

# Introduction to Graph Neural Networks

Minji Yoon

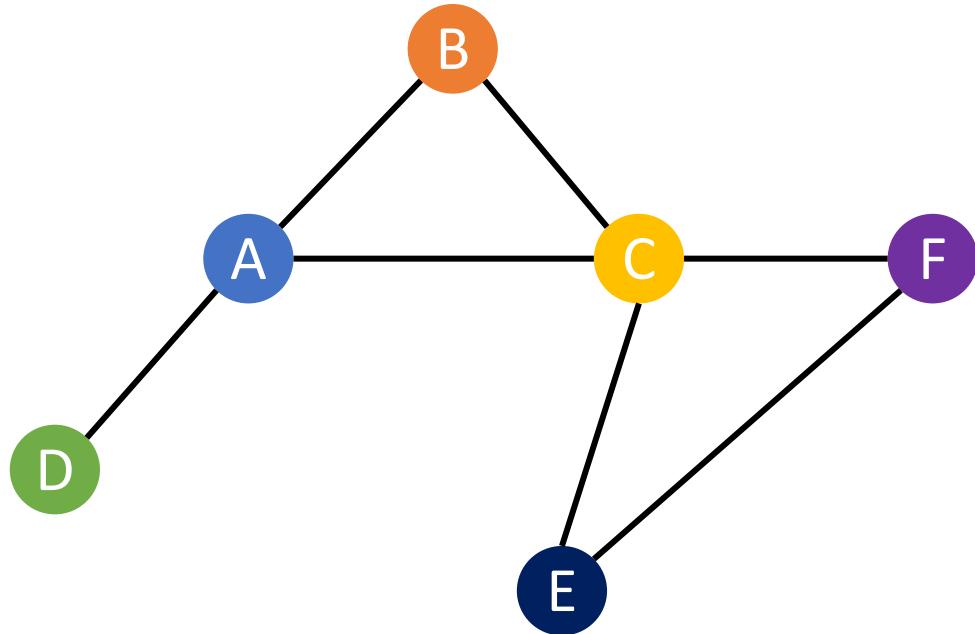
Computer Science Department

Carnegie Mellon University

# Talk objectives

- Introduce Graph Neural Networks (GNNs)
- Highlight interesting open research questions

# What is a graph?



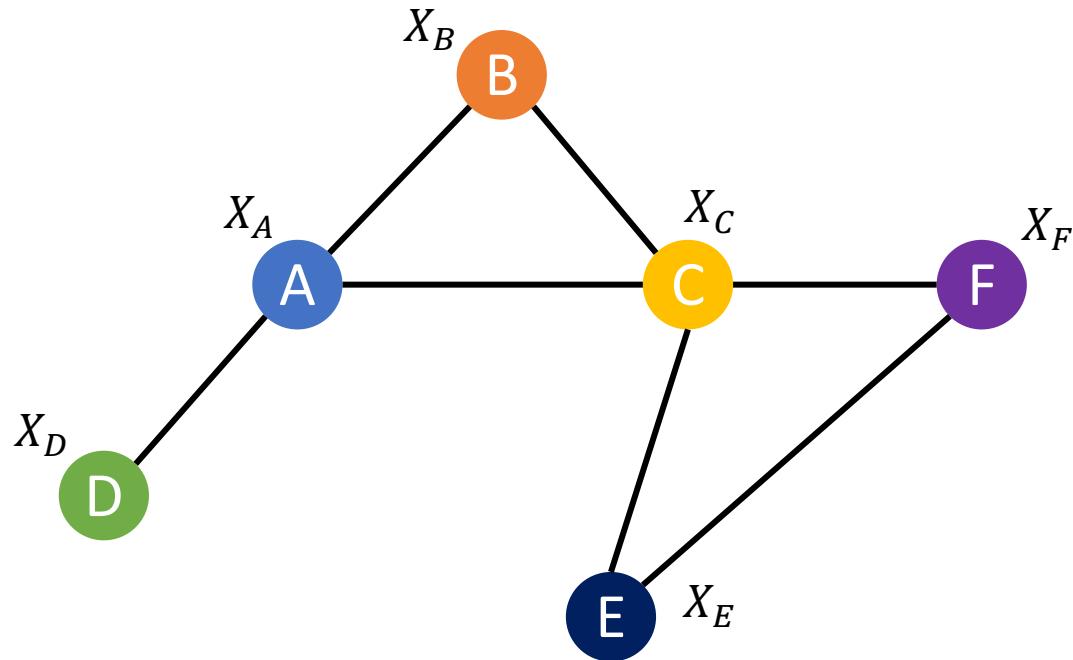
A graph is composed of

- **Nodes** (also called vertices)
- **Edges** connecting a pair of nodes

presented in an **adjacency matrix**

	A	B	C	D	E	F
A		1	1	1		
B	1			1		
C	1	1			1	1
D	1					
E			1			1
F			1	1		

# What is a graph?



A graph is composed of

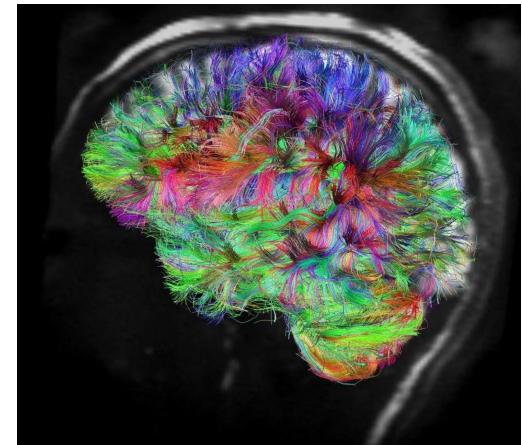
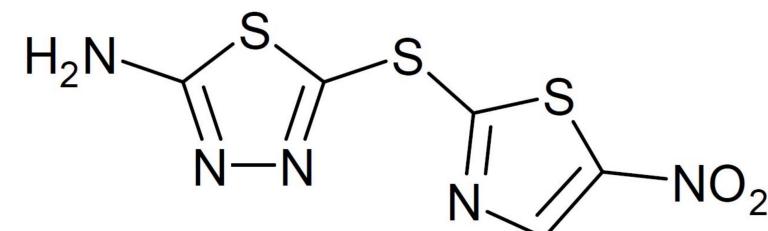
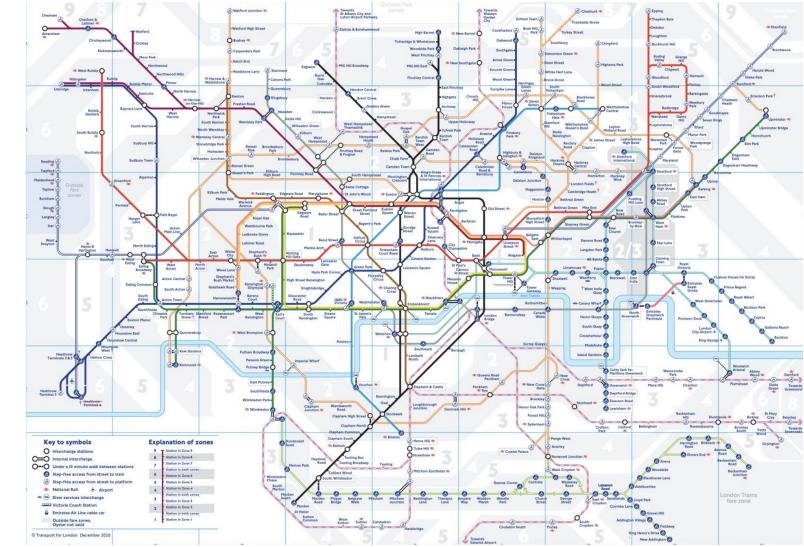
- **Nodes** (also called vertices)
- **Edges** connecting a pair of nodes

presented in an **adjacency matrix**

Nodes can have **feature vectors**

(A)	$X_A$
(B)	$X_B$
(C)	$X_C$
(D)	$X_D$
(E)	$X_E$
(F)	$X_F$

# Graphs are everywhere



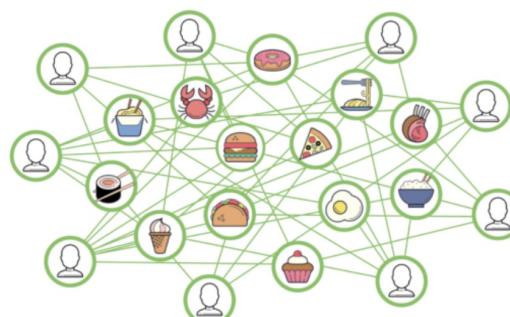
# Graph Neural Networks have a large impact on...

The image shows the DeepMind logo at the top left. To its right is a breadcrumb navigation path: 'Blog' > 'Traffic prediction with advanced Graph Neural Networks'. Below this is a large, colorful aerial photograph of a city at night, showing illuminated streets and buildings from a high vantage point.

# Food Discovery with Uber Eats: Using Graph Learning to Power Recommendations

Ankit Jain, Isaac Liu, Ankur Sarda, and Piero Molino

December 4, 201



Pinterest Engineering

Aug 15, 2018 · 8 min read

# PinSage: A new graph convolutional neural network for web-scale recommender systems

Ruining He | Pinterest engineer, Pinterest Labs



PUBLICATION

# Web image search gets better with graph neural networks

- to image search uses images returned by traditional search
- uses a graph neural network through which similarity signals are achieved, improving ranking in cross-modal retrieval.

---

ural Network

ER LABS Europe



# P-Companion: A principled framework for diversified complementary product recommendation

By Junheng Hao, Tong Zhao, Jin Li, Xin Luna Dong, Christos Faloutsos, Yizhou Sun, Wei Wang  
2020

# Graph Neural Networks have a large impact on...

GCN-RL Circuit Designer: Transferable Transistor Sizing with Graph Neural Networks and Reinforcement Learning

Hanrui Wang<sup>1</sup>, Kuan Wang<sup>1</sup>, Jiacheng Yang<sup>1</sup>, Linxiao Shen<sup>2</sup>, Nan Sun<sup>2</sup>, Hae-Seung Lee<sup>1</sup>, Song Han<sup>1</sup>

<sup>1</sup>Massachusetts Institute of Technology

<sup>2</sup>UT Austin



The next big thing: the use of graph neural networks to discover particles

September 24, 2020 | Zack Savitsky



Machine learning algorithms can beat the world's hardest video games in minutes and solve complex equations faster than the collective efforts of generations of physicists. But the conventional algorithms still struggle to pick out stop signs on a busy street.

Object identification continues to hamper the field of machine learning — especially when the pictures are multidimensional and complicated, like the ones particle detectors take of collisions in high-energy physics experiments. However, a new class of neural networks is helping these models boost their pattern recognition abilities, and the technology may soon be implemented in particle physics experiments to optimize data analysis.

npj | computational materials

Explore content ▾ About the journal ▾ Publish with us ▾

[nature](#) > [npj computational materials](#) > [articles](#) > [article](#)

Article | [Open Access](#) | Published: 03 June 2021

## Benchmarking graph neural networks for materials chemistry

[Victor Fung](#) [Jiaxin Zhang](#), [Eric Juarez](#) & [Bobby G. Sumpter](#)

[npj Computational Materials](#) 7, Article number: 84 (2021) | [Cite this article](#)

7807 Accesses | 7 Citations | 41 Altmetric | [Metrics](#)

nature

[View all journals](#)

[Search](#)

[Login](#)

Explore content ▾ About the journal ▾ Publish with us ▾

[nature](#) > [articles](#) > [article](#)

Article | Published: 09 June 2021

## A graph placement methodology for fast chip design

[Azalia Mirhoseini](#) [Anna Goldie](#) [Mustafa Yazgan](#), [Joe Wenjie Jiang](#), [Ebrahim Songhori](#), [Shen Wang](#), [Young-Joon Lee](#), [Eric Johnson](#), [Omkar Pathak](#), [Azade Nazi](#), [Jiwoo Pak](#), [Andy Tong](#), [Kavya Srinivasa](#), [William Hang](#), [Emre Tuncer](#), [Quoc V. Le](#), [James Laudon](#), [Richard Ho](#), [Roger Carpenter](#) & [Jeff Dean](#)

# Graph Neural Networks have a large impact on...

nature

Explore content ▾ About the journal ▾ Publish with us ▾ Subscribe

nature > news > article

NEWS | 01 December 2021

## DeepMind's AI helps untangle the mathematics of knots

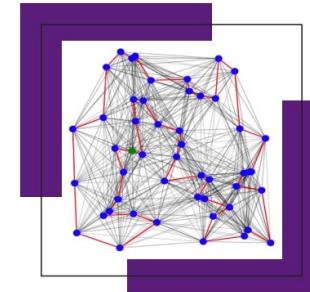
The machine-learning techniques could sets.

Patterns



## Deep Learning and Combinatorial Optimization

February 22 - 25, 2021



Opinion

## Neural algorithmic reasoning

Petar Veličković<sup>1,\*</sup> and Charles Blundell<sup>1</sup>

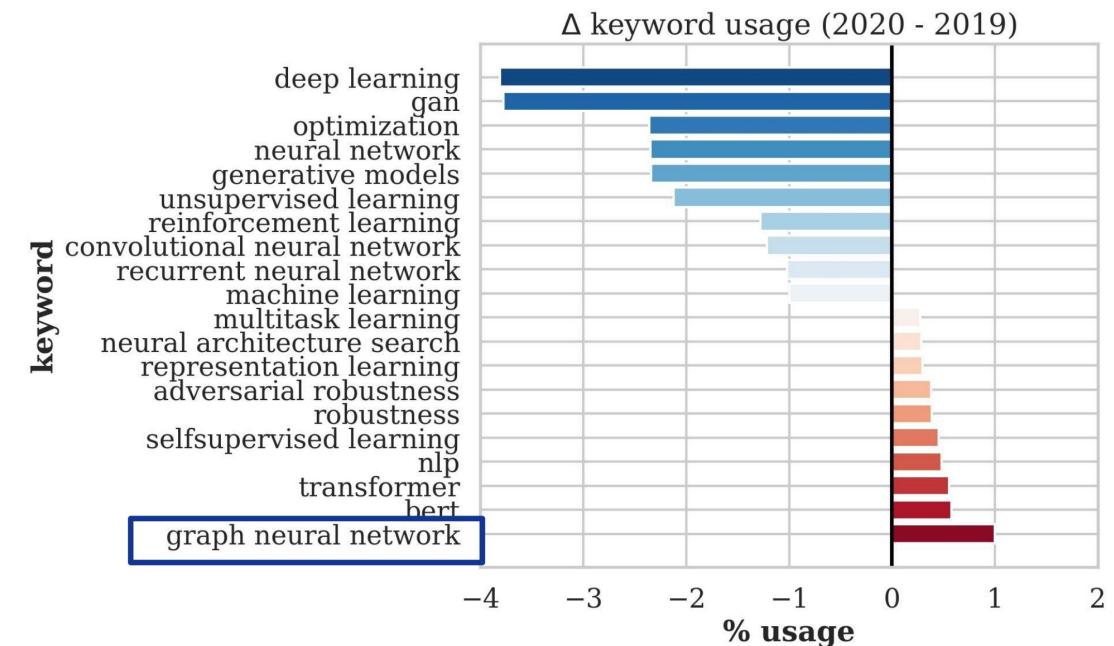
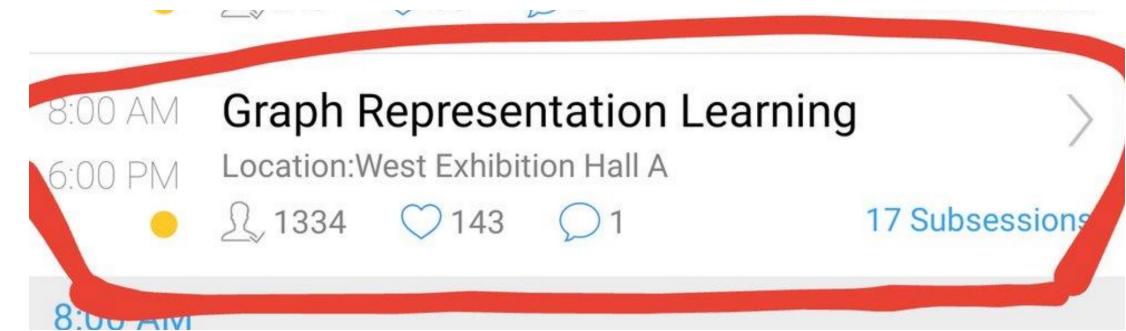
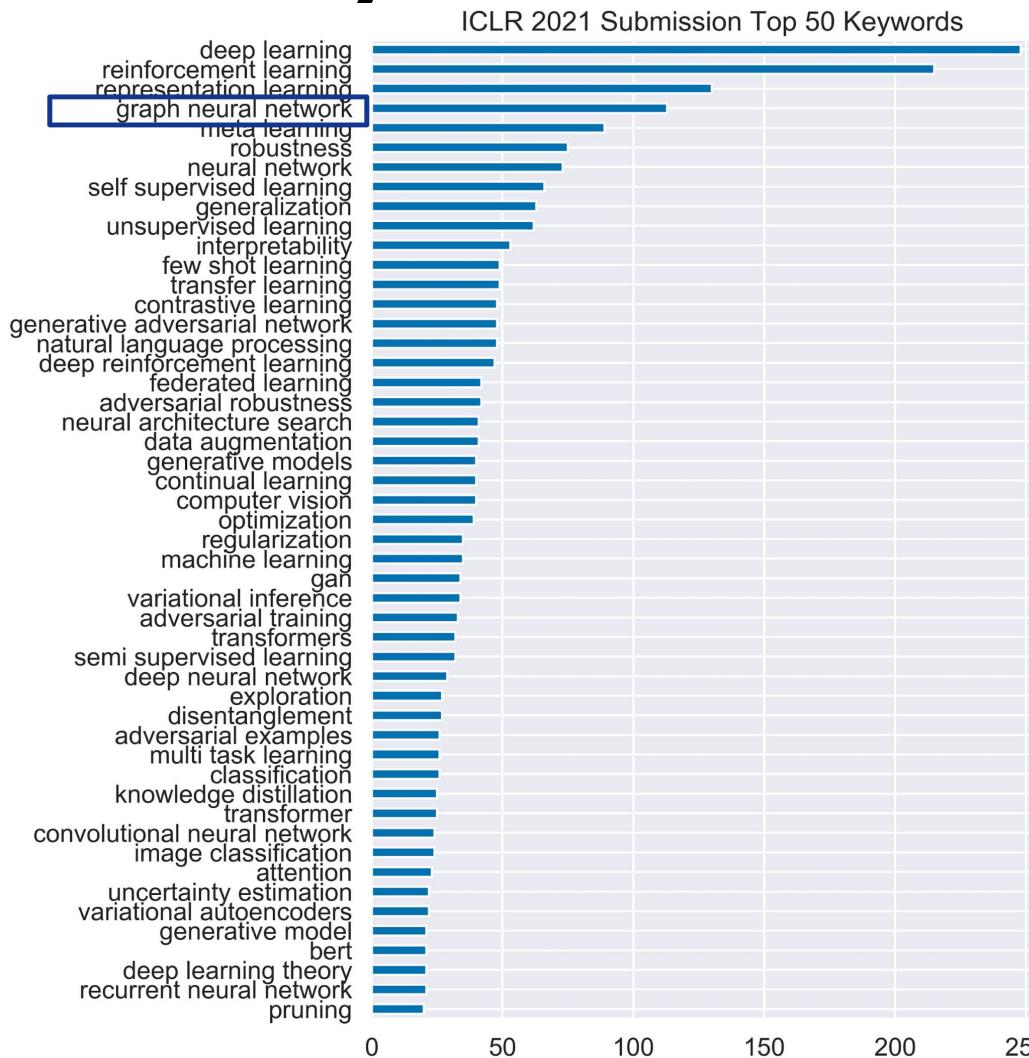
<sup>1</sup>DeepMind, London, Greater London, UK

\*Correspondence: [petarv@google.com](mailto:petarv@google.com)

<https://doi.org/10.1016/j.patter.2021.100273>

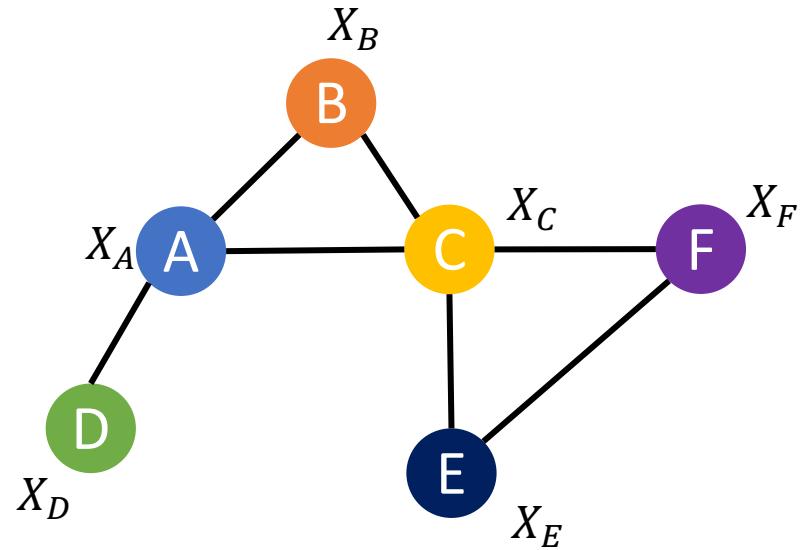
We present neural algorithmic reasoning—the art of building neural networks that are able to execute algorithmic computation—and provide our opinion on its transformative potential for running classical algorithms on inputs previously considered inaccessible to them.

# A very hot research topic



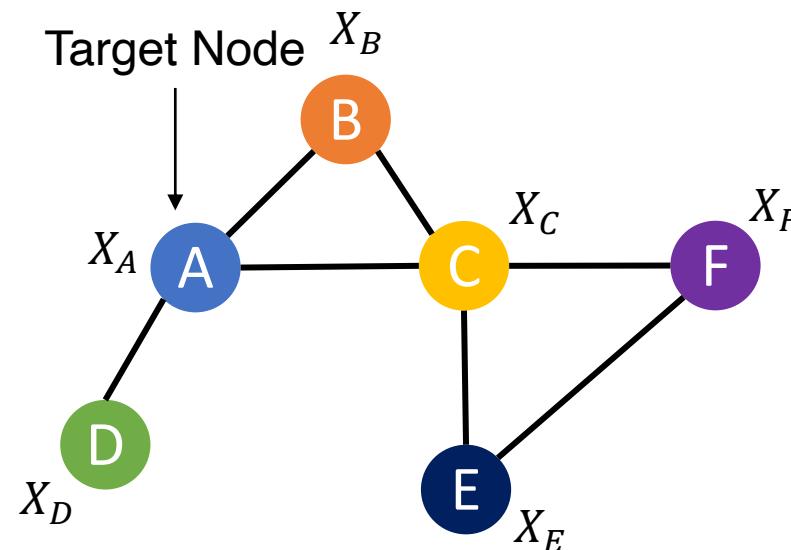
# What is Graph Neural Network?

# Problem definition



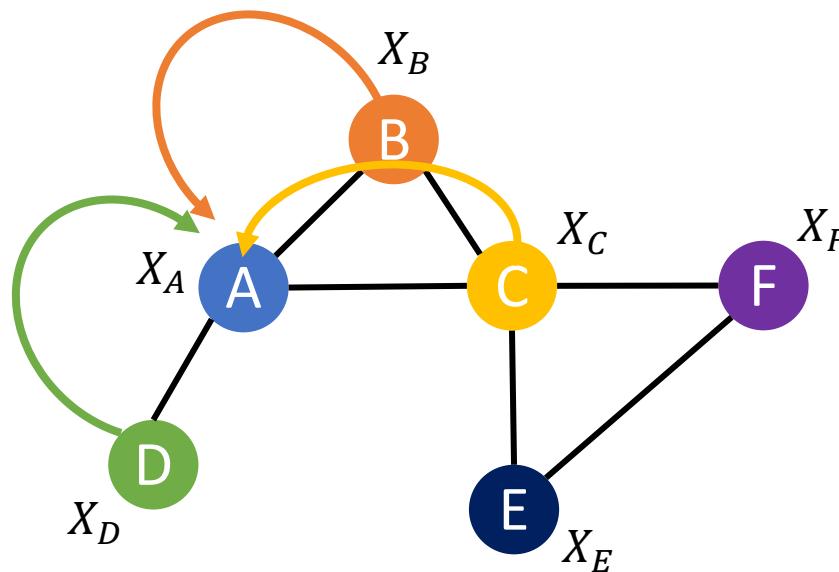
- **Given**
  - A graph
  - Node attributes
  - (part of nodes are labeled)
- **Find**
  - Node embeddings
- **Predict**
  - Labels for the remaining nodes

# Graph Neural Networks



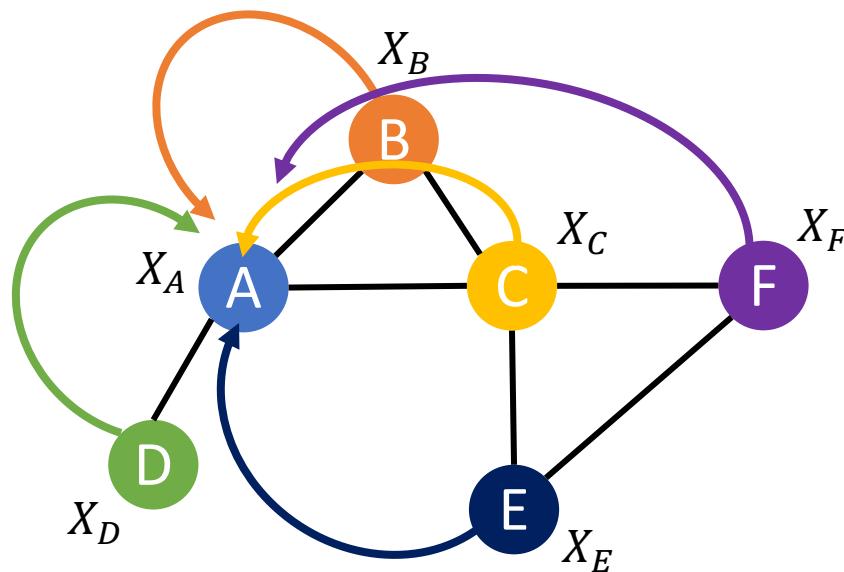
**“Homophily: connected nodes are related/informative/similar”**

# Graph Neural Networks



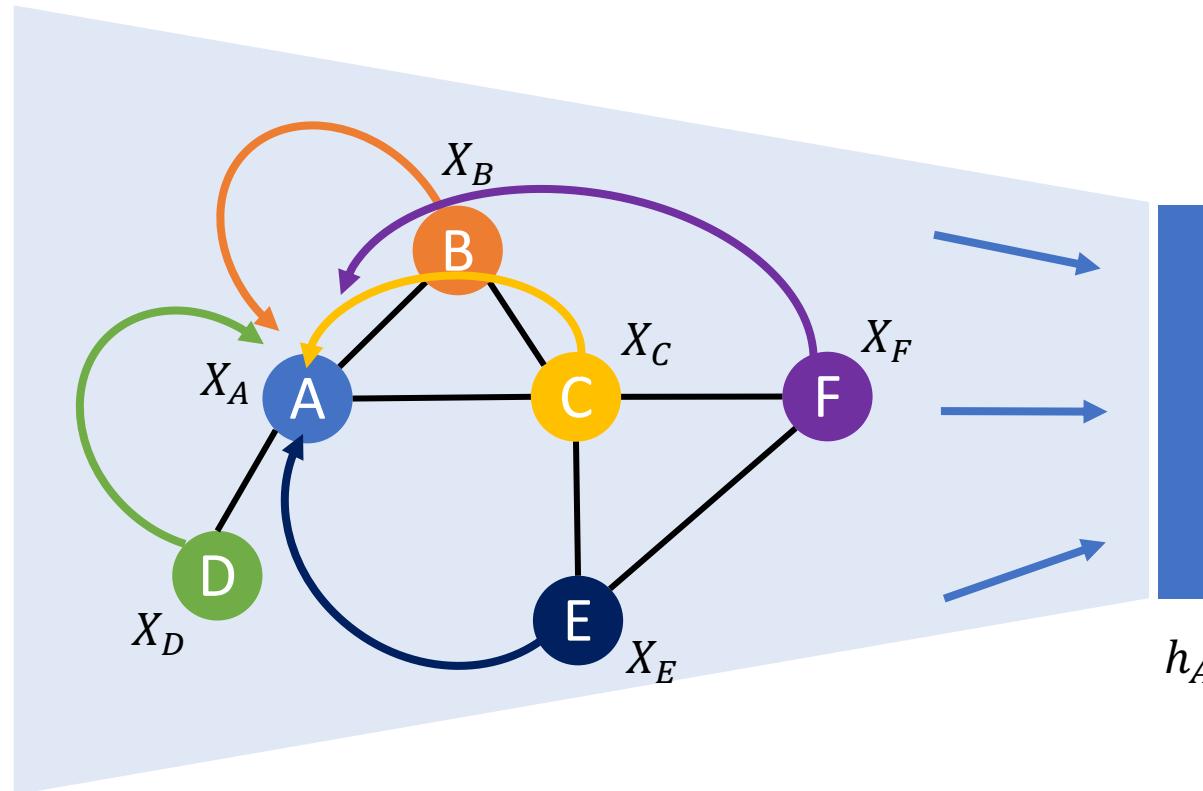
**“Homophily: connected nodes are related/informative/similar”**

