Darrick - Graph Laplacians

Note Title 5/16/2025

$G = (V, E)$ $\quad |V| = n$

nodes, edges $\quad E \subseteq V \times V$

Def: Adjacency matrix, $A^{n \times n}$, $A_{ij} = \begin{cases} 1, & i \sim j \\ 0, & \text{otherwise} \end{cases}$

$i \sim j$: adjacent.

Fact $(A^k)_{ij} = \#$ distinct paths i to j of length k

Degree $\quad d_i = |\{j : j \sim i\}|$, $\quad D_{ij} = \begin{cases} d_i & i = j \\ 0 & \text{oth.} \end{cases}$

Graph Laplacian $L := D - A$

$C^0 = \mathbb{R}^{|V|}$, $C^1 = \mathbb{R}^{|E|}$ $\quad s, t : E \to V$

$d : C^1 \longrightarrow C^0 \qquad \partial(e) = t(e) - s(e) \qquad \left(\partial = (\partial_{ie}) \right)$

$\partial \circ \partial^T : C^0 \longrightarrow C^0$

$$(\partial \circ \partial^T)_{ij} = \sum_e \partial_{ie} \partial_{je} = \begin{cases} d_i , & i = j \\ -1 , & i \sim j \\ 0 , & \text{oth.} \end{cases}$$

Thus $\boxed{\partial \circ \partial^T = L}$

Node Feature : function $f : \underset{\{v_1, \dots, v_n\}}{\underset{\parallel}{V}} \longrightarrow \mathbb{R}$

$$(Lf)(v_i) = \sum_{i \sim j} \left(f(v_i) - f(v_j) \right)$$

4) Symmetric Normalized Laplacian

$$\tilde{L} = D^{-1/2} L D^{-1/2} = \begin{cases} 1, & i=j \\ \frac{-1}{\sqrt{d_i}\sqrt{d_j}}, & i \sim j \\ 0 & \text{otherwise} \end{cases}$$

$\Rightarrow$ Symmetric, real, ≥ 0 evals

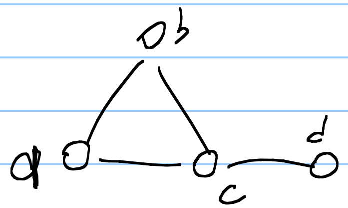
$L\mathbb{1} = 0$ $\quad L\mathbb{1}_{C}$ $\hookrightarrow$ connected components

Prop: For $\tilde{L}$, $\lambda_i \in [0, 2]$

2) Random Walk Laplacian

$$\tilde{L}_{rw} = D^{-1}L = I - D^{-1}A = \begin{cases} 1 & i = j \\ -1/d_i, & i \sim j \\ 0 & \text{otherwise} \end{cases}$$

$$(\tilde{L}_{rw} f)(v_i) = f(i) - \sum_{i \sim j} \frac{1}{d_i} f(j)$$



$$- D^{-1}A = \begin{array}{c} \\ a \\ b \\ c \\ d \end{array} \begin{array}{c} \begin{array}{cccc} a & b & c & d \end{array} \\ \begin{bmatrix} 0 & -1/2 & -1/2 & 0 \\ -1/2 & 0 & -1/2 & 0 \\ -1/3 & -1/3 & 0 & -1/3 \\ 0 & 0 & -1 & 0 \end{bmatrix} \end{array}$$

Graph diffusion (c.f. diffusion equation on $\mathbb{R}^n$ $\frac{\partial u(t,x)}{\partial t} = -\Delta_x u(t,x)$)

$$f_t - f_{t-1} = -\tilde{L}_{rw} f_{t-1} \quad , \quad f_t = \mathbb{R}^{|V|}$$

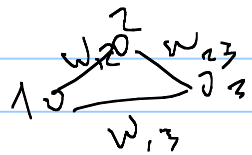
$$f_t = (I - \tilde{L}_{rw}) f_{t-1} \implies f_t = (D^{-1}A)^t f_0$$

