\varepsilon I + L_{11}) &= 1/\lambda_t(Y) < \varepsilon + \lambda_2 \\ \implies \varepsilon + \lambda_1(L_{11}) &< \varepsilon + \lambda_2 \end{aligned}$$

Hence $\lambda_1(L_{11}) < \lambda_2$. Similarly, $\lambda_1(L_{22}) < \lambda_2$.

If the eigenvectors corresponding to $\lambda_1(L_{11})$ and $\lambda_1(L_{22})$ are v_1 and v_2 respectively, then

$$\begin{bmatrix} L_{11} & 0 \\ 0 & L_{22} \end{bmatrix} \begin{bmatrix} v_1 \\ 0 \end{bmatrix} = \lambda_1(L_{11}) \begin{bmatrix} v_1 \\ 0 \end{bmatrix} \qquad \text{and} \qquad \begin{bmatrix} L_{11} & 0 \\ 0 & L_{22} \end{bmatrix} \begin{bmatrix} v_2 \\ 0 \end{bmatrix} = \lambda_1(L_{22}) \begin{bmatrix} v_2 \\ 0 \end{bmatrix}.$$

Thus the matrix $\begin{bmatrix} L_{11} & 0 \\ 0 & L_{22} \end{bmatrix}$ has two eigenvalues less than λ_2.

Theorem (Cauchy Interlacing theorem)

Let $A_{n\times n}$ be a symmetric matrix and $B_{m\times m}$ be a principal submatrix of A. Further, let the eigenvalues of A be $\lambda_1 \leq \cdots \leq \lambda_n$ and the eigenvalues of B be $\beta_1 \leq \cdots \leq \beta_m$. Then, for all $k \leq m$, the matrix A has at least k eigenvalues less than or equal to β_k.

By Cauchy Interlacing theorem, $\mathcal{L}$ has two eigenvalues less than λ_2, which is a contradiction!

Now we show that $(\varepsilon I + L_{11})$ is invertible and its inverse Y is positive.

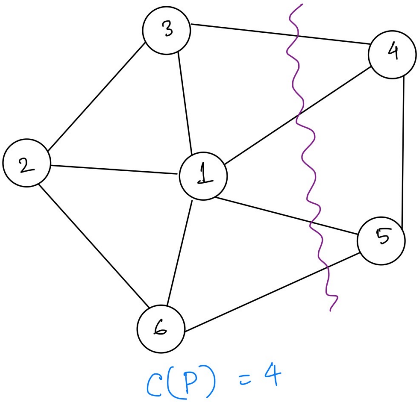
$$\begin{aligned}
&\varepsilon I + L_{11} \\
&= D - N \\
&= D^{1/2}(I - D^{-1/2} N D^{-1/2}) D^{1/2} \\
&= D^{1/2}(I - M) D^{1/2}
\end{aligned}$$

Because of some useful properties of M, it can be shown that $(I - M)^{-1} = \sum_{l=0}^{\infty} M^l$.

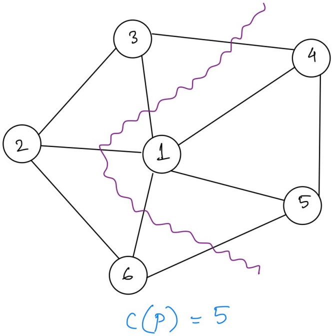
$$\begin{aligned}
\therefore Y &= (\varepsilon I + L_{11})^{-1} \\
&= D^{-1/2}(I - M)^{-1} D^{-1/2} \\
&= D^{-1/2} \cdot \sum_{l=0}^{\infty} M^l \cdot D^{-1/2}
\end{aligned}$$

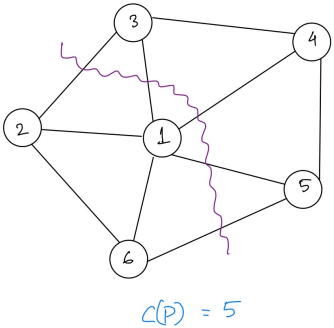
Y is positive as $\sum_{l=0}^{\infty} M^l$ is positive.

Example 1

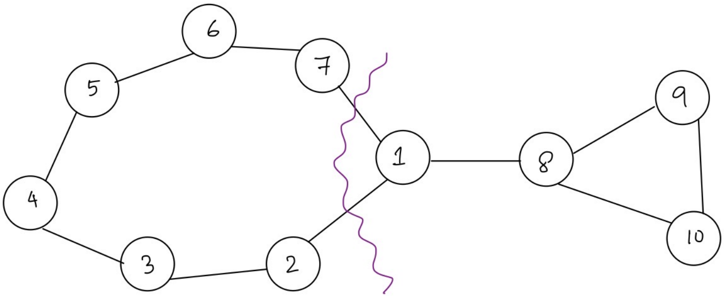


Example 1: But...



