Collaborative Filtering : From a Deep Learning Perspective

2025-07-31

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DMAIS

INDEX

- Recommender System
- Collaborative Filtering
- NeuMF
- VAE for CF
- LightGCN

Recommender system

Too Much Information

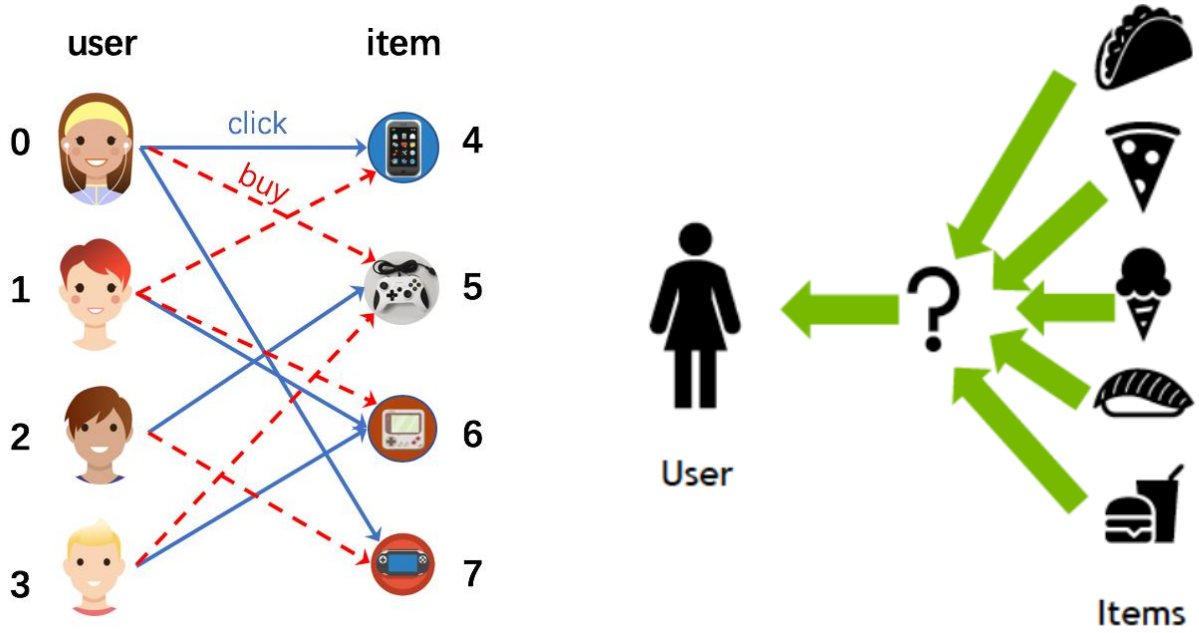
- So many options in the modern world
- We don’t have time to serf through everything

https://about.netflix.com/ko/news/continuing-our-games-journey
https://pixabay.com/ko/illustrations/youtube-%EC%8B%AC%EB%B2%8C-%EB%A7%88%ED%81%AC-5702765/
https://kr.freepik.com/free-photos-vectors/logo-amazon
https://medium.com/swlh/news-recommendation-system-a8efde3cb233 | https://insidebe.com/articles/choice-overload/

Recommender system

Need for Recommender System

- ☐ Variety of external data (e.g., click history, user social network, item meta data)
- ☐ Use them to predict user's preference

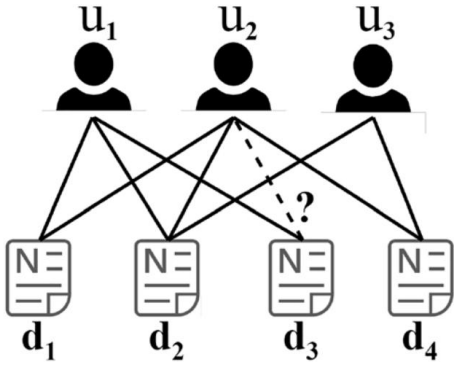


https://mdnice.com/writing/723f6890dd974898a1609ceaefe4ef1d
https://www.nvidia.com/en-us/glossary/recommendation-system/

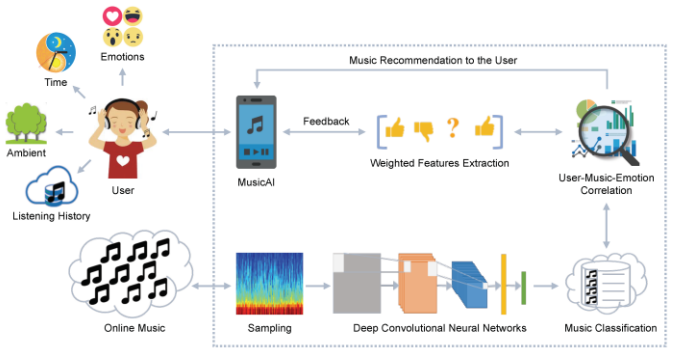
Recommender system

Recommender Systems In the Real-World

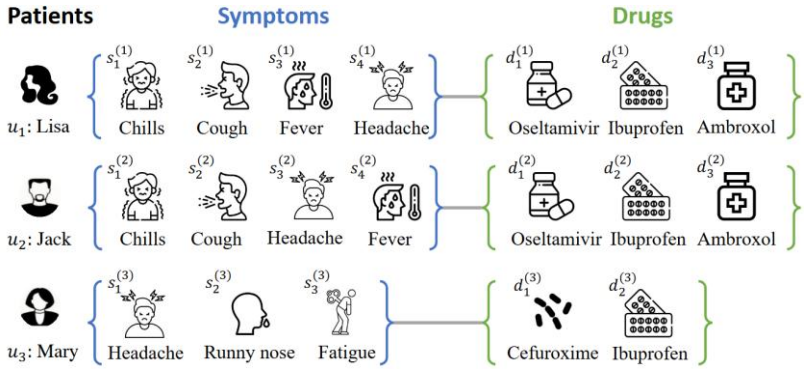
- **Core objective** : automatically recommend **items** to **users** based on data
- Applicable to various real-world problems



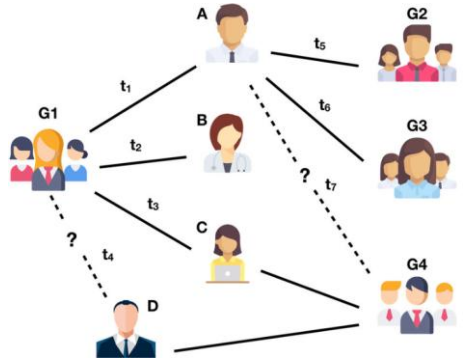
Personalized news recommendation



Personalized music recommendation



Set-to-set drug recommendation



Social network recommendation

Meng, Xiangfu, et al. "A survey of personalized news recommendation." *Data Science and Engineering* 8.4 (2023): 396-416..
Abdul, Ashu, et al. "An emotion-aware personalized music recommendation system using a convolutional neural networks approach." *Applied Sciences* 8.7 (2018): 1103.
Tan, Yanchao, et al. "4sdrug: Symptom-based set-to-set small and safe drug recommendation." *Proceedings of the 28th ACM SIGKDD Conference on Knowledge Discovery and Data Mining*. 2022.
Sha, Hao, Mohammad Al Hasan, and George Mohler. "Group link prediction using conditional variational autoencoder." *Proceedings of the International AAAI Conference on Web and Social Media*. Vol. 15. 2021.

Recommender system

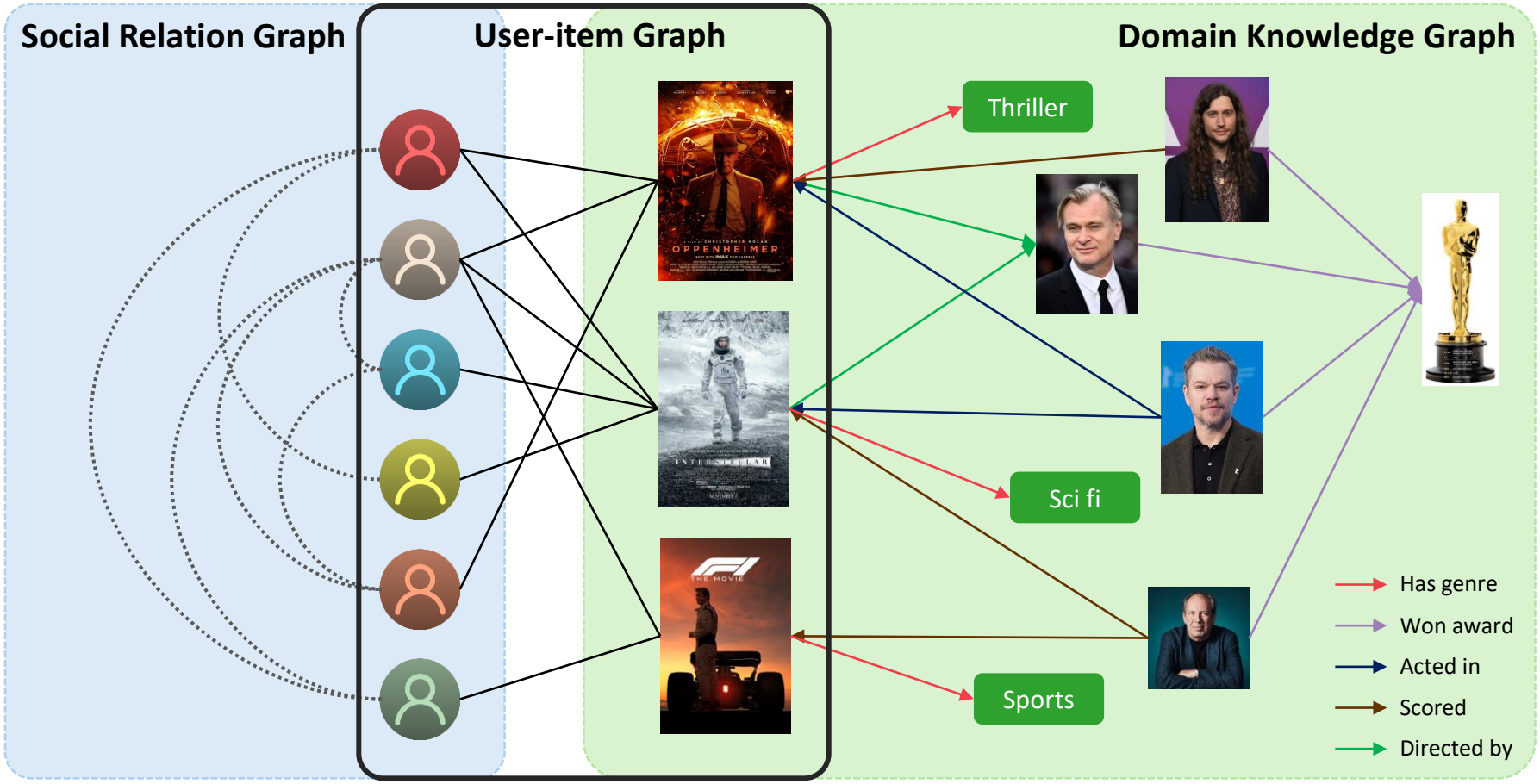
How Can We Approach This?

Content based filtering

Collaborative filtering

Hybrid recommendation

etc.



Recommender system

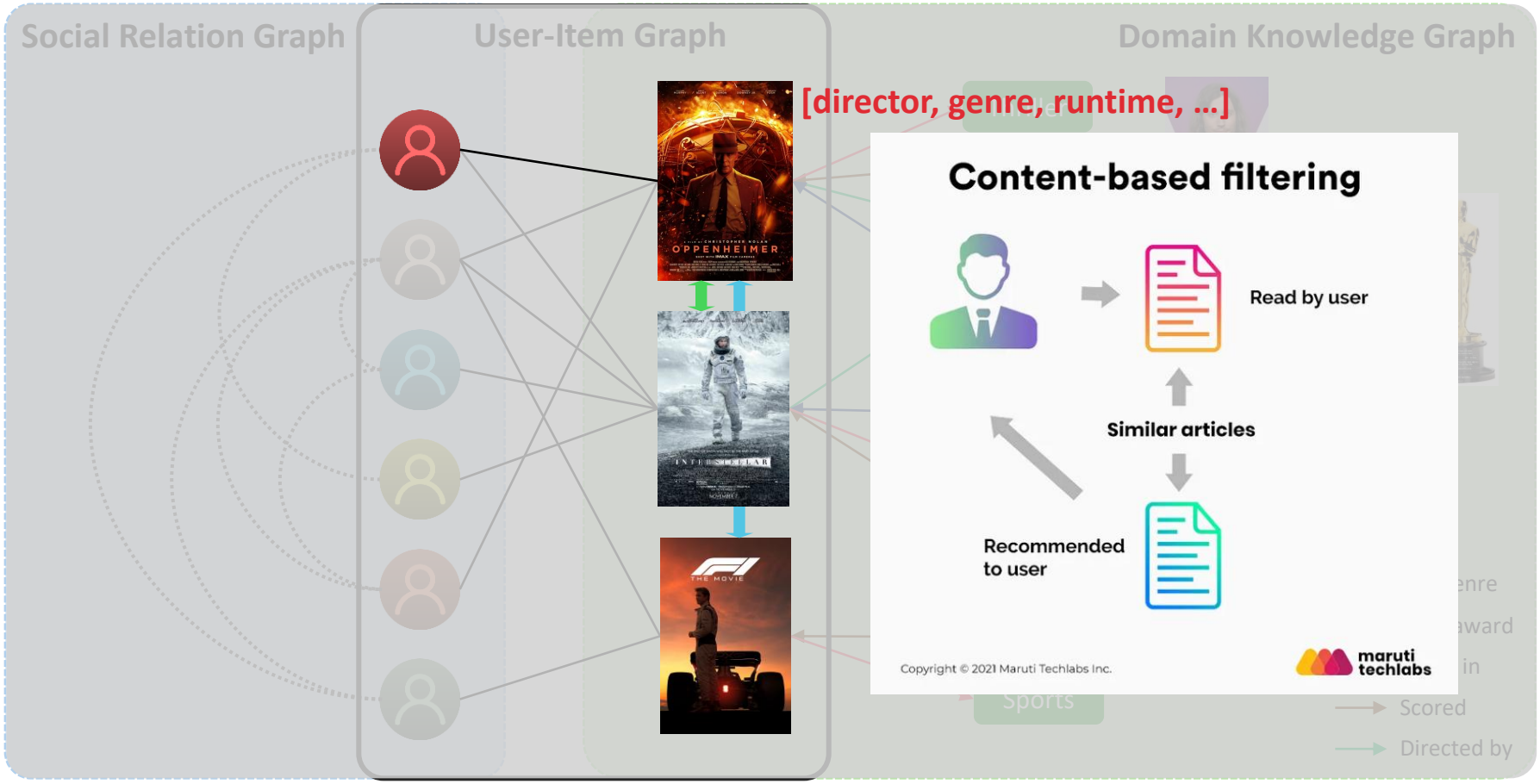
How Can We Approach This?

Content based filtering

Collaborative filtering

Hybrid recommendation

etc.



Recommender system

How Can We Approach This?

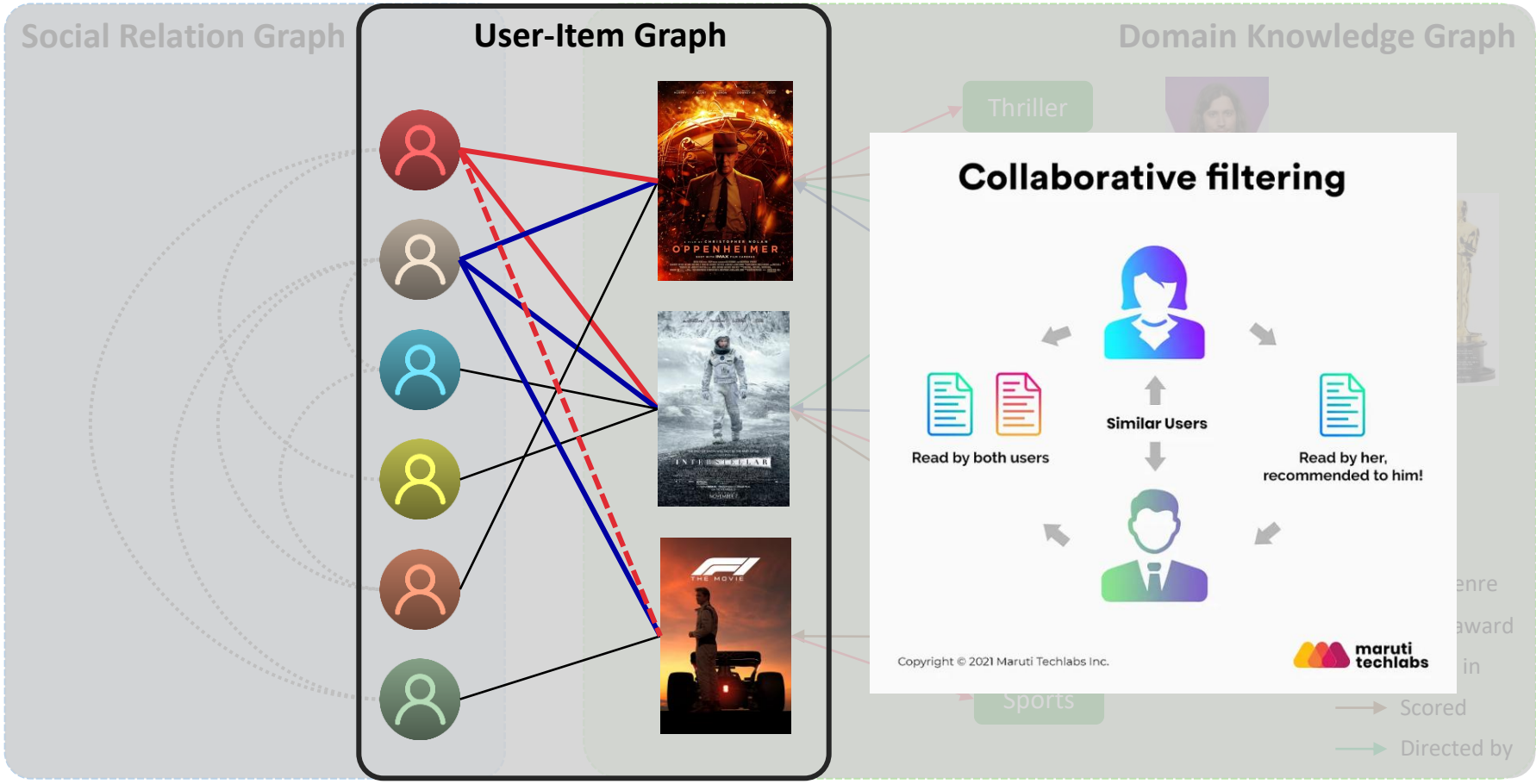
Content based filtering

Collaborative filtering

Hybrid recommendation

etc.

Bipartite graph



Recommender system

How Can We Approach This?

Content based filtering

Collaborative filtering

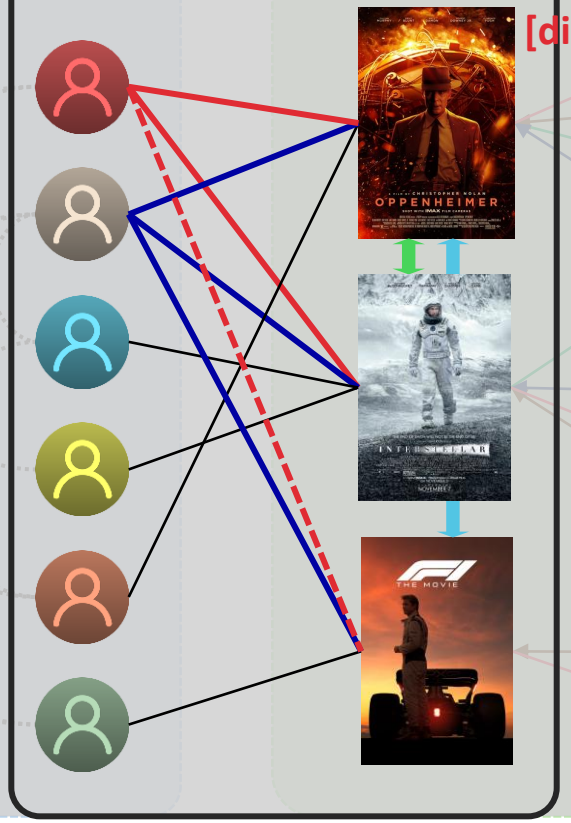
Hybrid recommendation

etc.

