Machine Learning on Graph for Recommendation and more

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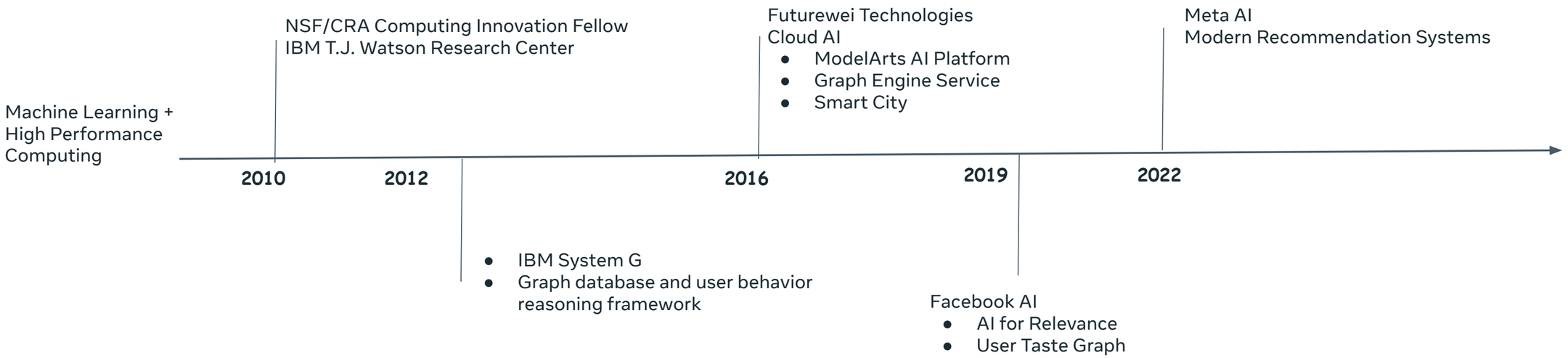
MRS, Meta

About me


Machine Learning +
High Performance
Computing
2010
NSF/CRA Computing Innovation Fellow
IBM T.J. Watson Research Center
2012
IBM System G
Graph database and user behavior reasoning framework
2016
Futurewei Technologies
Cloud AI
ModelArts AI Platform
Graph Engine Service
Smart City
2019
Facebook AI
AI for Relevance
User Taste Graph
2022
Meta AI
Modern Recommendation Systems

Agenda

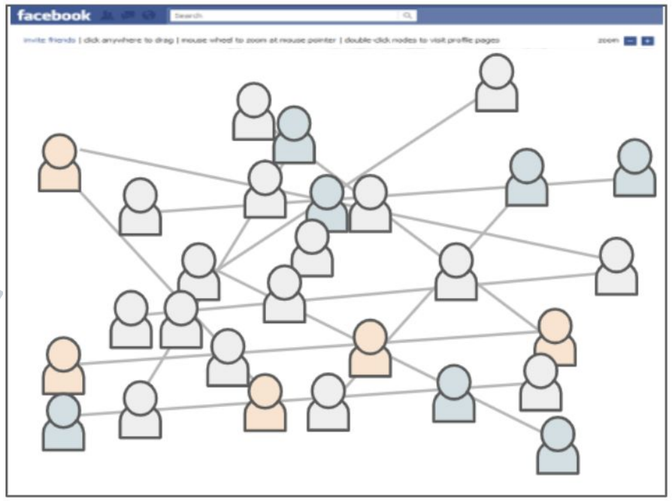
01 **Graph in RecSys**

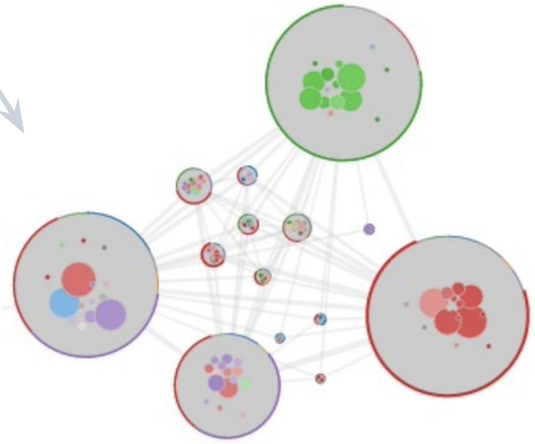
02 Graph sparse nodes in recommendation

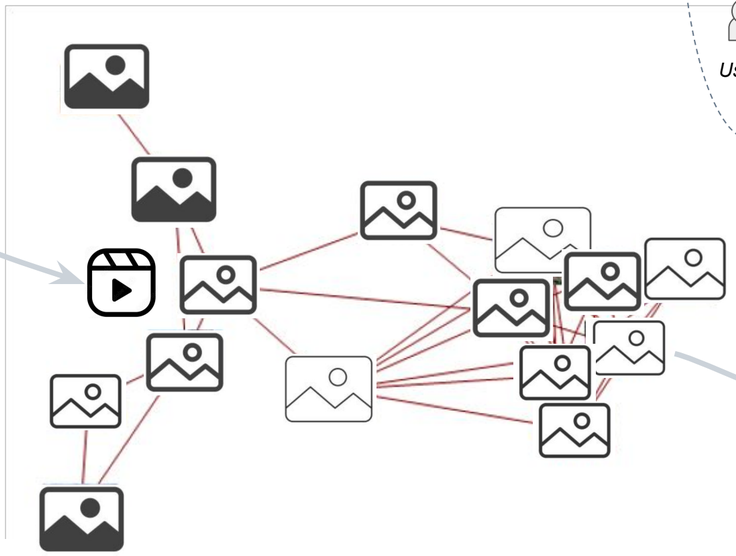
03 GNN expressiveness: depth, scope, & MoE

