

# **Stanford CS224W:** **GNNs for** **Recommender Systems**

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



# **Stanford CS224W:** **Recommender Systems:** **Task and Evaluation**

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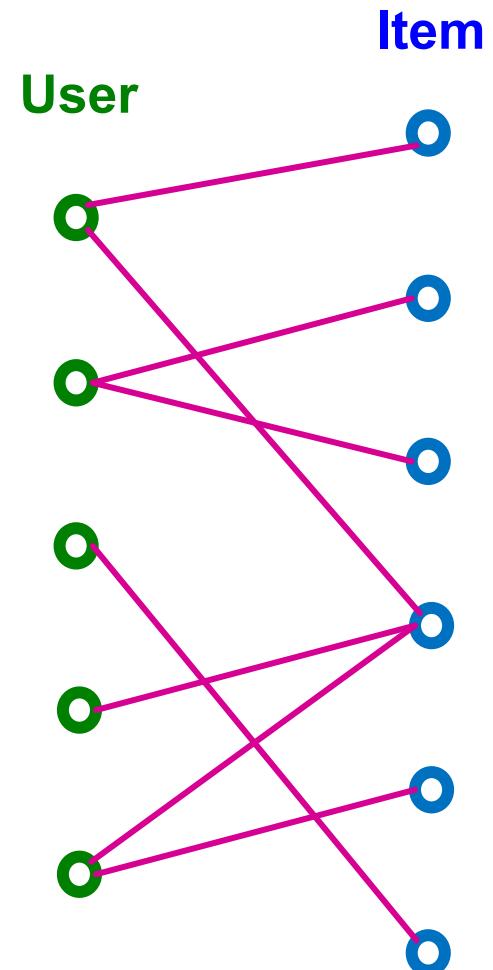


# Preliminary of Recommendation

- **Information Explosion in the era of Internet**
  - 10K+ movies in Netflix
  - 12M products in Amazon
  - 70M+ music tracks in Spotify
  - 10B+ videos on YouTube
  - 200B+ pins (images) in Pinterest
- **Personalized recommendation (i.e., suggesting a small number of interesting items for each user)** is critical for users to effectively explore the content of their interest.

# Recommender System as a Graph

- Recommender system can be naturally modeled as a **bipartite graph**
  - A graph with two node types: **users** and **items**.
  - **Edges** connect users and items
    - Indicates user-item interaction (e.g., click, purchase, review etc.)
    - Often associated with timestamp (timing of the interaction).



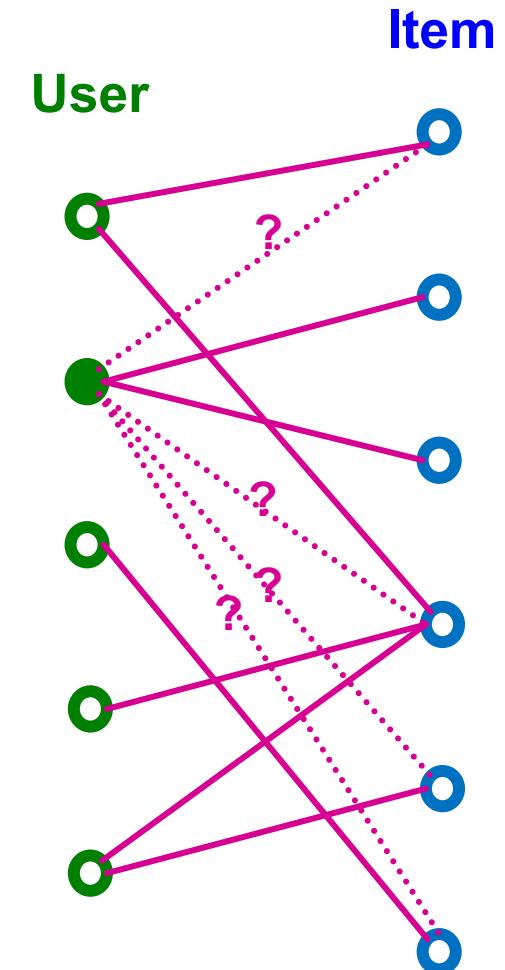
# Recommendation Task

## ■ Given

- Past user-item interactions

## ■ Task

- Predict new items each user will interact in the future.
- Can be cast as **link prediction** problem.
  - Predict new user-item interaction edges given the past edges.

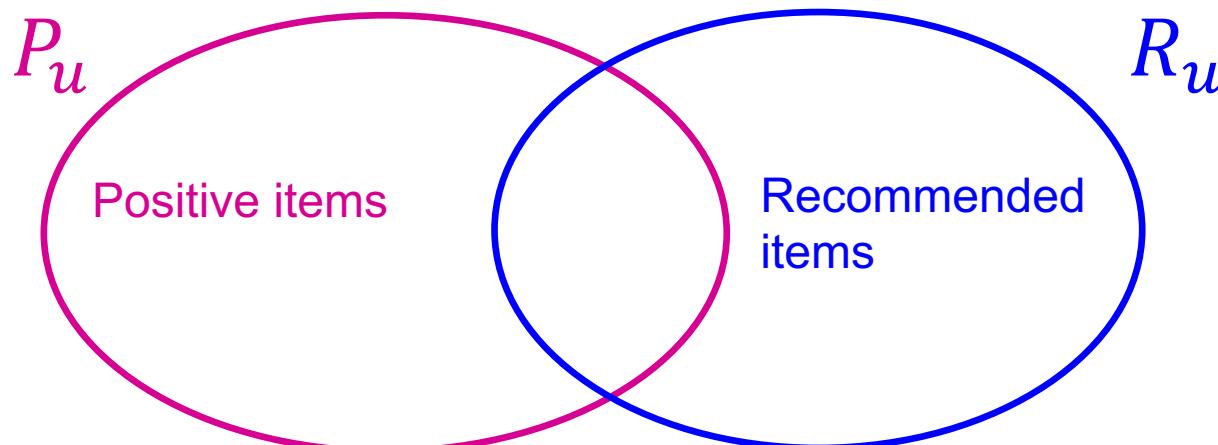


# Top- $K$ Recommendation

- For each user, we recommend  $K$  items.
  - In order for recommendation to be effective,  $K$  needs to be much smaller than the total number of items (up to billions)
  - $K$  is typically in the order of 10–100.
- The goal is to include as many **positive items** as possible in the top- $K$  recommended items.
  - **Positive items = Items that the user will interact with in the future.**
- **Evaluation metric:** Recall@ $K$  (defined next)

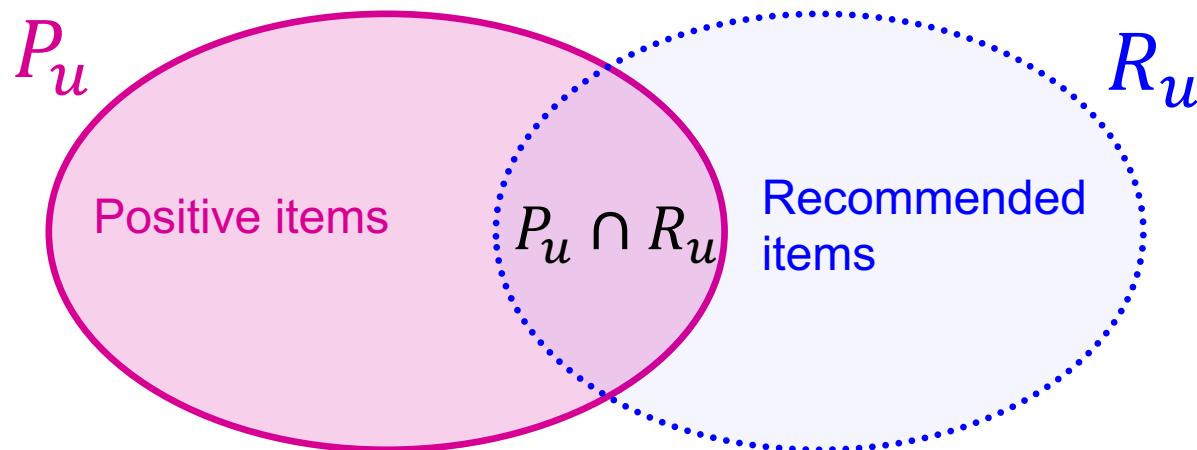
# Evaluation Metric: Recall@K (1)

- For each user  $u$ ,
  - Let  $P_u$  be a set of positive items the user will interact in the future.
  - Let  $R_u$  be a set of items recommended by the model.
    - In top- $K$  recommendation,  $|R_u| = K$ .
    - Items that the user has already interacted are excluded.



# Evaluation Metric: Recall@K (2)

- **Recall@K** for user  $u$  is  $|P_u \cap R_u|/|P_u|$ .
  - Higher value indicates more positive items are recommended in top- $K$  for user  $u$ .



- The final Recall@K is computed by averaging the recall values across all users.

