Graph Laplacian.

- basic properties
- graph connectivity
- graph partition
- spectral clustering.

Some linear algebra :

* **Rayleigh quotient.**

Let A be a ~~square~~ symmetric matrix.

Then all eigenvalues of A are real :

$$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n.$$

The Rayleigh quotient of A is of the form $\dfrac{\vec{x}^T A \vec{x}}{\vec{x}^T \vec{x}}$

and has the property

$$\lambda_1 = \min_{\vec{x} \neq 0} \frac{\vec{x}^T A \vec{x}}{\vec{x}^T \vec{x}}, \quad \lambda_n = \max_{\vec{x} \neq 0} \frac{\vec{x}^T A \vec{x}}{\vec{x}^T \vec{x}}.$$

- Reason: Suppose $\{\vec{v}_1, \ldots, \vec{v}_n\}$ are the unit eigenvectors for $\{\lambda_1, \ldots, \lambda_n\}$.

We may assume $|\vec{x}| = 1$ and $\vec{x} = c_1\vec{v}_1 + \cdots + c_n\vec{v}_n$.

$$\Rightarrow \vec{x}^T A \vec{x} = (c_1\vec{v}_1 + \cdots + c_n\vec{v}_n)^T (c_1\lambda_1\vec{v}_1 + \cdots + \cancel{c_n v_n}\; c_n\lambda_n\vec{v}_n)$$

$$= c_1^2\lambda_1 + c_2^2\lambda_2 + \cdots + c_n^2\lambda_n$$

$$(\,|\vec{v}_1| = \cdots = |\vec{v}_n| = 1\,)$$

* Courant–Fischer theorem

A : sym.

$\lambda_1 \le \cdots \le \lambda_n$: eigenvalues.

$$\lambda_k = \max_{\substack{S \\ \dim S = k-1}} \min_{\substack{\vec{x} \neq 0 \\ \vec{x} \in S^\perp}} \frac{\vec{x}^T A \vec{x}}{\vec{x}^T \vec{x}} = \min_{\substack{S \\ \dim S = n-k}} \max_{\substack{\vec{x} \neq 0 \\ \vec{x} \in S^\perp}} \frac{\vec{x}^T A \vec{x}}{\vec{x}^T \vec{x}}$$

~~eg~~.

maximized by $S = \mathrm{span}\{\vec{v}_1, \ldots, \vec{v}_{k-1}\}$

minimized by $S = \mathrm{span}\{\vec{v}_{k+1}, \ldots, \vec{v}_n\}$.

(Suppose $\vec{v}_1, \ldots, \vec{v}_n$ are eigenvectors of $\lambda_1, \ldots, \lambda_n$)

Corollary.

Let A be a sym matrix with eigenvalues $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$ and eigenvectors $\vec{v}_1, \ldots, \vec{v}_n$.

Then
$$\lambda_2 = \min_{\substack{\vec{x} \neq 0 \\ \vec{x} \perp \vec{v}_1}} \frac{\vec{x}^T A \vec{x}}{\vec{x}^T \vec{x}}.$$

* Cauchy interlacing theorem.

A: sym matrix

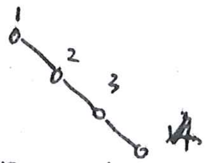
$A(i)$: $(n-1)\times(n-1)$ matrix by removing i-th row/column.

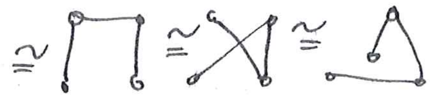
$\lambda_1 \le \cdots \le \lambda_n$: eigvals of A

$\mu_1 \le \cdots \le \mu_{n-1}$: eigvals of $A(i)$.

Then
$$\lambda_1 \le \mu_1 \le \lambda_2 \le \mu_2 \le \lambda_3 \cdots \lambda_{n-1} \le \mu_{n-1} \le \lambda_n.$$

Graph $G = (\underset{\text{vertices}}{V}, \underset{\text{edges}}{E})$.

e.g.  $V=\{1,2,3,4\}$. $E=\{12, 23, 34\}$. 位置不重要.



