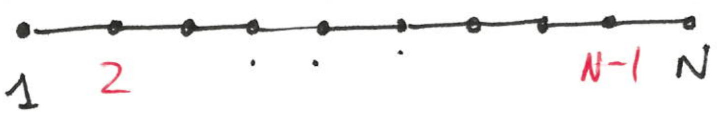
Equation becomes:

$$\frac{d\vec{u}}{dt} = \underbrace{\begin{pmatrix} -1 & 1 & & & & & & \\ 1 & -2 & 1 & & & 0 & & \\ & 1 & -2 & 1 & & & & \\ 0 & \cdots & 1 & -2 & 1 & 0 & \cdots & 0 \\ & & & 1 & -2 & 1 & & \\ & 0 & & & & \ddots & & \\ & & & & & & 1 & -1 \end{pmatrix}_{N\times N}}_{\boxed{\text{Laplacian matrix}} = -L} \begin{pmatrix} u_1 \\ \vdots \\ u_k \\ u_{k+1} \\ u_{k+2} \\ \vdots \\ u_N \end{pmatrix}$$

Graph:



$$-L = A - D$$

where $D = \mathrm{diag}(\vec{d}) = \mathrm{diag}(A\vec{1})$

Definition: $\boxed{\begin{array}{c}\text{Combinatorial graph Laplacian.} \\ L = D - A\end{array}}$

$$\boxed{\frac{d\vec{u}}{dt} = -L\vec{u}}$$

Heat equation on the graph.

Solution: $\vec{u}(t) = e^{-Lt}\vec{u}(0)$

Note that: ① $L\vec{1} = (D-A)\vec{1} = \vec{d}-\vec{d} = 0.$

i.e., $\vec{1}_{N\times 1}$ is an eigenvector of L with eigenvalue zero.

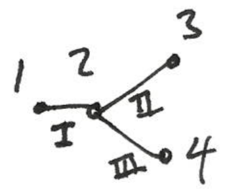
② So $\vec{1}$ is a stationary point of the heat equation.

...

②

$$\underset{N\times N}{L} = D - A = \underset{N\times E}{B^T}\ \underset{E\times N}{B}$$

B is the incidence matrix



$$B_{E\times N} = \begin{array}{c c} \begin{matrix} \quad ① & ② & ③ & ④ \end{matrix} & \\ \begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} & \begin{matrix} \mathrm{I} \\ \mathrm{II} \\ \mathrm{III} \end{matrix} \end{array}$$

$$B^T B = \begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} = L$$

$$\vec{u}^T L \vec{u} \qquad \vec{u} \in \mathbb{R}^N$$

$$\| $$

$$\vec{u}^T B^T B \vec{u} = \|B\vec{u}\|^2 \geq 0$$

Positive semidefinite matrix.

$$\vec{u}(t) = e^{-tL} \vec{u}(0)$$

$$L\vec{v}_i = \lambda_i \vec{v}_i$$

$$LV = V\Lambda \qquad \Lambda = \mathrm{diag}(\lambda_i)$$

$$V = (\vec{v}_1 \cdots \vec{v}_N)$$

$$VV^T = I$$

$$\underline{L = V\Lambda V^T}$$

$$e^{-tL} = \sum_{k=0}^{\infty} \frac{1}{k!} (-tL)^k$$

$$L^k = V\Lambda \underbrace{V^T V}_{I} \Lambda V^T \cdots V\Lambda V^T$$

$$= V\Lambda^k V^T$$

$$e^{-tL} = V \underbrace{\left[\sum_{k=0}^{\infty} \frac{(-t)^k}{k!} \Lambda^k \right]}_{\begin{pmatrix} \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} \lambda_1^k & & 0 \\ & \ddots & \\ 0 & & \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} \lambda_N^k \end{pmatrix}} V^T$$

$$= \begin{pmatrix} e^{-\lambda_1 t} & & \\ & \ddots & \\ & & e^{-\lambda_N t} \end{pmatrix}$$

$$= \mathrm{diag}\left(e^{-\lambda_i t}\right)$$

$$e^{-tL} = V \, \mathrm{diag}\left(e^{-\lambda_i t}\right) V^T$$

$$= \sum_{i=1}^{N} e^{-\lambda_i t} \vec{v_i} \vec{v_i}^T$$

$$\vec{u}(t) = e^{-tL}\vec{u}(0)$$

$$= \sum_{i=1}^{N} e^{-\lambda_i t}\,\vec{v}_i\left[\vec{v}_i^{T}\cdot\vec{u}(0)\right]$$

$$= \underbrace{\left(\vec{1}^{T}\cdot\vec{u}(0)\right)}\vec{1} + \sum_{i=2}^{N} e^{-\lambda_i t}\,\vec{v}_i\left(\vec{v}_i\cdot\vec{u}(0)\right)$$

As $t \to \infty$

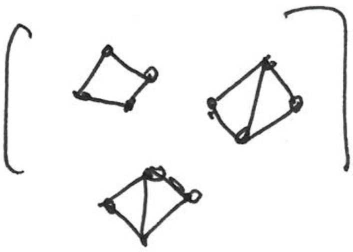
$$\vec{u}(t) - N\langle\vec{u}(0)\rangle\vec{1} \simeq e^{-\lambda_2 t}\,\vec{v}_2\left[\vec{v}_2\cdot\vec{u}(0)\right]$$

Spectral connectivity

Fiedler eigenvector.