# **Stanford CS224W:** **Recommender Systems:** **Embedding-Based Models**

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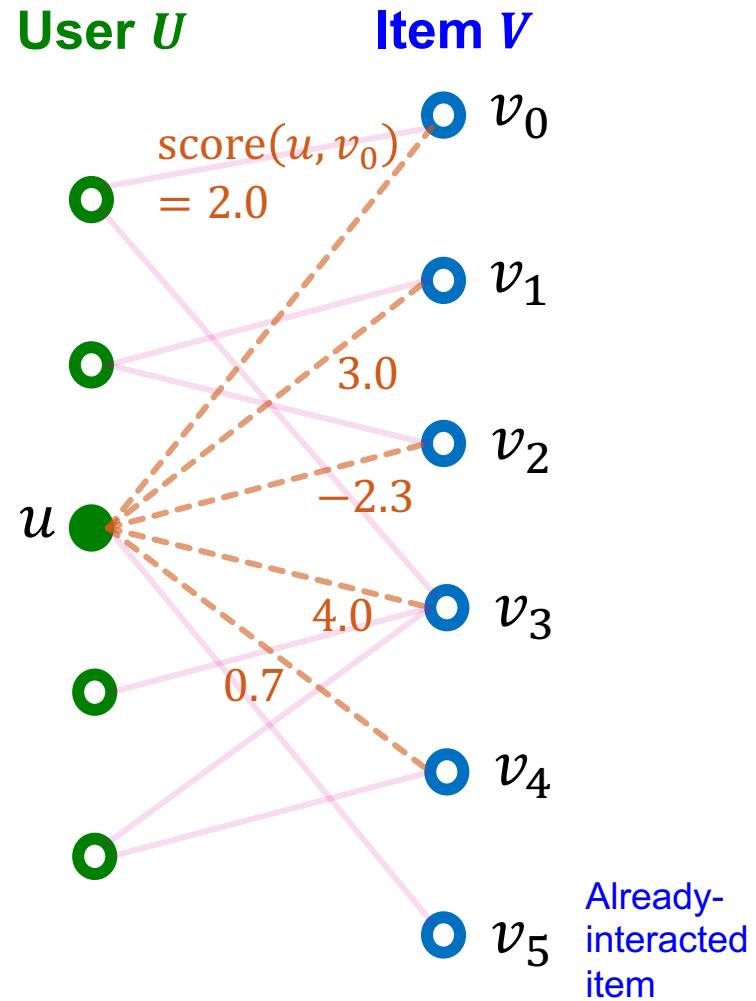


# Notation

- Notation:
  - $\mathbf{U}$ : A set of all users
  - $\mathbf{V}$ : A set of all items
  - $\mathbf{E}$ : A set of observed user-item interactions
    - $\mathbf{E} = \{(u, v) \mid u \in \mathbf{U}, v \in \mathbf{V}, u \text{ interacted with } v\}$

# Score Function

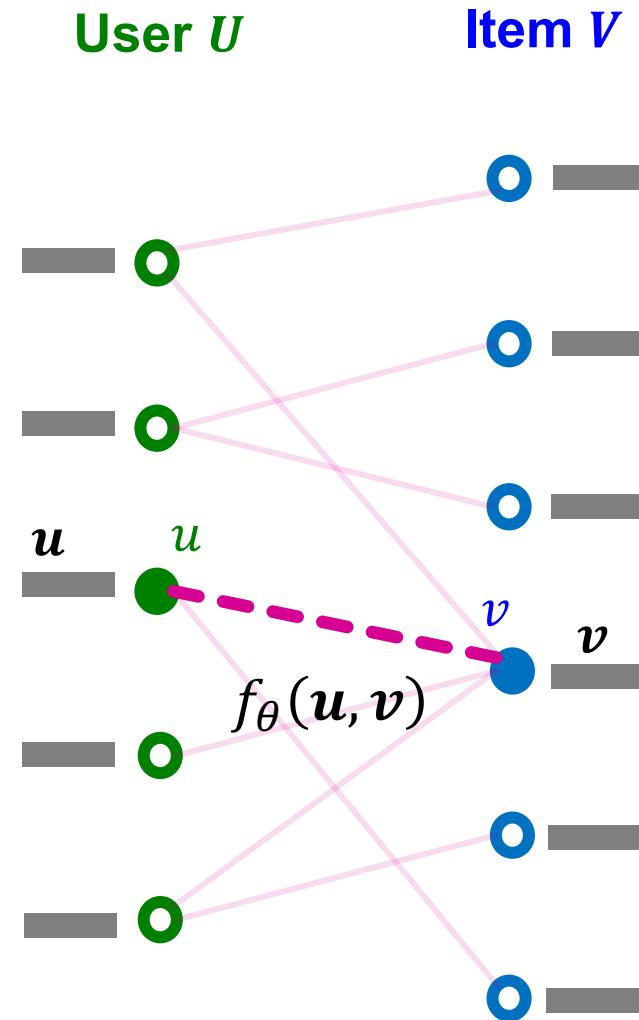
- To get the top- $K$  items, we need a score function for user-item interaction:
  - For  $u \in \mathbf{U}$ ,  $v \in \mathbf{V}$ , we need to get a real-valued scalar  $\text{score}(u, v)$ .
  - $K$  items with the largest scores for a given user  $u$  (excluding already-interacted items) are then recommended.**



For  $K = 2$ , recommended items for user  $u$  would be  $\{v_1, v_3\}$ .

# Embedding-Based Models

- We consider **embedding-based models** for scoring user-item interactions.
  - For each user  $u \in \mathcal{U}$ , let  $u \in \mathbb{R}^D$  be its  $D$ -dimensional embedding.
  - For each item  $v \in \mathcal{V}$ , let  $v \in \mathbb{R}^D$  be its  $D$ -dimensional embedding.
  - Let  $f_\theta(\cdot, \cdot): \mathbb{R}^D \times \mathbb{R}^D \rightarrow \mathbb{R}$  be a parametrized function.
  - Then,  $\text{score}(u, v) \equiv f_\theta(u, v)$



# Training Objective

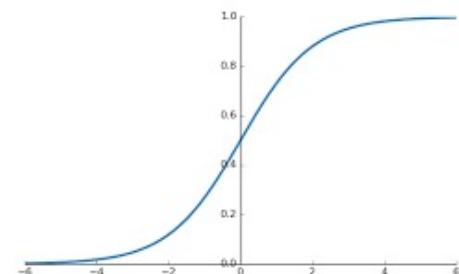
- Embedding-based models have three kinds of parameters:
  - An encoder to generate user embeddings  $\{u\}_{u \in U}$
  - An encoder to generate item embeddings  $\{v\}_{v \in V}$
  - Score function  $f_\theta(\cdot, \cdot)$
- **Training objective:** Optimize the model parameters to achieve high recall@ $K$  on *seen* (i.e., *training*) user-item interactions
  - We hope this objective would lead to high recall@ $K$  on *unseen* (i.e., *test*) interactions.

# Surrogate Loss Functions

- The vanilla training objective (training  $\text{recall}@K$ ) is **not differentiable**.
  - *Cannot* apply efficient gradient-based optimization.
- Two **surrogate loss functions** are widely-used to enable efficient gradient-based optimization.
  - Binary loss
  - Bayesian Personalized Ranking (BPR) loss
- Surrogate losses are **differentiable** and should **align well with the original training objective**.

# Binary Loss (1)

- Define **positive/negative edges**
  - A set of **positive edges**  $E$  (i.e., observed/training user-item interactions)
  - A set of **negative edges**  $E_{\text{neg}} = \{(u, v) \mid (u, v) \notin E, u \in U, v \in V\}$
- Define **sigmoid function**  $\sigma(x) \equiv \frac{1}{1+\exp(-x)}$ 
  - Maps real-valued scores into binary likelihood scores, i.e., in the range of [0,1].



# Binary Loss (2)

- **Binary loss**: Binary classification of **positive/negative** edges using  $\sigma(f_\theta(u, v))$ :

$$-\frac{1}{|\mathbf{E}|} \sum_{(u,v) \in \mathbf{E}} \log(\sigma(f_\theta(u, v))) - \frac{1}{|\mathbf{E}_{\text{neg}}|} \sum_{(u,v) \in \mathbf{E}_{\text{neg}}} \log(1 - \sigma(f_\theta(u, v)))$$

During training, these terms can be approximated using mini-batch of positive/negative edges

- Binary loss pushes the scores of **positive edges** higher than those of **negative edges**.
  - This aligns with the training recall metric since positive edges need to be recalled.

# Issue with Binary Loss (1)

- **Issue:** In the binary loss, the scores of ***ALL*** positive edges are pushed higher than those of ***ALL*** negative edges.
- This would unnecessarily penalize model predictions even if the training recall metric is perfect.
- **Why?** (example in the next slide)

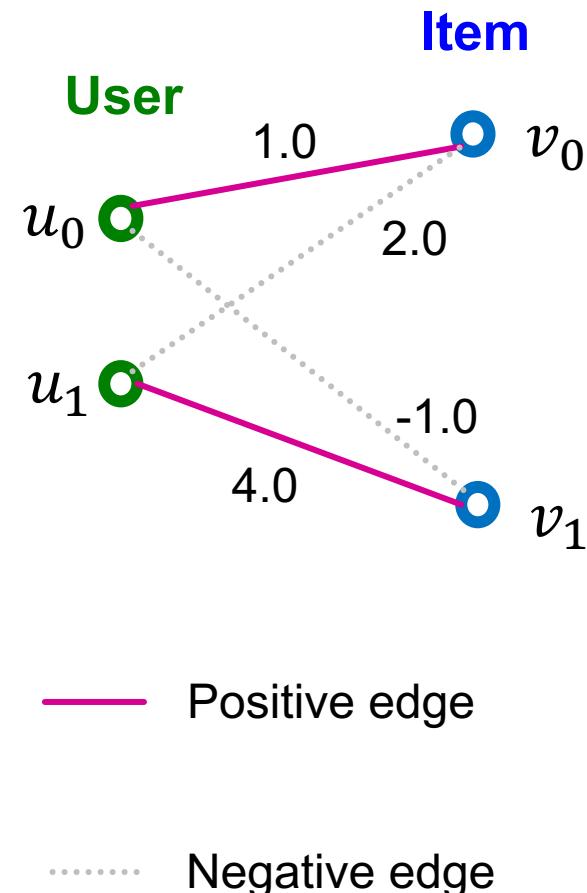
# Issue with Binary Loss (2)

- Let's consider the simplest case:

- Two users, two items
- Metric: Recall@1.
- A model assigns the score for every user-item pair (as shown in the right).

- Training **Recall@1 is 1.0** (perfect score), because  $v_0$  (resp.  $v_1$ ) is correctly recommended to  $u_0$  (resp.  $u_1$ ).

- However, **the binary loss would still penalize the model prediction** because the negative  $(u_1, v_0)$  edge gets the higher score than the positive edge  $(u_0, v_0)$ .

