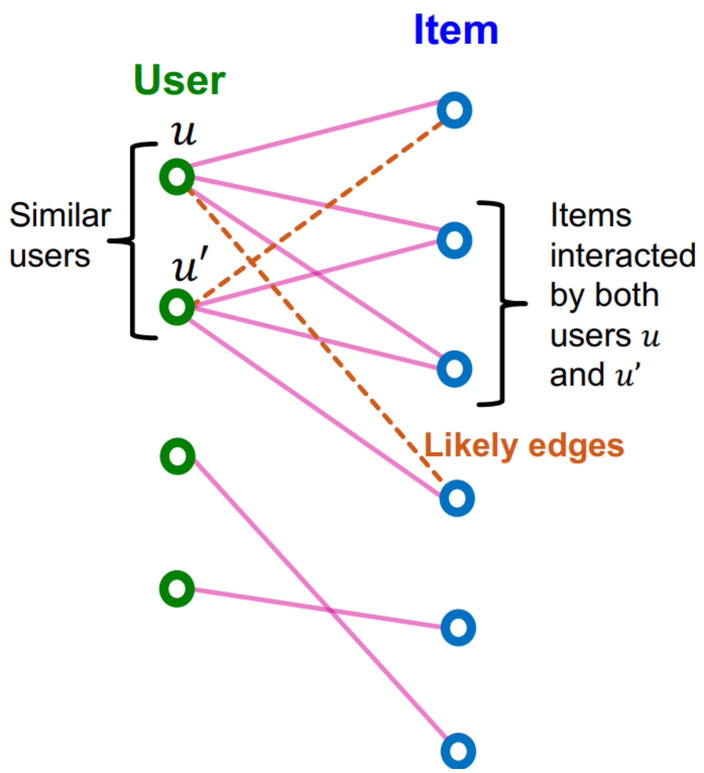
Recommender Systems with GNN



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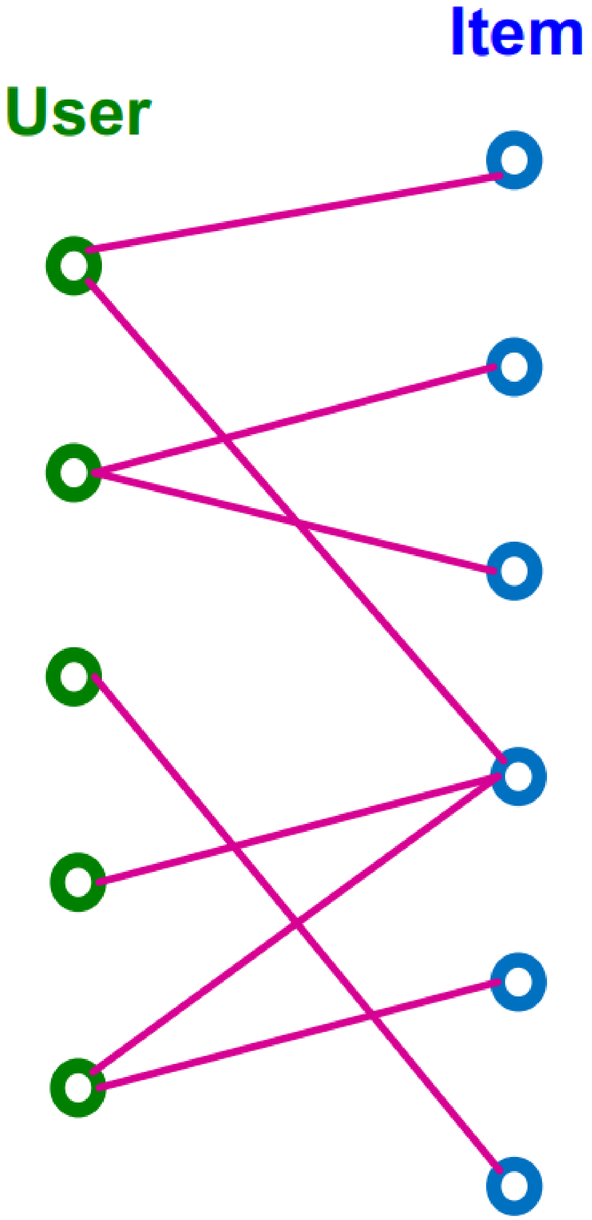
Recommender systems

