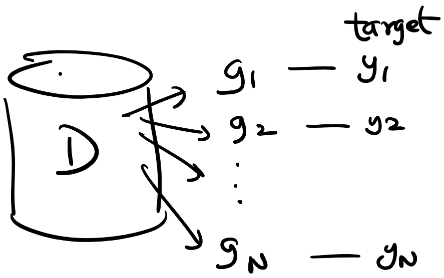
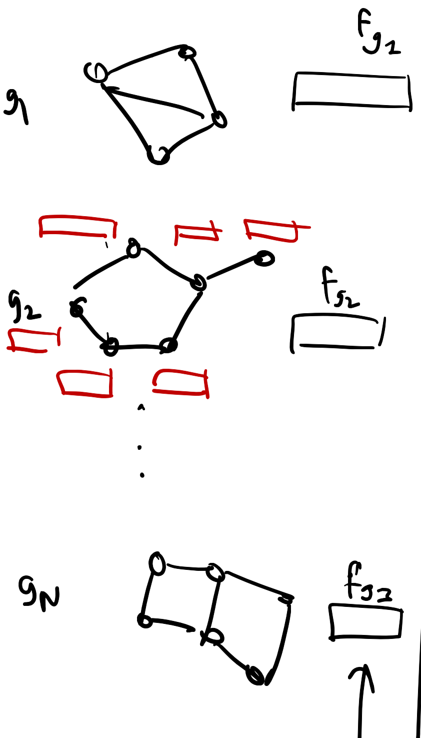
Graph Neural Networks

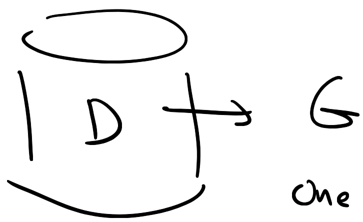


many different graphs

y_i → binary
y_i → k-class
y_i → real

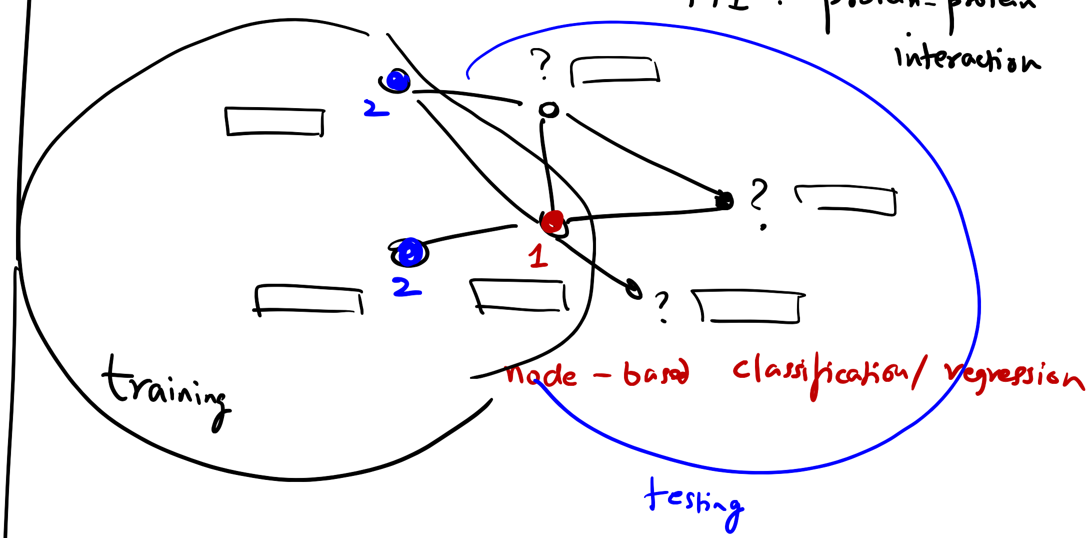


graph level embedding



One large graph

PPI : protein-protein interaction



Adjacency Matrix → A

symmetric < weighted / unweighted (binary)

$$A = \{a_{ij}\}_{i=1\ldots N,\ j=1\ldots N}$$

Degree Matrix D = $\begin{bmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_N \end{bmatrix}$