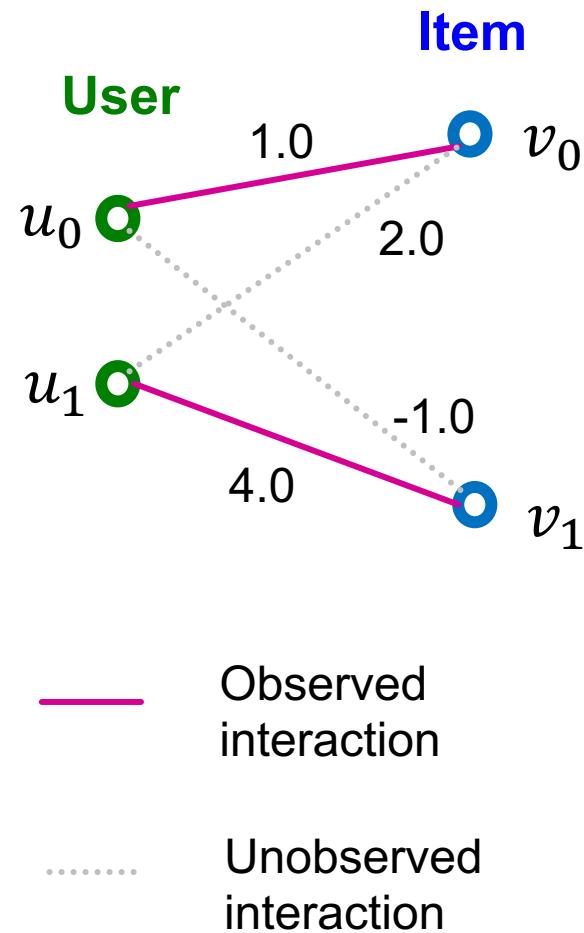


# Issue with Binary Loss (3)

- **Key insight:** The binary loss is **non-personalized** in the sense that the **positive/negative edges are considered across ALL users at once.**
- However, the recall metric is inherently **personalized (defined for each user).**
  - The non-personalized binary loss is overly-stringent for the personalized recall metric.

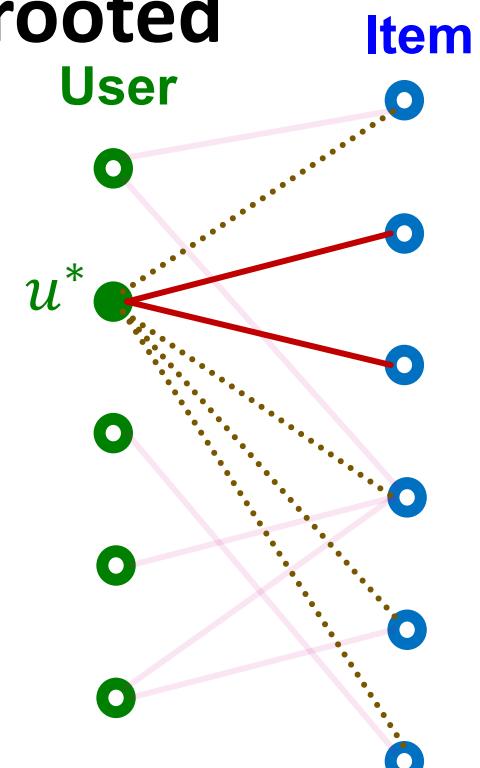
# Desirable Surrogate Loss

- **Lesson learned:** Surrogate loss function should be defined in a personalized manner.
  - For each user, we want the scores of positive items to be higher than those of the negative items
  - We do *not* care about the score ordering across users.
- Bayesian Personalized Ranking (BPR) loss achieves this!



# Loss Function: BPR Loss (1)

- **Bayesian Personalized Ranking (BPR) loss** is a personalized surrogate loss that aligns better with the recall@K metric.
- For each user  $u^* \in U$ , define the **rooted positive/negative edges** as
  - Positive edges rooted at  $u^*$ 
    - $E(u^*) \equiv \{(u^*, v) \mid (u^*, v) \in E\}$
  - Negative edges rooted at  $u^*$ 
    - $E_{\text{neg}}(u^*) \equiv \{(u^*, v) \mid (u^*, v) \in E_{\text{neg}}\}$



Note: The term “Bayesian” is not essential to the loss definition. The original paper [Rendle et al. 2009] considers the Bayesian prior over parameters (essentially acts as a parameter regularization), which we omit here.

# Loss Function: BPR Loss (2)

- **Training objective:** For each user  $u^*$ , we want the scores of rooted positive edges  $E(u^*)$  to be higher than those of rooted negative edges  $E_{\text{neg}}(u^*)$ .

■ Aligns with the personalized nature of the recall metric.

- **BPR Loss for user  $u^*$ :**

Encouraged to be positive for each user

=positive edge score is higher than negative edge score

$$\text{Loss}(u^*) = \frac{1}{|E| \cdot |E_{\text{neg}}|} \underbrace{\sum_{(u^*, v_{\text{pos}}) \in E(u^*)} \sum_{(u^*, v_{\text{neg}}) \in E_{\text{neg}}(u^*)} -\log \left( \sigma \left( f_{\theta}(u^*, v_{\text{pos}}) - f_{\theta}(u^*, v_{\text{neg}}) \right) \right)}_{\text{Can be approximated using mini-batch}}$$

- Final BPR Loss:  $\frac{1}{|U|} \sum_{u^* \in U} \text{Loss}(u^*)$

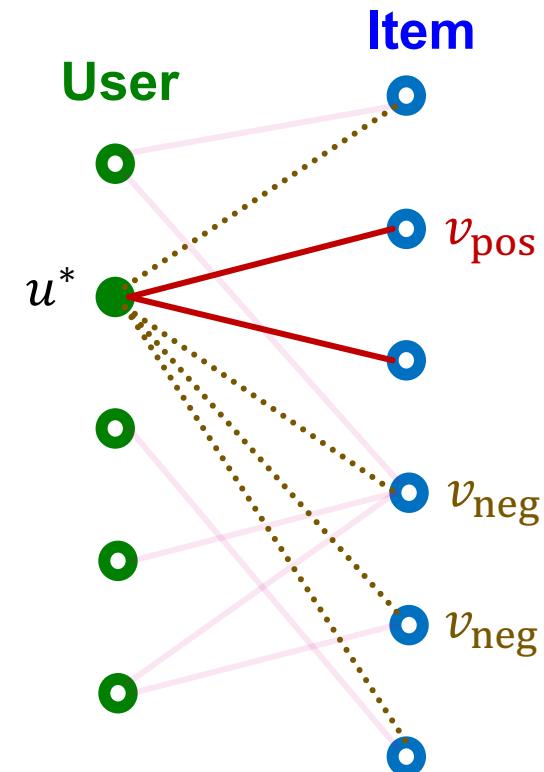
# Loss Function: BPR Loss (3)

## ■ Mini-batch training for the BPR loss:

- In each mini-batch, we sample a subset of users  $\mathbf{U}_{\text{mini}} \subset \mathbf{U}$ .
  - For each user  $u^* \in \mathbf{U}_{\text{mini}}$ , we sample one positive item  $v_{\text{pos}}$  and a set of sampled negative items  $V_{\text{neg}} = \{v_{\text{neg}}\}$ .
- The mini-batch loss is computed as

$$\boxed{\frac{1}{|\mathbf{U}_{\text{mini}}|} \sum_{u^* \in \mathbf{U}_{\text{mini}}} \frac{1}{|V_{\text{neg}}|} \sum_{v_{\text{neg}} \in V_{\text{neg}}} -\log(\sigma(f_\theta(u^*, v_{\text{pos}})) - \sigma(f_\theta(u^*, v_{\text{neg}})))}$$

Average over users  
in the mini-batch



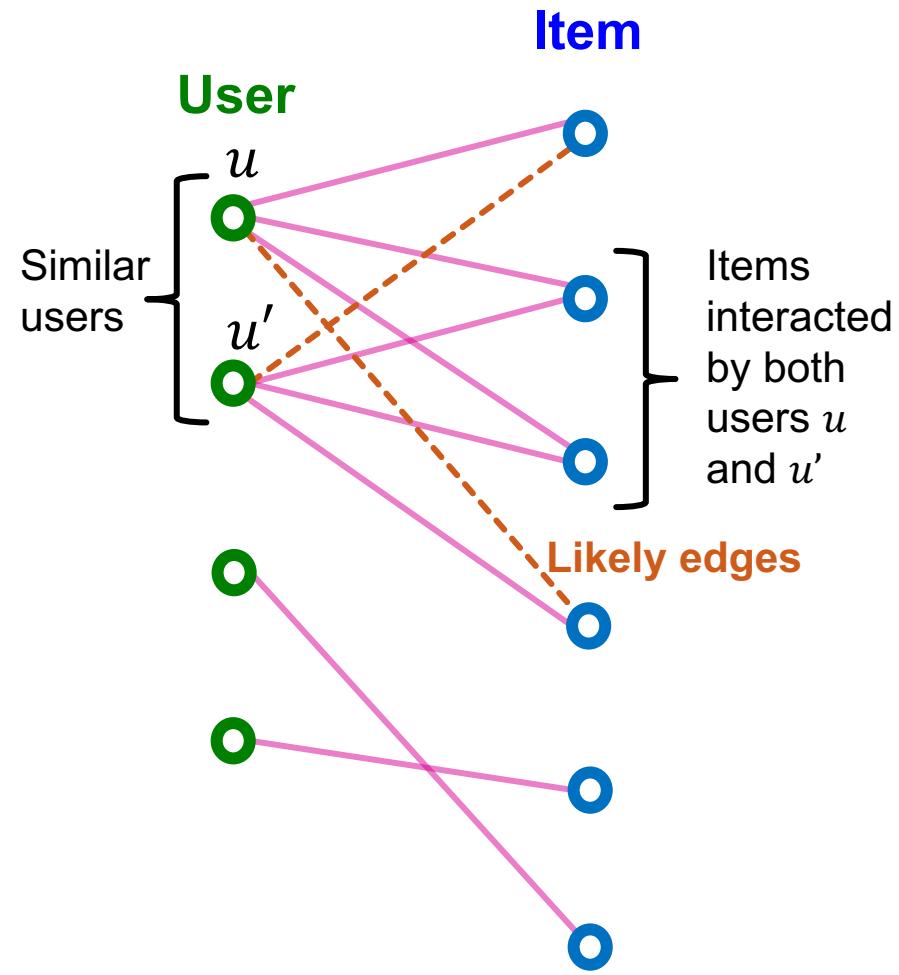
# Summary So Far

- **We have introduced**

- Recall@ $K$  as a metric for personalized recommendation
- Embedding-based models
  - Three kinds of parameters to learn
    - **user encoder** to generate user embeddings
    - **item encoder** to generate item embeddings
    - **score function** to predict the user-item interaction likelihood.
  - Surrogate loss functions to achieve the high recall metric.
- Embedding-based models have achieved SoTA in recommender systems.
  - **Why do they work so well?**

# Why Embedding Models Work?

- Underlying idea:  
**Collaborative filtering**
  - Recommend items for a user by **collecting preferences of many other similar users.**
  - **Similar users tend to prefer similar items.**
- Key question: **How to capture similarity between users/items?**



# Why Embedding Models Work?

- Embedding-based models can capture similarity of users/items!
  - Low-dimensional embeddings *cannot* simply memorize all user-item interaction data.
  - Embeddings are forced to **capture similarity between users/items to fit the data.**
  - This allows the models to make effective prediction on *unseen* user-item interactions.