- Information explosion in the era of the 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 helps users effectively explore content of interest

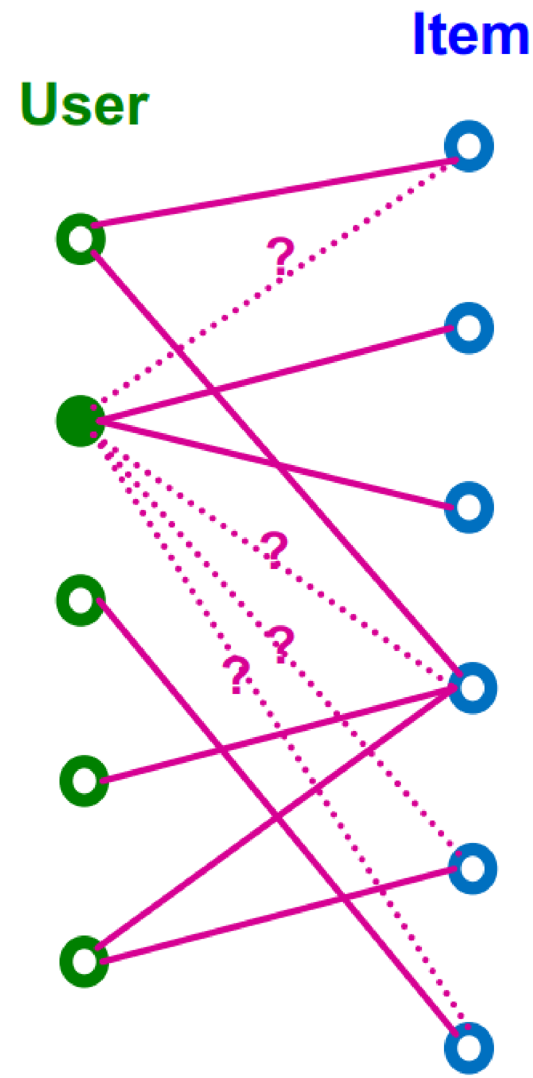
Bipartite graph

- Recommender systems can be naturally modelled as a bipartite graph
  - Nodes: users and items
  - Edges: interaction between users and items
    - Clicks, purchases, reviews etc.
    - Often have a timestamp



Task

- Given past user-item interactions, predict new items a user will interact with
  - Can be case as **link prediction**: predict new interaction given past edges

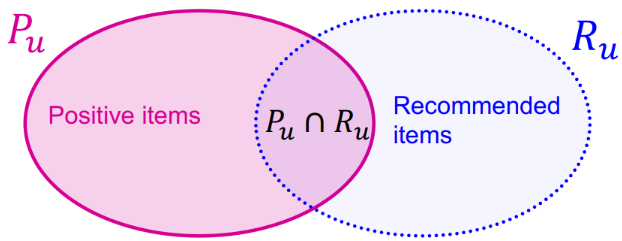


Top-K recommendations

- Recommend K items for each user
  - K needs to be low-is for the recommendations to make sense
  - Typically 10-100
- Goal: as many positive items as possible to be in the top-K recommendations
  - Positive items: items that the user will interact with in the future
- Evaluation metric: Recall@K

