NEURAL INFORMATION PROCESSING SYSTEMS

# Decoupling the Depth and Scope of Graph Neural Networks

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1. USC 2. PKU 3. Facebook AI 4. US-ARL

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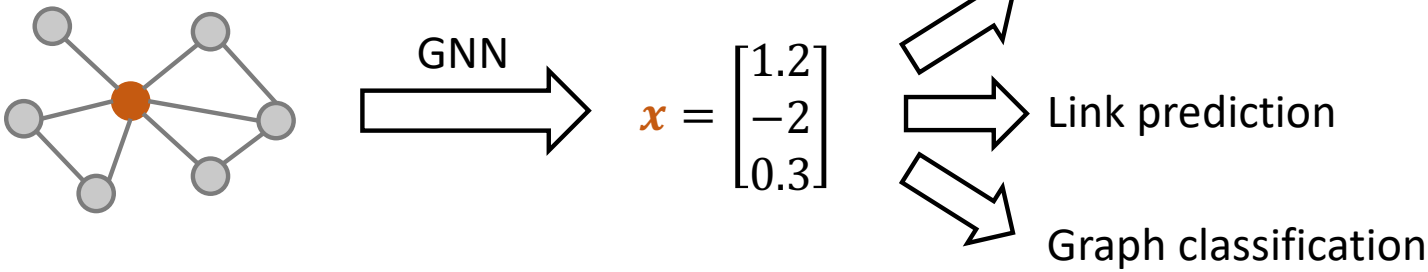
https://github.com/facebookresearch/shaDow_GNN

# Outline

- Background
- Depth-scope decoupling
- Theoretical justifications
- Architecture designs
- Evaluation
- Conclusion