Bipartite graph

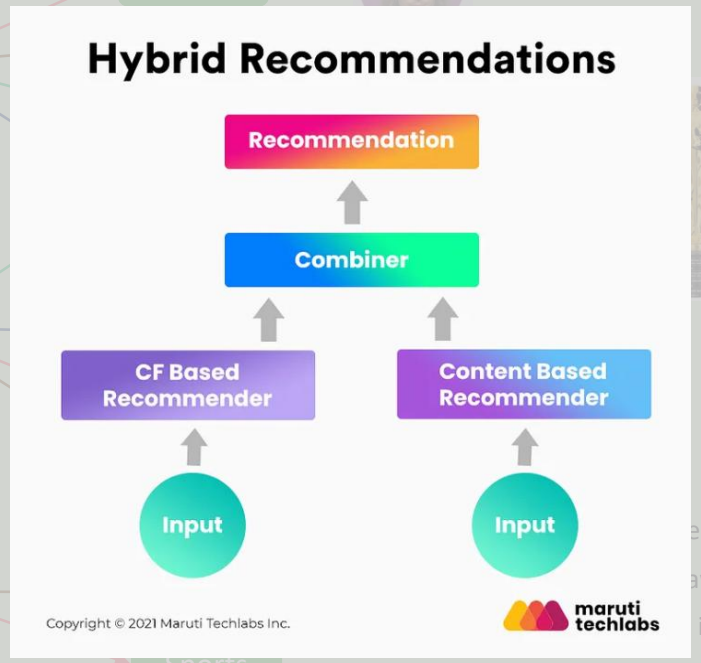
Social Relation Graph

User-Item Graph



Domain Knowledge Graph

[director, genre, runtime, …]



Scored

Directed by

Recommender system

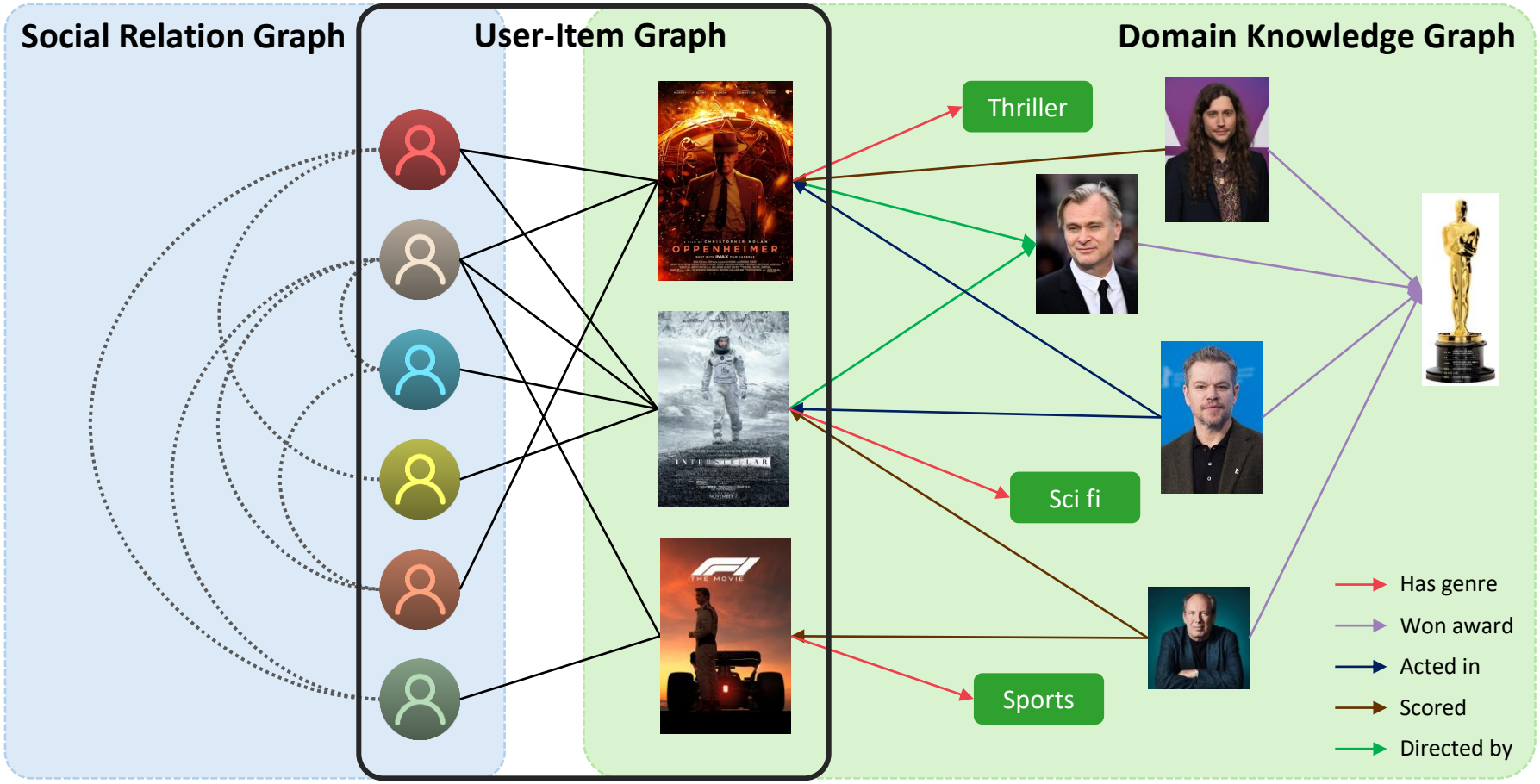
How Can We Approach This?

Content based filtering

Collaborative filtering

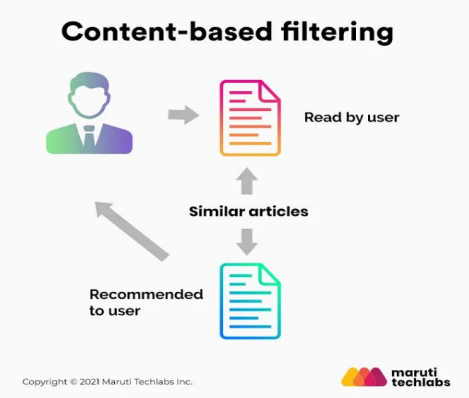
Hybrid recommendation

etc.



Collaborative Filtering

Why Collaborative Filtering (CF)?



Pros

- No external user data needed
- System easy to scale
- Relatively good at cold start

Cons

- Requires good feature constructions
- Can’t capture complex patterns across users

Pros

- No need for domain-specific features
- Find patterns directly from user behavior
- **Only requires user-item interaction matrix**

Cons

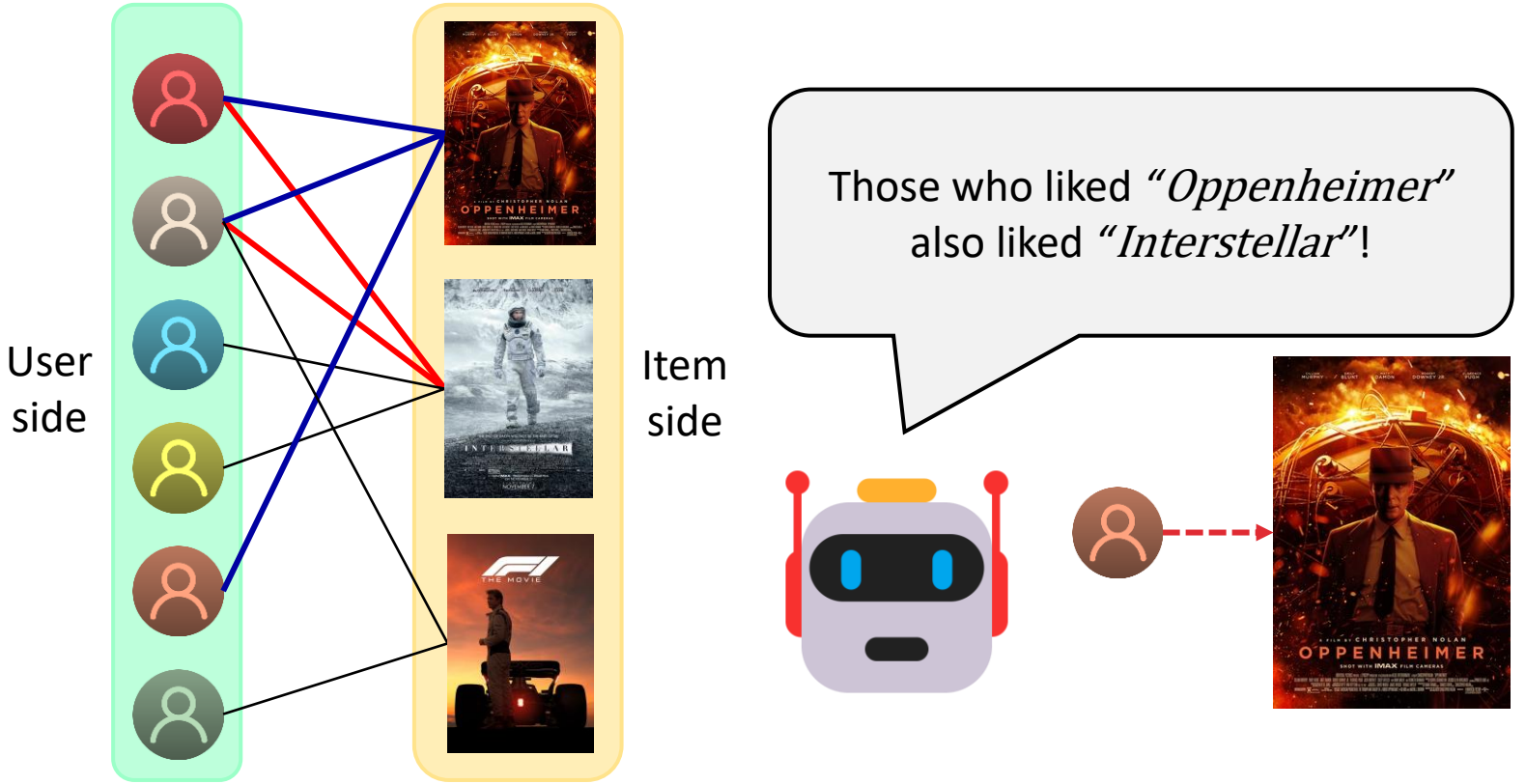
- Relatively struggles at cold start
- Scalability issues

Let’s focus on collaborative filtering!

Collaborative Filtering

Generalized Flow of CF

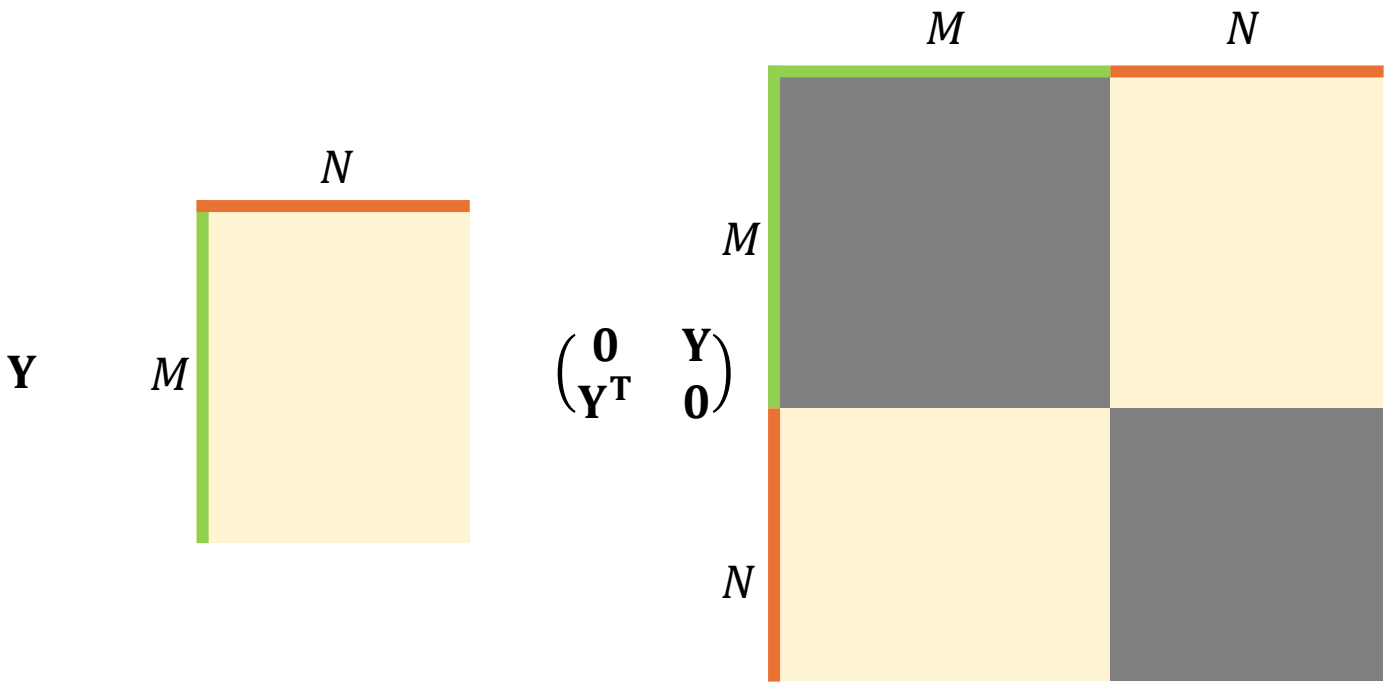
- Collaborative (**users influence each other**) filtering (**recommend items**)
- Underlying graph = bipartite graph, link = rating (e.g., 1 to 5) or interaction (e.g., 0 or 1)



Collaborative Filtering

Preliminaries : Notations

- User ($u \in U, |U| = M$), item ($i \in I, |I| = N$)
- User-item graph ($\mathbf{Y} \in \mathbb{R}^{M \times N}$)
- Binarized rating matrix = click matrix → **implicit feedback**



Collaborative Filtering

Preliminaries : Metrics

- Recall@K

$$\frac{\#of\ relevant\ items\ in\ top-K}{Total\ \#\ of\ relevant\ items}$$

- NDCG@K

$$normalize(\sum_{i=1}^{K}\frac{rel_i}{\log_2(i+1)})$$

- HR@K

$$\mathbb{I}[rank \leq K]$$

NeuMF

- ☐ Matrix Factorization
- ☐ General Framework
- ☐ Three Models
- ☐ Experiments
- ☐ Conclusion

Neural Collaborative Filtering*

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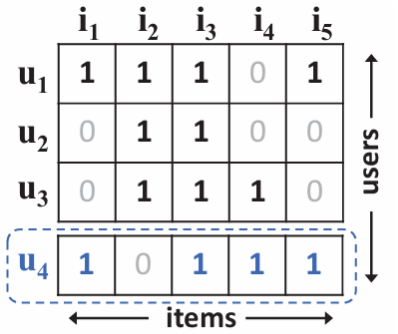
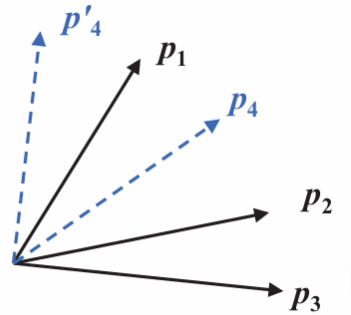
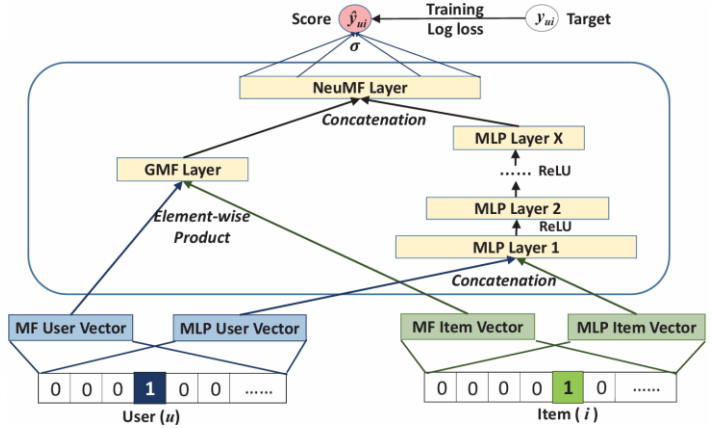


(a) user–item matrix



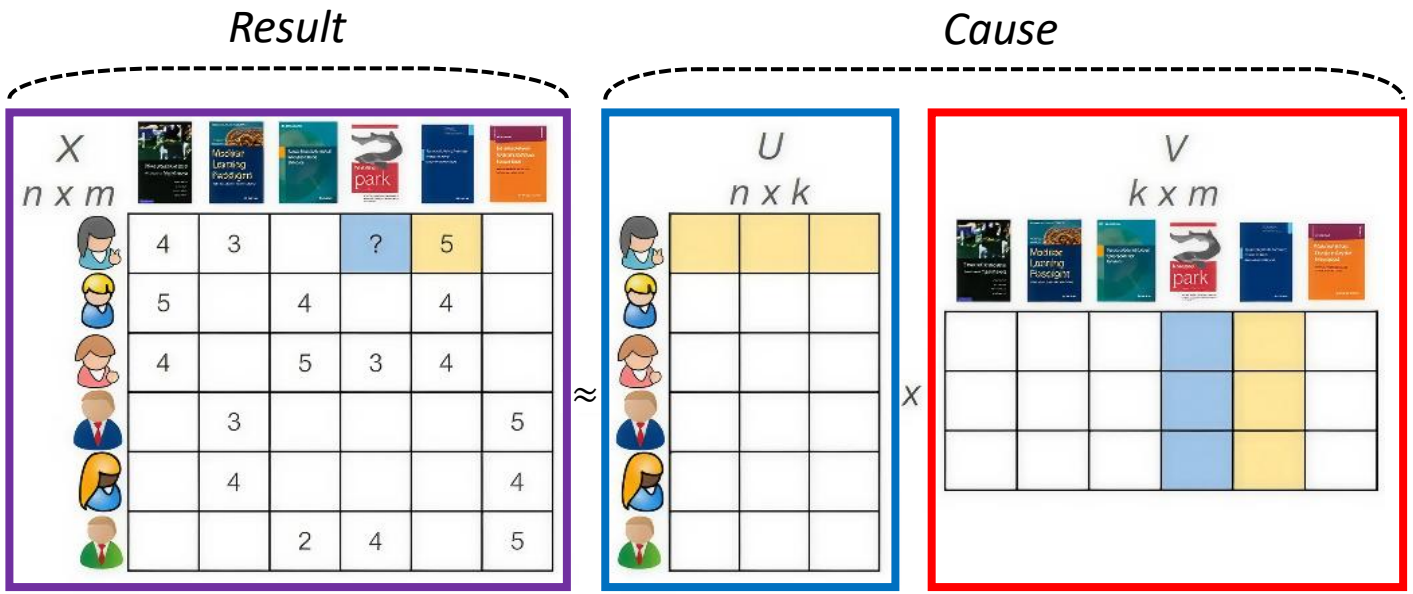
(b) user latent space

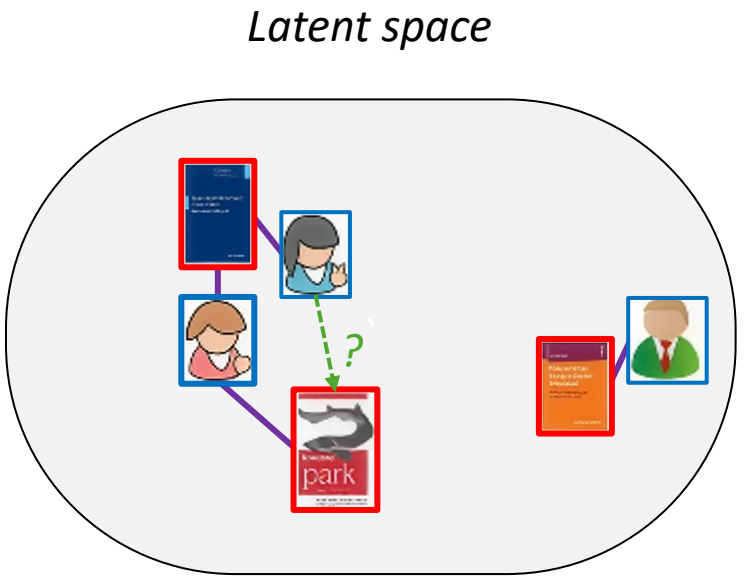


NeuMF / Matrix Factorization

Matrix Factorization : ‘De facto’ Approach of CF

- ☐ User-item matrix as explicit/implicit data
- ☐ User-item matrix ≈ user matrix × item matrix
- ☐ Modeling the cause for new recommendations