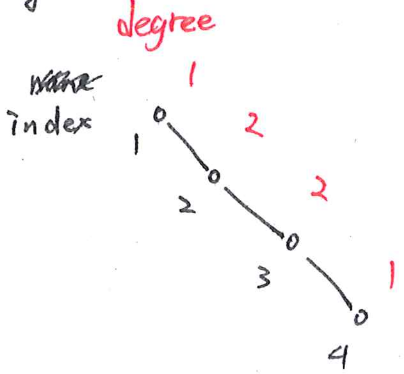
degeree: $\deg(i) = \#$ of edges incident to i.

For convenience, we assume $V=\{1,\dots,n\}$.

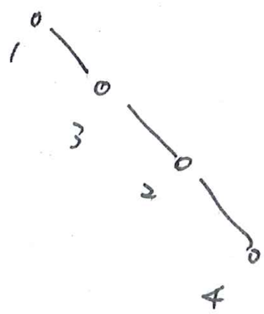
Laplacian matrix of a graph G

$$= L(G) := (l_{i,j}) \text{ with } \begin{cases} l_{i,j} = -1 & \text{if } ij \in E \\ l_{i,j} = \deg(i) & \text{if } i=j \\ l_{i,j} = 0 & \text{otherwise.} \end{cases}$$

e.g.



$$G \longleftrightarrow L(G) \quad \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix}$$



$$\longleftrightarrow \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 2 & -1 & -1 \\ -1 & -1 & 2 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}.$$

點的順序不影響 eigenvalue,
但影響 eigenvector 上 entry 的順序.

e.g.

$$\begin{pmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ \sqrt{2}-1 \\ -\sqrt{2}+1 \\ -1 \end{pmatrix} = (2-\sqrt{2}) \begin{pmatrix} 1 \\ \sqrt{2}-1 \\ -\sqrt{2}+1 \\ -1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 & -1 & 0 \\ 0 & 2 & -1 & -1 \\ -1 & -1 & 2 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ -\sqrt{2}+1 \\ \sqrt{2}-1 \\ -1 \end{pmatrix} = (2-\sqrt{2}) \begin{pmatrix} 1 \\ -\sqrt{2}+1 \\ \sqrt{2}-1 \\ -1 \end{pmatrix}$$

- Rayleigh quotient for Laplaciam matrix.

$L = L(G)$

$\vec{x} = (x_1, \dots, x_n)$

Then $$\frac{\vec{x}^T L \vec{x}}{\vec{x}\vec{x}} = \frac{\sum_{ij \in E} (x_i - x_j)^2}{\sum_{i=1}^{n} x_i^2}.$$

pf. $$\vec{x}^T L \vec{x} = \sum_{i=1}^{n} \deg(i) \cdot x_i^2 - 2\sum_{ij \in E} x_i x_j.$$

$$= \sum_{ij \in E} (x_i^2 + x_j^2 - 2x_i x_j)$$

x_i 被算了 $\deg(i)$ 次

$$\cancel{= \sum (x_i - x_j)^2}$$

$$= \sum_{ij \in E} (x_i - x_j)^2.$$

Observation

$$L \cdot \vec{1} = 0 \cdot \vec{1} = \vec{0}. \quad \text{for any } L = L(G).$$

Prop. Suppose $L = L(G)$.

Then ① L is positive semidefinite.

② 0 is an eigenvalue with eigenvector $\vec{1}$.

③ If G is connected, then $\text{nullity}(L) = 1$.

pf. ① Rayleigh quotient ≥ 0.

② By observation

有點 i 走不到點 j.

③

connected

not connected.

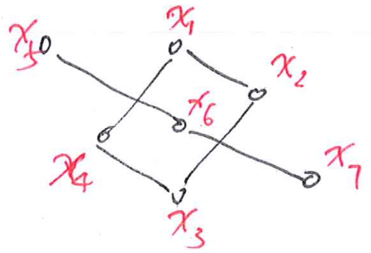
pf (continued). GL.

Suppose $\vec{x}$ is a unit null vector. (That is, $L\vec{x}=\vec{0}$).

