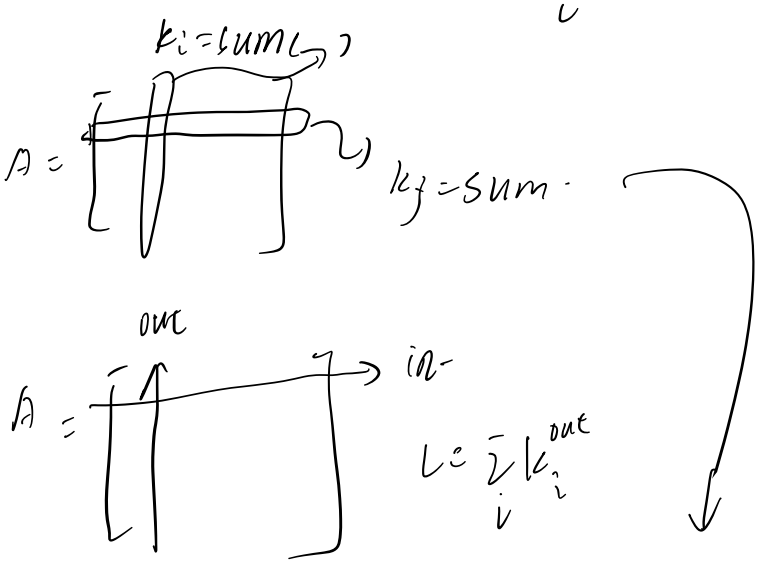
11. Intro.

Adj Matrix:

$L = \frac{1}{2}\sum_i k_i$

- undirect:



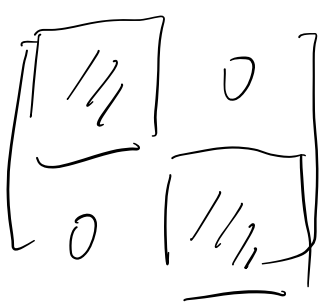
- direct:

平均度: $\bar{k} = \frac{2E}{N}$

weighted: $A = \begin{bmatrix} 0.1 & \cdots \\ 0.12 & \\ 1 & \end{bmatrix}$

$E = \frac{1}{2}\cdot\sum_{ij} B_{ij}$ $\quad$ $\bar{k} = 2\cdot\frac{E}{N}$

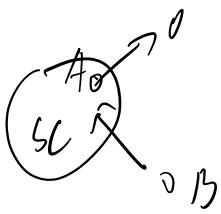
Disconnected:



Connectivity:

- Strongly connected: 任意2点间有通路 (A→B, B→A)
- Weakly ~ : ~ (不考虑方向)

SCCs:



A: In-component.

B: Out-component

L2, Feature learning.

- ML need features.

- Goal: learn Structure. position of a node.

Traditional Methods: { 1. Degree; 2, centrality; 3. Graphlets }

Node level:

- Degree: cons: can't capture importance of nodes.

- Centrality:

  - Degree: $C_d(v_i) = d_i$

$$\begin{cases} C_d^{norm}(v_i) = \frac{d_i}{n-1} \\ C_d^{max}(v_i) = \frac{d_i}{\max_j(d_j)} \\ C_d^{sum}(v_i) \approx \frac{d_i}{2|E|} \end{cases}$$

  - Betweenness:

$$C_B(v_i) = \sum_{j<k} \frac{g_{jk}(i)}{g_{jk}}$$

$g_{jk}(i)$ → paths j-k pass i

g_{jk} → all paths in j-k

$$C_B'(v_i) = \frac{C_B(v_i)}{\frac{(n-1)(n-2)}{2}}$$

- Closeness :

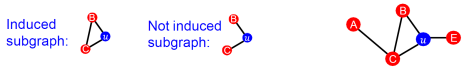
$$C_C(v_i) = \frac{N-1}{\sum_{j=1}^{N} d(i,j)}$$

Comparison:

	Low Degree	Low Closeness	Low Betweenness
High Degree		*Node is embedded in a community that is far from the rest of the network*	*Node's connections are redundant - communication bypasses the node*
High Closeness	*Key node connected to important/active alters*		*Probably multiple paths in the network, node is near many people, but so are many others*
High Betweenness	*Node's few ties are crucial for network flow*	*Very rare! Node monopolizes the ties from a small number of people to many others.*	

-Graphlets:

- Def: Induced subgraph is another graph, formed from a subset of vertices and *all* of the edges connecting the vertices in that subset.



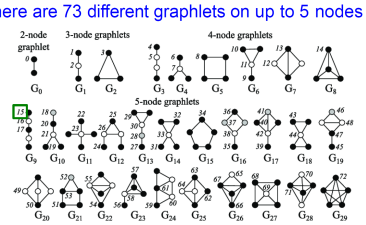
Homogeneous			Heterogenous					
Pattern	Graph	Count	Pattern	Graph	Count	Pattern	Graph	Count
		0			0			0
		12			4			1
		24			6			2

- Graphlets: Rooted connected induced non-isomorphic subgraphs:

There are 73 different graphlets on up to 5 nodes

Take some nodes and all the edges between them.

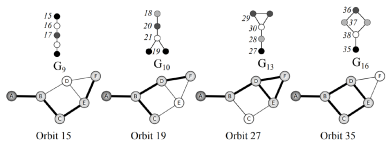
Graphlet id (Root / "position" of node *u*)



Note: Here is still on homogeneous graphs. Different colours distinguish different orbits and positions.

Graphlet Degree Vector

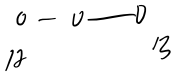
- Computation of the graphlet degree vector (GDV) of node A in the friendship network
  - GDV provides a measureof a node's local network topology
  - Comparing vectors of two nodes provides a more detailed measure of local topological similarity than node degrees



Orbit	0	1	2...3	4	5	6	7...14	15	16...18	19	20...26	27	28...34	35	36...72
GDV(A)	1	2	0...0	3	0	1	0...0	1	0...0	1	0...0	1	0...0	1	0...0

Link level: 預測 edge score : $C(x,y)$

1. Distance:



$S_{12,13} = 2$.

2. Local Neighbourhood Overlap:

$$\text{Jaccard} = \frac{N(12) \cap N(13)}{N(12) \cup N(13)}$$

L3 PageRank.

- $r = Mr$

- 计算：令 $r^0 = [1/n, \cdots 1/n]^T$

$$r^{k+1} = Mr^k$$

直至：$\|r^{k+1} - r^k\|_1 < \varepsilon$.

问题1：spider trap

→ ③ ②，会导致 PR 最高、其他为 0

Solution：

$$r^{k+1} = \beta \cdot M \cdot r^k + (1-\beta)\begin{bmatrix} 1/n \\ \vdots \\ 1/n \end{bmatrix}$$

（网页会随机跳到其它网页.

问题2：Dead End

→ ③，会导致 rank 全是 0. (Non-stochastic!)

Solution: $\begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 \\ 1/n \\ \vdots \\ 1/n \end{bmatrix}$

计算问题：M 非常 sparce. M 的空间太大. $M \approx 10N$ entries.

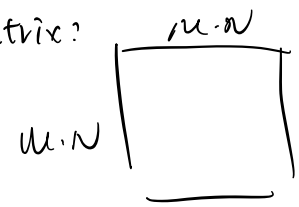
Solution：利用 adj list，encode M.

公式：$r \leftarrow \beta Mr + (1-\beta)[1/N]_N$

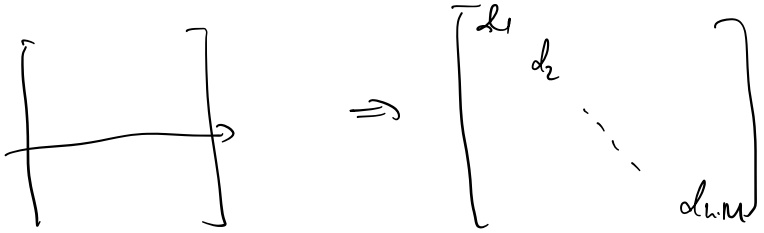
14. Graph Laplacian.

- similarity: $W_{ij} = e^{-\frac{\|x_{(i)} - x_{(j)}\|_2^2}{\sigma^2}}$

- Affinity Matrix:

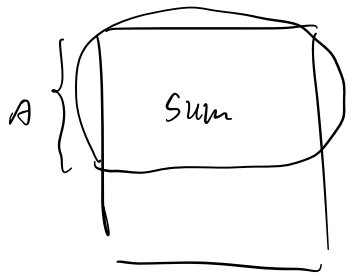


- Degree:



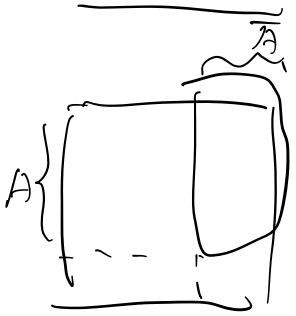
- Volume of set:

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



- Cuts:

$$Cut(A, \bar{A}) = \sum_{i \in A, j \in \bar{A}} W_{ij}$$



- Laplace: $L = D - W$

- Spetral Clustering:

- Min cut:

$$MinCut(A, B) = \min_{A,B} \sum_{u \in A, v \in B} w(u, v)$$

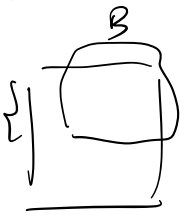
(intuition：两团体 i 间连接尽可能松)

—Normalized Cut:

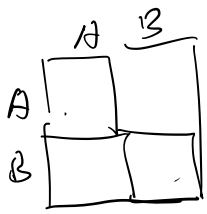
$$NCut(A,B) = Cut(A,B)\left(\frac{1}{Vol(A)} + \frac{1}{Vol(B)}\right)$$

排除小的 outlier 干扰

association: $assoc(A,B) = \sum_{u\in A, v\in B} w(u,v)$



$$Nassoc(A,B) = \frac{assoc(A,A)}{assoc(A,V)} + \frac{assoc(B,B)}{assoc(B,V)}$$



$$\Rightarrow Ncut(A,B) = 2 - Nassoc(A,B)$$

Problem: 2-clustering.

