15 Spectral clustering (cont.) 3

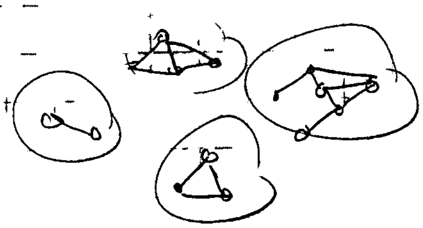
recall: $W_{n\times n}$, $W=W^T$ symmetric and $W_{ij}\ge 0$

$D=\text{diag}\{d_1,\dots,d_n\}$ where $d_i=\sum_j^n w_{ij}$

$\mathcal{L}_{un} = D-W$

$\mathcal{L}_{rw} = I-P$; $P=D^{-1}W$

If the graph has k connected components,



then the eigenspace of $\mathcal{L}_{un}$ associated with eigenvalue zero equals $\text{span}\{\mathbb{1}_{A_1},\dots,\mathbb{1}_{A_k}\}$

What if $\mathcal{L}_{rw}$?

$$\mathcal{L}_{rw}=\Psi(I-\Lambda)\Phi^T$$

$$P=\Psi\Lambda\Phi^T$$

$$\Psi^T D\Psi = I$$

$\Psi=[\psi_1,\dots,\psi_n]$, $\psi_k^T D\psi_k=1$

$\psi_k^T D\psi_l=0$ if $k\neq l$

and $P\psi_k=\lambda_k\psi_k$

If f is eigenvector of $\mathcal{L}_{un}$ with $\lambda=0$, $\mathcal{L}_{un}f=0\cdot f$ and $(D-W)f=0$.

If f is eigenvector of $\mathcal{L}_{rw}$ w/ $\lambda=0$,

$D^{-1}(D-W)f=0$ and $(D-W)f=0$

$\psi_1=c_1\cdot\mathbb{1}_{A_1},\dots,\psi_k=c_k\mathbb{1}_{A_k}$.

$$\Psi_{:,1:4}=\begin{array}{c c}\left[\begin{array}{c|c|c|c} c_1 & & & \\ \vdots & 0 & 0 & 0 \\ c_1 & & & \\ \hline & c_2 & & \\ 0 & \vdots & 0 & 0 \\ & c_2 & & \\ \hline & & c_3 & \\ 0 & 0 & \vdots & 0 \\ & & c_3 & \\ \hline & & & c_4 \\ 0 & 0 & 0 & \vdots \\ & & & c_4 \end{array}\right] & \begin{array}{l} \}n_1 \\ \\ \\ \}n_2 \\ \\ \\ \}n_3 \\ \\ \\ \}n_4 \\ \\ \\ \end{array}\end{array}$$

if $k=4$

$\psi_1=[c_1 -]$

$\psi_2=[-c_2-]$

What are the constants?

$$c_1=\sqrt{\frac{1}{\sum_{i\in C_1} d_i}}$$

$C_1=\{1,\dots,n_1\}$

$C_2=\{n_1+1,\dots,n_1+n_2\}$ ...

If $k=2$, $\Psi_{:,1:2}=\begin{array}{c c}\left[\begin{array}{c|c} c_1 & 0 \\ \hline 0 & c_2 \end{array}\right] & \begin{array}{l} n_1 \\ n_2 \end{array}\end{array}$

Need

$\tilde{\Psi}_{:,1}=\begin{bmatrix} c \\ \vdots \\ c\end{bmatrix}=\tilde{\psi}_1$, $\tilde{\Psi}_{:,2}==\tilde{\psi}_2$

$\tilde{\psi}_2=\alpha\psi_1+\beta\psi_2$

- $\tilde{\psi}_2^T D\tilde{\psi}_2=1 \Rightarrow \alpha^2+\beta^2=1$
- $\tilde{\psi}_2^T D\tilde{\psi}_1=0 \Rightarrow \tilde{\psi}_2^T d=0$

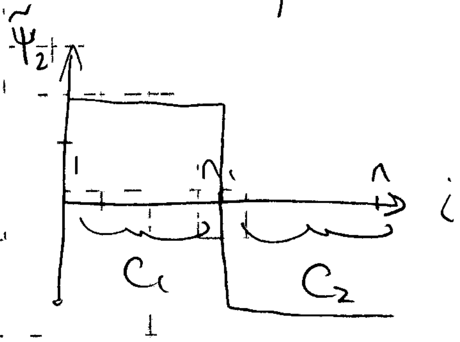
Since $d=\begin{bmatrix} d_1 \\ \vdots \\ d_n\end{bmatrix}$ so $\alpha(\psi_1^T d)+\beta(\psi_2^T d)=0$

and $\alpha\sqrt{\sum_{i\in C_1} d_i} + \beta\sqrt{\sum_{i\in C_2} d_i} = 0$

α and β should have different signs bc ...

