GNN Applications: Recommender Systems

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https://ulab-uiuc.github.io/CS598/

GNN Applications: Recommender Systems

Recommender Systems: Task and
Evaluation

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.

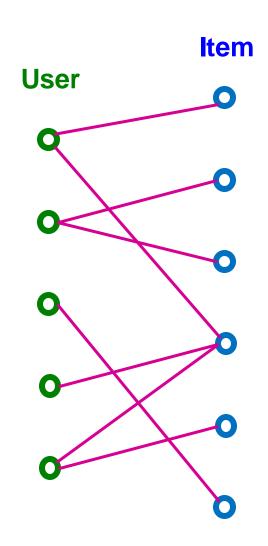
Notation

Notation:

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

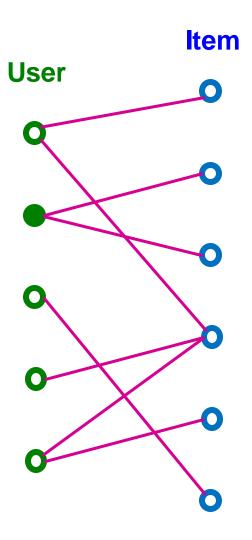
Recommender System as a Graph

- 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.
 - For $u \in U$, $v \in V$, we need to get a real-valued score f(u, v).



Modern Recommender System

- **Problem:** Cannot evaluate f(u, v) for every user u item v pair.
- Solution: 2-stage process:
 - Candidate generation (cheap, fast)
 - Ranking (slow, accurate)

 Search

 Recommendations

 Return top-10 items by score f(u, v)In the second of the s

Example f(u, v):

 $f(u,v) = z_u \cdot z_v$

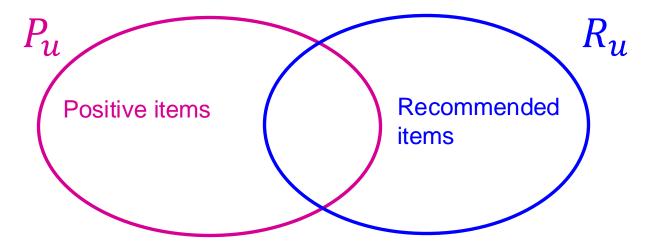
Top-K Recommendation

- For each user, we recommend *K* items.
 - 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)

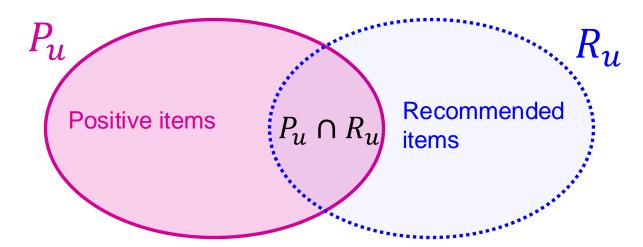
• For each user u,

- Let P_{μ} 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.



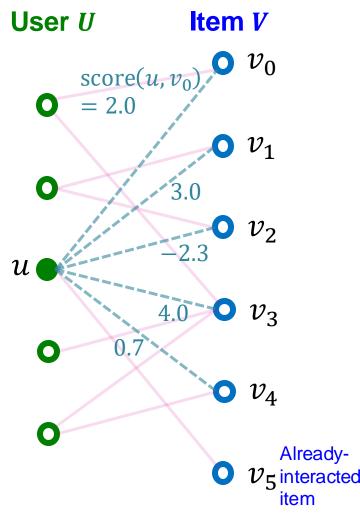
 The final Recall@K is computed by averaging the recall values across all users.

GNN Applications: Recommender Systems

Recommender Systems: Embedding-Based Models

Score Function

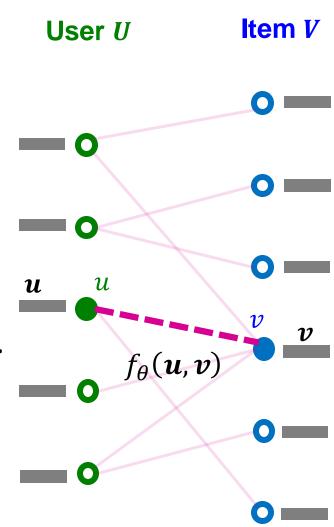
- To get the top-*K* items, we need a score function for user-item interaction:
 - For $u \in U$, $v \in V$, we need to get a real-valued scalar score(u, v).
 - *K* items with the largest scores for a given user *u* (excluding already-interacted items) are then recommended.