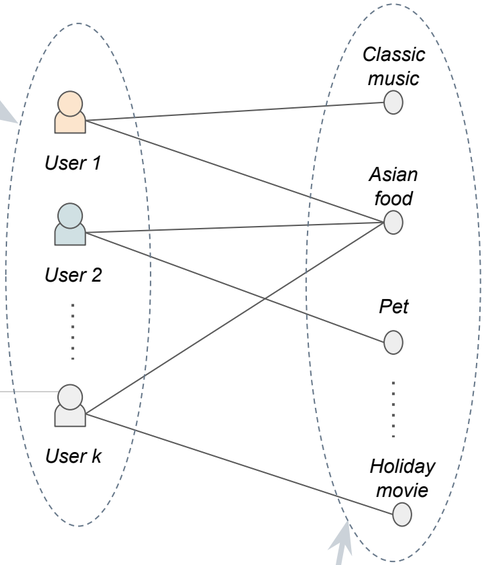
04 Conclusion & Opportunities

Graph is everywhere



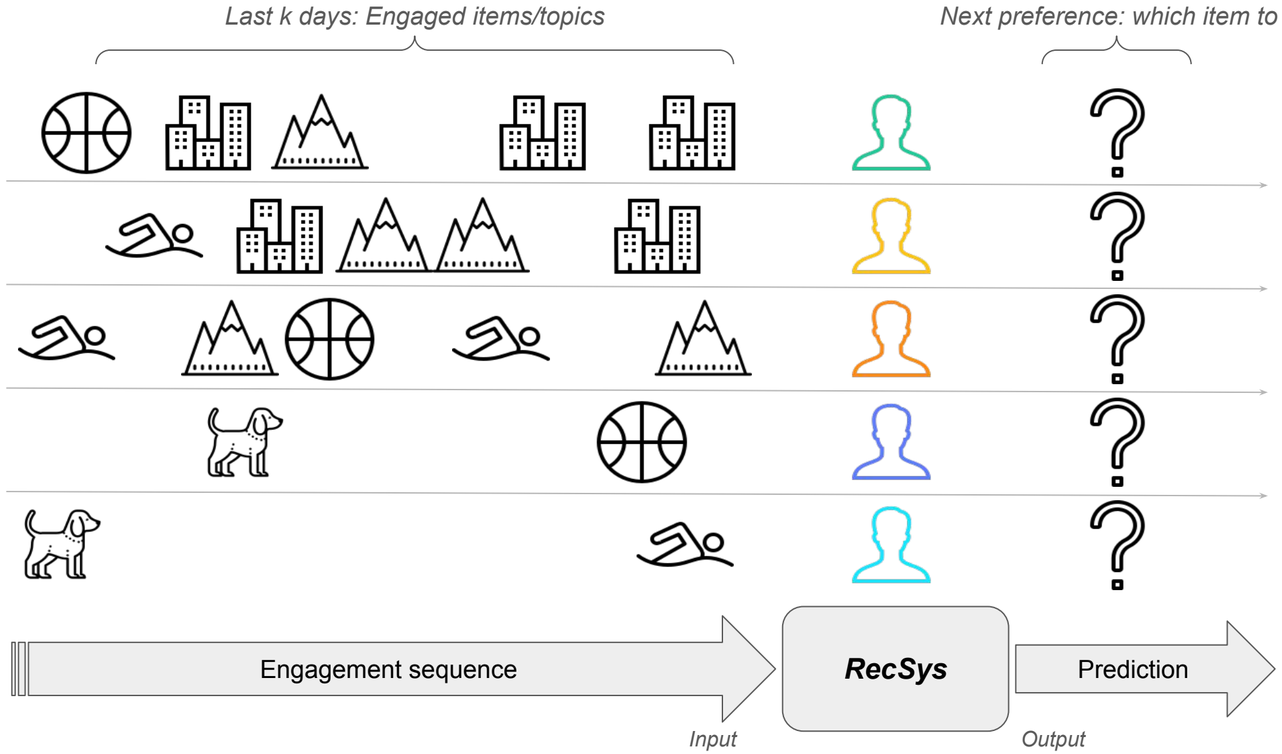




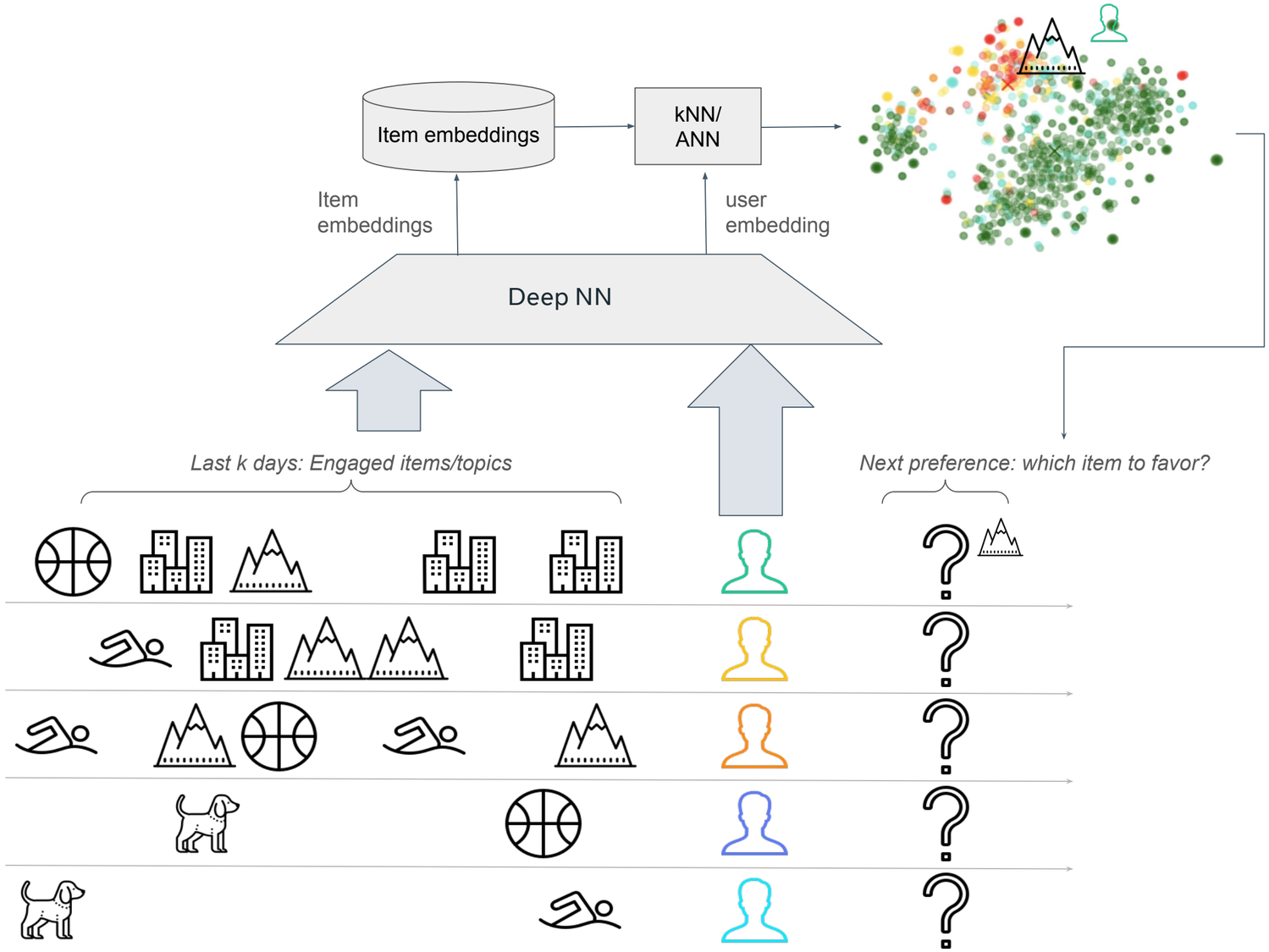


Recommendation system

A recsys is a subclass of information filtering system that provides suggestions for items that are most pertinent to a particular user.



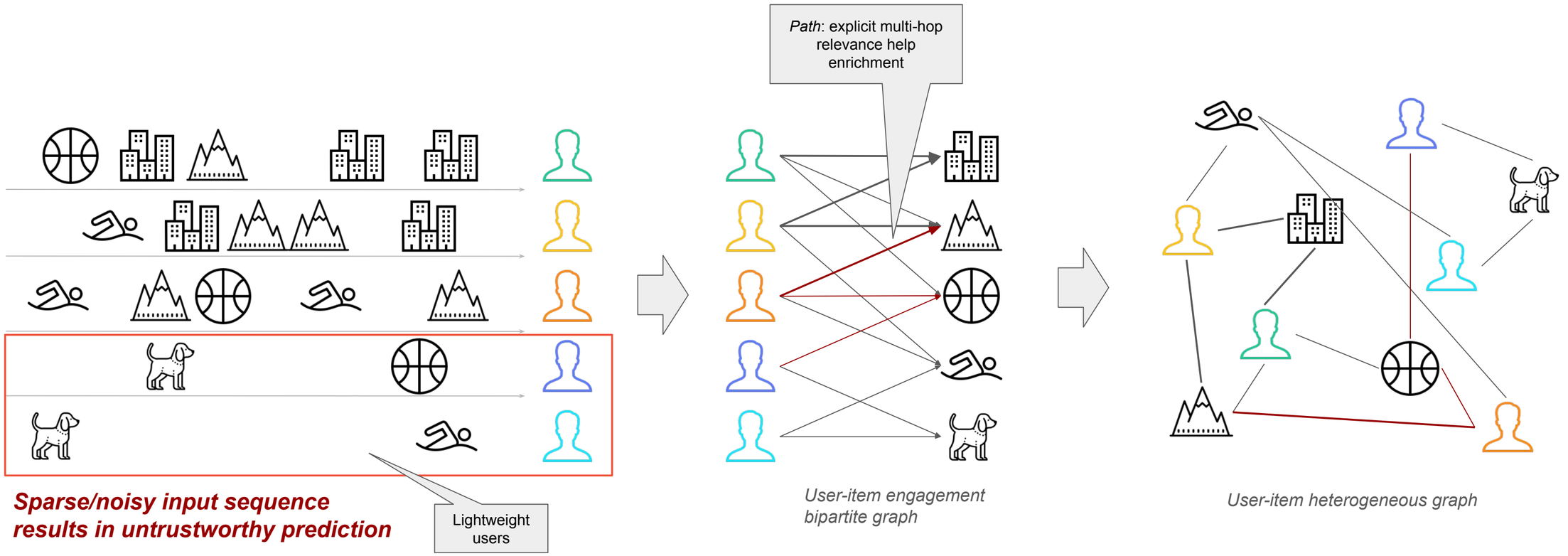
01 Graph in RecSys



Sequence vs Graph

ML101: "Garbage in, garbage out" (GIGO)

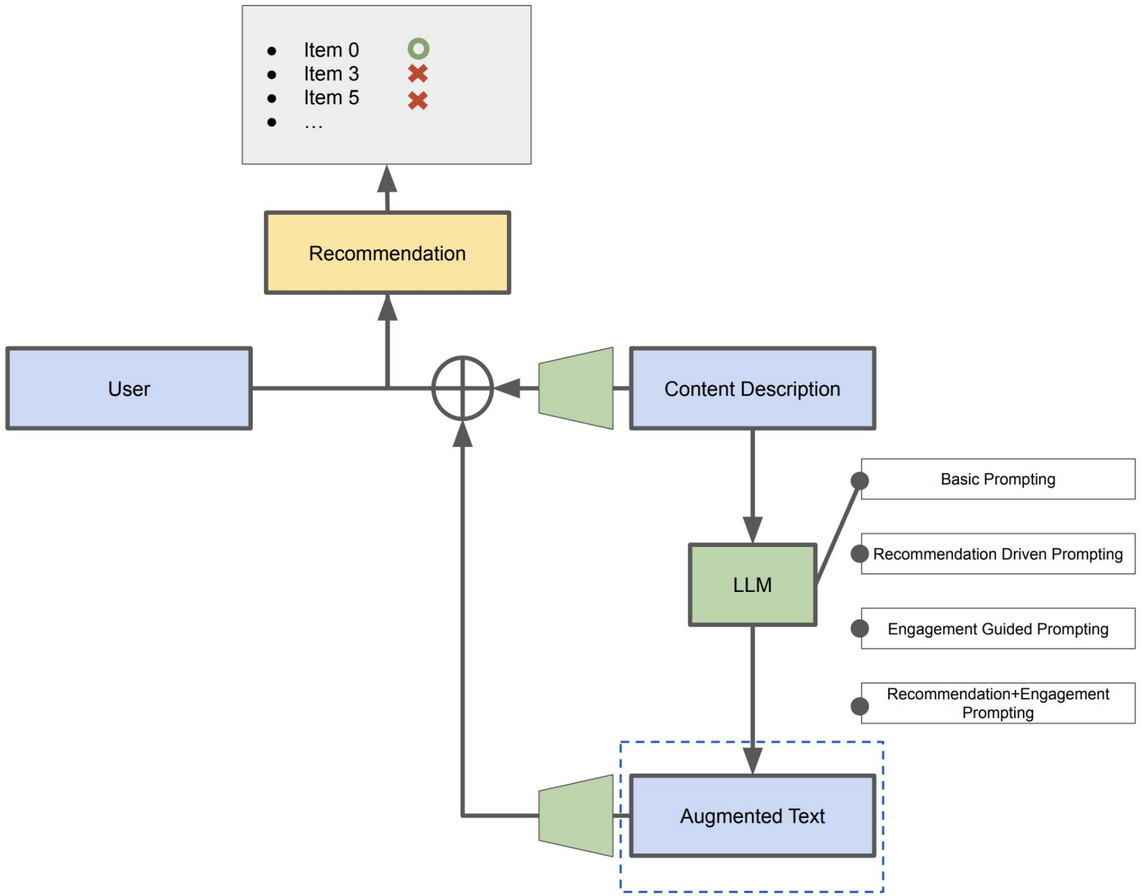
- RecSys prediction counts on user engagement history
- Cold start users have limited & noisy engagement history, if not unavailable
- How can we enrich user signals by leveraging latent relevance?

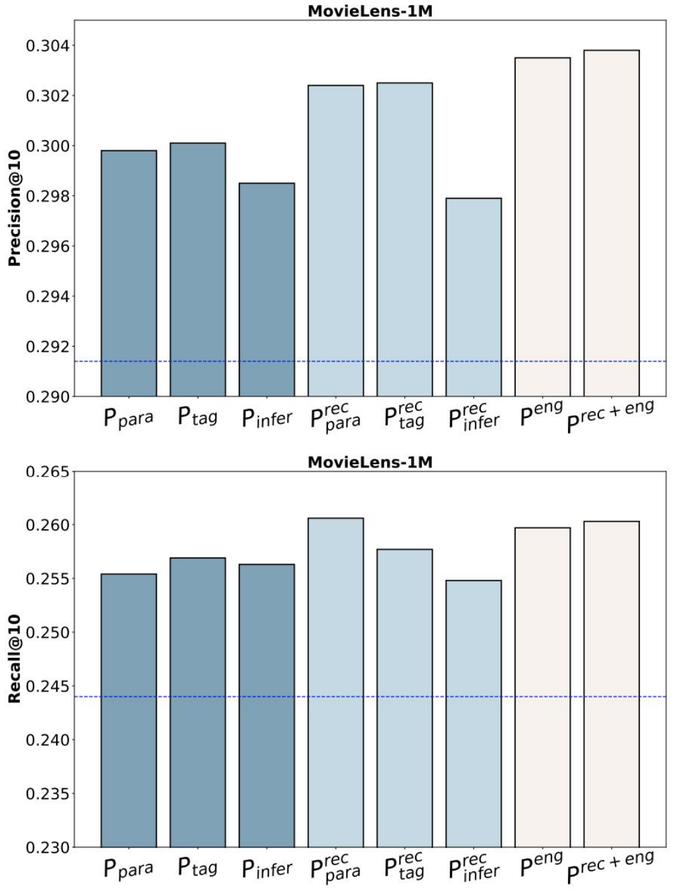


H. Zeng, Y. Xia, et al, LLM-Rec: Personalized Recommendation via Prompting Large Language Models, NAACL 2024

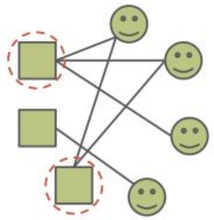
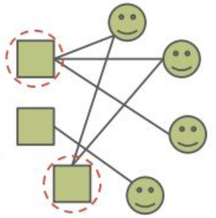
S. Jiang, Z. Shakeri, Y. Xia, et al, ResPROMPT: Residual Connection Prompting Advances Multi-Step Reasoning in Large Language Models, NAACL 2024