NeuMF / Matrix Factorization

ML with MF

- Objective : real rating(r_{ui}) ≈ predicted rating($\hat{r}_{ui}$)
- Inner product of user($\mathbf{p_u}$) and item($\mathbf{q_i}$) directly used for prediction
- Handcrafting all the features

$$\hat{r}_{ui} = \mu + b_u + b_i + \mathbf{p}_u^\top \mathbf{q}_i$$

Key Limitations

- (1) Inherent limitation of ML's **feature engineering**
- (2) Independency between features → prediction is a simple **linear combination**

$$\min_{\mathbf{p}_*,\mathbf{q}_*,b_*,\mathbf{v}_*} \sum_{(u,i)\in\mathcal{K}} (r_{ui}-\hat{r}_{ui})^2 + \lambda_1\left(\|\mathbf{p}_u\|^2+\|\mathbf{q}_i\|^2\right) + \lambda_2\left(b_u^2+b_i^2\right) + \lambda_3 \sum_{n\in N_i}\|\mathbf{v}_n\|^2 \quad (6)$$

$$\min_{\mathbf{p}_*,\mathbf{q}_*,b_*,\mathbf{v}_*,\mathbf{d}_*} \sum_{(u,i)\in\mathcal{K}} (r_{ui}-\hat{r}_{ui})^2 + \lambda_1\left(\|\mathbf{p}_u\|^2+\|\mathbf{q}_i\|^2\right) + \lambda_2\left(b_u^2+b_i^2\right) + \lambda_3\left(\sum_{n\in N_i}\|\mathbf{v}_n\|^2 + \sum_{c\in C_i}\|\mathbf{d}_c\|^2\right) \quad (7)$$

$$\min_{\mathbf{p}_*,\mathbf{q}_*,b_*,\mathbf{v}_*,\mathbf{d}_*} \sum_{(u,i)\in\mathcal{K}} (r_{ui}-\hat{r}_{ui})^2 + \lambda_1\left(\|\mathbf{p}_u\|^2 + \sum_{w\in R_i}\|\mathbf{q}_w\|^2\right) + \lambda_2\left(b_u^2+b_i^2\right) + \lambda_3\left(\sum_{n\in N_i}\|\mathbf{v}_n\|^2 + \sum_{c\in C_i}\|\mathbf{d}_c\|^2\right) \quad (8)$$

$$\min_{\mathbf{p}_*,\mathbf{q}_*,b_*,\mathbf{v}_*,\mathbf{d}_*,\beta_*} \sum_{(u,i)\in\mathcal{K}} (r_{ui}-\hat{r}_{ui})^2 + \lambda_1\left(\|\mathbf{p}_u\|^2 + \sum_{w\in R_i}\|\mathbf{q}_w\|^2\right) + \lambda_2\left(b_u^2+b_i^2+\beta_i^2+\beta_u^2\right) + \lambda_3\left(\sum_{n\in N_i}\|\mathbf{v}_n\|^2 + \sum_{c\in C_i}\|\mathbf{d}_c\|^2\right) \quad (9)$$

Hu, Longke, Aixin Sun, and Yong Liu. "Your neighbors affect your ratings: on geographical neighborhood influence to rating prediction." *Proceedings of the 37th international ACM SIGIR conference on Research & development in information retrieval*. 2014.

NeuMF / Matrix Factorization

Lack of Expressiveness

- ☐ WLOG, MF needs to recover similarity between two users (Jaccard Coefficient)
- ☐ Position of $\boldsymbol{p}_4$ can't be placed without ranking loss
- ☐ Higher dimension = solution? / Prone to overfit

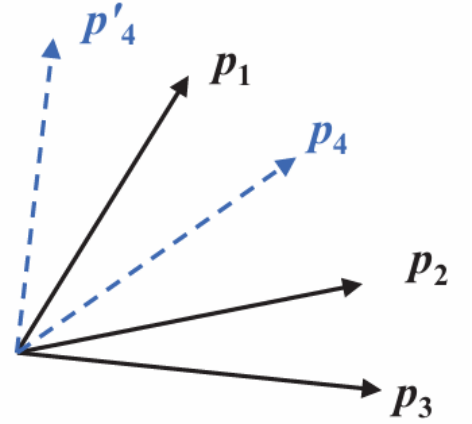
$$s_{ij} = \frac{|\mathcal{R}_i| \cap |\mathcal{R}_j|}{|\mathcal{R}_i| \cup |\mathcal{R}_j|} = \frac{\boldsymbol{AND}}{\boldsymbol{OR}}$$

	i_1	i_2	i_3	i_4	i_5
u_1	1	1	1	0	1
u_2	0	1	1	0	0
u_3	0	1	1	1	0
u_4	1	0	1	1	1

users

items

(a) user–item matrix



(b) user latent space

$$s_{23}(0.66) > s_{12}(0.5) > s_{13}(0.4)$$

Consider user 4

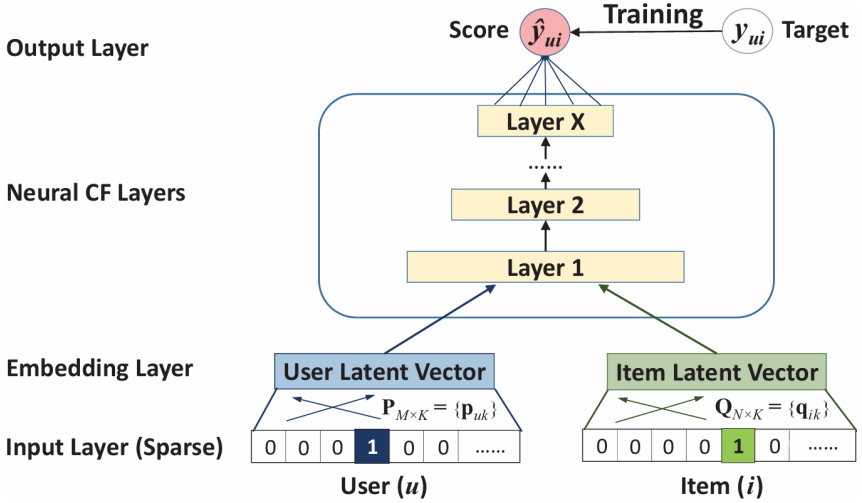
$$s_{41}(0.6) > s_{43}(0.4) > s_{42}(0.2)$$

NeuMF / General Framework

NCF's Predictive Model

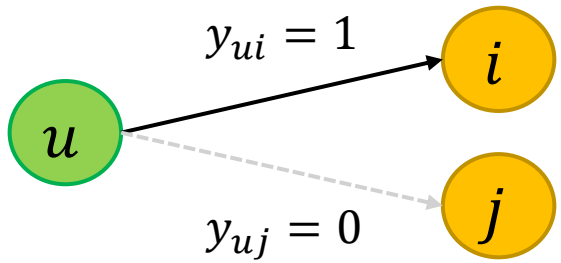
$$\hat{y}_{ui} = f(\mathbf{P}^T \mathbf{v}_u^U, \mathbf{Q}^T \mathbf{v}_i^I | \mathbf{P}, \mathbf{Q}, \Theta_f)$$

$$f(\mathbf{P}^T \mathbf{v}_u^U, \mathbf{Q}^T \mathbf{v}_i^I) = \phi_{out}(\phi_X(...\phi_2(\phi_1(\mathbf{P}^T \mathbf{v}_u^U, \mathbf{Q}^T \mathbf{v}_i^I))...))$$



Learning Objective for NCF

☐ Focus is on NN modeling → **consider only pointwise learning**



Pointwise : $\underset{\mathbf{P}, \mathbf{Q}, \Theta_f}{argmin} \ |y_{ui} - \hat{y}_{ui}|$

Pairwise : $\underset{\mathbf{P}, \mathbf{Q}, \Theta_f}{argmax} \ (\hat{y}_{ui} - \hat{y}_{uj})$

* The objective terms of argmin and argmax are abstract and can vary depending on the situation.

NeuMF / General Framework

Pointwise Learning NCF

- Assuming Gaussian distribution, existing methods used regression + squared loss
- However, recommendation is about recommend (1) or not (0) problem

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

⇩ *Binary cross entropy problem!*

$$L = -\sum_{(u,i) \in \mathcal{Y}} \log \hat{y}_{ui} - \sum_{(u,j) \in \mathcal{Y}^-} \log(1 - \hat{y}_{uj})$$

$$= -\sum_{(u,i) \in \mathcal{Y} \cup \mathcal{Y}^-} y_{ui} \log \hat{y}_{ui} + (1 - y_{ui}) \log(1 - \hat{y}_{ui})$$

NeuMF / Three Models

Generalized Matrix Factorization (GMF)

- Single layer ϕ_1 (dot product)
- If $a_{out}(x) = x$ (activation) and $\mathbf{h} = \mathbf{1} \in \mathbb{R}^K$ (edge weights of output layer)

$$\mathbf{p}_u = \mathbf{P}^T \mathbf{v}_u^U \quad \mathbf{q}_i = \mathbf{Q}^T \mathbf{v}_i^I$$

$$\phi_1(\mathbf{p}_u, \mathbf{q}_i) = \mathbf{p}_u \odot \mathbf{q}_i$$

$$\hat{y}_{ui} = a_{out}(\mathbf{h}^T(\mathbf{p}_u \odot \mathbf{q}_i))$$

Generalizes MF methods!

$$\hat{r}_{ui} = \mu + b_u + b_i + \mathbf{p}_u^\top \mathbf{q}_i$$

NeuMF / Three Models

Multi-Layer Perceptron (MLP)

- Concatenate → MLP
- Closer to the output layer, smaller the layer size (abstracting features)

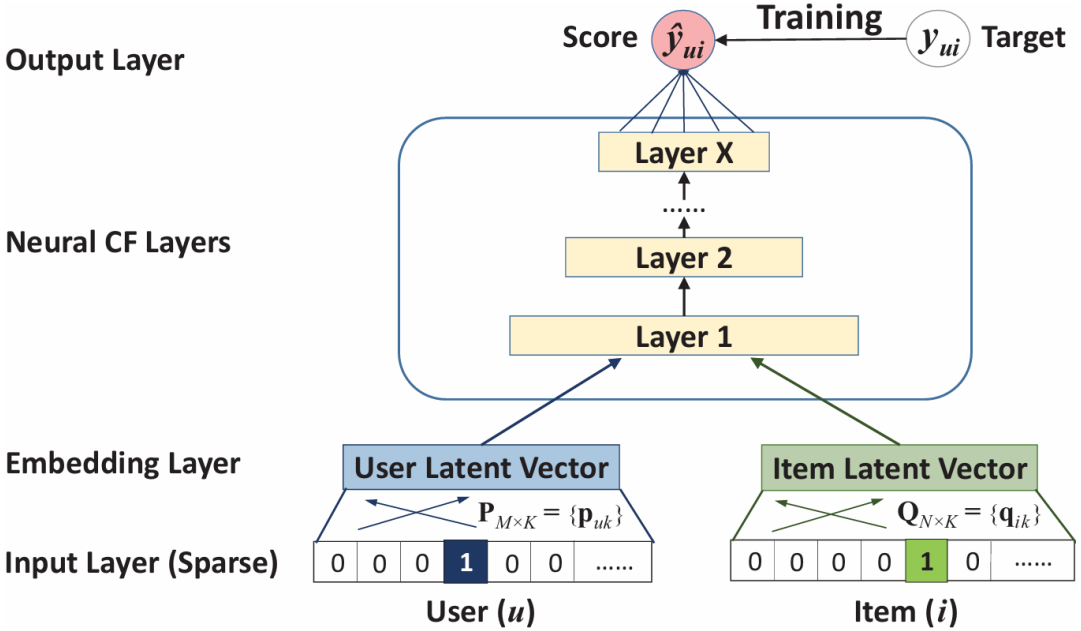
$$\mathbf{z}_1 = \phi_1(\mathbf{p}_u, \mathbf{q}_i) = \begin{bmatrix} \mathbf{p}_u \\ \mathbf{q}_i \end{bmatrix},$$

$$\phi_2(\mathbf{z}_1) = a_2(\mathbf{W}_2^T \mathbf{z}_1 + \mathbf{b}_2),$$

$$\ldots\ldots$$

$$\phi_L(\mathbf{z}_{L-1}) = a_L(\mathbf{W}_L^T \mathbf{z}_{L-1} + \mathbf{b}_L),$$

$$\hat{y}_{ui} = \sigma(\mathbf{h}^T \phi_L(\mathbf{z}_{L-1})),$$



NeuMF / Three Models

Fusion of GMF and MLP (NeuMF)

- Sharing embeddings of GMF and MLP limits the performance
- However, non-convexity of objective function leads to underfitting

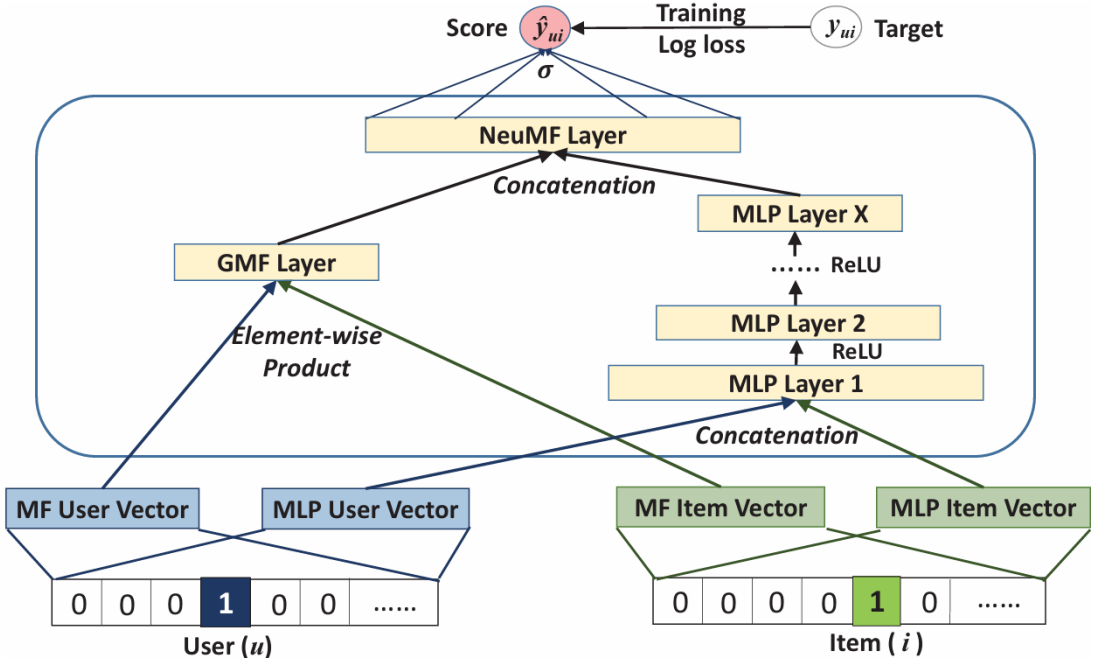
$$\hat{y}_{ui} = \sigma(\mathbf{h}^T a(\mathbf{p}_u \odot \mathbf{q}_i + \mathbf{W}\begin{bmatrix}\mathbf{p}_u \\ \mathbf{q}_i\end{bmatrix} + \mathbf{b}))$$

Manage own embeddings

$$\phi^{GMF} = \mathbf{p}_u^G \odot \mathbf{q}_i^G,$$

$$\phi^{MLP} = a_L(\mathbf{W}_L^T(a_{L-1}(...a_2(\mathbf{W}_2^T\begin{bmatrix}\mathbf{p}_u^M \\ \mathbf{q}_i^M\end{bmatrix} + \mathbf{b}_2)...)) + \mathbf{b}_L),$$

$$\hat{y}_{ui} = \sigma(\mathbf{h}^T\begin{bmatrix}\phi^{GMF} \\ \phi^{MLP}\end{bmatrix}),$$

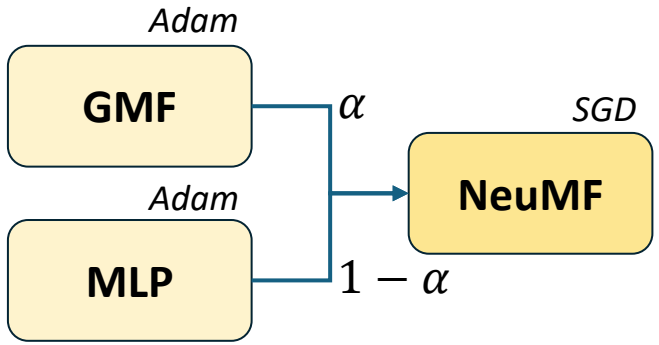


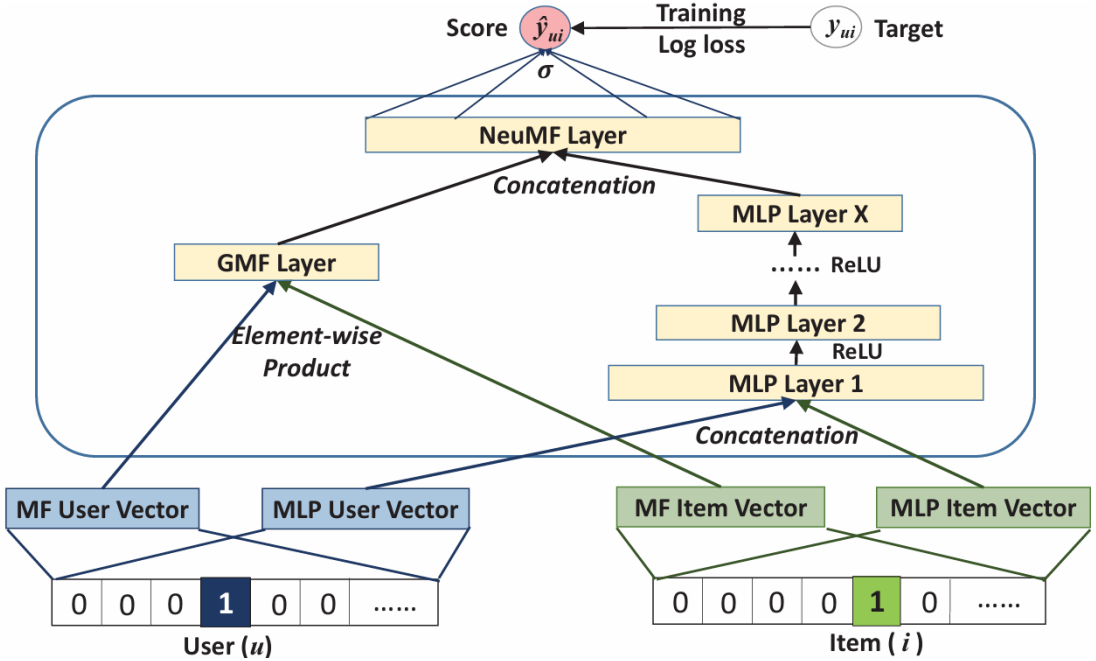
NeuMF / Three Models

Fusion of GMF and MLP (NeuMF) : Pre-Training

- Initialization is important (Erhan et al.) → initialize NeuMF with pretrained GMF and MLP
- Only NeuMF layer is updated

$$\mathbf{h} \leftarrow \begin{bmatrix} \alpha \mathbf{h}^{GMF} \\ (1-\alpha)\mathbf{h}^{MLP} \end{bmatrix}$$





D. Erhan, Y. Bengio, A. Courville, P.-A. Manzagol, P. Vincent, and S. Bengio. Why does unsupervised pre-training help deep learning? Journal of Machine Learning Research, 11:625–660, 2010.