# This Lecture: GNNs for Recsys

- In this lecture, we teach two representative GNN approaches for recommender systems.
- **Neural Graph Collaborative Filtering (NGCF)**  
[Wang et al. 2019], **LightGCN** [He et al. 2020]
  - Improve the conventional collaborative filtering models (i.e., matrix factorization) by explicitly modeling graph structure using GNNs.
- **PinSAGE** [Ying et al. 2018]
  - Use GNNs to generate high-quality embeddings by simultaneously capturing rich node attributes (e.g., images) and the graph structure.

# **Stanford CS224W:**

# **Neural Graph**

# **Collaborative Filtering**

CS224W: Machine Learning with Graphs

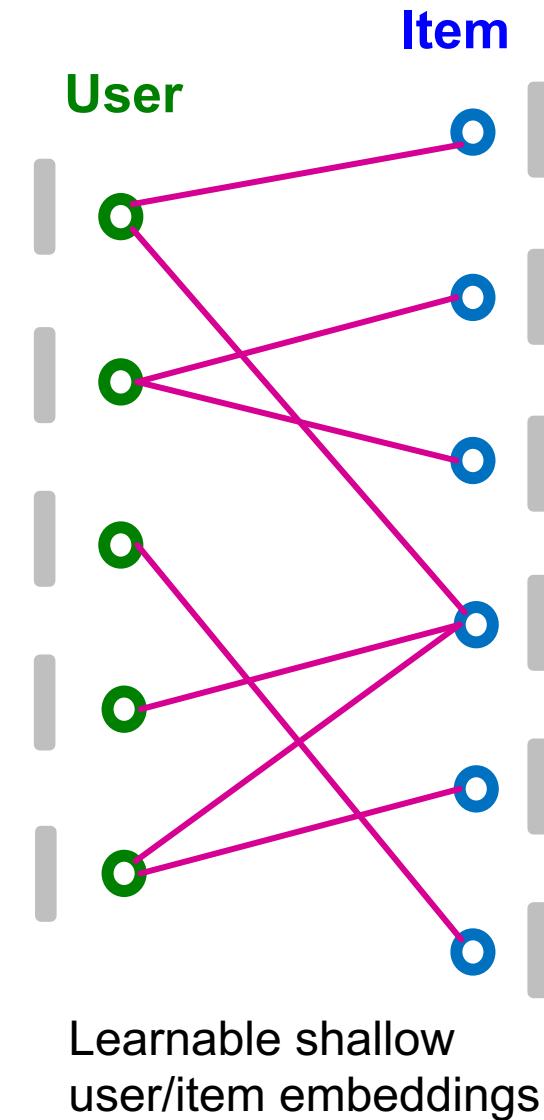
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# Conventional Collaborative Filtering

- Conventional collaborative filtering model is based on **Matrix Factorization (MF)**.
  - Use shallow encoders for users and items
    - For every  $u \in \mathcal{U}$  and  $v \in \mathcal{V}$ , we prepare shallow learnable embeddings  $\mathbf{u}, \mathbf{v} \in \mathbb{R}^D$ .
  - Score function for user  $u$  and item  $v$  is  $f_\theta(\mathbf{u}, \mathbf{v}) \equiv \mathbf{u}^T \mathbf{v}$ .



# Limitations of MF

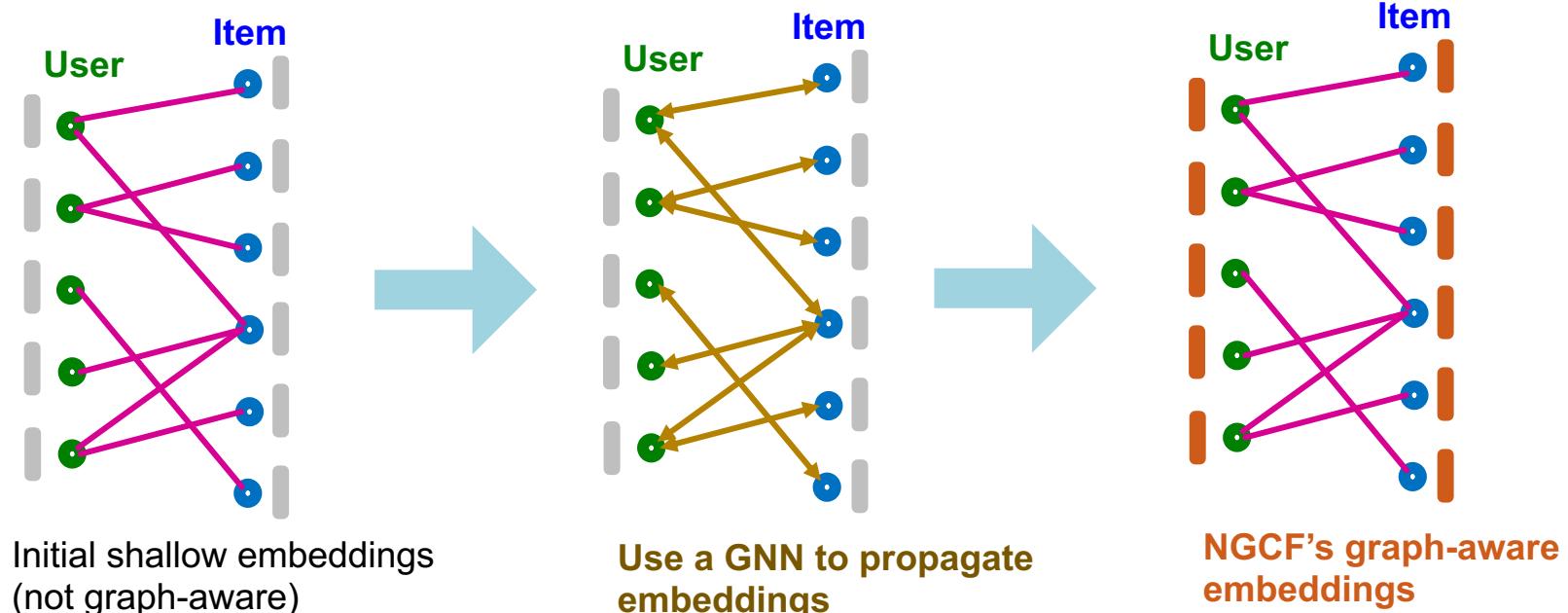
- The model itself does ***not explicitly*** capture graph structure
  - The graph structure is ***only implicitly*** captured in the training objective.
- Only the **first-order graph structure** (i.e., edges) is captured in the training objective.
  - **High-order graph structure** (e.g.,  $K$ -hop paths between two nodes) is ***not explicitly captured***.

# Motivation

- We want a model that...
  - **explicitly captures graph structure** (beyond implicitly through the training objective)
  - captures **high-order graph structure** (beyond the first-order edge connectivity structure)
- **GNNs are a natural approach to achieve both!**
  - Neural Graph Collaborative Filtering (NGCF) [Wang et al. 2019]
  - LightGCN [He et al. 2020]
    - A simplified and improved version of NGCF

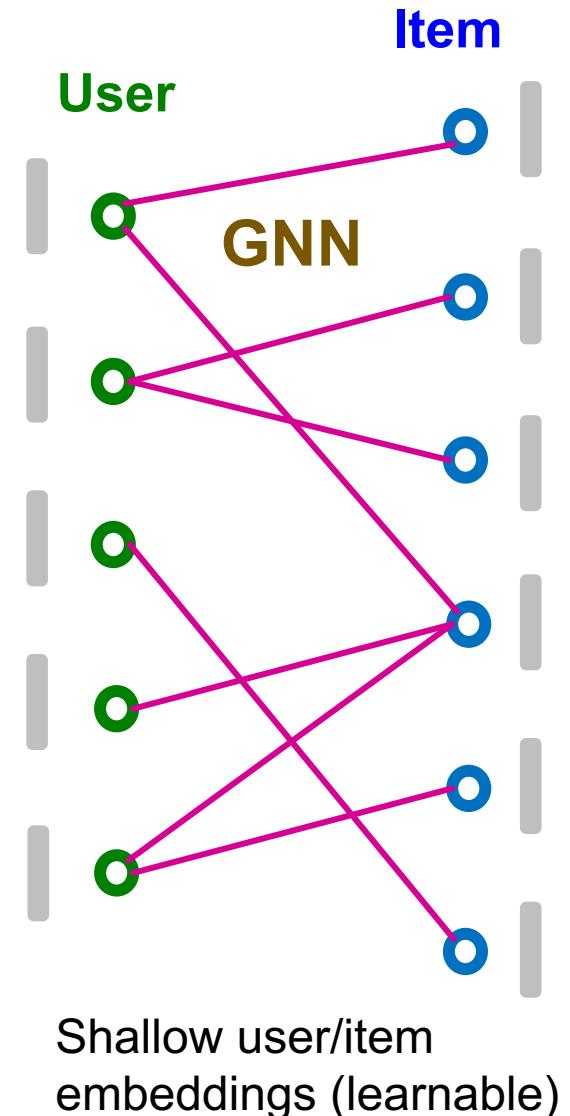
# NGCF: Overview

- **Neural Graph Collaborative Filtering (NGCF)** *explicitly* incorporates high-order graph structure when generating user/item embeddings.
- **Key idea:** Use a GNN to generate graph-aware user/item embeddings.