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 $u \in U$, let $u \in \mathbb{R}^D$ be its D-dimensional embedding.
 - For each item $v \in V$, let $v \in \mathbb{R}^D$ be its D-dimensional embedding.
 - Let $f_{\theta}(\cdot,\cdot)$: $\mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$ be a parametrized function.
 - Then, $score(u, v) \equiv f_{\theta}(u, v)$



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 original training objective (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.

Loss Function: Binary Loss

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

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

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.

Loss Function: BPR Loss

- 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 $E_{neg}(u^*)$.
 - 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

$$\operatorname{Loss}(u^*) = \frac{1}{|\boldsymbol{E}(u^*)| \cdot |\boldsymbol{E}_{\operatorname{neg}}(u^*)|} \sum_{(u^*, v_{\operatorname{pos}}) \in \boldsymbol{E}(u^*)} \sum_{(u^*, v_{\operatorname{neg}}) \in \boldsymbol{E}_{\operatorname{neg}}(u^*)} -\log(\sigma(f_{\theta}(\boldsymbol{u}^*, v_{\operatorname{pos}}) - f_{\theta}(\boldsymbol{u}^*, v_{\operatorname{neg}})))$$

Can be approximated using a mini-batch

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

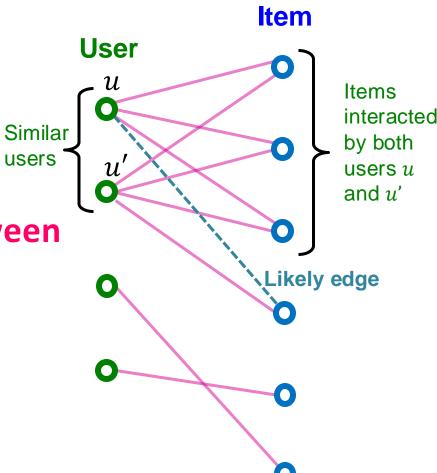
Summary So Far

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.

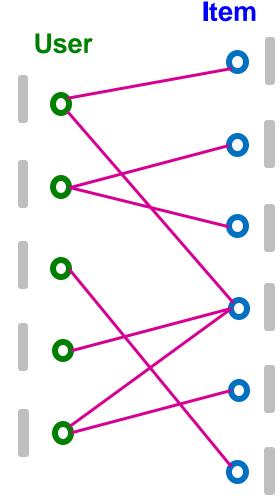
This Lecture: GNNs for Recsys

- In this lecture, we teach two representative GNN approaches for recommender systems.
- (1) Neural Graph Collab. Filtering (NGCF)
- **(2) LightGCN** [He et al. 2020]
 - Improve the conventional collaborative filtering models (i.e., shallow encoders) by explicitly modeling graph structure using GNNs.
 - Assumes no user/item features.
- 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.

GNN Applications: Recommender Systems Neural Graph Collaborative Filtering

Conventional Collaborative Filtering

- Conventional collaborative filtering model is based on shallow encoders:
 - No user/item features.
 - Use shallow encoders for users and items:
 - For every $u \in U$ and $v \in V$, we prepare shallow learnable embeddings $u, v \in \mathbb{R}^D$.
 - Score function for user u and item v is $f_{\theta}(u, v) \equiv z_u^T z_v$.



Learnable shallow user/item embeddings

Limitations of Shallow Encoders

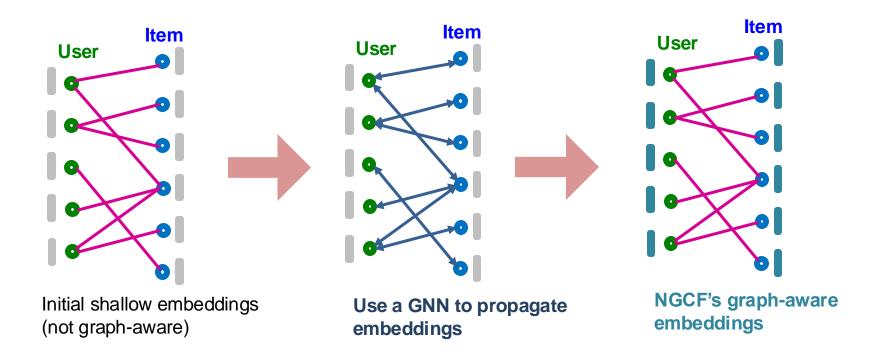
- The model itself does not explicitly capture graph structure
 - The graph structure is only implicitly captured in the training objective.
- Only the first-order graph structure (i.e., edges) is captured in the training objective.
 - High-order graph structure (e.g., K-hop paths between two nodes)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

