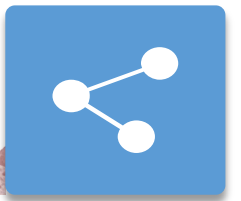




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# Profiling the Design Space for Graph Neural Networks based Collaborative Filtering

Zhenyi Wang<sup>1</sup>, Huan Zhao<sup>2</sup>, Chuan Shi<sup>1</sup>

<sup>1</sup>Beijing University of Posts and Telecommunications, China

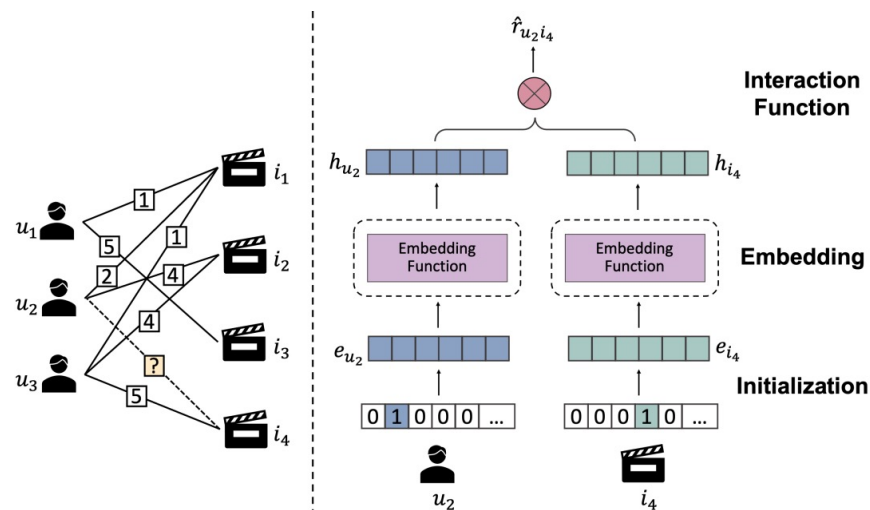
<sup>2</sup>4Paradigm Inc., China

- 1 Background**
- 2 The Design Space**
- 3 Evaluation**
- 4 Conclusions**

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- **Collaborative Filtering (CF)** has been one of the most popular recommender system (RS) methods
- **Graph Neural Networks (GNNs)** have been incorporated for the CF tasks, since the user-item interactions can be naturally modeled as a bipartite graph