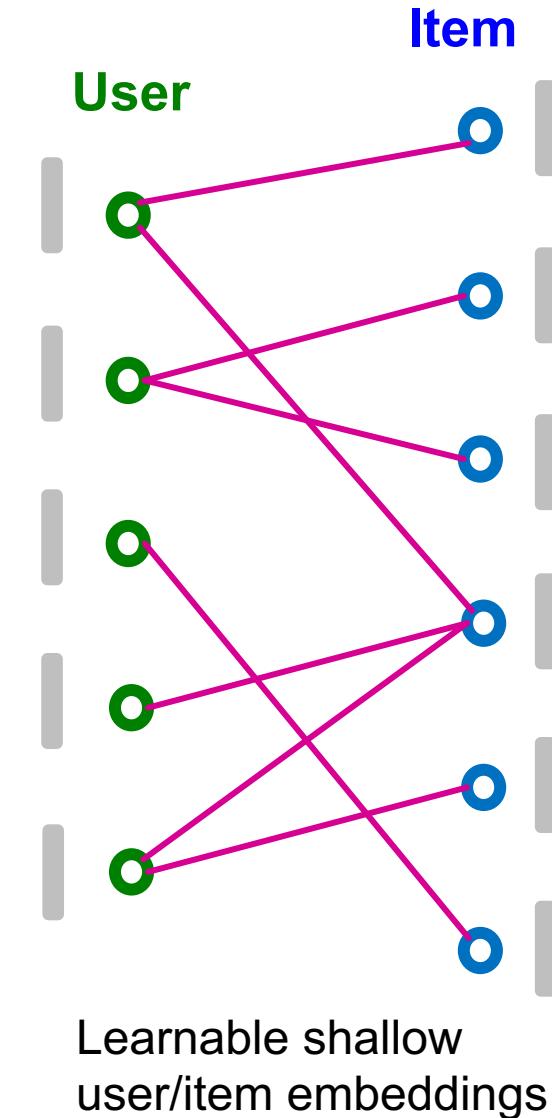
# NGCF Framework

- **Given:** User-item bipartite graph.
- **NGCF framework:**
  - Prepare shallow learnable embedding for each node.
  - Use multi-layer GNNs to propagate embeddings along the bipartite graph.
    - High-order graph structure is captured.
  - Final embeddings are *explicitly* graph-aware!
- **Two kinds of learnable params are jointly learned:**
  - Shallow user/item embeddings
  - GNN's parameters



# Initial Node Embeddings

- Set the shallow learnable embeddings as the initial node features.
  - For every user  $u \in \mathcal{U}$ , set  $\mathbf{h}_u^{(0)}$  as the user's shallow embedding.
  - For every item  $v \in \mathcal{V}$ , set  $\mathbf{h}_v^{(0)}$  as the item's shallow embedding.



# Neighbor Aggregation

- Iteratively update node embeddings using neighboring embeddings.

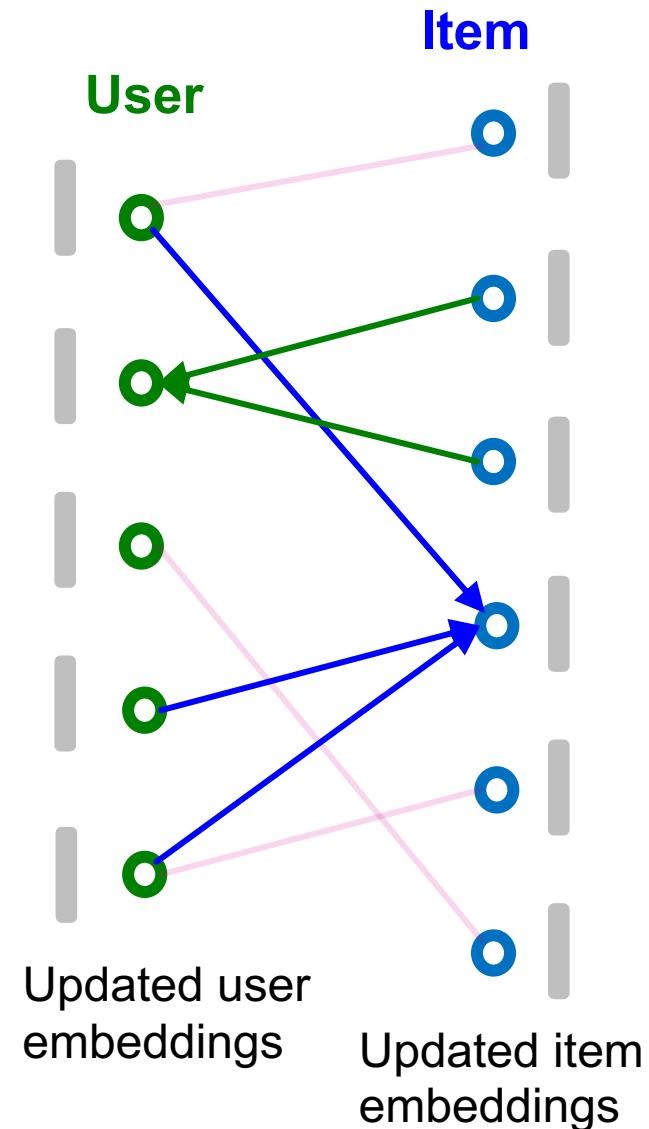
$$\mathbf{h}_v^{(k+1)} = \text{COMBINE} \left( \mathbf{h}_v^{(k)}, \text{AGGR} \left( \left\{ \mathbf{h}_u^{(k)} \right\}_{u \in N(v)} \right) \right)$$

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

High-order graph structure is captured through iterative neighbor aggregation.

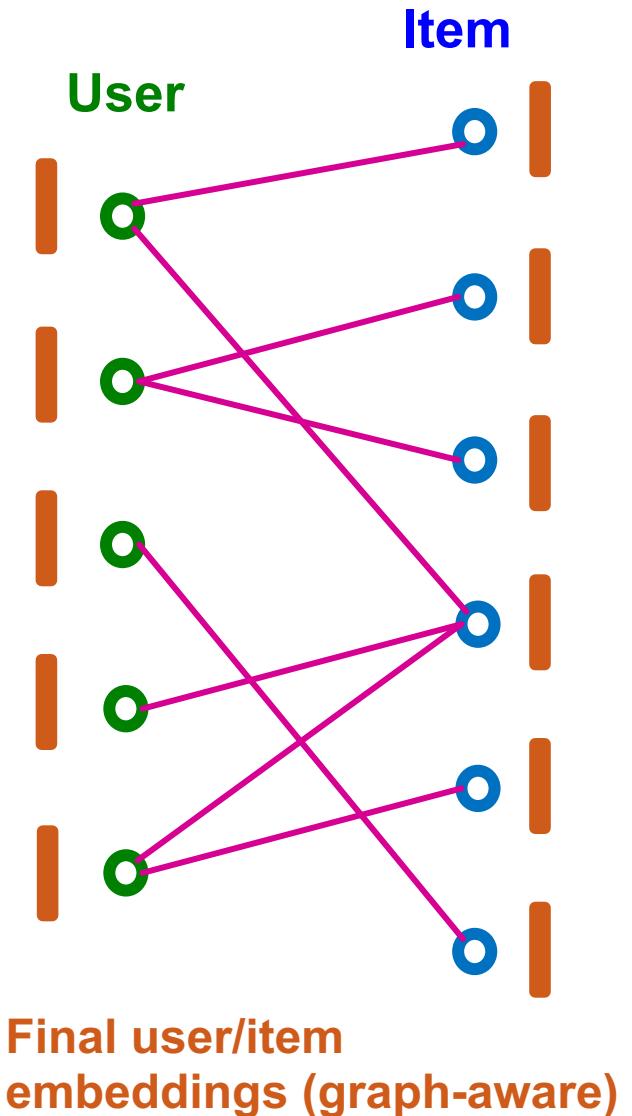
Different architecture choices are possible for AGGR and COMBINE.

- AGGR( $\cdot$ ) can be MEAN( $\cdot$ )
- COMBINE( $x, y$ ) can be  $\text{ReLU}(\text{Linear}(\text{Concat}(x, y)))$



# Final Embeddings and Score Function

- After  $K$  rounds of neighbor aggregation, we get the **final user/item embeddings**  $\mathbf{h}_u^{(K)}$  and  $\mathbf{h}_v^{(K)}$ .
- For all  $u \in \mathcal{U}, v \in \mathcal{V}$ , we set  $u \leftarrow \mathbf{h}_u^{(K)}, v \leftarrow \mathbf{h}_v^{(K)}$ .
- Score function is the inner product  
$$\text{score}(u, v) = \mathbf{u}^T \mathbf{v}$$



# NGCF: Summary

- Conventional collaborative filtering uses shallow user/item embeddings.
  - The embeddings do ***not explicitly model graph structure.***
  - The training objective ***does not model high-order graph structure.***
- **NGCF uses a GNN to propagate the shallow embeddings.**
  - The embeddings are ***explicitly aware of high-order graph structure.***

# Stanford CS224W: LightGCN

CS224W: Machine Learning with Graphs

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# LightGCN: Motivation (1)

- **Recall**: NGCF jointly learns two kinds of parameters:
  - Shallow user/item embeddings
  - GNN's parameters
- **Observation**: Shallow learnable embeddings are already quite expressive.
  - They are learned for every node.
  - Most of the parameter counts are in shallow embeddings when  $N$  (#nodes)  $\gg D$  (embedding dimensionality)
    - Shallow embeddings:  $O(ND)$ .
    - GNN:  $O(D^2)$ .

# LightGCN: Motivation (2)

- Can we simplify the GNN used in NGCF (e.g., remove its learnable parameters)?
  - **Answer:** Yes!
  - **Bonus:** Simplification improves the recommendation performance!
- **Overview of the idea:**
  - Adjacency matrix for a bipartite graph
  - Matrix formulation of GCN
  - Simplification of GCN by removing non-linearity
    - Related: SGC for scalable GNN [Wu et al. 2019]

# Adjacency and Embedding Matrices

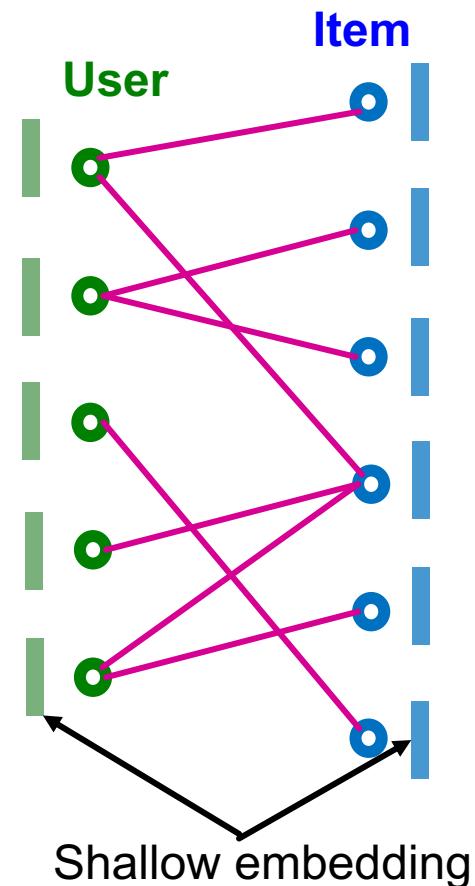
- **Adjacency matrix** of a (undirected) bipartite graph.
- **Shallow embedding matrix**.

