

# Graph Neural Network in Recommender Systems

Jiarui Qin

Apex Data & Knowledge Management Lab  
Shanghai Jiao Tong University

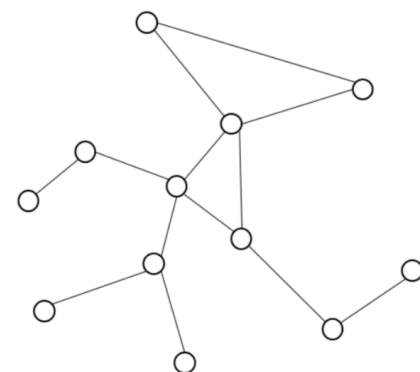


# Contents

- **Basics of GNN**
  - Graph Convolution Networks (GCN)
  - Graph Attention Networks (GAT)
- **GNN in Social Recommendation**
- **GNN in Knowledge Graph Recommendation**
- **GNN in User-Item Bipartite Graph**

# Graph Convolution Networks (GCN)

- Spectral method
- Non-spectral method:
  - Represent a node using its neighbors by an iterative manner
  - GCN
    - Aggregator:  $\mathbf{h}_{\mathcal{N}_v}^t = \mathbf{h}_v^{t-1} + \sum_{k=1}^{\mathcal{N}_v} \mathbf{h}_k^{t-1}$
    - Updater:  $\mathbf{h}_v^t = \sigma(\mathbf{h}_{\mathcal{N}_v}^t \mathbf{W}_L^{\mathcal{N}_v})$
  - GraphSAGE
    - Aggregator:  $\mathbf{h}_{\mathcal{N}_v}^t = \text{AGGREGATE}_t(\{\mathbf{h}_u^{t-1}, \forall u \in \mathcal{N}_v\})$
    - Updater:  $\mathbf{h}_v^t = \sigma(\mathbf{W}^t \cdot [\mathbf{h}_v^{t-1} \parallel \mathbf{h}_{\mathcal{N}_v}^t])$
    - AGGREGATE function: avg/max pooling, LSTM



J.Zhou et al. Graph Neural Networks: A Review of Methods and Applications

D.K.Duvenaud et al. Convolutional networks on graphs for learning molecular fingerprints. NIPS 2015

W.L.Hamilton et al. Inductive representation learning on large graphs. NIPS 2017

# Graph Attention Networks (GAT)

- Aggregator:

$$\alpha_{vk} = \frac{\exp(\text{LeakyReLU}(\mathbf{a}^T [\mathbf{W}\mathbf{h}_v \parallel \mathbf{W}\mathbf{h}_k]))}{\sum_{j \in \mathcal{N}_v} \exp(\text{LeakyReLU}(\mathbf{a}^T [\mathbf{W}\mathbf{h}_v \parallel \mathbf{W}\mathbf{h}_j]))}$$

$$\mathbf{h}_{\mathcal{N}_v}^t = \sigma \left( \sum_{k \in \mathcal{N}_v} \alpha_{vk} \mathbf{W}\mathbf{h}_k \right)$$

Multi-head concatenation:

$$\mathbf{h}_{\mathcal{N}_v}^t = \parallel_{m=1}^M \sigma \left( \sum_{k \in \mathcal{N}_v} \alpha_{vk}^m \mathbf{W}^m \mathbf{h}_k \right)$$