Graph meets LLM in RecSys

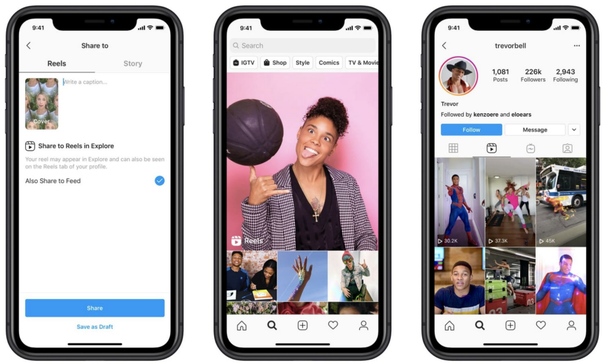




Description: *A group of toys embark on a journey of self-discovery as they learn the true meaning of friendship.*

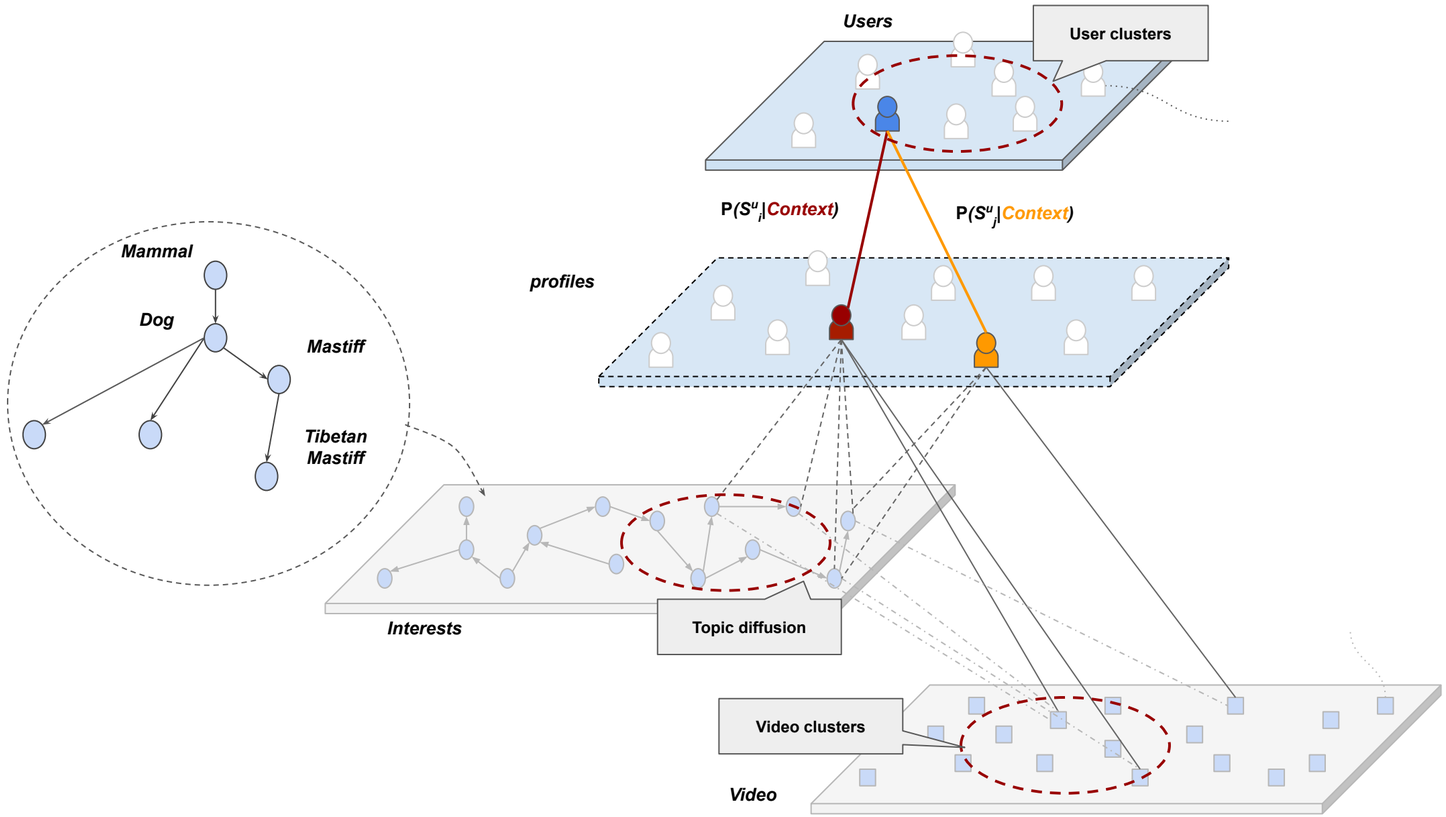
Basic Prompting	Recommendation-Driven Prompting	Engagement-Guided Prompting	Recommendation + Engagement
	… this is for recommendation …		… this is for recommendation … 
Model Input	**Model Input**	**Model Input**	**Model Input**
The description of an item is as follows: '{description}', paraphrase it	The description of an item is as follows: '{description}', what else should I say if I want to recommend it to others?	Summarize the commonalities among the following descriptions: '{description}'; '{descriptions of other important neighbors}'	The description of an item is as follows: '{description}'. What else should I say if I want to recommend it to others? This content is considered to hold some similar attractive characteristics as the following descriptions: '{descriptions of important neighbors}'
Model Output	**Model Output**	**Model Output**	**Model Output**
A collection of toys go on an adventure to understand the power of companionship.	This is a heartwarming story about friendship and self-discovery. It follows a group of toys on an exciting journey as they learn the importance of being there for each other. With its charming characters and captivating plot, this is a must-read for anyone looking for a fun and inspiring adventure.	The commonalities among the descriptions are that they all involve journeys, discovery, and comedic elements.	This item is a great choice for those looking for an entertaining and heartwarming story about friendship. It follows a group of toys on a journey of self-discovery as they learn the true meaning of friendship. It has a similar feel to classic films such as 'Being John Malkovich', 'Airplane!' and 'Monty Python and the Holy Grail', combining elements of comedy, adventure and fantasy. It's sure to be a hit with viewers of all ages!

Case study: Graph for user interest modeling



https://about.instagram.com/blog/announcements/introducing-instagram-reels-announcement

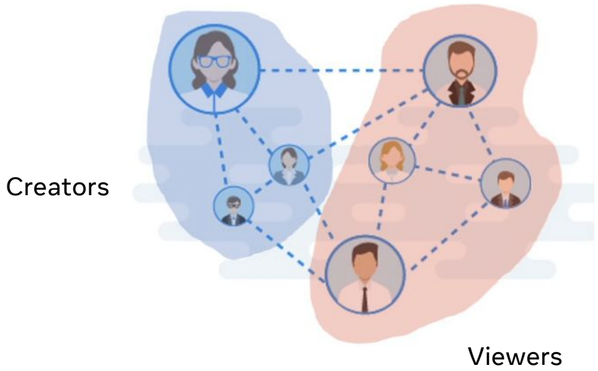
Graphs provide advanced modeling and system techniques for holistic user interest understanding and personalized recommendation, which provides interpretability to the output of some SOTA ML models, as well as supporting better user control over recommendations.



Case study: Graph ranking for audience matching

- Graph representation
  - Creator, viewer, media ⇒ heterogeneous nodes
  - Following, engagement, profile matching ⇒ edges

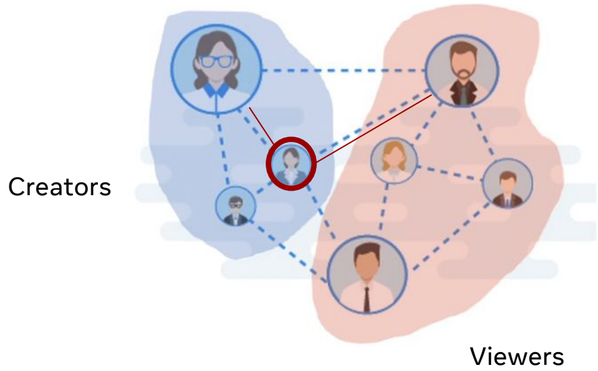
- Graph ranking
  - For a given creator (or a creator's newly shared media), rank the viewers within the neighborhood of the creator
    - Heterogeneous PPR with the creator as a root
    - GCN message passing with rich feature support



Case study: Graph ranking for audience matching (2)

- Personalized PageRank (PPR) helps find related creators for a given viewer (source node) in audience matching
  - r_s = (1 - c) * e_s + c * A * r_s

    ⇒ ppr_s(creator) = (1 - c) * e_s + c * $\Sigma_{\text{creator'} \in \text{path(creator-v-creator')}}$ ppr_s(creator') / deg(creator')
    - A: the adjacency matrix
    - s: the source node, say, a given viewer
    - c: damping factor, e.g. 0.85
    - e_s: biased teleportation vector, e.g. [0, 0, ….,1,..0] where e_s[s]=1
    - r_s: vector of probability showing the relevance of v to source,i.e., ppr[v]
    - deg(creator'): #path
  - What is missing?
    - deg(u) reflects interest match, not the size of connected followers
    - deg(u) does not reflect the "size/status" of a creator i.e. new /casual/power creator
  - Treatment?