Then $\dfrac{\vec{x}L\vec{x}}{\vec{x}^T\vec{x}}=0$ (assume $\vec{x}$ is a unit vector).

$$\Updownarrow$$

$$\sum_{ij\in E}(x_i-x_j)^2=0 \iff x_i=x_j \text{ for all } ij\in E.$$



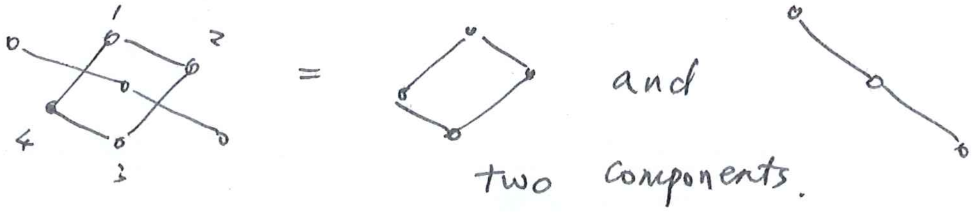
$$\begin{cases} x_1=x_2=x_3=x_4 \\ x_5=x_6=x_7 \end{cases}$$

If G is connected, then $\vec{x}=c\cdot\vec{1}$ (constant vector).

$\Rightarrow$ nullity $(G)=1$.

Defn. A <u>component</u> of a graph G. is

a maximal $\underbrace{\text{subgraph}}_{\text{connected}}$ ~~tha~~.



two components.

Defn. Let X be a subset of $[n]$.

The characteristic vector of X is

$$\phi_X=(\phi_1,\dots,\phi_n)$$

$$\phi_i=\begin{cases}1 & \text{if } i\in X\\ 0 & \text{if } i\notin X.\end{cases}$$

Corollary.

Suppose G has k components, whose vertex sets are $X_1, \dots, X_k$. Let $L = L(G)$.

Then $\text{nullity}(L) = k$, and

$$\text{nullspace}(L) = \text{span}\{\phi_{X_1}, \phi_{X_2}, \dots, \phi_{X_k}\}.$$

pf.

$$L(G) = \begin{pmatrix} \underbrace{\boxed{L(G_1)}}_{X_1} & & & \\ & \underbrace{\boxed{L(G_2)}}_{X_2} & & \\ & & \ddots & \\ & & & \underbrace{\boxed{L(G_k)}}_{X_k} \end{pmatrix}.$$

Laplacian vs Connectivity.

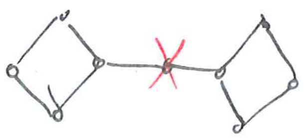
Let $L = L(G)$.

$\underset{0}{\underset{\shortparallel}{\lambda_1}} \le \lambda_2 \le \dots \le \lambda_n$: eig val's of L.

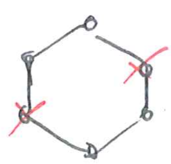
Then $\lambda_2 = 0 \iff G$ is not connected.

Also, $\lambda_2 = \min_{\substack{\vec{x} \neq 0 \\ \vec{x} \perp \vec{1}}} \dfrac{\vec{x}^T L \vec{x}}{\vec{x}^T \vec{x}}$

Defn. The <u>connectivity</u> of G is the minimum number of vertices such that removing them separate G, denoted as $\kappa(G)$.



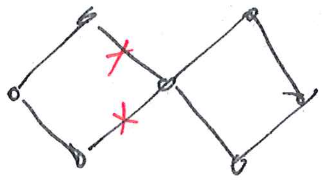
$\kappa = 1$



$\kappa = 2$

Defn. The <u>edge connectivity</u> of G is the min # of edges such that removing them separate G, denoted as $\cancel{\kappa(G)}$ $\lambda(G)$.

e.g.



$\kappa = 1$
$\lambda = 2$

~~$\lambda = 1$~~ ~~$\kappa = 2$~~

Thm. $\cancel{\lambda(G) \le \kappa(G)}$ $\kappa(G) \le \lambda(G)$ for any graph G.

Thm. Let $L = L(G)$,
$\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$: eigvals of L.
$\lambda_1 = 0$.

Then $\lambda_2 \le \kappa(G) \le \lambda(G)$.

pf. Claim: $\lambda_2(G) \le \lambda_2(G+e)$. [Consider e as a graph with $V(e) = V(G)$, $E(e) = \{e\}$.]