Goal: Find A,B. $\min_{A,B} Ncut(A,B)$

NP-hard

Solution: $\min_x Ncut(x) = \min_y \frac{y^T(D-W)y}{y^TDy}$, Subject to $y^TD\vec{1} = 0$

$\Leftrightarrow \min_y y^T(D-W)y$ subject to $y^TDy = 1$

$\Leftarrow \frac{\partial\, y^T(D-W)y - \lambda(y^TDy-1)}{\partial y} = 0$

$\Leftrightarrow (D-W)y - \lambda Dy = 0$

$(D-W)y = \lambda Dy$

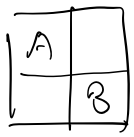
$\Rightarrow D^{-1}(D-W)y = \lambda y$

$(I - D^{-1}W)y = \lambda y$ $\Rightarrow$ eigenvector.

(second smallest)

$\sum_i y_i D_{ii} = 0$

- Avg association: $\max_{A,B} \left\{ \frac{assoc(A,A)}{|A|} + \frac{assoc(B,B)}{|B|} \right\}$



- Avg cut: $\min_{A,B} \left\{ \frac{Cut(A,B)}{|A|} + \frac{Cut(A,B)}{|B|} \right\}$

- Laplacian: $L = D - W$.

$$L_{sym} = D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}$$

$$L_{rw} = D^{-1}(D-W)$$

$$L_{sym} = D^{\frac{1}{2}} L_{rw} D^{-\frac{1}{2}}$$

- $y^T(D-W)y = \sum_{i,j} w_{ij}(y_i - y_j)^2$ — smoothness of G

$$y^T D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}} y = \sum_{i,j} w_{ij}\left(\frac{y_i}{\sqrt{D_{ii}}} - \frac{y_j}{\sqrt{D_{jj}}}\right)^2$$

- $(Ly)_i = \sum_{j \in N(i)} w_{ij}(y_i - y_j)$

- L^{-1} as operator:
  - $(D^{-1}W)^k$ k-th hop
  - $\sum_{k=0}^{\infty} (D^{-1}W)^k = I - D^{-1}W$

计算过程

$(Ay)_i = \sum_j A_{ij} y_j$

$\Rightarrow y^T Ay = \left(\sum_{ij} A_{ij} y_j\right) \cdot y_i$

$= \sum_{ij} A_{ij} y_j \cdot y_i$

$y^T Ay = \sum_i \sum_j A_{ij} y_i y_j$

$\frac{\partial y^T Ay}{\partial y_k} = \frac{\partial}{\partial y_k} \sum_i \sum_j A_{ij} y_i y_j$

$= \sum_{j \neq k} A_{kj} y_j + 2A_{kk} y_k + \sum_{i \neq k} A_{ik} y_i$

$= \sum_j A_{kj} y_j + \sum_i A_{ik} y_i$

$\therefore \frac{\partial y^T Ay}{\partial y} = y^T D + y^T D^T = y^T (D + D^T)$

$\frac{\partial y^T (D-W) y}{\partial y} = y^T \left[(D-W) + (D-W)^T\right]$

$= y^T (D - W + D^T - W^T)$

$= 2 y^T (D - W)$

$\Rightarrow (D-W) y - \lambda D y = 0$

$y^T (D-W) y$

$\left((D-W)y\right)_i = \sum_j (D-W)_{ij} y_j$

$\Rightarrow y^T (D-W) y = \left(\sum_j (D-W)_{ij} y_j\right) y_i$

$= \sum_{ij} D_{ij} y_i y_j - \sum_{ij} W_{ij} y_i y_j$

$= \sum_i D_{ii} y_i^2 - \sum_{ij} W_{ij} y_i y_j$

$= \sum_i \sum_j W_{ij} y_i^2 - \sum_{ij} W_{ij} y_i y_j$

$= \frac{1}{2} \sum_{ij} W_{ij} y_i^2 - \sum_{ij} W_{ij} y_i y_j + \frac{1}{2} \sum_{ij} W_{ij}$

$= \frac{1}{2} \sum_{ij} W_{ij} (y_i - y_j)^2$

Cuts Comparison:

Finding clumps ⟷ Finding splits

	Average association	Normalized Cut	Average cut
Discrete formulation	$\frac{asso(A,A)}{\lvert A\rvert} + \frac{asso(B,B)}{\lvert B\rvert}$	$\frac{cut(A,B)}{asso(A,V)} + \frac{cut(A,B)}{asso(B,V)}$ or $2 - \left(\frac{asso(A,A)}{asso(A,V)} + \frac{asso(B,B)}{asso(B,V)}\right)$	$\frac{cut(A,B)}{\lvert A\rvert} + \frac{cut(A,B)}{\lvert B\rvert}$
Continuous solution	$Wx = \bar{\lambda} x$	$(D-W)x = \bar{\lambda} D x$ or $W x = (1 - \bar{\lambda}) D x$	$(D-W)x = \bar{\lambda} x$

$$
\begin{aligned}
& f^T D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}} f \\
&= f^T f - f^T D^{-\frac{1}{2}} W D^{-\frac{1}{2}} f \\
&= \sum_{i=1}^{N} f_i^2 - \begin{bmatrix} \vdots \\ \frac{f_i}{\sqrt{D_{ii}}} \\ \vdots \end{bmatrix} \cdot \begin{bmatrix} \cdots & \sum_{j=1}^{N} \frac{f_j}{\sqrt{D_{jj}}} \cdot w_{ij} & \cdots \end{bmatrix} \rightarrow \text{i-th row} \\
&= \sum_{i=1}^{N} f_i^2 - \sum_{i=1}^{N} \frac{f_i}{\sqrt{D_{ii}}} \cdot \sum_{j=1}^{N} \frac{f_j}{\sqrt{D_{jj}}} w_{ij} \\
&= \sum_{i=1}^{N} \sum_{j=1}^{N} f_i^2 - \frac{f_i \cdot f_j}{\sqrt{D_{ii}} \cdot \sqrt{D_{jj}}} \cdot w_{ij} \\
&= \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij} \left(\frac{f_i^2}{D_{ii}} - \frac{2 f_i \cdot f_j}{\sqrt{D_{ii}} \sqrt{D_{jj}}} + \frac{f_j^2}{D_{jj}} \right) \\
&= \frac{1}{2} \sum_{i,j=1}^{N} w_{ij} \left(\frac{f_i}{\sqrt{D_{ii}}} - \frac{f_j}{\sqrt{D_{jj}}} \right)^2
\end{aligned}
$$

- Personalised PageRank:
  - $p^{t+1} = (1-\beta) q + \beta W p^t$ (不同的是，会有一定概率回到原点)
  - 用于 semi-supervised learning. (回到有 label 的地方)
  - eg: (2 classes)

    Formula: $f^{t+1} = (1-\alpha) y + \alpha S f^t$ ($S = D^{-\frac{1}{2}} W D^{-\frac{1}{2}}$)

    $\Rightarrow f^{t+1} = (1-\alpha) y + \alpha S((1-\alpha) y + \alpha S f^{t-1})$

$$= (1-\alpha)y \cdot \sum_{i=0}^{t} (\alpha S)^t + (\alpha S)^t y \quad (\to v)$$

$$\lim_{t\to\infty} \sum_{t} (\alpha S)^t = \frac{1-(\alpha S)^{t+1}}{1-\alpha S} = (1-\alpha S)^{-1}$$

$$\therefore f^* = \lim_{t\to\infty} f^t = (1-\alpha)\cdot y (1-\alpha S)^{-1}$$

In fact: $L(f) = \frac{1}{2}\left(\sum_{ij} w_{ij} \left| \frac{f_i}{\sqrt{D_{ii}}} - \frac{f_j}{\sqrt{D_{jj}}} \right|^2 + \mu \sum_i \| f_i - y_i \|^2 \right)$

$$= \frac{1}{2}\left(f^T D^{-\frac{1}{2}} (D-W) D^{-\frac{1}{2}} f + \mu \cdot (f-y)^T (f-y) \right)$$

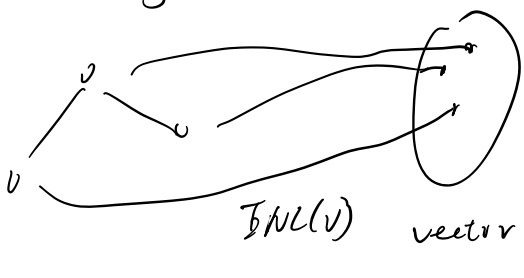
$$\frac{\partial L(f)}{\partial f} = 0 \iff \underbrace{D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}}_{A} f + \mu \cdot (f-y) = 0$$

$$\iff f^* = \mu y \cdot (D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}} + \mu \cdot I)^{-1}$$

(这是 GCN 之前 . semisupervised learning 的常规做法)

25. Node / Graph Embedding.

1. Node Embedding.



- $sim(z_1, z_2) \approx z_1^T z_2$
- learn structure feature, embedding for downstream task.
- 2种寻找nodes间关系的办法：

① Adj-based similarity:

$$-L = \sum_{(u,v) \in V \times V} \| z_u^T z_v - A_{u,v} \|^2$$

- 用SGD更新.
- Cons: 1. $O(|V|^2)$ time. (改进：由于是sparse图，对non-zero更新.)
  2. 只考虑local, direct连接

② Random Walk:

- why? 1. Expressive：考虑了local, high-order的信息.
  2. 只考虑Rand Walk上的node

· $N_R(u)$ — set of neighbur nodes. R — strategy

· objective: $\max_f \sum_{u \in V} \log P(N_R(u) | z_u)$

$$\Leftrightarrow L = -\sum_{u \in V} \sum_{v \in N(u)} \log P(v | z_u)$$

where $P(v|z_u) = \dfrac{\exp(z_v^T \cdot z_u)}{\sum_{k \in V} \exp(z_k^T \cdot z_u)}$

$$\Rightarrow L = -\sum_{u \in V} \sum_{v \in N(u)} \log \frac{\exp(z_v^T \cdot z_u)}{\sum_{k \in V} \exp(z_k^T \cdot z_u)}$$

$O(|V|^2)$!