NeuMF / Experiments

Research Questions

- **RQ1** : Do NCF methods outperform SOTA methods?
- **RQ2** : Does the log loss with negative sampling work?
- **RQ3** : Does deep learning help?

Dataset

Dataset	Interaction#	Item#	User#	Sparsity
MovieLens	1,000,209	3,706	6,040	95.53%
Pinterest	1,500,809	9,916	55,187	99.73%

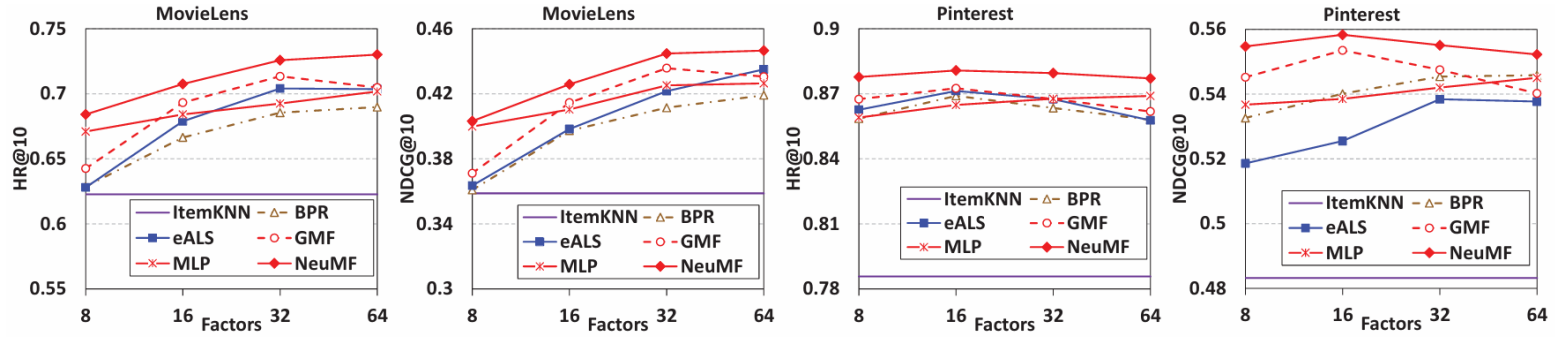
Evaluation Protocol

- User's latest interaction is in the test set
- Rank items : random sample 100 items not interacted by user
- Metrics : HR@K, NDCG@K

NeuMF / Experiments

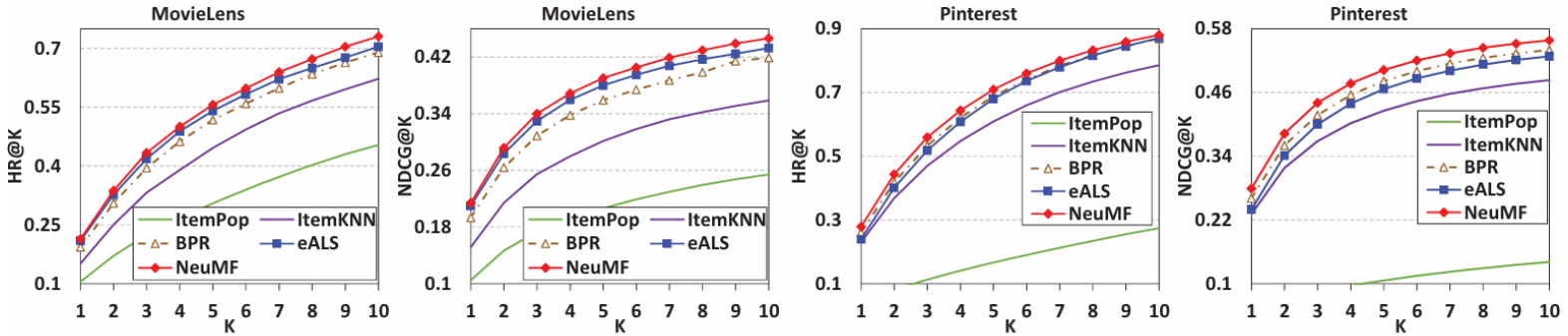
RQ1 : Do NCF Methods Outperform SOTA Methods?

- Predictive factor = last layer's dimension



(a) MovieLens — HR@10 (b) MovieLens — NDCG@10 (c) Pinterest — HR@10 (d) Pinterest — NDCG@10

Figure 4: Performance of HR@10 and NDCG@10 *w.r.t.* the number of predictive factors on the two datasets.



(a) MovieLens — HR@K (b) MovieLens — NDCG@K (c) Pinterest — HR@K (d) Pinterest — NDCG@K

Figure 5: Evaluation of Top-K item recommendation where K ranges from 1 to 10 on the two datasets.

NeuMF / Experiments

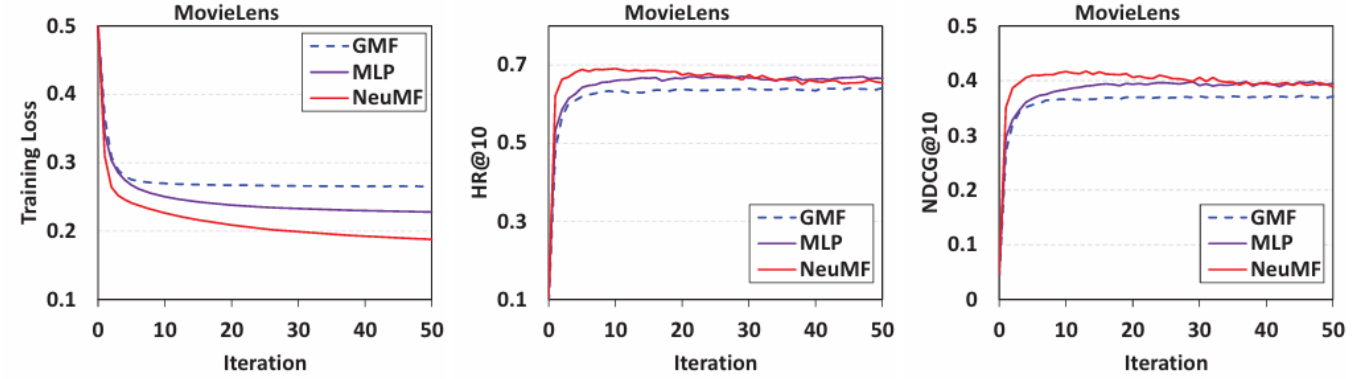
RQ1 : Do NCF Methods Outperform SOTA Methods?

- Affect of pre-training

	With Pre-training		Without Pre-training	
Factors	HR@10	NDCG@10	HR@10	NDCG@10
MovieLens				
8	0.684	0.403	**0.688**	**0.410**
16	**0.707**	**0.426**	0.696	0.420
32	**0.726**	**0.445**	0.701	0.425
64	**0.730**	**0.447**	0.705	0.426
Pinterest				
8	**0.878**	**0.555**	0.869	0.546
16	**0.880**	**0.558**	0.871	0.547
32	**0.879**	**0.555**	0.870	0.549
64	**0.877**	**0.552**	0.872	0.551

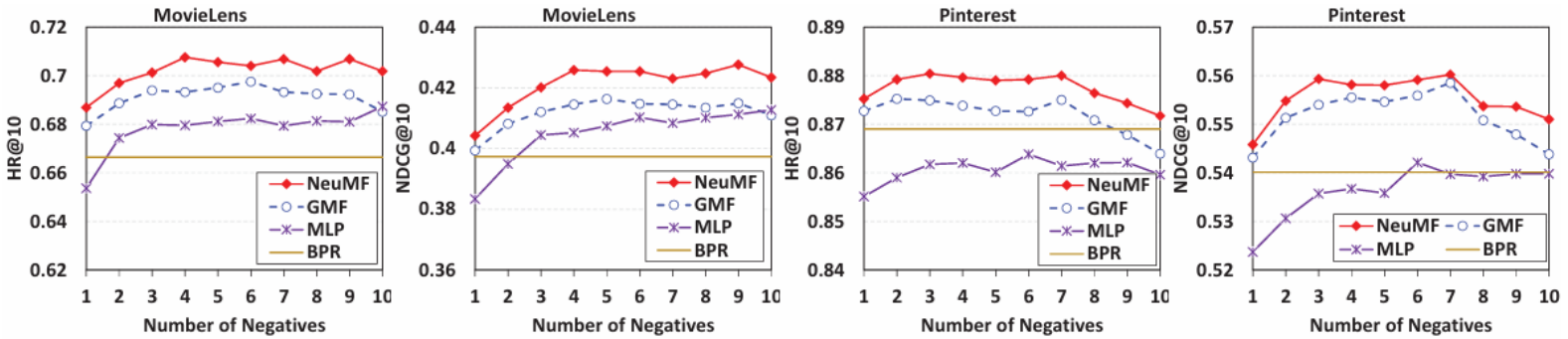
NeuMF / Experiments

RQ2 : Does the Log Loss with Negative Sampling Work?



(a) Training Loss (b) HR@10 (c) NDCG@10

Figure 6: Training loss and recommendation performance of NCF methods *w.r.t.* the number of iterations on MovieLens (factors=8).



(a) MovieLens — HR@10 (b) MovieLens — NDCG@10 (c) Pinterest — HR@10 (d) Pinterest — NDCG@10

Figure 7: Performance of NCF methods *w.r.t.* the number of negative samples per positive instance (factors=16). The performance of BPR is also shown, which samples only one negative instance to pair with a positive instance for learning.

NeuMF / Experiments

RQ3 : Does Deep Learning Help?

- MLP-0 : no hidden layers

Table 3: HR@10 of MLP with different layers.

Factors	MLP-0	MLP-1	MLP-2	MLP-3	MLP-4
MovieLens					
8	0.452	0.628	0.655	0.671	**0.678**
16	0.454	0.663	0.674	0.684	**0.690**
32	0.453	0.682	0.687	0.692	**0.699**
64	0.453	0.687	0.696	0.702	**0.707**
Pinterest					
8	0.275	0.848	0.855	0.859	**0.862**
16	0.274	0.855	0.861	0.865	**0.867**
32	0.273	0.861	0.863	**0.868**	0.867
64	0.274	0.864	0.867	0.869	**0.873**

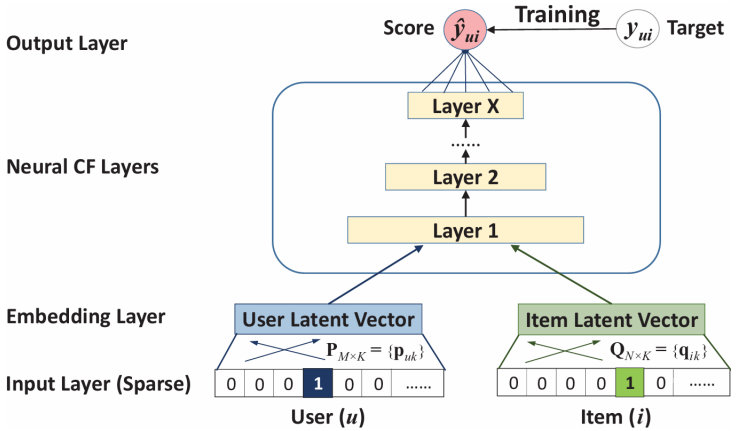
Table 4: NDCG@10 of MLP with different layers.

Factors	MLP-0	MLP-1	MLP-2	MLP-3	MLP-4
MovieLens					
8	0.253	0.359	0.383	0.399	**0.406**
16	0.252	0.391	0.402	0.410	**0.415**
32	0.252	0.406	0.410	**0.425**	0.423
64	0.251	0.409	0.417	0.426	**0.432**
Pinterest					
8	0.141	0.526	0.534	0.536	**0.539**
16	0.141	0.532	0.536	0.538	**0.544**
32	0.142	0.537	0.538	0.542	**0.546**
64	0.141	0.538	0.542	0.545	**0.550**

NeuMF / Conclusion

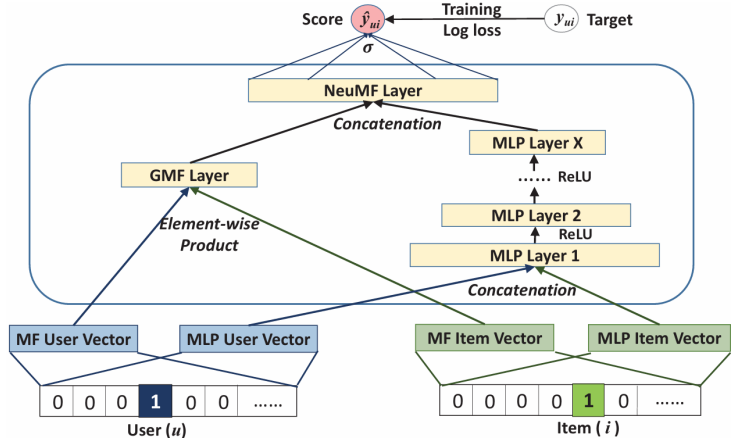
Neural Network into CF

- Proposed general framework NCF
- Generalized MF methods into NCF



NeuMF

- Proved that neural networks can help CF
- Modularized architecture enables greater flexibility and generality



Mult-VAE

- ☐ Non-Linearity for CF
- ☐ VAE for CF
- ☐ ELBO Variant
- ☐ General View of AE
- ☐ Experiments
- ☐ Conclusion

Variational Autoencoders for Collaborative Filtering

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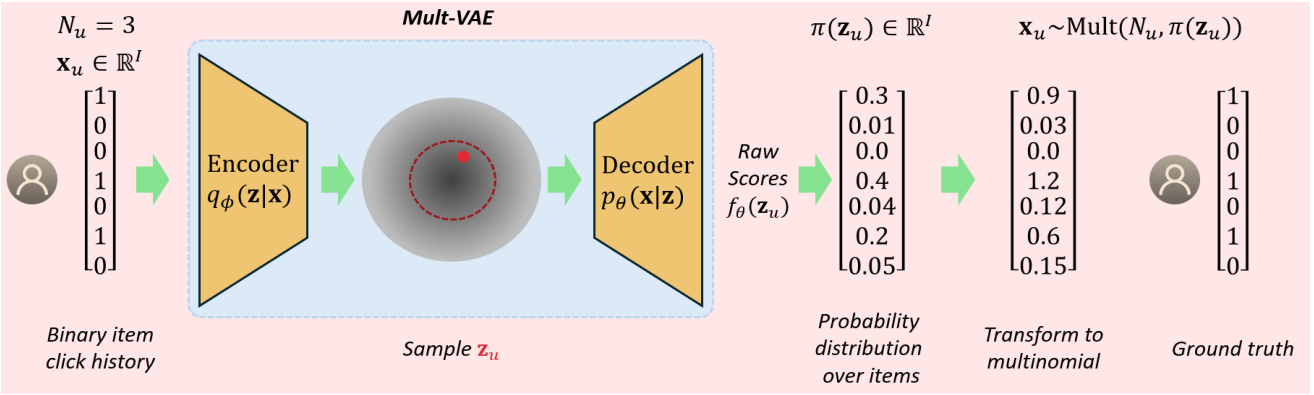
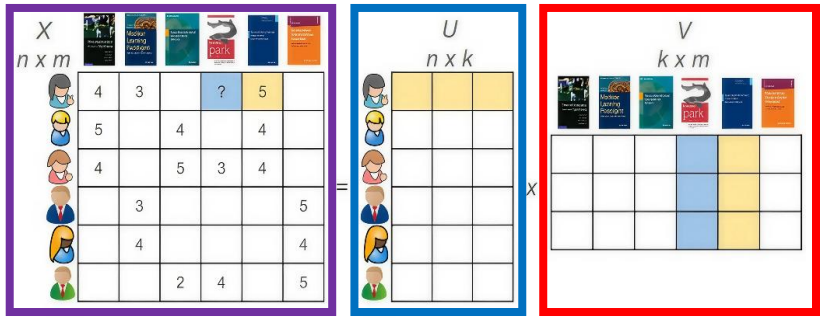


Mult-VAE / Non-Linearity for CF

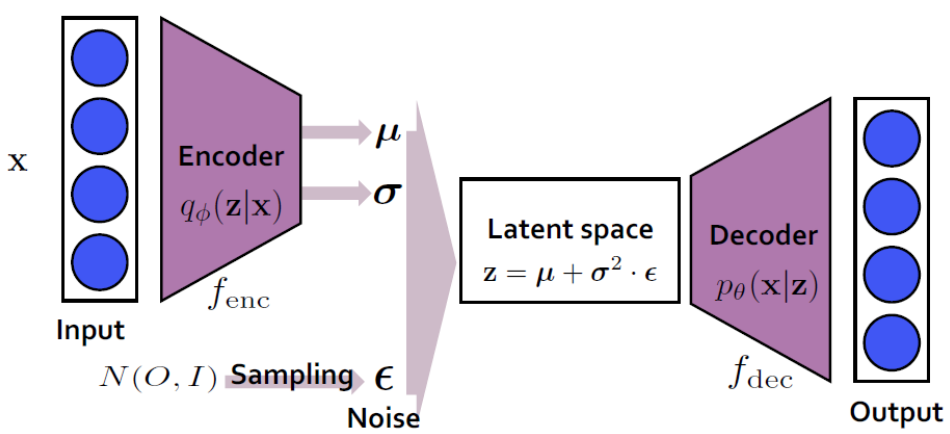
Linear Factor Models

- They did prove its simplicity and effectiveness
- However, inherent linearity limits its capacity



VAE for CF

- VAEs can generalize linear latent-factor models due to non-linearity
- **But how can we apply VAE for CF?**



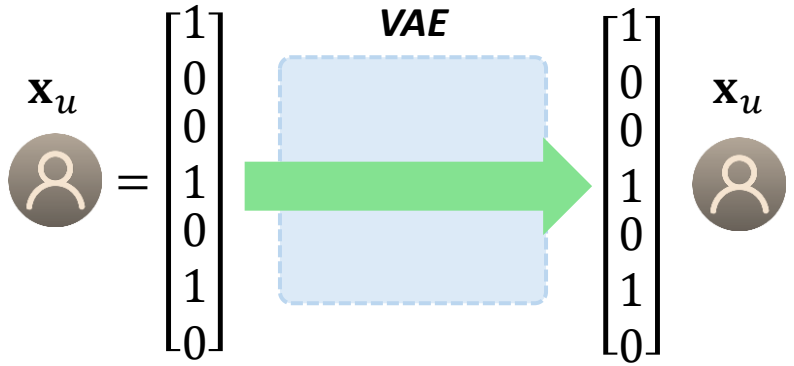
https://process-mining.tistory.com/161

Mult-VAE / Non-Linearity for CF

Input and Output?