# Graph Neural Networks

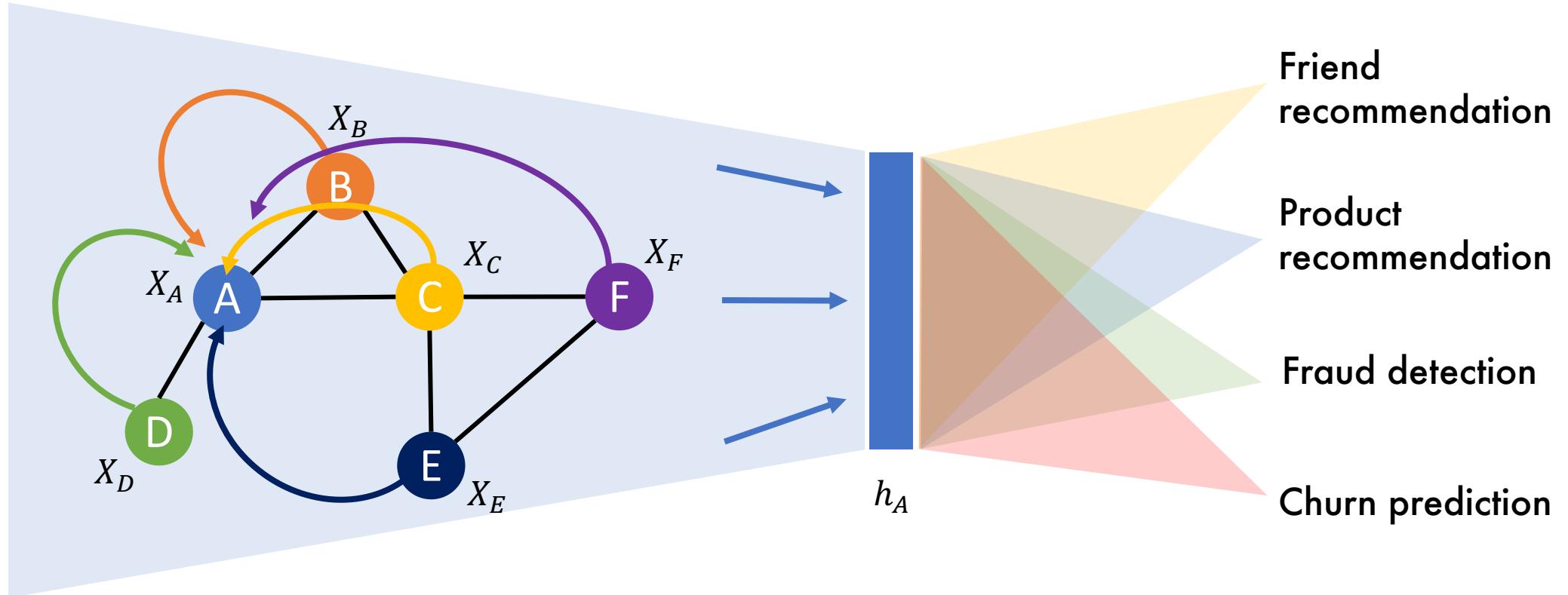


**“Homophily: connected nodes are related/informative/similar”**

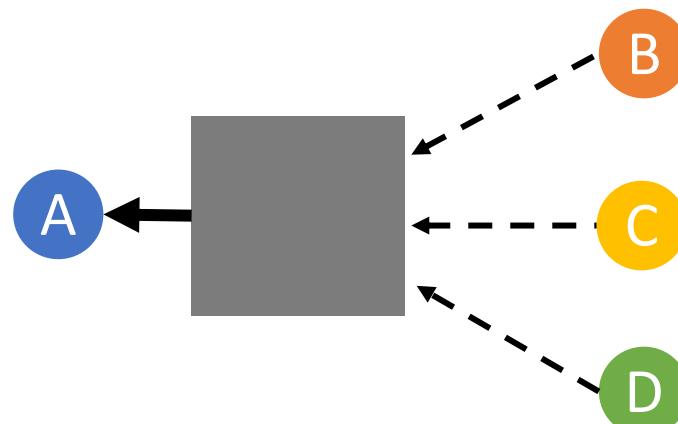
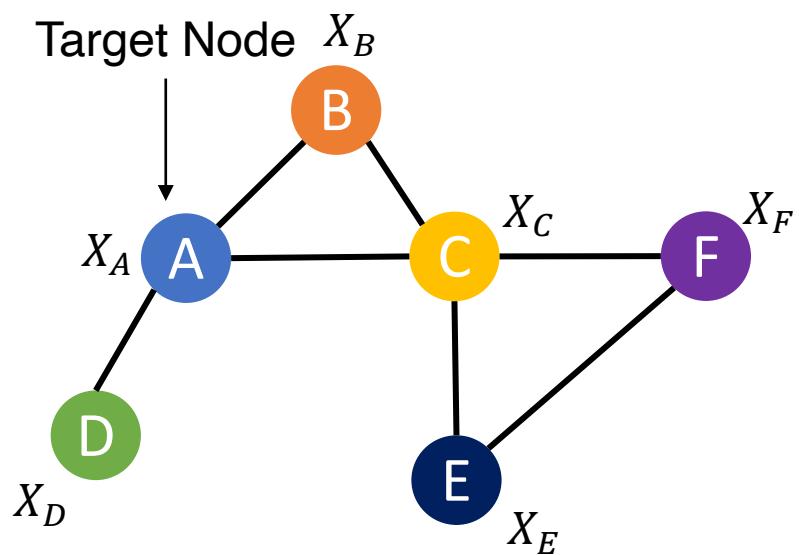
# Graph Neural Networks



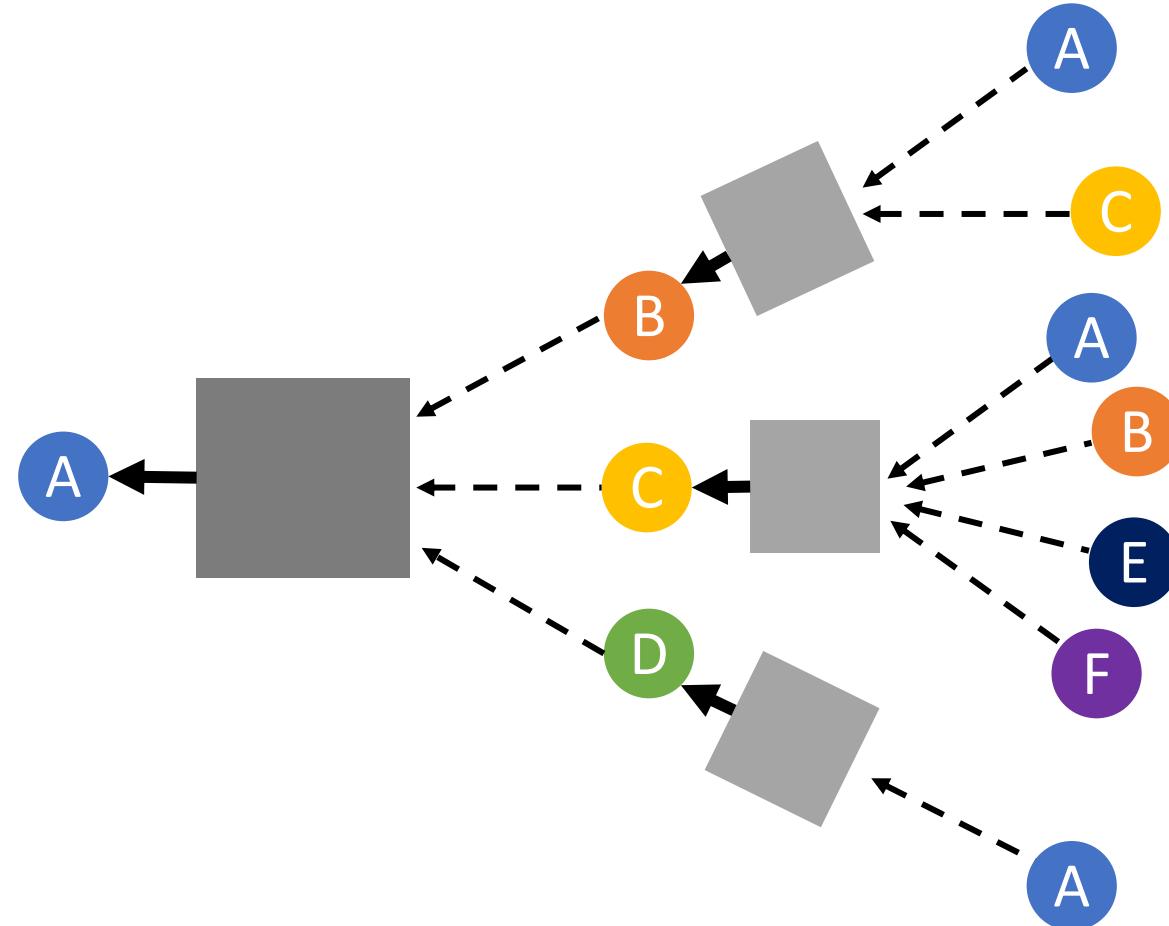
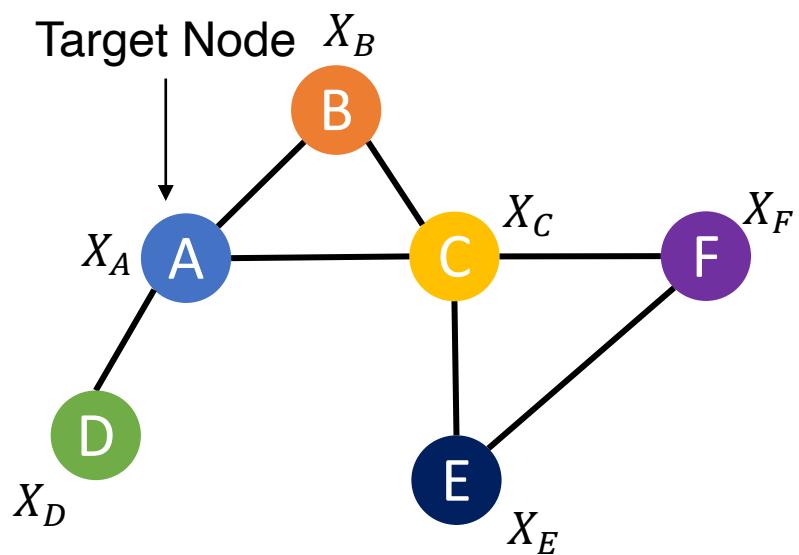
# Graph Neural Networks



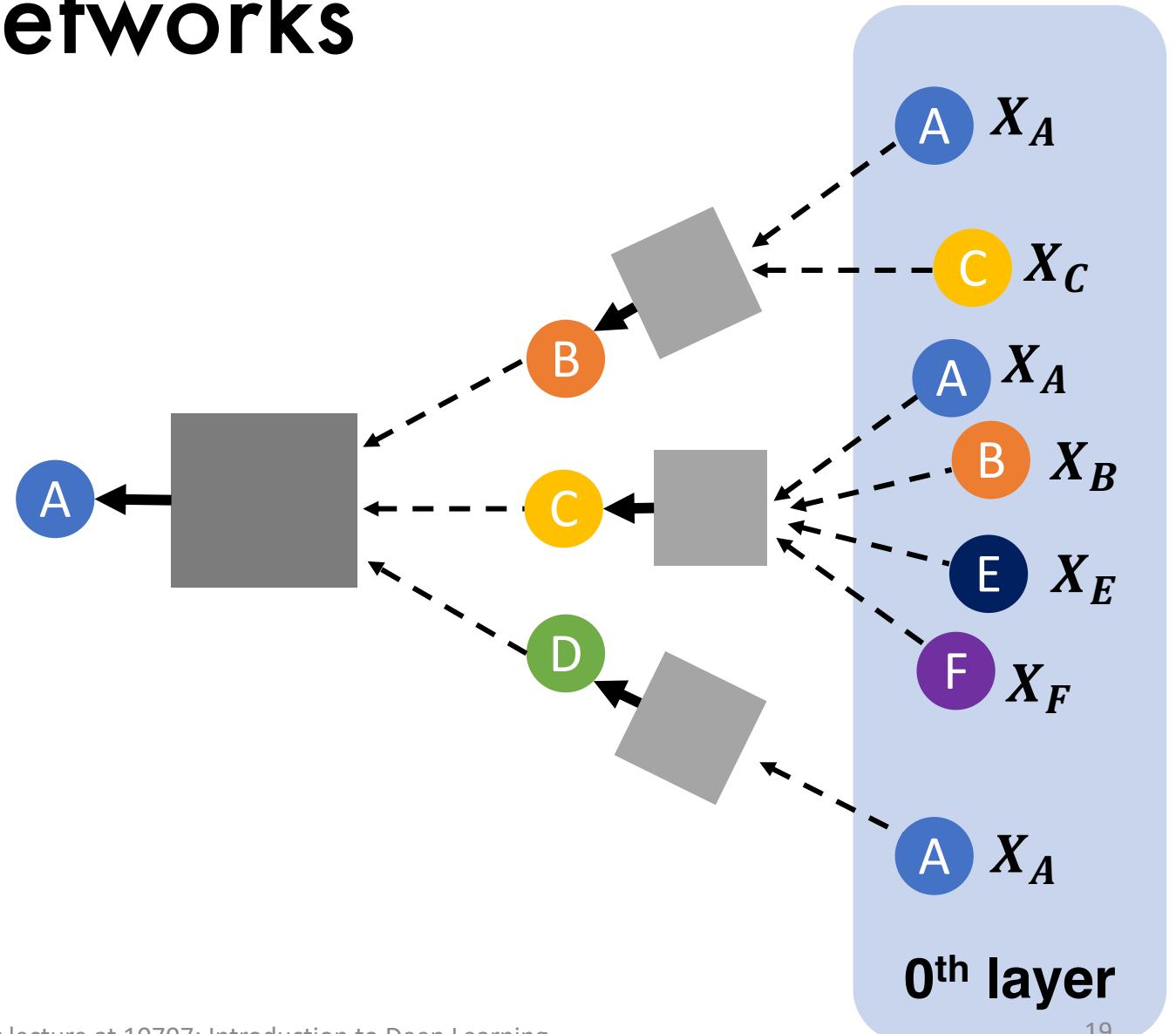
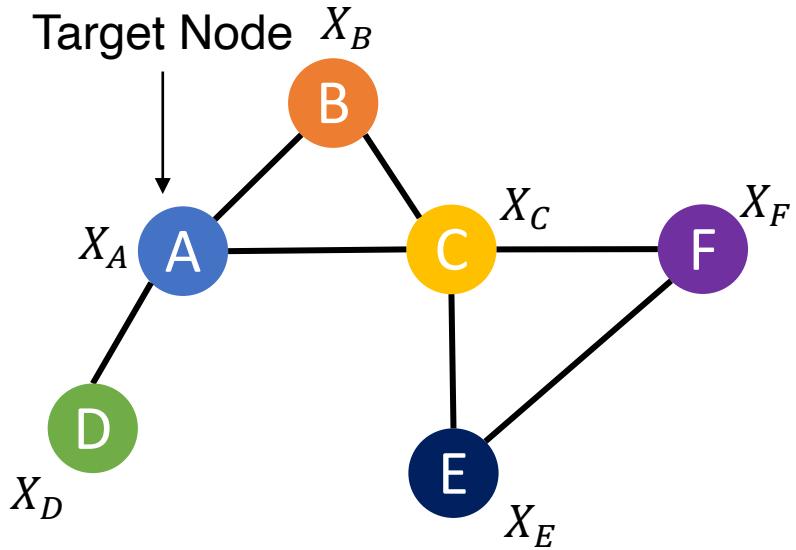
# Graph Neural Networks



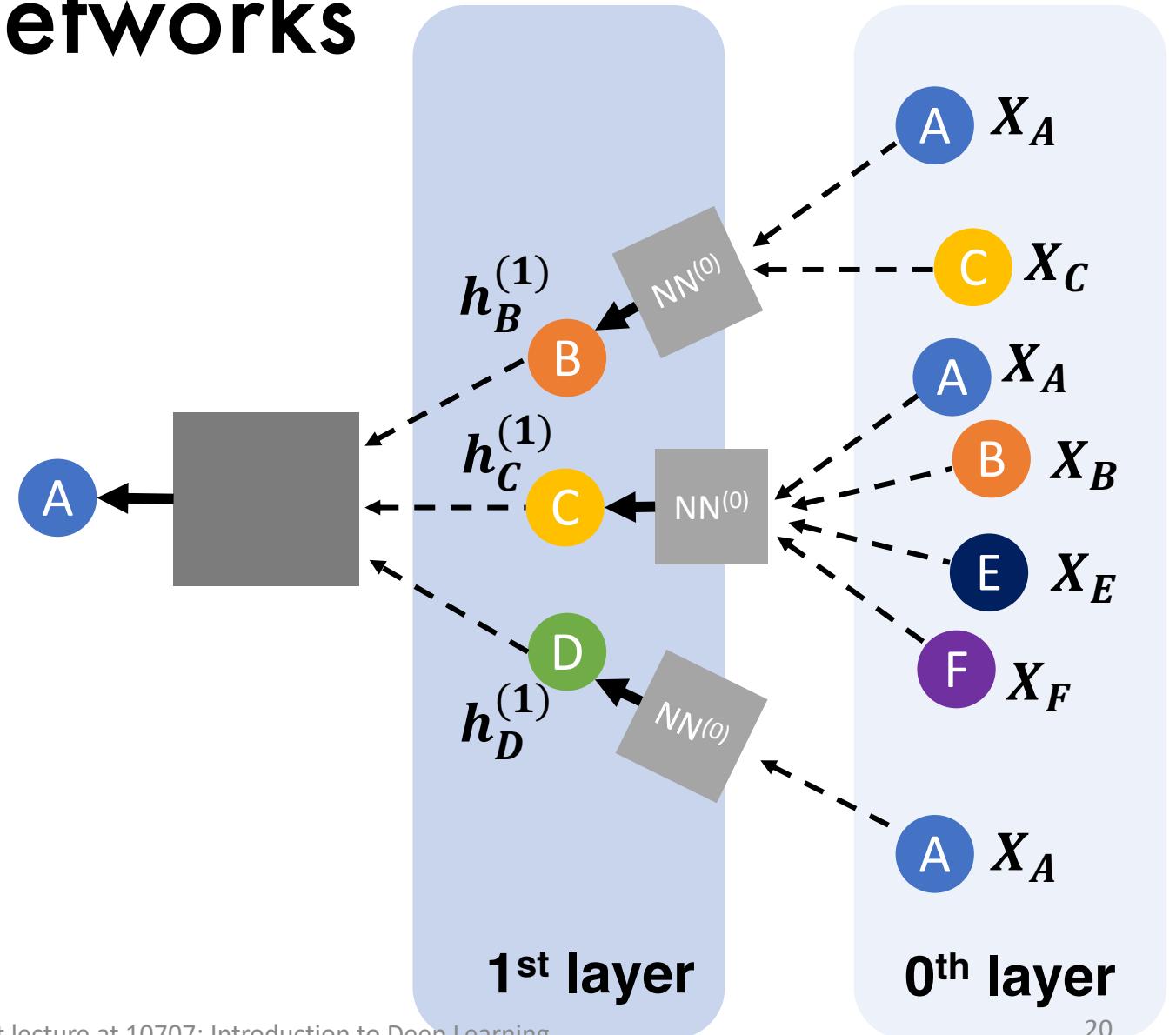
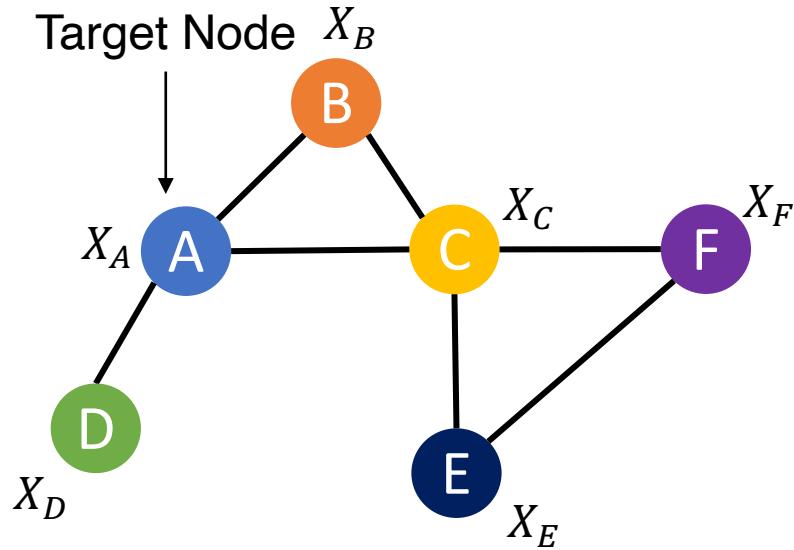
# Graph Neural Networks



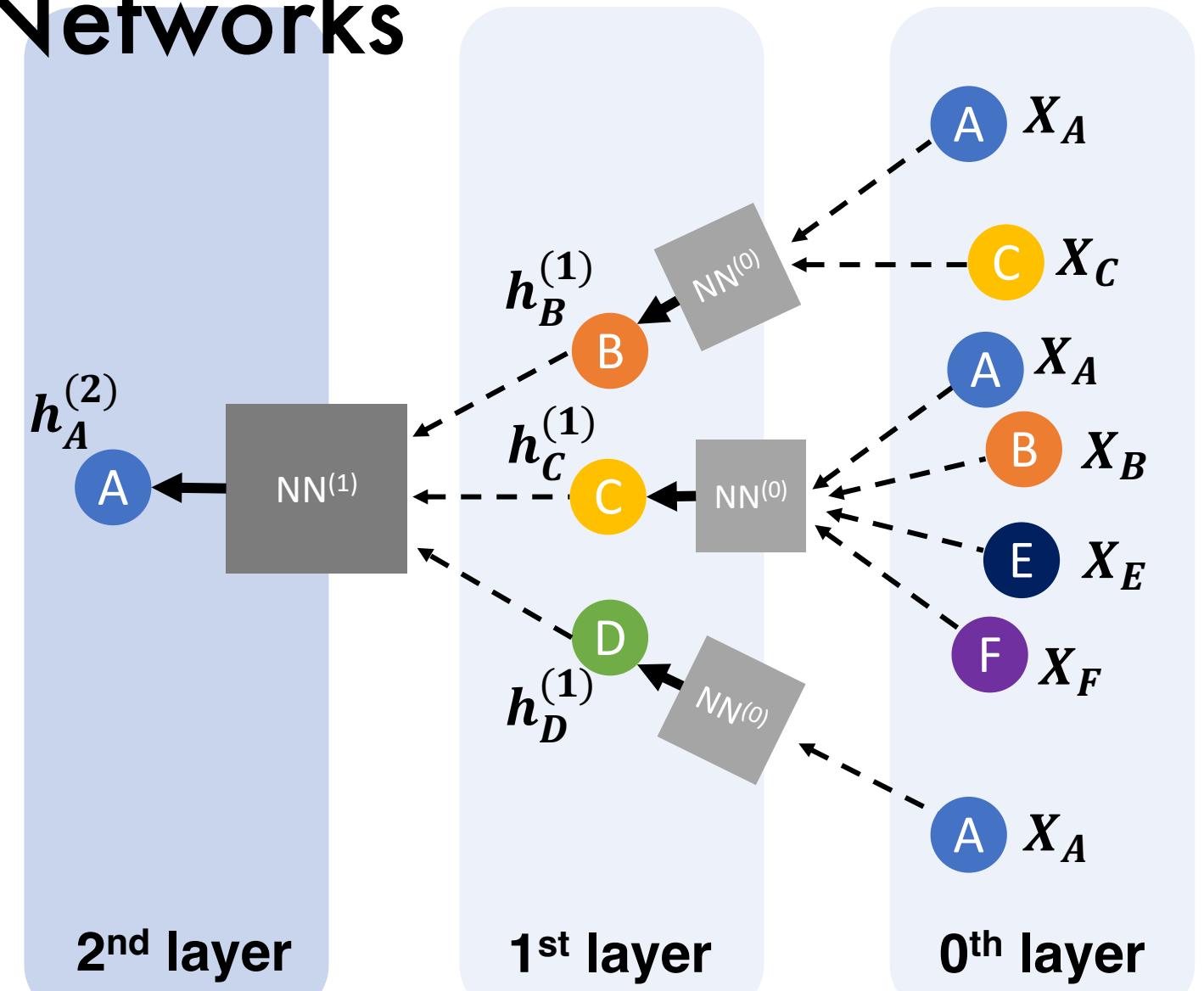
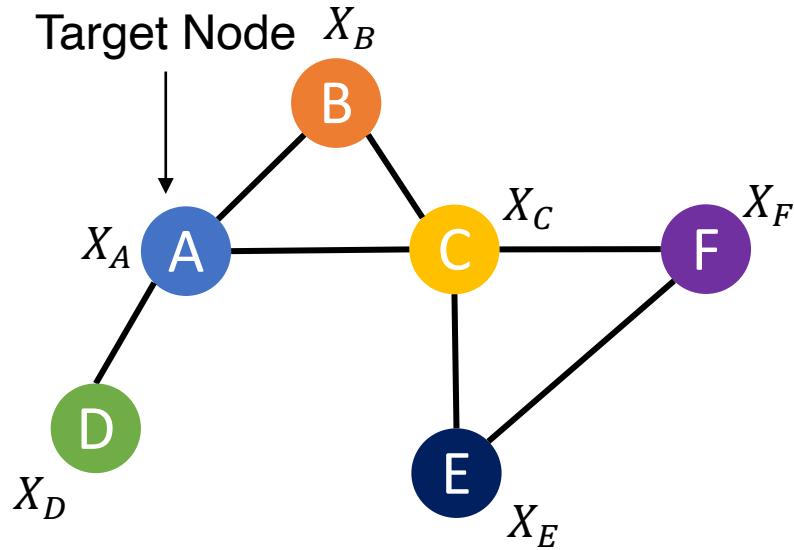
# Graph Neural Networks



# Graph Neural Networks



# Graph Neural Networks



# Graph Neural Networks

## 1. Aggregate messages from neighbors

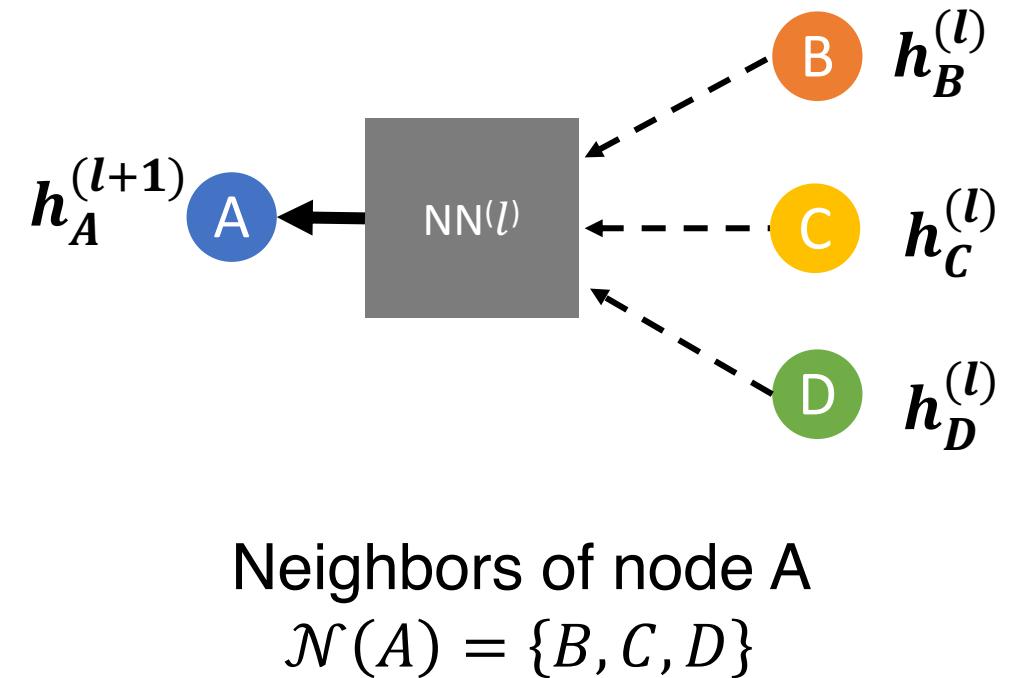
$h_v^{(l)}$ : node embedding of  $v$  at  $l$ -th layer

$\mathcal{N}(v)$  : neighboring nodes of  $v$

$f^{(l)}$ : aggregation function at  $l$ -th layer

$m_v^{(l)}$  : message vector of  $v$  at  $l$ -th layer

$$\begin{aligned} m_A^{(l)} &= f^{(l)} \left( h_A^{(l)}, \{h_u^{(l)} : u \in \mathcal{N}(A)\} \right) \\ &= f^{(l)} \left( h_A^{(l)}, h_B^{(l)}, h_C^{(l)}, h_D^{(l)} \right) \end{aligned}$$