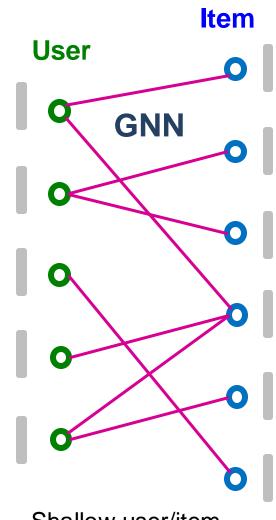
NGCF: Overview

- 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

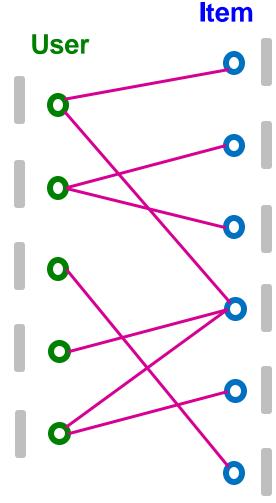
- Given: User-item bipartite graph.
- NGCF framework:
 - Prepare shallow learnable embedding for each node.
 - Use multi-layer GNNs to propagate embeddings along the bipartite graph.
 - High-order graph structure is captured.
 - Final embeddings are *explicitly* graph-aware!
- Two kinds of learnable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



Shallow user/item embeddings (learnable)

Initial Node Embeddings

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



Learnable shallow user/item embeddings

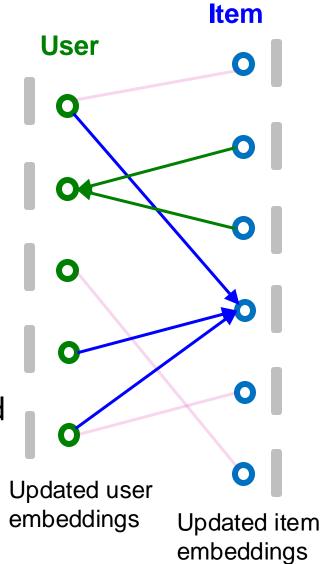
Neighbor Aggregation

 Iteratively update node embeddings using neighboring embeddings.

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

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 ReLU(Linear(Concat(x, y)))

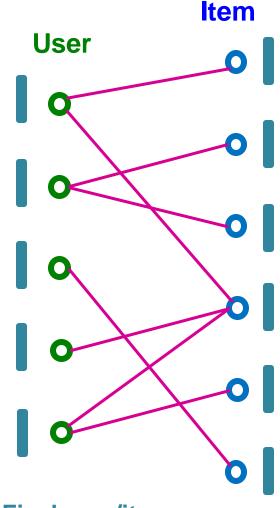


Final Embeddings and Score Function

- After K rounds of neighbor aggregation, we get the final user/item embeddings $\boldsymbol{h}_u^{(K)}$ and $\boldsymbol{h}_v^{(K)}$.
- For all $u \in U, v \in V$, we set

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

Score function is the inner product $score(u, v) = u^T v$



Final user/item embeddings (graph-aware)

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.

GNN Applications: Recommender Systems LightGCN

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 (user/item) node.
 - Most of the parameter counts are in shallow embeddings when N (#nodes) $\gg D$ (embedding dimensionality)
 - Shallow embeddings: O(ND).
 - GNN: $O(D^2)$.
 - The GNN parameters may not be so essential for performance.