Recall@K

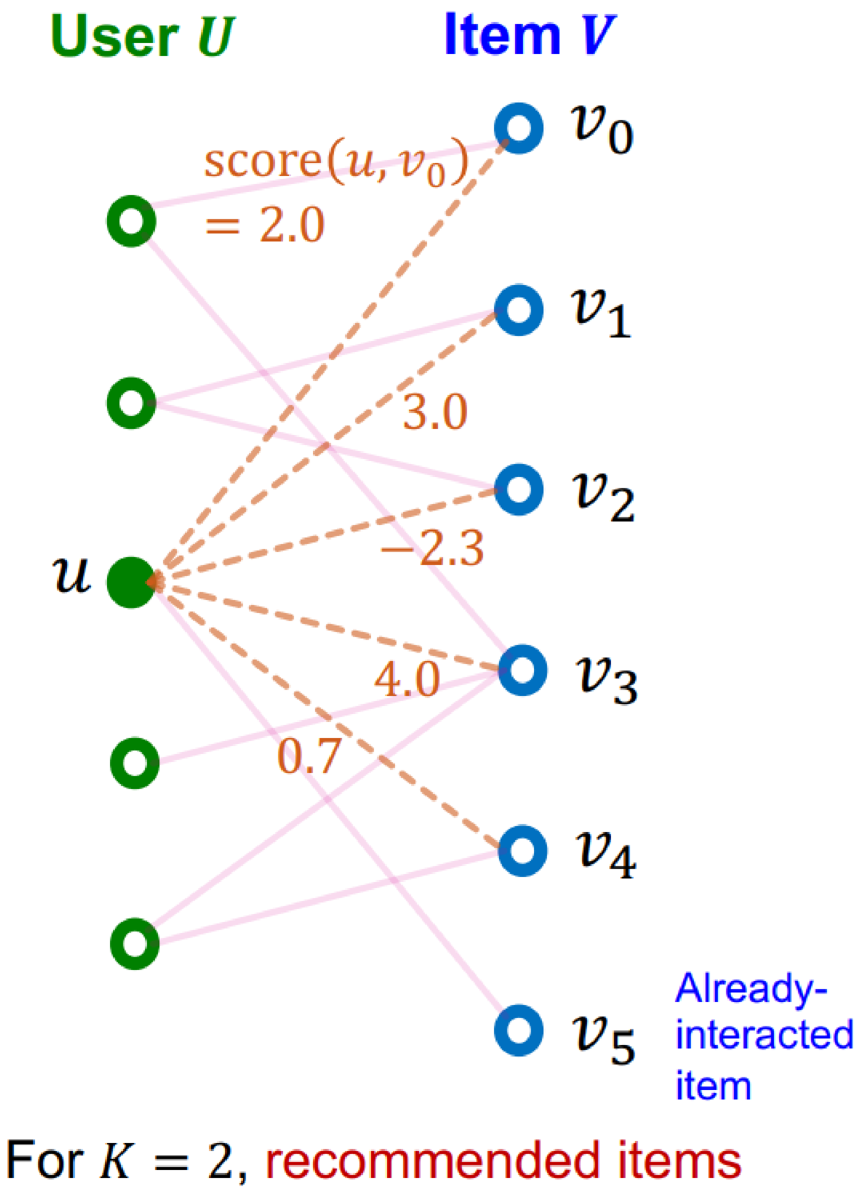
- For each user u,
  - Let P_u be a set of positive items the user will interact with in the future
  - Let R_u be the set of items recommended by the model
    - In top-K recommendation, $|R_u| = K$
    - Items the user has already interacted with are excluded



- Recall@K for user u is $|P_u \cap R_u| / |P_u|$
- Recall@K for the dataset is the averaged Recall@K across users