(3) Number of zero eigenvalues of L is equal to the number of disconnected components.

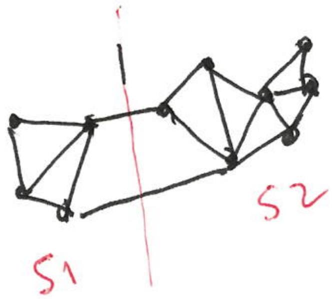
$n_1+n_2+n_3=N$



$$\begin{array}{cccc} & n_1 & n_2 & n_3 \\ L = & \multicolumn{3}{c}{\begin{bmatrix} \boxed{L_1} & & 0 \\ & \boxed{L_2} & \\ 0 & & \boxed{L_3} \end{bmatrix}} \end{array} = L_1 \oplus L_2 \oplus L_3$$

$$\underset{N\times N}{L}\vec{1} = 0 \qquad L_i\underset{n_i\times 1}{\vec{1}} = 0$$

Spectral clustering



Split the graph into K subgraphs with minimal cost but balanced cuts.

$K=2$

cost: $$C = \frac{1}{2} \sum_{\substack{i \in S_1 \\ j \in S_2}} A_{ij}$$

$$s_i = \begin{cases} +1 & \text{if } i \in S_1 \\ -1 & \text{if } i \in S_2 \end{cases}$$

$$t_{ij} = \frac{1}{2}(1 - s_i s_j) = \begin{cases} 1 & i,j \text{ are in different clusters} \\ 0 & i,j \text{ are in the same cluster} \end{cases}$$

$$C = \frac{1}{2} \sum_{i,j} t_{ij} A_{ij} = \frac{1}{4}\left(\sum_{i,j} A_{ij} - \sum_{i,j} A_{ij} s_i s_j \right)$$

Note that: $$\sum_{i,j} A_{ij} = \sum_i d_i = \sum_i d_i s_i^2 = \sum_{i,j} d_i s_i s_j \delta_{ij}$$

$$C = \frac{1}{4} \sum_{i,j} \Big(\underbrace{d_i \, \delta_{ij} - A_{ij}}_{L_{ij}} \Big) s_i s_j$$

$$\boxed{\min_{\vec{s}} \; \underline{C = \frac{1}{4} \vec{s}^T L \vec{s}} \qquad \vec{s} \in \mathbb{Z}^N, \quad s_i = \pm 1}$$

under these constraints:

$$\begin{cases} ① & \vec{s}^T \cdot \vec{s} = N = n_1 + n_2 \\ ② & \vec{s}^T \cdot \vec{1} = n_1 - n_2 \end{cases}$$

Relaxation : Solve the above for $\underline{\vec{s} \in \mathbb{R}^N}$ under ① & ②

$$\nabla_{\vec{s}} \left[\vec{s}^T L \vec{s} + \lambda \left(N - \vec{s}^T \cdot \vec{s} \right) + 2\mu \left((n_1 - n_2) - \vec{s}^T \cdot \vec{1} \right) \right]$$

$$\nabla_{\vec{s}} \left[\ldots \right] \Big|_{\vec{s}^*} = 0 \qquad \text{At } \vec{s}^* :$$

$$\underline{L \vec{s}^* = \lambda \vec{s}^* + \mu \vec{1}}$$

$$L\vec{1} = 0$$

$$\underbrace{\vec{1}^T L}_{= 0} \vec{s}^* = \lambda \underbrace{\vec{1}^T \cdot \vec{s}^*}_{(n_1 - n_2)} + \mu \underbrace{\vec{1}^T \cdot \vec{1}}_{N}$$

$$\frac{\mu}{\lambda} = -\frac{(n_1 - n_2)}{N}$$

$$L\vec{s}^* = \lambda\left(\vec{s}^* + \frac{\mu}{\lambda}\vec{1}\right)$$

$$= L\underbrace{\left(\vec{s}^* + \frac{\mu}{\lambda}\vec{1}\right)}_{\vec{v}}$$

$$\underline{\vec{v} = \vec{s}^* + \frac{\mu}{\lambda}\vec{1}}$$

$$L\vec{v} = \lambda\vec{v}$$

λ ← eigenvalue of L

$\vec{v}$ ↑ eigenvector of Laplacian

$$C = \frac{1}{4}\vec{s}^{*}L\vec{s}^{*} = \frac{1}{4}\vec{v}^{T}L\vec{v} = \frac{1}{4}\lambda\,\vec{v}^{T}\cdot\vec{v}$$

$\vec{v}_2$ associated with λ_2

Plugging in you get

$$C_{min} = \lambda_2 \frac{n_1 n_2}{N}$$

This vector $\vec{v}_2$ is called the Fiedler vector and indicates an optimal bipartition.

The quality of the bipartition is given by the eigenvalue λ_2, the algebraic connectivity of the graph.

If $\lambda_2 \ll$ ~~[illegible]~~
then there exists a good bipartition of the graph given by $\vec{v}_2$.