Agenda

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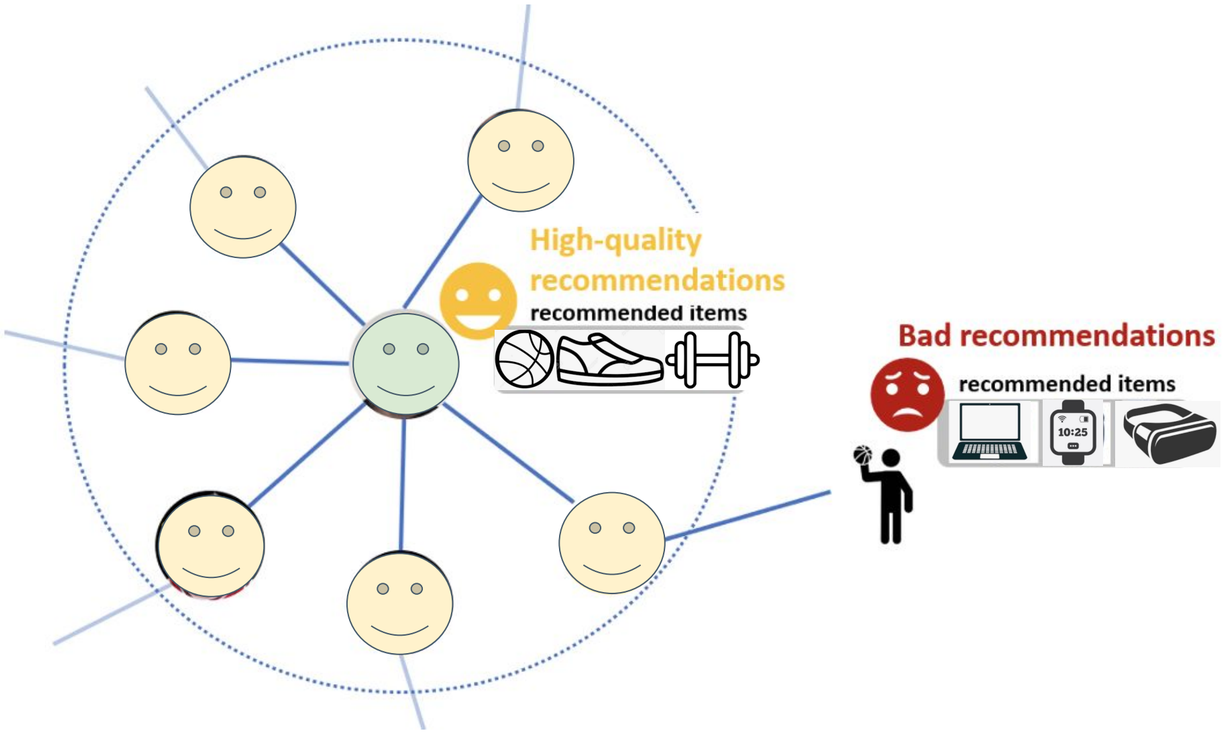
02 **Graph sparse nodes in recommendation**

03 GNN expressiveness: depth & scope

04 Conclusion & Opportunities

Disparity of node degrees in GCN

- Another example: Online advertising
  - Celebrities often enjoy high-quality recommendations
  - Grassroot users often suffer from bad recommendations



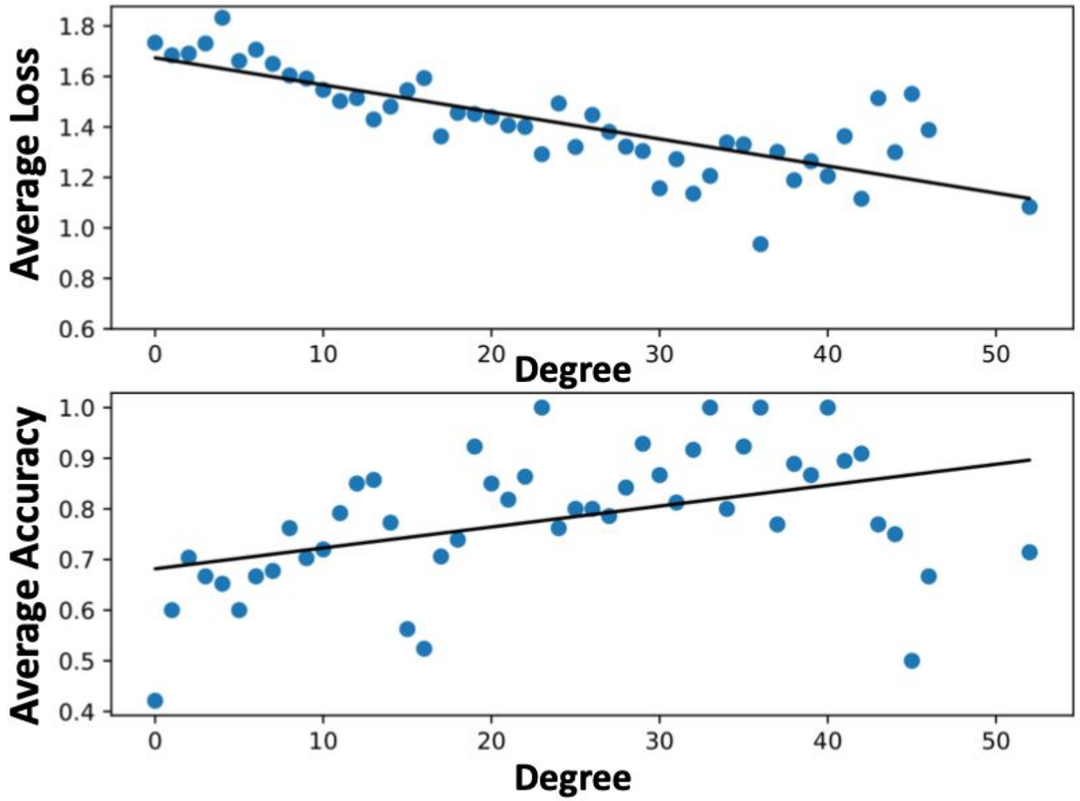
J. Kang, Y. Zhu, Y. Xia, J. Luo, and H. Tong, RawlsGCN: Towards Rawlsian Difference Principle on Graph Convolutional Network, TheWebConf'22

Disparity of node degrees in GCN

- Illustrative example
  - 2-layer GCN on Amazon-Photo
  - Average loss/accuracy of degree groups

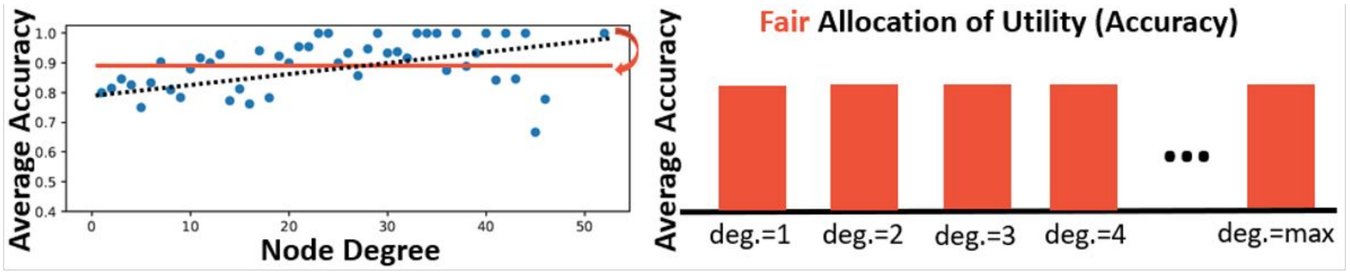
- Observation
  - Low-degree nodes suffer from higher loss and lower accuracy
  - Real-world graph is often long-tailed
  - GCN might be primarily beneficial to a few high-degree nodes

If small-sized creators are what we are interested in, then the GCN framework needs some remedy.



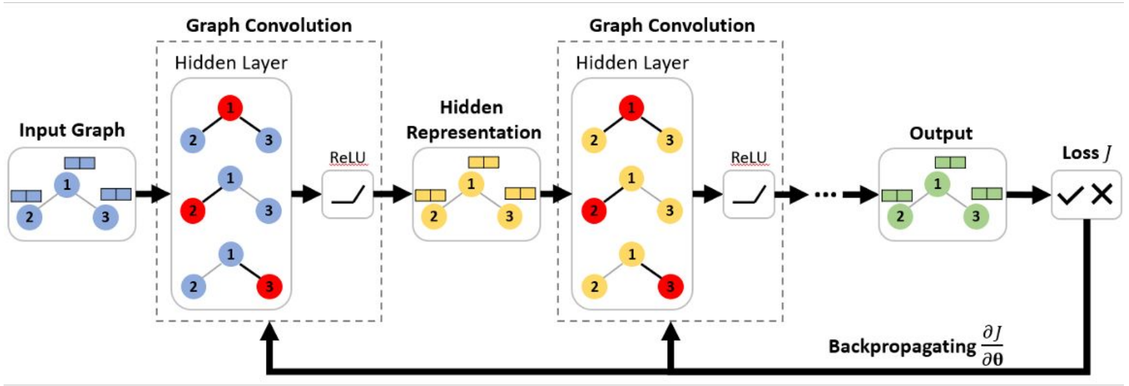
Rawlsian difference principle for GCN

- Given
  - An undirected graph $\mathcal{G}=(\mathbf{A},\mathbf{X})$
  - An L-layer GCN with weights $\boldsymbol{\theta}$
  - A task-specific loss J
- Find: A well-trained GCN that
  - Minimizes the task-specific loss
  - Achieves a fair allocation of utility for the groups of nodes with the same degree
- Key question:
  - When is the allocation of utility fair?



Understand the loss

- **Intuition:** Understand why the loss varies **after training**
- **What happens during training?**
  - –Extract node representations
  - –Predict the outcomes using the node representations
  - –Calculate the task-specific loss J
  - –Update model weights **θ** by the gradient $\partial J/\partial \boldsymbol{\theta}$ ← key component for training
- **Question:** Is the unfairness caused by the gradient?



Rawlsian difference principle for GCN

- Rawlsian difference principle
  - Equality principle in distributive justice
  - Equality ⇒ maximize welfare of worst-off grc

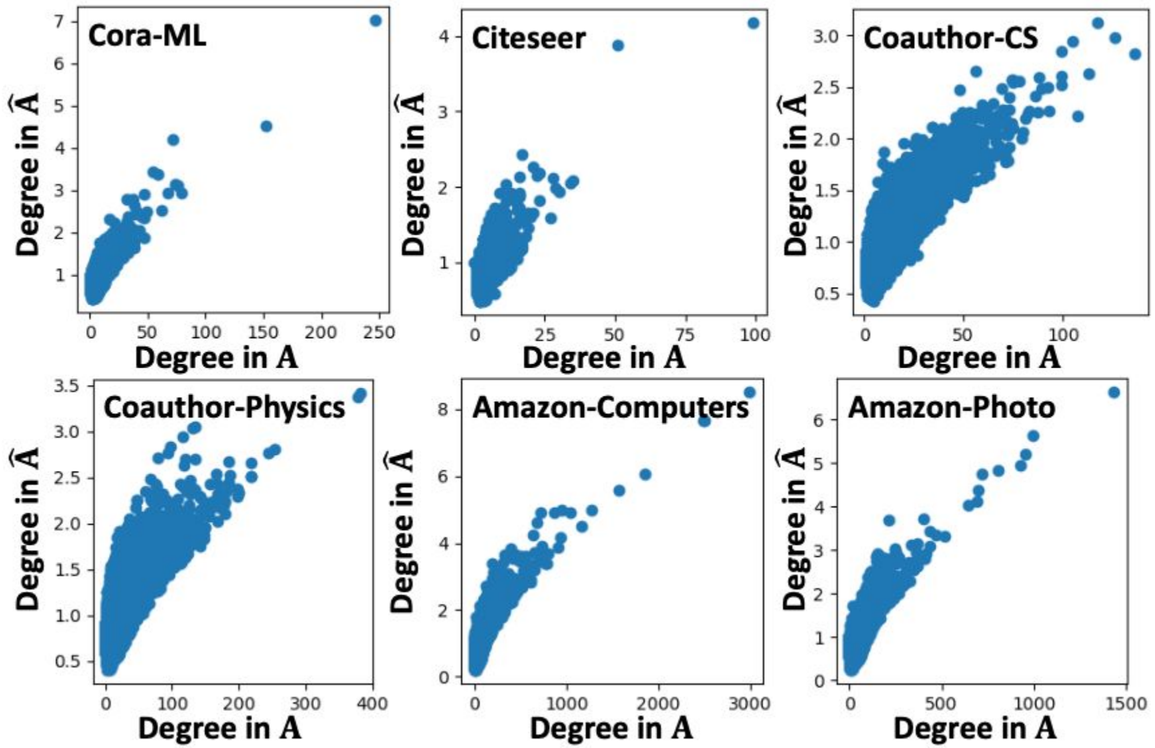
$$\min_{\theta} \quad \mathrm{Var}(\{U(\mathcal{D}_i, \theta) | i = 1, \ldots, h\})$$
$$\text{s.t.} \quad \theta = \operatorname{argmin} J(\mathcal{D}, \mathbf{Y}, \theta)$$

- Importance on the gradient
  - V ong nodes

$$\frac{\partial J}{\partial \mathbf{W}^{(l)}} = \sum_{j=1}^{n} deg_{\hat{\mathbf{A}}}(j)\mathbf{I}_j^{(row)} = \sum_{i=1}^{n} deg_{\hat{\mathbf{A}}}(i)\mathbf{I}_i^{(col)}$$

    - $\mathbf{I}_j$ is a degree-free influence of node j

Higher node degree in A, more importance it has on the gradient of the weight matrix.