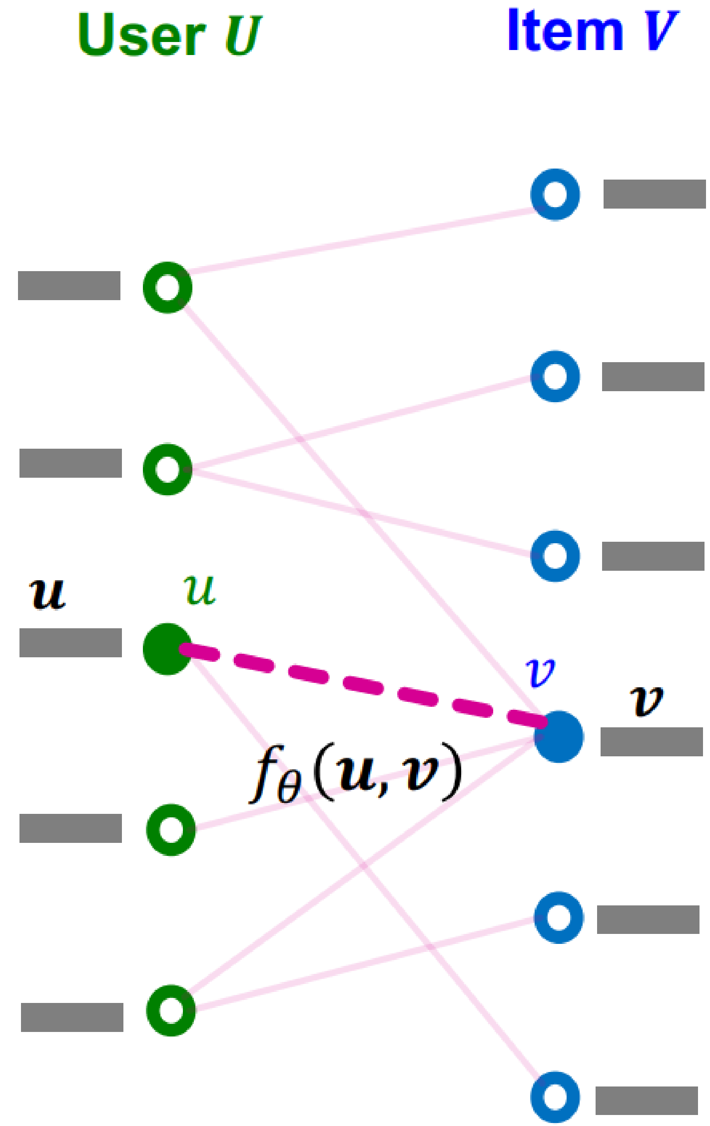
Score function

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



Emebedding-Based Models

- Embedding-based models for scoring user-item interactions:
  - Compute embeddings $z_u \in R^d$ and $z_v \in R^d$ for pairs (u, v) of users and items
  - Define $f_\theta(\cdot,\cdot): R^d \times R^d \to R$ to be a parameterized function
  - $score(u, v) = f_\theta(z_u, z_v)$



Training objective

- Optimize $\{z_u\}_{u \in U}, \{z_v\}_{v \in V}, \theta$ to achieve high recall@K on seen (i.e., training) user-item interactions
- Hope that would lead to high recall@K on unseen (i.e., test interactions)

Surrogate Loss functions

- recall@K is not a differentiable function, so cannot apply gradient-based optimization
- User *surrogate functions* to enable gradient based optimization
  - Binary loss
  - Bayesian Personalized Ranking (BPR) loss
- Surrogate losses should be
  - Differentiable
  - Aligned with the original training objective

Binary loss

- Sum over the positive edges E and negative edges E_{neg}
  - Negative edges are those that are absent in the training set