$\tilde{\varphi}_2 = \alpha c_1 \mathbb{1}_{A_1} + \beta c_2 \mathbb{1}_{A_2}$

$$\tilde{\varphi}_2(i) = \begin{cases} \alpha c_1 & \text{if } i \in C_1 \\ \beta c_2 & \text{if } i \in C_2 \end{cases}$$



we can use the signs of these to get the cluster. or more in general, we don't have to cut at zero but can tune to any cut-off

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How to know k in spectral clustering

Remark Spectral gap heuristic

the first k eigen values will be close to one, then there will be a "gap" after k.

(missing a lot here....)

Graph cut

def (cut)

$A \cap B = \emptyset$ where $A, B \subset V = \{1 \ldots n\}$

the cut $W(A,B) = \sum_{i \in A,\, j \in B} w_{ij}$

def (volume of set A)

$Vol(A) = \sum_{i \in A} d_i$ sum of degrees

def (normalized cut of partition C)

$\mathcal{C} = \{C_1, \ldots, C_k\}$

$$NCut(\mathcal{C}) = \sum_{l=1}^{k} \frac{W(C_l, C_l^c)}{Vol(C_l)}$$

where $A^c = V \setminus A$

Proposition

$$NCut(C) = \sum_{l=1}^{k} \varphi_l^T L \varphi_l$$

$\varphi_l = c_l \mathbb{1}_{C_l}, \quad l = 1 \ldots k$

$$c_l = \frac{1}{\sqrt{Vol(C_l)}}$$

Proof

$$\varphi_1^T L \varphi_1 = \frac{1}{2} \sum_{ij} w_{ij} (\varphi_1(i) - \varphi_1(j))^2$$

$$= \sum_{\substack{i \in C_1 \\ j \in C_1^c}} w_{ij} \left(\frac{1}{\sqrt{Vol(C_1)}} - 0 \right)^2$$

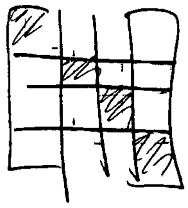
$$= \sum_{\substack{i \in C_1 \\ j \in C_1^c}} w_{ij} \frac{1}{Vol(C_1)} = \frac{W(C_1, C_1^c)}{Vol(C_1)}$$

Problem of min NCut

$$\min_{C} \; NCut(C) = Tr(\underbrace{H^T L H}_{\sum \psi_\ell^T L \psi_\ell})$$

introduce matrix $H = \begin{bmatrix} \psi_1 \dots \psi_k \end{bmatrix}$

as defined $\psi_\ell = c_\ell \mathbb{1}_{C_\ell}$

so we see $H =$  as

Seen previously: H is a function of C.

(min NCut)

$$\begin{cases} \min_H Tr(H^T L H) & \text{where } L = \mathcal{L}_{un} \\ H \text{ has the form above} \end{cases}$$

$\psi_k^T D \psi_\ell = \delta_{k\ell} \Rightarrow H^T D H = I_k$

spec-min-NCut

$$\begin{cases} \min_{H_{n\times k}} Tr(H^T L H) \\ \text{st. } H^T D H = I_k \end{cases}$$

Prop Solution of (spec-min-NCut) is the first k eigenvectors of $\mathcal{L}_{rw}$, normalized to be $\psi_k^T D \psi_k = 1$

exercise

$$RCut(C) = \sum_{\ell=1}^{k} \frac{W(C_\ell, C_\ell^c)}{|C_\ell|}$$

$|C_\ell|$ = number of nodes in C_ℓ.

spec-min-Rcut $\Leftrightarrow$ spectral clustering using $\mathcal{L}_{un}$

Which Laplacian to use between:

- $\mathcal{L}_{un}$
- $\mathcal{L}_{sym}$
- $\mathcal{L}_{rw}$

$\longrightarrow$ next class.