· Word2Vec 2种 model: v_1, v_2, v_3, v_4, v_5

1. CBOW: 背景词 → 中心词

$v_2 \uparrow \xrightarrow{z_{V \times N}} z_2 \searrow$

$\hat{z} = \frac{z_2 + z_4}{2} \xrightarrow{z_{N \times V}} \hat{y} \sim y_3$

$v_4 \uparrow \xrightarrow{z_{V \times N}} z_4 \nearrow$

2. SG: 中心词 → 背景词

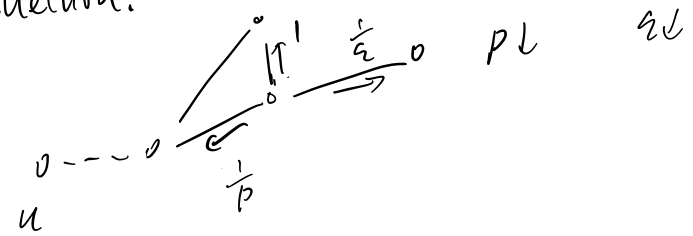
$v_3 \uparrow \xrightarrow{z_{V \times N}} z_3 \xrightarrow{z_{N \times V}} \hat{y} \sim y_2$ or y_4

- 如何解决 $O(|V|^2)$?
  - Approximation:

$$\log \frac{\exp(z_v^T \cdot z_u)}{\sum_{n \in V} (z_n^T \cdot z_u)} \approx \log \sigma(z_u^T z_v) - \sum_{k} \log \sigma(z_u^T z_k)$$

k 个 negative sample

  - k ↑, robust ↑
  - k nodes are not on the walks!
- Better strategy: Biased Walks.
  - why? trade off between local / global
  - Method:



$$\pi_{c_i|c_{i-1},c_{i-2}} = \begin{cases} 1, & d(c_{i-2}, c_i) = 1 \\ 1/p, & \sim = 2 \\ 1/q, & \sim = 0 \end{cases}$$

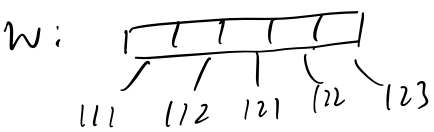
2. Graph Embedding:

法一：sum / avg of node embedding $z_G = \sum_{v \in G} z_v$

法二：virtual node, and run node embedding

法三：Anonymous Walk Embedding.

- 1. do m times random walk with len l
  2. record w_i counts
  3. normalize w vector. w is G embedding.



- How many walks?

$$m = \left\lceil \frac{2}{\varepsilon^2}\left(\log(2^\eta - 2) - \log(\delta)\right) \right\rceil$$

η: theoretically existed types of asym. walks of len l.

δ: $P(\#\text{errors} \le \varepsilon) < \delta$

2b GNN.

- Limitation of shallow Embedding:
  1. $O(|V|)$ params
  2. can't generate new embedding for new nodes.
  3. no data feature.
- Goal: Find $f: V \to R^d$

- Naive: MLP($[A_i, f_i]$)
  问题: 1. $O(|V|)$ parameters
  2. not invariant to node ordering
- GNN model should obey Permutation Equivariant/Invariant:
  1. Permutation Equivariant:
     同一幅图, 不同 order 的 (A, X), (A', X'), $f: G \to R^d$: vector
     对于同一个 node n: $f(A, X)_n = f(A, X')_n$
     $\Leftrightarrow$ f is permutation equivariant.
  2. Permutation Invariant:
     同一幅图, 不同 order 的 (A, X), (A', X'), $f: G \to k$: score.
     $f(A, X) = f(A', X')$
     $\Leftrightarrow$ f is Permutation Invariant.

· 2 Models:

1. Basic GNN:

· Math:

$$h_v^0 = x_v$$

$$h_v^k = \sigma\left(W_k \sum_{u \in N(v)} \frac{h_u^{k-1}}{|N(v)|} + B_k \cdot h_v^{k-1}\right), \forall k > 0$$

· Matrix Formulation:

$$H^{(k+1)} = \sigma\left(\tilde{D^{-1}A}H^{(k)} W_k^T + H^k B_k^T\right)$$

$\tilde{D^{-1}A}$: aggregation. W_k^T: projection

· Train:

1. unsupervised: 利用图结构, node similarity
   · DeepWalk, Adj sim
2. supervised: $f: R^n \to R$. classification.

- Pros: 1. share paras
  2. inductive

2. GraphSage:

· $h_v^{(k)} = \sigma\left([W_k \cdot AGG(h_u^{k-1}, \forall u \in N(v)), B_k h_v^{k-1}]\right)$

- 变化：1. $AGG(\cdot)$ generalization

  2. sum → concatenation.

- 3 种 AGG：

  1. Mean

  2. Pool：$\gamma\left(\{Qh_u^{k-1}, \forall u \in N(v)\}\right)$ → element-wise mean / max

  3. LSTM：$LSTM\left([h_u^{k-1}, \forall u \in \pi(N(v))]\right)$

     π：生成一个随机序列

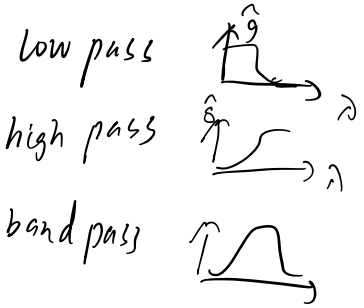
L7. GNN 2.

- Graph Signal: $f: V \to R^{N \times d}$
- Laplace Operator:
  1. $h = Lf$, $h(i) = \sum_{v_j \in N(v_i)} (f(i) - f(j))$
  2. $f^T L f = \frac{1}{2} \sum_{i,j=1}^{n} A_{ij} (f_i - f_j)^2$
- $L = U \Lambda U^T$
  - $\Lambda = [\lambda_0, \ldots, \lambda_{N-1}]$, where $0 = \lambda_0 \le \lambda_1 \cdots \le \lambda_{N-1}$.
    - $L \cdot 1 = 0 \cdot 1$ (trivial solution)

$u_0 \ldots u_{n-1}$ are based signals, $\lambda_0 \ldots \lambda_{n-1}$ are corresponding frequency.

- Graph Fourier Transform: smoothness: $Lu = \sum_{ij} w_{ij} (u_i - u_j)$
  - $L = U \Lambda U^T$ ($Lu = \lambda u$) → frequency. → $|U| = 1$
  - GFT: $\hat{f} = U^T f$
  - Inverse GFT: $f = U \hat{f}$
- GNN Framework:
  - Filter: $A \in R^{n \times n}$, $X \in R^{n \times d} \Rightarrow A \in R^{n \times n}$, $X \in R^{n \times d_{new}}$
  - Pooling: $A \in R^{n \times n}$, $X \in R^{n \times d} \Rightarrow A \times R^{n_p \times n_p}$, $X \in R^{n_p \times d_{new}}$

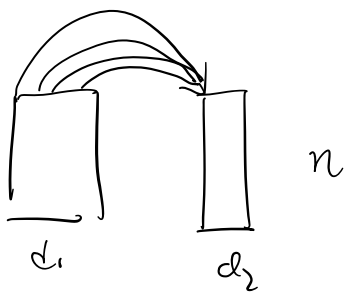
- Spectral Filtering:
  - $f \xrightarrow{GFT} U^T f \xrightarrow{\hat{g}(\Lambda)} g(\Lambda) U^T f \xrightarrow{IGFT} U \hat{g}(\Lambda) U^T f$
  - $\hat{g}(\Lambda) = \begin{bmatrix} \hat{g}(\lambda_0) & & \\ & \ddots & \\ & & \hat{g}(\lambda_{n-1}) \end{bmatrix}$



  - $f^* \leftarrow U \underbrace{g(\Lambda) U^T f}_{\hat{g}(L)}$
  - we learn $g(\Lambda)$ from data!

- Multi-channel signals:

$F_{in} \in \mathbb{R}^{n \times d_1} \rightarrow F_{out} \in \mathbb{R}^{n \times d_2}$



$$F_{out}[:, i] = \sum_{j=1}^{d_1} \hat{g}_{i,j}(L) \cdot F_{in}[:, j], \quad i = 1, \ldots, d_2$$

∴ we have $d_2 \times d_1$ filters.

- $g(\Lambda) = \begin{bmatrix} \theta_1 & & \\ & \ddots & \\ & & \theta_n \end{bmatrix} \Rightarrow d_2 \times d_1 \times N$ parameters.

- Polynomial Parameterized:

  - $\hat{g}(\Lambda) = \begin{bmatrix} \sum_{k=0}^{K} \theta_k \lambda_1^k & & \\ & \ddots & \\ & & \sum_{k=0}^{K} \theta_k \lambda_N^k \end{bmatrix}$

$$L^K = (U \Lambda U^T)^K = U \Lambda^K U^T \rightarrow \begin{bmatrix} \lambda_1^K & & \\ & \ddots & \\ & & \lambda_N^K \end{bmatrix}$$

  - $d_2 \times d_1 \times K$ params.