# Graph Neural Networks

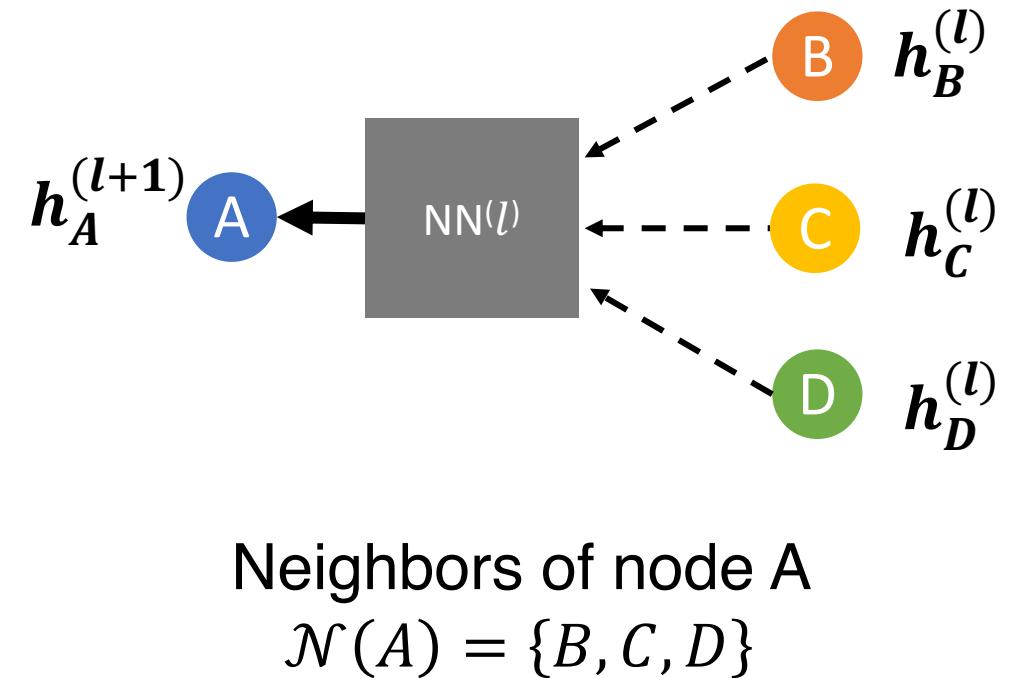
## 1. Aggregate messages from neighbors

$$\begin{aligned} m_A^{(l)} &= f^{(l)} \left( h_A^{(l)}, \{h_u^{(l)} : u \in \mathcal{N}(A)\} \right) \\ &= f^{(l)} \left( h_A^{(l)}, h_B^{(l)}, h_C^{(l)}, h_D^{(l)} \right) \end{aligned}$$

## 2. Transform messages

$g^{(l)}$ : transformation function at  $l$ -th layer

$$h_A^{(l+1)} = g^{(l)}(m_A^{(l)})$$



# Graph Neural Networks

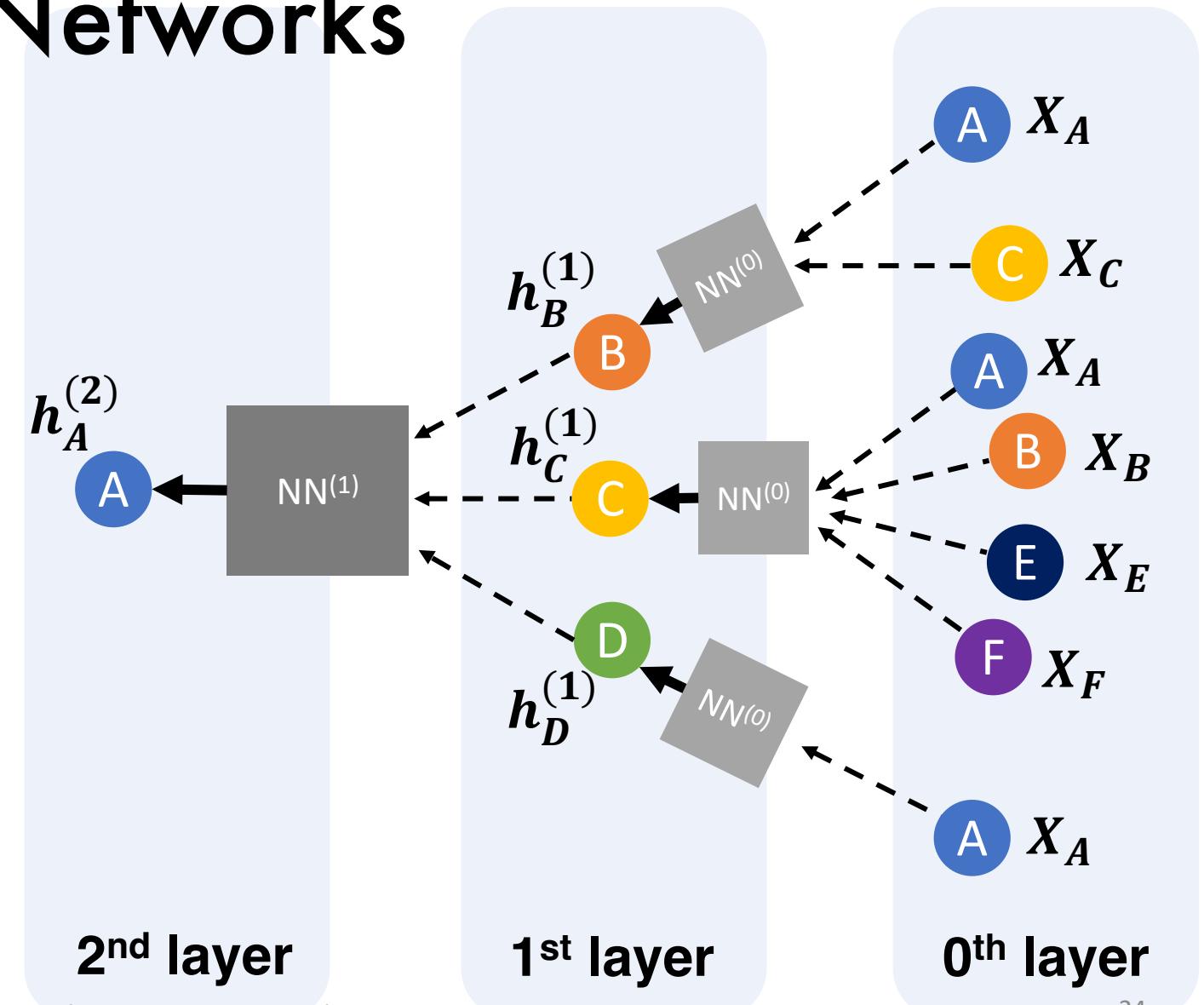
In each layer  $l$ ,  
for each target node  $v$ :

## 1. Aggregate messages

$$m_v^{(l)} = f^{(l)} \left( h_v^{(l)}, \{h_u^{(l)} : u \in \mathcal{N}(v)\} \right)$$

## 2. Transform messages

$$h_v^{(l+1)} = g^{(l)}(m_v^{(l)})$$



# Graph Neural Networks

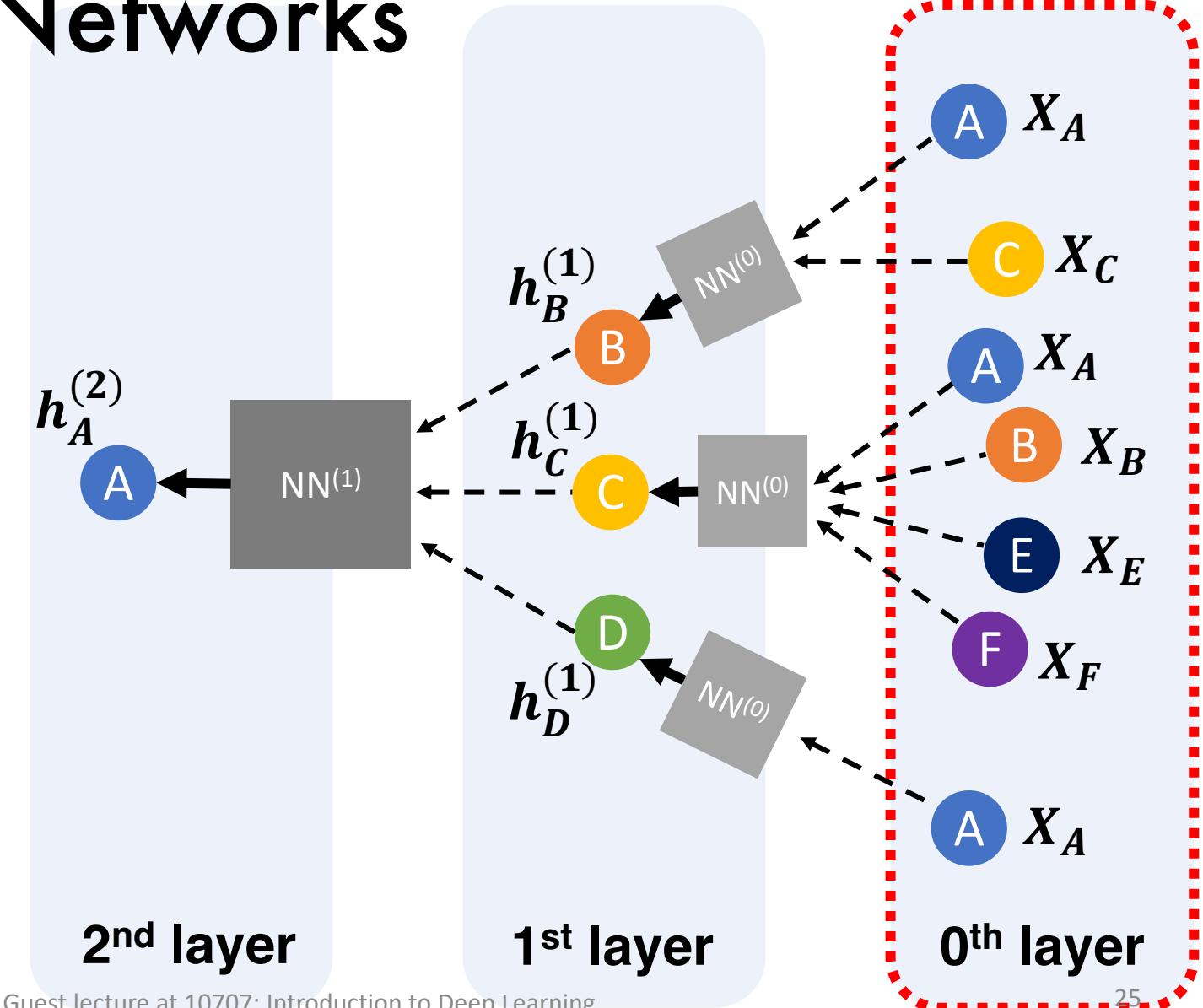
In each layer  $l$ ,  
for each target node  $v$ :

## 1. Aggregate messages

$$m_v^{(l)} = f^{(l)} \left( h_v^{(l)}, \{h_u^{(l)} : u \in \mathcal{N}(v)\} \right)$$

## 2. Transform messages

$$h_v^{(l+1)} = g^{(l)}(m_v^{(l)})$$



# Graph Neural Networks

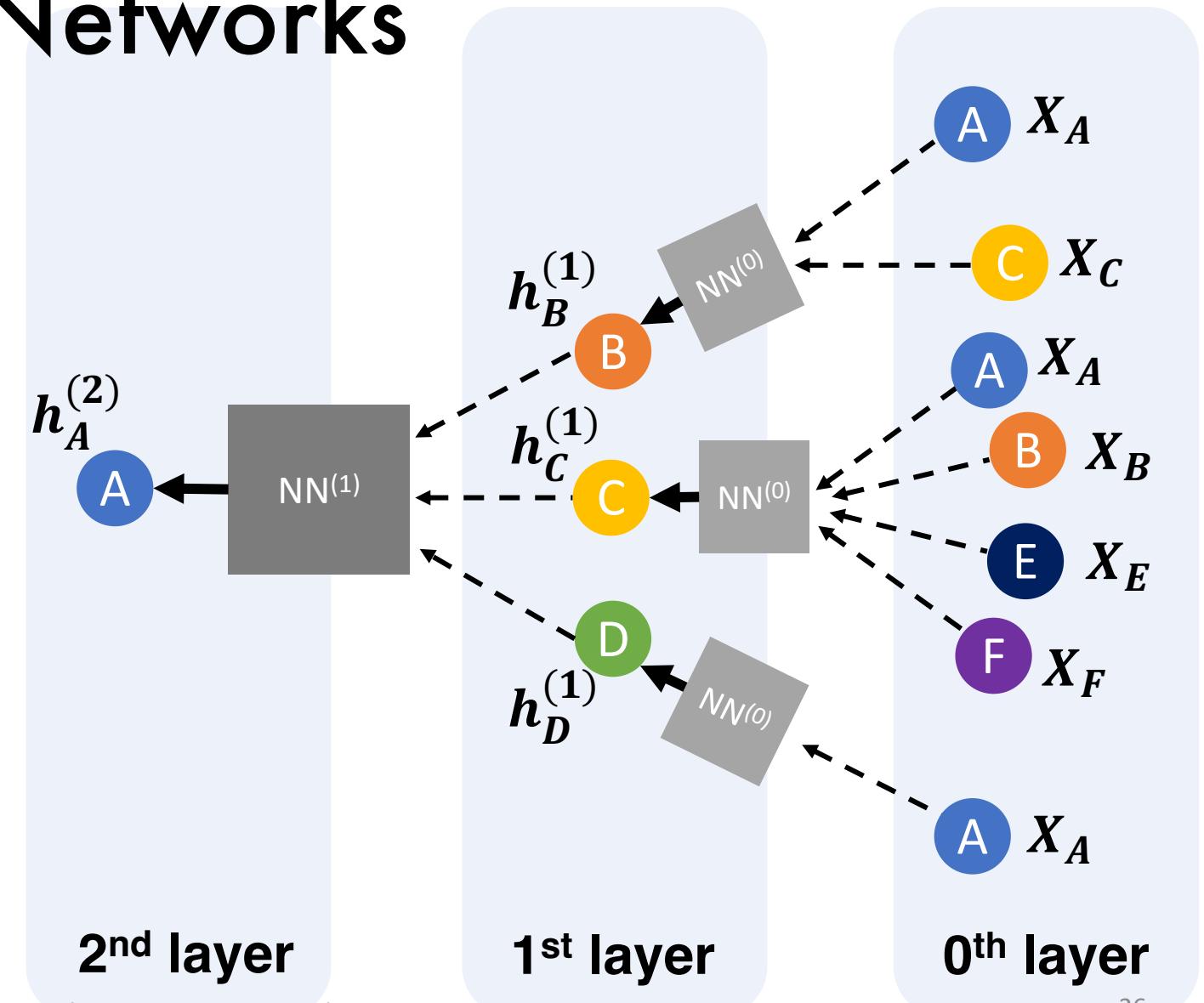
In each layer  $l$ ,  
for each target node  $v$ :

## 1. Aggregate messages

$$m_v^{(l)} = \boxed{f^{(l)}}\left(h_v^{(l)}, \{h_u^{(l)} : u \in \mathcal{N}(v)\}\right)$$

## 2. Transform messages

$$h_v^{(l+1)} = \boxed{g^{(l)}}(m_v^{(l)})$$



# Graph Neural Networks

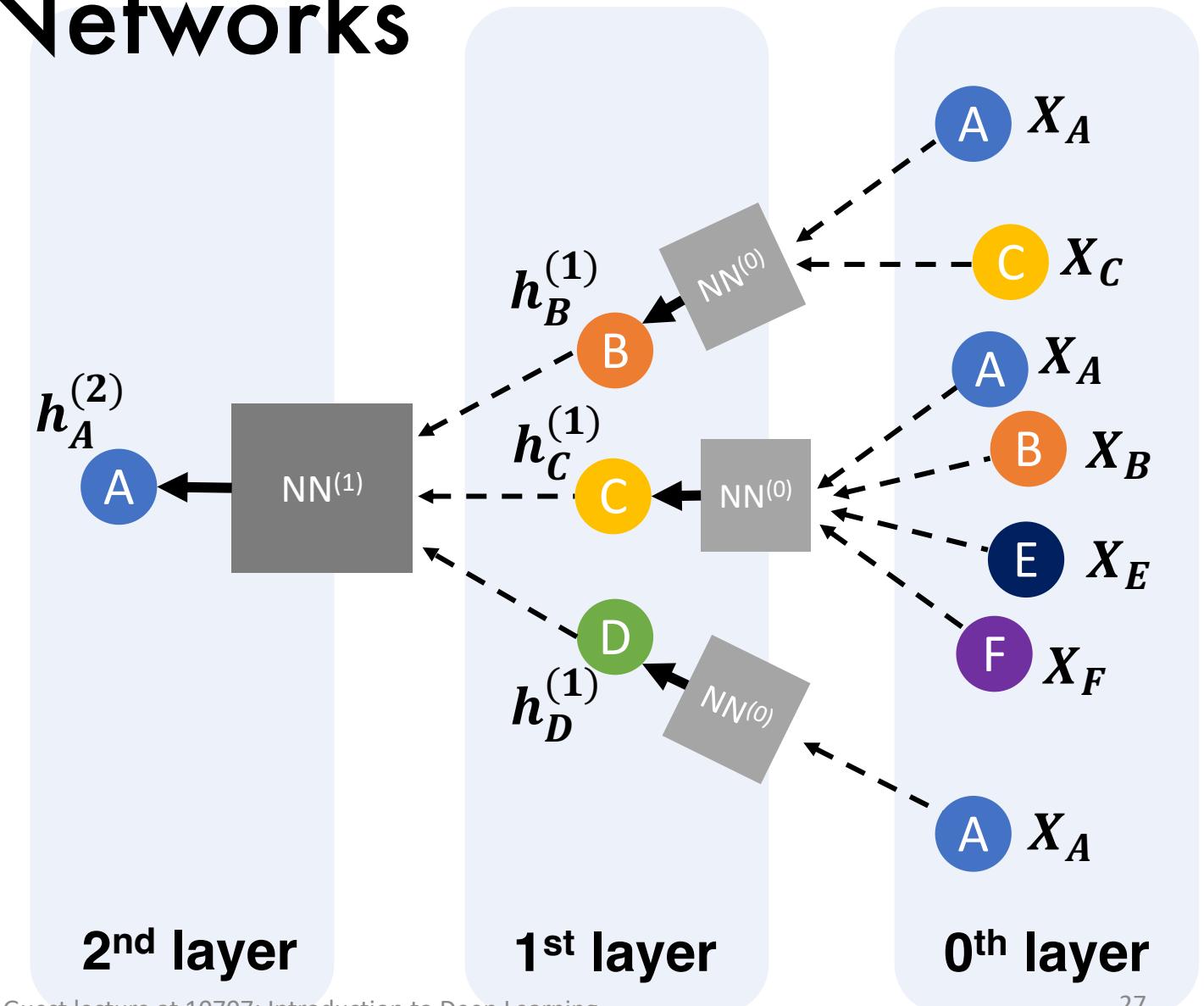
Graph Convolutional Networks<sup>[1]</sup>

## 1. Aggregate messages

$$m_v^{(l)} = \frac{1}{|\mathcal{N}(v) + 1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l)}$$

## 2. Transform messages

$$h_v^{(l+1)} = \sigma(W^{(l)} \circ m_v^{(l)})$$



[1] Kipf, Thomas N., et al. "Semi-supervised classification with graph convolutional networks."

# Graph Neural Networks

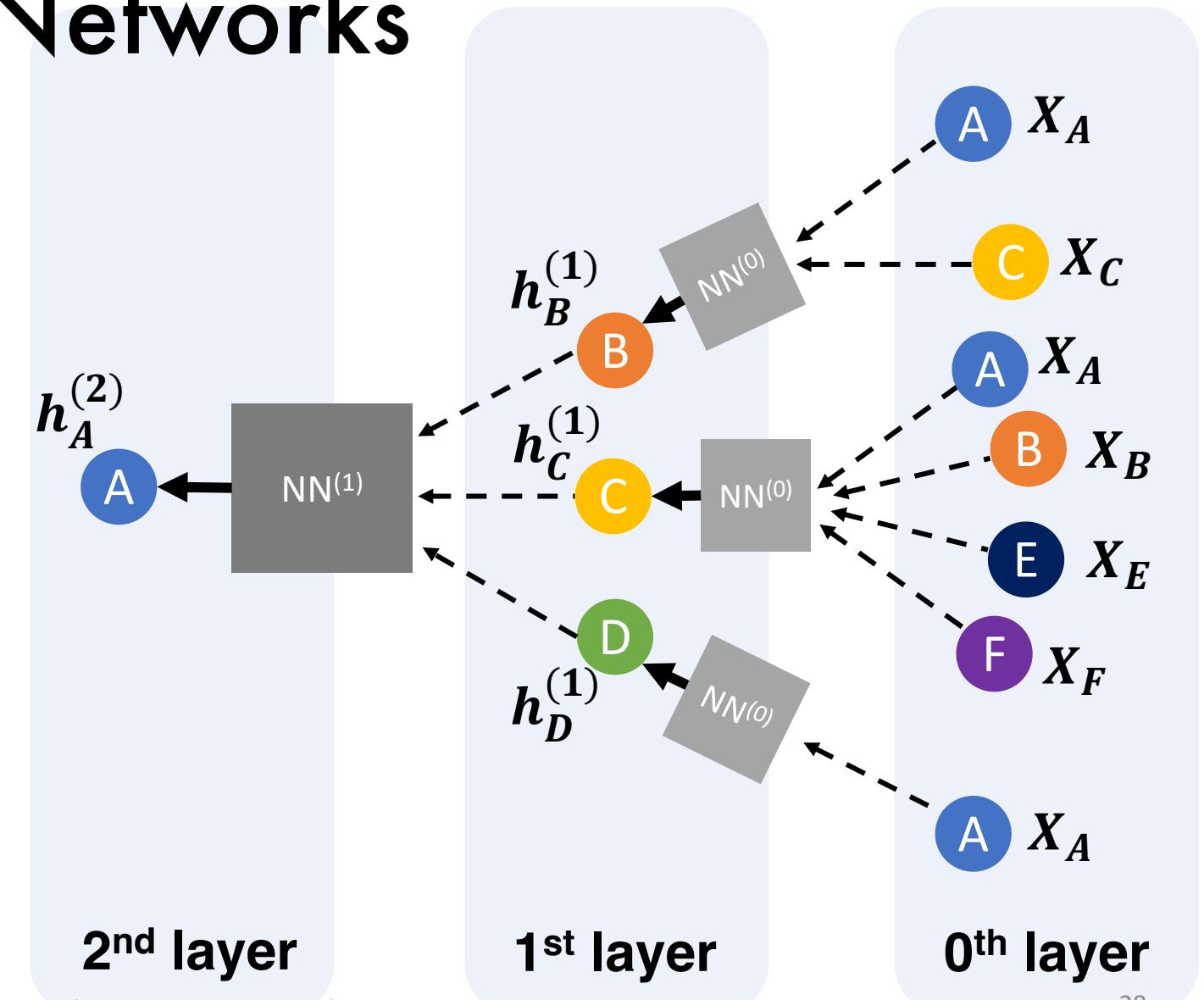
Graph Isomorphism Networks<sup>[2]</sup>

## 1. Aggregate messages

$$m_v^{(l)} = \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l)}$$

## 2. Transform messages

$$h_v^{(l+1)} = \sigma(W^{(l)} \circ m_v^{(l)})$$



[2] Xu, Keyulu, et al. "How powerful are graph neural networks?."

# Graph Neural Networks

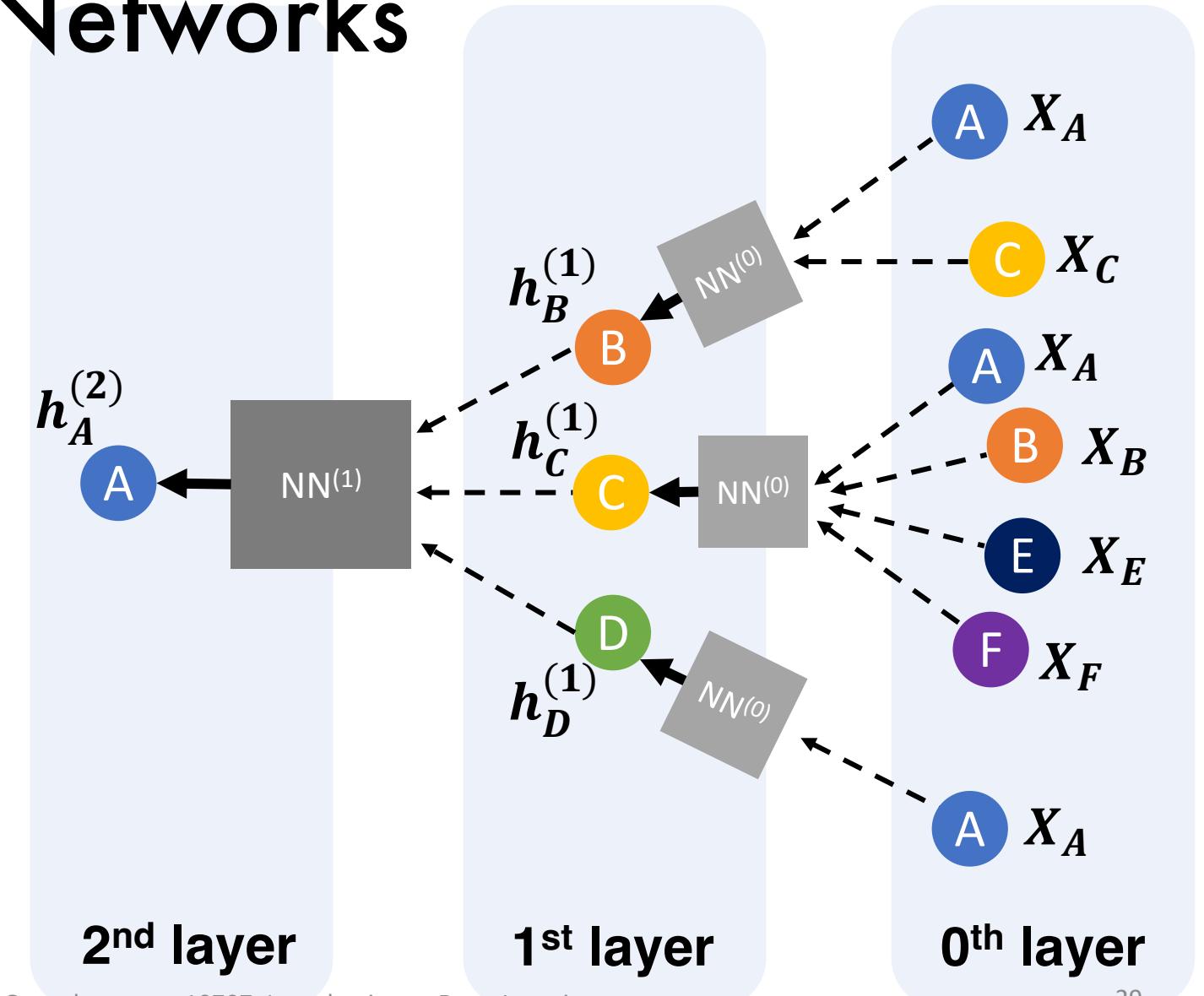
Simplified GCN<sup>[3]</sup>

## 1. Aggregate messages

$$m_v^{(l)} = \frac{1}{|\mathcal{N}(v) + 1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l)}$$