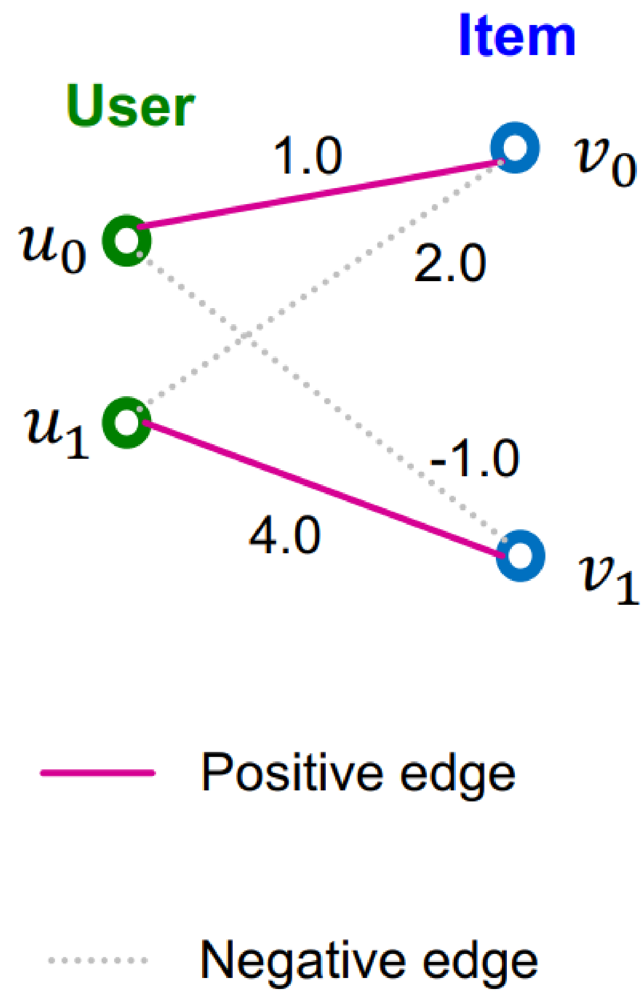
$$\underbrace{-\frac{1}{|\boldsymbol{E}|}\sum_{(u,v)\in \boldsymbol{E}} \log\left(\sigma(f_\theta(\boldsymbol{u},\boldsymbol{v}))\right)}\ \underbrace{-\frac{1}{|\boldsymbol{E}_{\mathbf{neg}}|}\sum_{(u,v)\in \boldsymbol{E}_{\mathbf{neg}}} \log\left(1-\sigma(f_\theta(\boldsymbol{u},\boldsymbol{v}))\right)}$$

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

- Make $f_\theta(u, v)$ high for observed edges (u, v), and low otherwise
- Aligns with recall@K in the sense that we are scoring positive edges higher

Binary loss: issue

- Binary loss pushes *all* negative edges down and *all* positive edges up
- But we can imagine a perfect recommender where some negative edges are higher than some positive edges
  - Only need for positive edges to be higher than negative edges for each particular user



Perfect recall@K, but high binary loss

BPR loss

- 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: $E(u^*) = \{(u^*, v) | (u^*, v) \in E\}$
  - Negative edges: $E_{neg}(u^*) = \left\{(u^*, v) \middle| (u^*, v) \in E_{neg}\right\}$

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.

Training objective: BPR loss

- For each user u^*, we want the scores of rooted positive edges $E(u^*)$ to be higher than those of rooted negative edges $E_{neg}(u^*)$
  - Aligns with what we want from maxmimizing recall@k
- BPR loss for user u^*:

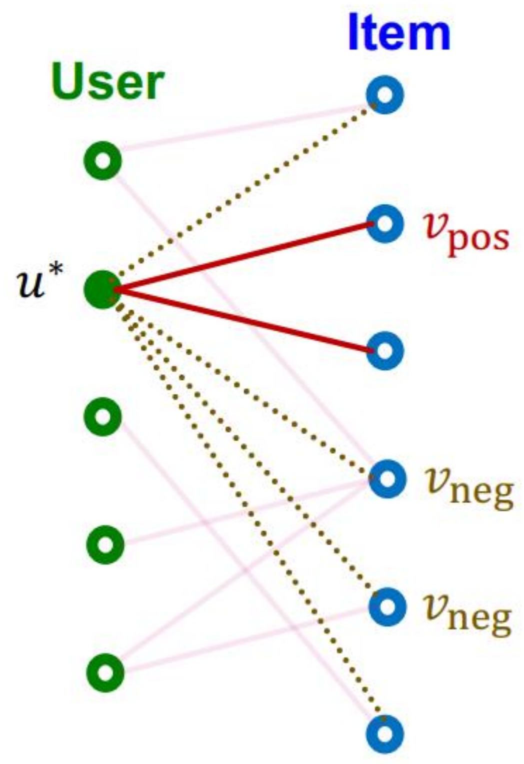
Encouraged to be positive for each user
=positive edge score is higher than negative edge score

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

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

BPR loss: mini-batch training

- Sample a subset of users $U_{min} \subset U$
  - For each user $u^* \in U_{mini}$, we sample one positive item v_{pos} and a set of sampled negative items V_{neg}
- Mini-batch loss:

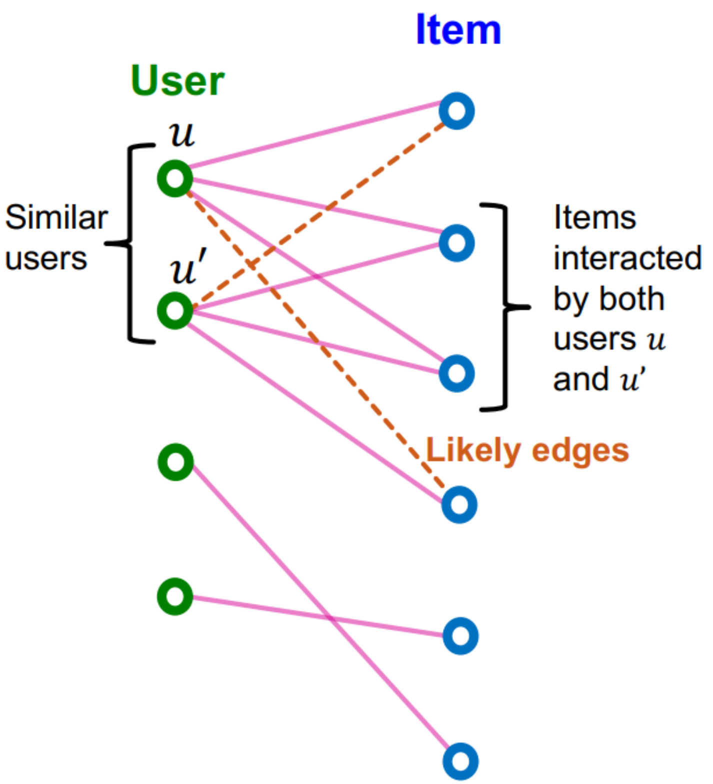


$$\boxed{\frac{1}{|\boldsymbol{U}_{\text{mini}}|}\sum_{u^*\in\boldsymbol{U}_{\text{mini}}}}\frac{1}{|\boldsymbol{V}_{\text{neg}}|}\sum_{v_{\text{neg}}\in\boldsymbol{V}_{\text{neg}}} -\log\left(\sigma\left(f_\theta(u^*,\boldsymbol{v}_{\text{pos}})\right)-\sigma\left(f_\theta(u^*,\boldsymbol{v}_{\text{neg}})\right)\right)$$

Average over users in the mini-batch

Embedding Models for Recommender Systems

- Underlying idea: "collaborative filtering"
  - Recommend items for a user by collecting preferences of many other similar users
  - Similar users tend to prefer similar items
- Graph embeddings capture similarity between users/items