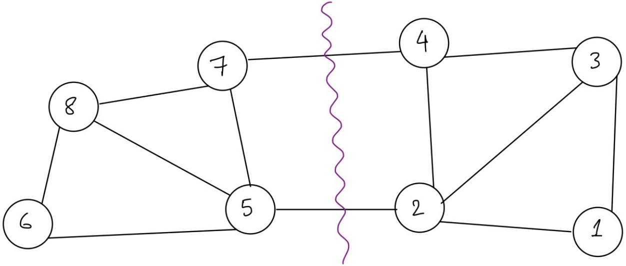


Example 2



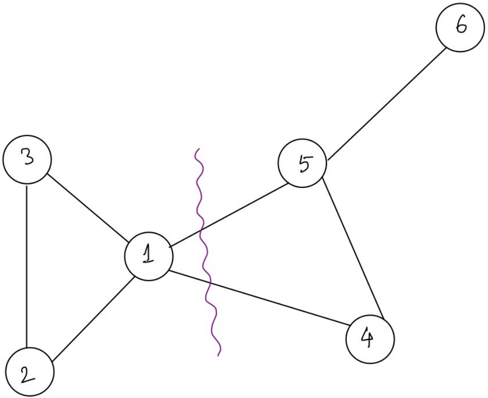
$C(P) = 2$

Example 3



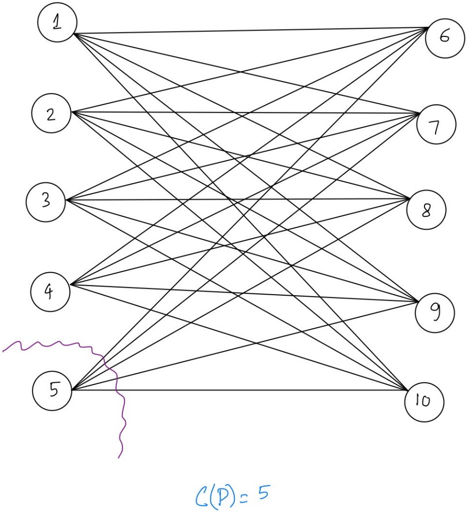
$C(P) = 2$

Example 4

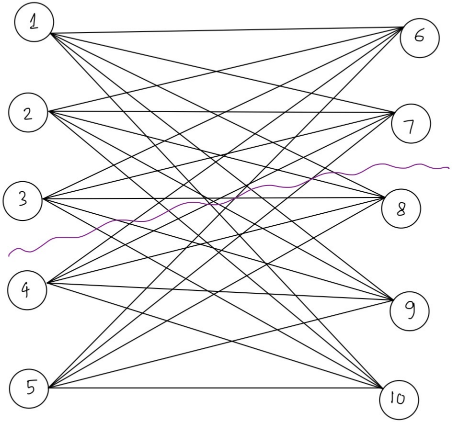


$c(P) = 2$

Example 5



Example 5: But...



$C(P) = 13$

What effect does connectedness have on λ_2?

Lemma

$\lambda_2 > 0 \iff$ *the graph connected.*

Proof.

If G has two connected components, then $(1 \cdots, 1, 0 \cdots, 0)$ and $(1 \cdots, 1, 0 \cdots, 0)$ are LI eigenvectors for 0.
If G is connected, then use $\boldsymbol{v}^t \mathcal{L} \boldsymbol{v} = \sum_{\{i,j\} \in E} (v_i - v_j)^2$ to show that geometric (=algebraic) multiplicity of 0 is one. ∎

Terminology

λ_2 is also called the algebraic connectivity of the graph.

What if all components are positive?

Say $\mathcal{L}\boldsymbol{v} = \lambda \boldsymbol{v}$ with $\lambda > 0$.

$$l_{11}v_1 + \cdots + l_{1n}v_n = \lambda v_1$$
$$\vdots$$
$$l_{n1}v_1 + \cdots + l_{nn}v_n = \lambda v_n$$

Adding these gives $\sum_{i=1}^{n} l_{i1}v_1 + \cdots + \sum_{i=1}^{n} l_{in}v_n = \lambda \sum_{i=1}^{n} v_i$. All the red sums are 0 because of the way $\mathcal{L}$ is defined. It follows that $\sum_i v_i = 0$ because $\lambda > 0$.

How to balance so many 0's (if at all)?

What do we do if there are only a few nonzero components of the Fiedler vector and a bunch of 0's?

One conjecture we made was

For a connected graph G with Laplacian $\mathcal{L}$, let $\boldsymbol{v}$ be a Fiedler vector. Look at $S = \{i : v_i = 0\}$. Then for each $i \in S, \exists j, k$ such that $v_j > 0, v_k < 0$ and both j and k are neighbours of i.

The above conjecture is false. A counterexample is $K_{n,n}$, the complete bipartite graph on $2n$ vertices.