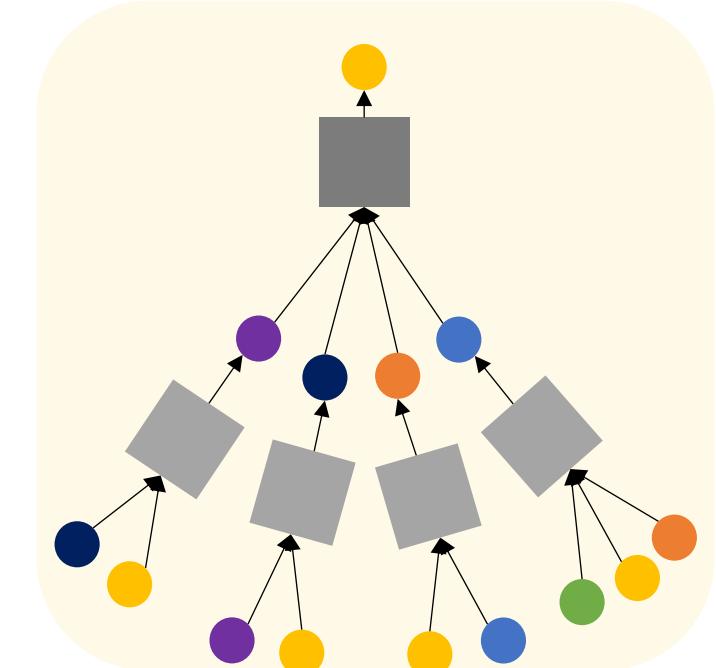
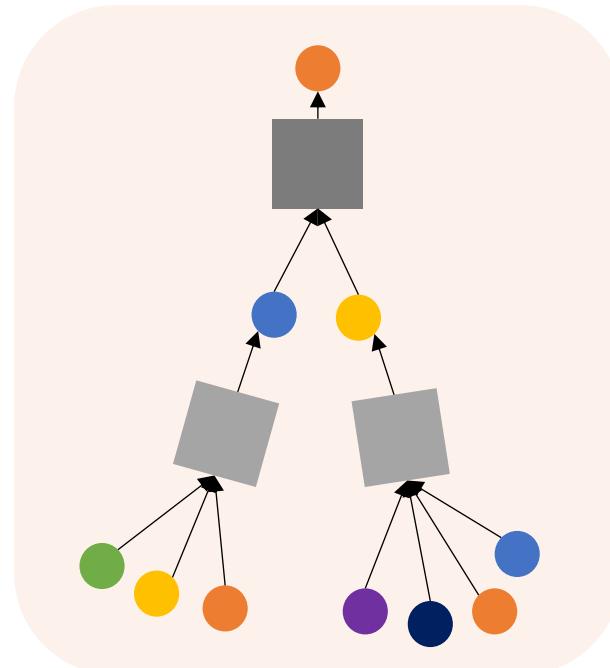
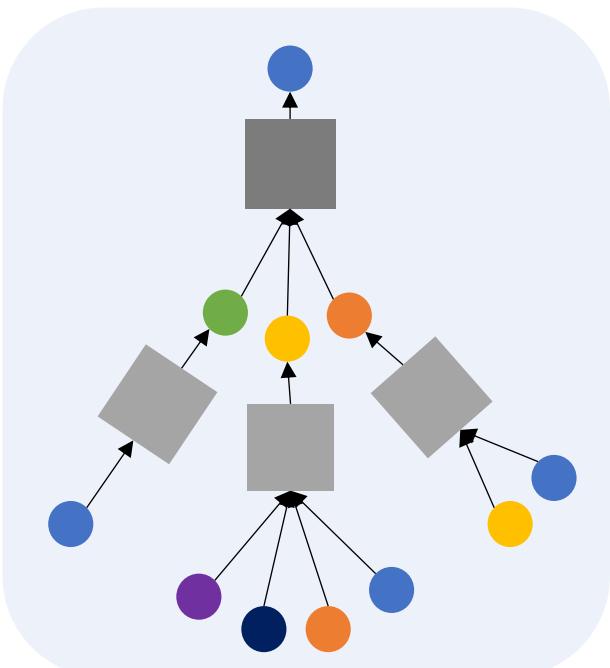
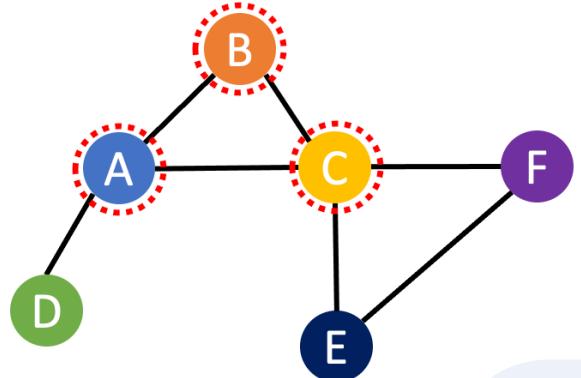
## 2. Transform messages

$$h_v^{(l+1)} = W^{(l)} \circ m_v^{(l)}$$

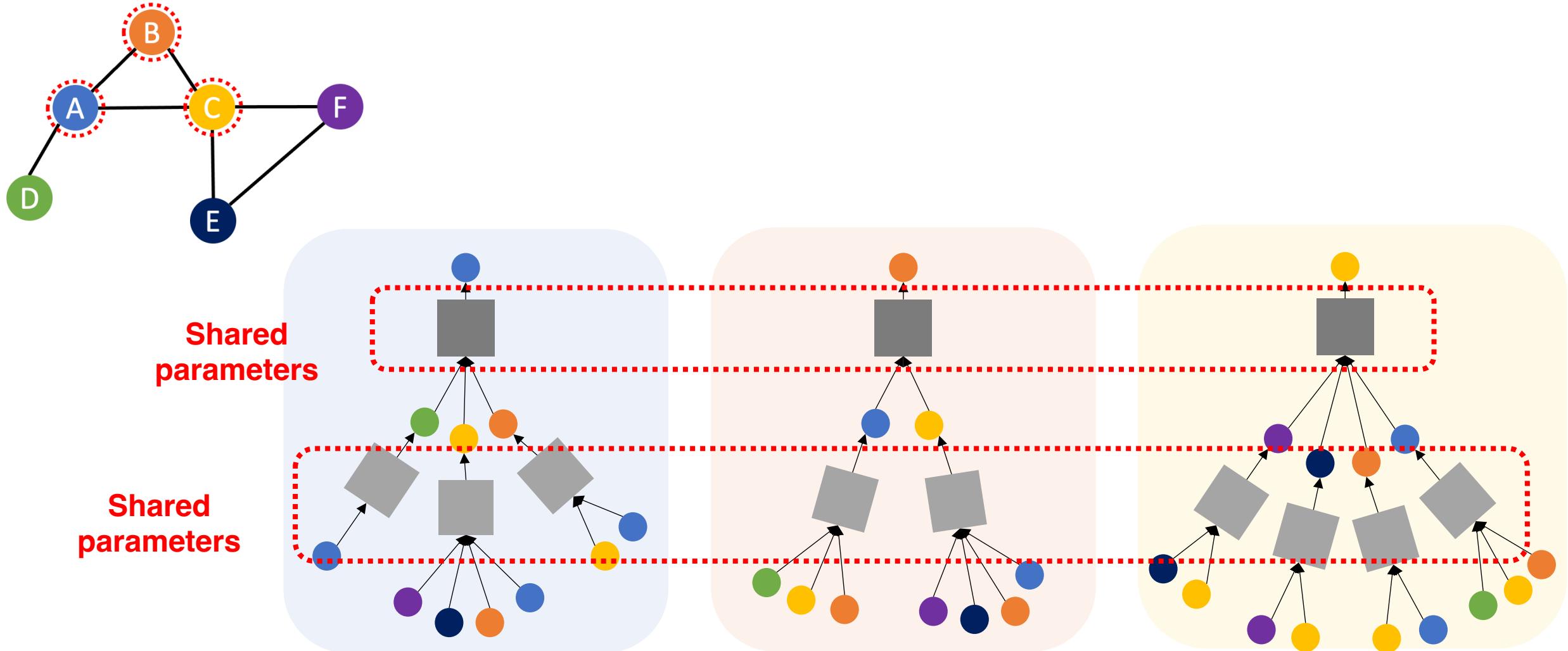


[3] Wu, Felix, et al. "Simplifying graph convolutional networks."

# Computation graphs

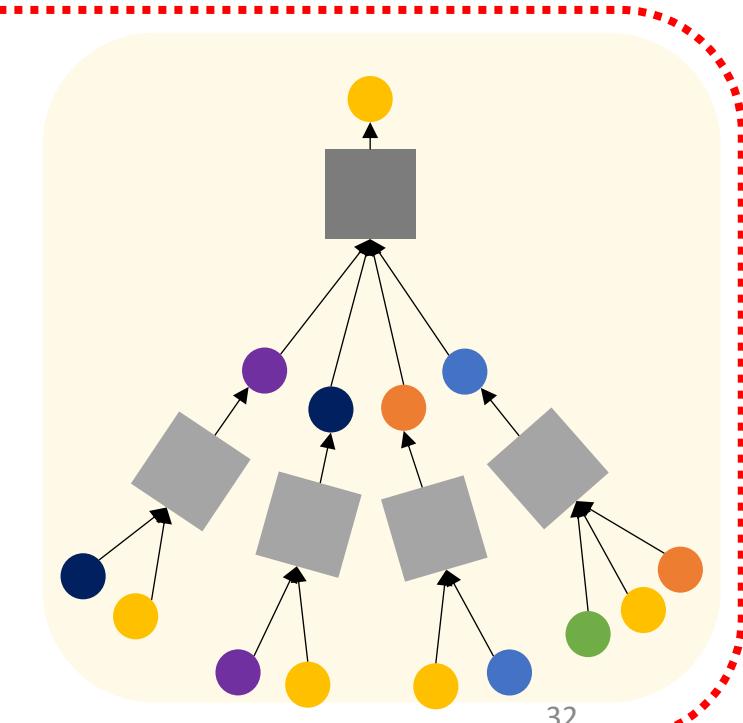
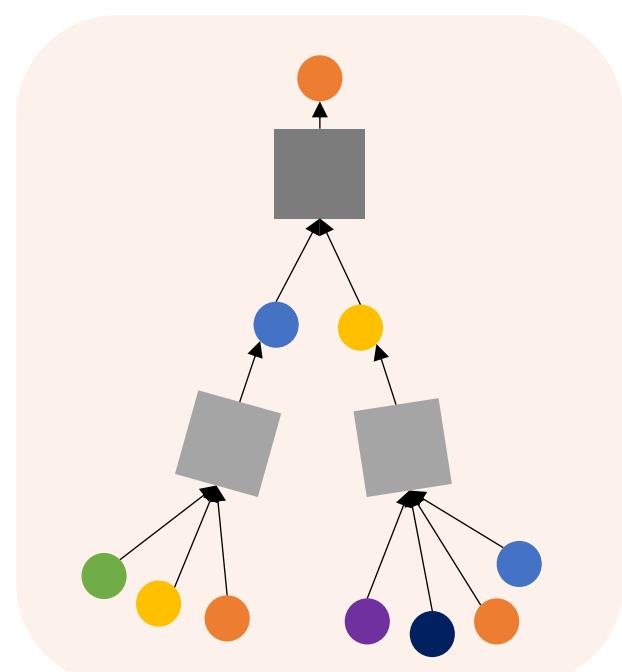
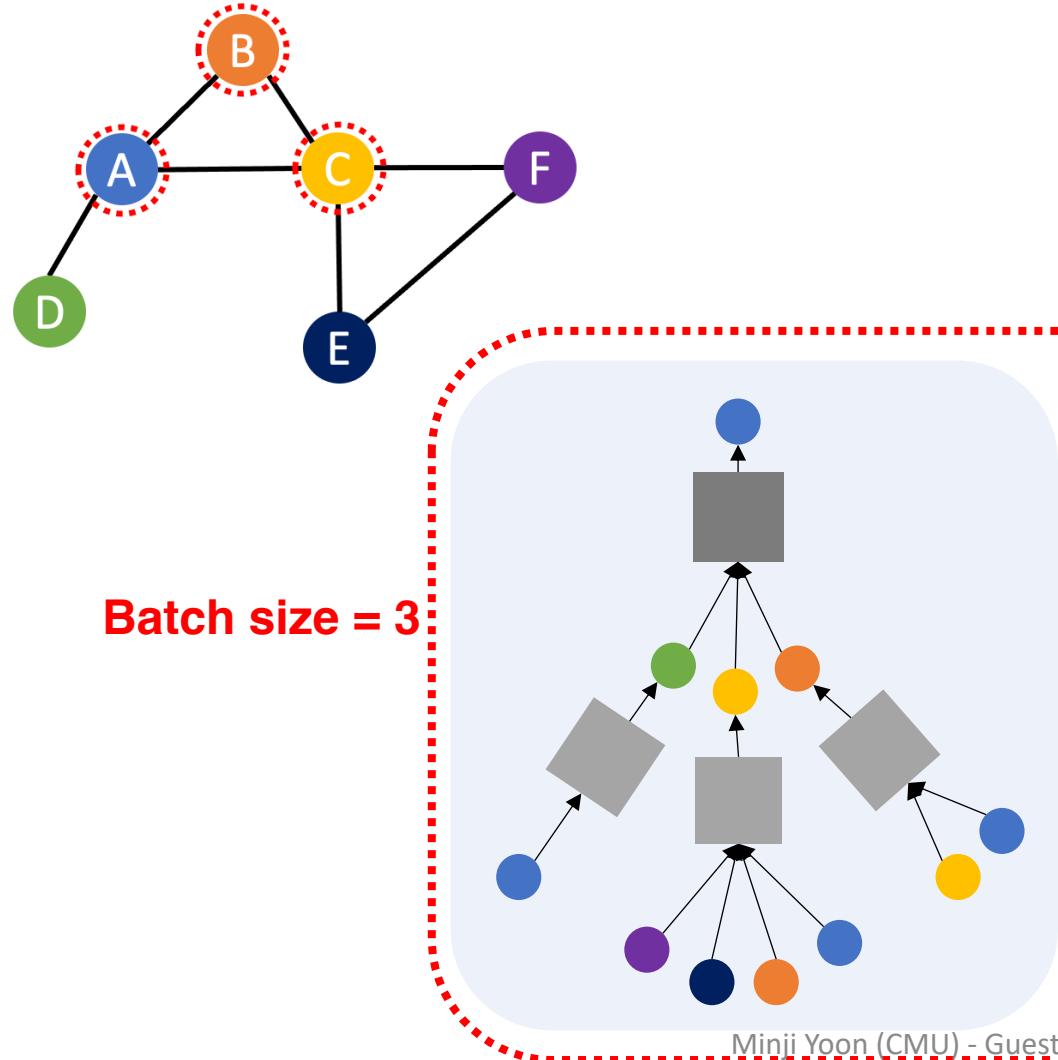


# Computation graphs

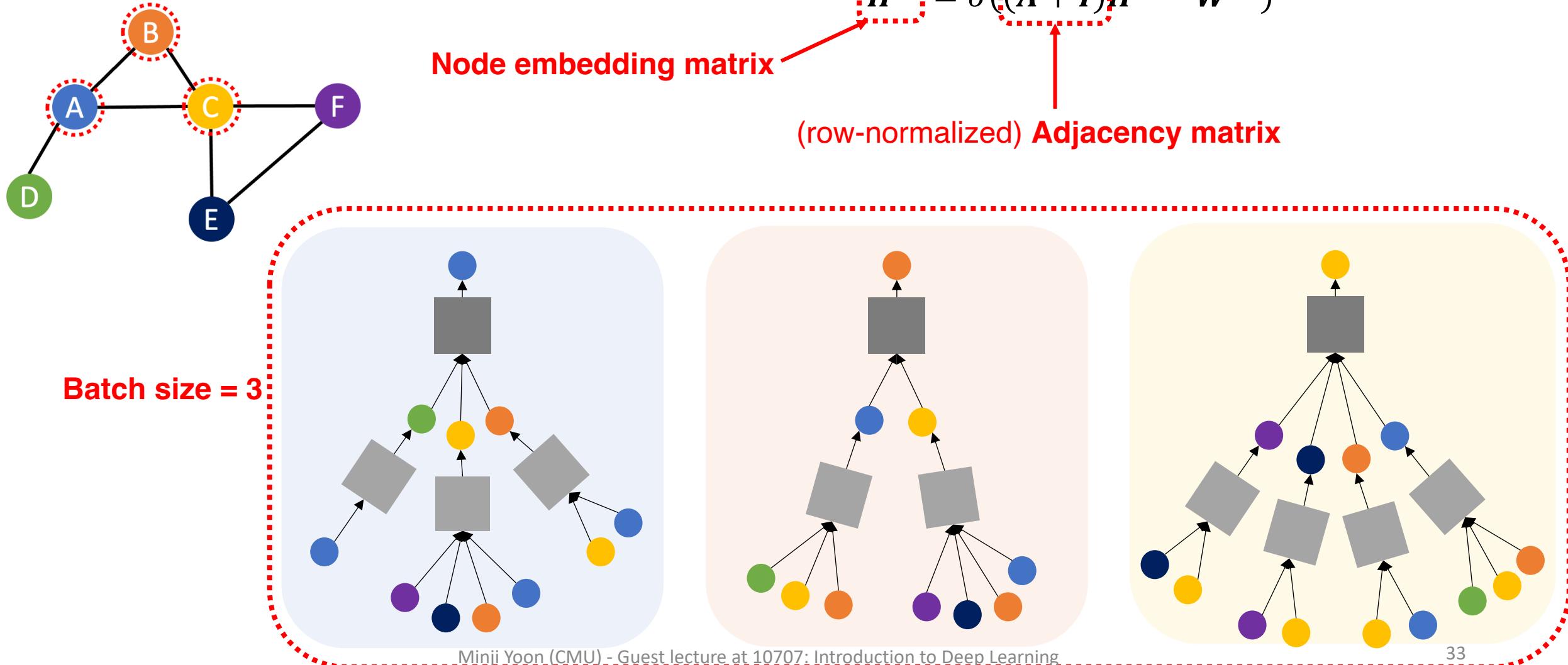


# Batch execution

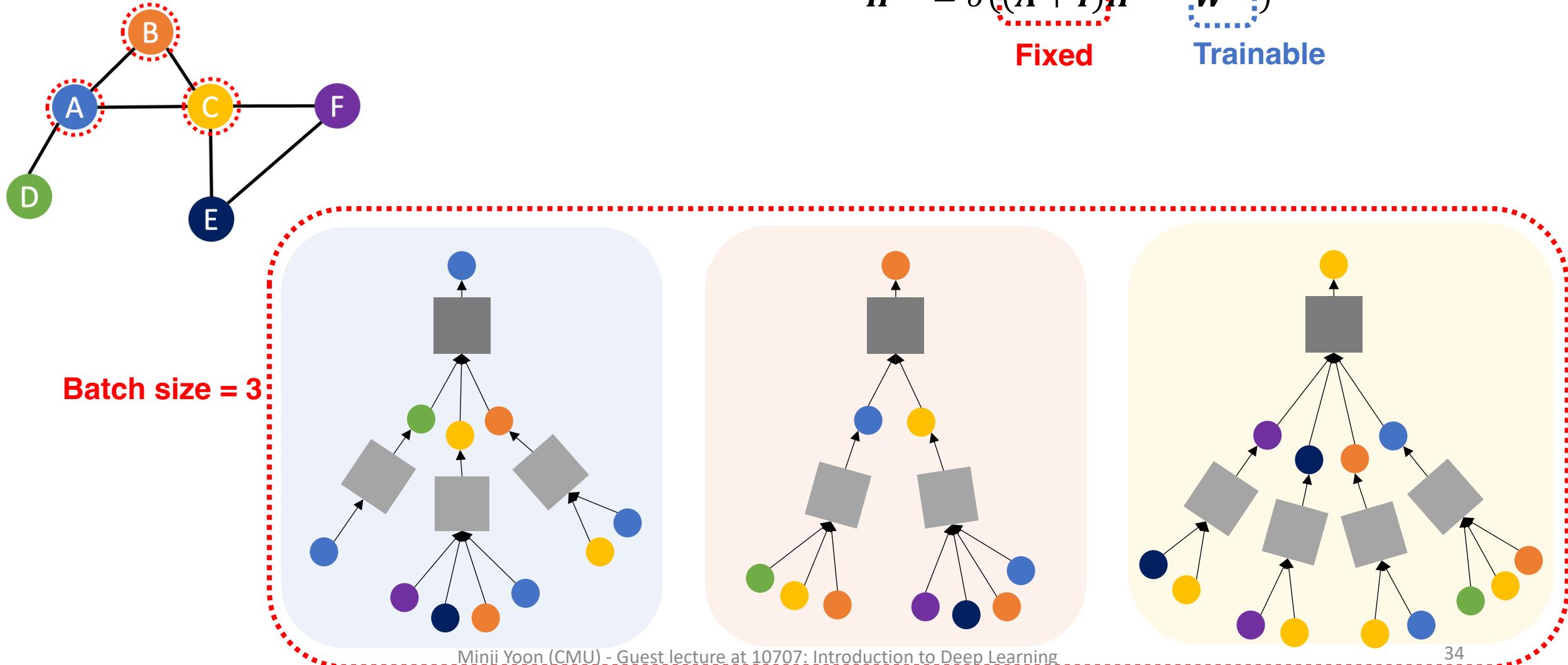
$$h_v^{(l)} = \sigma(\mathbf{W}^{(l)} \circ (\frac{1}{|\mathcal{N}(v)+1|} \sum_{u \in \mathcal{N}(v) \cup \{v\}} h_u^{(l-1)}))$$



# Batch execution

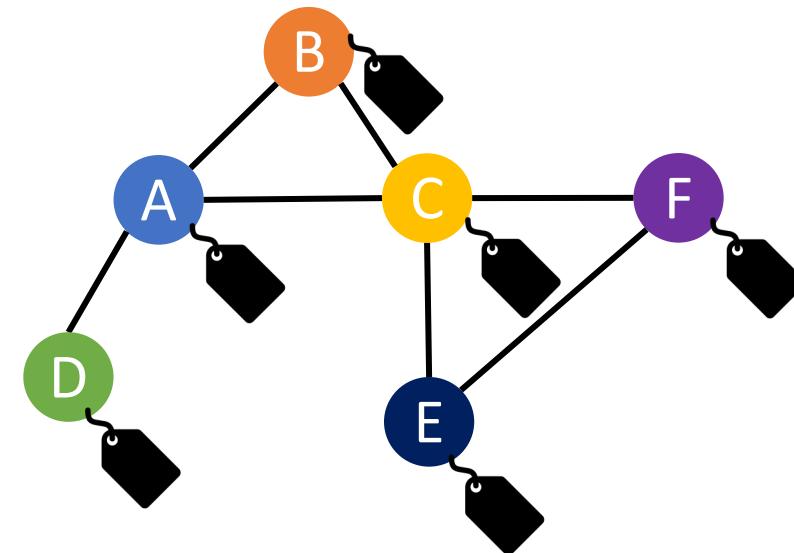


# Batch execution



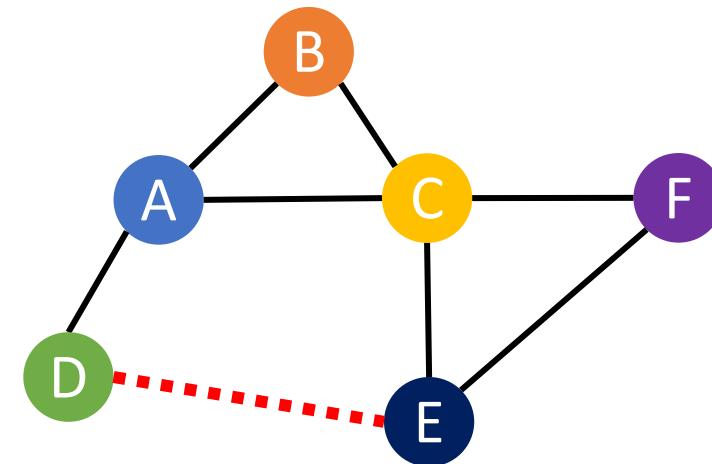
# Downstream tasks

- Node-level prediction



# Downstream tasks

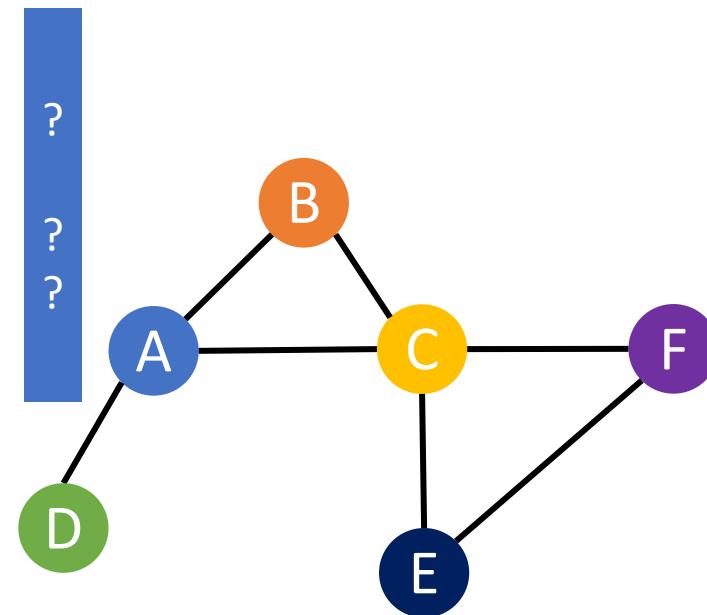
- Node-level prediction
- Edge-level prediction



D and E are related enough  
to be connected?

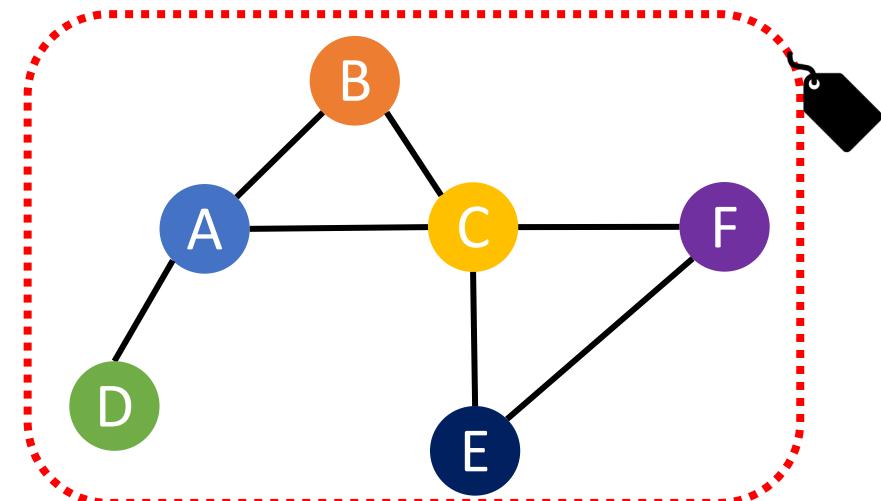
# Downstream tasks

- Node-level prediction
- Edge-level prediction
- Attribute-level prediction



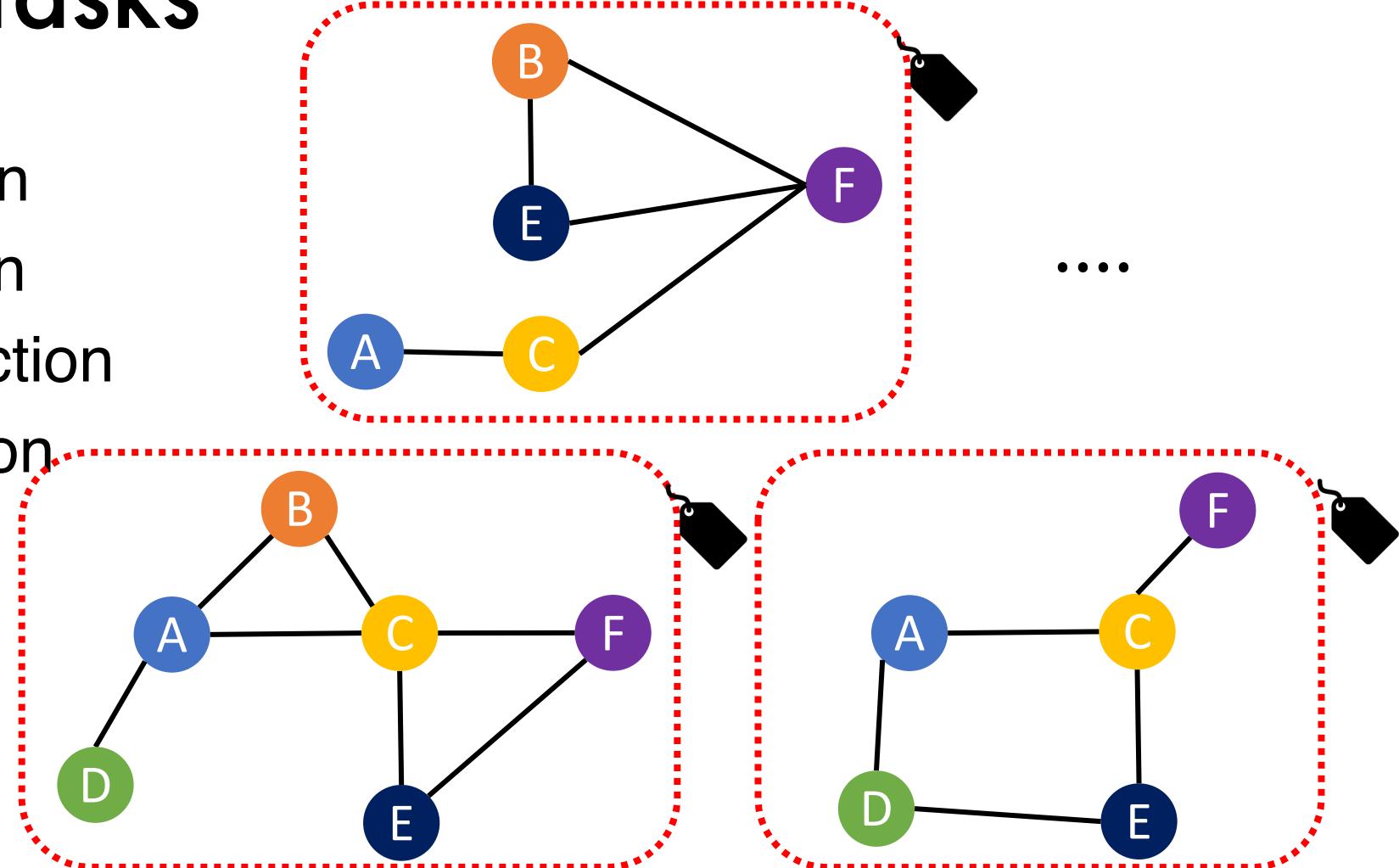
# Downstream tasks

- Node-level prediction
- Edge-level prediction
- Attribute-level prediction
- Graph-level prediction