Rawlsian GCN

- Doubly Stochastic Matrix Computation Normalize the importance of influence matrices to mitigate the node degree-related unfairness, so that each node will have equal importance in updating the weight parameters
  - Computing the doubly stochastic matrix is nontrivial, so we adopt the Sinkhorn-Knopp
- Rawlsian GCN
  - Gradient is computed using the doubly stochastic matrix, so that all nodes will have equal importance in determining the gradient

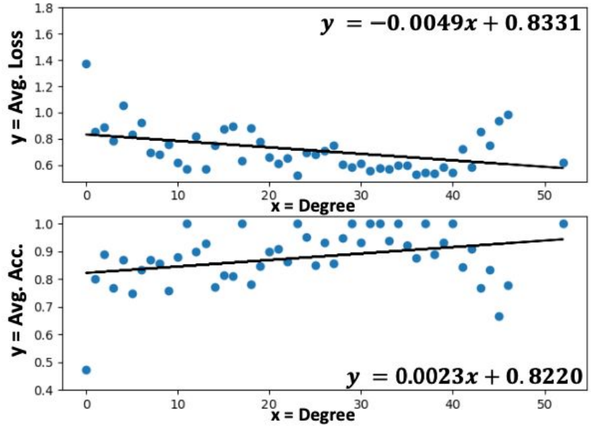
$$\frac{\partial J}{\partial \mathbf{W}^{(l)}}_{\text{fair}} = (\mathbf{H}^{(l-1)})^T \hat{\mathbf{A}}_{DS}^T \frac{\partial J}{\partial \mathbf{E}^{(l)}}$$

where $\mathbf{E}^{(l)} = \hat{\mathbf{A}}\mathbf{H}^{(l-1)}\mathbf{W}^{(l)}$.

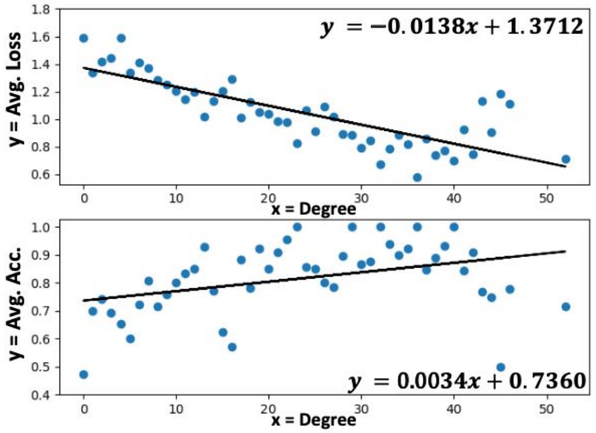
Experiments

Method	Cora-ML		Citeseer		Coauthor-CS	
	Acc.	Bias	Acc.	Bias	Acc.	Bias
GCN	80.10 ± 0.812	0.392 ± 0.046	68.60 ± 0.341	0.353 ± 0.040	93.28 ± 0.194	0.075 ± 0.004
DEMO-Net	61.60 ± 0.687	0.181 ± 0.015	60.26 ± 0.408	0.315 ± 0.022	65.90 ± 0.583	0.164 ± 0.006
DSGCN	30.26 ± 5.690	8.003 ± 2.766	31.42 ± 3.257	6.887 ± 1.947	44.20 ± 7.155	1.460 ± 0.397
Tail-GNN	78.54 ± 0.582	0.503 ± 0.284	66.34 ± 0.009	0.655 ± 0.382	92.66 ± 0.196	0.052 ± 0.031
AdvFair	67.56 ± 2.594	10.01 ± 2.480	50.26 ± 6.277	3.146 ± 2.425	84.82 ± 2.254	12.26 ± 6.797
REDRESS	75.70 ± 0.620	0.955 ± 0.213	65.80 ± 0.518	0.944 ± 0.077	92.44 ± 0.233	0.028 ± 0.003
RawlsGCN-Graph (Ours)	76.96 ± 1.098	0.105 ± 0.012	69.34 ± 0.745	0.196 ± 0.013	92.52 ± 0.264	0.043 ± 0.002
RawlsGCN-Grad (Ours)	79.34 ± 1.247	0.232 ± 0.065	68.81 ± 0.462	0.283 ± 0.047	92.68 ± 0.240	0.058 ± 0.007

Method	Coauthor-Physics		Amazon-Computers		Amazon-Photo	
	Acc.	Bias	Acc.	Bias	Acc.	Bias
GCN	93.96 ± 0.367	0.023 ± 0.001	64.84 ± 0.641	0.353 ± 0.026	79.58 ± 1.507	0.646 ± 0.038
DEMO-Net	77.50 ± 0.566	0.084 ± 0.010	26.48 ± 3.455	0.456 ± 0.021	39.92 ± 1.242	0.243 ± 0.013
DSGCN	79.08 ± 1.533	0.262 ± 0.075	27.68 ± 1.663	1.407 ± 0.685	26.76 ± 3.387	0.921 ± 0.805
Tail-GNN	OOM	OOM	76.24 ± 1.491	1.547 ± 0.670	86.00 ± 2.715	0.471 ± 0.264
AdvFair	87.44 ± 1.132	0.892 ± 0.502	53.50 ± 5.362	4.395 ± 1.102	75.80 ± 3.563	51.24 ± 39.94
REDRESS	94.48 ± 0.172	0.019 ± 0.001	80.36 ± 0.206	0.455 ± 0.032	89.00 ± 0.369	0.186 ± 0.030
RawlsGCN-Graph (Ours)	94.06 ± 0.196	0.016 ± 0.000	80.16 ± 0.859	0.121 ± 0.010	88.58 ± 1.116	0.071 ± 0.006
RawlsGCN-Grad (Ours)	94.18 ± 0.306	0.021 ± 0.002	74.18 ± 2.530	0.195 ± 0.029	83.70 ± 0.672	0.186 ± 0.068



Rawlsian GCN



GCN

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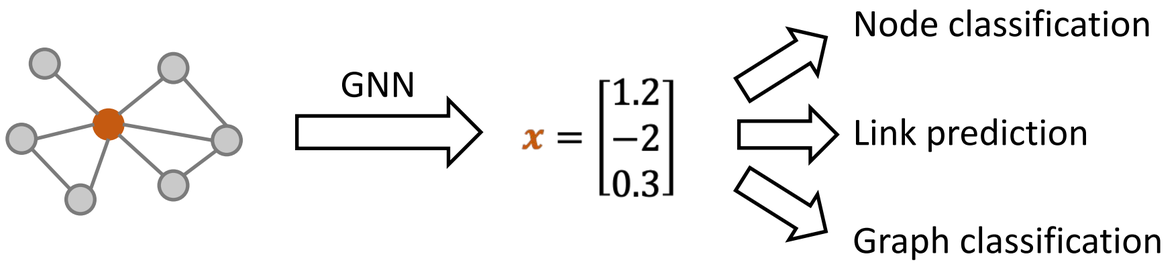
03 **GNN expressiveness: depth & scope**

04 Conclusion & Opportunities

Hanqing Zeng, Muhan Zhang, Yinglong Xia, Ajitesh Srivastava, Andrey Malevich, Rajgopal Kannan, Viktor Prasanna, Long Jin, Ren Chen, Decoupling the Depth and Scope of Graph Neural Networks, NeurIPS'21

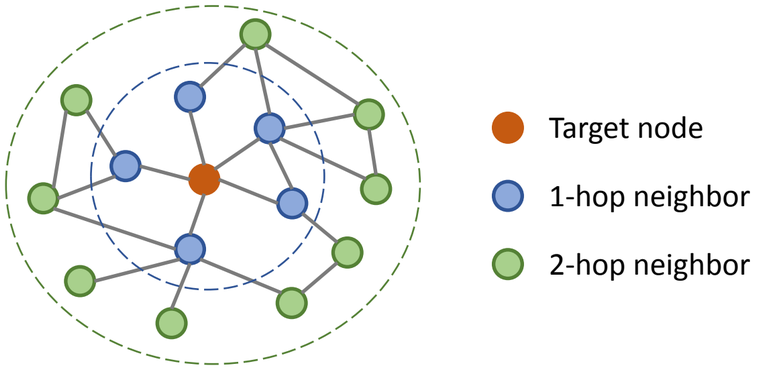
Recap: Graph Neural Networks

Graph representation learning



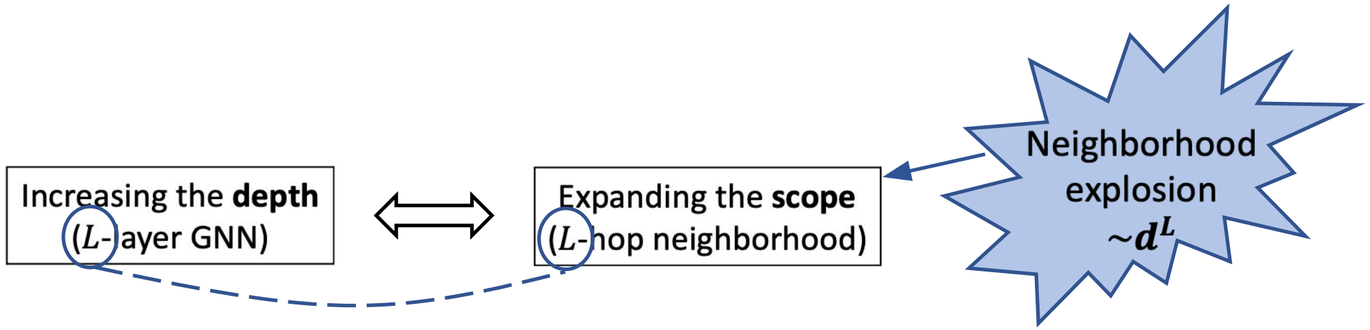
Message passing in GNNs

- **Scope**: from what neighbors?
- **Depth**: by how many iterations / layers?