  - $U \hat{g}(\Lambda) U^T f = \sum_{k=0}^{K} \theta_k L^k f$ (no eigen-decomposition needed)

  - Spatial View: $L^K f$: smoothness within k-hops.

- Chebyshev Polynomial:

  - $T_0(x) = 1$, $T_1(x) = x$, $T_{n+1}(x) = 2 \cdot T_n(x) - T_{n-1}(x)$

  - Moivre's formula: $(\cos x + i \cdot \sin x)^n = \cos nx + i \sin nx$

    (proved by induction.)

  - Othogonal polynomial (def)

    w/ integrable, $w(x) \geq 0$, $\langle f_m, f_n \rangle = \int_a^b f_m(x) \cdot f_n(x) w(x) \, dx$

$\langle f_m, f_n \rangle = 0$ for $m \neq n$.

- Gram-Schmidt orthonormalization:

$$\text{proj}_u(v) \overset{\text{def}}{=} \frac{\langle u, v \rangle}{\langle u, u \rangle} \cdot \vec{u}$$

$$u_1 = v_1$$
$$u_2 = v_2 - \text{proj}_{u_1} v_2$$
$$u_3 = v_3 - \text{proj}_{u_1} v_3 - \text{proj}_{u_2} v_3$$
$$\vdots$$
$$u_k = v_k - \sum_{i=1}^{k-1} \text{proj}_{u_i} v_k$$

then normalize $\{u_i\}_{i=1}^{k}$

- Def by trigonometric function:

$$T_n(\cos\theta) = \cos(n\theta)$$

- Proof correctness of chebyshev polynomials are orthogonal:

$$\langle T_n, T_m \rangle = \int_{-1}^{1} T_n(x) \cdot T_m(x) \underbrace{\frac{1}{\sqrt{1-x^2}}}_{\to w(x)} dx$$

$$= \int_{-1}^{1} \cos(n \cdot \arccos x) \cdot \cos(m \cdot \arccos x) \frac{1}{\sqrt{1-x^2}} dx$$

$$= \int_{-1}^{1} \cos(n \cdot \arccos x) \cdot \cos(m \cdot \arccos x) \, d\arccos x$$

$$= \int_{\pi}^{0} \cos(ny)\cos(my) \, dy$$

$$= \int_{-1}^{1} \left(\cos((m-n)y) + \cos((m+n)y) \right) dy$$

$$= 0 \qquad (m \neq n).$$

∴ orthogonal!

普通多项式，x值可能特别大/小，造成数值问题

- ChebNet: (stable under perturbation of coefficients)

  → $x \in [-1, 1]$, $y \in [-1, 1]$

  - Chebyshev polynomial: $T_0 = 1,\ T_1 = x,\ T_{n+1}(x) = 2T_n(x) - T_{n-1}(x)$

    $g(\Lambda) = \theta_0 T_0(x) + \theta_1 \cdot T_1(x)$ + ...

    → Initialization for Cheb poly, $x \in [-1, 1]$.

  - $\hat{\Lambda} = \frac{2\Lambda}{\lambda_{max}} - I$, $\hat{g}(\Lambda) = \sum_{k=0}^{K} \theta_k T_k(\hat{\Lambda})$

    → recursive def

  ∴ $U \hat{g}(\Lambda) U^T f = \sum_{k=0}^{K} \theta_k T_k(\hat{L}) f$, where $\hat{L} = \frac{2L}{\lambda_{max}} - I$.

- GCN: set $k=1$, $\lambda_{max} = 2$ for ChebNet.

  - $\hat{g}(\Lambda) = \theta_0 + \theta_1(\Lambda - I)$

    Generally we want GCN be a low-pass filter for $\hat{L}$

    let $-\theta_1 = \theta_0 = \theta$ (further constrain)

    $\hat{g}(\Lambda) = \theta(2I - \Lambda)$

    ∴ $U \hat{g}(\Lambda) U^T f = \theta(2I - L) f = \theta(2I - D^{-\frac{1}{2}}(D - A)D^{-\frac{1}{2}}) f$

    $= \theta(I + D^{-\frac{1}{2}} A D^{-\frac{1}{2}}) f$

    renormalization: $U \hat{g}(\Lambda) U^T f = \theta(D^{-\frac{1}{2}} \hat{A} D^{-\frac{1}{2}}) f$, where $\hat{A} = A + I$

- multi-channel GCN:

In general: $F_{out}[:, i] = \sum_{j=1}^{d_1} g_{i,j}(L) \cdot F_{in}[:, j],\ i = 1 \dots d_2$.

GCN: $F_{out}[:, i] = \sum_{j=1}^{d_1} \theta_{i,j} (D^{-\frac{1}{2}} \hat{A} D^{-\frac{1}{2}}) F_{in}[:, j]$ $i = 1 \dots d_2$

Matrix form: $F_{out} = (D^{-\frac{1}{2}} \hat{A} D^{-\frac{1}{2}}) F_{in} \cdot \theta$ $\theta \in R^{d_1 \times d_2}$.

- Spatial view for GCN:

let $C = D^{-\frac{1}{2}} \hat{A} D^{-\frac{1}{2}}$

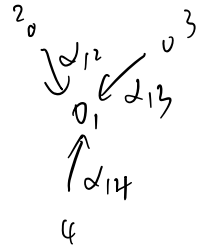
$F_{out} = C F_{in} \theta$

we know that: $C[i, j]$ if $v_j \notin N(v_i) \cup \{v_i\}$.

$\Rightarrow F_{out}[i, :] = \sum_{v_j \in N(v_i) \cup \{v_i\}} C[i, j] \cdot F_{in}[j, :] \theta$.

Aggregation. Feature transformation.

- GAT:



$$\alpha_{ij} = \frac{\exp(\sigma(a^T \cdot [Wh_i, Wh_j]))}{\sum_{k \in N_i} \exp(\sigma(a^T [Wh_i, Wh_k]))}$$

σ is LeakyRelu.

· MPNN：(考虑edge embedding)

$$m_i^{(k+1)} = \sum_{v_j \in N(v_i)} M_k(h_i^k, h_j^k, e_{ij})$$

$$h_i^{k+1} = U_k(h_i^k, m_i^{k+1}) \quad \text{, where } M_k, U_k \text{ need to be designed.}$$

· Graph Pooling：
- gPool：考虑 node importance
- DiffPool：考虑 clustering
- EigenPooling：利用滤波器 GFT，得到更好的 Hidden H_f

1. gPool：$v_i \to y_i$，$y_i = \frac{h_i^T \cdot p}{\|p\|}$ ⟶ Importance Ranking

$idx \leftarrow rank(y, n_p)$

$A_p \leftarrow A[idx, idx]$ ⟶ new Adj Matrix

$H_p \leftarrow H[idx, :] \odot \sigma(y[idx])$ ⟶ new hidden

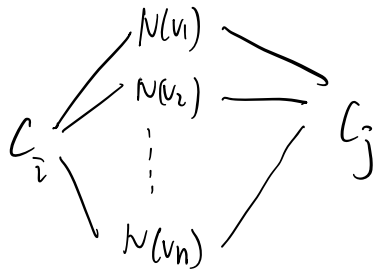
Cons：没考虑聚合性，使得 sample 的 node 连接性不强

2、DiffPool：

$H \in R^{n \times d}$ → W_1 → $H_a \in R^{n \times n_p}$ → $A_p = H_a^T A H_a$

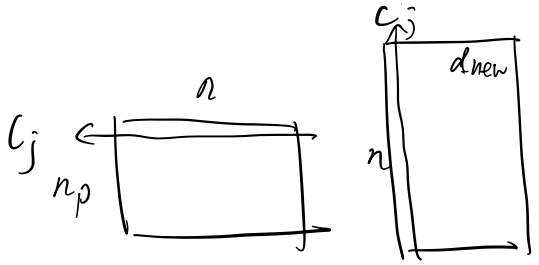
$H \in R^{n \times d}$ → W_2 → $H_f \in R^{n \times d_{new}}$ → $H_p = H_a^T H_f$

原理：1. $A_p = H_a^T A H_a$



cluster ⟷ nodes & N(v) ⟷ cluster.

2. $H_p = H_a^T H_f$



Hidden feature of C_j is from weighted sum of H_p

↓

"weight" is prob of node i & N(i) in C_j

3. Eigen pooling: Step 1: learn Ap like DiffPool

Step 2: use GFT to learn a better H_p.

subgraph G_i $\xrightarrow{GFT}$ $\hat{f}$ ⟶ Truncate some $\hat{f}_i$

*

- Eigen-decomposition is $O(N^3)$!!!