Adjacency matrix  $A$

User	Item
User	$R$
Item	$R^T$

$R_{uv} = 1$  if user  $u$  interacts with item  $v$ ,  
 $R_{uv} = 0$  otherwise.

Embedding matrix  $E$



# Matrix Formulation of GCN

- **Recall:** Diffusion matrix of C&S.
- Let  $D$  be the degree matrix of  $A$ .
- Define the normalized adjacency matrix  $\tilde{A}$  as

$$\tilde{A} \equiv D^{-1/2} A D^{-1/2}$$

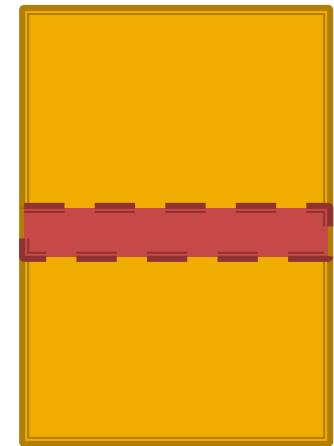
**Note:** Different from the original GCN, self-connection is omitted here.

- Let  $E^{(k)}$  be the embedding matrix at  $k$ -th layer.
- Each layer of GCN's aggregation can be written in a matrix form:

$$E^{(k+1)} = \text{ReLU}(\tilde{A}E^{(k)}W^{(k)})$$

**Neighbor aggregation**    **Learnable linear transformation**

Matrix of node embeddings  $E^{(k)}$



Each row stores node embedding

# Simplifying GCN (1)

- Simplify GCN by removing ReLU non-linearity:

$$\mathbf{E}^{(k+1)} = \tilde{\mathbf{A}} \mathbf{E}^{(k)} \mathbf{W}^{(k)}$$

Original idea from  
SGC [Wu et al. 2019]

- The final node embedding matrix is given as

$$\mathbf{E}^{(K)} = \tilde{\mathbf{A}} \underbrace{\mathbf{E}^{(K-1)} \mathbf{W}^{(K-1)}}_{\downarrow}$$

$$= \tilde{\mathbf{A}} (\underbrace{\tilde{\mathbf{A}} \mathbf{E}^{(K-2)} \mathbf{W}^{(K-2)}}_{\downarrow}) \mathbf{W}^{(K-1)}$$

$$= \tilde{\mathbf{A}} (\underbrace{\tilde{\mathbf{A}} (\cdots (\underbrace{\tilde{\mathbf{A}} \mathbf{E}^{(0)} \mathbf{W}^{(0)}}_{\downarrow} \cdots) \mathbf{W}^{(K-2)})}_{\text{Red bracket}} \mathbf{W}^{(K-1)})$$

Set  $\mathbf{E}$  as input  
embedding  $\mathbf{E}^{(0)}$

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

# Simplifying GCN (2)

- Removing ReLU significantly simplifies GCN!

$$\mathbf{E}^{(K)} = \boxed{\tilde{\mathbf{A}}^K \mathbf{E}} \mathbf{W}$$

Diffusing node embeddings  
along the graph

$$\mathbf{W} \equiv \mathbf{W}^{(0)} \dots \mathbf{W}^{(K-1)}$$

(similar to C&S that diffuses  
soft labels along the graph)

- **Algorithm:** Apply  $\mathbf{E} \leftarrow \tilde{\mathbf{A}} \mathbf{E}$  for  $K$  times.

- Each matrix multiplication diffuses the current embeddings to their one-hop neighbors.
- **Note:**  $\tilde{\mathbf{A}}^K$  is dense and never gets materialized. Instead, the above iterative matrix-vector product is used to compute  $\tilde{\mathbf{A}}^K \mathbf{E}$ .

# Multi-Scale Diffusion

- We can consider **multi-scale diffusion**

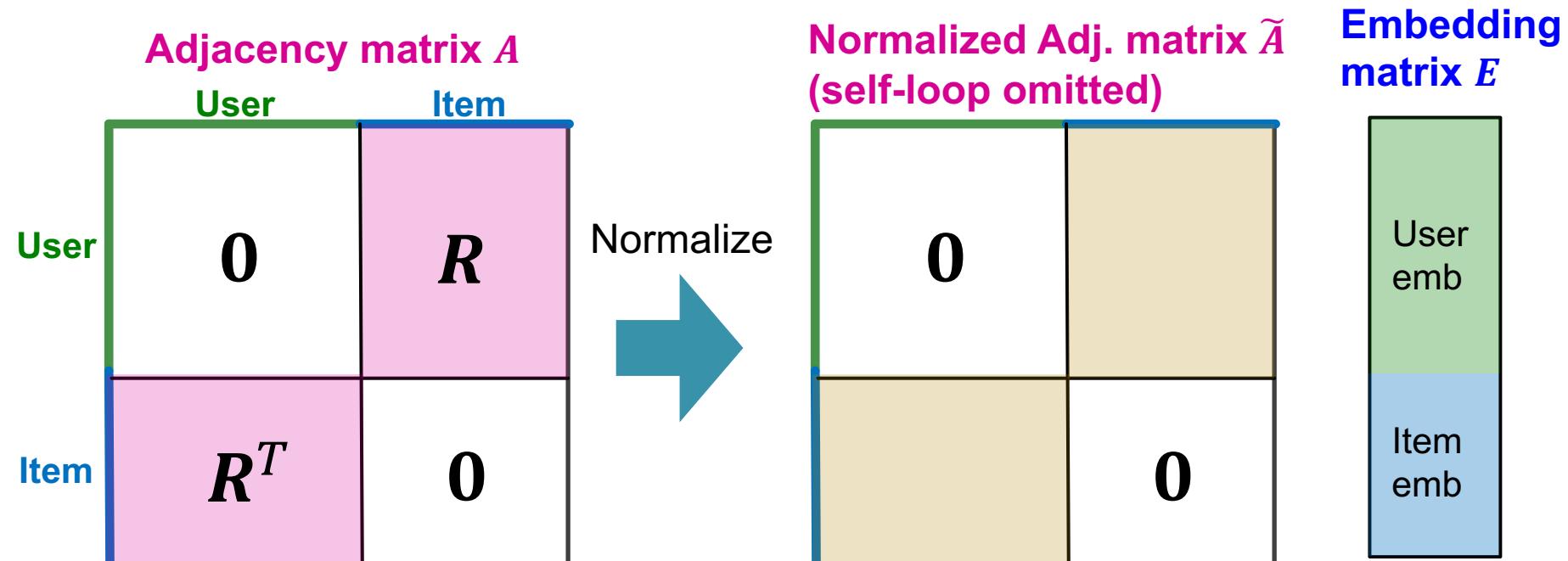
$$\alpha_0 E^{(0)} + \alpha_1 E^{(1)} + \alpha_2 E^{(2)} + \dots + \alpha_K E^{(K)}$$

- The above includes embeddings diffused at multiple hop scales.
- $\alpha_0 E^{(0)} = \alpha_0 \tilde{A}^0 E^{(0)}$  acts as a self-connection (that is omitted in the definition  $\tilde{A}$ )
- The coefficients,  $\alpha_0, \dots, \alpha_K$ , are hyper-parameters.
- For simplicity, LightGCN uses the uniform coefficient, i.e.,  $\alpha_k = \frac{1}{K+1}$  for  $k = 0, \dots, K$ .

# LightGCN: Model Overview (1)

## Given:

- Adjacency matrix  $A$
- Initial learnable embedding matrix  $E$



# LightGCN: Model Overview (2)

- Iteratively diffuse embedding matrix  $E$  using  $\tilde{A}$

For  $k = 0 \dots K - 1$ ,

Embedding  
matrix  $E^{(k+1)}$

User emb  
Item emb

Normalized Adj. matrix  $\tilde{A}$   
(self-loop omitted)



0	
	0

Embedding  
matrix  $E^{(k)}$   
( $E^{(0)}$  is set to  $E$ )

User emb  
Item emb

# LightGCN: Model Overview (3)

- Average the embedding matrices at different scales.

Embedding matrix  $E_{\text{final}}$

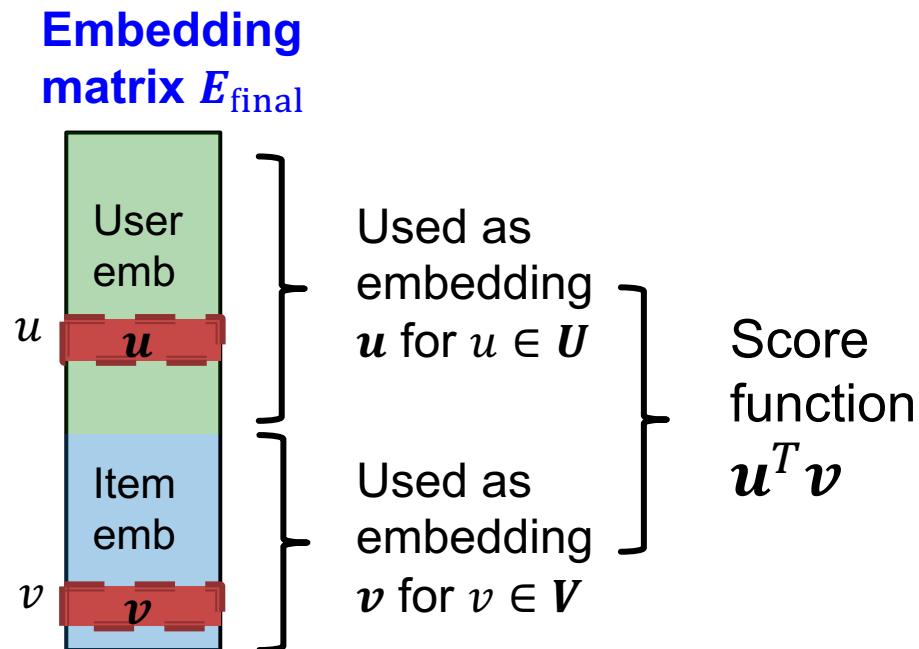
$$\leftarrow \frac{1}{K+1} \left( E^{(0)} + E^{(1)} + \dots + E^{(K)} \right)$$

The diagram illustrates the computation of the final embedding matrix  $E_{\text{final}}$ . It shows a large green arrow pointing left, followed by the formula  $\frac{1}{K+1} \left( E^{(0)} + E^{(1)} + \dots + E^{(K)} \right)$ . To the left of the formula is a vertical rectangle divided into two horizontal sections: a green "User emb" section at the top and a blue "Item emb" section at the bottom. This represents the final embedding matrix  $E_{\text{final}}$ . To the right of the formula, there is a series of three vertical rectangles, each representing an intermediate embedding matrix  $E^{(0)}$ ,  $E^{(1)}$ , and  $E^{(K)}$ . Each of these intermediate matrices is also divided into "User emb" (green) and "Item emb" (blue) sections. Brackets above the matrices group them into pairs: a large bracket groups all three matrices ( $E^{(0)}, E^{(1)}, E^{(K)}$ ), and a smaller bracket groups the first two ( $E^{(0)}, E^{(1)}$ ). Plus signs are placed between the first pair and between the last pair, indicating the summation step in the formula.