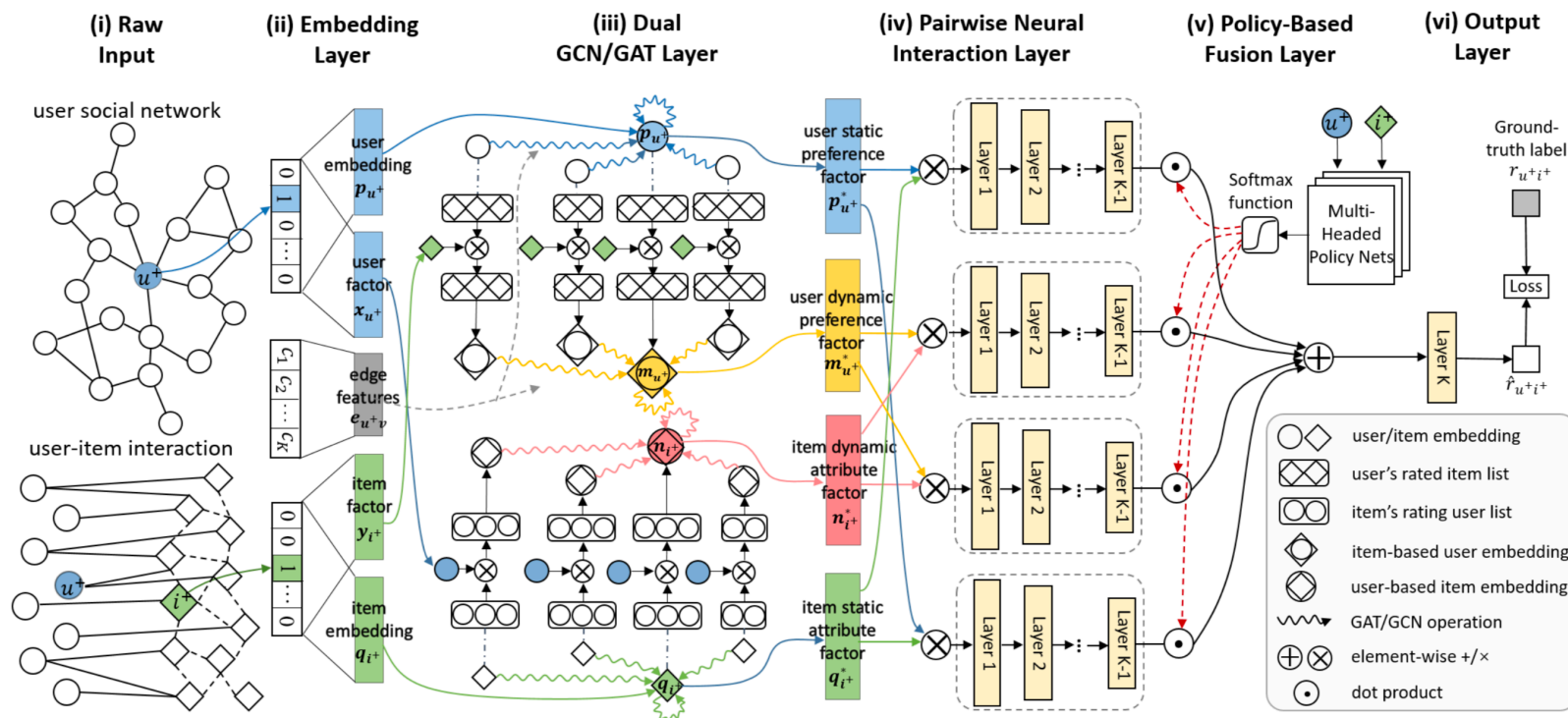
Multi-head average:

$$\mathbf{h}_{\mathcal{N}_v}^t = \sigma \left( \frac{1}{M} \sum_{m=1}^M \sum_{k \in \mathcal{N}_v} \alpha_{vk}^m \mathbf{W}^m \mathbf{h}_k \right)$$

- Updater:

$$\mathbf{h}_v^t = \mathbf{h}_{\mathcal{N}_v}^t$$

# GNN in Social Recommendation (DANSER)



- Three Graphs:
  - user-item interaction;
  - user social network;
  - item-item network (attract same user)

Q. Wu et al. Dual Graph Attention Networks for Deep Latent Representation of Multifaceted Social Effects in Recommender Systems. WWW 2019

# GNN in Social Recommendation (DANSER)

- GAT to capture social/item-item homophily

$$\mathbf{P}^* = \sigma(\mathbf{A}_P(G_U)\mathbf{P}\mathbf{W}_P^T + \mathbf{b}_P)$$

$$\alpha_{uv}^P = \frac{\text{attn}_U(\mathbf{W}_P\mathbf{p}_u, \mathbf{W}_P\mathbf{p}_v, \mathbf{W}_E\mathbf{e}_{uv})}{\sum_{w \in \Gamma_U(u)} \text{attn}_U(\mathbf{W}_P\mathbf{p}_u, \mathbf{W}_P\mathbf{p}_w, \mathbf{W}_E\mathbf{e}_{uw})}, v \in \Gamma_U(u).$$

- GAT to capture social/item-item influence

$$\mathbf{M}_{i^+}^* = \sigma(\mathbf{A}_M(G_U)\mathbf{M}\mathbf{W}_M^T + \mathbf{b}_M), \mathbf{A}_M(G_U) = \{\alpha_{uv, i^+}^M\}_{M \times M},$$

$$\alpha_{uv, i^+}^M = \frac{\text{attn}_U(\mathbf{W}_M\mathbf{m}_u^{i^+}, \mathbf{W}_M\mathbf{m}_v^{i^+}, \mathbf{W}_E\mathbf{e}_{uv})}{\sum_{w \in \Gamma_U(u)} \text{attn}_U(\mathbf{W}_M\mathbf{m}_u^{i^+}, \mathbf{W}_M\mathbf{m}_w^{i^+}, \mathbf{W}_E\mathbf{e}_{uw})},$$

$$m_{ud}^{i^+} = \max_{j \in R_I(u)} \{y_{jd} \cdot y_{i^+d}\} \quad \forall d = 1, \dots, D$$