d_i = degree of vertex v_i = $\sum_{j=1}^{N} a_{ij}$

Transition Matrix $M = D^{-1} A$ = row-stochastic matrix

(Normalized adjacency) $= \left\{ \frac{a_{ij}}{d_i} \right\}_{i,j=1,\dots,N}$

a symmetric matrix

Laplacian Matrix

$$L = D - A$$

$$= \begin{bmatrix} d_1 & & & 0 \\ & d_2 & & \\ & & \ddots & \\ 0 & & & d_N \end{bmatrix} - \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1N} \\ a_{21} & a_{22} & \cdots & a_{2N} \\ & & & \\ a_{N1} & a_{N2} & \cdots & a_{NN} \end{bmatrix}$$

$$= \begin{bmatrix} \sum_{j=1}^{N} a_{1j} - a_{11} & -a_{12} & -a_{13} & \cdots & -a_{1N} \\ & \ddots & & & \\ & & \ddots & & \end{bmatrix}$$

$\boxed{\text{Symmetric, PSD : positive semi-definite}}$

Normalized Laplacian : $L_a = D^{-1} L$

asymmetric

$$= \begin{bmatrix} 1/d_1 & & & \\ & 1/d_2 & & \\ & & \ddots & \\ & & & 1/d_N \end{bmatrix} \begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{bmatrix}$$

D^{-1} $\quad$ L

L_a : behaves like PSD

(all eigenvalue are non-negative)

Symmetric Normalized Laplacian

$$L_s = D^{-1/2} L D^{-1/2}$$

$$= \begin{bmatrix} 1/\sqrt{d_1} & & & 0 \\ & 1/\sqrt{d_2} & & \\ & & \ddots & \\ 0 & & & 1/\sqrt{d_N} \end{bmatrix} L \begin{bmatrix} 1/\sqrt{d_1} & & & 0 \\ & 1/\sqrt{d_2} & & \\ & & \ddots & \\ 0 & & & 1/\sqrt{d_N} \end{bmatrix}$$

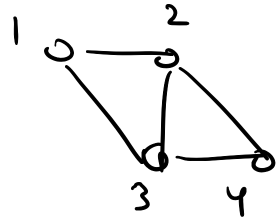
$D^{-1/2}$

row-operations $\qquad$ col-operations

$$= \left\{ \frac{l_{ij}}{\sqrt{d_i}\sqrt{d_j}} \right\}_{i=1..N,\ j=1..N}$$

$L = \{ l_{ij} \}$ $\qquad$ $L_s = \left\{ \frac{l_{ij}}{\sqrt{d_i}\sqrt{d_j}} \right\}$ $\qquad$ $L_a = \left\{ \frac{l_{ij}}{d_i} \right\}$

symmetric, PSD $\qquad$ $\Downarrow$ symmetric, PSD $\qquad$ asymmetric, PSD



$$A = \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 1 & 0 \\ 2 & 1 & 0 & 1 & 1 \\ 3 & 1 & 1 & 0 & 1 \\ 4 & 0 & 1 & 1 & 0 \end{array} \qquad D = \begin{bmatrix} 2 & & & 0 \\ & 3 & & \\ & & 3 & \\ 0 & & & 2 \end{bmatrix}$$

$$M = D^{-1}A = \begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$$

$$L = D - A = \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & 3 & 4 \end{array} \\ \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix} \end{array} \qquad D \; \begin{bmatrix} 2 & & & \\ & 3 & & \\ & & 3 & \\ & & & 2 \end{bmatrix}$$

$$L_s = D^{-1/2}(L)D^{-1/2}$$

$$= D^{-1/2}(D - A)D^{-1/2}$$

$$= \underbrace{D^{-1/2} D D^{-1/2}}_{} - D^{-1/2} A D^{-1/2}$$

$$\boxed{L = I - \underbrace{D^{-1/2} A D^{-1/2}}_{\text{Normalized symmetric adjacency matrix}}}$$

$$\begin{bmatrix} \frac{2}{\sqrt{2}\sqrt{2}} & \frac{-1}{\sqrt{2}\sqrt{3}} & \frac{-1}{\sqrt{2}\sqrt{3}} & \frac{0}{\sqrt{2}\sqrt{2}} \\ & \vdots & & \\ & & & \end{bmatrix}$$

$$\Downarrow$$

$$\begin{bmatrix} 1 & -1/\sqrt{6} & -1/\sqrt{6} & 0 \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