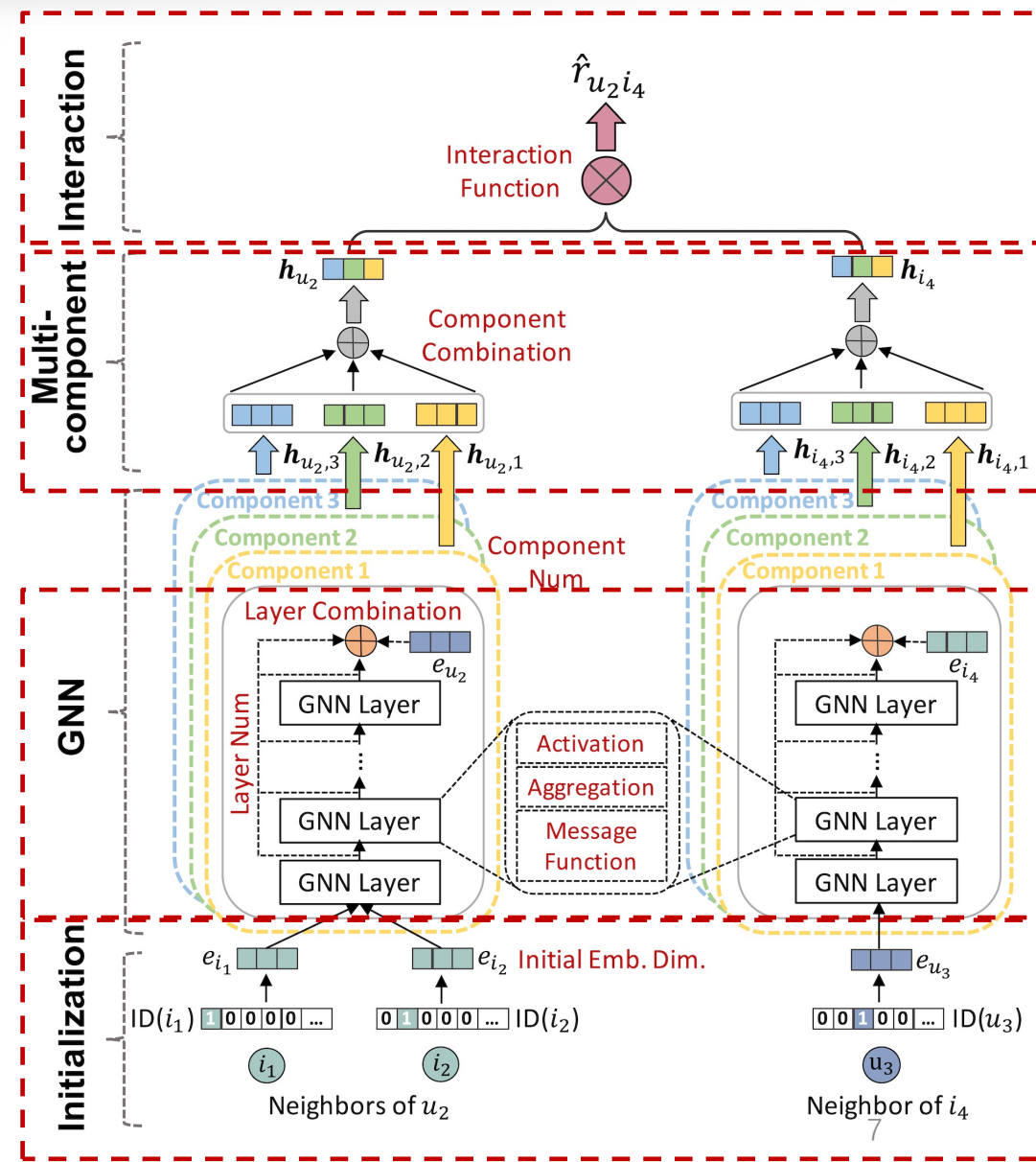
- Existing GNN-based methods are mainly limited to designing a single best architecture for a specific scenario
- Little has been done to systematically understand the influences of different design dimensions of GNN-based CF on recommendation performance

We propose to profile the **design space** of existing GNN-based methods for CF

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- 4 modules of the unified framework:
  - **Initialization** performs embedding matrix ID-lookup
  - **GNN** refines the embeddings via the propagation of GNN layers
  - **Multi-component** models diverse user interests from different aspects
  - **Interaction** predicts the rating value of the user-item pair
- Covers extensive popular GNN-based CF models
- On top of the framework, 9 **design dimensions** can be extracted





## ■ Popular choices in the 9 design dimensions:

Design Dimension	Choices
Initial Embedding Dimension $d$	64, 128, 256
Message Function $m(\cdot)$	Identity, Hadamard
Aggregation $f(\cdot)$	None, GCN, GAT, GIN, GraphSAGE
Activation $\sigma(\cdot)$	Identity, Sigmoid, Tanh, ReLU, PReLU, LeakyReLU
Layer Number $L$	1, 2, 3, 4
Layer Combination $g(\cdot)$	Stack, Concat, Sum, Mean
Component Number $K$	1, 2, 3, 4
Component Combination $c(\cdot)$	Concat, Mean, Att
Interaction Function $p(\cdot)$	Dot Product, Concat+MLP, Sum+MLP

$$\mathbf{h}_u^{(l+1)} = \sigma \left( \hat{r}_{ui} = \boxed{p}(\mathbf{h}_u, \mathbf{h}_i) \cdot \{ \mathbf{h}_u^{(l)} \} \right)$$

non-learnable interaction functions, Dot Product  
 4 GNN aggregators and None to enlarge the  
 capacity of the design space to include those  
 non-GNN-based models

## ■ To explore the impacts of different design dimensions, we propose to profile the **design space**, defined as the Cartesian product of design dimensions<sup>[1]</sup>

[1] J. You et al. Design space for graph neural networks. NeurIPS 2020.