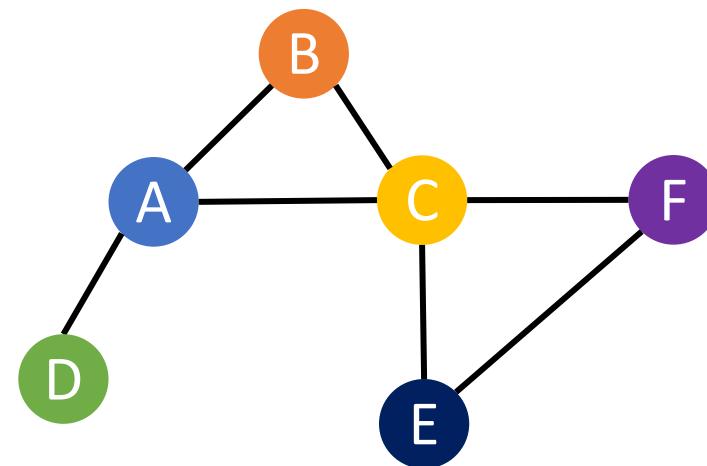
# Downstream tasks

- Node-level prediction
- Edge-level prediction
- Attribute-level prediction
- Graph-level prediction



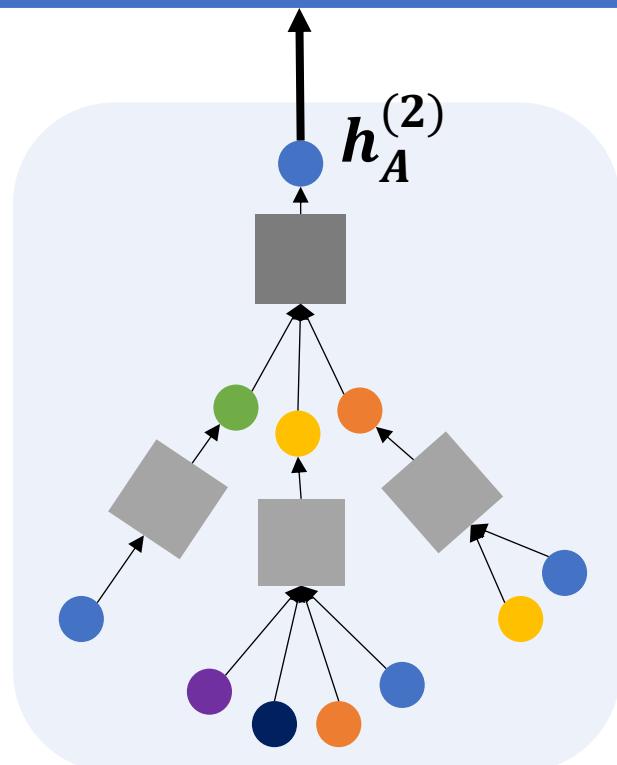
# Downstream tasks

- **Node-level prediction**
- Edge-level prediction
- Attribute-level prediction
- **Graph-level prediction**



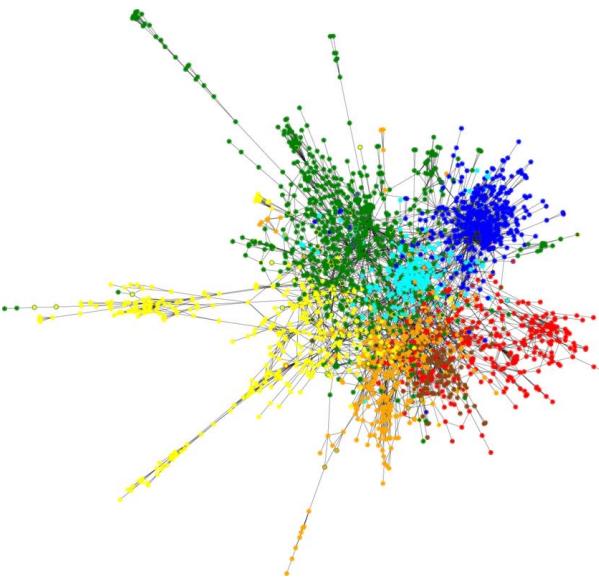
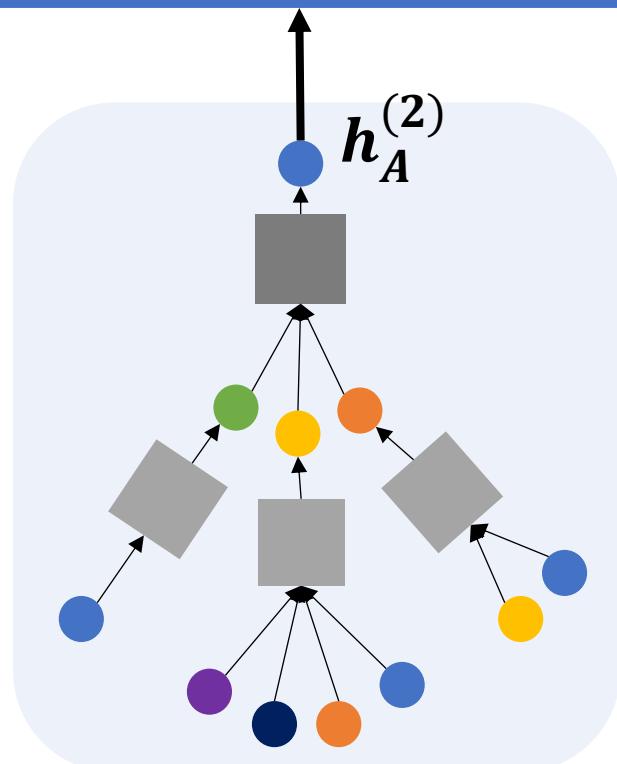
# Node-level prediction tasks

Node  
classification



# Node-level prediction tasks

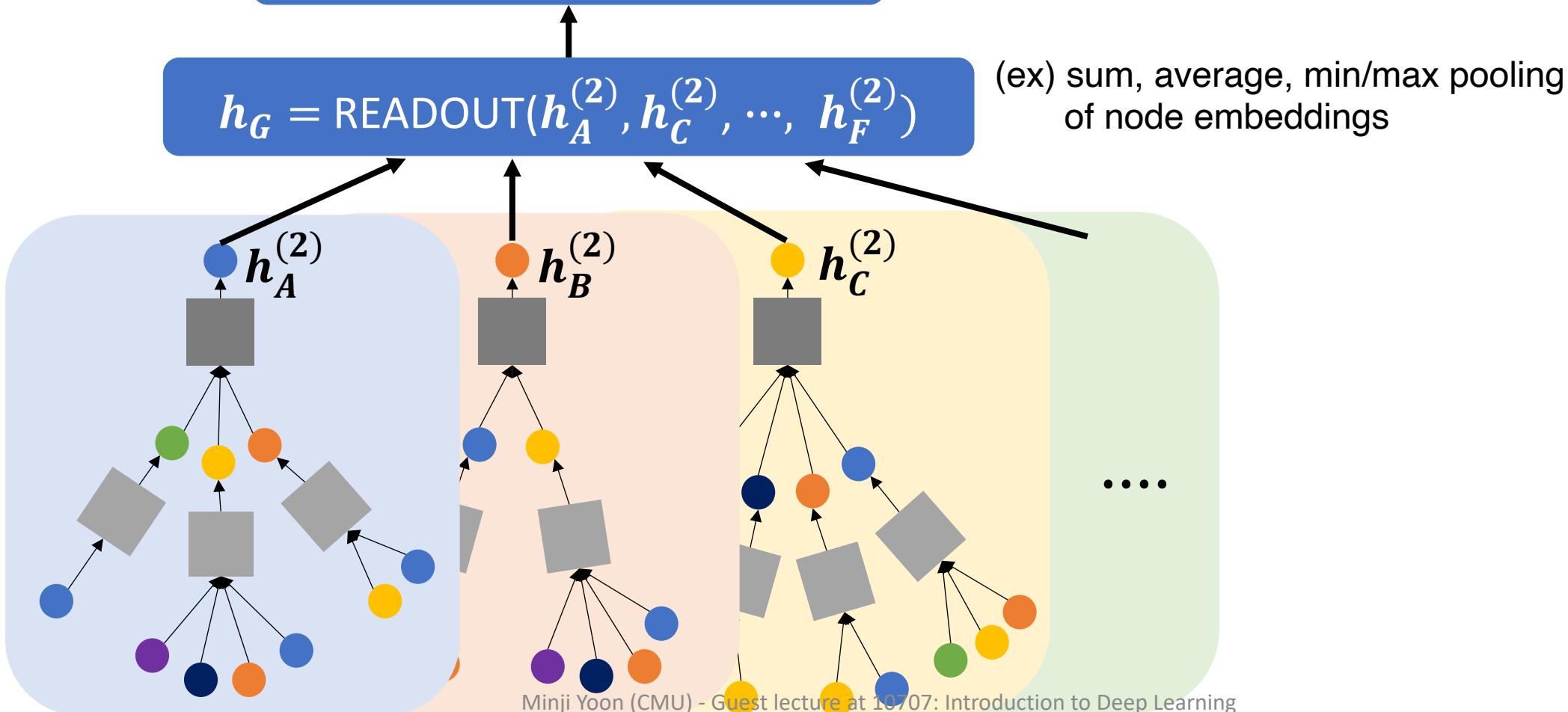
Node classification



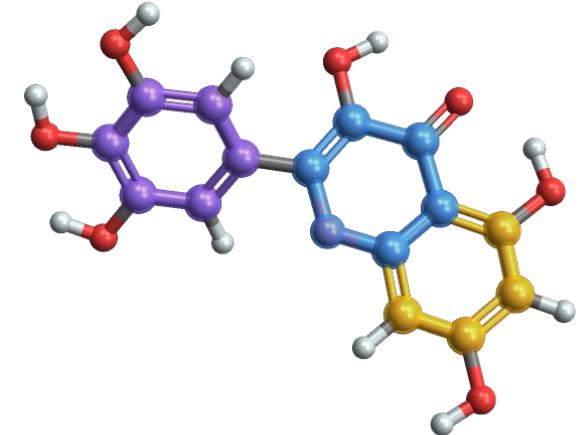
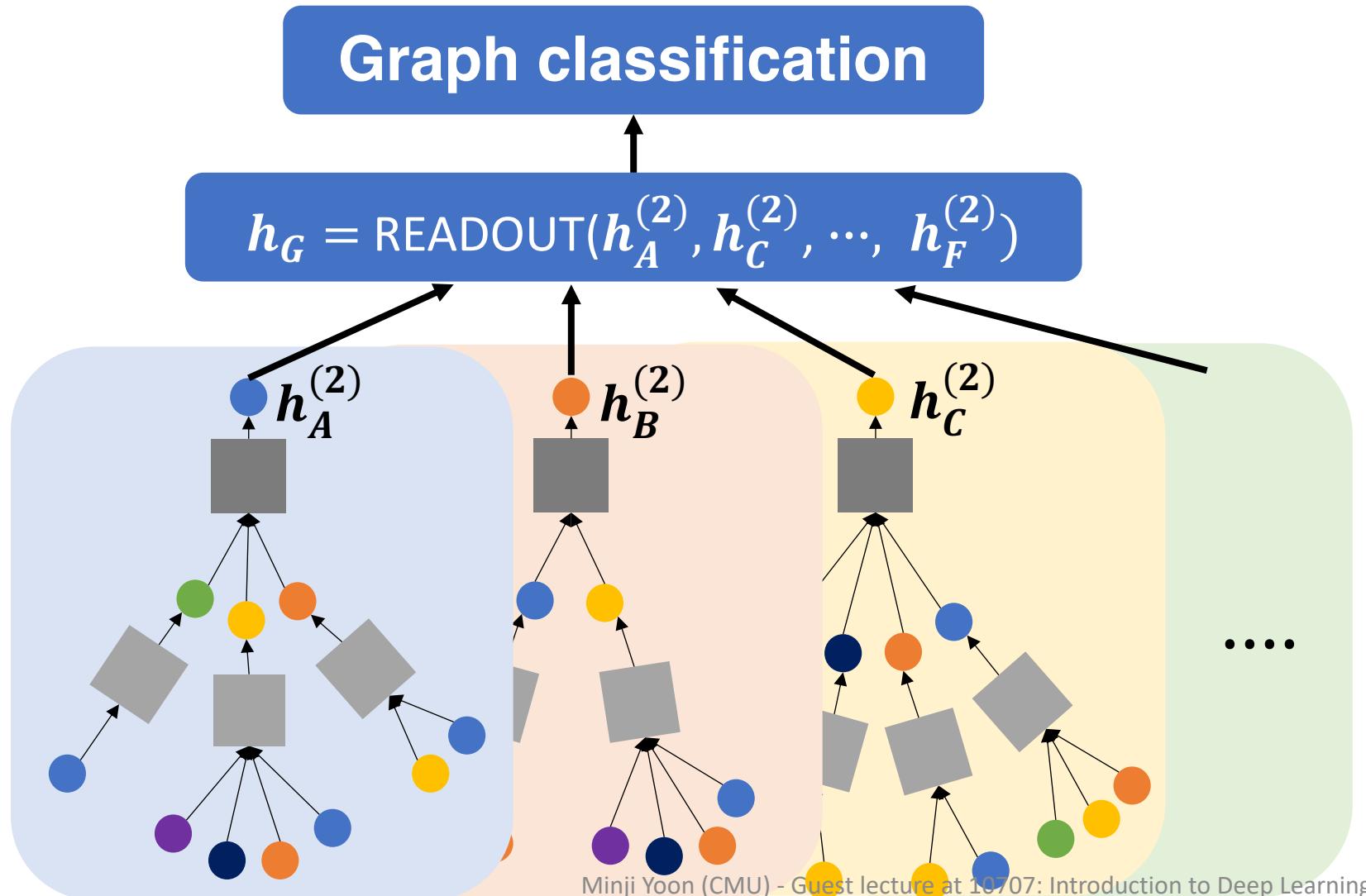
- Classify **papers** into topics on **citation networks**
- Cluster **posts** into subgroups on **Reddit networks**
- Classify **products** into categories on **Amazon co-purchase graphs**

# Graph-level prediction tasks

## Graph classification



# Graph-level prediction tasks



- Predict **properties of a molecule (graph)** where nodes are atoms and edges are chemical bonds

# So far, we have talked about..

## 1. Graph Neural Network

- Problem definition
- Skeleton
  - Aggregation operation
  - Transformation operation

## 2. Implementation

- Computation graph
- Batch execution

## 3. Downstream tasks

- Node-level prediction
- Graph-level prediction

# So far, we have talked about..

## 1. Graph Neural Network

- Problem definition
- Skeleton
  - Aggregation operation
  - Transformation operation

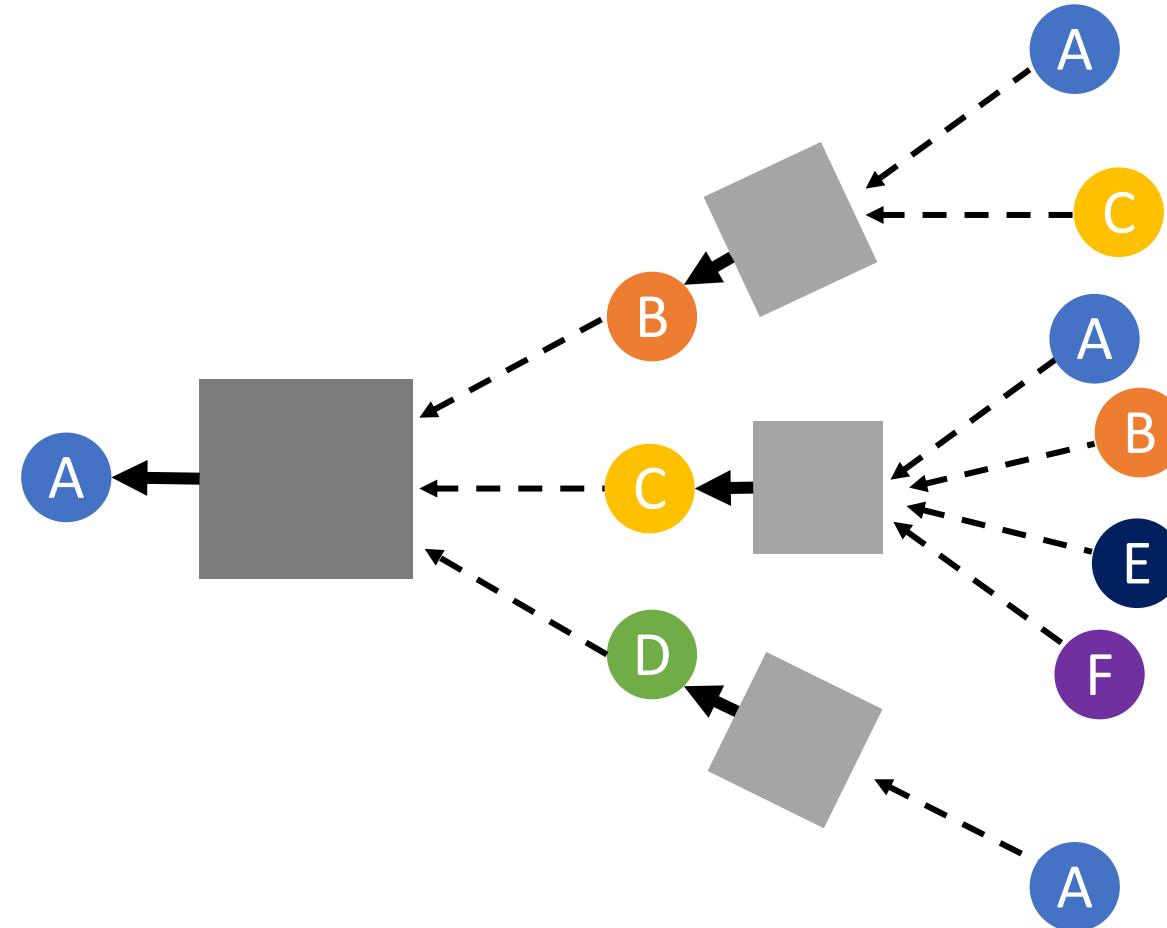
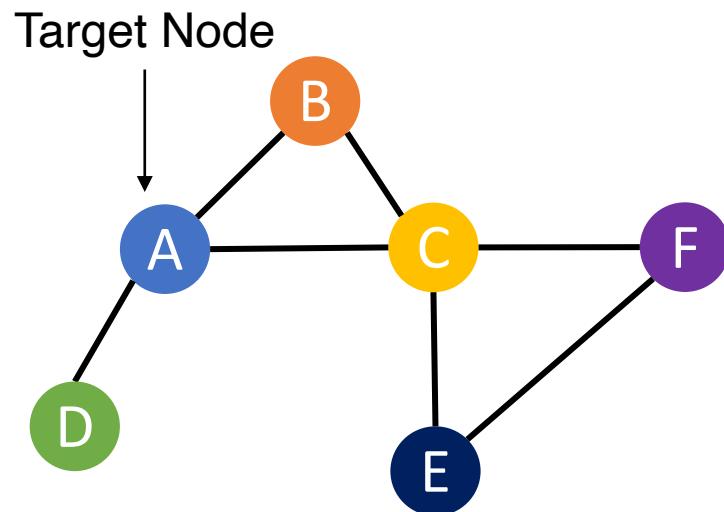
## 2. Implementation

- Computation graph
- Batch execution

## 3. Downstream tasks

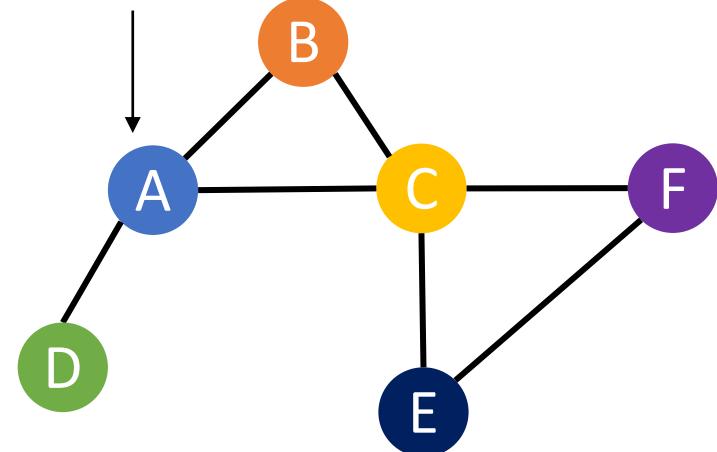
- Node-level prediction
- Graph-level prediction

# Graph Neural Networks

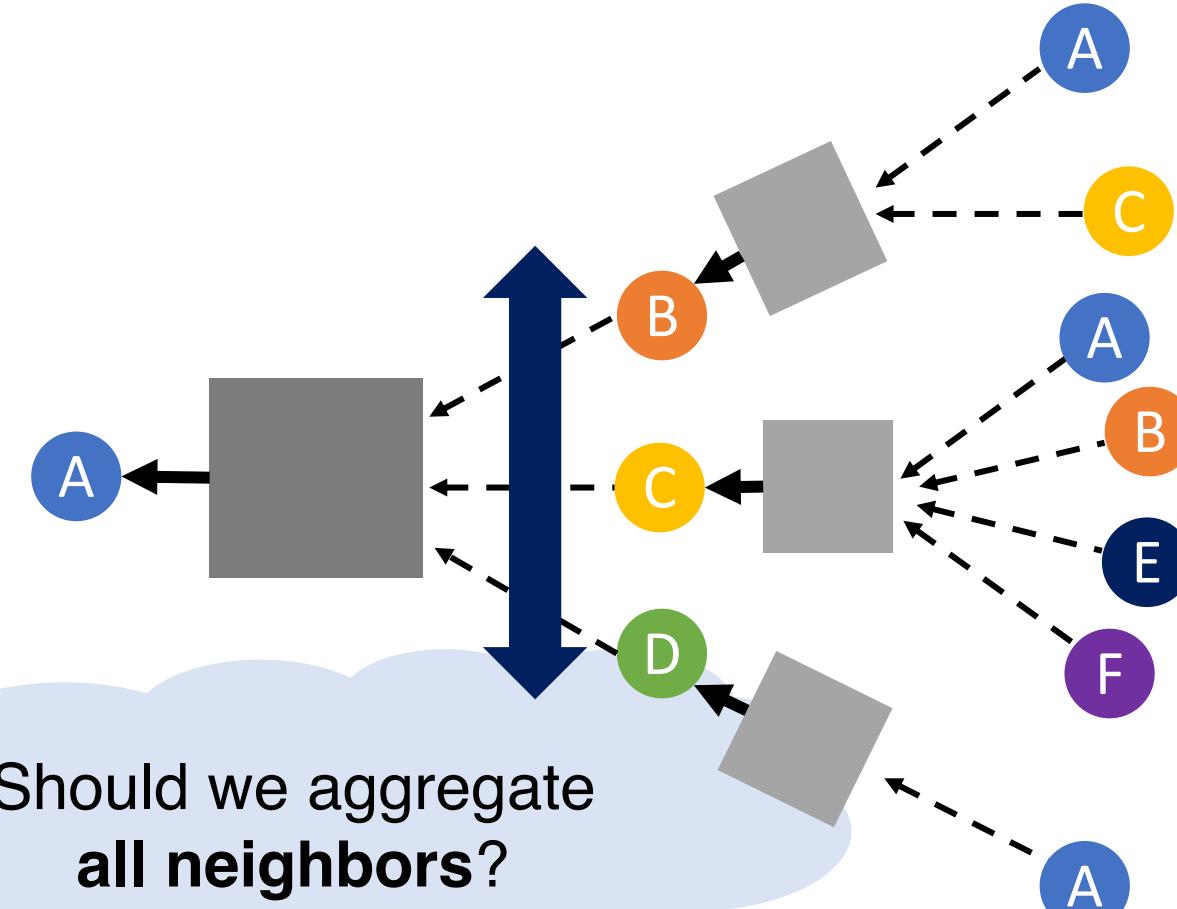


# Graph Neural Networks - Width

Target Node

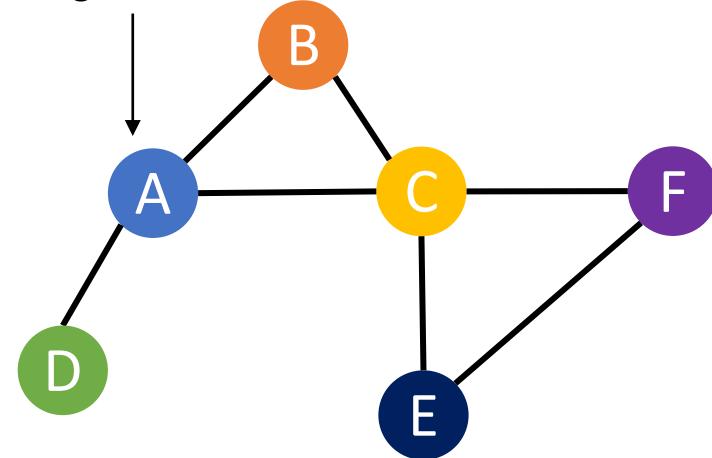


Should we aggregate  
all neighbors?

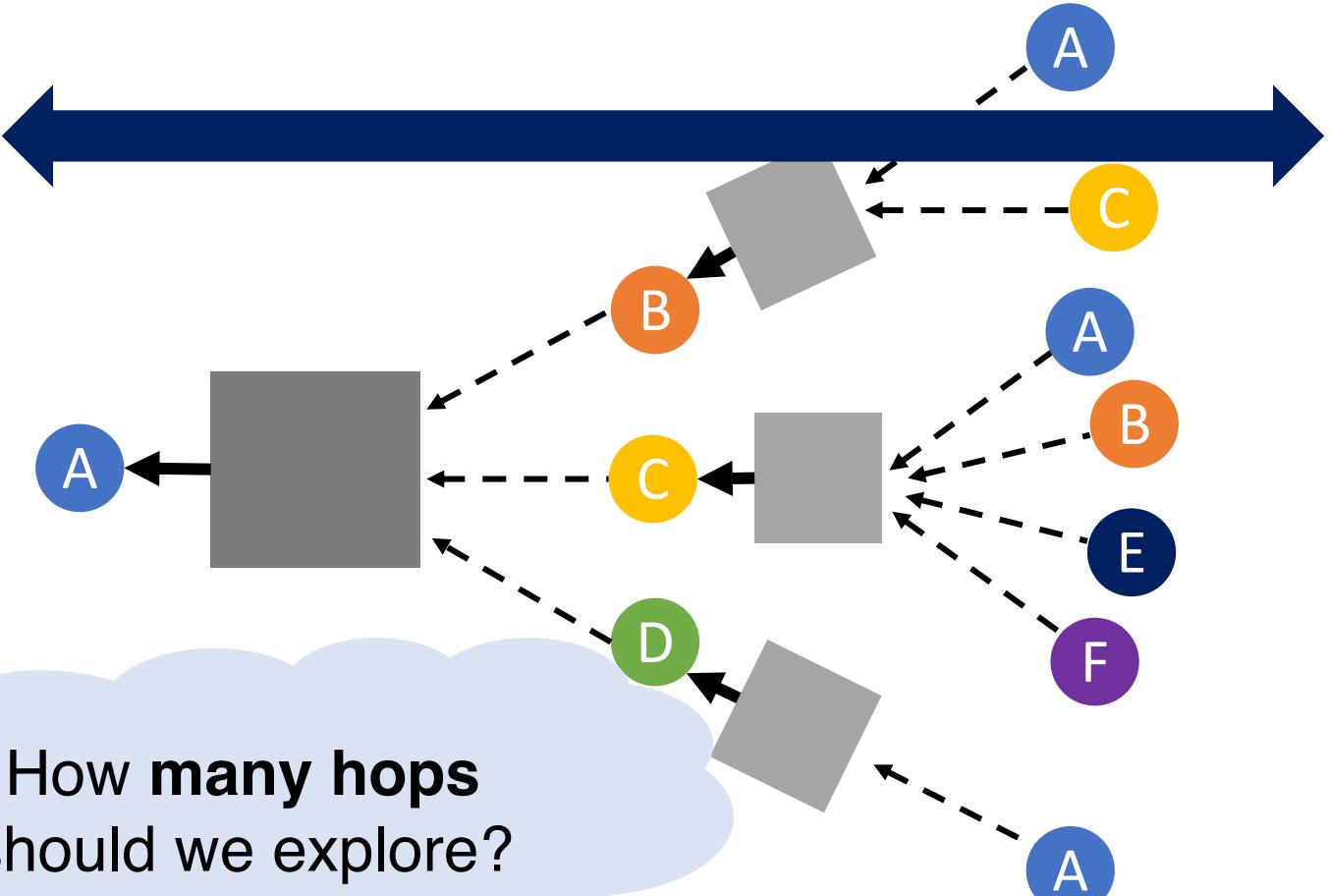


# Graph Neural Networks - Depth

Target Node

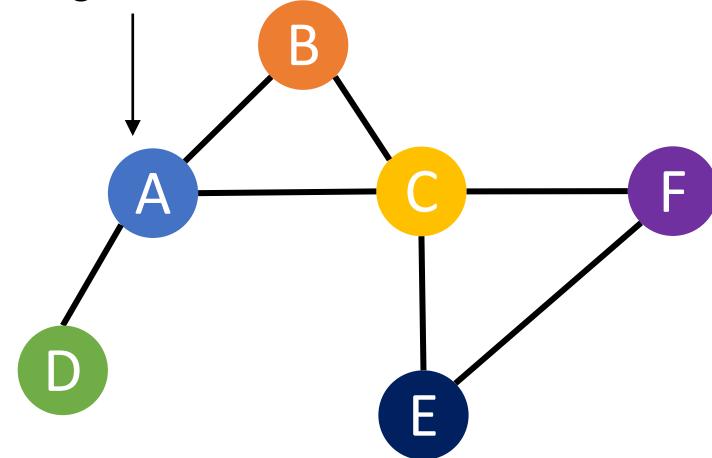


How **many hops**  
should we explore?