# GNN in Social Recommendation (DANSER)

- Pairwise Neural Interaction Layer

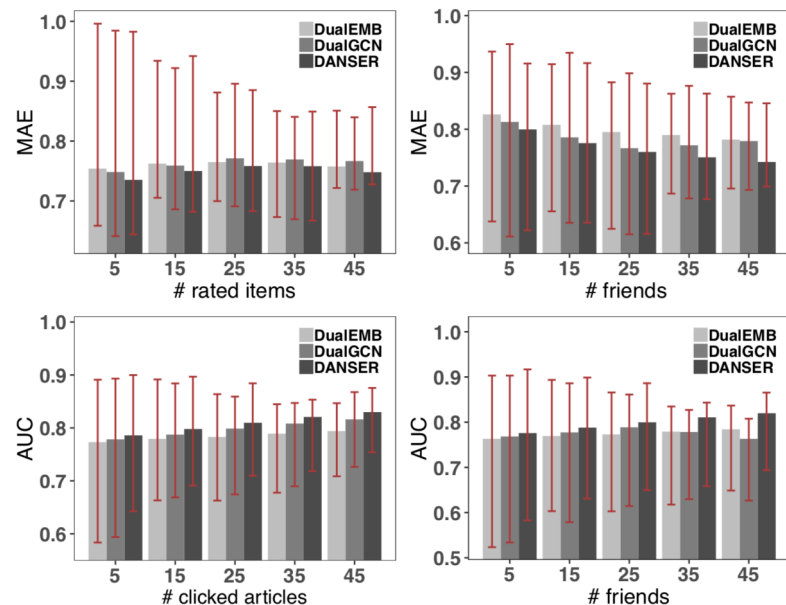
$$\begin{aligned}s_a &= \phi_K^a(\cdots \phi_2^a(\phi_1^a(z_0[a]))), \\ \phi_k^a(z_{k-1}) &= \tanh(\mathbf{W}_k^a \mathbf{z}_{k-1}^a + \mathbf{b}_k^a), k \in [1, K-1], \\ \mathbf{z}_0 &= [\mathbf{p}_u^* \oplus \mathbf{q}_i^*, \mathbf{p}_u^* \oplus \mathbf{n}_i^*, \mathbf{m}_u^* \oplus \mathbf{q}_i^*, \mathbf{m}_u^* \oplus \mathbf{n}_i^*],\end{aligned}$$

- Policy-Based Fusion Layer

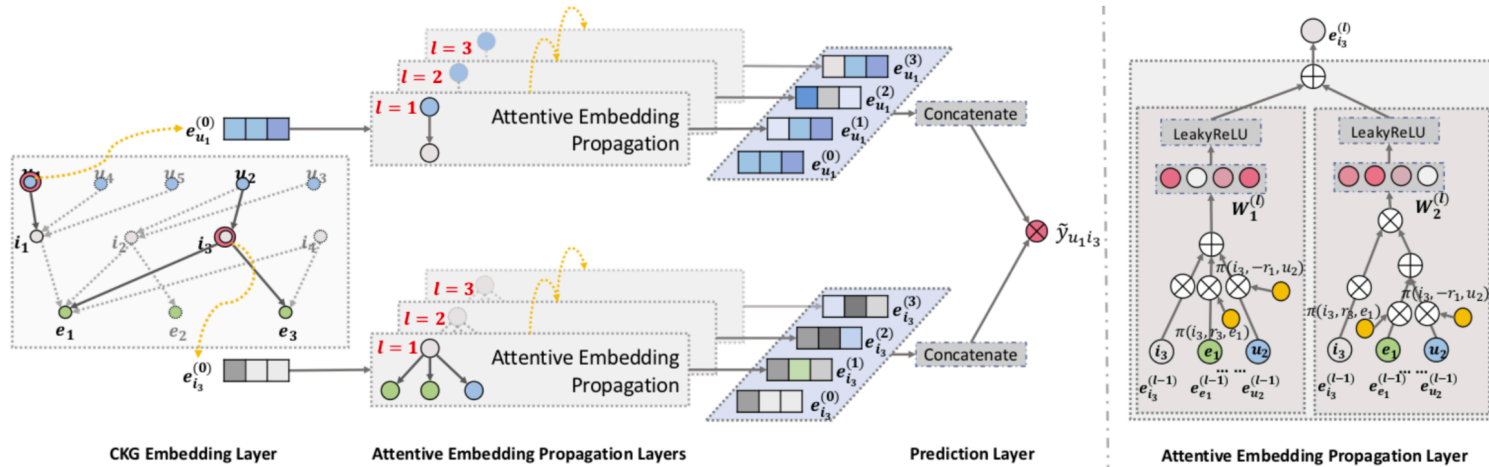
$$\begin{aligned}e_\gamma &= \mathbf{W}_F^2 \tanh(\mathbf{W}_F^1(\mathbf{p}_u || \mathbf{q}_i) + \mathbf{b}_F^1) + \mathbf{b}_F^2. \\ p(\gamma | \mathbf{p}_u, \mathbf{q}_i) &= \frac{\exp(e_\gamma)}{\sum_{a=1}^4 \exp(e_a)}. \\ \mathbf{s} &= \mathbb{E}_{\gamma \sim p(\gamma | \mathbf{p}_u, \mathbf{q}_i)}(\mathbf{s}_\gamma) = \sum_{\gamma=1}^4 p(\gamma | \mathbf{p}_u, \mathbf{q}_i) \cdot \mathbf{s}_\gamma.\end{aligned}$$