# LightGCN: Model Overview (4)

## Score function:

- Use user/item vectors from  $E_{\text{final}}$  to score user-item interaction



# LightGCN: Intuition

- **Question:** Why does the simple diffusion propagation work well?
- **Answer:** The diffusion directly encourages the embeddings of similar users/items to be similar.
  - Similar users share many common neighbors (items) and are expected to have similar future preferences (interact with similar items).

# LightGCN and GCN/C&S

- The embedding propagation of LightGCN is closely related to GCN/C&S.
- **Recall:** GCN/C&S (neighbor aggregation part)

$$\mathbf{h}_v^{(k+1)} = \sum_{u \in N(v)} \frac{1}{\sqrt{d_u} \sqrt{d_v}} \cdot \mathbf{h}_u^{(k)}$$

Node degree

- Self-loop is added in the neighborhood definition.
- LightGCN uses the same equation except that
  - Self-loop is *not* added in the neighborhood definition.
  - Final embedding takes the average of embeddings from all the layers:  $\mathbf{h}_v = \frac{1}{K+1} \sum_{k=0}^K \mathbf{h}_v^{(k)}$ .

# LightGCN and MF: Comparison

- Both LightGCN and Matrix Factorization (MF) **learn a unique embedding for each user/item.**
- The difference is that
  - MF directly uses the shallow user/item embeddings for scoring.
  - LightGCN uses the **diffused** user/item embeddings for scoring.
- LightGCN performs better than MF but are also more computationally expensive due to the additional diffusion step.
  - The final embedding of a user/item is obtained by aggregating embeddings of its multi-hop neighboring nodes.

# LightGCN: Summary

- LightGCN simplifies NGCF by **removing the learnable parameters of GNNs**.
- **Learnable parameters are all in the shallow input node embeddings.**
  - Diffusion propagation only involves matrix-vector multiplication.
  - The simplification leads to better empirical performance than NGCF.

# **Stanford CS224W:**

# **PinSAGE**

CS224W: Machine Learning with Graphs

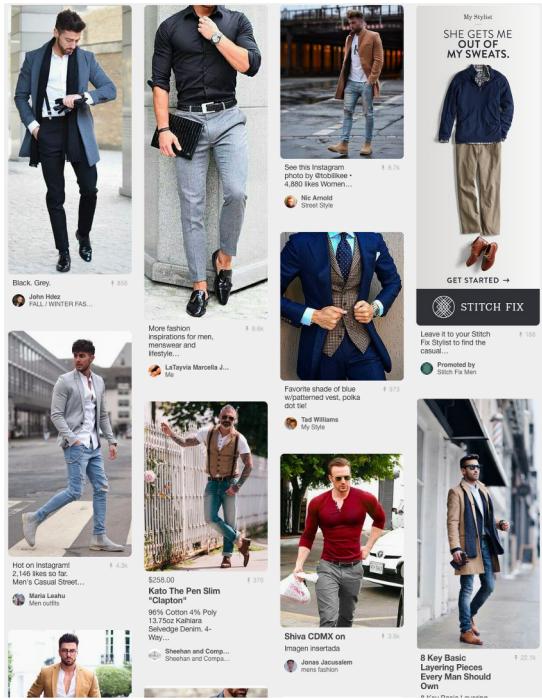
Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



# Motivation

## ■ P2P recommendation



# PinSAGE: Pin Embedding

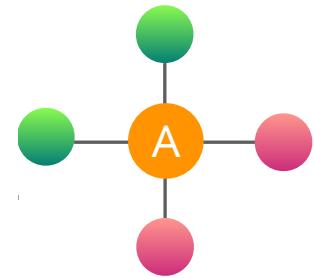
- ❑ Unifies visual, textual, and graph information.
- ❑ The largest industry deployment of a Graph Convolutional Networks
- ❑ Huge Adoption across Pinterest
- ❑ Works for fresh content and is available in a few seconds after pin creation



# Application: Pinterest

## PinSage graph convolutional network:

- **Goal:** Generate embeddings for nodes in a large-scale Pinterest graph containing billions of objects
- **Key Idea:** Borrow information from nearby nodes
  - E.g., bed rail Pin might look like a garden fence, but gates and beds are rarely adjacent in the graph



- Pin embeddings are essential to various tasks like recommendation of Pins, classification, ranking
  - Services like “Related Pins”, “Search”, “Shopping”, “Ads”

# Harnessing Pins and Boards



Very ape blue  
structured coat  
Nitty Gritty

Picked for you  
Street style



Hans Wegner chair  
Room and Board

Promoted by  
Room & Board



This is just a beautiful  
image for thoughts.  
Yay or nay, your choice.

+\$14

Annie Teng  
Plantation



mid century modern ...  
MJL I -



Man Style  
Gavin Jones



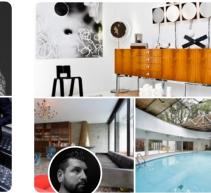
men + style I  
FIG + SALT



Plants  
HelloSandwich



Men's Style  
Andrea Sempi



Mid century modern  
Tyler Goodro



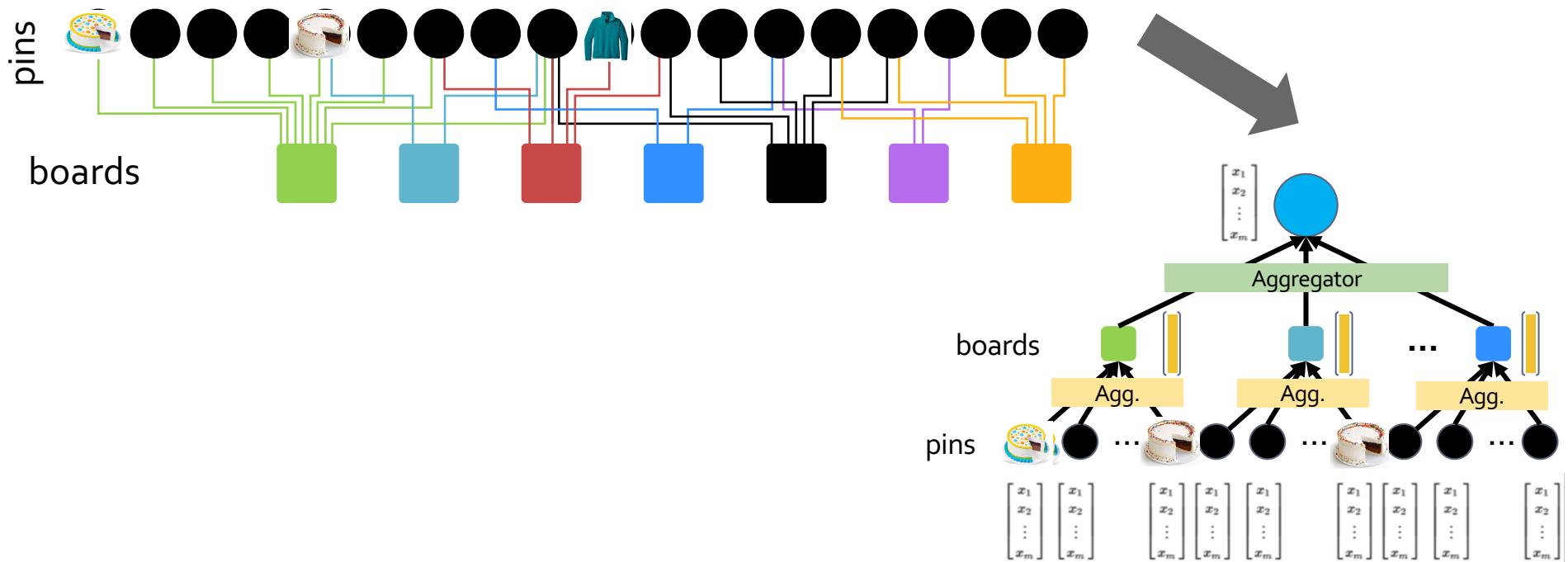
Plants  
Moorea Seal



Mid century modern ...  
Prettygreen tea

# PinSAGE:Graph Neural Network

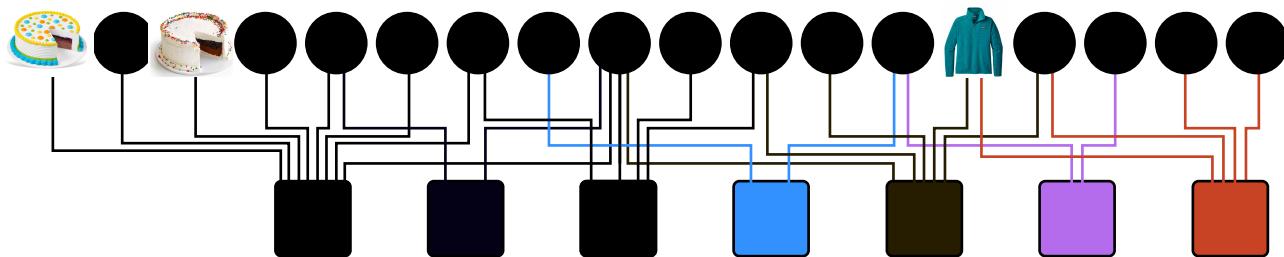
- Graph has tens of billions of nodes and edges
- Further resolves embeddings across the Pinterest graph