- Popular CF methods that can be instantiated from the proposed design space:

Category	Model	$m(\cdot)$	$f(\cdot)$	$\sigma(\cdot)$	$g(\cdot)$	$c(\cdot)$	$p(\cdot)$	Single-/Multi-component
Classic	MF [16, 24]	Identity	None	Identity	Stack	-	Dot Product	Single
	LLORMA [18, 46]	Identity	None	Identity	Stack	Att	Dot Product	Multiple
MLP-based	NCF [11]	Identity	None	ReLU	Stack	-	Concat+MLP	Single
GNN-based	NGCF [36]	Hadamard	GCN	LeakyReLU	Concat	-	Dot Product	Single
	LightGCN [10]	Identity	GCN	Identity	Mean	-	Dot Product	Single
	LR-GCCF [2]	Identity	GCN	Identity	Concat	-	Dot Product	Single
	SMOG-CF [43]	Hadamard	GCN	ReLU	Concat	-	Dot Product	Single
	PinSage [41]	Identity	GraphSAGE	ReLU	Stack	-	Dot Product	Single
	MCCF [38]	Identity	GAT	ReLU	Stack	Att	Concat+MLP	Multiple
	DGCF [37]	Identity	GCN	Tanh	Sum	Concat	Dot Product	Multiple

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## ■ Datasets

Dataset	# of Users	# of Items	# of Interactions	Rating Scale	Density
Yelp <sup>1</sup>	58,069	31,721	1,160,605	[1,5]	0.063%
Amazon-CDs [9]	31,296	24,379	622,163	[1,5]	0.082%
Amazon-Movies [9]	44,439	25,047	1,070,860	[1,5]	0.096%
YahooMusic [5, 25]	1,357	1,363	5,335	[1,100]	0.28%
Amazon-Beauty [9]	7,068	3,570	79,506	[1,5]	0.32%
Flixster[13, 25]	2,341	2,956	26,173	[0.5,5]	0.38%
Douban [23, 25]	2,999	3,000	136,891	[1,5]	1.52%
MovieLens-1M <sup>2</sup>	6,040	3,706	1,000,209	[1,5]	4.47%
MovieLens-100K <sup>3</sup>	943	1,682	100,000	[1,5]	6.31%

<sup>1</sup> <https://www.yelp.com/dataset/>

<sup>2</sup> <https://grouplens.org/datasets/movielens/100k/>

<sup>3</sup> <https://grouplens.org/datasets/movielens/1m/>

## ■ Evaluation technique: *controlled random search*<sup>[1]</sup>

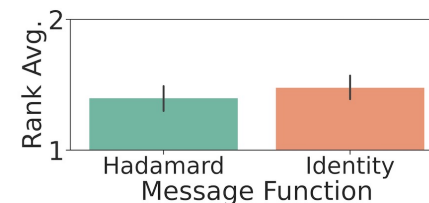
Group No.	Configuration Space					Experimental Results	
	Message Function	Activation	...	Interaction Function	Dataset	Performance	Ranking
1	Identity	ReLU	...	Dot Product	Yelp	0.8996	2
	Hadamard					0.8665	1
2	Identity	Sigmoid	...	Concat+MLP	Amazon-CDs	0.7636	1
	Hadamard					0.7812	2
...							
S	Identity	Tanh	...	Sum+MLP	MovieLens-1M	0.8231	1(tie)
	Hadamard					0.8231	1(tie)