$(D^{-1}A)^t_{ij}$ = prob. of r.w. starting at i ending at j

$$f_t(v_i) = (D^{-1}A)^t f_0(v_i) = \mathbb{E}[f_0(B_t) \mid B_0 \text{ r.w. starting at } i]$$

B_t: R.W. after t steps

Modifications for weighted graphs, $w: E \to (0,\infty)$



$$\text{Adjacency} = A_{ij} = \begin{cases} w_{ij}, & i \sim j \\ 0 & \text{otherwise} \end{cases}$$

$$D = \begin{cases} d_i = \sum_{i \sim j} w_{ij} & i = j \\ 0 & \text{oth.} \end{cases}$$

Everything works the same after the modification

2. Manifold Learning

Manifold Hypothesis: Real data sets are concentrated about lower dim submanifold $M \subset \mathbb{R}^N$, $N \gg 1$

Setting $M \subset \mathbb{R}^N$, $X^{(n)} = \{x_1, \ldots, x_n\}$ iid samples from volume measure of M.

Define $G = (X^{(n)}, E, w^t)$ for $t > 0$, $w_{ij}^t = \exp\left(\frac{-\|x_i - x_j\|^2}{4t}\right)$
fully connected

Graph Laplacian: $L_{ij}^{t,n} = \begin{cases} -w_{ij}^t, & i \neq j \\ \sum_k w_{ik}^t, & i = j \end{cases}$

$f : X^{(m)} \to \mathbb{R}$, $L^{t,n} f(x_i) = \sum_j \big(f(x_i) - f(x_j)\big) w_{ij}^t$

$\tilde{f} : M \to \mathbb{R}$, $L^{t,n} f(x) = \sum_j \big(f(x) - f(x_j)\big) \exp\left(\frac{-\|x - x_j\|^2}{4t}\right)$

<u>Thm</u> (Belkin, Niyogi, 2007)

$M \subset \mathbb{R}^N$ compact, $\dim(M) = k$, $t_n = n^{\frac{-1}{k+2+\alpha}}$ $\alpha > 0$

$$\lim_{n \to \infty} \frac{1}{n t_n (4\pi t)^{k/2}} L^{t,n} f(x) = \frac{1}{vol(M)} \Delta_M f(x)$$

in probability.

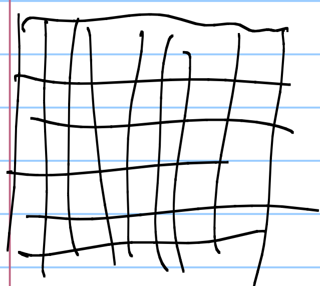
$\lambda_i^{t,n}$ evals of $L^{t,n}$

$\varphi_i^{t,n}$ evectors of $L^{t,n}$

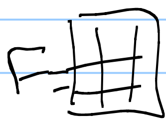
$$\phi = (\varphi_1^{t,n}, \ldots\ldots, \varphi_t^{t,n}) : \mathbb{R}^N \to \mathbb{R}^k$$

Graph Neural Networks

Convolutional Neural Networks



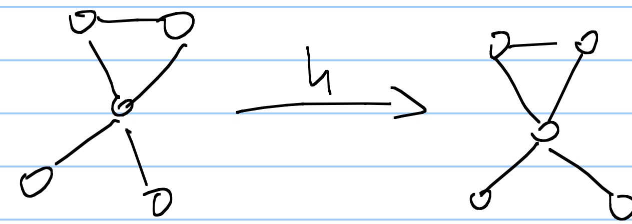
$n \times n$ grid of values in $\mathbb{R}^3$



3×3 grid of $\mathbb{R}$ (convolutional filter)

$$h = \sigma(X * F)$$

Graph Neural Networks



$f_0 : V \to \mathbb{R}^{n_0}$

$f_1 : V \to \mathbb{R}^{n_1}$

Eg $f_1 = \sigma(\tilde{L} f_0 \Theta)$ (Graph conv network)