- If we want to develop a low-pass filter simply:

$$\hat{g}(\Lambda) = \begin{bmatrix} \lambda_{max} - \lambda_0 = \lambda_{max} & & & \\ & \lambda_{max} - \lambda_1 & & \\ & & \ddots & \\ & & & \lambda_{max} - \lambda_N \\ & & & \| \\ & & & 0 \end{bmatrix} \quad \begin{matrix} \leftarrow \text{low } f \\ \\ U^T f \\ \\ \leftarrow \text{high } f \end{matrix}$$

*

- Empirically LeakyRelu > Relu

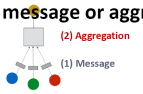
· 18 GNN 3:

- **GNN Layer:**
  - Transformation + Aggregation
  - Classic GNN layers: GCN, GraphSAGE, GAT
- **Layer connectivity:**
  - Deciding number of layers
  - Skip connections
- **Graph Manipulation:**
  - Feature augmentation
  - Structure manipulation

1. GNN Layer:

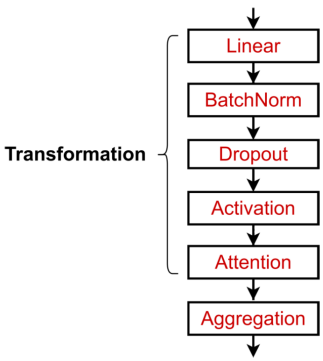
A Single GNN Layer

- **Putting things together:**
  - **(1) Message**: each node computes a mes: $\mathbf{m}_u^{(l)} = \text{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$
  - **(2) Aggregation**: aggregate messages from neighb $\mathbf{h}_v^{(l)} = \text{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}, \mathbf{m}_v^{(l)}\right)$
  - **Nonlinearity (activation):** Adds expressiveness
    - Often written as $\sigma(\cdot)$: $\text{ReLU}(\cdot)$, $\text{Sigmoid}(\cdot)$, ...
    - Can be added to **message or aggregation**



DNN Tricks: (in a linear layer)

A suggested GNN Layer



2. More Layers

- Add More layers ⇒ Over Smooth Problem. (Embedding are the same for different nodes)

原因

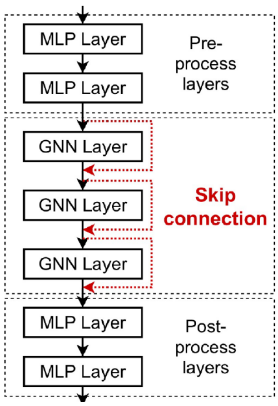
- **Receptive field:** the set of nodes that determine the embedding of a node of interest

- We knew **the embedding of a node is determined by its** receptive field
  - If two nodes **have highly-overlapped receptive fields, then their embeddings are highly similar**

- Stack many GNN layers → **nodes will have highly- overlapped receptive fields** → **node embeddings will be highly similar** → **suffer from the over-smoothing problem**

1. 假设前提1：决定合理的层数.

- **Step 1: Analyze the necessary receptive field** to solve your problem. E.g., by computing the diameter of the graph
- **Step 2:** Set number of GNN layers L to be a bit more than the receptive field we like. **Do not set L to be unnecessarily large**!



2. 改变model结构:

① Skip-Connection Formula

- **A standard GCN layer**

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}\right)$$

This is our $F(\mathbf{x})$

- **A GCN layer with skip connection**

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|} + \mathbf{h}_v^{(l-1)}\right)$$

$F(\mathbf{x})$ + $\mathbf{x}$

Other commonly used augmented features:

- **PageRank**
- **Centrality**

② 加强GNN之外的表达

Pre-processing layers: Important when encoding node features is necessary.
E.g., when nodes represent images/text

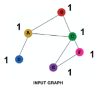
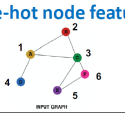
Post-processing layers: Important when reasoning / transformation over node embeddings are needed
E.g., graph classification, knowledge graphs

③ GNN layer 减少. 单个layer 加深

3. Augmentation. { Feature / Structure

- **Graph Feature manipulation**
  - The input graph **lacks features** → **feature augmentation**
- **Graph Structure manipulation**
  - The graph is **too sparse** → **Add virtual nodes / edges**
  - The graph is **too dense** → **Sample neighbors when doing message passing**
  - The graph is **too large** → **Sample subgraphs to compute embeddings**

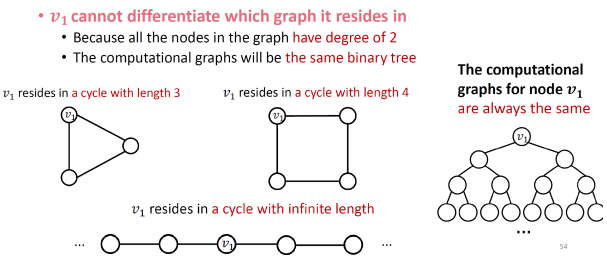
1. Feature Augment

	Constant node feature	One-hot node feature
		
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a unique ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple to generalize to new nodes: we assign constant feature to them, then apply our GNN	**Low**. Cannot generalize to new nodes: new nodes introduce new IDs, GNN doesn't know how to embed unseen IDs
Computational cost	**Low**. Only 1 dimensional feature	**High**. O V dimensional feature, cannot apply to large graphs
Use cases	Any graph, inductive settings (generalize to new nodes)	Small graph, transductive settings (no new nodes)

Why Feature Aug?

① Input hasn't any features. more expressive (表达)

② Some structures are hard to learn



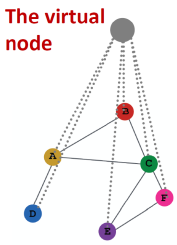
other Feature Aug Tricks: PageRank, Centrality ...

2. Structure augmentation

I. Add virtual edges: K-hops: $\tilde{A} = \sum_{k} A^k$

II. Add virtual nodes:

improve message passing in sparse graph.



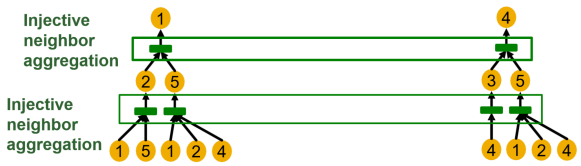
Why we need these augmentation?

- Our assumption so far has been **Raw input graph = computational graph**
- **Reasons for breaking this assumption**
  - **Feature level:**
    - The input graph **lacks features** → feature augmentation
  - **Structure level:**
    - The graph is **too sparse** → inefficient message passing
    - The graph is **too dense** → message passing is too costly
    - The graph is **too large** → cannot fit the computational graph into a GPU

29 Graph Isomorphism Network.

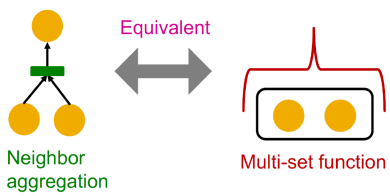
(研究的是：GNN对于structure的表达能力)

- More expressive: Injective neighbor aggregation:



Every step of aggregation is injective ⇒ GNN is injective ⇒ most expressive

- Multi-set-function:



Injective function can distinguish multi-sets!

- Fail Examples:

- **GCN** (mean-pool) [Kipf & Welling, ICLR 2017]
  - Uses **element-wise** mean pooling over neighboring node features

$$\text{Mean}(\{x_u\}_{u \in N(v)})$$

- **GraphSAGE** (max-pool) [Hamilton et al. NeurIPS 2017]
  - Uses **element-wise** max pooling over neighboring node features

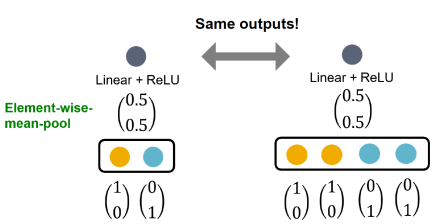
$$\text{Max}(\{x_u\}_{u \in N(v)})$$

① GCN:

Theorem [Xu et al. ICLR 2019]

- GCN's aggregation **function cannot distinguish different multi-sets with the same color proportion.**

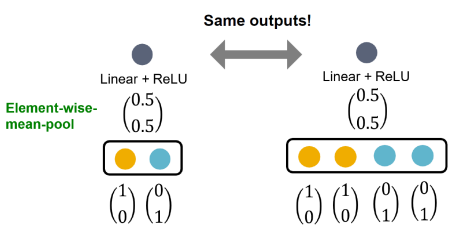
Failure case illustration



② GraphSAGE (max pool)

- GraphSAGE's aggregation **function cannot distinguish different multi-sets with the same set of distinct colors.**

Failure case illustration



· Injective Multi-set function:

· Thm: Injective function can be expressed as: $\Phi\left(\sum_{x \in S} f(x)\right)$

non-linear; linear; multi-set.

· How to model Φ, f? MLP.

Thm (Universal Approximation Thm):

MLP(hidden = 1) with $\sigma(\cdot)$ can approximate any continuous function.

$\Rightarrow$ Injective function $\Leftrightarrow$ $MLP_\Phi\left(\sum_{x \in S} MLP_f(x)\right)$

· GIN: $MLP_\Phi\left(\sum_{x \in S} MLP_f(x)\right)$

· Thm: GIN's aggregation is injective.

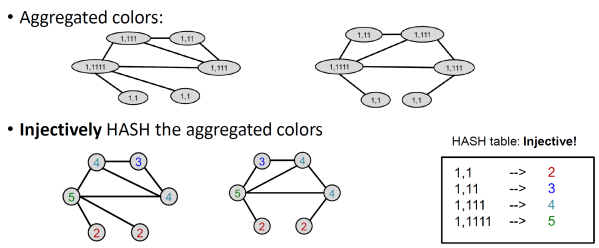
$\Rightarrow$ GIN is most expressive!

· WL graph kernal:

· Checking isomorphism is NP-hard!

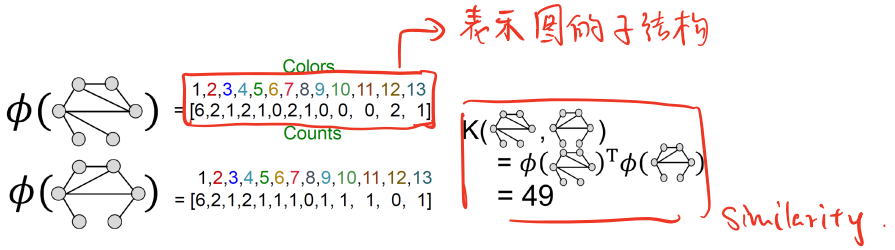
· WL kernal can distinguish most of the real-world graphs.