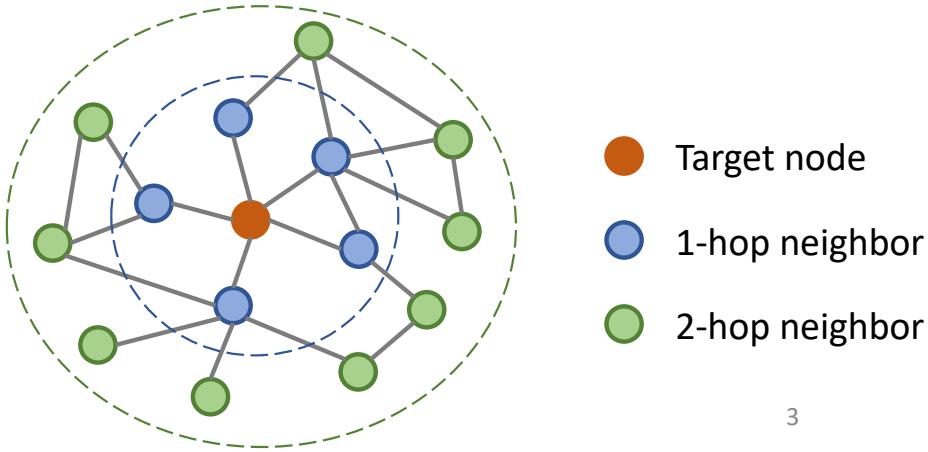
# Background: Graph Neural Networks

Graph representation learning



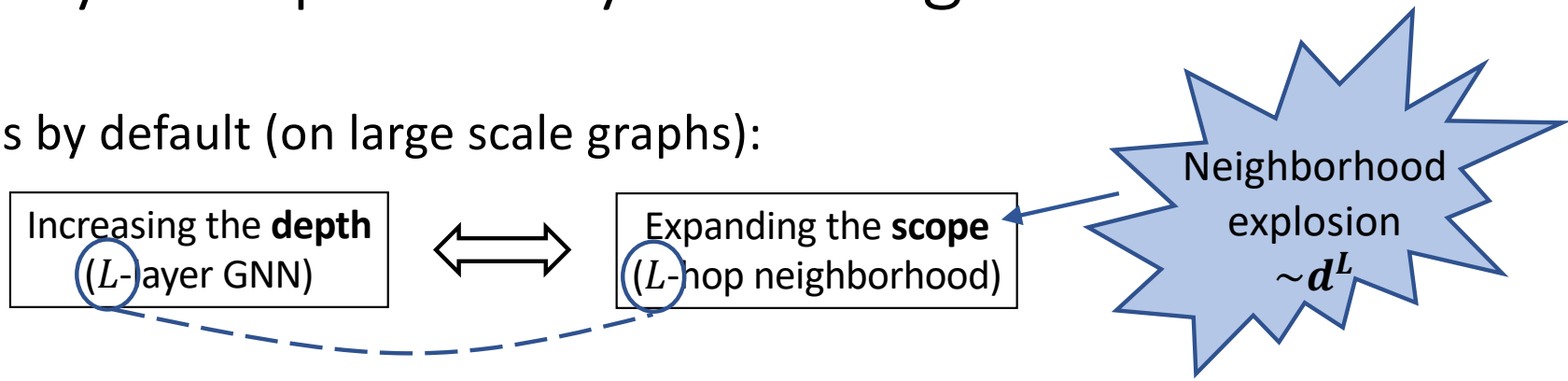

Message passing in GNNs

- **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 $\mathcal{G}$

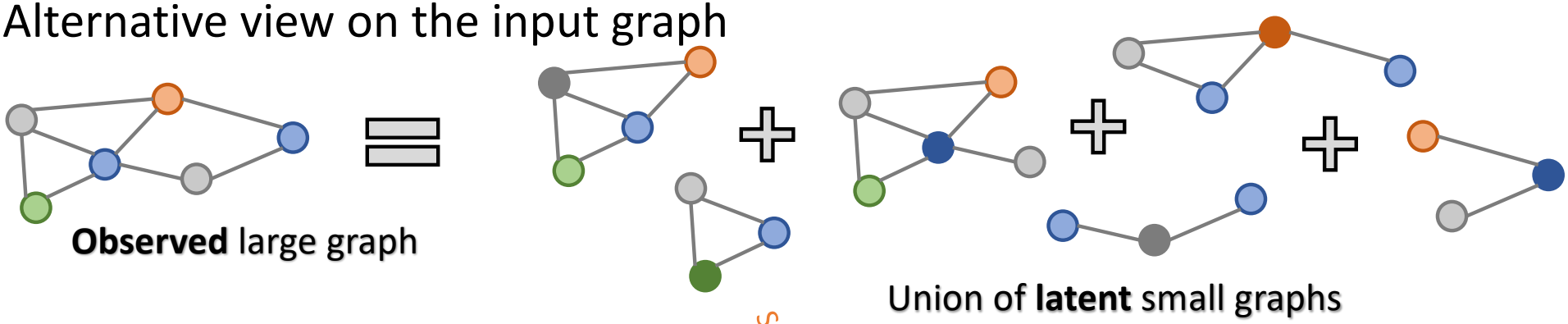
1. Extract a subgraph $\mathcal{G}_{[v]}$ around $v$
2. for round $i = 1$ to $L'$:
   Perform message passing along all edges in $\mathcal{G}_{[v]}$
3. Take $v$'s embedding from all node embeddings of $\mathcal{G}_{[v]}$

# Depth-Scope Decoupling

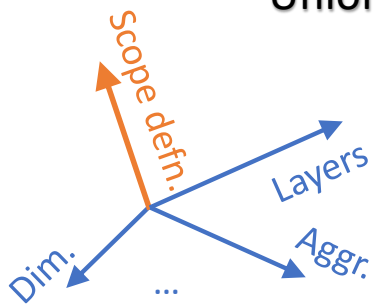
Interpretation

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

Alternative view on the input graph




Enlarging the GNN design space



# Theoretical Justifications: Overview

**Decoupling improves GNN expressive power**, from the perspectives of

- Graph signal processing: decoupled-GCN avoids oversmoothing
- Function approximator: decoupled-SAGE learns some target function
- Topological information: decoupled-GIN exceeds 1-WL test

**Decoupling improves GNN scalability**

- Deep model + large graph ≠ Exploding scope
- With fixed-size scope, complexity is linear with the model depth