# Experiments

	Epinions		WeChat	
	MAE	RMSE	P@10	AUC
SVD++ [15]	0.8321	1.0772	0.0653	0.7304
DELFI [2]	0.8115	1.0561	<u>0.0752</u>	<u>0.7818</u>
TrustPro [37]	0.9130	1.1124	0.0561	0.6482
TrustMF [36]	0.8214	1.0715	0.0625	0.7005
TrustSVD [10]	0.8144	1.0492	0.0664	0.7325
NSCR [31]	0.8044	1.0425	0.0736	0.7727
SREPS [16]	<u>0.8014</u>	<u>1.0393</u>	0.0725	0.7745
DANSER	<b>0.7781</b>	<b>1.0268</b>	<b>0.0823</b>	<b>0.8165</b>
Impv. <sup>1</sup>	2.87%	1.25%	9.33%	4.48%



# GNN in Knowledge Graph Recommendation (KGAT)



- Collaborative Knowledge Graph: Add the user-item bipartite graph to the original KG
- Embedding Layer:
  - TransR:  $g(h, r, t) = \|\mathbf{W}_r \mathbf{e}_h + \mathbf{e}_r - \mathbf{W}_r \mathbf{e}_t\|_2^2$
- Attentive Embedding Propagation Layers
  - Information Propagation:  $\mathbf{e}_{N_h} = \sum_{(h, r, t) \in N_h} \pi(h, r, t) \mathbf{e}_t$
  - Knowledge-aware Attention:  $\pi(h, r, t) = (\mathbf{W}_r \mathbf{e}_t)^\top \tanh((\mathbf{W}_r \mathbf{e}_h + \mathbf{e}_r))$
  - Information Aggregation:  $f_{\text{GCN}} = \text{LeakyReLU}(\mathbf{W}(\mathbf{e}_h + \mathbf{e}_{N_h}))$

$$\mathcal{L}_{\text{KG}} = \sum_{(h, r, t, t') \in \mathcal{T}} -\ln \sigma(g(h, r, t') - g(h, r, t))$$

# GNN in Knowledge Graph Recommendation (KGAT)

- High-order Propagation:

$$\begin{aligned} \mathbf{e}_h^{(l)} &= f\left(\mathbf{e}_h^{(l-1)}, \mathbf{e}_{\mathcal{N}_h}^{(l-1)}\right), \\ \mathbf{e}_{\mathcal{N}_h}^{(l-1)} &= \sum_{(h,r,t) \in \mathcal{N}_h} \pi(h,r,t) \mathbf{e}_t^{(l-1)}, \\ \mathbf{e}_u^* &= \mathbf{e}_u^{(0)} \parallel \cdots \parallel \mathbf{e}_u^{(L)}, \quad \mathbf{e}_i^* = \mathbf{e}_i^{(0)} \parallel \cdots \parallel \mathbf{e}_i^{(L)}. \end{aligned}$$

- Model Prediction:  $\hat{y}(u, i) = \mathbf{e}_u^{* \top} \mathbf{e}_i^*$ .
- Optimization: BPR ranking loss + TransR loss, optimize the two loss alternatively

$$\begin{aligned} \mathcal{L}_{\text{CF}} &= \sum_{(u,i,j) \in \mathcal{O}} -\ln \sigma\left(\hat{y}(u, i) - \hat{y}(u, j)\right) \\ \mathcal{L}_{\text{KGAT}} &= \mathcal{L}_{\text{KG}} + \mathcal{L}_{\text{CF}} + \lambda \|\Theta\|_2^2 \end{aligned}$$

# Experiments

**Table 2: Overall Performance Comparison.**

	Amazon-Book		Last-FM		Yelp2018	
	recall	ndcg	recall	ndcg	recall	ndcg
FM	0.1345	0.0886	0.0778	0.1181	0.0627	0.0768
NFM	<b>0.1366</b>	0.0913	<b>0.0829</b>	0.1214	0.0660	0.0810
CKE	0.1343	0.0885	0.0736	0.1184	0.0657	0.0805
CFKG	0.1142	0.0770	0.0723	0.1143	0.0522	0.0644
MCTRec	0.1113	0.0783	-	-	-	-
RippleNet	0.1336	0.0910	0.0791	0.1238	<b>0.0664</b>	<b>0.0822</b>
GC-MC	0.1316	0.0874	0.0818	<b>0.1253</b>	0.0659	0.0790
KGAT	<b>0.1489*</b>	<b>0.1006*</b>	<b>0.0870*</b>	<b>0.1325*</b>	<b>0.0712*</b>	<b>0.0867*</b>
%Improv.	8.95%	10.05%	4.93%	5.77%	7.18%	5.54%

**Table 3: Effect of embedding propagation layer numbers ( $L$ ).**

	Amazon-Book		Last-FM		Yelp2018	
	recall	ndcg	recall	ndcg	recall	ndcg
KGAT-1	0.1393	0.0948	0.0834	0.1286	0.0693	0.0848
KGAT-2	0.1464	0.1002	0.0863	0.1318	0.0714	<b>0.0872</b>
KGAT-3	0.1489	0.1006	0.0870	0.1325	0.0712	0.0867
KGAT-4	<b>0.1503</b>	<b>0.1015</b>	<b>0.0871</b>	<b>0.1329</b>	<b>0.0722</b>	0.0871