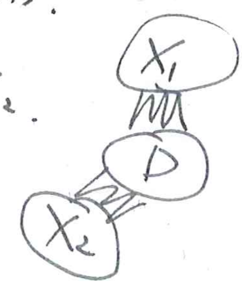
Let $\vec{x}$ be the unit eigvector of $L(G+e)$ for λ_2.

Then $\vec{x}^T L(G+e)\vec{x} = \vec{x}^T L(G)\vec{x} + \vec{x}^T L(e)\vec{x}$

$$\ge \lambda_2(G) + \lambda_2(e)$$

~~Let~~ Suppose $G \setminus D$ has two disconnected parts.

Let $H = G +$ all edges between D and $X_1 \cup X_2$.



Let $\vec{v} = |X_2|\phi_{X_1} - |X_1|\phi_{X_2}$ $\Rightarrow$ $\vec{v} \perp \vec{1}$.

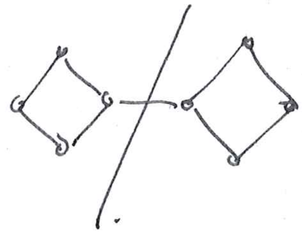
Also, $\lambda_2(H) \le \dfrac{\vec{v}^T L(H)\vec{v}}{\vec{v}^T\vec{v}} = \dfrac{|X_2|^2 |D| + |X_1|^2 |D|}{|X_1|^2 + |X_2|^2} = |D|$

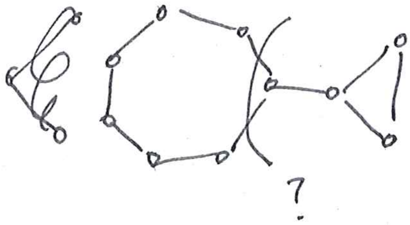
$\Rightarrow$ $\lambda_2(G) \le \lambda_2(H) \le |D|$.

Laplacian vs partition.

Goal: partition the graph into balanced two parts with minimum edges in between.

e.g.





* Fiedler's partition.

Suppose G is a connected graph.

$L = L(G)$. $\lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$: eig vals
$\lambda_1 = 0$, $\lambda_2 \uparrow \vec{v}$: eigvec. ← called ~~Fielde~~ Fiedler vector

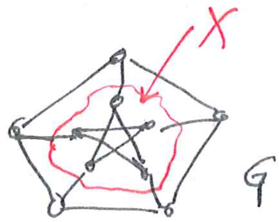
Assume multiplicity of λ_2 is one.

Separate $V = \{1, \ldots, n\}$ into three parts.

$N_+ = \{ i : v_i > 0 \}$

$N_- = \{ i : v_i < 0 \}$ Here $\vec{v} = (v_1, \ldots, v_n)$

$N_0 = \{ i : v_i = 0 \}$



~~Thm [Fiedl~~

Defn. $X \subseteq V$: a subset of vertices.
The induced subgraph G is $G[X]$.

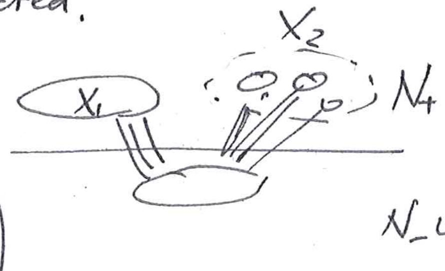
Thm [Fiedler].

$G[N_+]$, $G[N_- \cup N_0]$ are both connected.

GL.

pf. By contradiction.

Suppose $N_+^* = X_1 \dot\cup X_2$. such that $G[N_+]$ is not connected.



Then

$$L - \lambda_2 I = \begin{array}{c} \begin{pmatrix} L_{1,1} - \lambda_2 I & 0 & L_{1,3} \\ 0 & L_{2,2} - \lambda_2 I & L_{2,3} \\ L_{3,1} & L_{3,2} & L_{3,3} \end{pmatrix} \\ \begin{array}{ccc} \underbrace{\quad\quad}_{X_1} & \underbrace{\quad\quad}_{X_2} & \underbrace{\quad\quad}_{N_- \cup N_0} \end{array} \end{array}$$

$$\vec{v} = \begin{pmatrix} \vec{v}_1 \\ \vec{v}_2 \\ \vec{v}_3 \end{pmatrix} \begin{array}{l} \}\, X_1 \\ \}\, X_2 \\ \}\, N_- \cup N_0 \end{array}$$