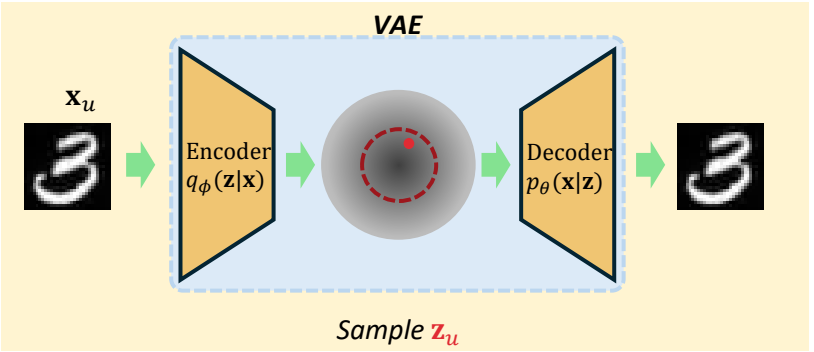
- ☐ Input = user, output = predicted preference (i.e., probabilities) over all items
- ☐ However, input = output in VAEs
- ☐ Solution : binarized click history = input = output = $\mathbf{x}_u$
- ☐ **Objective : generate the multinomial distribution!!!**

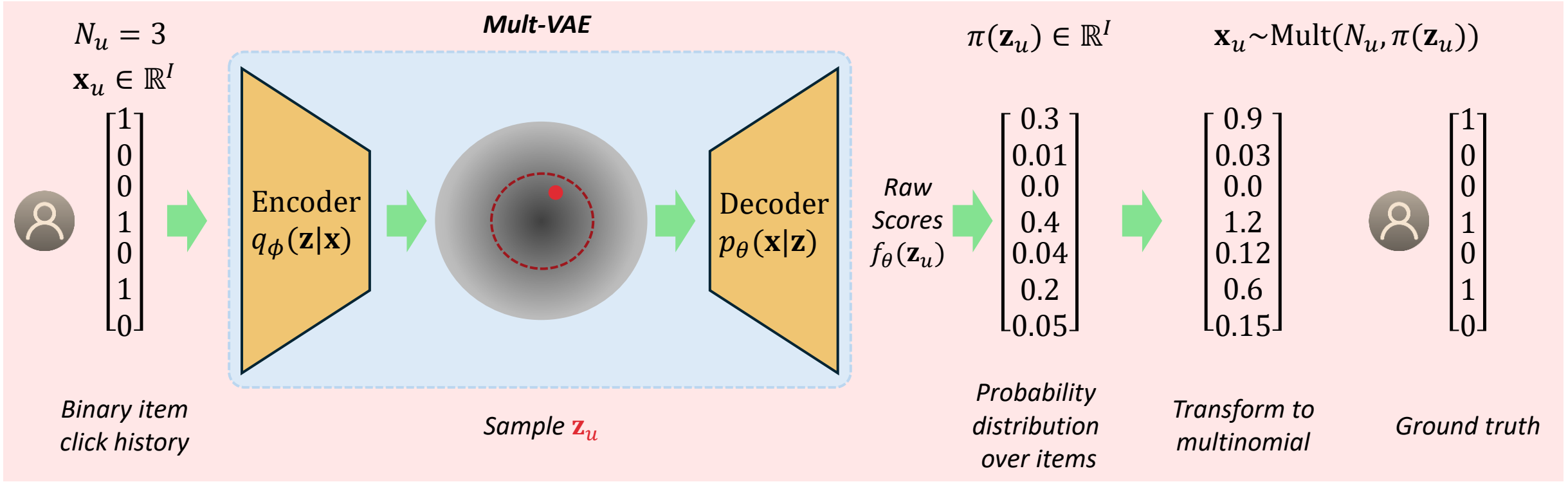
$$\mathbf{x}_u \sim \text{Mult}(\{total\ clicks\}, \{click\ probability\ for\ each\ item\})$$



Mult-VAE / VAE for CF

Overview of Mult-VAE





Mult-VAE / VAE for CF

Optimization Process of Mult-VAE

- Based on ELBO, lower bound of the log marginal likelihood

Similarity between encoded input and decoded output (↑)

$$\log p(\mathbf{x}_u;\theta) \geq \mathbb{E}_{q_\phi(\mathbf{z}_u \mid \mathbf{x}_u)}\left[\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u)\right] - \mathrm{KL}(q_\phi(\mathbf{z}_u \mid \mathbf{x}_u) \| p(\mathbf{z}_u))$$

∗ $p(\mathbf{z}_u)$ is assumed to be $\mathcal{N}(\mathbf{0}, \mathbf{I})$ and is approximated with $q_\phi(\mathbf{z}_u|\mathbf{x}_u)$

Acts as a **regularization** so that encoded distribution(q_ϕ) doesn't deviate too much from the prior(p) (↓)

Mult-VAE / VAE for CF

Negative Reconstruction Loss

$$\log p(\mathbf{x}_u;\theta) \geq \mathbb{E}_{q_\phi(\mathbf{z}_u \mid \mathbf{x}_u)}[\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u)] - \mathrm{KL}(q_\phi(\mathbf{z}_u \mid \mathbf{x}_u) \| p(\mathbf{z}_u))$$

- Assumed multinomial environment → multinomial likelihood most natural
- Gaussian log-likelihood and logistic log-likelihood also possible
- **Author's claim** : multinomial likelihood models click data better

Multinomial likelihood

$$\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u) \overset{c}{=} \sum_i x_{ui} \log \pi_i(\mathbf{z}_u)$$

Gaussian likelihood

$$\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u) \overset{c}{=} -\sum_i \frac{c_{ui}}{2}(x_{ui} - f_{ui})^2$$

Logistic log-likelihood

$$\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u) = \sum_i x_{ui} \log \sigma(f_{ui}) + (1 - x_{ui}) \log(1 - \sigma(f_{ui}))$$

Mult-VAE / ELBO Variant

Balancing Between Two Terms

$$\log p(\mathbf{x}_u;\theta) \geq \mathbb{E}_{q_\phi(\mathbf{z}_u \mid \mathbf{x}_u)}[\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u)] - \mathrm{KL}(q_\phi(\mathbf{z}_u \mid \mathbf{x}_u) \| p(\mathbf{z}_u))$$

- **Primary goal** : good recommendation (i.e., good reconstruction)
- Do need to follow up ELBO → partially regularized VAE

$$\textbf{Mult} - \textbf{VAE}^{\textbf{PR}}$$

$$\mathcal{L}_\beta(\mathbf{x}_u;\theta,\phi) \equiv \mathbb{E}_{q_\phi(\mathbf{z}_u \mid \mathbf{x}_u)}[\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u)] - \beta \cdot \mathrm{KL}(q_\phi(\mathbf{z}_u \mid \mathbf{x}_u) \| p(\mathbf{z}_u))$$

Weaker regularization
(Stronger reconstruction)

↓ ↑

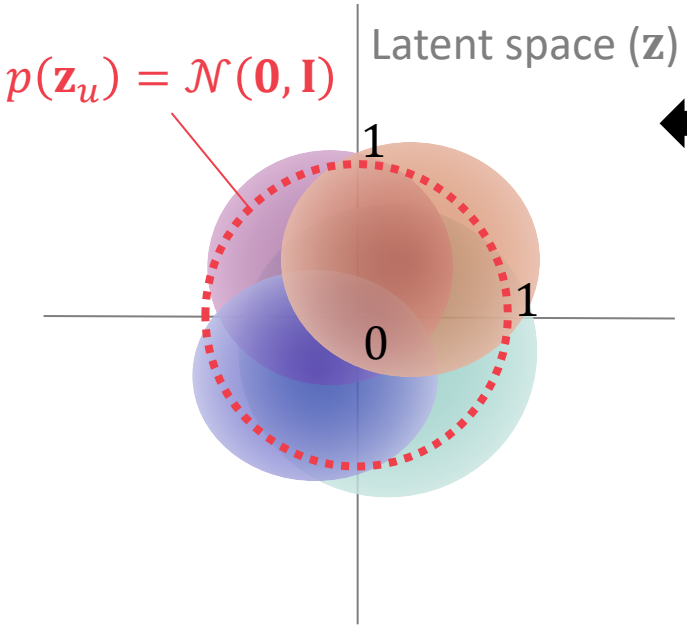
Stronger regularization
(Weaker reconstruction)

Mult-VAE / ELBO Variant

What Does β Control?

- $\beta > 1$ (left): posterior $q_\phi(\mathbf{z}_u|\mathbf{x}_u)$ is close to the prior $p(\mathbf{z}_u) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
- $\beta < 1$ (right): posterior $q_\phi(\mathbf{z}_u|\mathbf{x}_u)$ is far away from the prior $p(\mathbf{z}_u) = \mathcal{N}(\mathbf{0}, \mathbf{I})$

$$\beta \cdot \mathrm{KL}(q_\phi(\mathbf{z}_u|\mathbf{x}_u) \,\|\, p(\mathbf{z}_u))$$

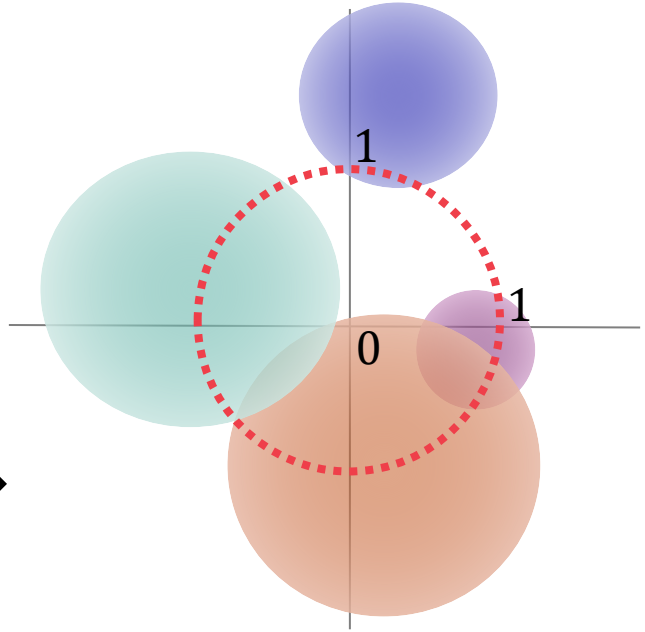


Smoother interpolation → Favorable in learning disentangled representations (Higgins, Irina, et al.)

Close resemblance to input data is hard to generate

Good reconstruction → Favorable when reconstruction is more important

Not a proper "generative model"
Suited for recommendation!!!



Higgins, Irina, et al. "beta-vae: Learning basic visual concepts with a constrained variational framework." *International conference on learning representations*. 2017.

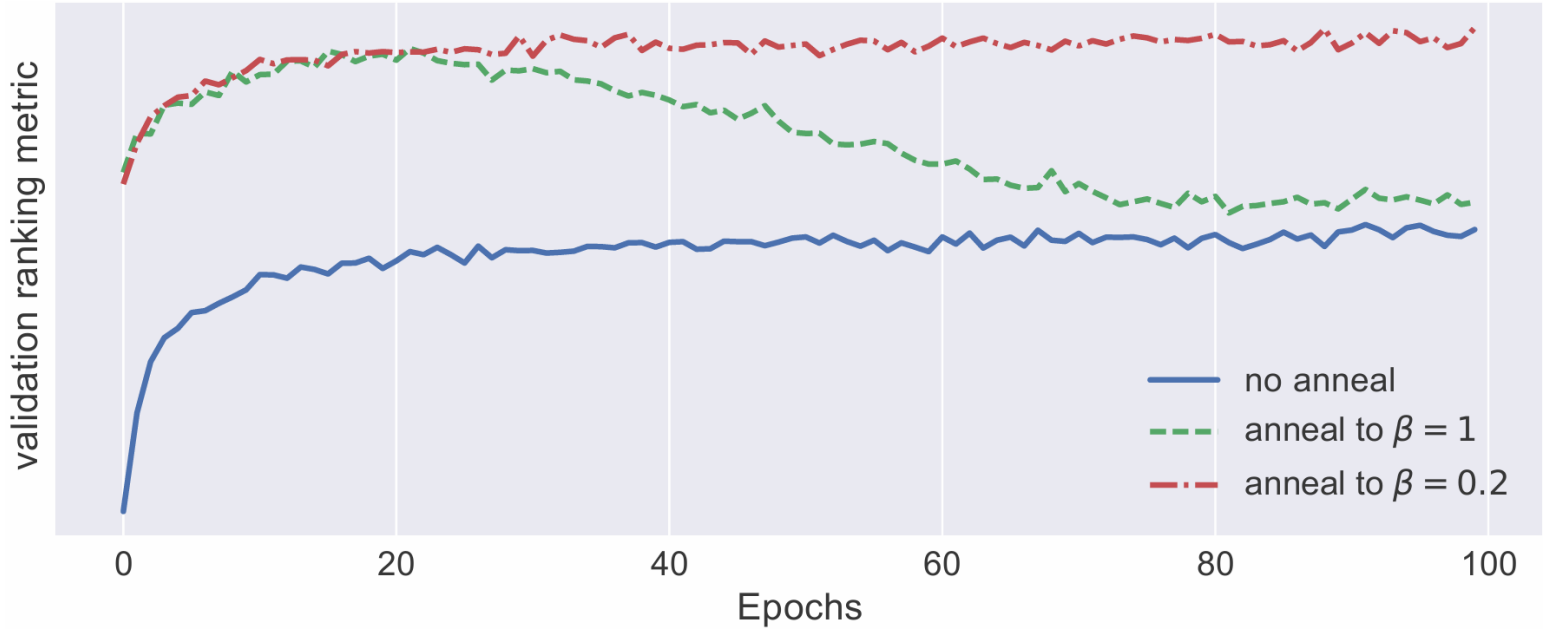
Mult-VAE / ELBO Variant

Annealing β

- Increase β from 0 to 1 until validation metric decreases → fix β afterwards (**annealing**)
- Inherently sub-optimal scheduling, but no additional tuning required

Analysis on Annealing β

- Model focusses on reconstruction at initial stage of learning
- When reconstruction is hindered by regularization (e.g., epoch 20), fix β



Mult-VAE / General View of AE

Autoencoders (AEs)

- ☐ Let's look through other types of AEs
- ☐ Maximum-likelihood estimation of AE is as follows

$$\theta^{\text{AE}}, \phi^{\text{AE}} = \arg\max_{\theta,\phi} \sum_{u} \mathbb{E}_{\delta(\mathbf{z}_u - g_\phi(\mathbf{x}_u))} \left[\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u)\right]$$

$$= \arg\max_{\theta,\phi} \sum_{u} \log p_\theta(\mathbf{x}_u \mid g_\phi(\mathbf{x}_u))$$

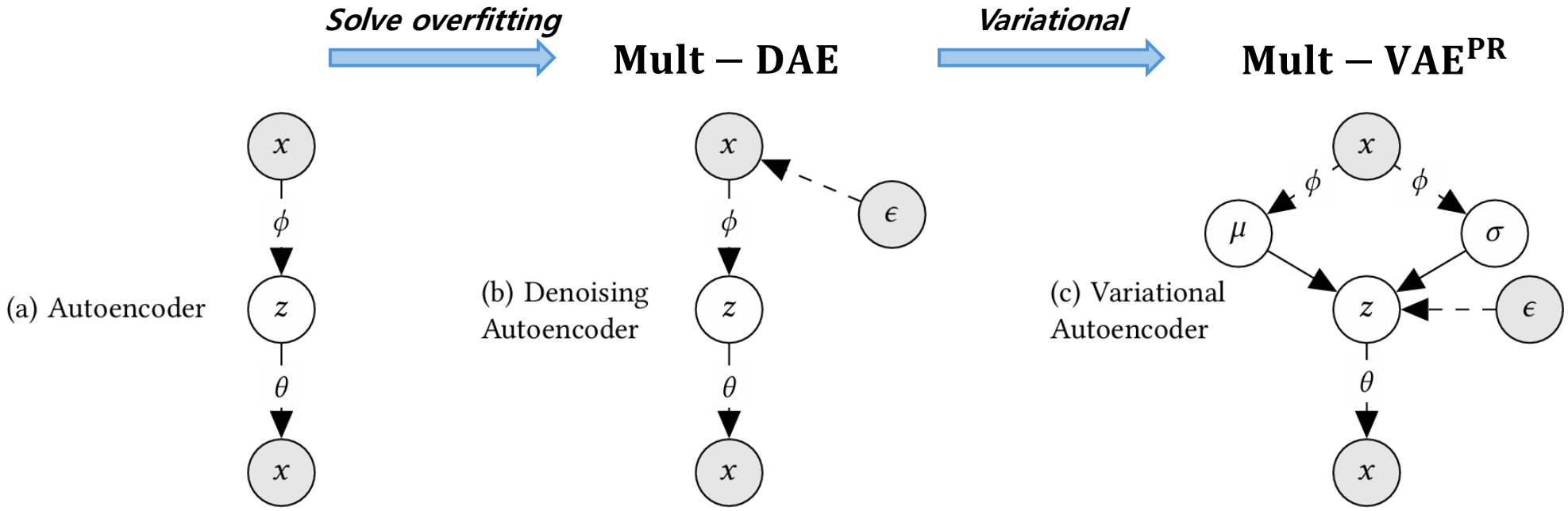
Unit pulse (δ) has value only when $\mathbf{z}_u = g_\phi(\mathbf{x}_u)$

No regularization (KLD) since AEs project single point to latent space

Mult-VAE / General View of AE

AE Variants

- ☐ AEs are prone to overfit : put all the probability mass to non-zero entries in $\mathbf{x}_u$
- ☐ Mixing AE with dropout, denoising AE (DAE) achieves better results



Mult-VAE / Experiments

Prediction

- Input : user click history / Output : multinomial probability
- Advantage of AEs : recommendation possible for users not seen in training data

Experiment Setup

- # of interactions : density of user-item click matrix
- # of held-out users : number of users on in training data

	ML-20M	Netflix	MSD
# of users	136,677	463,435	571,355
# of items	20,108	17,769	41,140
# of interactions	10.0M	56.9M	33.6M
% of interactions	0.36%	0.69%	0.14%
# of held-out users	10,000	40,000	50,000

Mult-VAE / Experiments

Comparison with Baselines

- NCF (=NeuMF) only compatible in ML-1M, Pinterest dataset

(a) ML-20M

	Recall@20	Recall@50	NDCG@100
Mult-VAE^{PR}	**0.395**	**0.537**	**0.426**
Mult-DAE	0.387	0.524	0.419
WMF	0.360	0.498	0.386
SLIM	0.370	0.495	0.401
CDAE	0.391	0.523	0.418

(b) Netflix

	Recall@20	Recall@50	NDCG@100
Mult-VAE^{PR}	**0.351**	**0.444**	**0.386**
Mult-DAE	0.344	0.438	0.380
WMF	0.316	0.404	0.351
SLIM	0.347	0.428	0.379
CDAE	0.343	0.428	0.376

(c) MSD

	Recall@20	Recall@50	NDCG@100
Mult-VAE^{PR}	**0.266**	**0.364**	**0.316**
Mult-DAE	**0.266**	**0.363**	0.313
WMF	0.211	0.312	0.257
SLIM	—	—	—
CDAE	0.188	0.283	0.237

(a) ML-1M

	NCF	NCF (pre-train)	Mult-DAE
Recall@10	0.705	**0.730**	0.722
NDCG@10	0.426	**0.447**	0.446