Spectral properties

↳ eigenvalues / eigenvectors

$$L = D - A$$

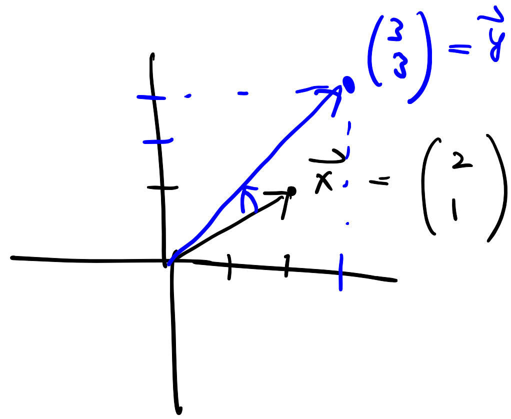
symmetric matrix
$n \times n$ ← square matrix

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

$\vec{u} \in \mathbb{R}^n$

n-dim vector

$$Z\vec{x} = \vec{y}$$



$$Z = \begin{bmatrix} 2 & -1 \\ -1 & 5 \end{bmatrix}$$

$$Z\vec{x} = \begin{bmatrix} 3 \\ 3 \end{bmatrix} = \vec{y}$$

$$\boxed{L\vec{u} = \lambda\vec{u}}$$

no-change in the vector "direction"

n solutions

$$L\vec{u}_1 = \lambda_1\vec{u}_1$$
$$L\vec{u}_2 = \lambda_2\vec{u}_2$$
$$\vdots$$
$$L\vec{u}_n = \lambda_n\vec{u}_n$$

$\vec{u}_1 \; \vec{u}_2 \; \cdots \; \vec{u}_n$ ⟸ eigenvectors ← unit vectors

$\lambda_1 \; \lambda_2 \; \cdots \; \lambda_n$ ⟸ eigenvalue

in decreasing order of λ_i

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

L : PSD

$$\boxed{\begin{gathered} \text{all} \quad \lambda_i \geq 0 \\ \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0 \\ \text{smallest eigen value is zero} \\ \lambda_1 \geq \lambda_2 \dots \geq \lambda_n = 0 \end{gathered}}$$

$\lambda_n = 0 \leftarrow$

$$\vec{u}_n = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$L = D - A$$

$$= \begin{bmatrix} d_1 & -a_{12} & -a_{13} & \dots & -a_{1N} \\ & & \vdots & & \\ & & & & \\ & & & & \end{bmatrix} \underbrace{\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} / \sqrt{n}}_{\vec{u}_n} = \underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}}_{\vec{0}}$$

$$L$$

$$= 0 \cdot \vec{u}_n$$

$$\vec{u}_n = (1\,1\,1\,1 \dots 1)^T / \sqrt{n} \qquad \lambda_n = 0$$

L : symmetric

$$\Rightarrow \quad \vec{u}_i^T \vec{u}_j = 0 \leftarrow$$

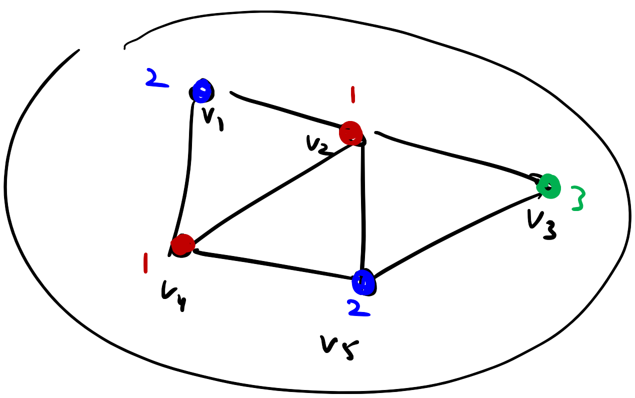
$$\vec{u}_i^T \vec{u}_i = 1$$

$$U = \underbrace{\begin{bmatrix} | & | & & | \\ \vec{u}_1 & \vec{u}_2 & \dots & \vec{u}_n \\ | & | & & | \end{bmatrix}}_{\text{cols are the eigenvectors}} \qquad U^T U = U U^T = I$$