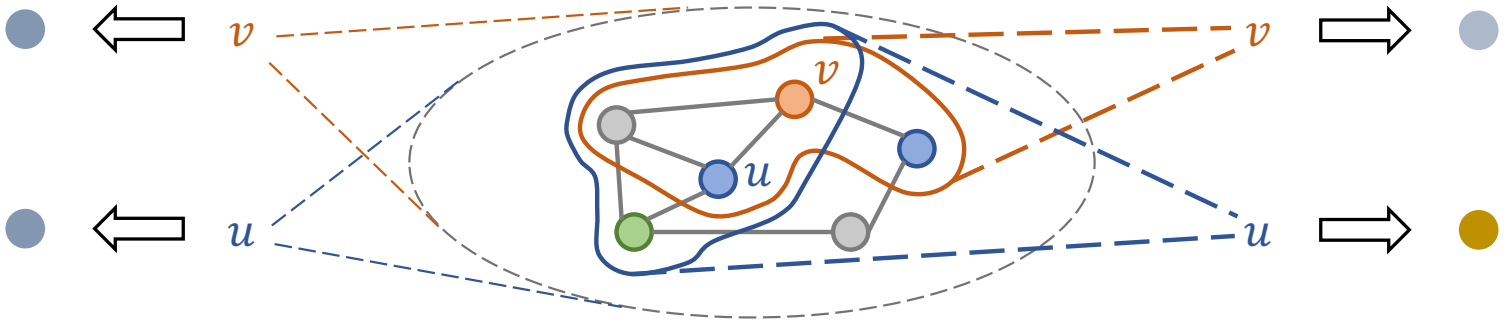
# Theoretical Justification: Graph Signal Processing Perspective

**Oversmoothing of GCN**

- Each GCN layer smooths features of direct neighbors
- For $u \neq v$, their scopes are both the full graph $\mathcal{G}$
- Many GCN layers smooths features of the full graph $\mathcal{G}$

**Non-smoothing of decoupled-GCN**

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



# Theoretical Justification: Function Approximator Perspective

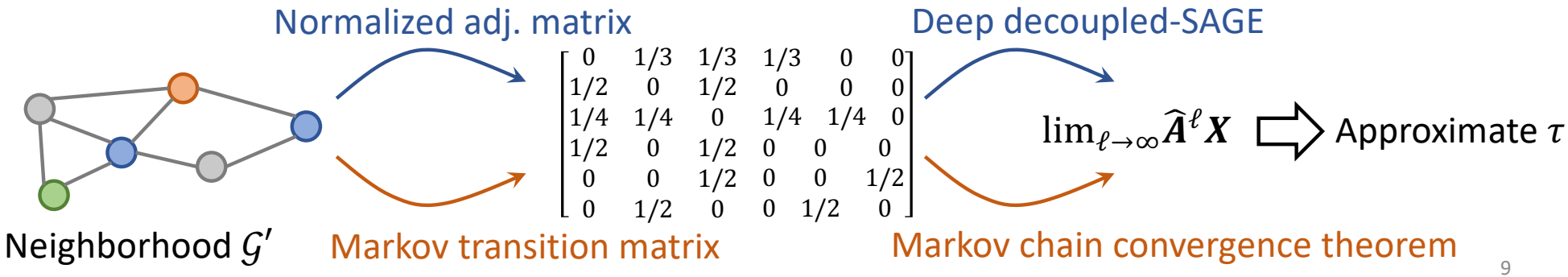
**Decoupled-SAGE is more expressive than GraphSAGE**

Consider neighborhood $\mathcal{G}'$ & function $\tau$ for linear comb. of $\mathcal{G}'$ features

- GraphSAGE cannot approximate $\tau$ well, even if $\mathcal{G}'$ is $L$-hop neighborhood
- Decoupled-SAGE can approximate $\tau$ where

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

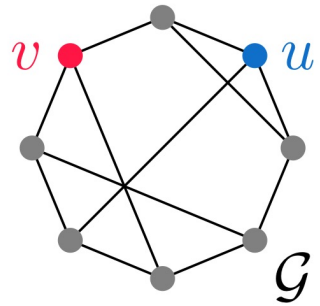
**Depth** reduces the error exponentially



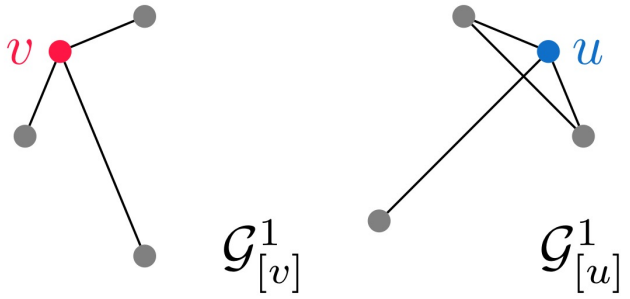
# Theoretical Justification: Topology Information Perspective