# Experiments

## Better Performance in Sparse Recommendation

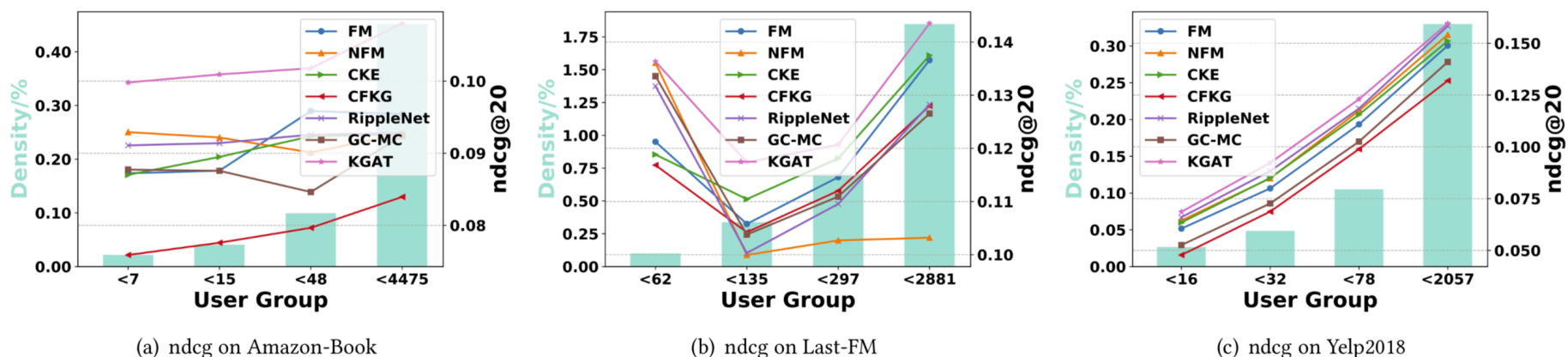
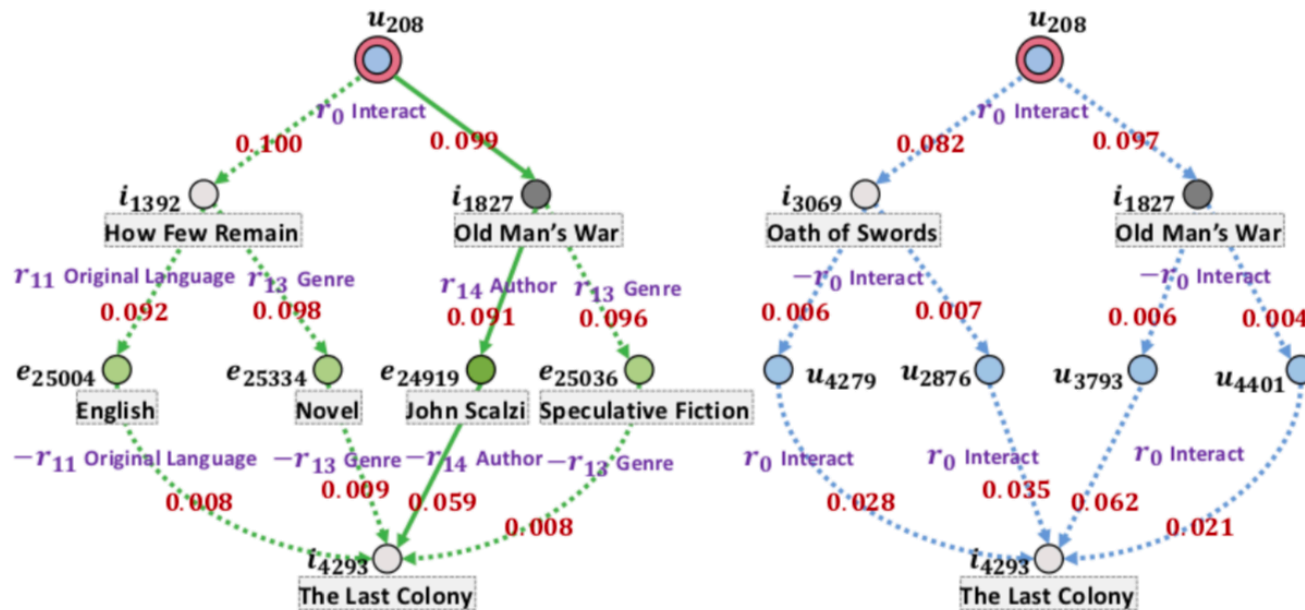