$$\Rightarrow (L_{1,1} - \lambda_2 I)\,\vec{v}_1 = -L_{1,3}\vec{v}_3$$

$$(L_{2,2} - \lambda_2 I)\,\vec{v}_2 = -L_{2,3}\vec{v}_3$$

Let $\vec{y} = \begin{pmatrix} \langle \vec{v}_2, \vec{1} \rangle \cdot \vec{v}_1 \\ -\langle \vec{v}_1, \vec{1} \rangle\, \vec{v}_2 \\ 0 \end{pmatrix} \rightarrow \vec{y} \perp \vec{1} = 0.$

Now. $\vec{y}^T (L - \lambda_2 I)\vec{y} = -(\langle \vec{v}_2, \vec{1} \rangle)^2 \cdot \vec{v}_1^T L_{1,3} \vec{v}_3 - (\langle \vec{v}_1, \vec{1} \rangle)^2 \cdot \vec{v}_2^T L_{2,3} \vec{v}_3$

≤ 0

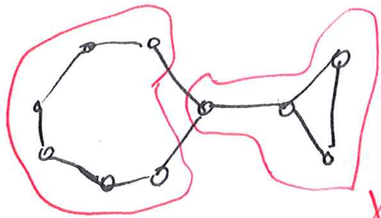
$\Rightarrow$ $\vec{y}$ is an eigvector of λ_2 indep of $\vec{v}$ $\rightarrow\leftarrow$

(we assumed multi = 1)

Cut

Defn. X_1, X_2 two subsets of vertices V.

$W(X_1, X_2) = \#$ of edges between X_1 and X_2.



Q : Find a partition $V = X_1 \dot{\cup} X_2$ with $|X_1| = |X_2|$ that minimized $W(X_1, X_2)$.

Let $B = \{$ all vectors in $\mathbb{R}^n$ with $\frac{n}{2}$ 1's and $\frac{n}{2}$ -1's $\}$.

That is, every vector in B is of the form

$$\phi_{X_1} - \phi_{X_2}, \quad V = X_1 \dot{\cup} X_2, \quad |X_1| = |X_2|.$$

Then for $\vec{v}_0 \in B$,

$$\frac{\vec{v}^T L \vec{v}}{\vec{v}^T \vec{v}} = \frac{\sum_{ij \in E} (v_i - v_j)^2}{\sum_{i=1}^n v_i^2}$$

$$= \frac{1}{n} \cdot \left[\sum_{\substack{ij \in E \\ \binom{i \in X_1}{j \in X_2} \text{ or } \binom{i \in X_2}{j \in X_1}}} 2^2 + \sum_{\substack{ij \in E \\ (i,j \in X_1) \\ \text{or} \\ (i,j \in X_2)}} 0^2 \right] = \frac{4}{n} \cdot W(X_1, X_2).$$

So

$$\min_{|X_1| = |X_2|} W(X_1, X_2) = \frac{n}{4} \cdot \min_{\substack{\vec{v} \in B \\ \vec{v} \perp 1}} \frac{\vec{v}^T L \vec{v}}{\vec{v}^T \vec{v}} \geq \lambda_2.$$

Spectral clustering

Sketch:

(1). Construct a similarity graph

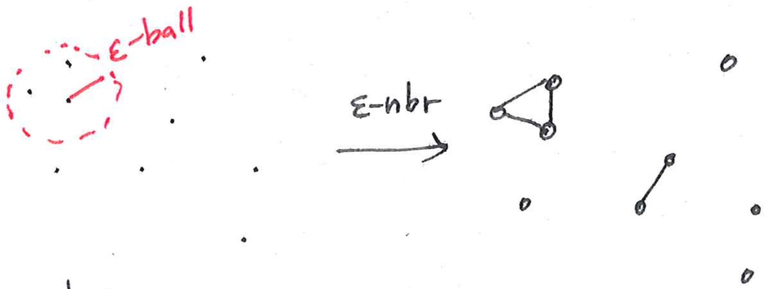
(2). Spectral reduction. (e.g. Laplacian eigenmap)

(3). clustering (e.g. k-mean).