Scalability & Expressivity Challenges

GNN designs by default (on large scale graphs):



Dilemma in deep GNN: scalability-expressivity tradeoff

- **Depth is important**: Experience from general deep learning
- **Depth is expensive**: Observation from graph message passing
- **Depth can cause training challenges**: Oversmoothing in GCN

Solution: Don’t forget the scope!

Depth-Scope Decoupling

Define ***scope*** independent of ***depth***

- Intuitions
  - Some neighbors are irrelevant → no need to pass their messages
  - Some neighbors are extra important → worth passing their messages many times
- Example: Deep (L'-layer) GNN on shallow (L-hop) subgraph

Algorithm: generate embedding for a target node v of the full graph $\mathcal{G}$

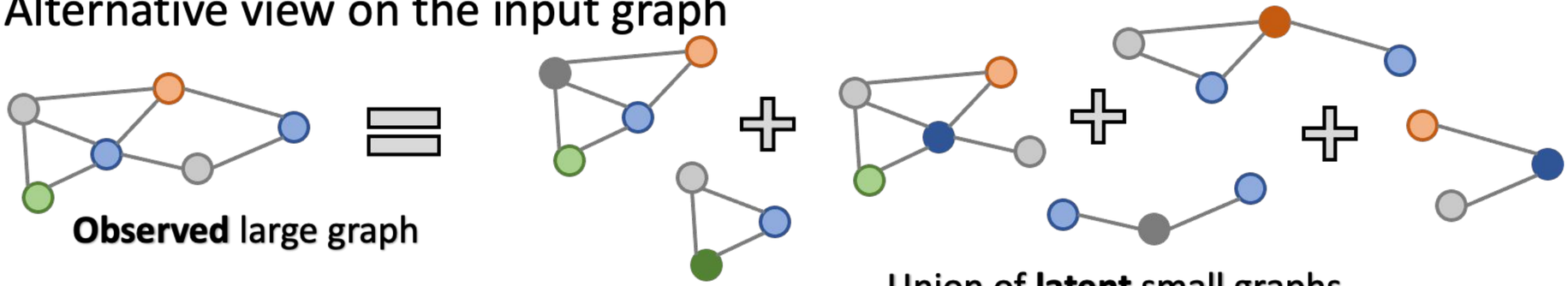
1. Extract a subgraph $\mathcal{G}_{[v]}$ around v
2. for round $i = 1$ to L':
   Perform message passing along all edges in $\mathcal{G}_{[v]}$
3. Take v's embedding from all node embeddings of $\mathcal{G}_{[v]}$

Depth-Scope Decoupling

Interpretation

Scope, Depth } is a property of the { Data, Model

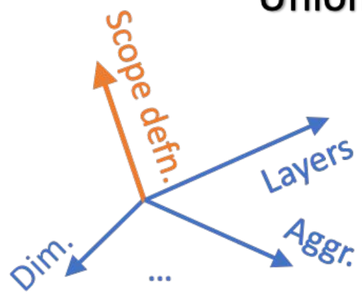
Alternative view on the input graph



Observed large graph

Union of **latent** small graphs

Enlarging the GNN design space



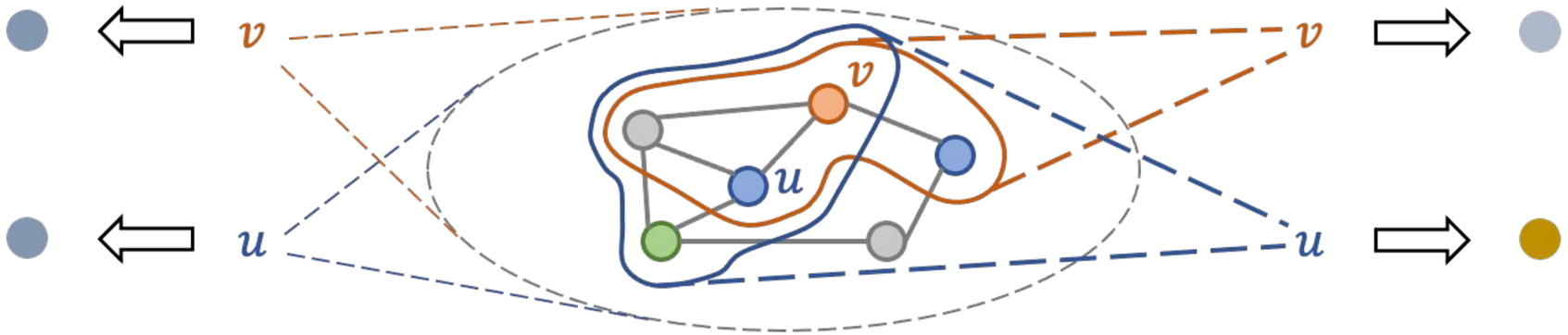
Theoretical Justification: Graph Signal Processing Perspective

Oversmoothing of GCN

- Each GCN layer smooths features of direct neighbors
- For u≠v, their scopes are both the full graph G
- Many GCN layers smooths features of the full graph G

Non-smoothing of decoupled-GCN

- GCN layers only smooths the features within $G_{[v]}$
- For u≠v, their scopes can be different $G_{[u]} \neq G_{[v]}$
- Smoothing different set of features produces distinctive embeddings



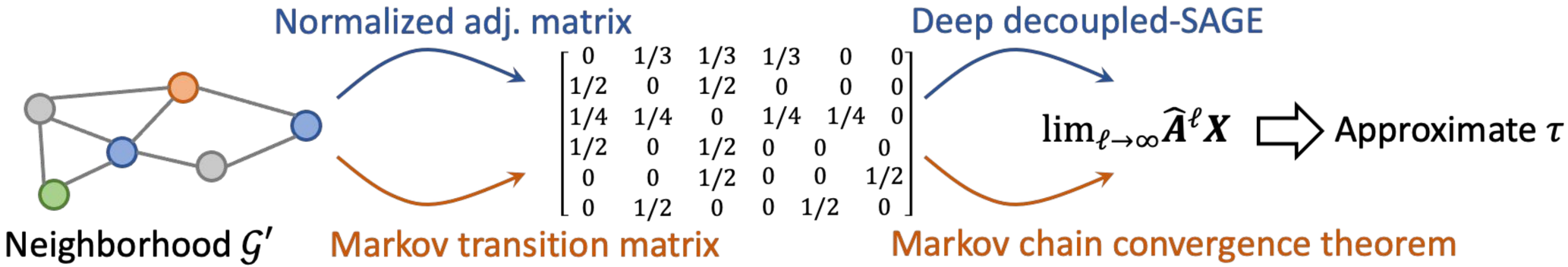
Theoretical Justification: Function Approximator Perspective

Decoupled-SAGE is more expressive than GraphSAGE

- Consider neighborhood G′ & function τ for linear comb. of G′ features
- GraphSAGE cannot approximate τ well, even if G′ is L-hop neighborhood
- Decoupled-SAGE can approximate τ where

Scope $\mathcal{G}_{[v]} = \mathcal{G}'$

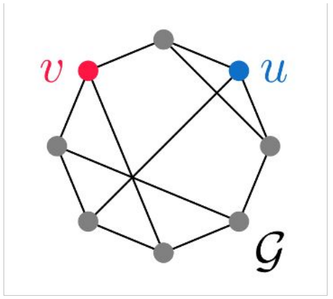
Depth reduces the error exponentially



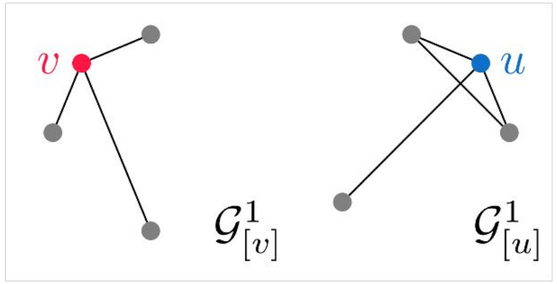
Theoretical Justification: Topology Information Perspective

Decoupled-GIN is more expressive than GIN/1-WL

- Challenge for GIN/1-WL: non-isomorphic regular graphs
- Benefit of decoupling: *subgraphs of a regular graph may not be regular*



Example 3-regular graph where GIN cannot distinguish u and v



Decoupled-GIN can distinguish u and v

Scope = 1-hop

Depth = 2

Evaluation: Setup

Datasets 7 graphs (up to 111M nodes)
inductive & transductive

Backbone models 5 aggregation functions & residue connection

Tasks node classification & link prediction

Training of baselines full batch & GraphSAINT minibatch

Training of proposed minibatch of independently constructed $G_{[v]}$

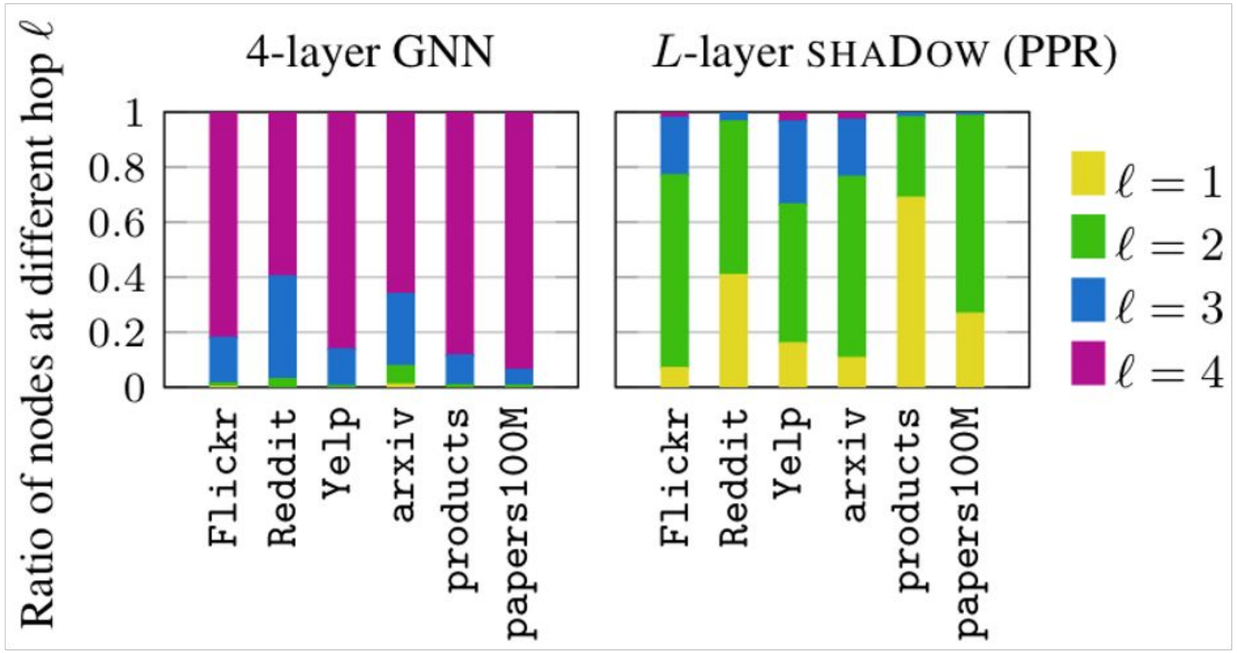
Practical design: **shaDow-GNN** (Decoupled GNN on shallow subgraphs)

- Scope: based on 2-hop / PPR (top 200 nodes)
- Depth: 3- / 5-layer

Evaluation: Neighborhood Composition

How many neighbors are ℓ hops away from the target node?