LightGCN: Motivation (2)

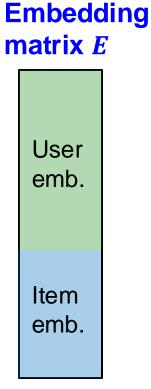
- Can we simplify the GNN used in NGCF (e.g., remove its learnable parameters)?
 - Answer: Yes!
 - Bonus: Simplification improves the recommendation performance!
- Overview of the idea:
 - Adjacency matrix for a bipartite graph
 - Matrix formulation of GCN
 - Simplification of GCN by removing non-linearity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

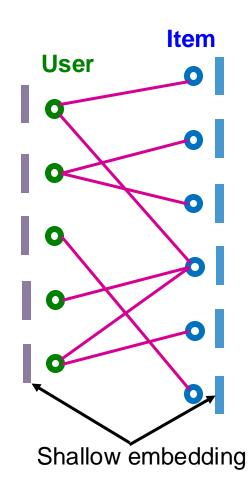
Recall: Adjacency and Embedding Matrices

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

Adjacency matrix A

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





Recall: Matrix Formulation of GCN

- Recall: The diffusion matrix of C&S.
- Let **D** be the degree matrix of **A**.
- Define the normalized adjacency matrix \widetilde{A} as

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

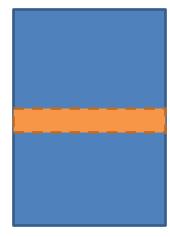
Note: Different from the original GCN, selfconnection is omitted here.

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

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

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:

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

Original idea from SGC [Wu et al. 2019]

The final node embedding matrix is given as

$$E^{(K)} = \widetilde{A} E^{(K-1)} W^{(K-1)}$$

$$= \widetilde{A} (\widetilde{A} E^{(K-2)} W^{(K-2)}) W^{(K-1)}$$

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

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

Simplifying GCN (2)

Removing ReLU significantly simplifies GCN!

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

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

Diffusing node embeddings along the graph

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

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

Multi-Scale Diffusion

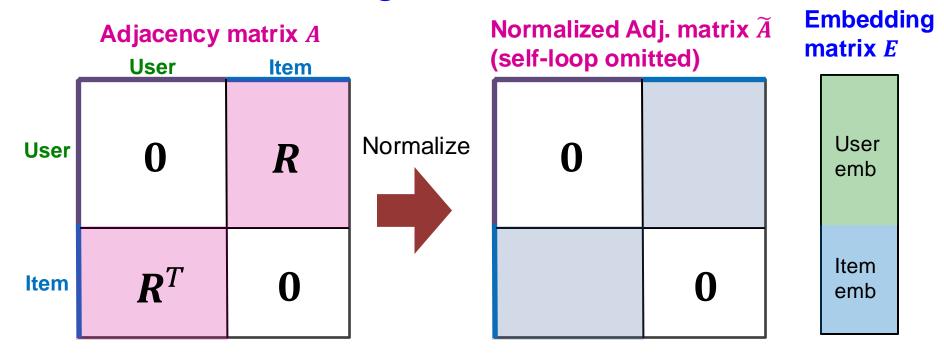
We can consider multi-scale diffusion

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

- The above includes embeddings diffused at multiple hop scales.
- $\alpha_0 E^{(0)} = \alpha_0 \widetilde{A}^0 E^{(0)}$ acts as a self-connection (that is omitted in the definition \widetilde{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 $k=0,\ldots,K$.

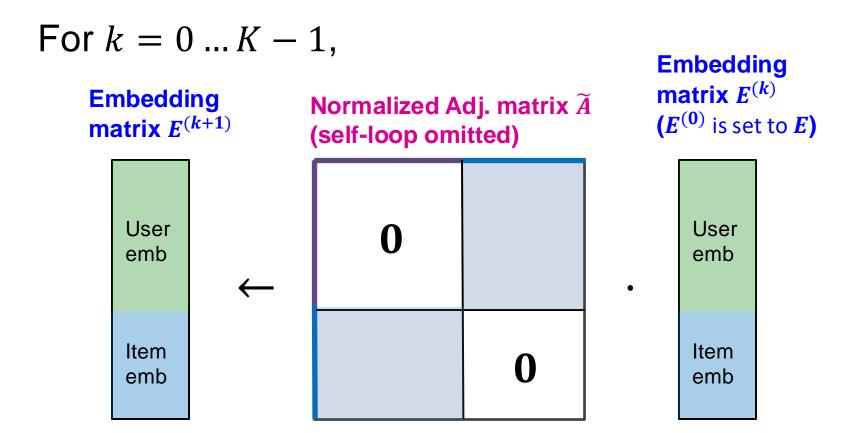
LightGCN: Model Overview (1)