· Color refinement: $c^{(k+1)}(v) = HASH\left(c^{(k)}(v), \{c^{(k)}(u)\}_{u \in N(v)}\right)$



HASH is injective!

· Iterate till: no difference between nodes in a Graph in iteration $i+1$.



- KL kernel can somehow show the similarity.
  However $\phi(G_1) = \phi(G_2)$ doesn't imply isomorphism!

- $O(|E|)$ algorithm.
  (since there are $2|E|$ multiplication for each iteration)

- GIN model: use NN to model the HASH function
  - $MLP_\phi\left((1+\varepsilon)\cdot MLP_f(c^{k}(v)) + \sum_{u\in N(v)} MLP_f(c^{(k)}(u))\right)$
  - Since MLP can provide "one-hot" input for next layer:

$$GINConv\left(c^{k}(v), \{c^{k}(u)\}_{u\in N(v)}\right) = MLP_\phi\left((1+\varepsilon)\cdot c^{k}(v) + \sum_{u\in N(v)} c^{(k)}(u)\right)$$

- Iteratively update node vectors by (Differentiable color HASH function)

$$c^{(k+1)}(v) = \text{GINConv}\left(\{c^{(k)}(v), \{c^{(k)}(u)\}_{u\in N(v)}\}\right),$$

- **GIN can be understood as differentiable neural version of the WL graph Kernel:**

	Update target	Update function
WL Graph Kernel	Node colors (one-hot)	HASH
GIN	Node embeddings (low-dim vectors)	GINConv

↳ Capture fine-grained similarity of different nodes.

- Rank of expression: Sum > mean > max

L10 Heterogeneous Graphs, Knowledge Graphs.

1. Heterogeneous Graphs

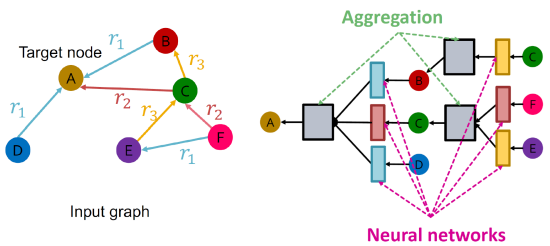
A heterogeneous graph is defined as

- $\boldsymbol{G} = (\boldsymbol{V}, \boldsymbol{E}, \boldsymbol{R}, \boldsymbol{T})$

- Nodes with node types $v_i \in V$
- Edges with relation types $(v_i, r, v_j) \in E$
- Node type $T(v_i)$
- Relation type $r \in R$

· Method: Relational GCN.

- Use different neural network weights for different relation types.



$$h_v^{(l+1)} = \sigma\left(\sum_{r \in R} \sum_{u \in N_v^r} \frac{1}{c_{v,r}} W_r^{(l)} h_u^{(l)} + W_0^{(l)} h_v^{(l)}\right)$$

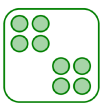
· params: $\{W_r^1, \cdots W_r^L\}_{r \in R}$.

⇒ too many params, overfitting

· Solution:

① block diagonal Matrix:

- **Key insight**: make the weights **sparse**!
- Use **block diagonal matrices** for $\mathbf{W}_r^{(l)}$

$\mathbf{W}_r =$ 

Limitation: only nearby neurons/dimensions can interact through W

- If use B low-dimensional matrices, then # param reduces from $d^{(l+1)} \times d^{(l)}$ to $B \times \frac{d^{(l+1)}}{B} \times \frac{d^{(l)}}{B}$

② Basis learning:

$W_r = \sum_{b=1}^{B} a_{rb} \cdot V_b$ → basis matrix; a_{rb} → importance.

2. knowledge Graph

- KG completion : given (h, r) , predict tails.

  that is $\arg\max_{\theta} \prod_{i,j,k \in N} P(X_{ijk}=1 \mid \theta, G)$, $X_{ijk}=1$ means $i \Rightarrow k$ is plausible.

- Methods:

  - Path Rank Alg: (Random Walk)

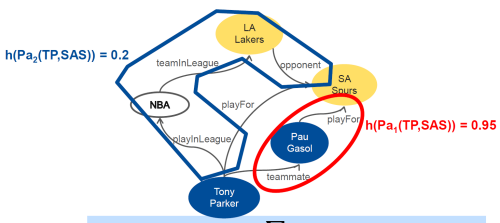
    $$S(A,r,B) = \sum_{p \in paths(A \to B)} \theta_r^p \cdot Pr(p)$$

    $$rel = \arg\max_{r \in rels} S(A,r,B)$$

    $$obj = \arg\max_{e \in ents} S(A,R,e)$$

Path Ranking Algorithm [Lao et al., 11]

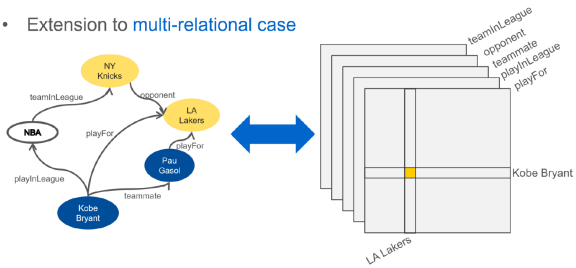
- Random walks on the graph are used to sample paths
- Paths are weighted with probability of reaching target from source
- Paths are used as ranking experts in a scoring function



$$S(TP, playFor, SAS) = \sum_{i \in paths} \theta^i_{playFor} h(pa_i(TP, SAS))$$

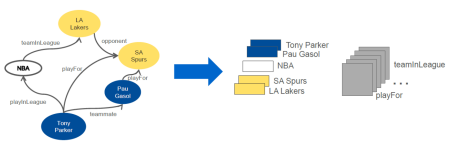
  - Factorization:

    - Extension to multi-relational case



  - Embedding:

    - Related to Deep Learning methods
    - Entities are vectors (low-dimensional sparse)
    - Relation types are operators on these vectors



Embeddings trained to define a **similarity score** on triples such that

$$S(KB, playFor, LAL) > S(KB, playFor, NYK)$$

- KG Embeding : (h, r, t).

  Goal : (h, r) ≈ t

Relation Patterns

- **Symmetric (Antisymmetric) Relations:** $r(h,t) \Rightarrow r(t,h)$ $(r(h,t) \Rightarrow \neg r(t,h))$ $\forall h,t$
  - **Example**:
    - Symmetric: Family, Roommate
    - Antisymmetric: Hypernym
- **Inverse Relations:** $r_2(h,t) \Rightarrow r_1(t,h)$
  - **Example** : (Advisor, Advisee)
- **Composition (Transitive) Relations:** $r_1(x,y) \wedge r_2(y,z) \Rightarrow r_3(x,z)$ $\forall x,y,z$
  - **Example**: My mother's husband is my father.
- **1-to-N relations:** $r(h,t_1), r(h,t_2), \ldots, r(h,t_n)$ are all True.
  - **Example**: r is "StudentsOf"

1. TransE: $h + r \approx t$

Score: $f_r(h,t) = -d_r(h,t) = -\|h+r-t\|$

Loss function: $L(h,r,t) = \max(0, \gamma + d_{r,pos} - d_{r,neg})$

$= \max(0, \gamma + f_{r,neg} - f_{r,pos})$

Algorithm 1 Learning TransE

input Training set $S = \{(h,\ell,t)\}$, entities and rel. sets E and L, margin γ, embeddings dim. k.

1: **initialize** $\ell \leftarrow$ uniform$(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$ for each $\ell \in L$
2: $\ell \leftarrow \ell / \|\ell\|$ for each $\ell \in L$
3: $\mathbf{e} \leftarrow$ uniform$(-\frac{6}{\sqrt{k}}, \frac{6}{\sqrt{k}})$ for each entity $e \in E$

Entities and relations are initialized uniformly, and normalized

4: **loop**
5: $\mathbf{e} \leftarrow \mathbf{e} / \|\mathbf{e}\|$ for each entity $e \in E$
6: $S_{batch} \leftarrow$ sample(S, b) // sample a minibatch of size b
7: $T_{batch} \leftarrow \emptyset$ // initialize the set of pairs of triplets
8: **for** $(h,\ell,t) \in S_{batch}$ **do**
9: $(h',\ell,t') \leftarrow$ sample$(S'_{(h,\ell,t)})$ // sample a corrupted triplet

Negative sampling with triplet that does not appear in the KG

10: $T_{batch} \leftarrow T_{batch} \cup \{((h,\ell,t),(h',\ell,t'))\}$
11: **end for**
12: Update embeddings w.r.t. $\sum_{((h,\ell,t),(h',\ell,t')) \in T_{batch}} \nabla[\gamma + d(\boldsymbol{h}+\boldsymbol{\ell},\boldsymbol{t}) - d(\boldsymbol{h'}+\boldsymbol{\ell},\boldsymbol{t'})]_+$

d represents distance (negative of score)

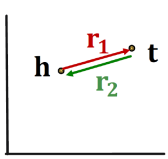
positive sample / negative sample

13: **end loop**

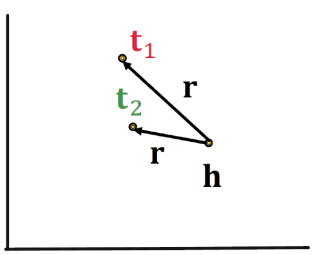
Contrastive loss: favors lower distance (or higher score) for valid triplets, high distance (or lower score) for corrupted ones

Inverse (✓)

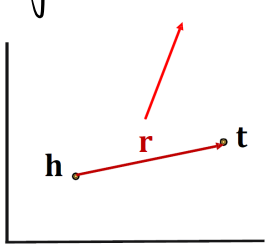
$\mathbf{h} + \mathbf{r}_2 = \mathbf{t}$, we can set $\mathbf{r}_1 = -\mathbf{r}_2$