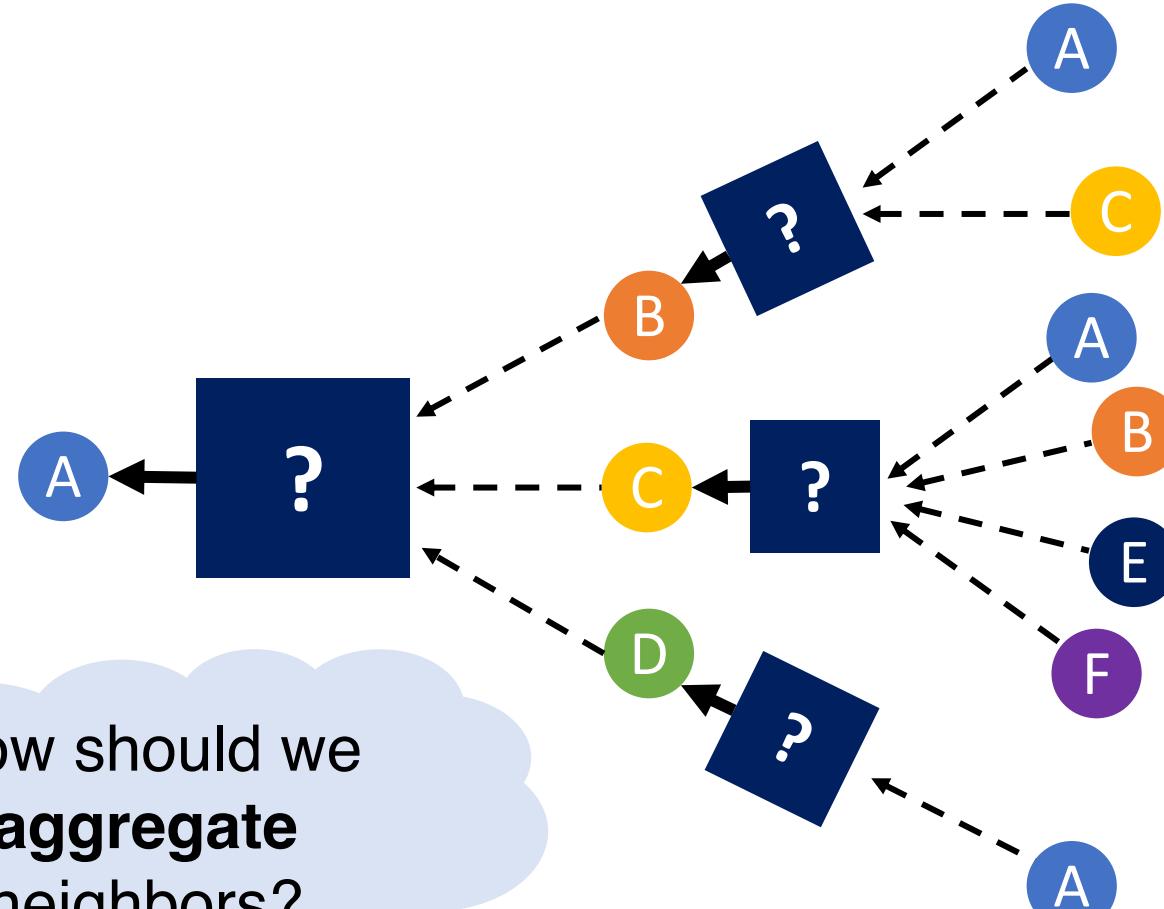


# Graph Neural Networks - Aggregation

Target Node

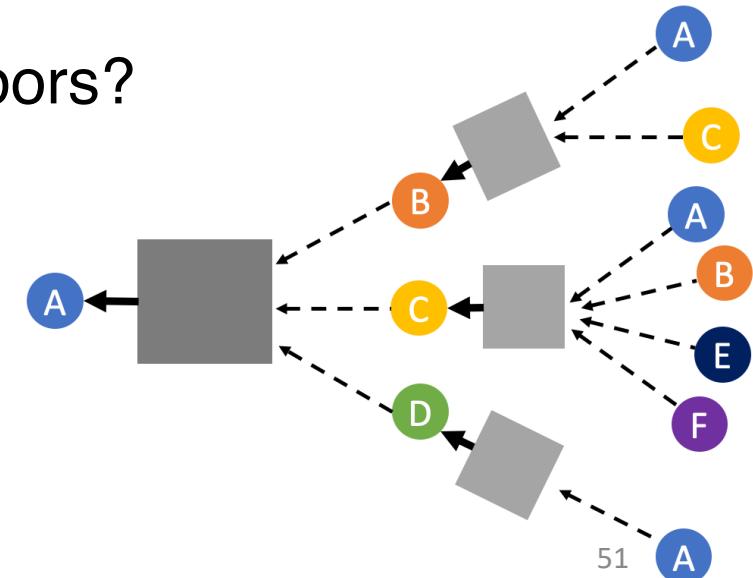


How should we  
**aggregate**  
neighbors?



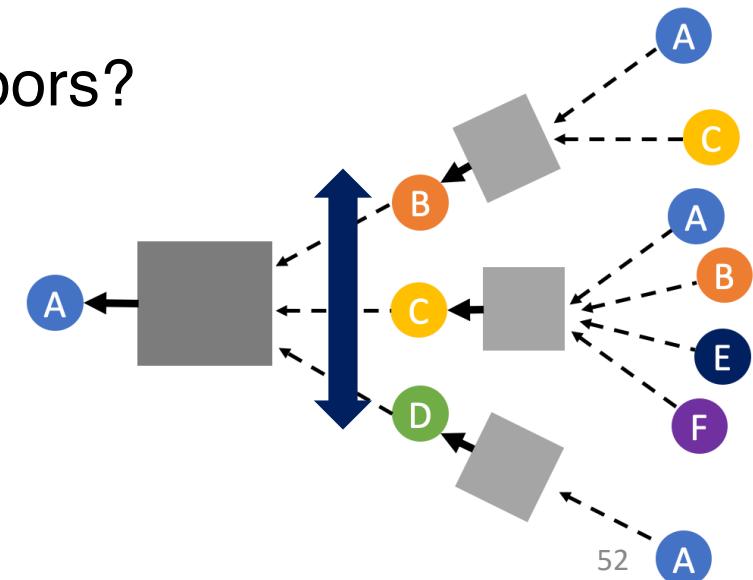
# Graph Neural Network Architectures

- Width
  - Which neighbors should we aggregate messages from?
- Depth
  - How many hops should we check?
- Aggregation
  - How should we aggregate messages from neighbors?



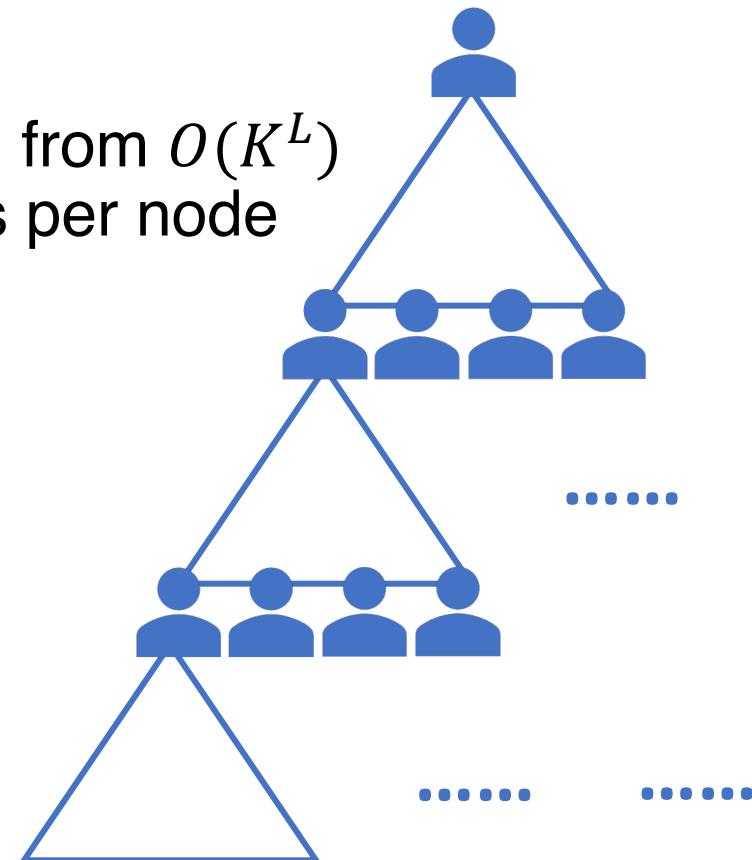
# Graph Neural Network Architectures

- Width
  - Which neighbors should we aggregate messages from?
- Depth
  - How many hops should we check?
- Aggregation
  - How should we aggregate messages from neighbors?



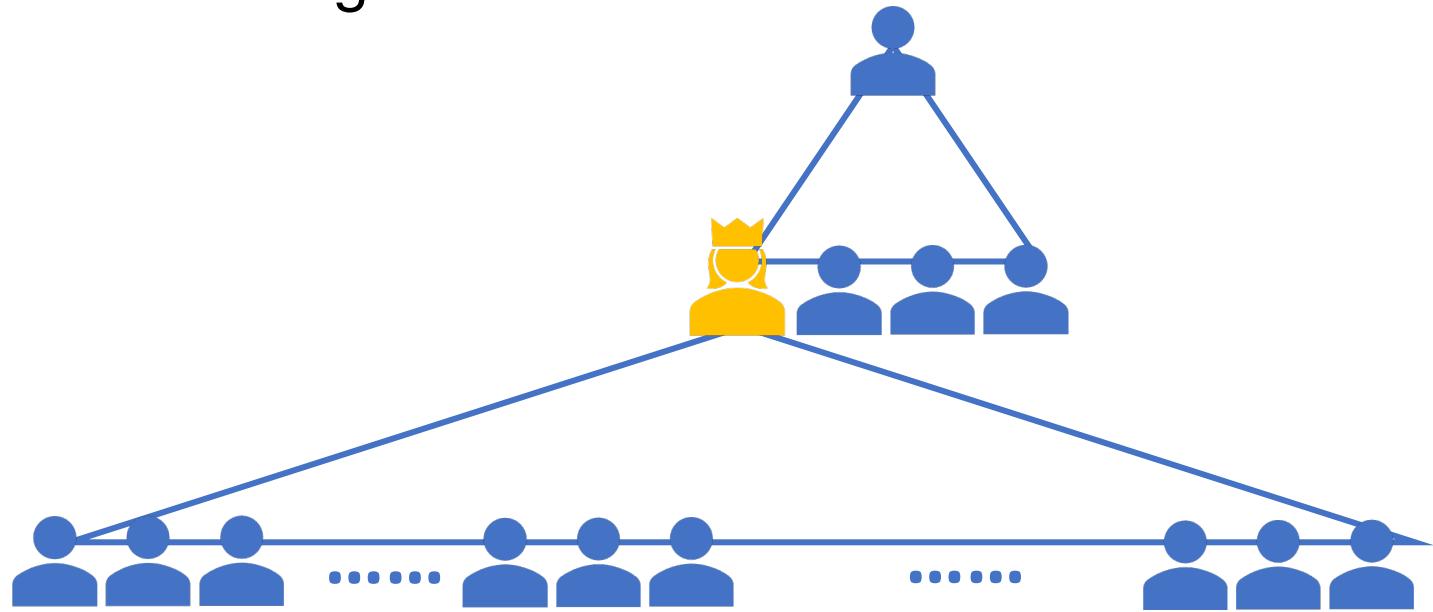
# Aggregation Width in GNNs

- If we aggregate all neighbors, GNNs have scalability issues
- Neighbor explosion
  - In  $L$ -layer GNNs, one node aggregates information from  $O(K^L)$  nodes where  $K$  is the average number of neighbors per node



# Aggregation Width in GNNs

- If we aggregate all neighbors, GNNs have scalability issues
- Neighbor explosion
  - Hub nodes who are connected to a huge number of nodes



# Aggregation Width in GNNs

- Limit the neighborhood expansion by **sampling** a fixed number of neighbors



# Aggregation Width in GNNs

- Random sampling
  - Assign **same** sampling probabilities to all neighbors
  - *GraphSage*<sup>[4]</sup>
- Importance sampling
  - Assign **different** sampling probabilities to all neighbors
  - *FastGCM*<sup>[5]</sup>, *LADIES*<sup>[6]</sup>, *AS-GCM*<sup>[7]</sup>, *GCN-BS*<sup>[8]</sup>, *PASS*<sup>[9]</sup>

[4] Will Hamilton, et al. “Inductive representation learning on large graphs”

[5] Jie Chen, et al. “Fastgcn: fast learning with graph convolutional networks via importance sampling”

[6] Difan Zou, et al. “Layer-Dependent Importance Sampling for Training Deep and Large Graph Convolutional Networks”

[7] Wenbing Huang, et al. “Adaptive sampling towards fast graph representation learning”

[8] Ziqi Liu, et al. “Bandit Samplers for Training Graph Neural Networks”

[9] Minji Yoon, et al. “Performance-Adaptive Sampling Strategy Towards Fast and Accurate Graph Neural Networks”

# Aggregation Width in GNNs

## Importance sampling

: assign *higher sampling probabilities to neighbors who*

- **Minimize variance in sampling**
  - *FastGCN<sup>[5]</sup>, LADIES<sup>[6]</sup>, AS-GCN<sup>[7]</sup>, GCN-BS<sup>[8]</sup>*
- **Maximize GNN performance**
  - *PASS<sup>[9]</sup>*

[4] Will Hamilton, et al. “Inductive representation learning on large graphs”

[5] Jie Chen, et al. “Fastgcn: fast learning with graph convolutional networks via importance sampling”

[6] Difan Zou, et al. “Layer-Dependent Importance Sampling for Training Deep and Large Graph Convolutional Networks”

[7] Wenbing Huang, et al. “Adaptive sampling towards fast graph representation learning”

[8] Ziqi Liu, et al. “Bandit Samplers for Training Graph Neural Networks”

[9] Minji Yoon, et al. “Performance-Adaptive Sampling Strategy Towards Fast and Accurate Graph Neural Networks”

# Aggregation Width in GNNs

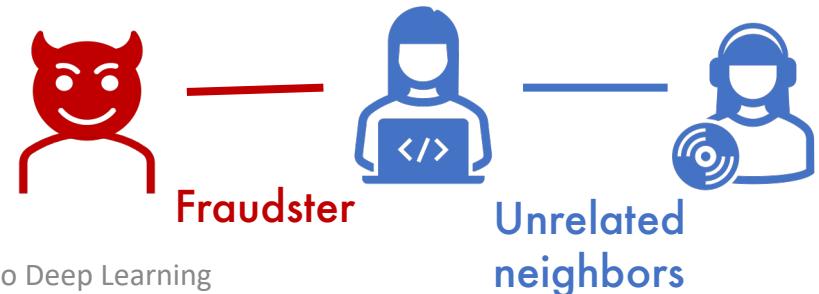
Method	Cora	Citeseer	Pubmed	AmazonC	AmazonP	MsCS	MsPhysics
FastGCN	0.582	0.496	0.569	0.480	0.542	0.520	0.638
AS-GCN	0.462	0.387	0.502	0.419	0.480	0.403	0.516
GraphSage	0.788	0.698	0.792	0.707	0.787	0.766	0.875
GCN-BS	0.788	0.693	0.809	0.736	0.800	0.780	0.887
PASS	<b>0.821</b>	<b>0.715</b>	<b>0.858</b>	<b>0.757</b>	<b>0.855</b>	<b>0.884</b>	<b>0.934</b>

- Node classification task on 7 different real-world graphs
- PASS outperforms all variance-minimizing methods by up to 10.4%

# Aggregation Width in GNNs

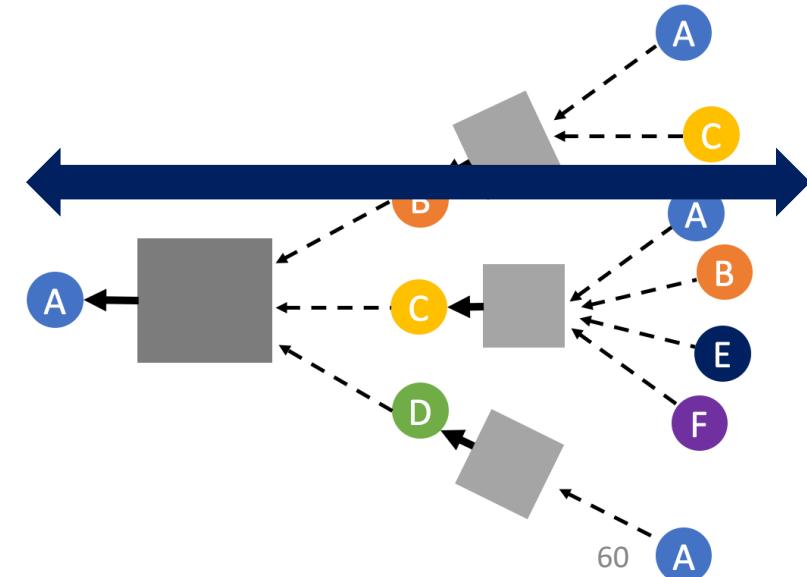
Method	Cora	Citeseer	Pubmed	AmazonC	AmazonP	MsCS	MsPhysics
FastGCN	0.582	0.496	0.569	0.480	0.542	0.520	0.638
AS-GCN	0.462	0.387	0.502	0.419	0.480	0.403	0.516
GraphSage	0.788	0.698	0.792	0.707	0.787	0.766	0.875
GCN-BS	0.788	0.693	0.809	0.736	0.800	0.780	0.887
PASS	<b>0.821</b>	<b>0.715</b>	<b>0.858</b>	<b>0.757</b>	<b>0.855</b>	<b>0.884</b>	<b>0.934</b>

Real-world graphs are noisy!!



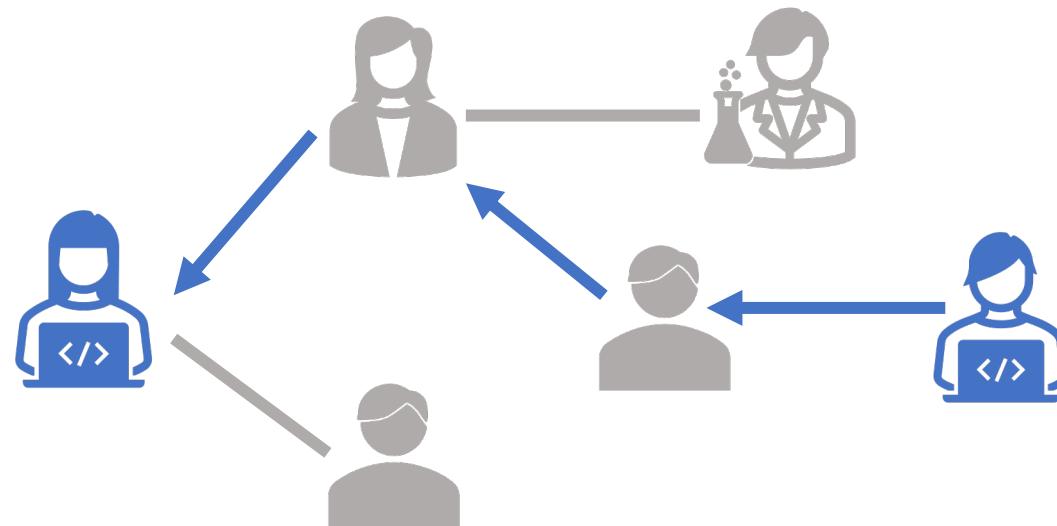
# Graph Neural Network Architectures

- Width
  - Which neighbors should we aggregate messages from?
- Depth
  - **How many hops should we check?**
- Aggregation
  - How should we aggregate messages from neighbors?



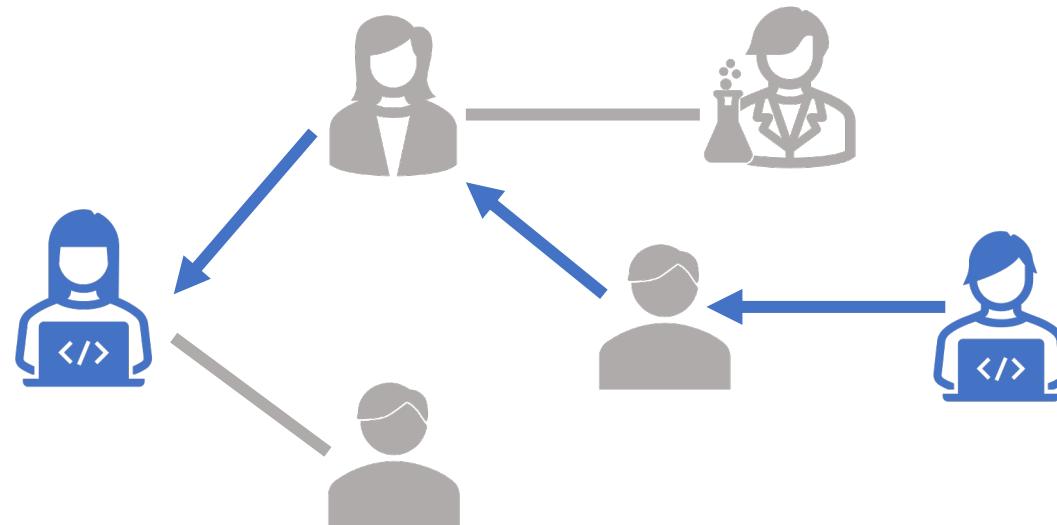
# Aggregation Depth in GNNs

- Informative neighbors could be indirectly connected with a target node



# Aggregation Depth in GNNs

- Informative neighbors could be indirectly connected with a target node
- Can't we just look multiple hops away from the target node?



# Aggregation Depth in GNNs

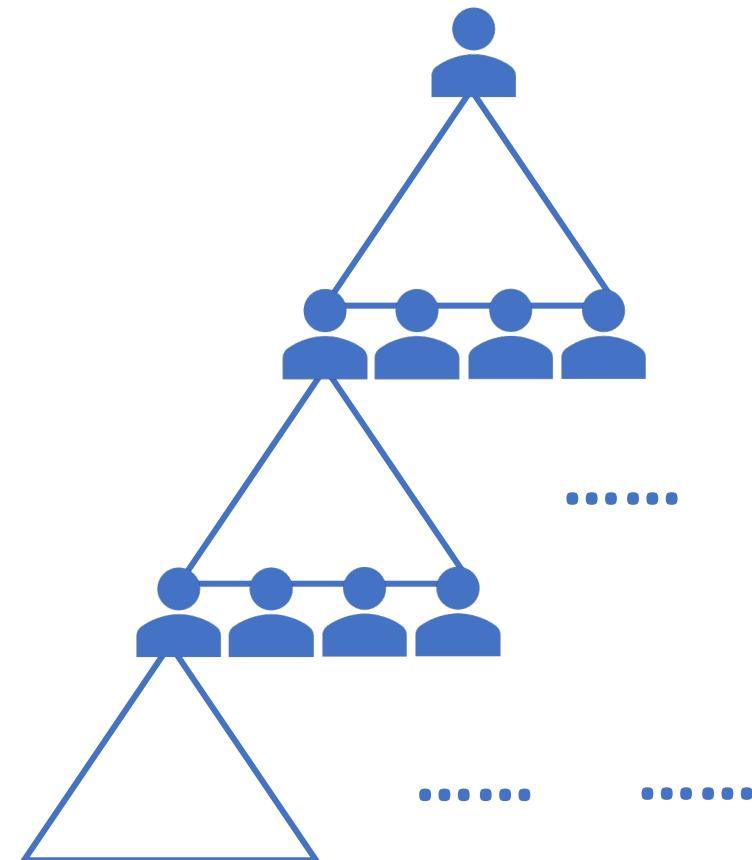
- 2-layer or 3-layer GNNs are commonly used in real worlds



**Wasn't it Deeeep Learning?**

# Aggregation Depth in GNNs

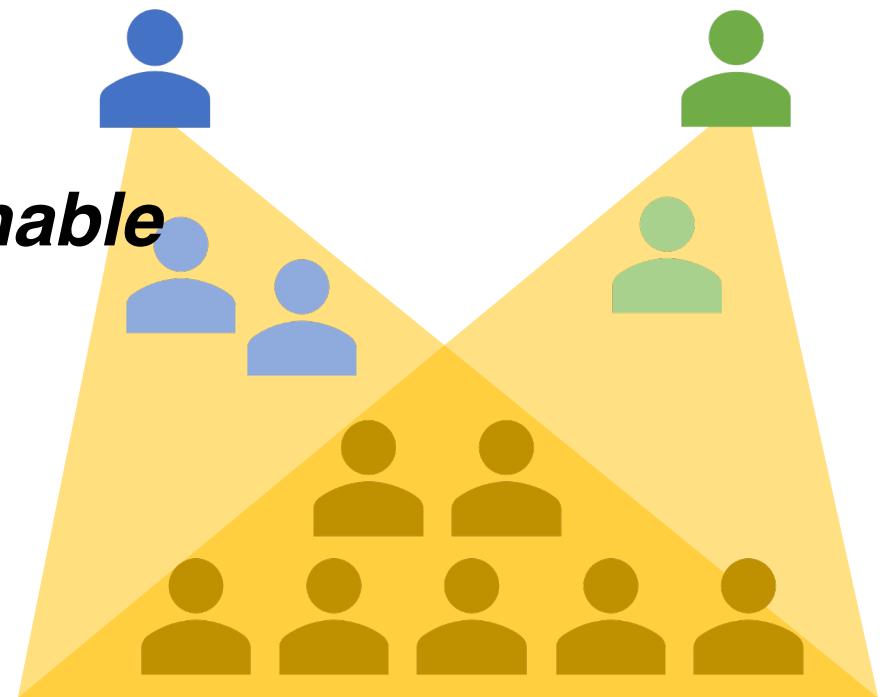
- When we increase the depth  $L$  more than this, GNNs face neighbor explosion  $O(K^L)$ 
  - Over-smoothing
  - Over-squashing



# Aggregation Depth in GNNs

## Over-smoothing<sup>[10]</sup>

- When GNNs become deep,  
nodes share many neighbors
- Node embeddings become *indistinguishable*

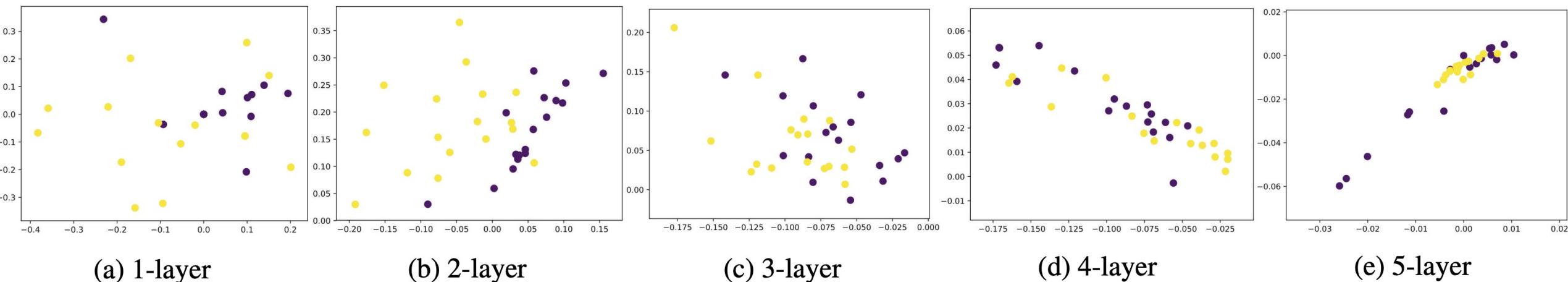


[10] Qimai Li, et al. "Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning"

# Aggregation Depth in GNNs

## Over-smoothing<sup>[10]</sup>

- Node embeddings of Zachary's karate club network with GNNs



[10] Qimai Li, et al. "Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning"

# Aggregation Depth in GNNs

## Mitigate over-smoothing

PairNorm<sup>[11]</sup>

- Keep total pairwise squared distance (TPSD) **constant** across layers
- Push away pairs that are not connected

$$\text{TPSD}(\dot{X}) = \sum_{(i,j) \in \mathcal{E}} \|\dot{x}_i - \dot{x}_j\|_2^2 + \sum_{(i,j) \notin \mathcal{E}} \|\dot{x}_i - \dot{x}_j\|_2^2 = C$$

Connected pairs      Disconnected pairs

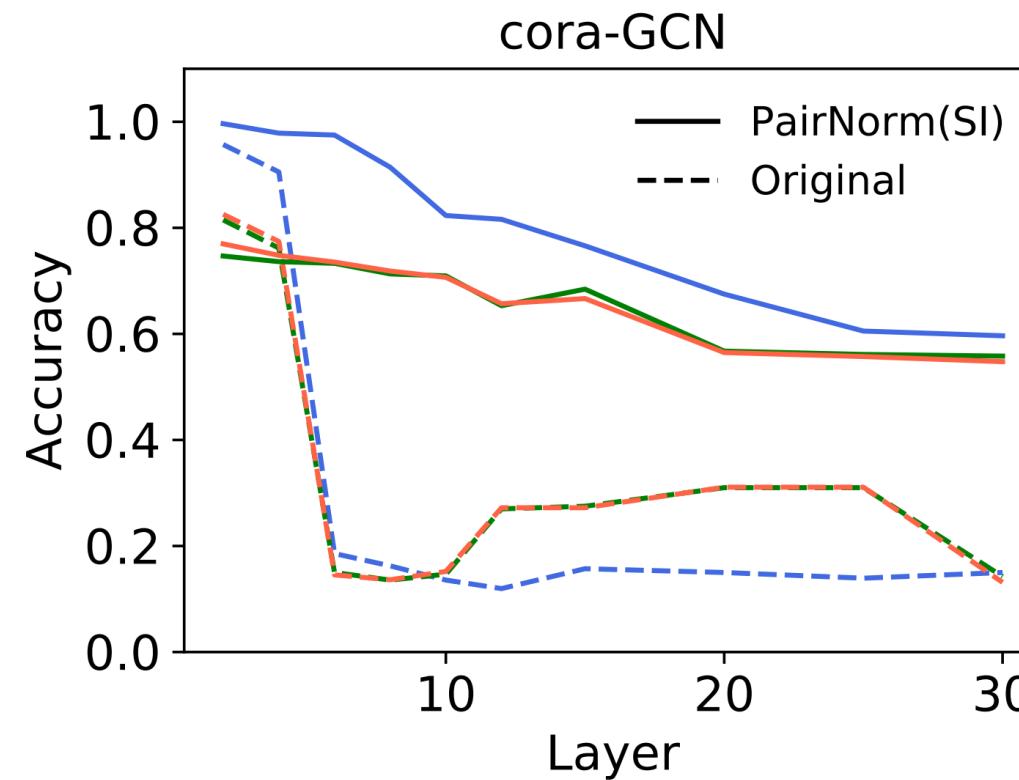
The diagram illustrates the decomposition of the Total Pairwise Squared Distance (TPSD) into two components. A red dotted rectangle encloses the first term of the equation, which represents the sum over connected pairs  $(i,j) \in \mathcal{E}$ . A blue dotted rectangle encloses the second term, which represents the sum over disconnected pairs  $(i,j) \notin \mathcal{E}$ .