# PinSAGE: Methods for Scaling Up

- In addition to the GNN model, the PinSAGE paper introduces several methods to scale the GNN to a billion-scale recommender system (e.g., Pinterest).
  - Shared negative samples across users in a mini-batch
  - Hard negative samples
  - Curriculum learning
  - Mini-batch training of GNNs on a large-graph (to be covered in the future lecture)

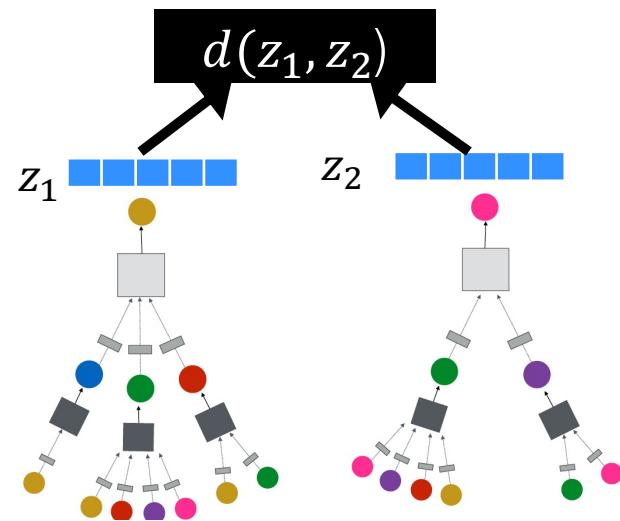
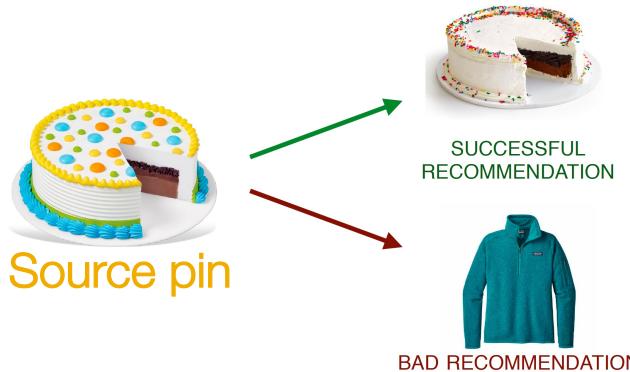
# PinSAGE Model



**Task: Recommend related pins to users**

Learn node embeddings  $z_i$  such that

$$d(z_{cake1}, z_{cake2}) < d(z_{cake1}, z_{sweater})$$



# Training Data

1+B repin pairs:

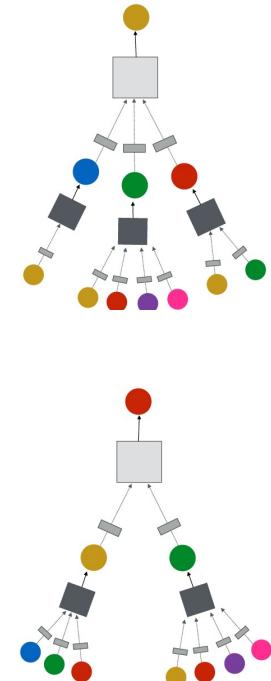
- From Related Pins surface
- Capture semantic relatedness
- Goal: Embed such pairs to be “neighbors”

Example positive training pairs (Q,X):



# Shared Negative Samples (1)

- **Recall**: In BPR loss, for each user  $u^* \in U_{\text{mini}}$ , we sample one positive item  $v_{\text{pos}}$  and a set of sampled negative items  $V_{\text{neg}} = \{v_{\text{neg}}\}$ .
- Using more negative samples per user improves the recommendation performance, but is also expensive.
  - We need to generate  $|U_{\text{mini}}| \cdot |V_{\text{neg}}|$  embeddings for negative nodes.
  - We need to apply  $|U_{\text{mini}}| \cdot |V_{\text{neg}}|$  GNN computational graphs (see right), which is expensive.



# Shared Negative Samples (2)

- **Key idea:** We can share the same set of negative samples  $V_{\text{neg}} = \{\nu_{\text{neg}}\}$  **across all users**  $U_{\text{mini}}$  in the mini-batch.
- This way, we only need to generate  $|V_{\text{neg}}|$  embeddings for negative nodes.
  - This saves the node embedding generation computation **by a factor of  $|U_{\text{mini}}|$ !**
  - Empirically, the performance stays similar to the non-shared negative sampling scheme.

# Curriculum Learning

- **Key insight:** It is effective **to make the negative samples *gradually harder* in the process of training.**
- At  $n$ -th epoch, we add  $n - 1$  hard negative items.
  - #(Hard negatives) gradually increases in the process of training.
- The model will gradually learn to make finer-grained predictions.

# PinSAGE: Curriculum Learning

- Idea: use harder and harder negative samples
- Include more and more hard negative samples for each epoch



Source pin



Positive



Easy negative



Hard negative

# Hard Negatives (1)

- **Challenge:** Industrial recsys needs to make **extremely fine-grained predictions**.
  - #Total items: Up to billions.
  - #Items to recommend for each user: 10 to 100.
- **Issue:** The shared negative items are randomly sampled from all items
  - Most of them are “**easy negatives**”, i.e., a model does not need to be fine-grained to distinguish them from positive items.
- We need a way to sample “**hard negatives**” to force the model to be fine-grained!

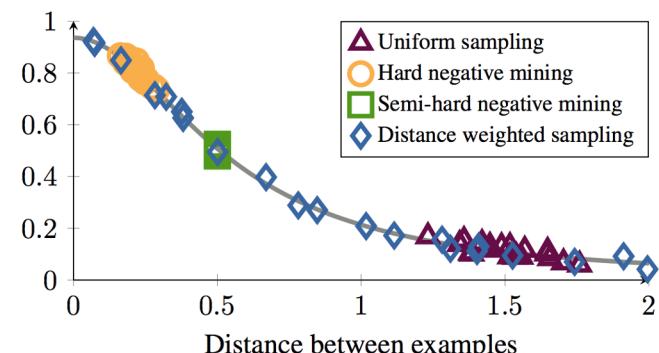
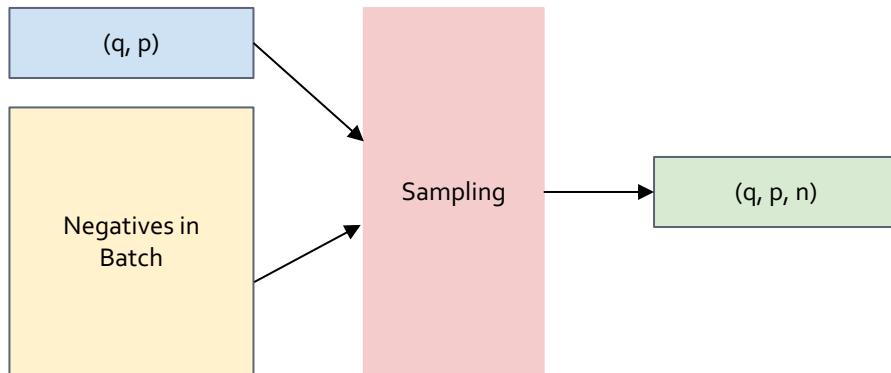
# Hard Negatives (2)

- For each user node, the hard negatives are item nodes that are close (but not connected) to the user node in the graph.
- Hard negatives for user  $u \in \mathcal{U}$  are obtained as follows:
  - Compute personalized page rank (PPR) for user  $u$ .
  - Sort items in the descending order of their PPR scores.
  - Randomly sample item nodes that are ranked high but not too high, e.g., 2000<sup>th</sup> — 5000<sup>th</sup>.
    - Item nodes that are close but not too close (connected) to the user node.
- The hard negatives for each user are used in addition to the shared negatives.

# PinSAGE: Negative Sampling

$(q, p)$  positive pairs are given but various methods to sample negatives to form  $(q, p, n)$

- Distance Weighted Sampling ([Wu et al., 2017](#))
  - Sample negatives so that query-negative distance distribution is approx  $U[0.5, 1.4]$



(b) Sample distribution for different strategies.

# Fine-Grained Object Similarity

Query



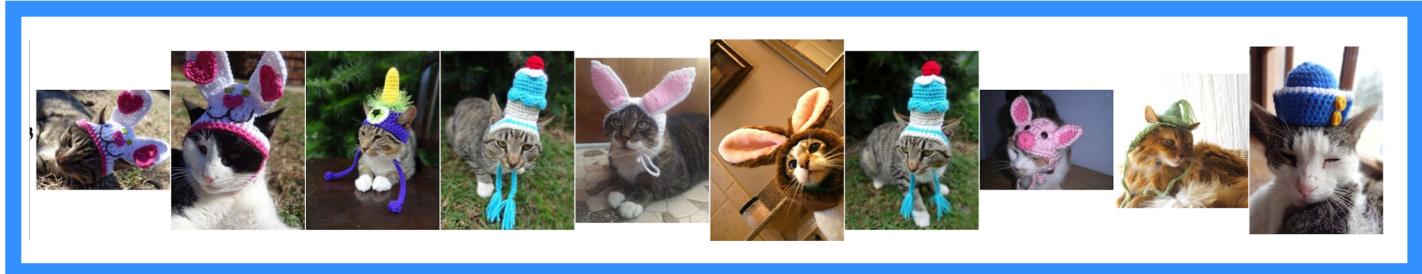
Visual only

PinSAGE



# Compare against Prod

Query



# PinSAGE: Summary

- PinSAGE uses GNNs to generate high-quality user/item embeddings that capture both the rich node attributes and graph structure.
- The PinSAGE model is effectively trained using sophisticated negative sampling strategies.
- PinSAGE is successfully deployed at Pinterest, a billion-scale image content recommendation service.
  - Uncovered in this lecture: How to scale up GNNs to large-scale graphs. Will be covered in a later lecture.