(b) Pinterest

	NCF	NCF (pre-train)	Mult-DAE
Recall@10	0.872	0.880	**0.886**
NDCG@10	0.551	0.558	**0.580**

Mult-VAE / Experiments

Reconstruction Losses

Mult

$$\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u) \overset{c}{=} \sum_i x_{ui} \log \pi_i(\mathbf{z}_u)$$

Gaussian

$$\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u) \overset{c}{=} -\sum_i \frac{c_{ui}}{2}(x_{ui} - f_{ui})^2$$

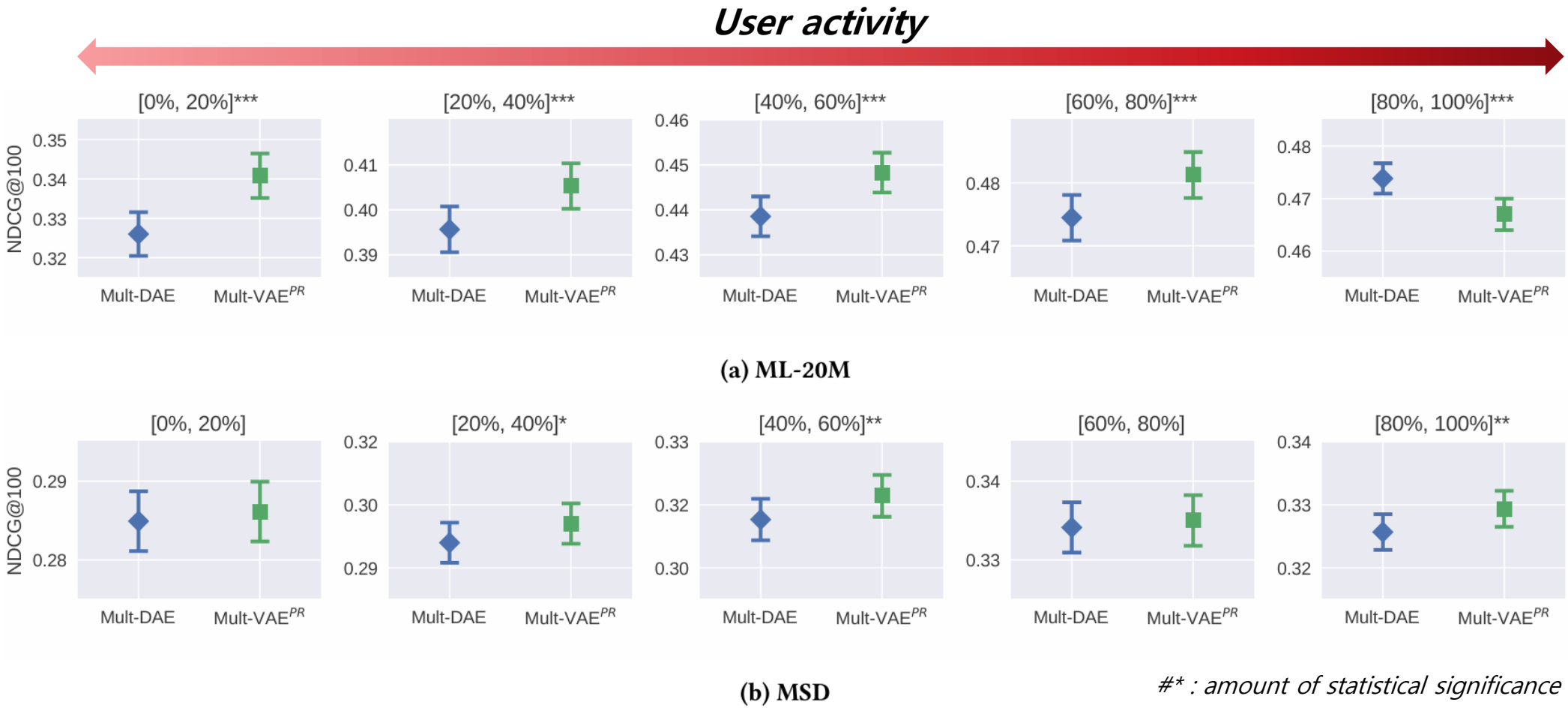
Logistic

$$\log p_\theta(\mathbf{x}_u \mid \mathbf{z}_u) = \sum_i x_{ui} \log \sigma(f_{ui}) + (1 - x_{ui}) \log(1 - \sigma(f_{ui}))$$

	ML-20M		
	Recall@20	Recall@50	NDCG@100
Mult-VAE^{PR}	**0.395**	**0.537**	**0.426**
Gaussian-VAE^{PR}	0.383	0.523	0.415
Logistic-VAE^{PR}	0.388	0.523	0.419
Mult-DAE	**0.387**	**0.524**	**0.419**
Gaussian-DAE	0.376	0.515	0.409
Logistic-DAE	0.381	0.516	0.414

Mult-VAE / Experiments

DAE vs VAE

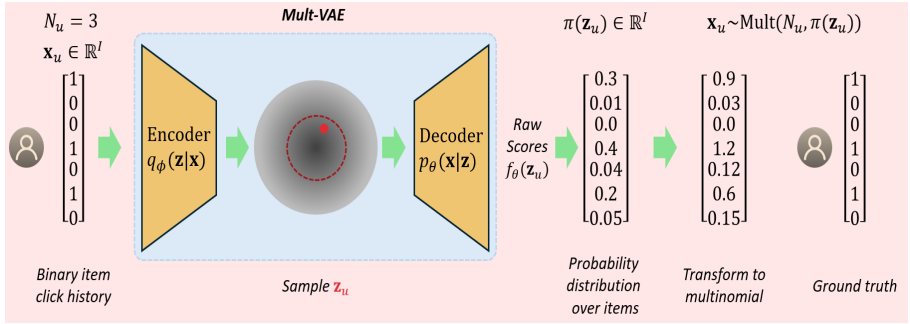


: amount of statistical significance*

Mult-VAE / Conclusion

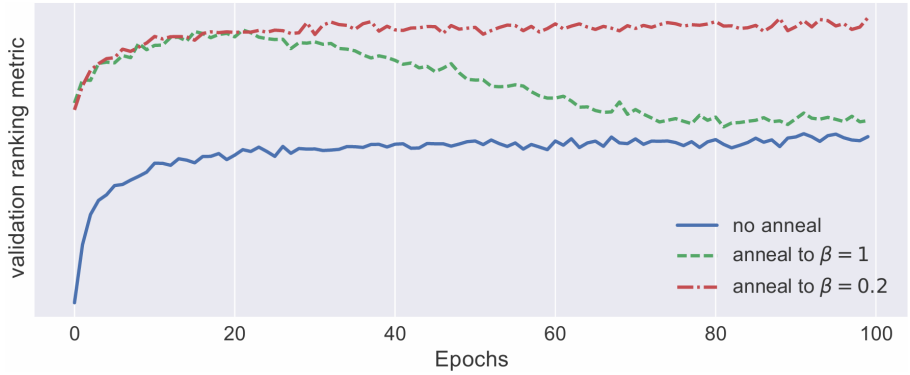
VAE for CF

- ☐ Incorporated generative models to CF
- ☐ Performed promising results based on multinomial view



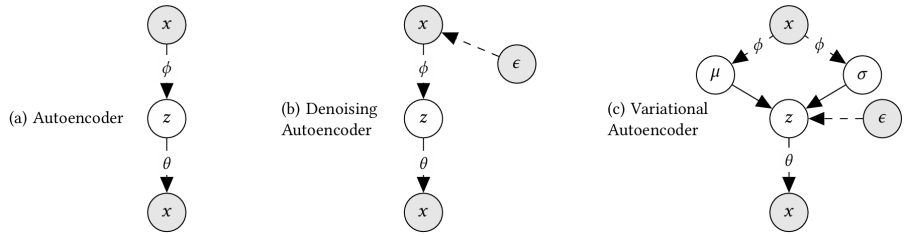
Information Theory Connections

- ☐ Provided re-interpretation of ELBO in this literature
- ☐ Showed connection to other domains



Investigation of AEs

- ☐ Identified pros and cons of both Mult-VAE^{PR} and Mult-DAE
- ☐ Showed robustness of principled Bayesian approach



LightGCN

- ☐ GCN for CF
- ☐ Too Heavy!
- ☐ Architecture
- ☐ Analysis
- ☐ Experiments
- ☐ Conclusion

LightGCN: Simplifying and Powering Graph Convolution Network for Recommendation

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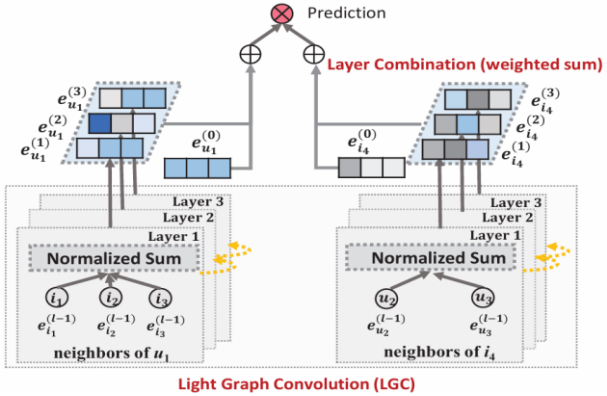
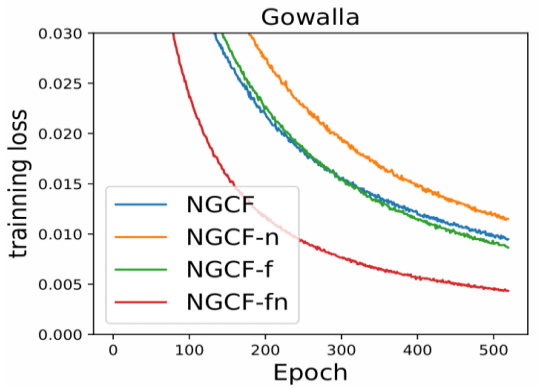
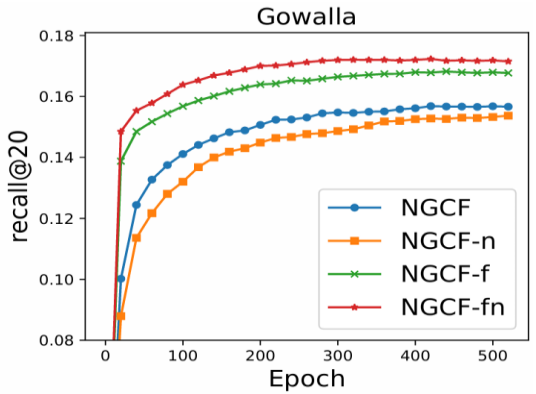
SIGIR 2020





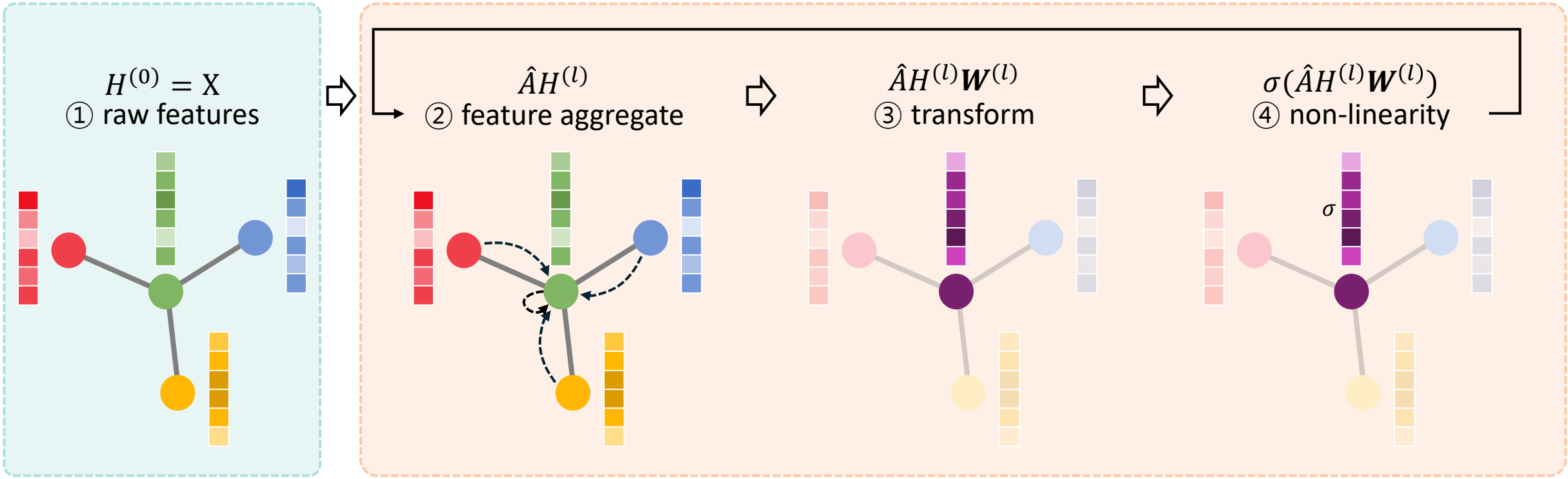


LightGCN / GCN for CF

Graph Convolution Network (GCN)

- GCN : rising star in many graph representation learning tasks
- Node-wise learning view of GCN is as follows

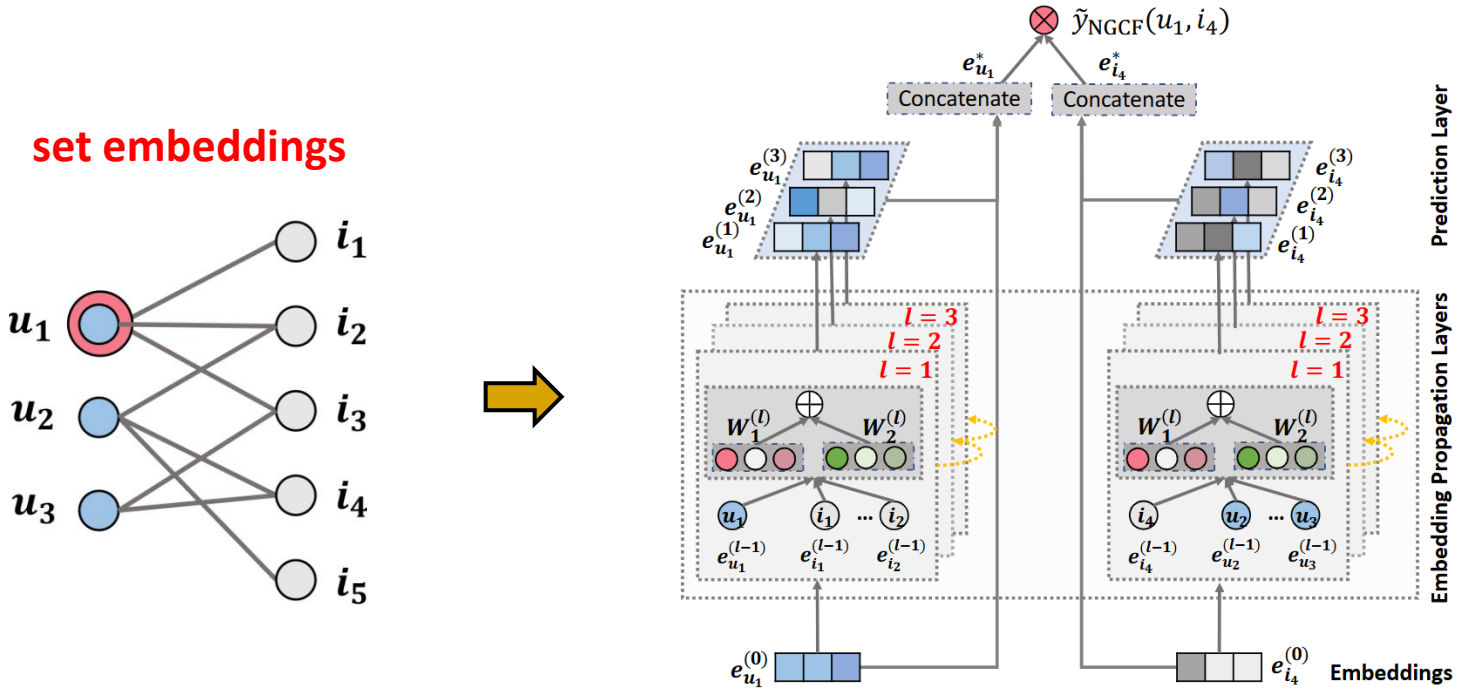
$$H^{(l+1)} = \sigma(\hat{A}H^{(l)}\boldsymbol{W}^{(l)})$$



LightGCN / GCN for CF

Inspired by GCN, Creation of NGCF

- ☐ Incorporated every GCN architecture to CF
- ☐ Major difference : no initial raw features for users and items



LightGCN / GCN for CF

Posing Doubt on NGCF Architecture

- ☐ Environment between node classification(GCN) and CF(NGCF) is different
- ☐ This should lead in architecture change, rather than naively copying GCN
- ☐ Authors point out 2 problematic components of NGCF → $\mathbf{W}_1, \mathbf{W}_2$ and $\sigma(\cdot)$

Embedding update formulas (NGCF)

$$\mathbf{e}_u^{(k+1)} = \sigma\left(\mathbf{W}_1\mathbf{e}_u^{(k)} + \sum_{i\in\mathcal{N}_u} \frac{1}{\sqrt{|\mathcal{N}_u||\mathcal{N}_i|}}(\mathbf{W}_1\mathbf{e}_i^{(k)} + \mathbf{W}_2(\mathbf{e}_i^{(k)} \odot \mathbf{e}_u^{(k)}))\right)$$

$$\mathbf{e}_i^{(k+1)} = \sigma\left(\mathbf{W}_1\mathbf{e}_i^{(k)} + \sum_{u\in\mathcal{N}_i} \frac{1}{\sqrt{|\mathcal{N}_u||\mathcal{N}_i|}}(\mathbf{W}_1\mathbf{e}_u^{(k)} + \mathbf{W}_2(\mathbf{e}_u^{(k)} \odot \mathbf{e}_i^{(k)}))\right)$$

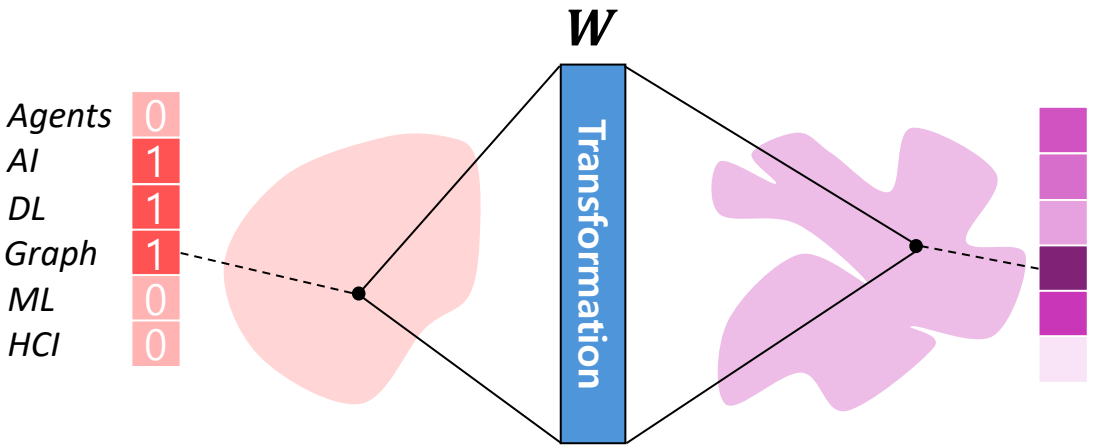
LightGCN / Too Heavy!

Do We Even Need W?