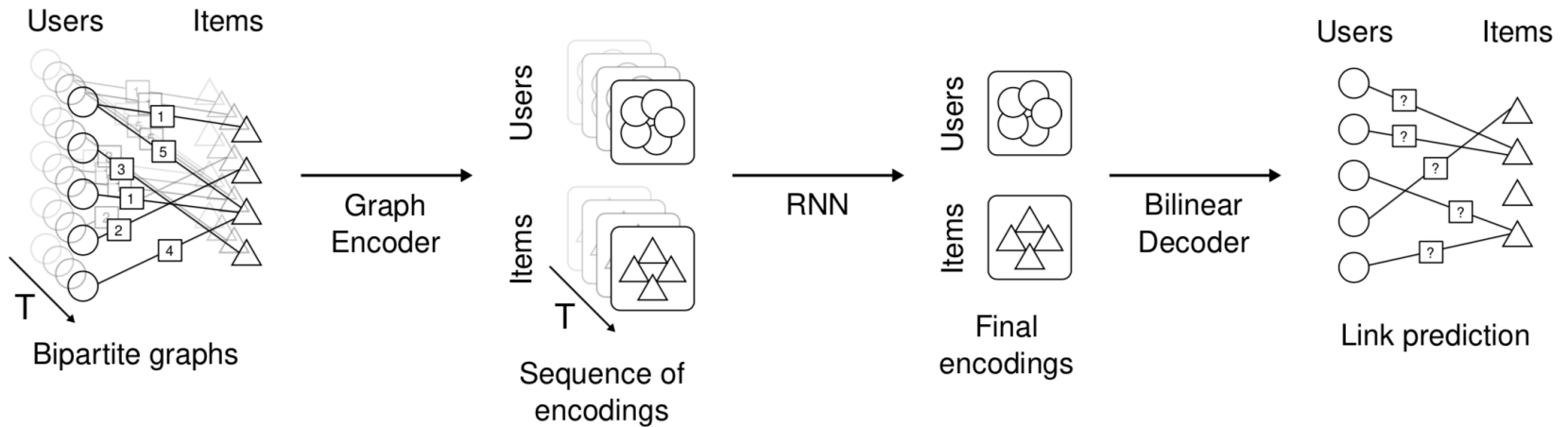
Figure 3: Performance comparison over the sparsity distribution of user groups on different datasets. The background histograms indicate the density of each user group; meanwhile, the lines demonstrate the performance *w.r.t.* ndcg@20.

# Experiments

Case study: Explainability



# GNN in User-Item Bipartite Graph (GCMC)



- Regard the sequential recommendation as a dynamic graph link prediction problem
- Use GCN as graph information aggregator:

$$\mathbf{h}_{u_i} = \xi \left( \text{accum}_{r \in \mathcal{R}} \left\{ \sum_{j \in \mathcal{N}_{i,r}} \frac{1}{c_{ij}} W_r \mathbf{x}_{v_j} \right\} \right),$$

$$\mathbf{z}_{u_i} = \xi(W \mathbf{h}_{u_i}),$$

# GNN in User-Item Bipartite Graph (SCoRe)

- Traditional CF models:
  - No sequential dynamics
  - Collaborative information is used in an implicit manner
- Sequential recommendation models:
  - Just use user-side temporal dynamics
  - Ignorance of collaborative information
- Sequential incremental graph models:
  - Lack of high-order propagation
  - Graph aggregator is simple and not effective enough
- Sequential Collaborative Recommender:
  - Spatial: uses collaborative information explicitly by exploiting high-order relations
  - Temporal: models both user- and item-side temporal dynamics

# GNN in User-Item Bipartite Graph (SCoRe)

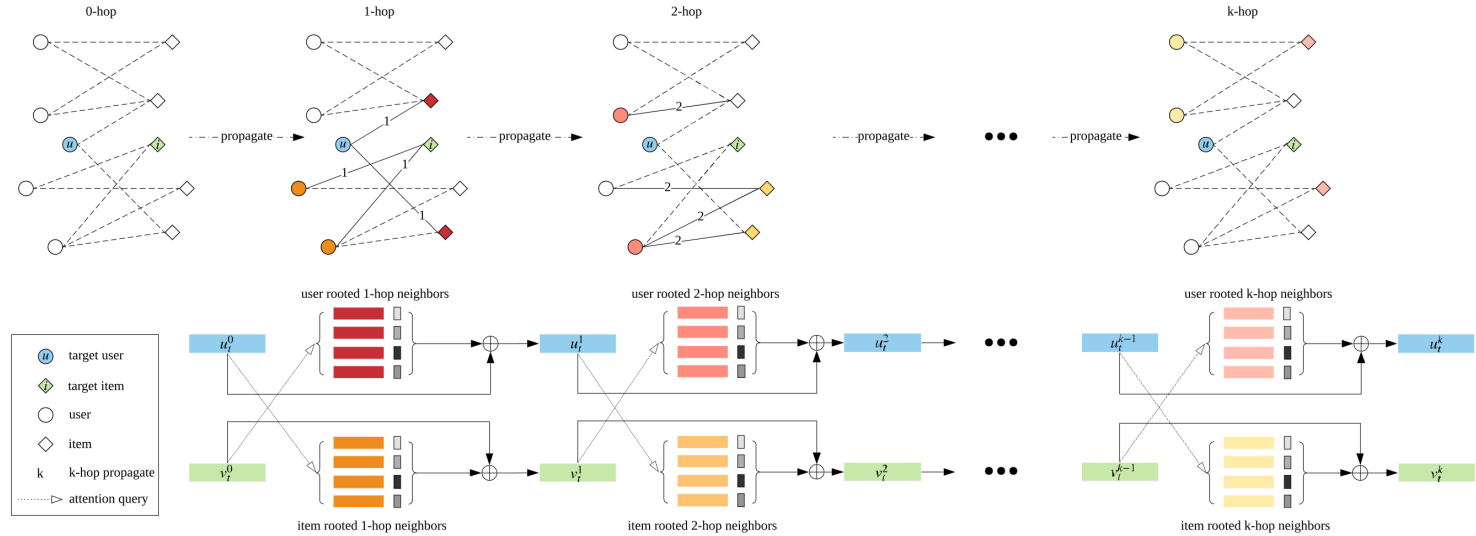


Figure 2: Multi-hop Co-Attention Graph Network calculation process.