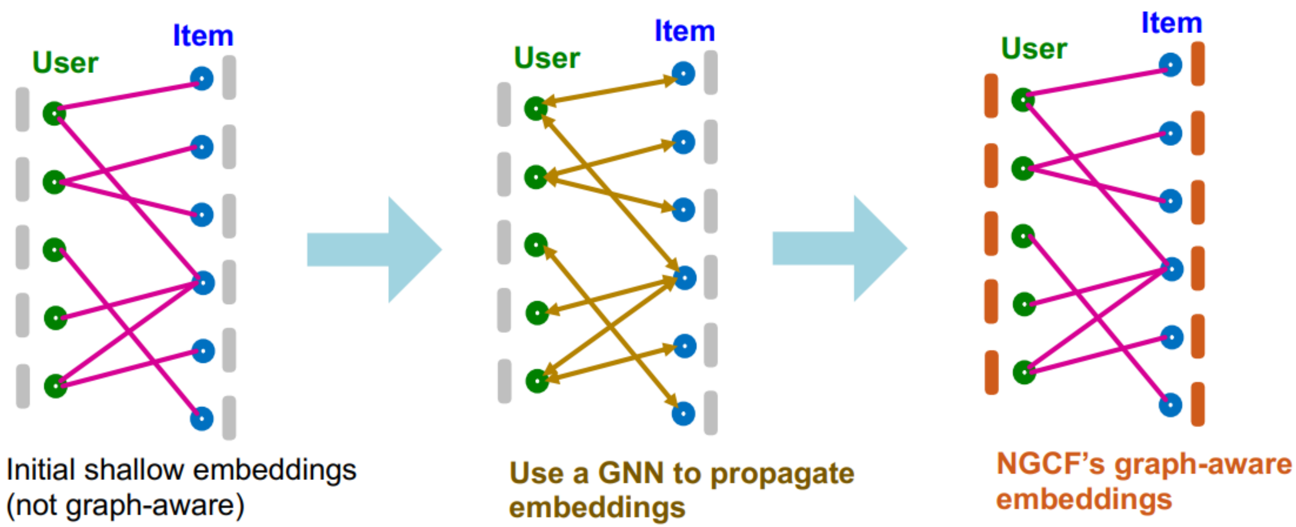


Embedding Models for Recommender Systems

- 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

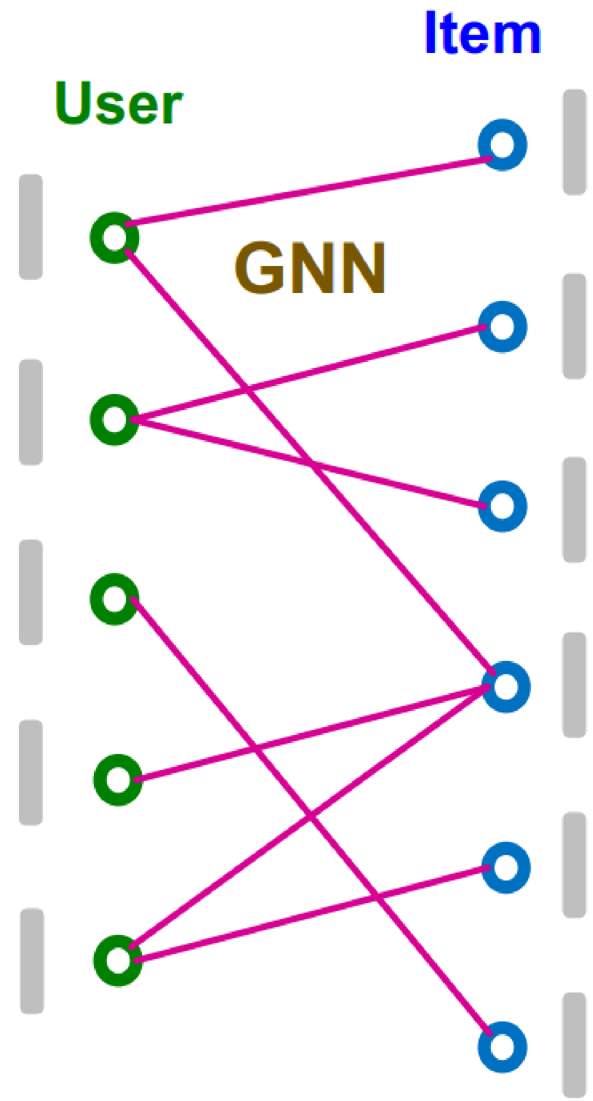
Neural Graph Collaborative Filtering

- Explicitly incorporates high-order graph structure (i.e., neighbourhood information rather than just edges) when generating user/item embeddings
- Key idea: user a GNN to generate graph-aware user/item embeddings



NGCF Framework

- Start with a user-item bipartite graph
- NGCF framework:
  - Prepare shallow learnable embedding for each node
  - User multi-layer GNNs to propagate embeddings along the bipartite graph
    - Capture higher-order structure
  - Final embeddings are explicitly graph-aware
- Jointly learn:
  - Shallow user/item embeddings
  - GNN's parameters



Shallow user/item embeddings (learnable)