- When do we need feature transformation?
- Transformation allows rich attributes to be mapped into meaningful latent space

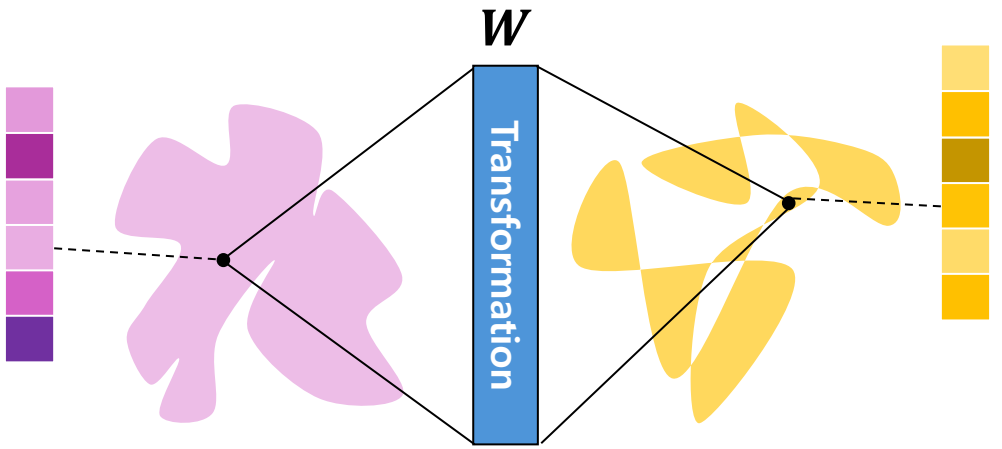
GCN

Mapping useful information



NGCF

*Mapping **not useful** information*



* The feature scenario of GCN is based on CiteSeer dataset

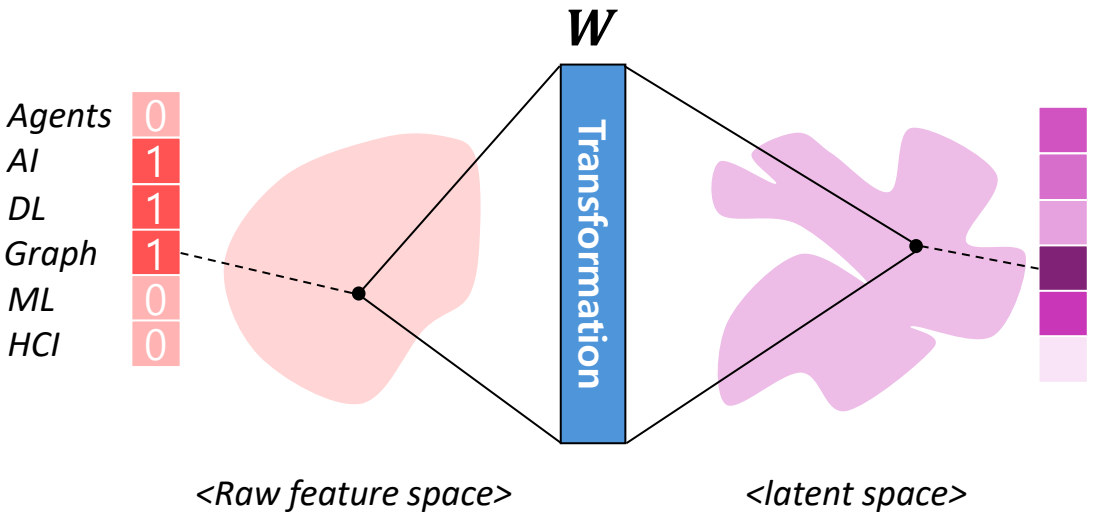
LightGCN / Too Heavy!

No Need for Feature Transformation W

- ☐ Node classification (GCN) : node has rich attributes
- ☐ Collaborative filtering (NGCF) : node ID (only attribute) is nothing but an identifier

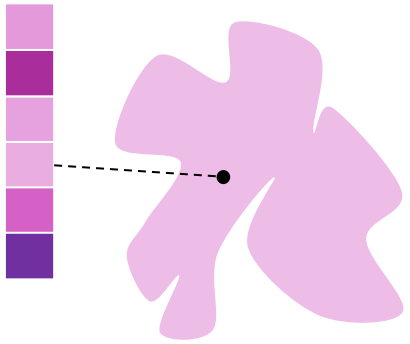
GCN

Mapping useful information

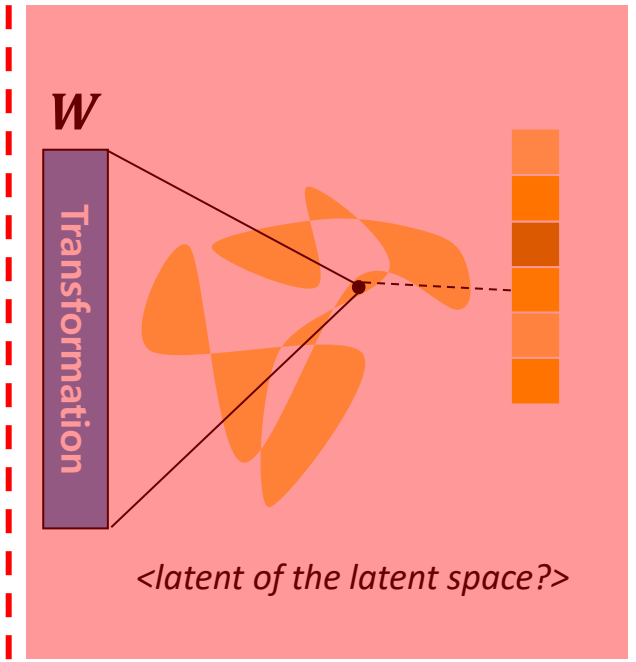


LightGCN

Identifier is enough



Redundant!!!



* The feature scenario of GCN is based on CiteSeer dataset

LightGCN / Too Heavy!

Hypothesis on W and $\sigma(\cdot)$

- ☐ e_u and e_i serves as identity and latent traits → **no need for feature transformation**
- ☐ No need for feature transformation → **no need for nonlinear activation**

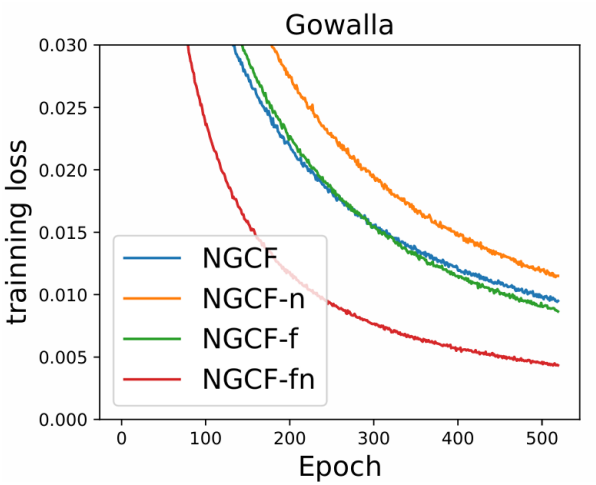
$$\mathbf{e}_u^{(k+1)} = \sigma\left(\mathbf{W}_1\mathbf{e}_u^{(k)} + \sum_{i\in\mathcal{N}_u}\frac{1}{\sqrt{|\mathcal{N}_u||\mathcal{N}_i|}}\left(\mathbf{W}_1\mathbf{e}_i^{(k)} + \mathbf{W}_2(\mathbf{e}_i^{(k)}\odot\mathbf{e}_u^{(k)})\right)\right)$$

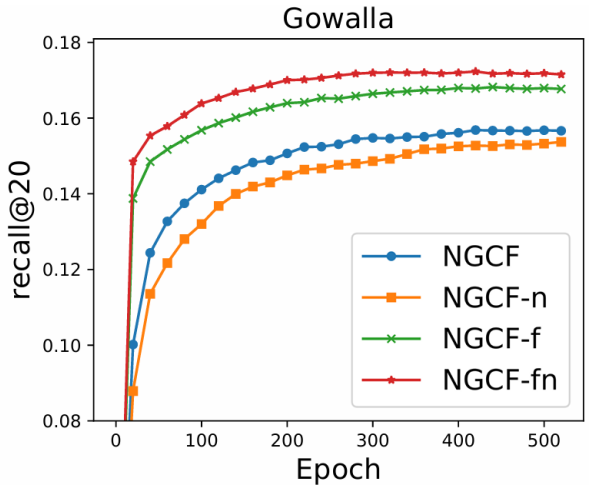
$$\mathbf{e}_i^{(k+1)} = \sigma\left(\mathbf{W}_1\mathbf{e}_i^{(k)} + \sum_{u\in\mathcal{N}_i}\frac{1}{\sqrt{|\mathcal{N}_u||\mathcal{N}_i|}}\left(\mathbf{W}_1\mathbf{e}_u^{(k)} + \mathbf{W}_2(\mathbf{e}_u^{(k)}\odot\mathbf{e}_i^{(k)})\right)\right)$$

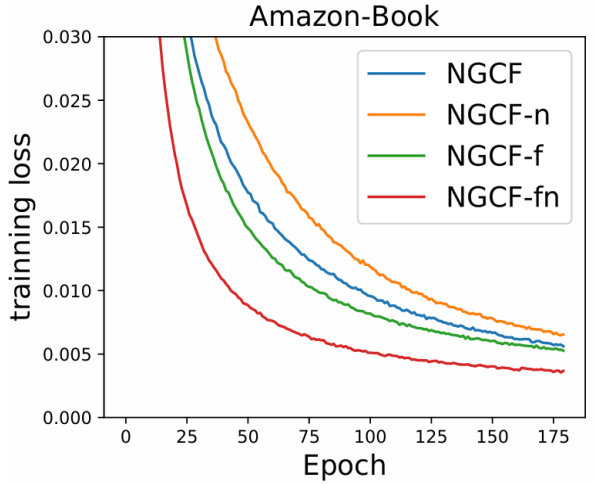
LightGCN / Too Heavy!

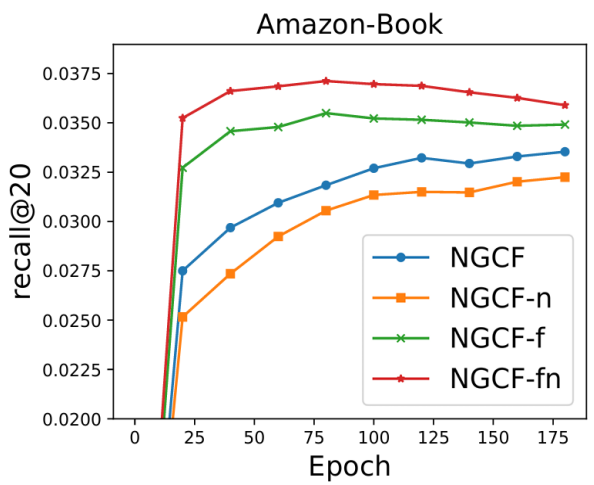
Ablation : NGCF with 3 Variants

☐ Don’t increase the training difficulty!!!









NGCF, original

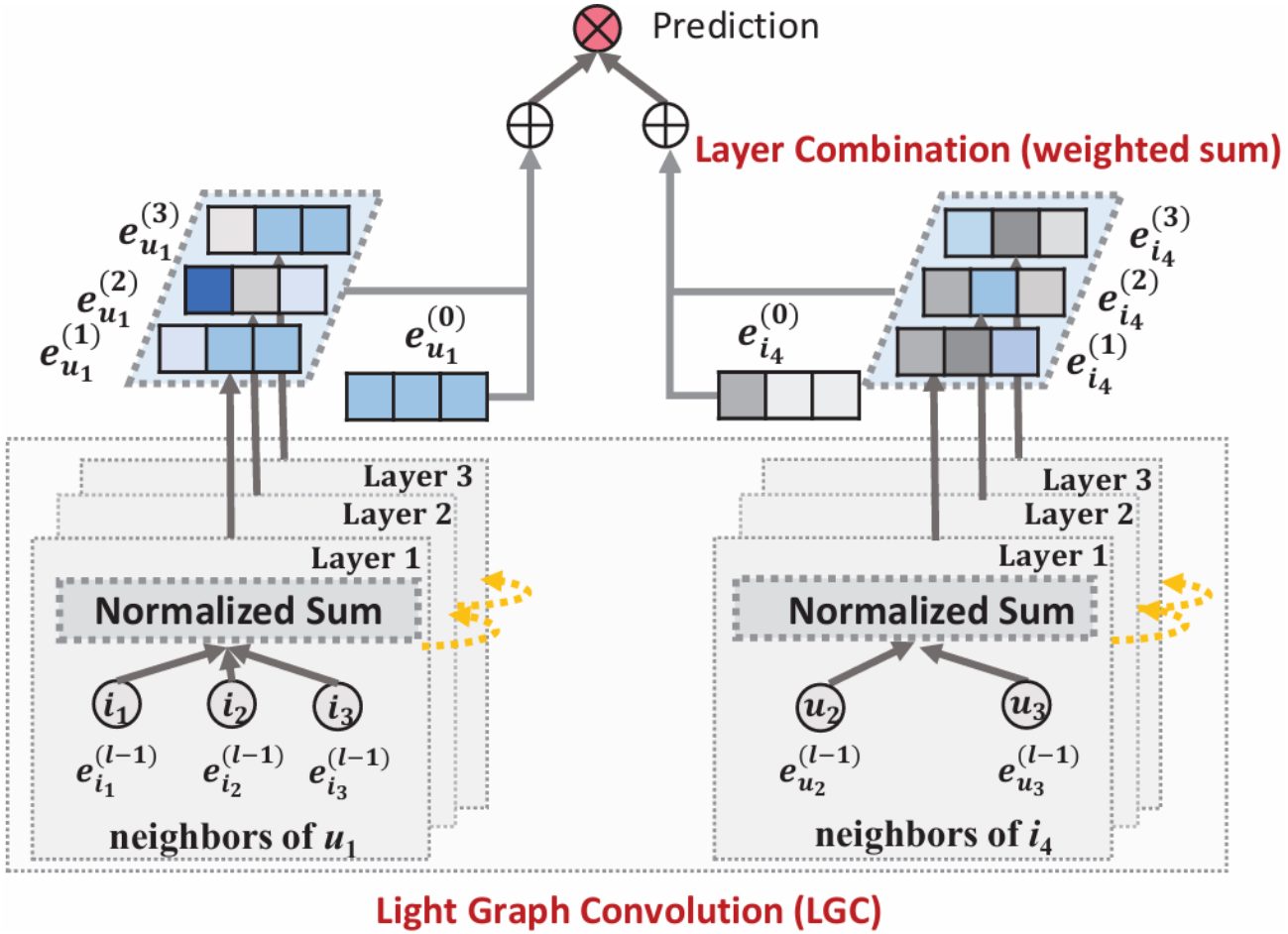
NGCF-f, remove $\mathbf{W}_1, \mathbf{W}_2$ → improved result : the absence of meaningless transformation

NGCF-n, remove σ → degraded result : linearity of transformations

NGCF-fn, remove $\mathbf{W}_1, \mathbf{W}_2$ and σ → improved result : **removing every meaningless counterparts**

LightGCN / Architecture

Overview of LightGCN



LightGCN / Architecture

Light Graph Convolution (LGC)

- Aggregation module of LightGCN
- Symmetric normalization follows standard GCN
- Other options are possible, later experimented

$$\mathbf{e}_u^{(k+1)} = \sum_{i \in \mathcal{N}_u} \frac{1}{\sqrt{|\mathcal{N}_u|}\sqrt{|\mathcal{N}_i|}} \mathbf{e}_i^{(k)},$$

$$\mathbf{e}_i^{(k+1)} = \sum_{u \in \mathcal{N}_i} \frac{1}{\sqrt{|\mathcal{N}_i|}\sqrt{|\mathcal{N}_u|}} \mathbf{e}_u^{(k)}.$$

No self-connection?

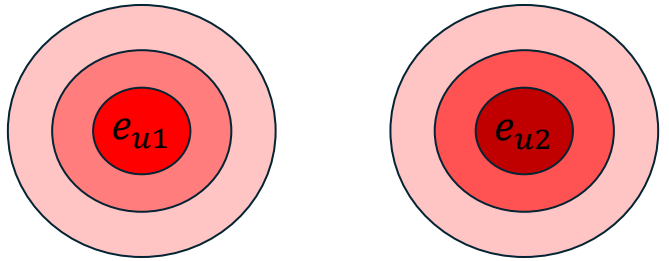
Controls the influence of super nodes

LightGCN / Architecture

Layer Combination

- Final node representation = weighted (α_k) sum over **all layer (hop) representations**
- Weights uniformly set to $1/(K+1)$ to maintain simplicity

$$\mathbf{e}_u = \sum_{k=0}^{K} \alpha_k \mathbf{e}_u^{(k)}; \quad \mathbf{e}_i = \sum_{k=0}^{K} \alpha_k \mathbf{e}_i^{(k)}$$



Prediction

- Dot product, used for ranking score

$$\hat{y}_{ui} = \mathbf{e}_u^T \mathbf{e}_i$$

LightGCN / Analysis

Is the Simple Design Okay?

- Authors investigate the rationality behind LightGCN
- **1) Connections with other GCN variants**
- **2) Second-order embedding smoothness**

$$\mathbf{R} \in \mathbb{R}^{M \times N}$$

$$\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{R} \\ \mathbf{R}^T & \mathbf{0} \end{pmatrix}$$

$$\mathbf{E}^{(k+1)} = (\mathbf{D}^{-\frac{1}{2}}\mathbf{A}\mathbf{D}^{-\frac{1}{2}})\mathbf{E}^{(k)}$$

$$\Rightarrow \quad \mathbf{E} = \alpha_0\mathbf{E}^{(0)} + \alpha_1\mathbf{E}^{(1)} + \alpha_2\mathbf{E}^{(2)} + \ldots + \alpha_K\mathbf{E}^{(K)}$$

$$= \alpha_0\mathbf{E}^{(0)} + \alpha_1\tilde{\mathbf{A}}\mathbf{E}^{(0)} + \alpha_2\tilde{\mathbf{A}}^2\mathbf{E}^{(0)} + \ldots + \alpha_K\tilde{\mathbf{A}}^K\mathbf{E}^{(0)}$$

LightGCN / Analysis

Connections with Other GCN Variants (SGCN)

☐ Simplified GCN : removed nonlinearities + collapse weight metrices into one

Self-connection

SGCN

$$\mathbf{E}^{(k+1)} = (\mathbf{D}+\mathbf{I})^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})(\mathbf{D}+\mathbf{I})^{-\frac{1}{2}}\mathbf{E}^{(k)}$$

$(\mathbf{D}+\mathbf{I})^{-\frac{1}{2}}$ *only rescales*

$$\mathbf{E}^{(K)} = (\mathbf{A}+\mathbf{I})\mathbf{E}^{(K-1)} = (\mathbf{A}+\mathbf{I})^{K}\mathbf{E}^{(0)}$$

$$= \binom{K}{0}\mathbf{E}^{(0)} + \binom{K}{1}\mathbf{A}\mathbf{E}^{(0)} + \binom{K}{2}\mathbf{A}^{2}\mathbf{E}^{(0)} + \ldots + \binom{K}{K}\mathbf{A}^{K}\mathbf{E}^{(0)}$$

Essentially equivalent!

LightGCN

$$\mathbf{E} = \alpha_0\mathbf{E}^{(0)} + \alpha_1\tilde{\mathbf{A}}\mathbf{E}^{(0)} + \alpha_2\tilde{\mathbf{A}}^{2}\mathbf{E}^{(0)} + \ldots + \alpha_K\tilde{\mathbf{A}}^{K}\mathbf{E}^{(0)}$$

LightGCN subsumes self-connection!

The weight matrix in SGCN can be absorbed into the 0-th layer embedding parameters, thus it is omitted in the analysis.