- Given:
 - Adjacency matrix A
 - Initial learnable embedding matrix E



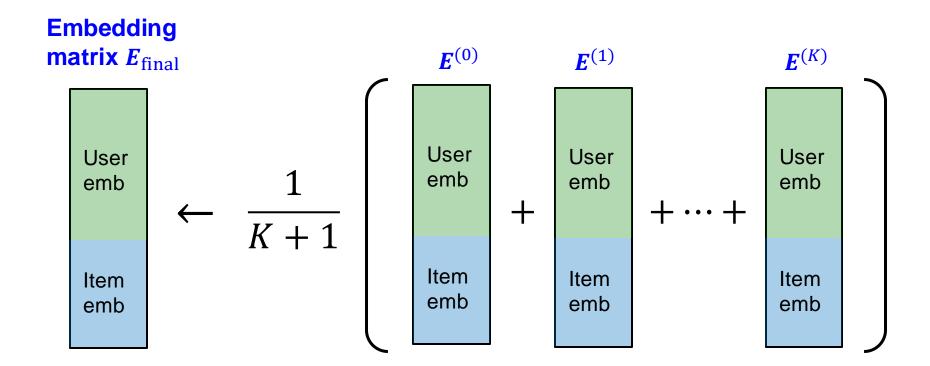
LightGCN: Model Overview (2)

• Iteratively diffuse embedding matrix E using \widetilde{A}



LightGCN: Model Overview (3)

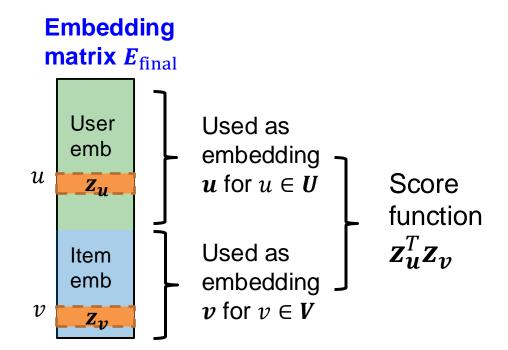
Average the embedding matrices at different scales.



LightGCN: Model Overview (4)

Score function:

• Use user/item vectors from E_{final} to score user-item interaction



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.
 - Key insight: the diffusion directly encourages the embeddings of similar users/items to be similar
 - The simplification leads to better empirical performance than NGCF.

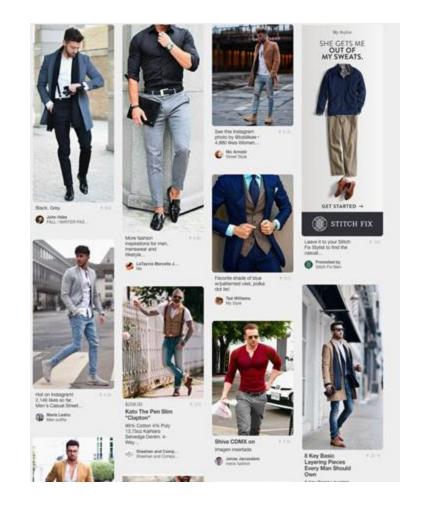
GNN Applications: Recommender Systems PinSAGE