- Scope of normal GNN
  - Dominated by distant neighbors
  - Size grows rapidly
- Scope of shaDow-GNN
  - Consists of nearby neighbors
  - Size is small regardless of number of layers (< 200 neighbors)



Evaluation: Baseline Comparisons

- Decoupling improves **accuracy** at lower computation **cost**
- Decoupling is a general design principle applicable to **various backbones**
- **Subgraph extraction** algorithms are important

Method	Layers	Flickr		Reddit		Yelp		ogbn-arxiv		ogbn-products	
		Accuracy	Cost	Accuracy	Cost	F1-micro	Cost	Accuracy	Cost	Accuracy	Cost
GCN	3	0.5159±0.0017	2E0	0.9532±0.0003	6E1	0.4028±0.0019	2E1	0.7170±0.0026	1E1	0.7567±0.0018	5E0
	5	0.5217±0.0016	2E2	0.9495±0.0012	1E3	OOM	1E3	0.7186±0.0017	1E3	OOM	9E2
GCN	3	0.5155±0.0027	2E0	0.9523±0.0003	6E1	0.5110±0.0012	2E1	0.7093±0.0003	1E1	**0.8003**±0.0024	5E0
+ GraphSAINT-RW	5	0.5165±0.0026	2E2	0.9523±0.0012	1E3	0.5012±0.0021	1E3	0.7039±0.0020	1E3	0.7992±0.0021	9E2
SHADOW-GCN	3	0.5262±0.0018	**(1)**	0.9581±0.0004	**(1)**	0.5255±0.0012	**(1)**	0.7192±0.0025	**(1)**	0.7778±0.0030	**(1)**
+PPR	5	**0.5270**±0.0024	1E0	**0.9583**±0.0002	1E0	**0.5272**±0.0018	2E0	**0.7207**±0.0030	2E0	0.7844±0.0029	2E0
GraphSAGE	3	0.5140±0.0014	3E0	0.9653±0.0002	5E1	0.6178±0.0033	2E1	0.7192±0.0027	1E1	0.7858±0.0013	4E0
	5	0.5154±0.0052	2E2	0.9626±0.0004	1E3	OOM	2E3	0.7193±0.0037	1E3	OOM	1E3
GraphSAGE	3	0.5176±0.0032	3E0	0.9671±0.0003	5E1	0.6453±0.0011	2E1	0.7107±0.0003	1E1	0.7923±0.0023	4E0
+ GraphSAINT-RW	5	0.5201±0.0032	2E2	0.9670±0.0010	1E3	0.6394±0.0003	2E3	0.7013±0.0021	1E3	0.7964±0.0022	1E3
SHADOW-SAGE	3	0.5288±0.0014	1E0	0.9660±0.0003	1E0	0.6493±0.0001	1E0	0.7163±0.0012	1E0	0.7993±0.0012	1E0
+ 2-hop	5	0.5338±0.0038	2E0	0.9661±0.0002	2E0	0.6503±0.0001	2E0	0.7183±0.0012	2E0	0.8014±0.0020	2E0
SHADOW-SAGE	3	0.5344±0.0028	**(1)**	**0.9693**±0.0002	**(1)**	**0.6512**±0.0002	**(1)**	0.7234±0.0032	**(1)**	0.7945±0.0021	**(1)**
+ PPR	5	**0.5424**±0.0025	2E0	0.9691±0.0003	2E0	0.6502±0.0001	2E0	**0.7255**±0.0013	2E0	**0.8043**±0.0026	2E0
GAT	3	0.5070±0.0032	2E1	OOM	3E2	OOM	2E2	0.7201±0.0011	1E2	OOM	3E1
	5	0.5164±0.0033	2E2	OOM	2E3	OOM	2E3	OOM	3E3	OOM	2E3
GAT	3	0.5225±0.0053	2E1	0.9671±0.0003	3E2	0.6459±0.0002	2E2	0.6977±0.0003	1E2	0.8027±0.0028	3E1
+ GraphSAINT-RW	5	0.5153±0.0034	2E2	0.9651±0.0024	2E3	0.6478±0.0012	2E3	0.6954±0.0013	3E3	0.7990±0.0072	2E3
SHADOW-GAT	3	**0.5383**±0.0032	**(1)**	0.9703±0.0010	**(1)**	**0.6549**±0.0002	**(1)**	0.7243±0.0011	**(1)**	0.8014±0.0012	**(1)**
+ PPR	5	0.5342±0.0023	2E0	**0.9710**±0.0008	2E0	0.6537±0.0004	2E0	**0.7283**±0.0027	2E0	**0.8094**±0.0034	2E0

Evaluation: Scaling to 100M-Node Graph

OGB Leaderboard comparison

- Higher accuracy
- Orders of magnitude smaller neighborhood size

Table 2: Leaderboard comparison on `papers100M`

Method	Test accuracy	Val accuracy	Neigh size
GraphSAGE+incep	0.6707±0.0017	0.7032±0.0011	4E5
SIGN-XL	0.6606±0.0019	0.6984±0.0006	> 4E5
SGC	0.6329±0.0019	0.6648±0.0020	> 4E5
SHADOW-GAT$_{200}$	0.6681±0.0016	0.7019±0.0011	2E2
SHADOW-GAT$_{400}$	**0.6710**±0.0015	**0.7067**±0.0012	3E2

Memory consumption

- Lowest in both CPU and GPU
- Train & inference the 100M graph on a low-end server

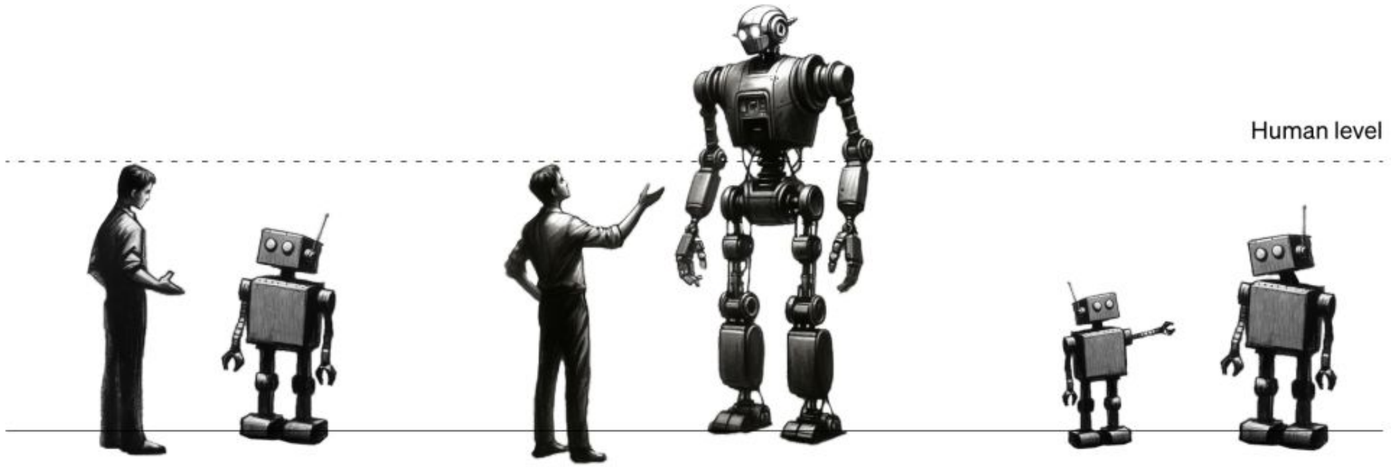
Memory consumption of the `ogbn-papers100M` leaderboard methods

Method	CPU RAM	GPU memory
GraphSAGE+incep	80GB	16GB
SIGN-XL	>682GB	4GB
SGC	>137GB	4GB
SHADOW-GAT	**80GB**	**4GB**

H. Zeng, H. Lyu, D. Hu, Y. Xia, J. Luo, Mixture of Weak and Strong Experts on Graphs, ICLR'24 (to appear)

Mixture of Weak and Strong on Graph

- Mixture-of-Experts (MoE) system has effectively improved model capacity
- Improve model capacity without significant trade-offs in computation overhead and optimization difficulty
- Achieve high expressive power, coming at the cost of minor computation overhead