1-to-N (✗)

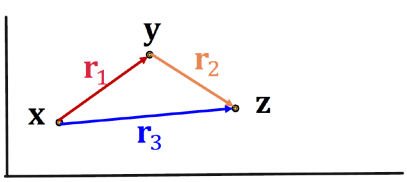


Symmetric (✗)

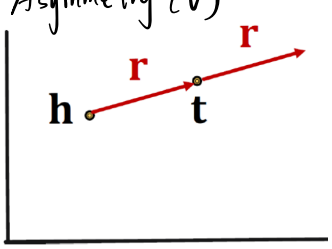


Composition (✓)

- $\mathbf{r}_1 = \mathbf{r}_2 + \mathbf{r}_3$

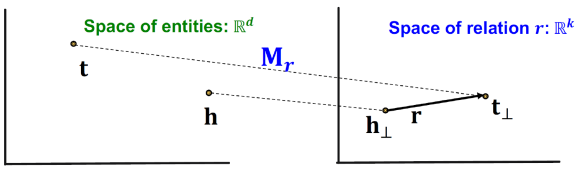


Asymmetry (✓)



2. TransR: entity space $\mathbb{R}^d$ $\xrightarrow{M_r \in \mathbb{R}^{k \times d}}$ relation space $\mathbb{R}^k$

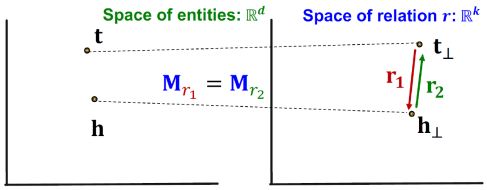
- $h_\perp = M_r h$, $t_\perp = M_r t$
- Score: $-\|h_\perp + r - t_\perp\|$



Inverse: ✓

$$\mathbf{r}_2 = -\mathbf{r}_1, \mathbf{M}_{r_1} = \mathbf{M}_{r_2}$$

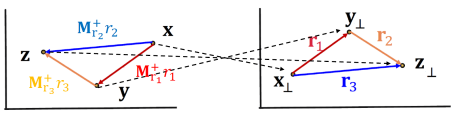
$$\mathbf{M}_{r_1}\mathbf{t} + \mathbf{r}_1 = \mathbf{M}_{r_1}\mathbf{h} \quad \mathbf{M}_{r_2}\mathbf{h} + \mathbf{r}_2 = \mathbf{M}_{r_2}\mathbf{t}$$



Composition ✓

- TransR can model composition relations ✓

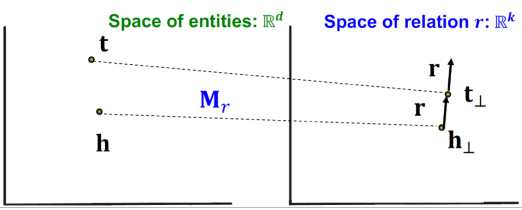
$\mathbf{M}_{r_i}^+ = \mathbf{M}_{r_i}^T(\mathbf{M}_{r_i}\mathbf{M}_{r_i}^T)^{-1}$ is the Moore–Penrose inverse (pseudoinverse) of $\mathbf{M}_{r_i}$ where $\mathbf{M}_{r_i}\mathbf{M}_{r_i}^T$ is invertible (full rank); so that $\mathbf{M}_{r_i}\mathbf{M}_{r_i}^+ = I$



Asymmetry: ✓

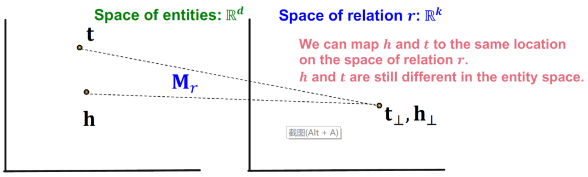
$$\mathbf{r} \neq 0, \mathbf{M}_r\mathbf{h} + \mathbf{r} = \mathbf{M}_r\mathbf{t},$$

Then $\mathbf{M}_r\mathbf{t} + \mathbf{r} \neq \mathbf{M}_r\mathbf{h}$ ✓



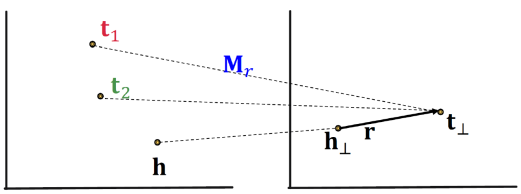
Symmetric: ✓

$$\mathbf{r} = 0,\ \mathbf{h}_\perp = \mathbf{M}_r\mathbf{h} = \mathbf{M}_r\mathbf{t} = \mathbf{t}_\perp$$ ✓



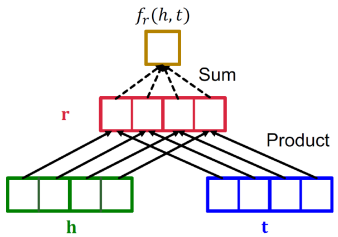
1-to-N: ✓

- We can learn $\mathbf{M}_r$ so that $\mathbf{t}_\perp = \mathbf{M}_r\mathbf{t}_1 = \mathbf{M}_r\mathbf{t}_2$
- Note that $\mathbf{t}_1$ does not need to be equal to $\mathbf{t}_2$!



3. DistMult: (bilinear Modeling)

- $h, r, t \in \mathbb{R}^k$
- score: $f_r(h,t) = \langle h, r, t \rangle = \sum_i h_i \cdot r_i \cdot t_i$
- Intuition: dot product of $h \cdot r$ and t.



Symmetric: (✓)

DistMult can naturally model symmetric relations

$$f_r(h,t) = \langle \mathbf{h}, \mathbf{r}, \mathbf{t} \rangle = \sum_i \mathbf{h}_i \cdot \mathbf{r}_i \cdot \mathbf{t}_i = \langle \mathbf{t}, \mathbf{r}, \mathbf{h} \rangle = f_r(t,h)$$

Inverse (X)

DistMult cannot model inverse relations

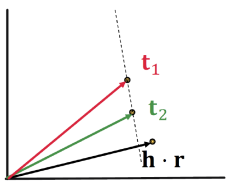
- If it does model inverse relations:

$$f_{r_2}(h,t) = \langle \mathbf{h}, \mathbf{r}_2, \mathbf{t} \rangle = \langle \mathbf{t}, \mathbf{r}_1, \mathbf{h} \rangle = f_{r_1}(t,h)$$

- This means $r_1 = r_2$

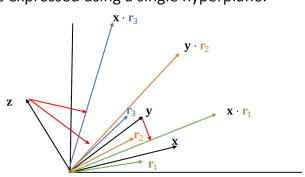
1-to-N (✓)

$$\langle \mathbf{h}, \mathbf{r}, \mathbf{t}_1 \rangle = \langle \mathbf{h}, \mathbf{r}, \mathbf{t}_2 \rangle$$



Composition (X)

- **Intuition:** **DistMult** defines a hyperplane for each (head, relation), the union of the hyperplanes induced by multihops of relations, e.g., (r_1, r_2), cannot be expressed using a single hyperplane.



5 Embedding Alg:

Model	Sym.	Antisym.	Inv.	Compos.	1-to-N
TransE	✗	✓	✓	✓	✗
TransR	✓	✓	✓	✓	✓
DistMult	✓	✗	✗	✗	✓
ComplEx	✓	✓	✓	✗	✓
RotatE	✓	✓	✓	✓	✓

L10.11 Recommendation System.

1. Collebrative Filetering (CF)

- input : user-item matrix.
- output : recommended items.

缺点：

- A popular similarity measure in user-based CF: **Pearson correlation**
  - a, b : users
  - $r_{a,p}$: rating of user a for item p
  - P : set of items, rated both by a and b
  - $sim(a,b) = \frac{\sum_{p \in P}(r_{a,p} - \bar{r}_a)(r_{b,p} - \bar{r}_b)}{\sqrt{\sum_{p \in P}(r_{a,p} - \bar{r}_a)^2}\sqrt{\sum_{p \in P}(r_{b,p} - \bar{r}_b)^2}}$
- Possible similarity values between −1 and 1

	Item1	Item2	Item3	Item4	Item5	
Alice	5	3	4	4	?	
User1	3	1	2	3	3	sim = 0.85
User2	4	3	4	3	5	sim = 0.70
User3	3	3	1	5	4	sim = 0.00
User4	1	5	5	2	1	sim = -0.79

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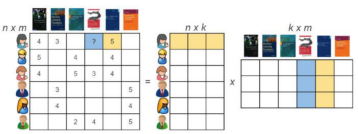
$$pred(a,p) = \overline{r_a} + \frac{\sum_{b \in N} sim(a,b) * (r_{b,p} - \overline{r_b})}{\sum_{b \in N} |sim(a,b)|}$$

优点：

- Matrix Factorization is one of the most popular methods for collaborative filtering
  - Given rating matrix Y
  - Each row represents an user u
  - While each column an item i

Regularization of p and q should be applied



$$\hat{y}_{ui} = f(u,i|\mathbf{p}_u, \mathbf{q}_i) = \mathbf{p}_u^T \mathbf{q}_i = \sum_{k=1}^{K} p_{uk} q_{ik}$$

$$L_{sqr} = \sum_{(u,i) \in \mathcal{Y} \cup \mathcal{Y}^-} w_{ui}(y_{ui} - \hat{y}_{ui})^2$$