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





Hans Wegner chair
Room and Board

FIG+SALT



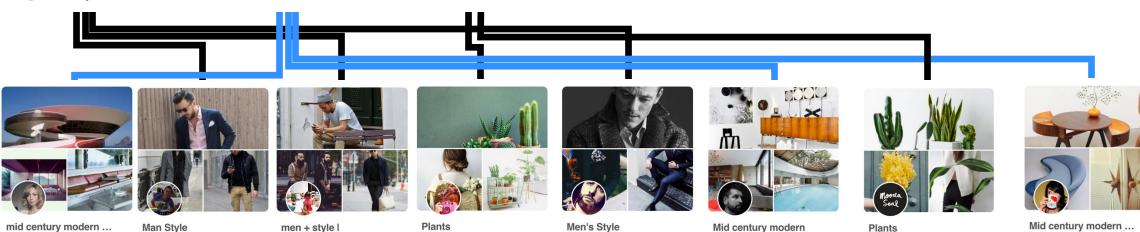
Gavin Jones



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



HelloSandwich



Andrea Sempi

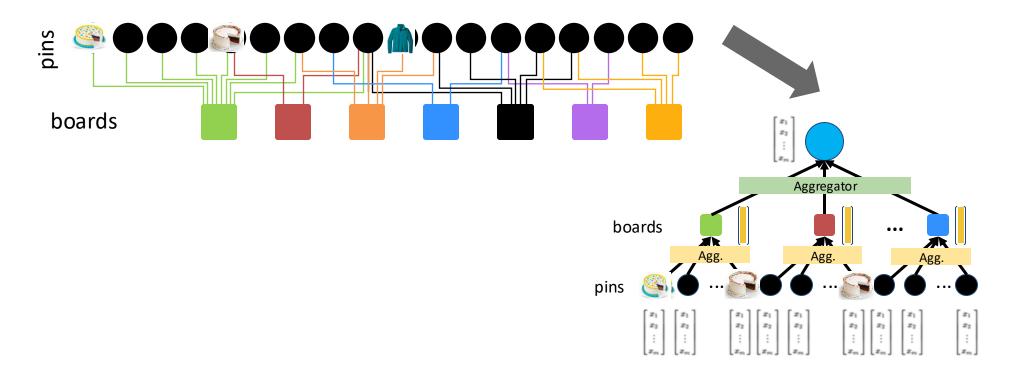
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Prettygreentea

PinSAGE:Graph Neural Network

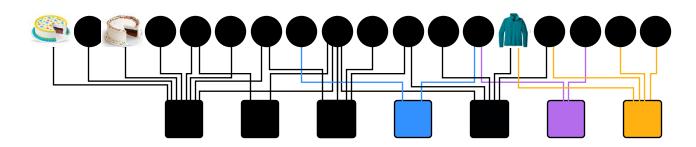
- Graph has tens of billions of nodes and edges
- Further resolves embeddings across the Pinterest graph



PinSAGE: Scaling Up and Considerations

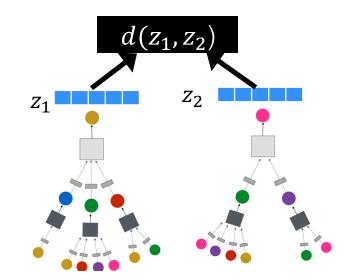
- In addition to the GNN model, the PinSAGE paper introduces several methods to scale the GNN to a billion-scale recommender system (e.g., Pinterest).
 - Mini-batch training of GNNs on a large-graph
 - Shared negative samples across users in a mini-batch
 - Hard negative samples
 - Curriculum learning

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):





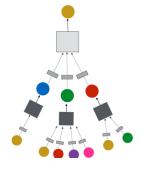


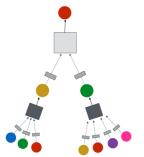




Shared Negative Samples (1)

- Recall: In BPR loss, for each user $u^* \in U_{\min}$, we sample one positive item v_{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 $| \pmb{U}_{\min i} | \cdot | \pmb{V}_{neg} |$ embeddings for negative nodes.
 - We need to apply $|U_{\min i}| \cdot |V_{\text{neg}}|$ GNN computational graphs (see right), which is expensive.





Shared Negative Samples (2)

- Key idea: We can share the same set of negative samples $V_{\rm neg} = \{v_{\rm neg}\}$ across all users $U_{\rm mini}$ 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 $|U_{\min}|!$
 - Empirically, the performance stays similar to the non-shared negative sampling scheme.

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 finegrained to distinguish them from positive items.
- We need a way to sample "hard negatives" to force the model to be fine-grained!

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

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.

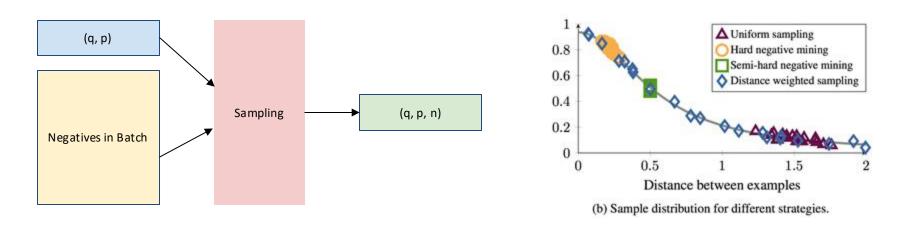
Hard Negatives (2)

- 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 $u \in U$ 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., $2000^{th} 5000^{th}$.
 - 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]



Fine-Grained Object Similarity

Visual only









Compare against Production Model

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.