Ref: OpenAI WEAK-TO-STRONG GENERALIZATION

3. Mixture of weak and strong

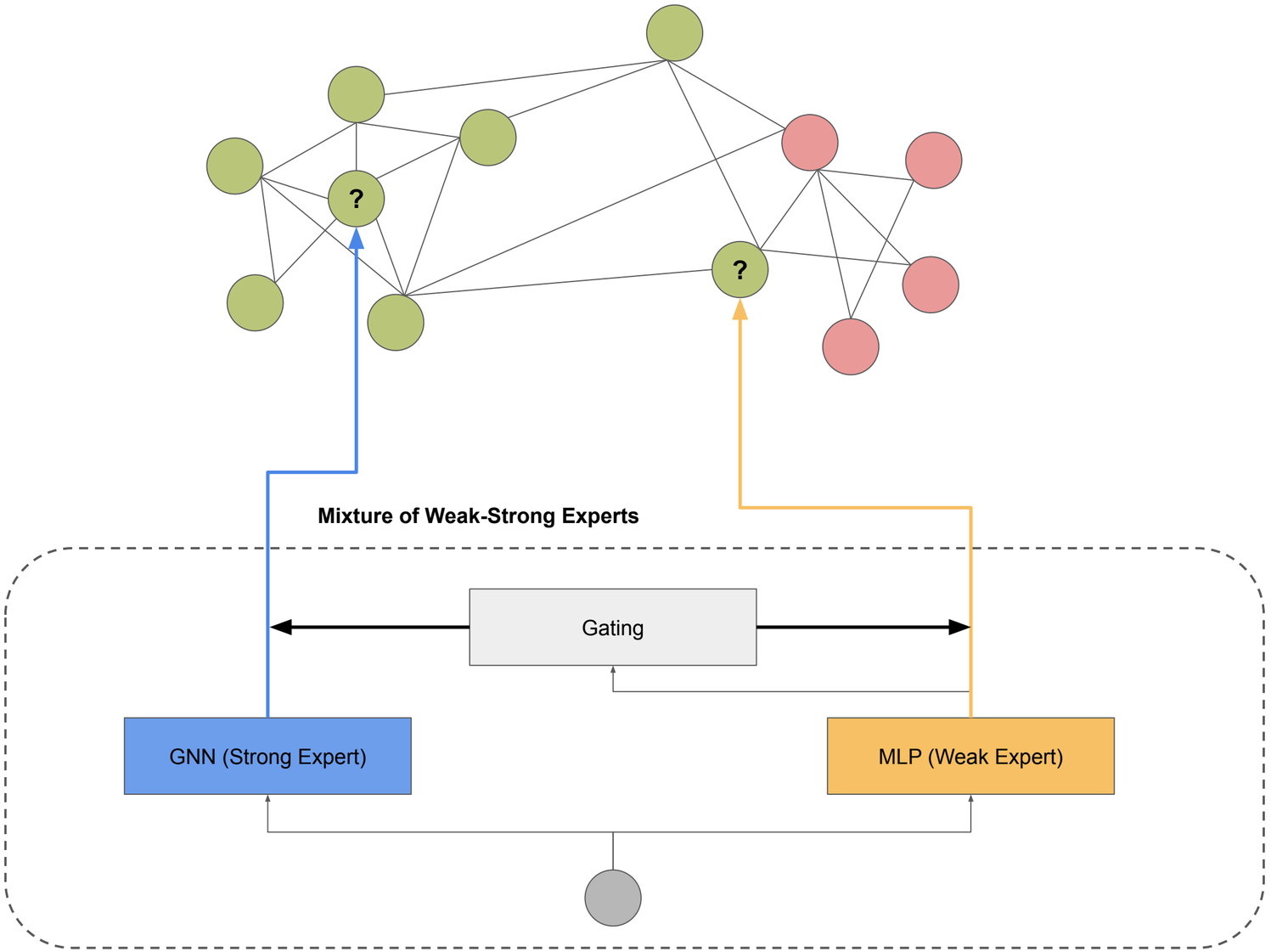
A novel mixture-of-experts design to combine a weak MLP expert with a strong GNN expert for decoupling the self-feature and neighbor structure modalities in graphs.

- Weak expert is a light-weight Multi-layer Perceptron (MLP)
- Strong expert is an off-the-shelf GNN

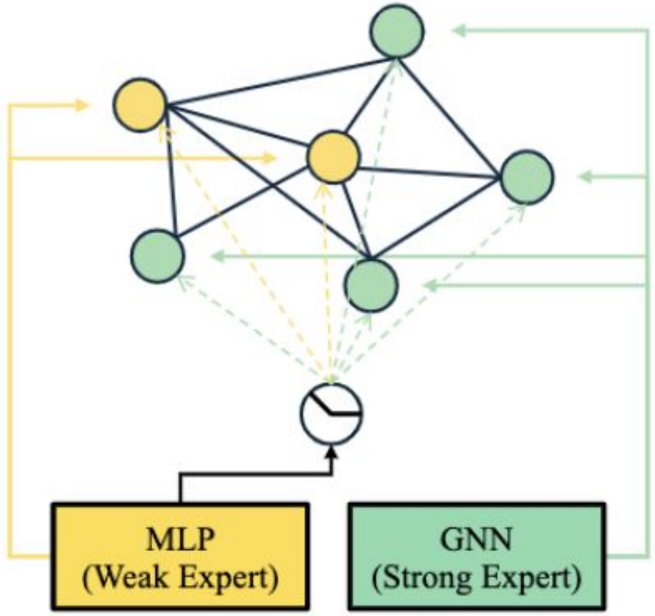
A “confidence” gating mechanism based on the dispersion of the weak expert’s prediction logits.

$$L = \frac{1}{|\mathcal{V}|} \sum_{v \in \mathcal{V}} \left(C\left(\boldsymbol{p}_v\right) \cdot L\left(\boldsymbol{p}_v, \boldsymbol{y}_v\right) + \left(1 - C\left(\boldsymbol{p}_v\right)\right) \cdot L\left(\boldsymbol{p}'_v, \boldsymbol{y}_v\right) \right)$$

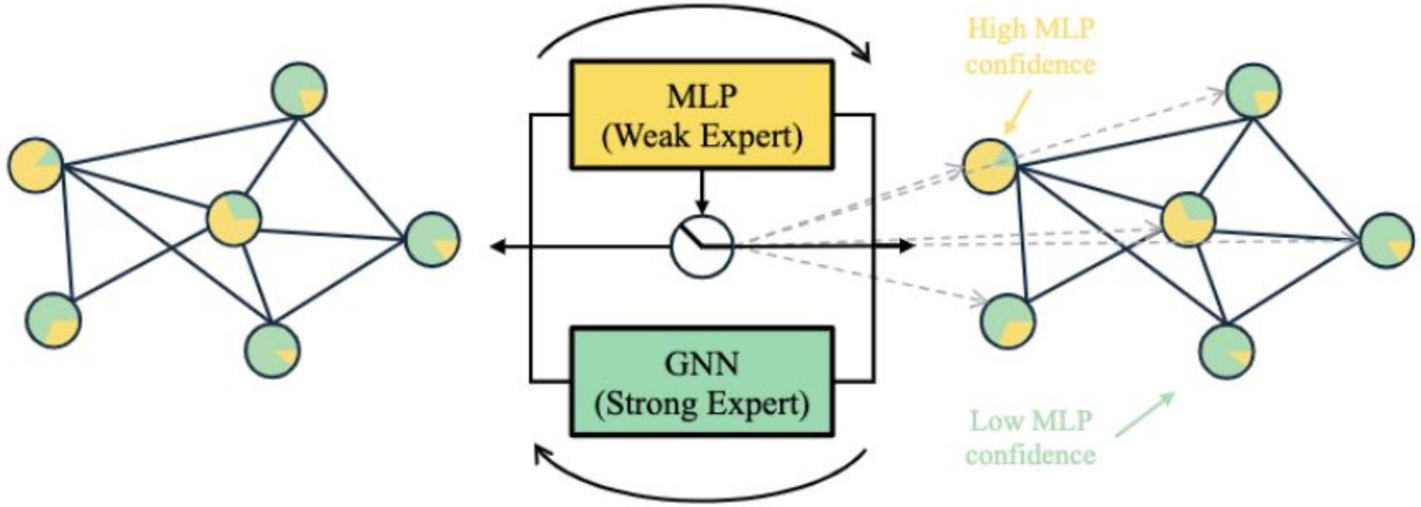
$$\boldsymbol{p}_v = \texttt{MLP}\left(\boldsymbol{x}_v; \boldsymbol{\theta}\right) \text{ and } \boldsymbol{p}'_v = \texttt{GNN}\left(\boldsymbol{x}_v; \boldsymbol{\theta}'\right)$$



3. Mixture of weak and strong

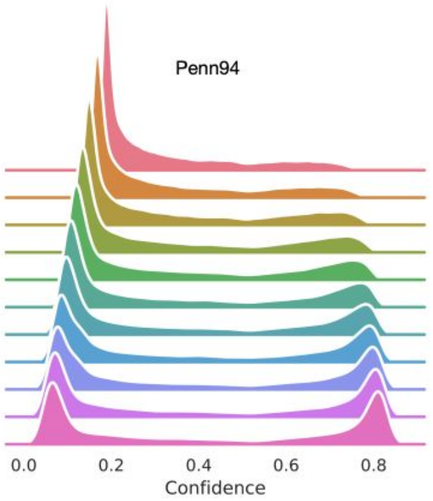


Fix GNN weights; Train MLP and Gating Module; Gating module computes MLP's confidence

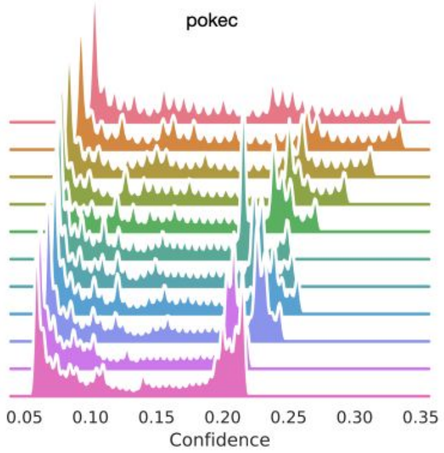


Fix MLP and Gating module weights; Learn GNN; GNN focuses on nodes that MLP is *not* confident

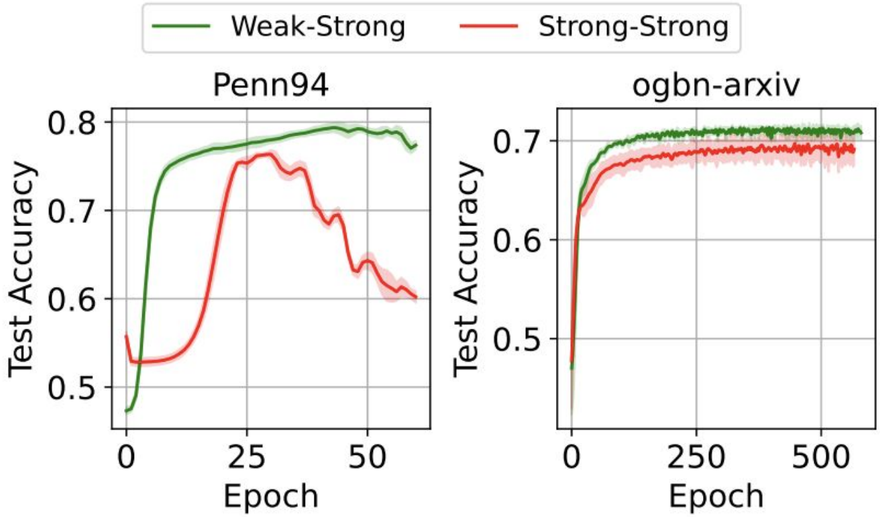
Evaluation



On Penn94, the GNN dominates initially. The MLP gradually learns to specialize on a significant portion of the data. Eventually, the whole graph is clearly split between the two experts



For pokec, the specialization is not so strong. When training progresses, the MLP becomes less confidence when the GNN is optimized better; For different graphs, the two experts will adapt their extent of collaboration by minimizing the confidence-weighted loss.



On both Penn94 and ogbn-arxiv, we observe that the convergence quality of the “strong-strong” variant is much worse. The per-epoch execution time for “strong-strong” is also significantly longer, indicating an even longer overall convergence time than the “weak-strong” model.

Agenda

01 Graph in RecSys

02 Graph sparse nodes in recommendation

03 GNN expressiveness: depth & scope

04 Conclusion & Opportunities

Conclusion

- Graph learning is not only a buzzword in academia research, but also finds increasing impacts in industry
- When graph learning meets industry, vanilla models usually need modifications to meet the product needs
- When graph learning meets industry, novel frameworks must be developed to address the challenges in expressity and scalability

- Speaker info: https://research.facebook.com/people/xia-yinglong/
- Open source: https://github.com/facebookresearch/shaDow_GNN

Opportunity

Yinglong Xia
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