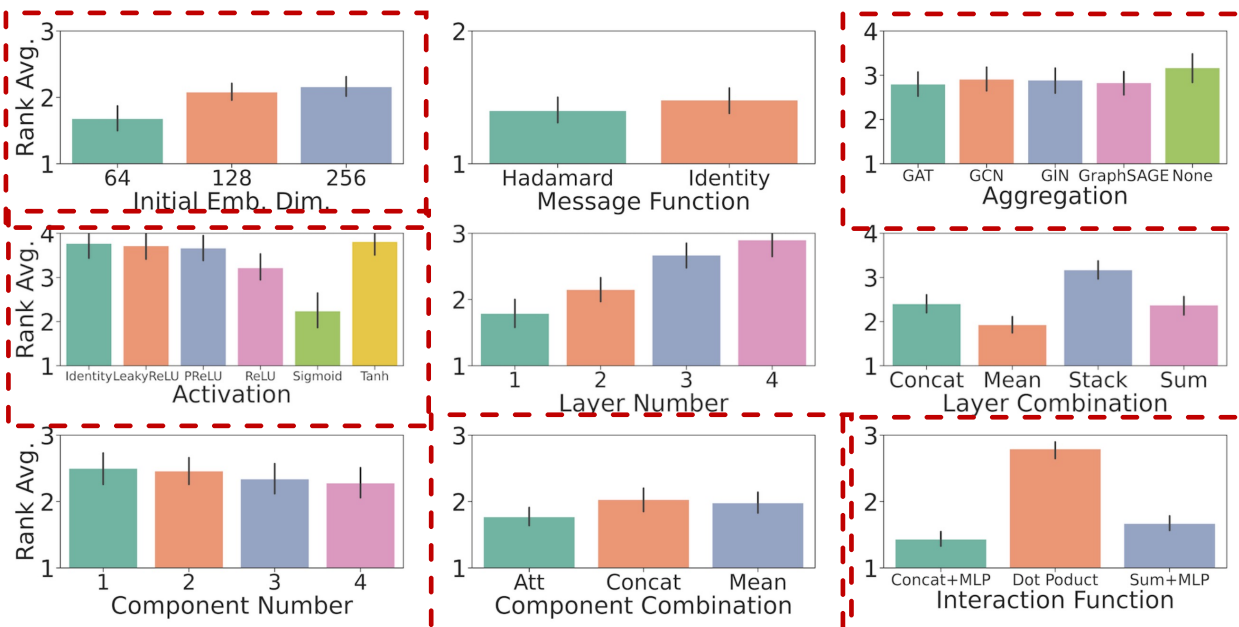
## ■ Loss: *MSE*

$$L = \frac{\sum_{(u,i) \in O_t} (\hat{r}_{ui} - r_{ui})^2}{|O_t|} + \lambda \|\Theta\|^2$$

## ■ Evaluation Metric: *RMSE*

$$RMSE = \sqrt{\frac{\sum_{(u,i) \in O_e} (\hat{r}_{ui} - r_{ui})^2}{|O_e|}}$$





- The experimental findings provide valuable insights for effectively designing top-performing models

- GAT and GraphSAGE slightly outperform, and None is competitive
- Sigmoid stands out
- Att is the preferable multi-component combination
- Neural interaction is superior to Dot Product
- ...

- There exists some **redundancy** in the design space
- The vanilla design space can be further **pruned**
  - e.g., the initial embedding dimension can be fixed as 64
- Boost the searching efficiency of top-performing models



- By remaining favorable design choices, the pruned design space contains **a higher concentration of top-performing models**
- Choices in the design dimensions of the pruned design space:

Design Dimension	Choices
Initial Embedding Dimension $d$	64
Message Function $m(\cdot)$	Identity, Hadamard
Aggregation $f(\cdot)$	None, GraphSAGE
Activation $\sigma(\cdot)$	Identity, Sigmoid, ReLU
Layer Number $L$	1, 2
Layer Combination $g(\cdot)$	Mean
Component Number $K$	1, 4
Component Combination $c(\cdot)$	Att
Interaction Function $h(\cdot)$	Concat+MLP, Sum+MLP

- 96 v.s. 103,680, reduction of three orders of magnitude (1,080x)