**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

# Architecture: Subgraph Extraction

Define scope $\mathcal{G}_{[v]}$ by extracting subgraphs around $v$

**General approaches** to preserve neighborhood characteristics

Heuristic based | Model based | Learning based

**Example** heuristic-based extraction function

- Identify important neighbors by Personalized PageRank (PPR) scores

1. Compute PPR score with target $v$ as the root node
2. Take $B$ neighbors $\mathcal{N}_{[v]}$ with top PPR scores
3. Construct node-induced subgraph $\mathcal{G}_{[v]}$ from $\mathcal{N}_{[v]}$

# Architecture: READOUT & Ensemble

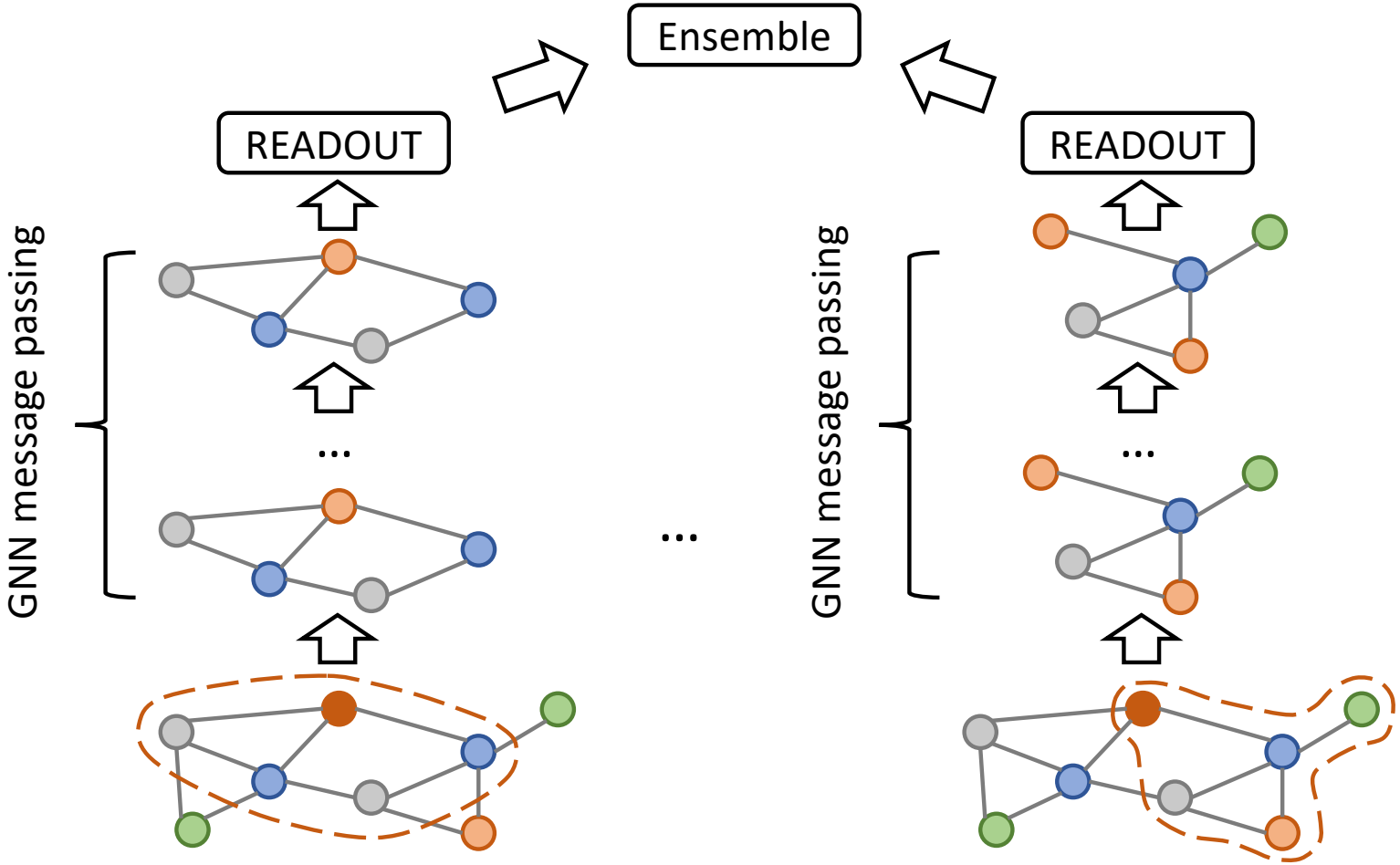
**READOUT** for node-& link-level tasks

- Two $L$-hop neighbors may only talk to each other after $2L$ layers
- Deep GNN on a shallow subgraph: each node of $\mathcal{G}_{[v]}$ sees the complete information of $\mathcal{G}_{[v]}$
- READOUT all embeddings of $\mathcal{G}_{[v]}$ nodes as the final embedding of $v$

**Ensemble** of different subgraphs

- Different graph metrics captures different neighbor importance
- Design a single complicated subgraph extraction function?
- Ensemble multiple simple subgraph extraction functions
  - e.g., [$L$-hop] + [PPR]

# Architecture: Full Picture



# Evaluation: Setup

| | |
|---|---|
| **Datasets** | 7 graphs (up to 111M nodes)<br>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 $\mathcal{G}_{[v]}$ |

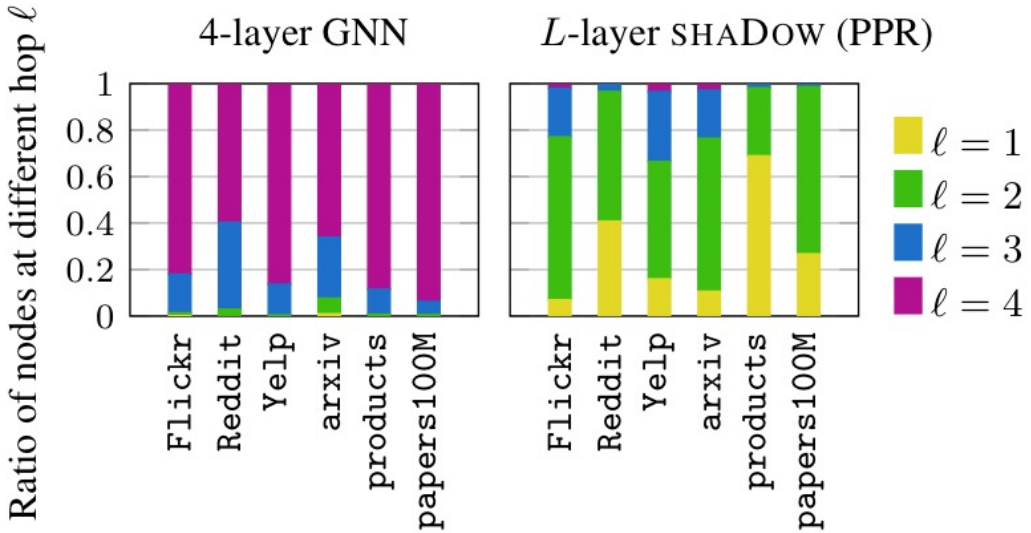
**Practical design:** **shaDow-GNN** (Decoupled GNN on shallow subgraphs)

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

# Evaluation: Neighborhood Composition

*How many neighbors are $\ell$ 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 + GraphSAINT-RW | 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 |
| | 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 +PPR | 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)** |
| | 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 + GraphSAINT-RW | 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 |
| | 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 + 2-hop | 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 |
| | 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 + PPR | 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)** |
| | 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 + GraphSAINT-RW | 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 |
| | 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 + PPR | 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)** |
| | 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** |

# Conclusion

General design principle to decouple the depth & scope of GNNs

- Theoretical benefits in expressivity & scalability
- Empirical performance gain in accuracy & cost
- Flexibility w.r.t. GNN architecture, subgraph extraction algorithms & learning tasks

Public implementations

- Official code:

  https://github.com/facebookresearch/shaDow_GNN

- PyG version:

  https://pytorch-geometric.readthedocs.io/en/2.0.0/modules/loader.html?#torch_geometric.loader.ShaDowKHopSampler

Thank you!