LightGCN / Analysis

Connections with Other GCN Variants (APPNP)

- APPNP : restart design into GCN to alleviate oversmoothing
- APPNP adds self-connection (already discussed)

Restart prob

APPNP

$$\mathbf{E}^{(k+1)} = \beta\mathbf{E}^{(0)} + (1-\beta)\tilde{\mathbf{A}}\mathbf{E}^{(k)}$$

$$\mathbf{E}^{(K)} = \beta\mathbf{E}^{(0)} + (1-\beta)\tilde{\mathbf{A}}\mathbf{E}^{(K-1)},$$

$$= \beta\mathbf{E}^{(0)} + \beta(1-\beta)\tilde{\mathbf{A}}\mathbf{E}^{(0)} + (1-\beta)^2\tilde{\mathbf{A}}^2\mathbf{E}^{(K-2)}$$

$$= \beta\mathbf{E}^{(0)} + \beta(1-\beta)\tilde{\mathbf{A}}\mathbf{E}^{(0)} + \beta(1-\beta)^2\tilde{\mathbf{A}}^2\mathbf{E}^{(0)} + \ldots + (1-\beta)^K\tilde{\mathbf{A}}^K\mathbf{E}^{(0)}.$$

Essentially equivalent!

LightGCN

$$\mathbf{E} = \alpha_0\mathbf{E}^{(0)} + \alpha_1\tilde{\mathbf{A}}\mathbf{E}^{(0)} + \alpha_2\tilde{\mathbf{A}}^2\mathbf{E}^{(0)} + \ldots + \alpha_K\tilde{\mathbf{A}}^K\mathbf{E}^{(0)}$$

LightGCN can allow long-range modeling

LightGCN / Analysis

Second-Order Embedding Smoothness

- How much smoothening happen between two users (u, v)?
- Smoothness strength ($c_{v \to u}$) : $\mathbf{e}_u^{(2)} = \sum_v c_{v \to u} \mathbf{e}_v^{(0)}$

$$\mathbf{e}_u^{(2)} = \sum_{i \in \mathcal{N}_u} \frac{1}{\sqrt{|\mathcal{N}_u|}\sqrt{|\mathcal{N}_i|}} \mathbf{e}_i^{(1)} = \sum_{i \in \mathcal{N}_u} \frac{1}{|\mathcal{N}_i|} \sum_{v \in \mathcal{N}_i} \frac{1}{\sqrt{|\mathcal{N}_u|}\sqrt{|\mathcal{N}_v|}} \mathbf{e}_v^{(0)}$$

$$c_{v->u} = \frac{1}{\sqrt{|\mathcal{N}_u|}\sqrt{|\mathcal{N}_v|}} \sum_{i \in \mathcal{N}_u \cap \mathcal{N}_v} \frac{1}{|\mathcal{N}_i|}$$

⇒ ***Explains well on CF measuring user (item) similarity***

LightGCN / Experiments

Model Training

- Bayesian Personalized Ranking loss (pairwise)

$$L_{BPR} = -\sum_{u=1}^{M} \sum_{i \in \mathcal{N}_u} \sum_{j \notin \mathcal{N}_u} \ln \sigma(\hat{y}_{ui} - \hat{y}_{uj}) + \lambda ||\mathbf{E}^{(0)}||^2$$

Datasets

Table 2: Statistics of the experimented data.

Dataset	User #	Item #	Interaction #	Density
Gowalla	29, 858	40, 981	1, 027, 370	0.00084
Yelp2018	31, 668	38, 048	1, 561, 406	0.00130
Amazon-Book	52, 643	91, 599	2, 984, 108	0.00062

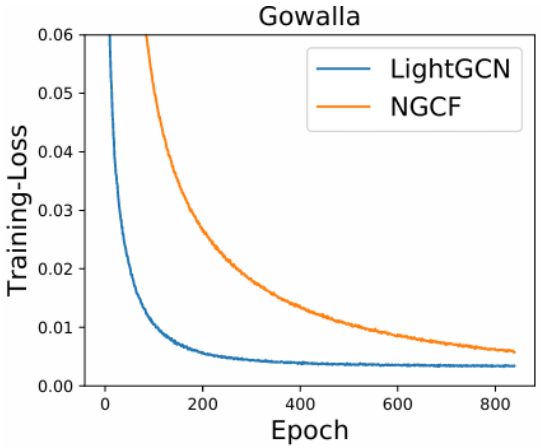
Metrics

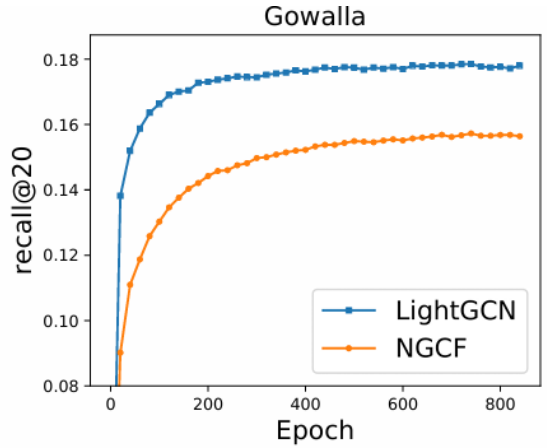
- Recall@20, NDCG@20

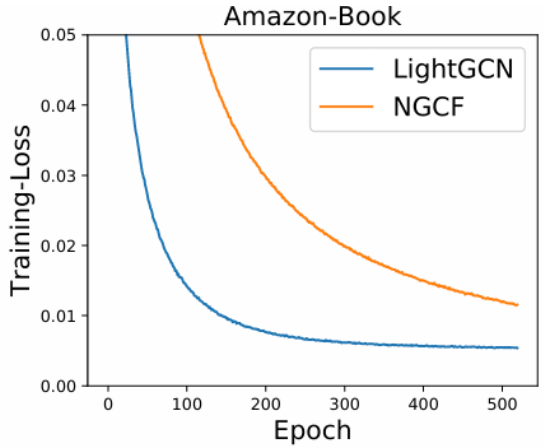
LightGCN / Experiments

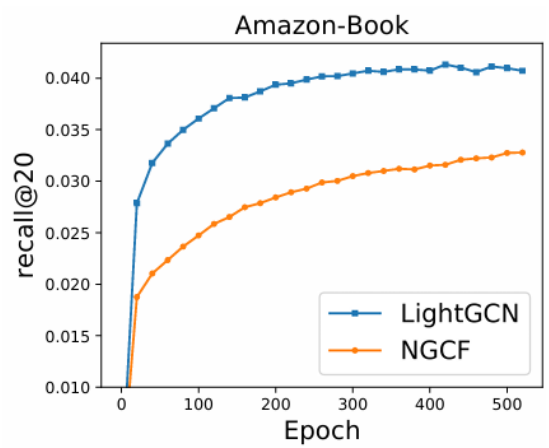
NGCF vs LightGCN with Different Layers

Dataset		Gowalla		Yelp2018		Amazon-Book	
Layer #	Method	recall	ndcg	recall	ndcg	recall	ndcg
1 Layer	NGCF	0.1556	0.1315	0.0543	0.0442	0.0313	0.0241
	LightGCN	0.1755(+12.79%)	0.1492(+13.46%)	0.0631(+16.20%)	0.0515(+16.51%)	0.0384(+22.68%)	0.0298(+23.65%)
2 Layers	NGCF	0.1547	0.1307	0.0566	0.0465	0.0330	0.0254
	LightGCN	0.1777(+14.84%)	0.1524(+16.60%)	0.0622(+9.89%)	0.0504(+8.38%)	0.0411(+24.54%)	0.0315(+24.02%)
3 Layers	NGCF	0.1569	0.1327	0.0579	0.0477	0.0337	0.0261
	LightGCN	0.1823(+16.19%)	0.1555(+17.18%)	0.0639(+10.38%)	0.0525(+10.06%)	0.0410(+21.66%)	0.0318(+21.84%)
4 Layers	NGCF	0.1570	0.1327	0.0566	0.0461	0.0344	0.0263
	LightGCN	0.1830(+16.56%)	0.1550(+16.80%)	0.0649(+14.58%)	0.530(+15.02%)	0.0406(+17.92%)	0.0313(+18.92%)









LightGCN / Experiments

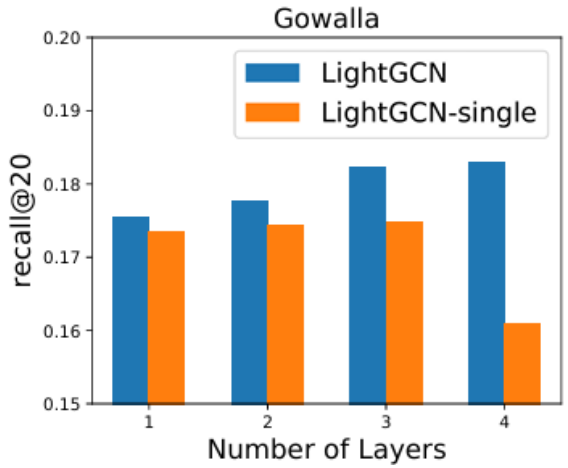
LightGCN vs Different Models

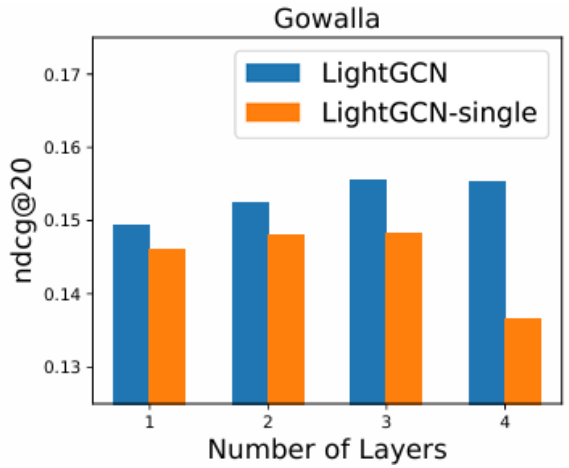
Dataset	Gowalla		Yelp2018		Amazon-Book	
Method	recall	ndcg	recall	ndcg	recall	ndcg
NGCF	0.1570	0.1327	0.0579	0.0477	0.0344	0.0263
Mult-VAE	0.1641	0.1335	0.0584	0.0450	0.0407	0.0315
GRMF	0.1477	0.1205	0.0571	0.0462	0.0354	0.0270
GRMF-norm	0.1557	0.1261	0.0561	0.0454	0.0352	0.0269
LightGCN	**0.1830**	**0.1554**	**0.0649**	**0.0530**	**0.0411**	**0.0315**

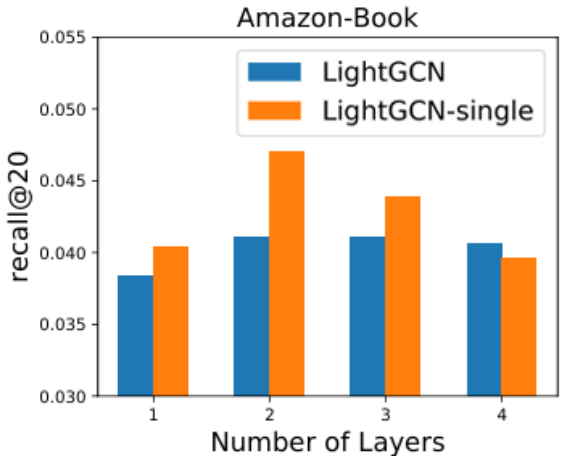
LightGCN / Experiments

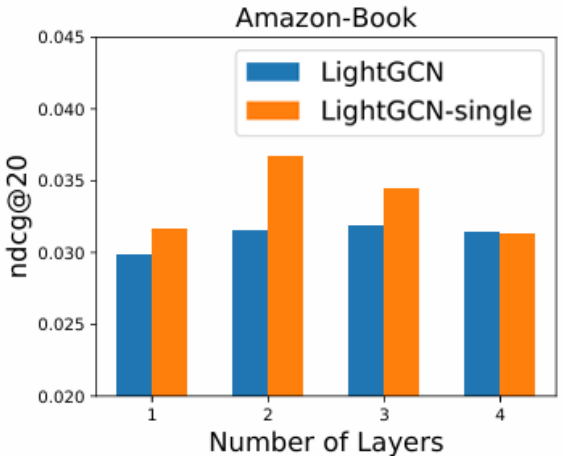
Ablation : Layer Combination

- LightGCN-single : only use the last embedding $\mathbf{E}^{(K)}$ for prediction
- LightGCN tackles oversmoothing









LightGCN / Experiments

Ablation : Others

- -L : target node's coefficient / -R : neighbor node's coefficient

Table 5: Performance of the 3-layer LightGCN with different choices of normalization schemes in graph convolution.

Dataset	Gowalla		Yelp2018		Amazon-Book	
Method	**recall**	**ndcg**	**recall**	**ndcg**	**recall**	**ndcg**
LightGCN-L_1-L	0.1724	0.1414	0.0630	0.0511	**0.0419**	**0.0320**
LightGCN-L_1-R	0.1578	0.1348	0.0587	0.0477	0.0334	0.0259
LightGCN-L_1	0.159	0.1319	0.0573	0.0465	0.0361	0.0275
LightGCN-L	0.1589	0.1317	0.0619	0.0509	0.0383	0.0299
LightGCN-R	0.1420	0.1156	0.0521	0.0401	0.0252	0.0196
LightGCN	**0.1830**	**0.1554**	**0.0649**	**0.0530**	0.0411	0.0315

Method notation: -L means only the left-side norm is used, -R means only the right-side norm is used, and -L_1 means the L_1 norm is used.

$$S_U = \sum_{u=1}^{M}\sum_{v=1}^{M} c_{v\to u}\left(\frac{\mathbf{e}_u}{||\mathbf{e}_u||^2} - \frac{\mathbf{e}_v}{||\mathbf{e}_v||^2}\right)^2$$

Table 6: Smoothness loss of the embeddings learned by LightGCN and MF (the lower the smoother).

Dataset	Gowalla	Yelp2018	Amazon-book
	Smoothness of User Embeddings		
MF	15449.3	16258.2	38034.2
LightGCN-single	12872.7	10091.7	32191.1
	Smoothness of Item Embeddings		
MF	12106.7	16632.1	28307.9
LightGCN-single	5829.0	6459.8	16866.0

LightGCN / Experiments

Hyper-Parameter Sensitivity

$$L_{BPR} = -\sum_{u=1}^{M} \sum_{i \in \mathcal{N}_u} \sum_{j \notin \mathcal{N}_u} \ln \sigma(\hat{y}_{ui} - \hat{y}_{uj}) + \lambda ||\mathbf{E}^{(0)}||^2$$

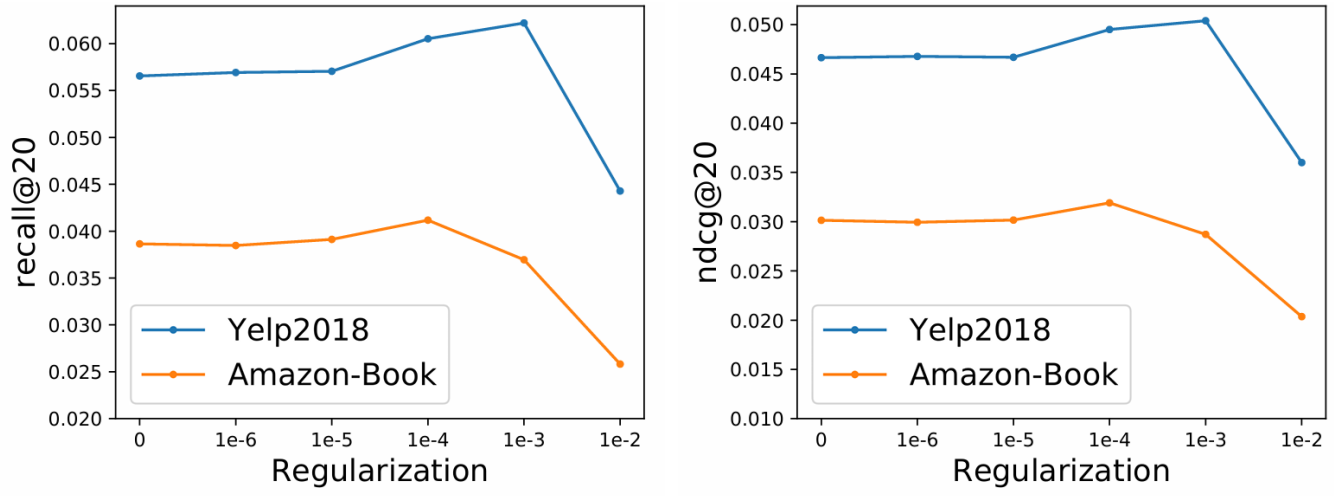


Figure 5: Performance of 2-layer LightGCN w.r.t. different regularization coefficient λ on Yelp and Amazon-Book.

LightGCN / Conclusion

LightGCN

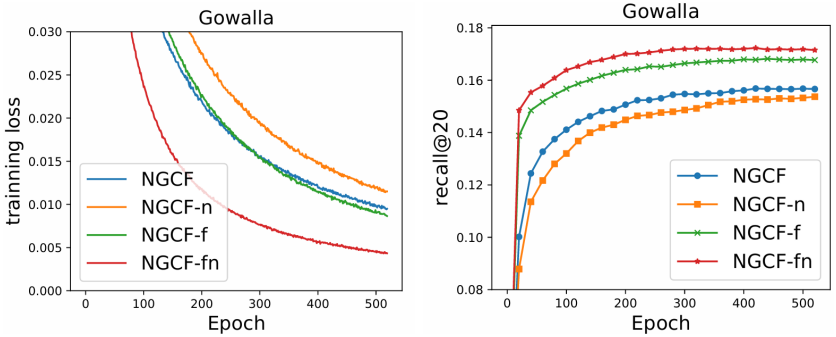
- ☐ Motivated by the CF environment, simplified NGCF
- ☐ Proved that complicated designs are unnecessary for CF

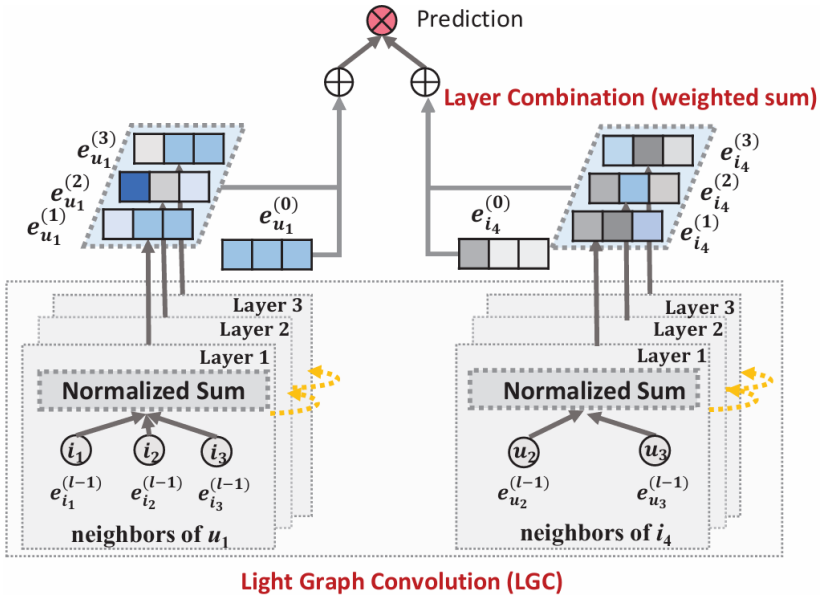
Advantages of Simplicity

- ☐ Simple structure allows for more interpretability
- ☐ Proved LightGCN subsumes the effect of self-connection
- ☐ Proved LightGCN has rational smoothing mechanism

Lessons

- ☐ Ablations critical for understanding the impact of each operation
- ☐ Performance doesn't stem from complexity





Thank you

Q&A