U : Orthogonal matrix $\rightarrow$ orthogonal cols
$\rightarrow$ unit vectors (normal)

$$U^T = \begin{bmatrix} — u_1^T — \\ — u_2^T — \\ \vdots \\ — u_n^T — \end{bmatrix} \quad U = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_n \\ | & | & & | \end{bmatrix}$$

$$U^T U = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ 0 & 0 & \cdots & 1 \end{bmatrix} = I$$



$$\vec{f} = \begin{bmatrix} 2 \\ 1 \\ 3 \\ 1 \\ 2 \end{bmatrix} \in \mathbb{R}^n$$

# of nodes

forward: $\hat{f} = U^T f$

$$= \begin{bmatrix} — u_1^T — \\ — u_2^T — \\ \vdots \\ — u_n^T — \end{bmatrix} \vec{f} = \begin{bmatrix} \vec{u}_1^T f \\ \vec{u}_2^T f \\ \vdots \\ \vec{u}_n^T f \end{bmatrix}$$

graph fourier transform

$$\Big(\underbrace{\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_n}_{\text{basis vectors}} \Big)$$

orthogonal / unit vectors

Inverse mapping:

$$\hat{f} = U^T f$$

$$U\hat{f} = UU^T f = I \cdot f = f$$

forward U^T

inverse U

$$\boxed{L\vec{u}_i = \lambda_i \vec{u}_i \qquad i = 1, \dots, n}$$

$$U = \begin{bmatrix} | & | & & | \\ \vec{u}_1 & \vec{u}_2 & \cdots & \vec{u}_n \\ | & | & & | \end{bmatrix} \qquad \Lambda = \begin{bmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{bmatrix}$$

$$LU = U\Lambda$$

$$L\underline{UU^T} = U\Lambda U^T$$

$$\boxed{L = U\Lambda U^T} = \sum_{i=1}^{n} \lambda_i (u_i u_i^T)$$

$$= \lambda_1 u_1 u_1^T + \lambda_2 u_2 u_2^T + \dots + \lambda_n \vec{u}_n \vec{u}_n^T$$

$$= \lambda_1 \square_{n}^{n} + \lambda_2 \square_{n}^{n} + \dots + \lambda_n \square_{n}^{n}$$

$$Lf$$

$$\vec{h} = L \begin{bmatrix} 2 \\ 1 \\ 3 \\ 1 \\ 2 \end{bmatrix} = \underline{\underline{Lf}}$$

$$\vec{h} = (D - A)\vec{f}$$

what about node v_i

$$\vec{h}[i] = \left(d_i - \sum_{j=1}^{n} a_{ij}\right) \vec{f}[i]$$

$$= \sum_{v_j \in N(v_i)} \left(f[i] - f[j] \right)$$

$N(v_i)$ = set of neighbors of node v_i

$$f^T L f = \sum_{v_i} f[i] \left(Lf \right)[i]$$

$$\vdots$$

$$\boxed{f^T L f = \frac{1}{2} \sum_{v_i} \sum_{v_j \in N(v_i)} \left(f[i] - f[j] \right)^2} \geq 0$$

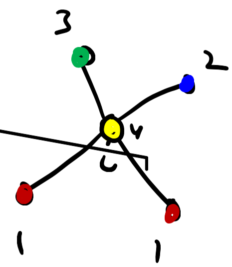
PSD: a matrix L $(n \times n)$ is PSD iff

$$\forall \vec{x} \in \mathbb{R}^n$$

$$\vec{x}^T L \vec{x} \geq 0$$

$f[i] = 4$

$\{1, 1, 2, 3\}$



$$\vec{v}_1^T L \vec{v}_1 = v_1^T \left(\lambda_1 \vec{v}_1 \right) = \lambda_1 v_1^T v_1 = \lambda_1$$

$$\vdots$$

$$\vec{v}_n L \vec{v}_n = v_n^T \lambda_n \vec{v}_n = \lambda_n v_n^T v_n = \lambda_n \geq 0$$

$$\vec{v}_n = \begin{pmatrix} 1/\sqrt{n} \\ 1/\sqrt{n} \\ \vdots \\ 1/\sqrt{n} \end{pmatrix}$$

eigenvalue represent "smoothness" of the basis

$$\vec{f} = \begin{pmatrix} 3 \\ 1 \\ 2 \\ 1 \\ 3 \end{pmatrix}$$

$$\underline{\underline{U^T}}\vec{f} = \hat{f}$$

$U^T f$ represents projections of $\vec{f}$ along the different basis vectors