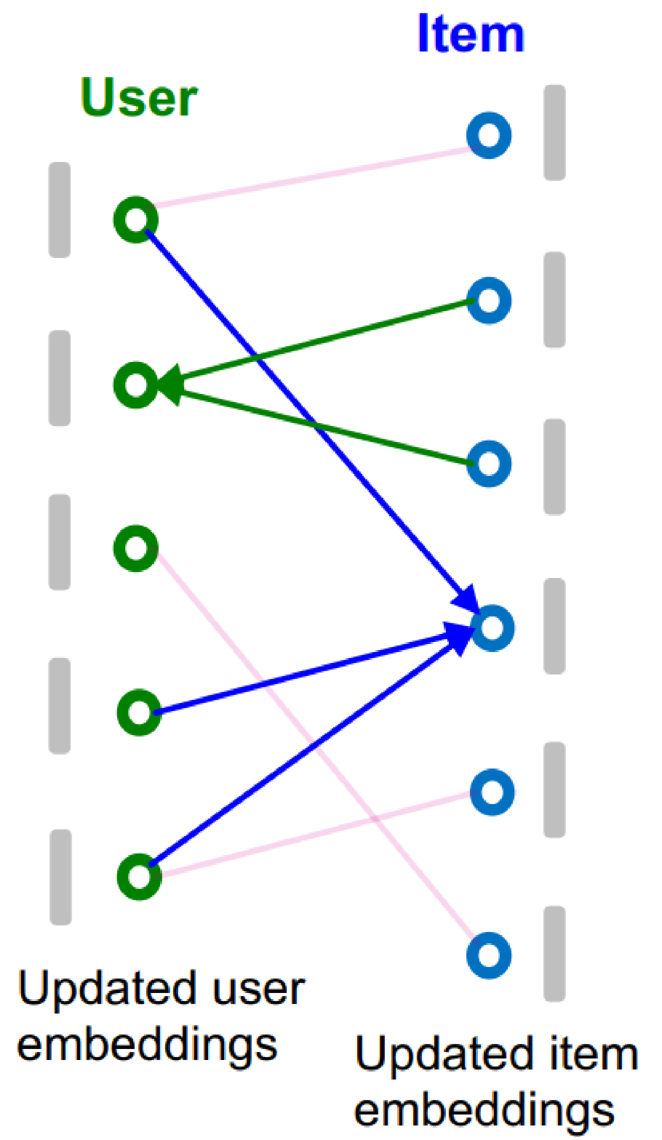
NGCF learning

- Initialize shallow embeddings
- Iteratively update node embedding using neighbouring embeddings

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

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

- AGGR() can be MEAN(), COMBINE(x, y) can be ReLU(Linear(Contact(x, y))



NGCF learning

- After K rounds of aggregation, get final user/item embeddings $h_u^{(K)}$ and $h_v^{(k)}$
- $score(u, v) = h_u^{(K)} \cdot h_v^{(k)}$
- Can now compute BPR and backpropagate

PinSAGE: Scaling Up NGCF

- Data: Pinterest pins
- Pin embedding unifies visual, textual, and graph information
- Embeddings for new content available within seconds

PinSAGE: Scaling Up

- Shared negative samples across users in a mini-batch
- Mining for hard negative samples
- Curriculum learning
- Mini-batch training of GNNs on a large graph

Shared negative samples

- In BPR loss, we sampled a set of negative edges for each positive edge
- Costs $O(|U_{mini}||V_{neg}|)$ to sample and compute the loss for the negative edges
- Idea: sample $V_{neg} = \{v_{neg}\}$ across all users in the minibatch U_{mini}
  - Only compute $|V_{neg}|$ embeddings

Curriculum learning

- Idea: make the negative samples *gradually harder* in the process of training
- At the n-th epoch, add n-1 hard negative items
- The model will gradually learn to make finer-grained predictions

Curriculum learning II

- Idea: use harder and hard negative samples

Source pin

Positive

Easy negative

Hard negative

Hard negatives

- Most negatives that are sampled are “easy negatives”
- Hard negatives are nodes that are close (but not connected) to the user node in the graph
- Obtain hard negatives for u:
  - Compute Personalized Page Rank (PPR) for user u
    - PPR is the probability of v occurs on a random walk starting at u
    - Sample item notes that are ranked high but not too high by PPR to U
      - Item nodes that are close not not connected to user node