Spectral

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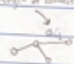
spectral embedding

similarity

strength of connection. normally $a_{ij} \in \{0,1\}$ for simple graph. but cld be kernel.



A: adjacency matrix. element (i,j) is similarity of nodes (i,j)

D: degree matrix

Laplacian matrix $L := D - A$

let $\vec{x}_i$ be node feature we wish to discover based on graph connectivity

$$\begin{bmatrix} | & & | \\ \vec{x}_1 & \cdots & \vec{x}_N \\ | & & | \end{bmatrix} = X \quad \leftarrow d \times n$$

node embeddings of the N graphs.

learn X via:

$$\min_X \sum_{(i,j)} a_{ij} \|\vec{x}_i - \vec{x}_j\|^2$$

sum over all pairs $a_{ij} = 0$ if no edge

aside:

$$(\vec{x}_i - \vec{x}_j)^T (\vec{x}_i - \vec{x}_j)^2 = \|x_i - x_j\|^2$$
$$\vec{x}_i^T \vec{x}_i - 2\vec{x}_i^T \vec{x}_j - \vec{x}_j^T \vec{x}_j$$

if nodes i,j strongly connected, place their latent repr nearby

without a constraint, we would have $\vec{x}_i = \vec{x}_j \;\; \forall (i,j)$.

$\Rightarrow$ constraint $\underset{(d \times n)(n \times d)}{X X^T} = \underset{d \times d}{I} \Rightarrow \sum_{i=1}^{N} \vec{x}_i[d]^2 = 1$ ← gives budget for each dimension.

$$\begin{bmatrix} \vec{x}_1 & \cdots & \vec{x}_N \end{bmatrix} \begin{bmatrix} - x_1 - \\ \vdots \\ - x_N - \end{bmatrix} = \begin{bmatrix} 1 & \\ & 1 \end{bmatrix}$$

e.g. $d = 1 \Rightarrow [x_1 \cdots x_N] \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = [1]$

$$\sum_{i=1}^{N} x_i^2 = 1$$ spaces them out.

feature number of node i

objective in terms of L:

sums over all pairs

$$= \frac{1}{2} \sum_i \sum_j a_{ij} \left[x_i^T x_i + x_j^T x_j - 2 \vec{x}_j \vec{x}_i \right]$$

$$= \frac{1}{2} \left[\sum_i \sum_j a_{ij} x_i \cdot x_i + \sum_i \sum_j a_{ij} \vec{x}_j \cdot \vec{x}_j - 2 \sum_i \sum_j x_i \cdot x_j \right]$$

← switch i,j

b/c symmetry $a_{ij} = a_{ji}$

$$= \left(\sum_i \sum_j a_{ij} \left[x_i \cdot x_i - x_i \cdot x_j \right] \right)$$

d_i, degree of node i

$$= \sum_i x_i \cdot \left(\sum_j a_{ij} (x_i - x_j) \right) = \sum_i x_i \cdot \left(x_i \sum_j a_{ij} - \sum_j a_{ij} x_j \right)$$

$$[a \; b] \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} = \begin{bmatrix} a\alpha + b\gamma & \beta a + b\delta \end{bmatrix}$$

$$= a[\alpha \; \beta] + b[\gamma \; \delta]$$

$$= \sum_i \vec{x}_i \cdot \left(\vec{x}_i d_i - \sum_j a_{ij} \vec{x}_j \right)$$

row i of $(D-A) X^T = L X^T$

$$= tr(X L X^T)$$

$A X^T$. el

⇒ rov

b/c

$X (L X^T)$ element i,i is

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