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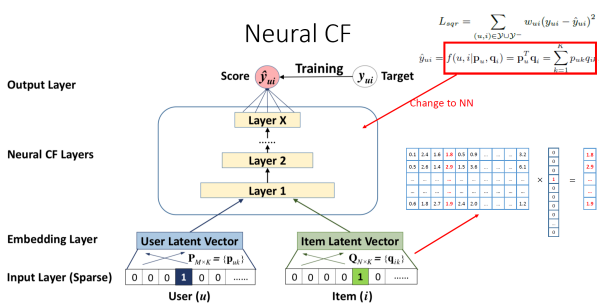
Metric:

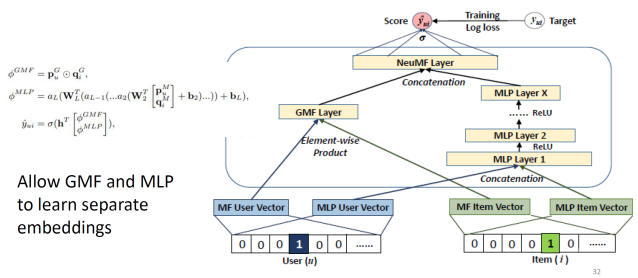
$$MAE = \frac{1}{n}\sum_{i=1}^{n}|p_i - r_i|$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(p_i - r_i)^2}$$

- Pros:
  - well-understood, works well in some domains, no knowledge engineering required
- Cons:
  - requires user community, sparsity problems, no integration of other knowledge sources, no explanation of results

2. Neural Collaborative Filtering (NLF)





Allow GMF and MLP to learn separate embeddings

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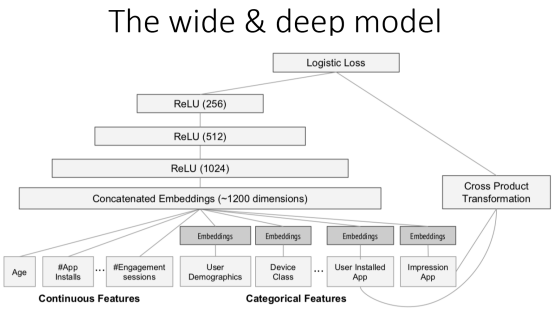
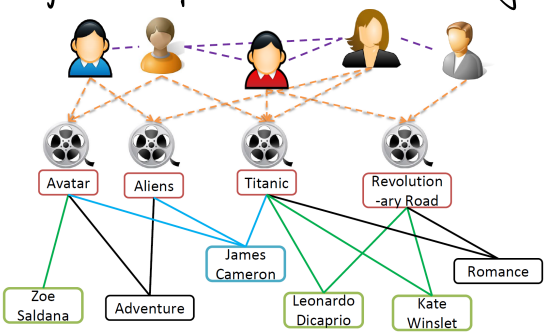
3. Wide. Deep learning



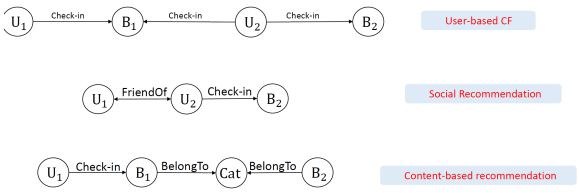
$$P(Y=1|\mathbf{x}) = \sigma(\mathbf{w}_{wide}^T[\mathbf{x}, \phi(\mathbf{x})] + \mathbf{w}_{deep}^T a^{(l_f)} + b)$$

4. Heterogeneous Info for Recommendation System.

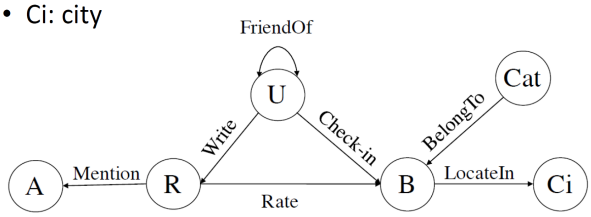


Metapath based RS

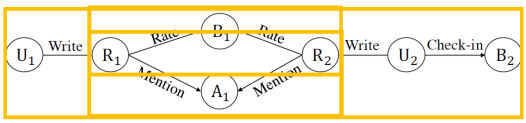
- Metapath → Recommending Strategy.



- R: reviews;
- U: users;
- B: business;
- Cat: category of item;
- Ci: city



Compute Similarity based on a Meta-graph



Compute $\mathbf{C}_{P_1}$: $\mathbf{C}_{P_1} = \mathbf{W}_{RB} \cdot \mathbf{W}_{RB}^\top$;
Compute $\mathbf{C}_{P_2}$: $\mathbf{C}_{P_2} = \mathbf{W}_{RA} \cdot \mathbf{W}_{RA}^\top$;
Compute $\mathbf{C}_{S_r}$: $\mathbf{C}_{S_r} = \mathbf{C}_{P_1} \odot \mathbf{C}_{P_2}$;
Compute $\mathbf{C}_{M_9}$ $\mathbf{C}_{M_9} = \mathbf{W}_{UR} \cdot \mathbf{C}_{S_r} \cdot \mathbf{W}_{UR}^\top \cdot \mathbf{W}_{UB}$;

L12 Recommendation Sys 2.

· Problem: MF doesn't explicitly use graph structure.

⇒ Only First-order graph structure capture in training objective

· Solution : GNN (explicitly, high order)

1. NGCF : NGCF jointly learn :

1. GNN 2. node shallow embedding

- Iteratively update node embeddings using neighboring embeddings.

$$\boldsymbol{h}_v^{(k+1)} = \text{COMBINE}\left(\boldsymbol{h}_v^{(k)}, \text{AGGR}\left(\left\{\boldsymbol{h}_u^{(k)}\right\}_{u \in N(v)}\right)\right)$$

$$\boldsymbol{h}_u^{(k+1)} = \text{COMBINE}\left(\boldsymbol{h}_u^{(k)}, \text{AGGR}\left(\left\{\boldsymbol{h}_v^{(k)}\right\}_{v \in N(u)}\right)\right)$$

$\sigma(W \cdot [x, y])$ Mean

· Finally : At k^{th} iteration :

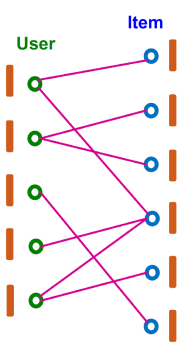
- For all $u \in \boldsymbol{U}$, $v \in \boldsymbol{V}$, we set

$$\boldsymbol{u} \leftarrow \boldsymbol{h}_v^{(K)}, \ \boldsymbol{v} \leftarrow \boldsymbol{h}_v^{(K)}.$$

- Score function is the inner product:

$$\text{Score}(u, v) = \boldsymbol{u}^{\mathrm{T}}\boldsymbol{v}$$

· User - item - User : very informative



2. LightGCN.

- Shallow embedding : $O(ND)$
- GNN : $O(D^2)$ $\quad f: R^D \to R^D$

- Simplifying GCN

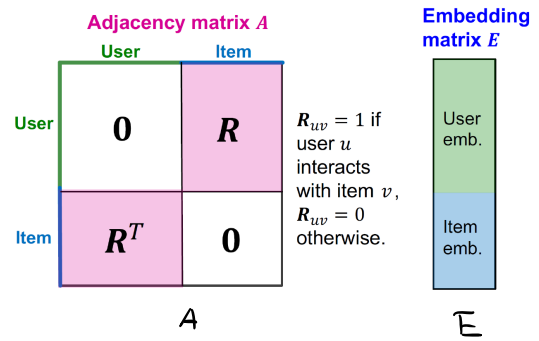
- GCN: $E^{(k+1)} = \sigma(\tilde{A} E^{(k)} W^{(k)})$, $\tilde{A} = D^{-1/2} A D^{-1/2}$

- Simplify GCN by removing ReLU:

$$E^k = \tilde{A} E^{k-1} W^{k-1}$$
$$= \tilde{A}(\tilde{A} E^{k-2}) W^{k-2} W^{k-1}$$
$$\cdots$$
$$= \tilde{A}^k E^0 (W^0 \cdots W^{k-1})$$

($W^0 \cdots W^{k-1} = W$)

$$\Rightarrow E^k = \hat{A}^k E W$$

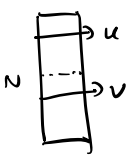


- Alg: $E \leftarrow \hat{A} E$ for every k.

- Final E: $E_{final} = \alpha_0 E^0 + \alpha_1 E^1 + \cdots + \alpha_k E^k \quad \left(\alpha = \frac{1}{k+1}\right)$

$$= \frac{1}{k+1} \sum_k \alpha_k E^k$$

- E_{final} for score: $u^T v \quad (u, v \in E)$



- Remember: Normalized Laplace: $D^{-1}(D-W)$, $D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}$

$$\sum_{k=0}^{\infty} \tilde{A}^k = (I - \tilde{A})^{-1} = \left(D^{-\frac{1}{2}}(D-W)D^{-\frac{1}{2}}\right)^{-1} = L^{-1}$$

LightGCN

$L = U \Lambda U^T$, $L^{-1} = U \Lambda^{-1} U^T$ ($Lu = \lambda u \Rightarrow L^{-1} L u = \lambda L u \Rightarrow L^{-1} u = \frac{1}{\lambda} u$)

Low-pass filter

∴ LightGCN can be thought as a low-pass filter. $\left(\sum_k A^k\right) \cdot E = L^{-1} E$

- Simplification leads to better performance. (than NGCF)

3. PinSAGE:

- Learn embeddings z_i: $d(z_{cake1}, z_{cake2}) < d(z_{cake}, z_{sweater})$

- Share Negative Sample: V_{neg} for a batch U_{mini} (performance stay similar!)

- Curriculum learning : make negative gradually harder
    - At n-th epoch , Add n-1 hard negative items
- Hard Negatives : close but not connected!
    - method: Run PageRank , random sample from high ranking item (but not too high)