[11] Lingxiao Zhao, et al. "PAIRNORM: TACKLING OVERSMOOTHING IN GNNS"

# Aggregation Depth in GNNs

Mitigate over-smoothing

PairNorm<sup>[11]</sup>

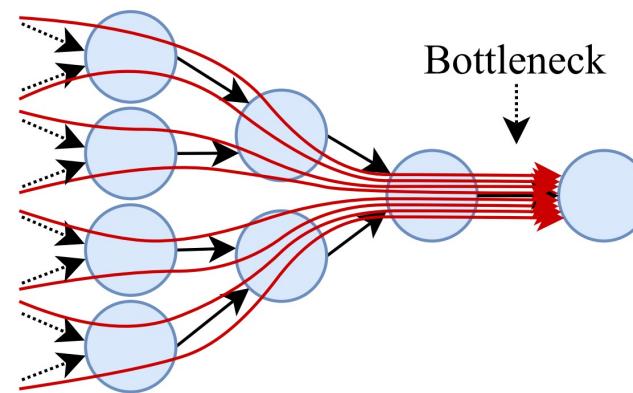


[11] Lingxiao Zhao, et al. “PAIRNORM: TACKLING OVERSMOOTHING IN GNNS”

# Aggregation Depth in GNNs

## Over-squashing<sup>[12]</sup>

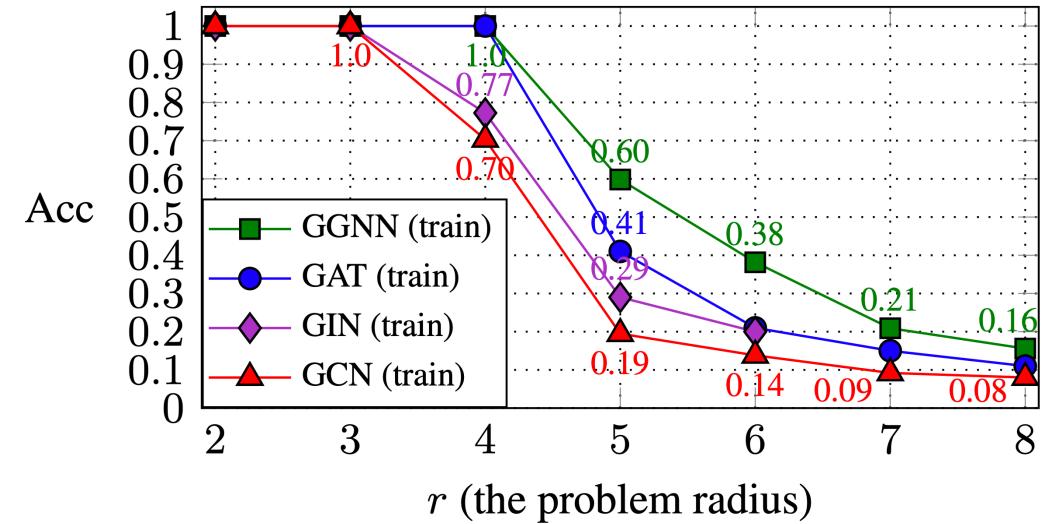
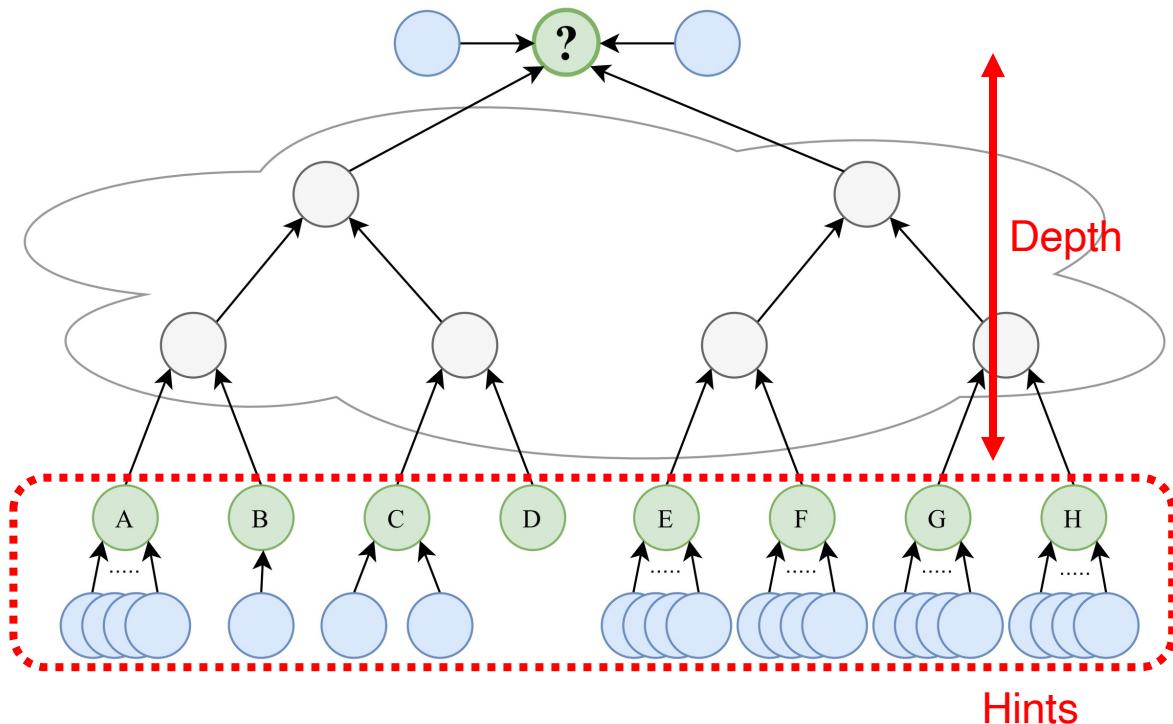
- A node's exponentially-growing neighborhood is compressed into a fixed-size vector



[12] Uri Alon, et al. "ON THE BOTTLENECK OF GRAPH NEURAL NETWORKS AND ITS PRACTICAL IMPLICATIONS"

# Aggregation Depth in GNNs

## Over-squashing<sup>[12]</sup>



[12] Uri Alon, et al. "ON THE BOTTLENECK OF GRAPH NEURAL NETWORKS AND ITS PRACTICAL IMPLICATIONS"

# Aggregation Depth in GNNs

Decoupling the two concepts of depths in GNNs<sup>[13]</sup>

- **Depth-1:** neighborhood that each node aggregates information from
- **Depth-2:** number of layers in GNNs

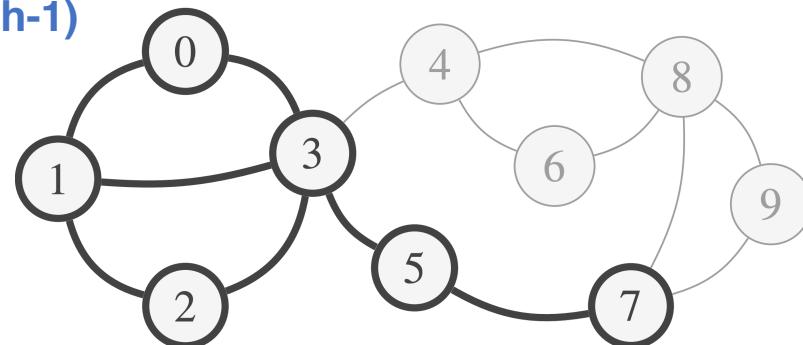
[13] Hanqing Zeng, et al. “Decoupling the Depth and Scope of Graph Neural Networks”

# Aggregation Depth in GNNs

Decoupling the two concepts of depths in GNNs<sup>[13]</sup>

- **Depth-1:** neighborhood that each node aggregates information from
- **Depth-2:** number of layers in GNNs

Depth of neighborhood  
(Depth-1)



$$\mathcal{G}_s = \text{SAMPLE}(\mathcal{G})$$

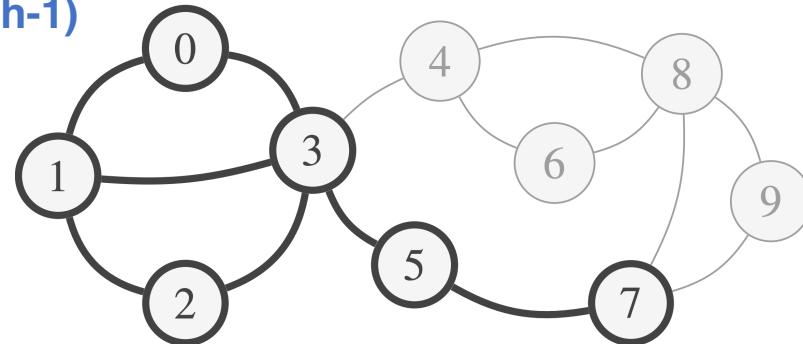
[13] Hanqing Zeng, et al. "Decoupling the Depth and Scope of Graph Neural Networks"

# Aggregation Depth in GNNs

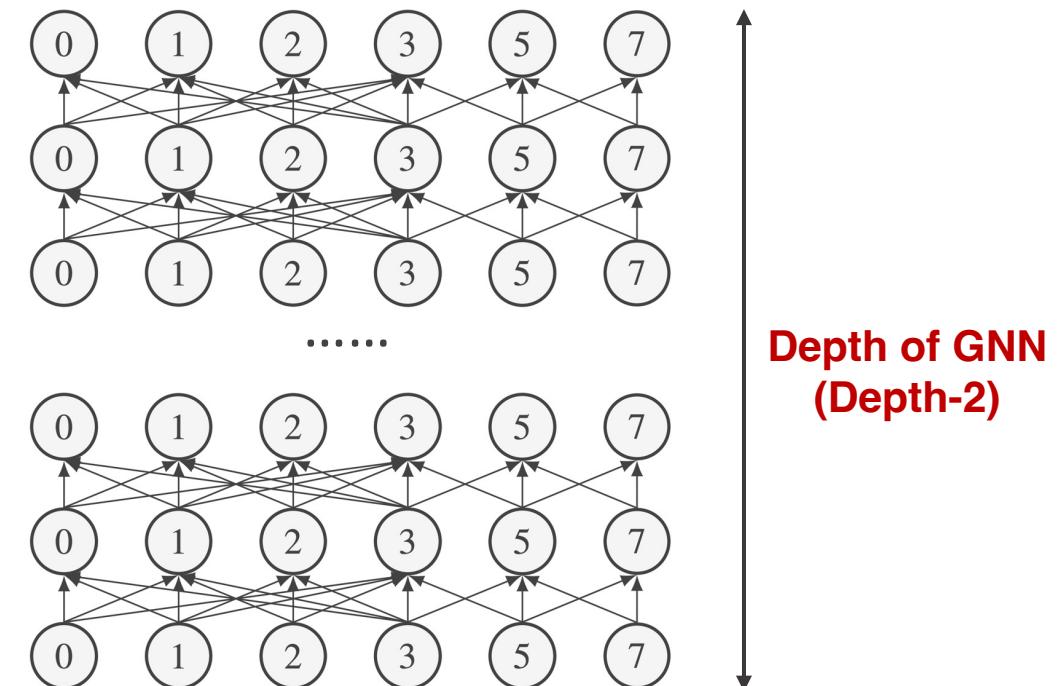
Decoupling the two concepts of depths in GNNs<sup>[13]</sup>

- **Depth-1:** neighborhood that each node aggregates information from
- **Depth-2:** number of layers in GNNs

Depth of neighborhood  
(Depth-1)



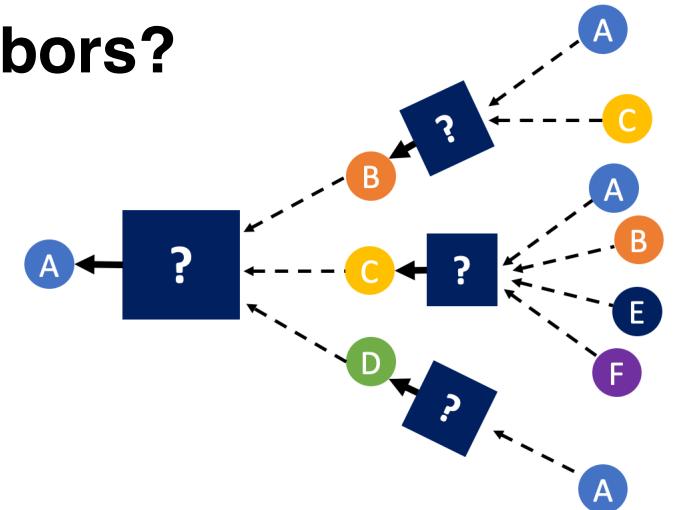
Depth of GNN  
(Depth-2)



[13] Hanqing Zeng, et al. "Decoupling the Depth and Scope of Graph Neural Networks"

# Graph Neural Network Architectures

- Width
  - Which neighbors should we aggregate messages from?
- Depth
  - How many hops should we check?
- Aggregation
  - **How should we aggregate messages from neighbors?**



# Aggregation strategy in GNNs

In each layer  $l$  :

**Aggregate** over neighbors

$$m_v^{(l-1)} = \boxed{f}^{(l)} \left( h_v^{(l-1)}, \left\{ h_u^{(l-1)} : u \in \mathcal{N}(v) \right\} \right)$$

**Transform** messages

$$h_v^{(l)} = g^{(l)}(m_v^{(l-1)})$$

# Aggregation strategy in GNNs

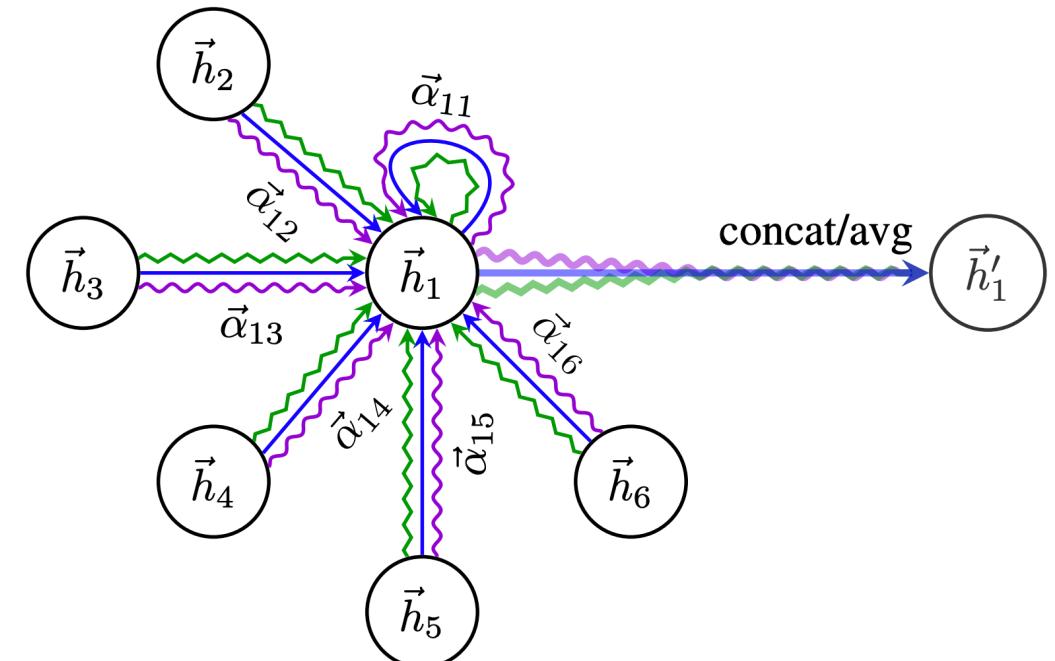
- GCN<sup>[1]</sup>
  - Average embeddings of neighboring nodes

[1] Kipf, Thomas N., et al. "Semi-supervised classification with graph convolutional networks."

# Aggregation strategy in GNNs

- GAT<sup>[14]</sup>
  - Different weights to different nodes in a neighborhood
  - Multi-head attention

$$\alpha_{ij} = \frac{\exp \left( \text{LeakyReLU} \left( \vec{\mathbf{a}}^T [\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j] \right) \right)}{\sum_{k \in \mathcal{N}_i} \exp \left( \text{LeakyReLU} \left( \vec{\mathbf{a}}^T [\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k] \right) \right)}$$



[14] Petar Veličković., et al. "GRAPH ATTENTION NETWORKS."

# Aggregation strategy in GNNs

In each layer  $l$  :

**Aggregate** over neighbors

$$m_v^{(l-1)} = \boxed{f}^{(l)} \left( h_v^{(l-1)}, \{h_u^{(l-1)} : u \in \mathcal{N}(v)\} \right)$$

Core part of GNNs

**Transform** messages

$$h_v^{(l)} = \boxed{g}^{(l)}(m_v^{(l-1)})$$

Any neural network module can fit in  
1-layer MLP is commonly used

# Aggregation strategy in GNNs

Power of **GNNs**

=

Power of **aggregation strategies**

# Aggregation strategy in GNNs

- By measuring the power of GNNs, we can find the best aggregation strategy!!



# Aggregation strategy in GNNs

- By measuring the expressive power of GNNs, we can find the best aggregation strategy!!
- *But.. what is the power of GNNs and how can we measure it?*



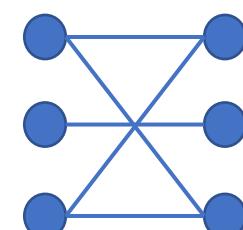
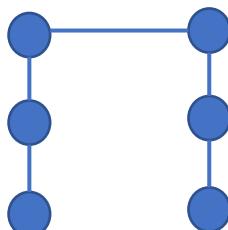
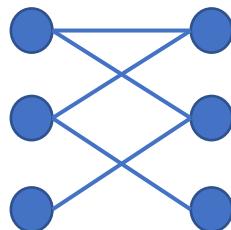
# Aggregation strategy in GNNs

- How powerful are Graph Neural Networks?<sup>[2]</sup>
- Metric
  - Graph-level prediction task
  - Can a GNN model distinguish two non-isomorphic graphs?

[2] Keyulu Xu., et al. "HOW POWERFUL ARE GRAPH NEURAL NETWORKS?"

# Aggregation strategy in GNNs

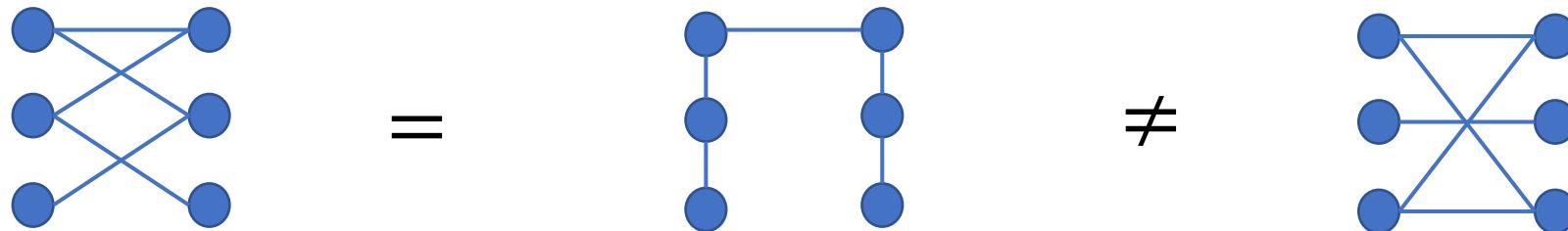
- How powerful are Graph Neural Networks?<sup>[2]</sup>
- Metric
  - Graph-level prediction task
  - Can a GNN model distinguish two non-isomorphic graphs?



[2] Keyulu Xu., et al. "HOW POWERFUL ARE GRAPH NEURAL NETWORKS?"

# Aggregation strategy in GNNs

- How powerful are Graph Neural Networks?<sup>[2]</sup>
- Metric
  - Graph-level prediction task
  - Can a GNN model distinguish two non-isomorphic graphs?



[2] Keyulu Xu., et al. "HOW POWERFUL ARE GRAPH NEURAL NETWORKS?"

# Aggregation strategy in GNNs

- How powerful are Graph Neural Networks?<sup>[2]</sup>
  - Any aggregation-based GNN is at most as powerful as the **WL test**<sup>[15]</sup>
  - Maximum power = aggregation strategy is injective

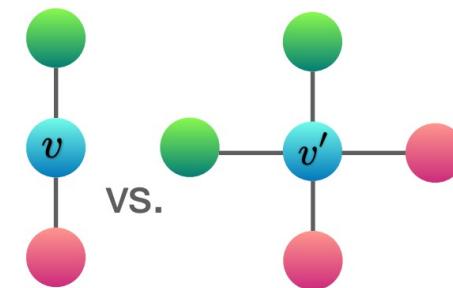
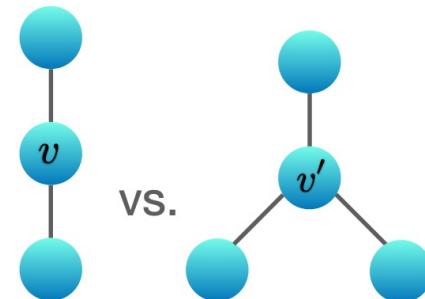
$$f(x_1) = f(x_2) \Rightarrow x_1 = x_2$$


[2] Keyulu Xu., et al. "HOW POWERFUL ARE GRAPH NEURAL NETWORKS?"

[15] Boris Weisfeiler and AA Leman. "A reduction of a graph to a canonical form and an algebra arising during this reduction"

# Aggregation strategy in GNNs

- How powerful are Graph Neural Networks?<sup>[2]</sup>
  - Any aggregation-based GNN is at most as powerful as the **WL test**<sup>[15]</sup>
  - Maximum power = aggregation strategy is injective
  - (ex) summation



**Mean and Max both fail, while Sum can distinguish them!!**

[2] Keyulu Xu., et al. "HOW POWERFUL ARE GRAPH NEURAL NETWORKS?"

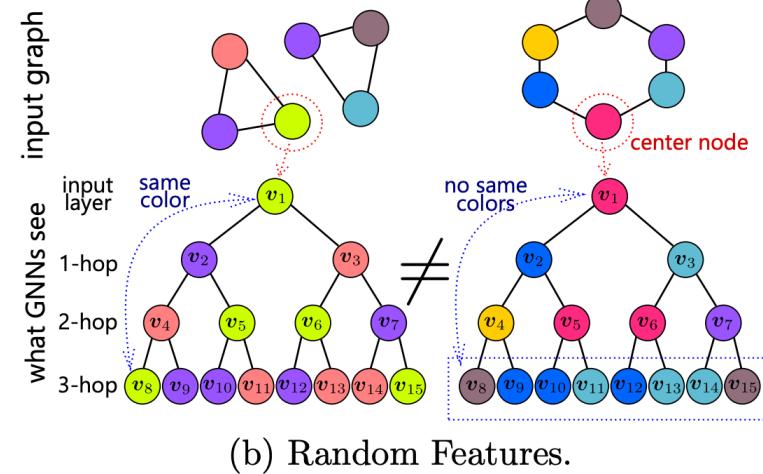
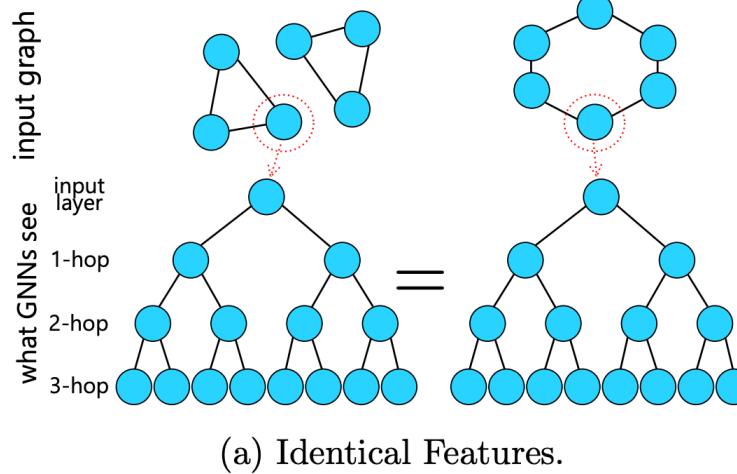
[15] Boris Weisfeiler and AA Leman. "A reduction of a graph to a canonical form and an algebra arising during this reduction"

# Aggregation strategy in GNNs

- Can we make more powerful GNNs?
  - Very active area, with many open problems

# Aggregation strategy in GNNs

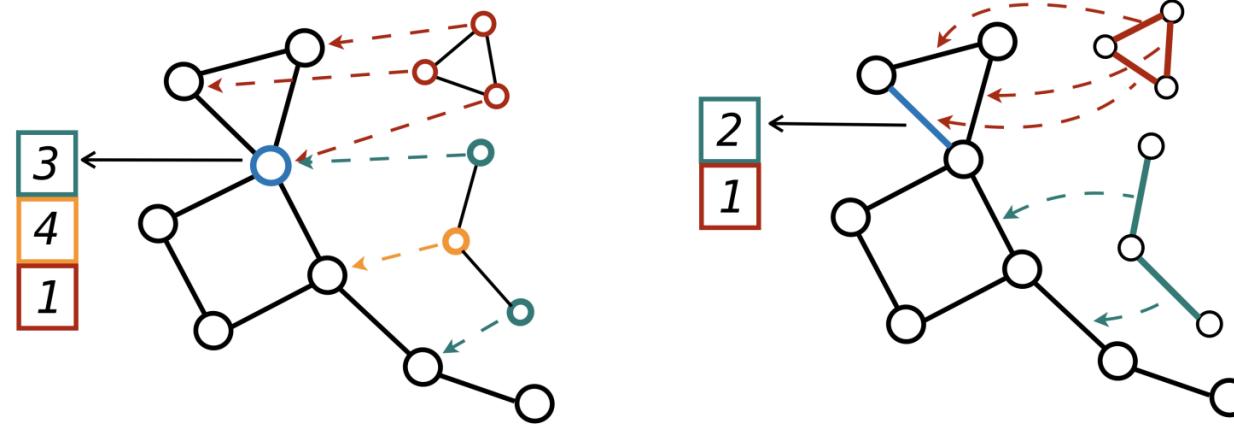
- Can we make more powerful GNNs?
- Augment nodes with randomized/positional features<sup>[16]</sup>



[16] Ryoma Sato, et al. "Random Features Strengthen Graph Neural Networks"

# Aggregation strategy in GNNs

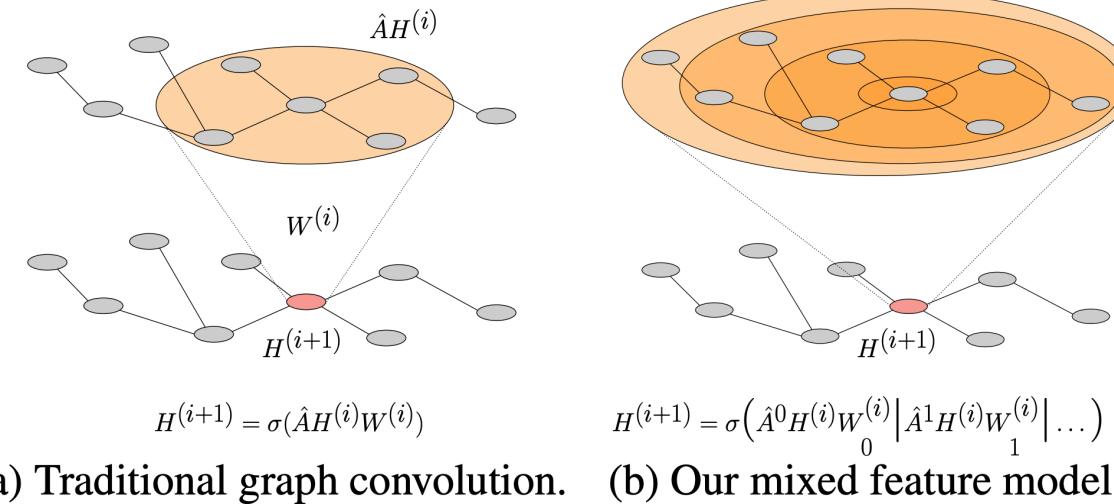
- Can we make more powerful GNNs?
- Augment nodes with handcrafted subgraph-based features<sup>[17]</sup>