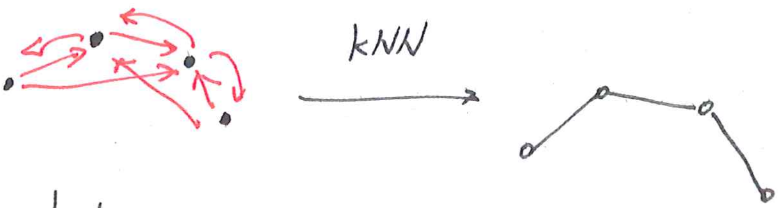
Workflow:

$$\text{data} \xrightarrow[\varepsilon\text{-nbr}]{kNN} \text{similarity graph} \xrightarrow{\text{embedding}} \text{data} \xrightarrow{\text{clustering}} \text{groups.}$$

reduction.



data graph



data

[Similarity graph ~~mixes~~ loses the distance info, unless you put weight on graph]

~~Ee~~ Embedding.

Laplacian eigenmap ???

Goal: Given a graph G, find an embedding

$$f: V \longrightarrow \mathbb{R}^d$$
$$i \longmapsto \vec{y}_i$$

such that $\sum_{ij \in E} |\vec{y}_i - \vec{y}_j|^2$ is minimized.

(Subject to $Y = \begin{pmatrix} | & & | \\ \vec{v}_1 & \cdots & \vec{v}_d \\ | & & | \end{pmatrix} = \begin{pmatrix} - \vec{y}_1 - \\ \vdots \\ - \vec{y}_n - \end{pmatrix}$

has $1^T Y = \vec{0}$ [置中].

and $Y^T Y = I$).

Algorithm:

Input: G : similarity graph

d : desired dimension.

Output: $Y \leftarrow n \times d$ matrix with $1^T Y = 0$ and $Y^T Y = I$.

(then the rows of Y are the new coordinates.)

Steps:

$$\overset{\overset{0}{\parallel}}{\lambda_0} \le \lambda_1 \le \lambda_2 \le \cdots \le \lambda_d \le \cdots \le \lambda_n$$

第二小的 eigval.

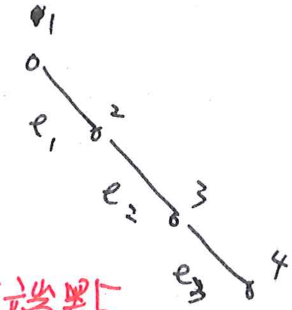
1. $L = L(G)$.
2. Compute the unit eigenvectors $\vec{v}_1, \vec{v}_2, \ldots, \vec{v}_d$
3. $Y = \begin{pmatrix} | & & | \\ \vec{v}_1 & \cdots & \vec{v}_d \\ | & & | \end{pmatrix} = \begin{pmatrix} - \vec{y}_1 - \\ \vdots \\ - \vec{y}_n - \end{pmatrix}$.

And vertex $i \longmapsto \vec{y}_i$.

Reason :

① Incidence matrix : Q.

$$\begin{array}{c} \\ e_1 \\ e_2 \\ e_3 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{pmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & 1 & -1 \end{pmatrix} \end{array}$$



e_i 的兩端點 放 1, -1. 哪個是1都行.

prop. ① Q has zero row sums. $\Rightarrow Q\mathbf{1} = \vec{0}$.

② $Q^TQ = L$.

$$\begin{pmatrix} 1 & & \\ -1 & 1 & \\ & -1 & 1 \\ & & -1 \end{pmatrix} \begin{pmatrix} 1 & -1 & & \\ & 1 & -1 & \\ & & 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 1 \end{pmatrix}$$

③ $$QY = \begin{pmatrix} \text{—} \ \vec{y}_i - \vec{y}_j \ \text{—} \\ \vdots \\ \text{—} \ \vec{y}_i - \vec{y}_j \ \text{—} \end{pmatrix}$$

i, j 是 e 的兩端點 (different in each row).

$$\|QY\|^2 = \sum_{ij \in E} |y_i - y_j|^2$$

So the goal is to minimize $\operatorname{tr}(Y^TQ^TQY)$
subject to $\mathbf{1}^TY = \vec{0}$ and $Y^TY = I$.

$\longrightarrow$ use the eigenvectors.

[Now think about ~~the~~ Fiedler's partition thm.]