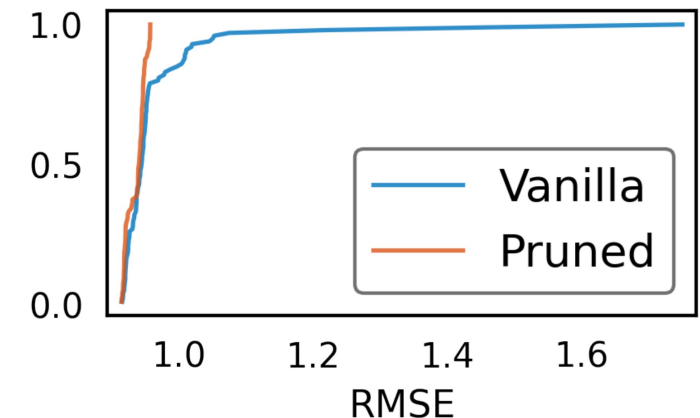
## Evaluation technique

- *RMSE empirical distribution function (EDF)*<sup>[1]</sup>

- Suppose **1** as the indicator function,  $n$  as the number of sampled models, each with RMSE  $x_i$ . The RMSE EDF is given by:

$$F(x) = \frac{1}{n} \sum_{i=1}^n \mathbf{1}[x_i < x]$$

- $F(x)$  gives the fraction of models with RMSE less than  $x$

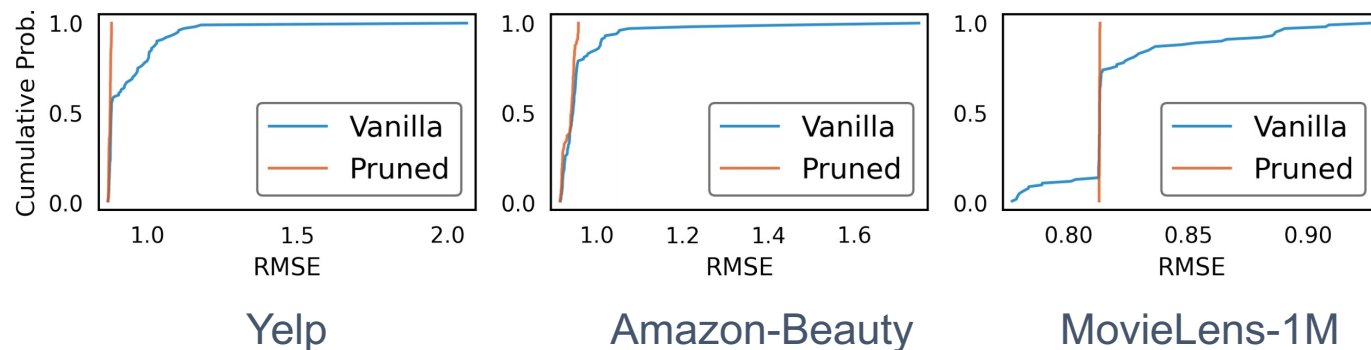


- Comparing distributions can help to obtain more robust and informative conclusions