- Co-Attention Graph Network to aggregate high-order spatial information:

$$\mathbf{u}_t^k = \mathbf{u}_t^{k-1} + \sum_i \alpha_{ui}^k \mathbf{e}_i^k$$

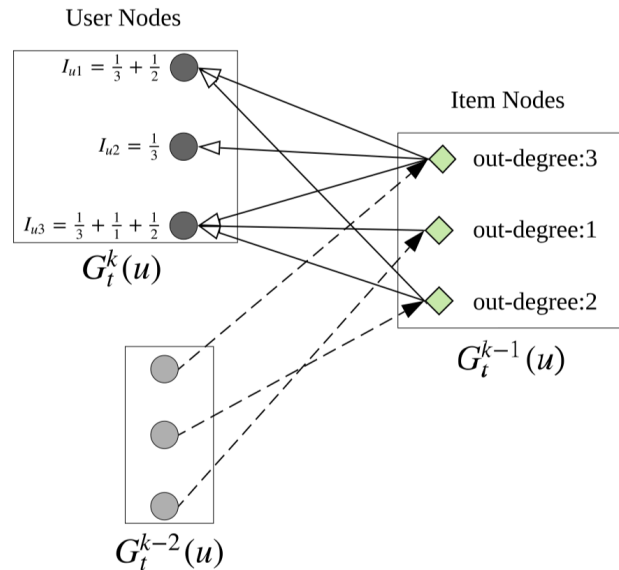
$$\mathbf{v}_t^k = \mathbf{v}_t^{k-1} + \sum_i \alpha_{vi}^k \mathbf{e}_i^k$$

$$\alpha_{ui} = \frac{\exp(\text{LeakyReLU}(\mathbf{a}^T [\mathbf{W} \mathbf{e}_i^k || \mathbf{W} \mathbf{v}_t^{k-1}]))}{\sum_{\mathbf{e}_j^k \in G^k(u)} \exp(\text{LeakyReLU}(\mathbf{a}^T [\mathbf{W} \mathbf{e}_j^k || \mathbf{W} \mathbf{v}_t^{k-1}]))}$$

$$\alpha_{vi} = \frac{\exp(\text{LeakyReLU}(\mathbf{a}^T [\mathbf{W} \mathbf{e}_i^k || \mathbf{W} \mathbf{u}_t^{k-1}]))}{\sum_{\mathbf{e}_j^k \in G^k(v)} \exp(\text{LeakyReLU}(\mathbf{a}^T [\mathbf{W} \mathbf{e}_j^k || \mathbf{W} \mathbf{u}_t^{k-1}]))}$$

# GNN in User-Item Bipartite Graph (SCoRe)

- Importance Sampling Strategy to reduce noise:

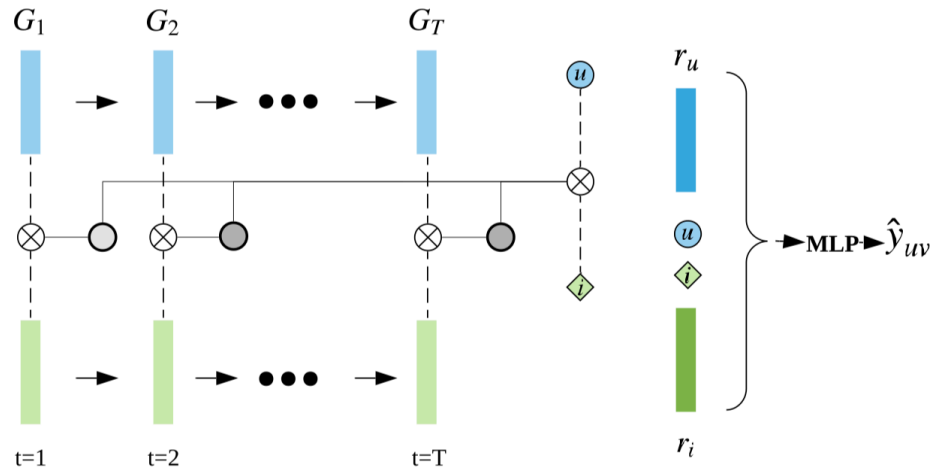


$$I_p = \sum_{q \in \text{pre}(p)} \frac{1}{\text{out-degree}(q)}$$

$$\text{Pr}_p = \frac{\exp(I_p)}{\sum_{n \in G_t^k(u)} \exp(I_n)}.$$

# GNN in User-Item Bipartite Graph (SCoRe)

- Temporal Interactive Dual Sequence Modeling:



$$relation_t = \sigma(Q_2(\sigma(Q_1((h_t^u \odot h_t^v) || (u \odot v))))))$$

$$\beta_t = \frac{\exp(relation_t)}{\sum_{i=1}^T \exp(relation_i)}$$

$$r_u = \sum_{t=1}^T \beta_t h_t^u, r_v = \sum_{t=1}^T \beta_t h_t^v$$

# Experiments

Dataset	Metric	Group 1		Group 2			Group 3		
		SVD++	DELFL	GRU4Rec	Caser	SASRec	RRN	GCMC	SCoRe
CCMR	HR@1	0.2378	0.6536	0.6703	0.6777	<u>0.6979</u>	0.6633	0.6591	<b>0.7001</b>
	HR@5	0.4288	0.9087	0.8911	0.8907	0.9047	0.903	<u>0.9063</u>	<b>0.9118</b>
	HR@10	0.5462	0.9586	0.9268	0.9184	0.9361	0.9469	<u>0.9508</u>	<b>0.9583</b>
	NDCG@5	0.3356	0.7919	0.7917	0.7954	<u>0.8123</u>	0.7957	0.7946	<b>0.8161</b>
	NDCG@10	0.3735	0.8084	0.8034	0.8045	<u>0.8226</u>	0.8101	0.8092	<b>0.8281</b>
	MRR	0.3375	0.7617	0.7662	0.7699	<u>0.7878</u>	0.7681	0.7652	<b>0.7913</b>
Tmall	HR@1	0.1229	0.2001	0.1979	0.2029	0.3312	0.4177	<u>0.4254</u>	<b>0.4764</b>
	HR@5	0.3098	0.3765	0.3818	0.4037	0.6307	<u>0.6452</u>	0.6449	<b>0.6806</b>
	HR@10	0.3438	0.4573	0.4713	0.4925	0.7072	0.7449	<u>0.7512</u>	<b>0.7632</b>
	NDCG@5	0.2112	0.2975	0.2947	0.3089	0.4935	0.5368	<u>0.5403</u>	<b>0.5842</b>
	NDCG@10	0.2342	0.3130	0.3236	0.3376	0.5184	0.5691	<u>0.5747</u>	<b>0.6109</b>
	MRR	0.1373	0.2990	0.2950	0.3058	0.4676	0.5257	<u>0.5314</u>	<b>0.5734</b>
Taobao	HR@1	0.0705	0.1299	0.1117	0.1292	0.1897	0.2138	<u>0.2164</u>	<b>0.2431</b>
	HR@5	0.1539	0.2999	0.3001	0.3022	0.3871	<u>0.4695</u>	0.4672	<b>0.4991</b>
	HR@10	0.2063	0.4656	0.4395	0.4539	0.5331	<u>0.6213</u>	0.6156	<b>0.6467</b>
	NDCG@5	0.0998	0.1719	0.1667	0.1724	0.2512	0.3447	<u>0.3449</u>	<b>0.3590</b>
	NDCG@10	0.1082	0.2008	0.1995	0.2013	0.2788	<u>0.3937</u>	0.3929	<b>0.4112</b>
	MRR	0.0935	0.1203	0.1119	0.1232	0.2198	0.3402	<u>0.3411</u>	<b>0.3786</b>

# Experiments

**Table 5: Performance comparison on different size of user/item-rooted interaction set.**

Dataset	Metric	Size of Interaction Set			
		5	10	15	20
CCMR	HR@10	<b>0.9583</b>	0.9555	0.9498	0.9423
	NDCG@10	<b>0.8281</b>	0.8239	0.8232	0.8221
	MRR	<b>0.7913</b>	0.7909	0.7895	0.7829
Tmall	HR@10	0.7589	<b>0.7632</b>	0.7619	0.7607
	NDCG@10	0.6091	<b>0.6109</b>	0.6087	0.6052
	MRR	0.5658	<b>0.5734</b>	0.5698	0.5611
Taobao	HR@10	0.6288	<b>0.6467</b>	0.6319	0.6299
	NDCG@10	0.4068	<b>0.4112</b>	0.4081	0.4027
	MRR	0.3679	<b>0.3786</b>	0.3673	0.3648

**Table 6: Performance comparison of ablation study**

Dataset	Metric	models				
		RIA	Single-hop	GAT	RS	SCoRe
CCMR	HR@10	0.9509	0.9296	0.9358	0.9452	<b>0.9583</b>
	NDCG@10	0.8157	0.8011	0.8104	0.8217	<b>0.8281</b>
	MRR	0.7741	0.7621	0.7724	0.7841	<b>0.7913</b>
Tmall	HR@10	0.7620	0.7632	0.7287	0.7431	<b>0.7632</b>
	NDCG@10	0.5893	0.6029	0.5866	0.6032	<b>0.6109</b>
	MRR	0.5567	0.5633	0.5543	0.5662	<b>0.5734</b>
Taobao	HR@10	0.6216	0.6172	0.6201	0.6212	<b>0.6467</b>
	NDCG@10	0.4001	0.3991	0.4017	0.4015	<b>0.4112</b>
	MRR	0.3575	0.3456	0.3498	0.3523	<b>0.3786</b>

# Experiments