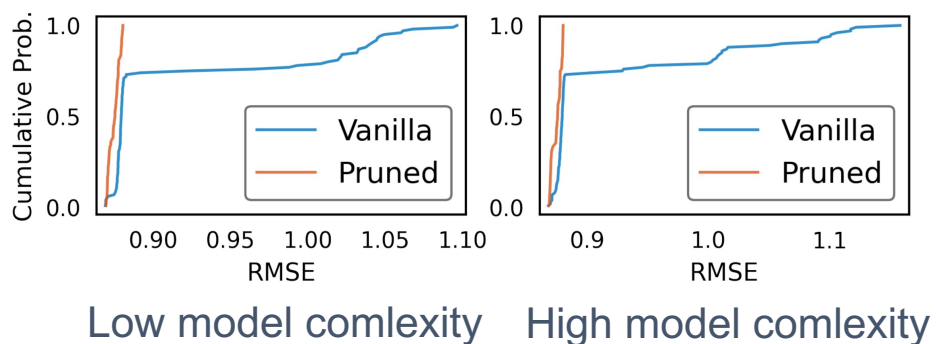
## Generalization evaluation

### Different levels of density

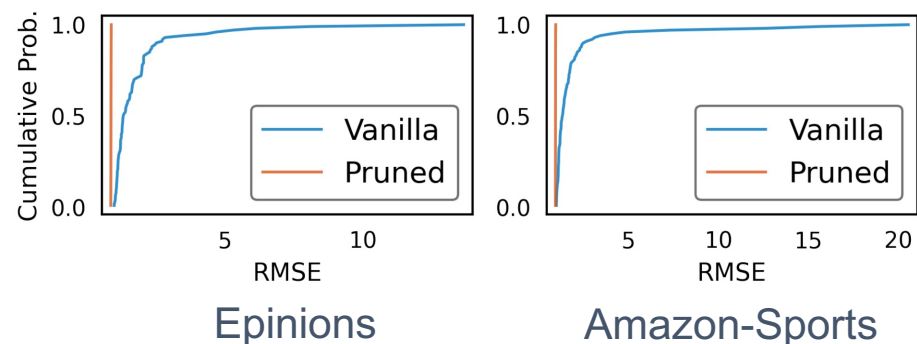


Dataset	Density
Yelp <sup>1</sup>	0.063%
Amazon-CDs [9]	0.082%
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Douban [23, 25]	1.52%
MovieLens-1M <sup>2</sup>	4.47%
MovieLens-100K <sup>3</sup>	6.31%

### Different model complexity



### Generalization to new datasets



The pruned design space consistently holds **better quality**, which demonstrates its **strong generalization** to various new settings.



- We perform random search on the pruned design space
  - The searched model architectures on new datasets :

Dataset	$m(\cdot)$	$f(\cdot)$	$\sigma(\cdot)$	$L$	$K$	$p(\cdot)$
Epinions	Hadamard	None	ReLU	1	1	Sum+MLP
Amazon-Sports	Identity	GraphSAGE	Sigmoid	1	4	Sum+MLP

- Performance comparisons with baselines:

Model	Epinions	Amazon-Sports
MF [16]	$0.9945 \pm 0.0000$	$0.9882 \pm 0.0007$
NCF [11]	$1.0070 \pm 0.0055$	$0.9342 \pm 0.0008$
NGCF [36]	$1.1437 \pm 0.0240$	$1.0668 \pm 0.0038$
LightGCN [10]	$0.9926 \pm 0.0001$	$0.9705 \pm 0.0003$
DGCF [37]	$1.6800 \pm 0.2272$	$0.9894 \pm 0.0000$
RS-10	$0.8729 \pm 0.0014$	$0.9327 \pm 0.0006$

- The randomly searched models outperform all the baselines
- The pruned design space helps to **efficiently** design top-performing models for **new recommendation scenarios**

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## ■ Problem

- The **first attempt** to profile the design space of GNN-based CF

## ■ Evaluation of the Design Space

- Propose **a unified framework** covering popular GNN-based CF models
- Develop a design space and **evaluate** it by extensive experiments

## ■ Evaluation of the Pruned Design Space

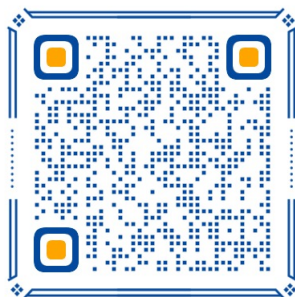
- Prune the design space for **a higher concentration** of top-performing models
- Empirical studies demonstrate its **high quality** and **strong generalization ability**



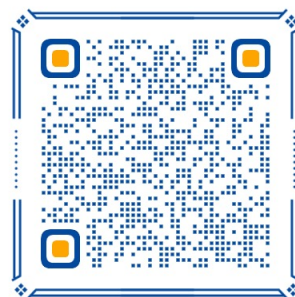
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## Thank you!



Paper



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Contact: Zhenyi Wang, [zy\\_wang@bupt.edu.cn](mailto:zy_wang@bupt.edu.cn)