[17] Giorgos Bouritsas, et al. "Improving Graph Neural Network Expressivity via Subgraph Isomorphism Counting"

# Aggregation strategy in GNNs

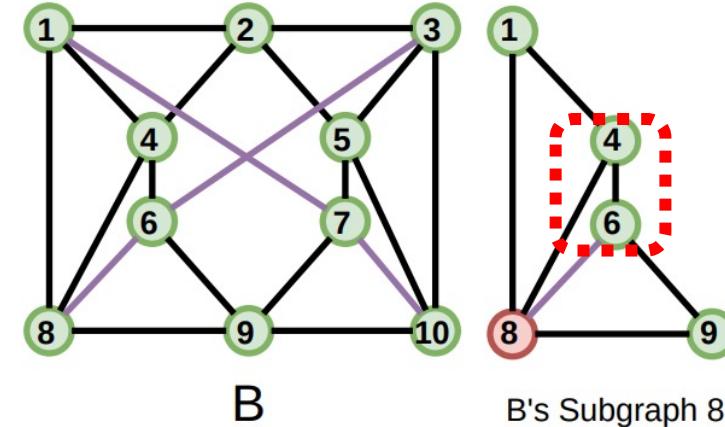
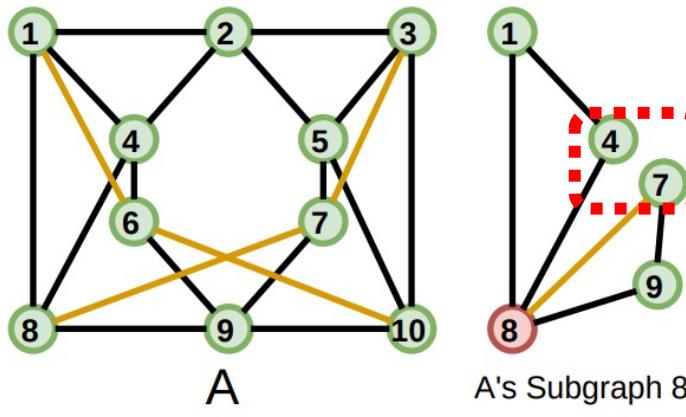
- Can we make more powerful GNNs?
- Directly aggregates k-hop information by using adjacency matrix powers<sup>[18]</sup>



[18] Sami Abu-El-Haija, et al. "MixHop: Higher-Order Graph Convolutional Architectures via Sparsified Neighborhood Mixing"

# Aggregation strategy in GNNs

- Can we make more powerful GNNs?
- Extending local aggregation in GNNs from star patterns to general subgraph patterns<sup>[19]</sup>



[19] Lingxiao Zhao, et al. "FROM STARS TO SUBGRAPHS: UPLIFTING ANY GNN WITH LOCAL STRUCTURE AWARENESS"

# Aggregation strategy in GNNs

- [20] proves that *there isn't* a clear single “winner” aggregator

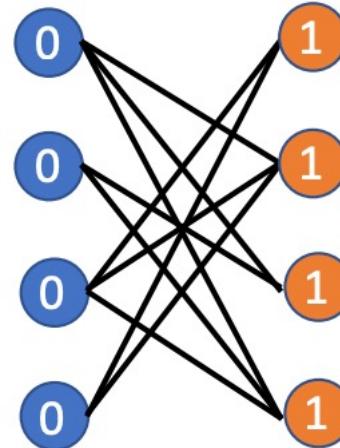
**Theorem 1** (Number of aggregators needed). *In order to discriminate between multisets of size  $n$  whose underlying set is  $\mathbb{R}$ , at least  $n$  aggregators are needed.*

# Aggregation strategy in GNNs

- Homophily assumption
  - Connected nodes are similar/related/informative

# Aggregation strategy in GNNs

- Homophily assumption
  - Connected nodes are similar/related/informative
- How can we deal with **heterophilous networks**?<sup>[21,22]</sup>
  - Connected nodes have different class labels and dissimilar features

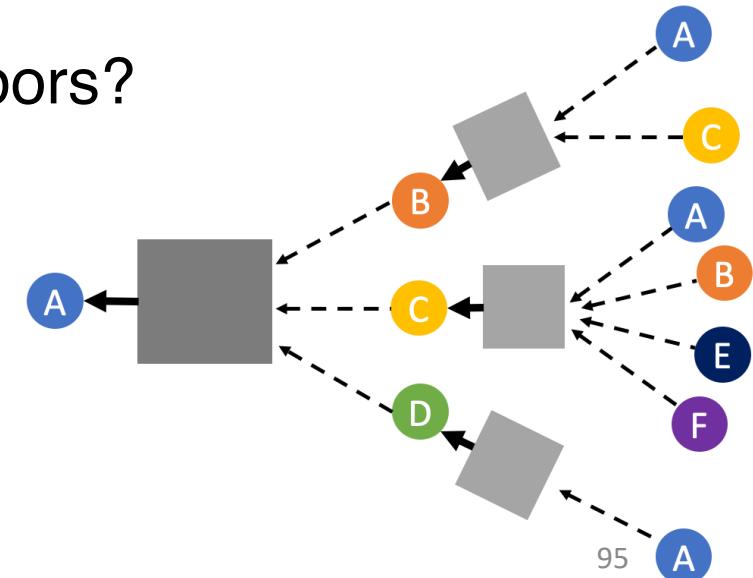


[21] Jiong Zhu., et al. "Beyond Homophily in Graph Neural Networks: Current Limitations and Effective Designs"

[22] Yao Ma, et al. "IS HOMOPHILY A NECESSITY FOR GRAPH NEURAL NETWORKS?"

# Graph Neural Network Architectures

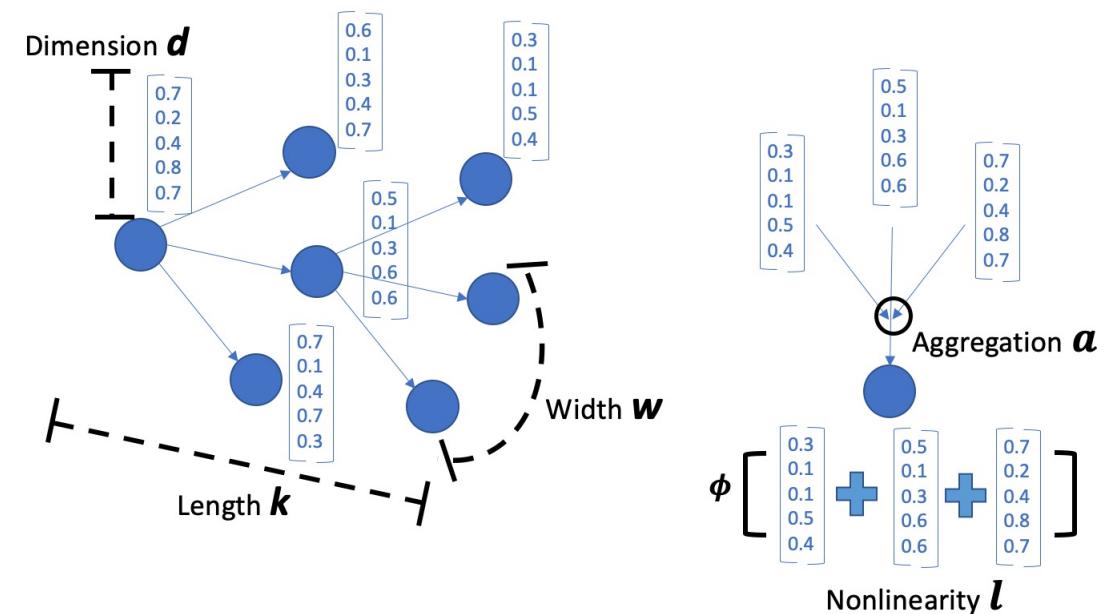
- Width
  - Which neighbors should we aggregate messages from?
- Depth
  - How many hops should we check?
- Aggregation
  - How should we aggregate messages from neighbors?



# Neural Architecture Search for GNNs

- Which *width*, *depth*, and *aggregation strategy* are proper for a given graph and task?

Width?  
Depth?  
Aggregation?



# Neural Architecture Search for GNNs

- Finding proper *width, depth, and aggregation strategy* for a given graph and task **automatically**<sup>[1,2,3]</sup>

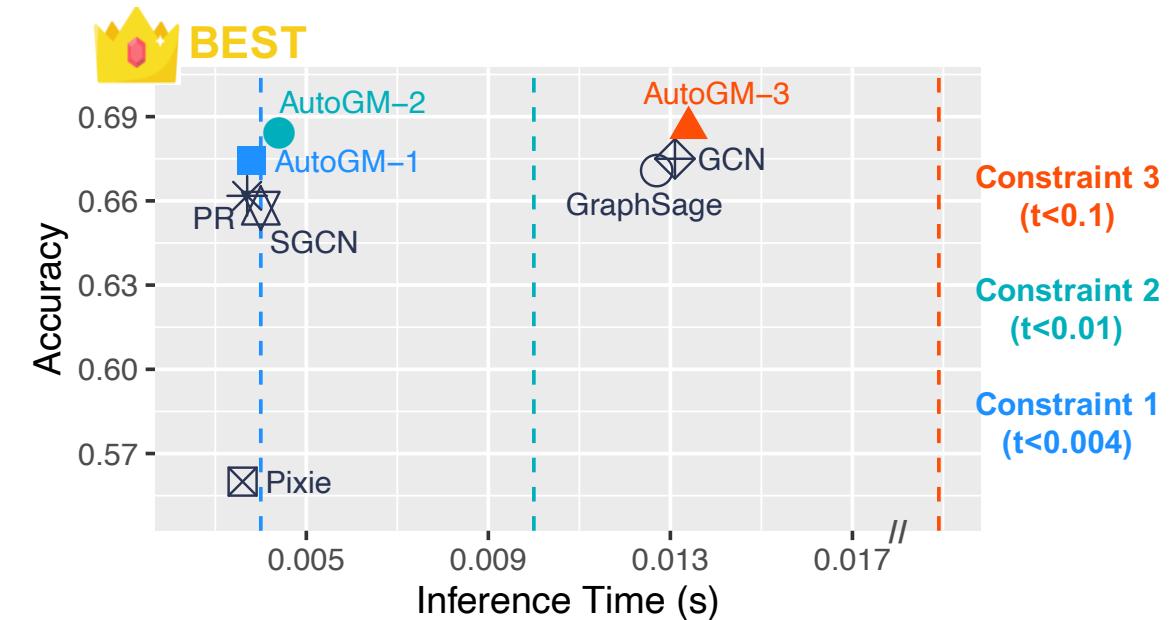
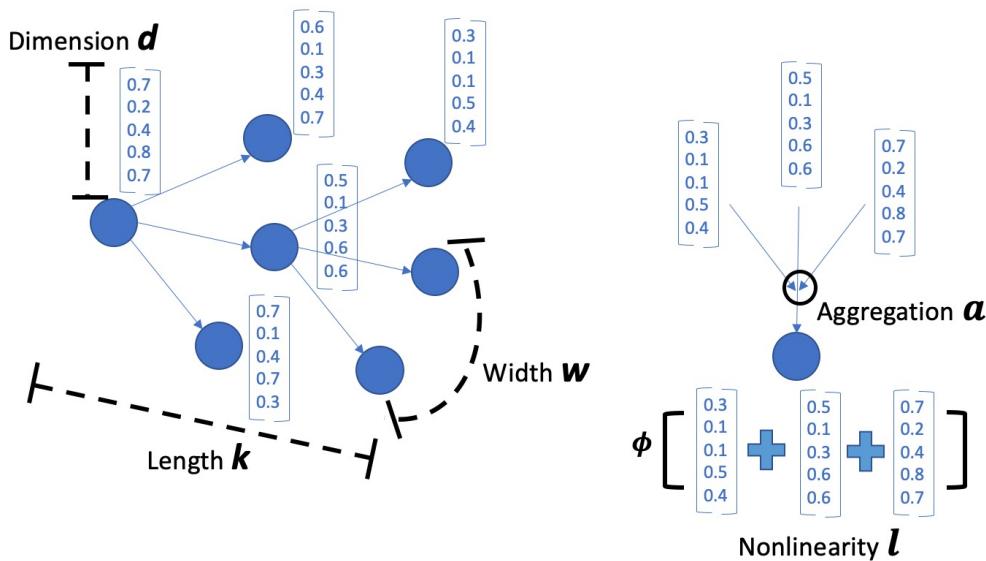
Here is the GNN you requested



- [23] Minji Yoon., et al. "Autonomous Graph Mining Algorithm Search with Best Speed/Accuracy Trade-off"  
[24] Kaixiong Zhou, et al. "Auto-GNN: Neural Architecture Search of Graph Neural Networks"  
[25] Yang Gao, et al. "GraphNAS: Graph Neural Architecture Search with Reinforcement Learning"

# Neural Architecture Search for GNNs

- AutoGM<sup>[23]</sup>



Step 1: define a hyperparameter space

Step 2: explore the space efficiently

[23] Minji Yoon., et al. "Autonomous Graph Mining Algorithm Search with Best Speed/Accuracy Trade-off"

# So far, we have talked about..

## 1. Graph Neural Network

- Problem definition
- Skeleton: aggregation, transformation operations

## 2. Open research questions in GNN architectures

- Width
- Depth
- Aggregation

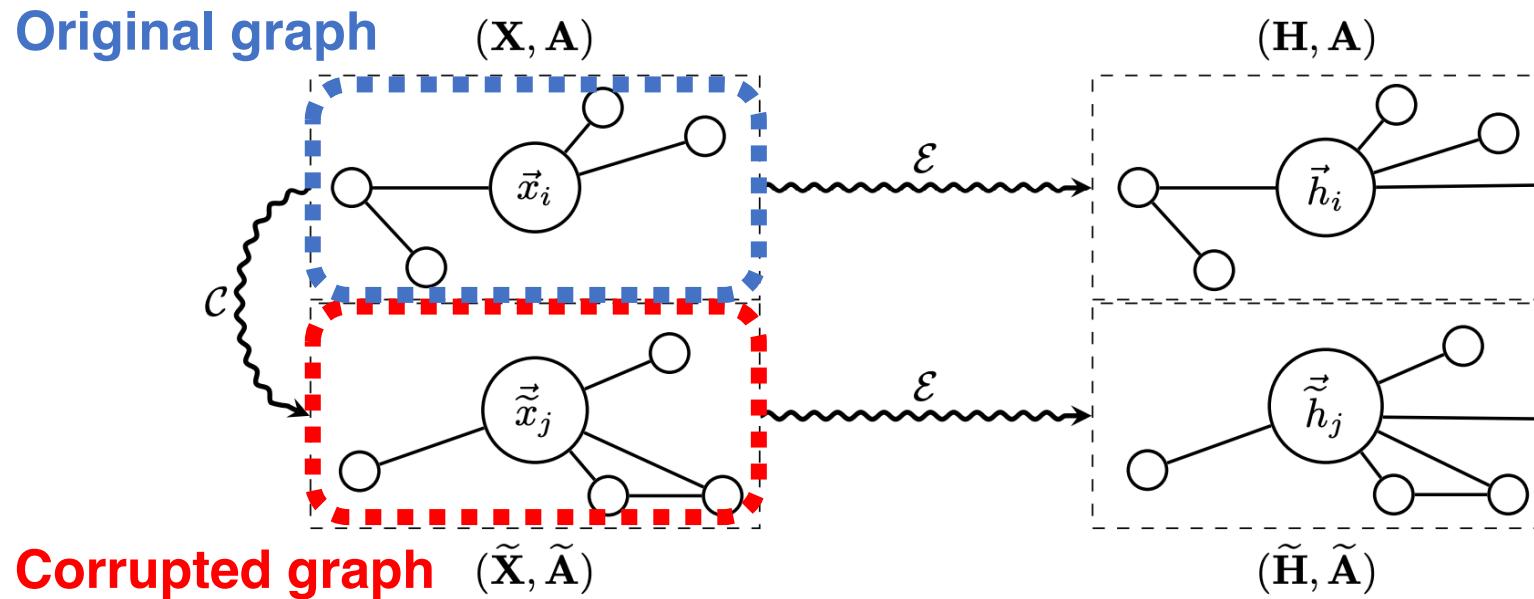
## 3. GNN training strategy

# How to train GNNs

- Semi-supervised learning
  - Input node features are given for all nodes in a graph
  - Only a subset of nodes have labels

# How to train GNNs

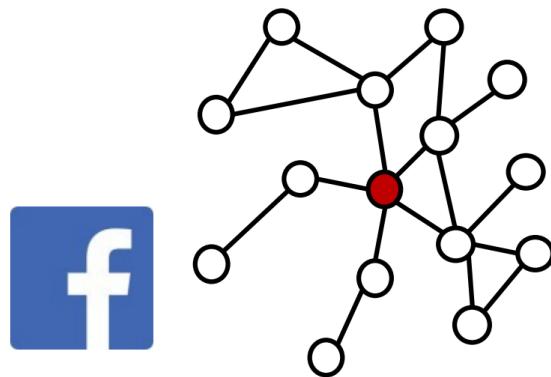
- Unsupervised learning<sup>[26]</sup>
  - Contrastive learning



[26] Petar Veličković., et al. "DEEP GRAPH INFOMAX"

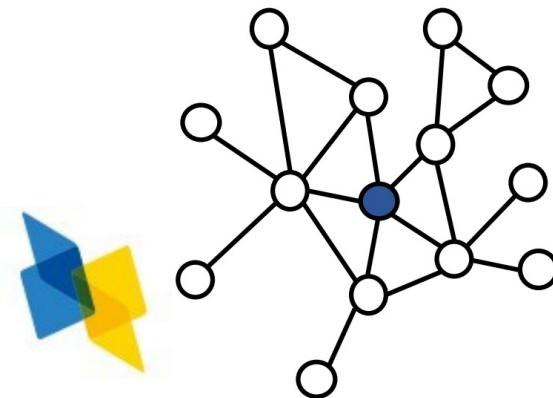
# How to train GNNs

- Transfer learning
  - Transfer a pre-trained GNN model between graphs<sup>[27]</sup>



Facebook network

Pre-trained GNN  $f$

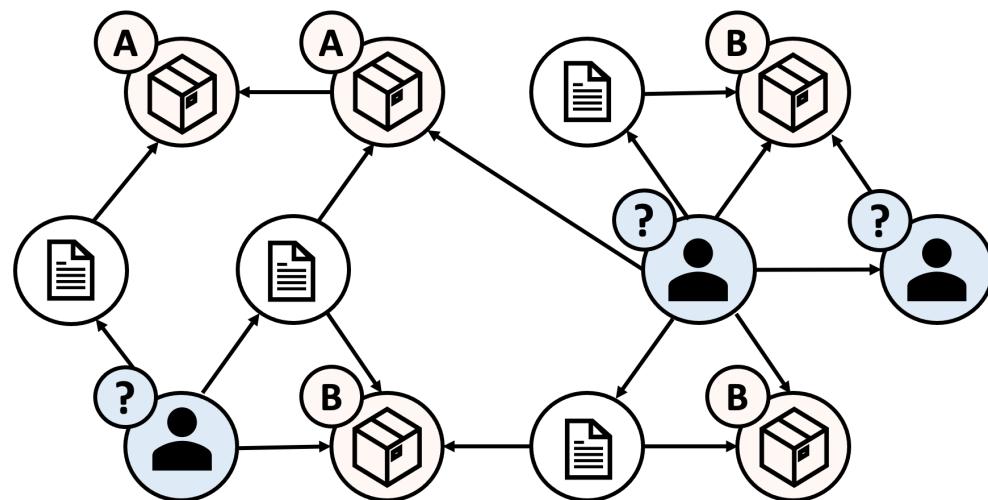


DBLP co-authorship network

[27] Jiezhong Qiu, et al. "GCC: Graph Contrastive Coding for Graph Neural Network Pre-Training"

# How to train GNNs

- Transfer learning
  - Transfer between different node types across a **heterogeneous graph**<sup>[28]</sup>



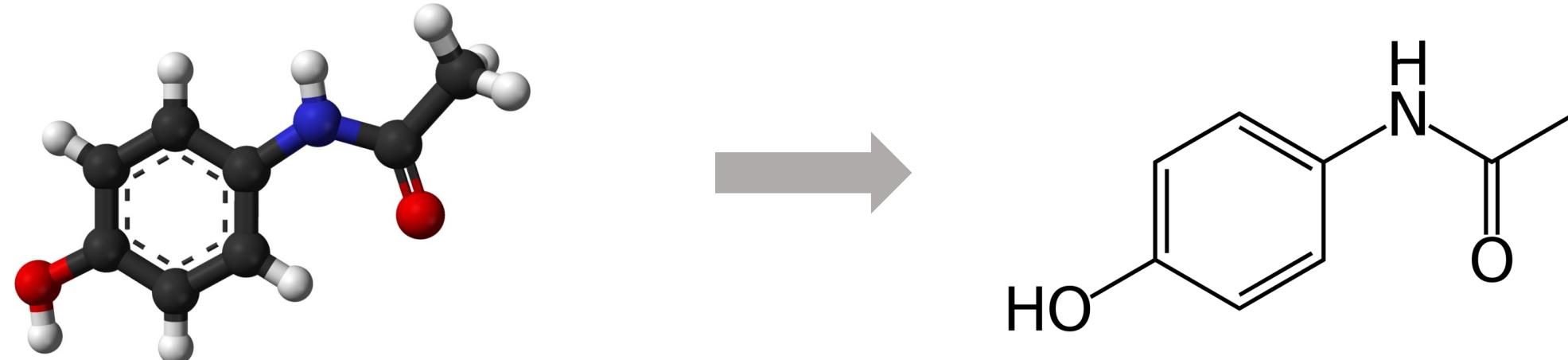
[28] Minji Yoon, et al. "Zero-shot Domain Adaptation of Heterogeneous Graphs via Knowledge Transfer Networks "

# **So far, we have talked about..**

- 1. Graph Neural Network**
- 2. Open research questions in GNN architectures**
- 3. GNN training strategy**
- 4. Application**

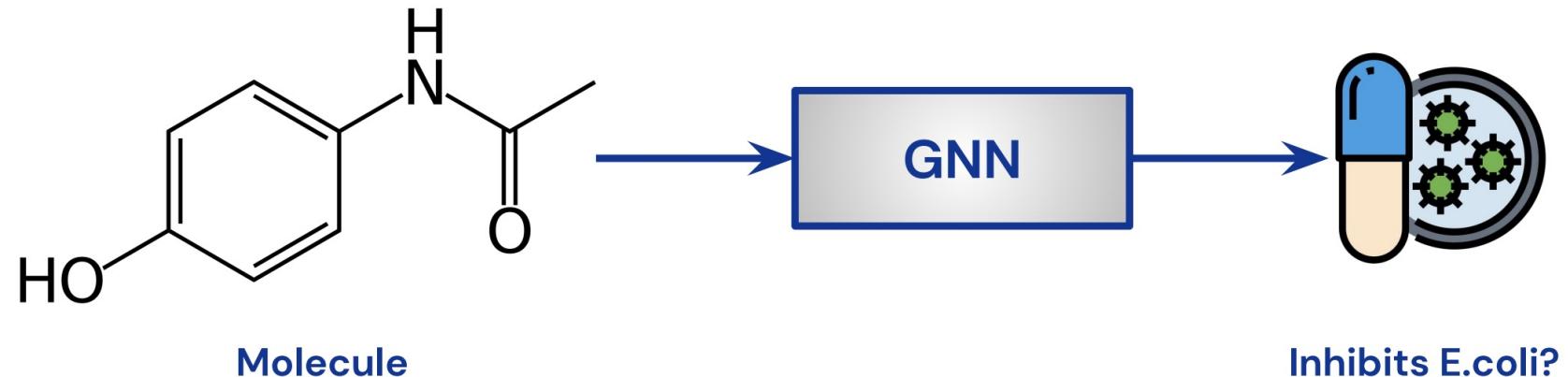
# Impactful applications in science

- GNNs for molecule classification
- Molecule
  - Node: atoms
  - Edge: bonds
  - Input features: atom type, charge, bond type



# Impactful applications in science

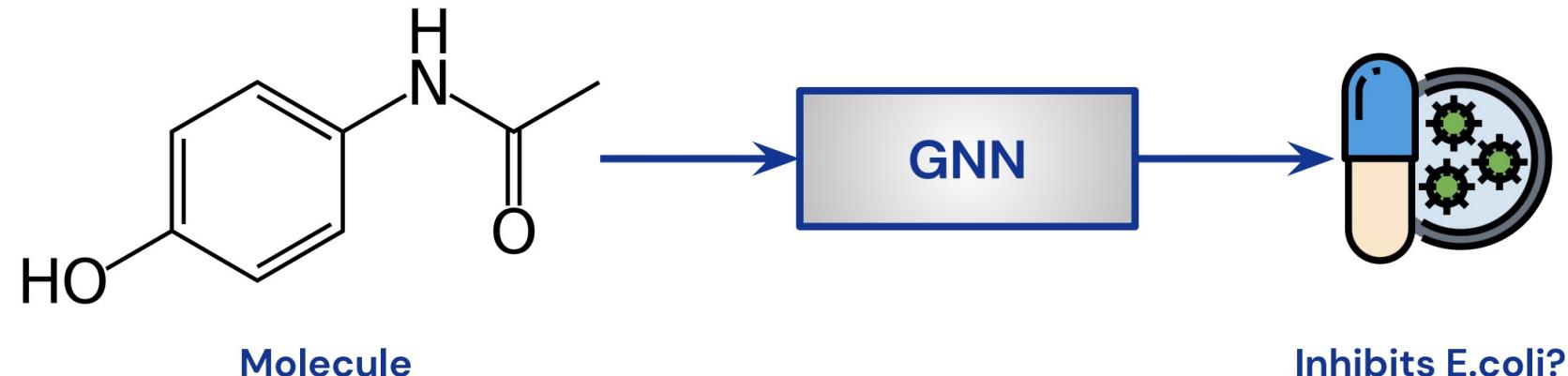
- Graph-level prediction: whether the molecule is a potent **drug**<sup>[29]</sup>
  - Binary classification on whether the drug will inhibit certain bacteria



[29] Jonathan M.Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

# Impactful applications in science

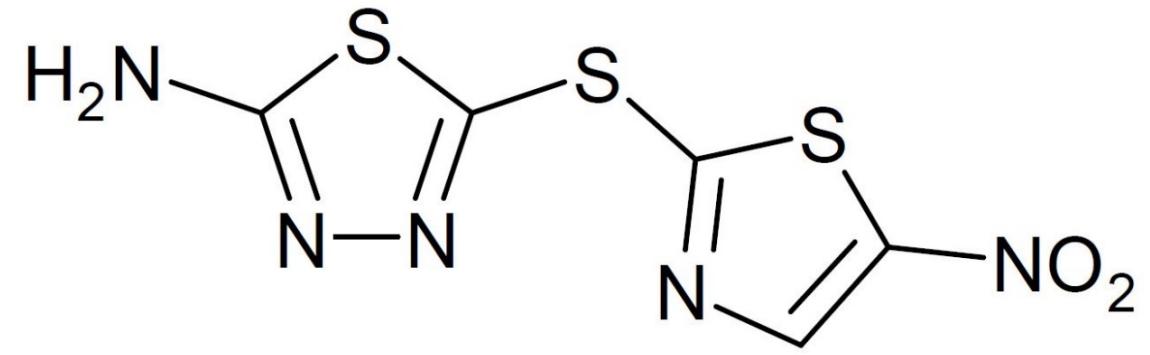
- Graph-level prediction: whether the molecule is a potent **drug**<sup>[29]</sup>
  - Execute on a large dataset of known candidate molecules
  - Select the ~ *top-100* candidates from the GNN model
  - Have chemists thoroughly investigate those



[29] Jonathan M.Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

# Impactful applications in science

- Discover a previously overlooked compound that is a **highly potent antibiotic**<sup>[29]</sup>



Halicin

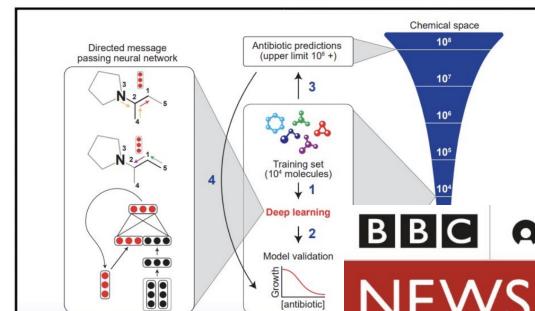
[29] Jonathan M.Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

# Impactful applications in science

Cell

## A Deep Learning Approach to Antibiotic Discovery

### Graphical Abstract



### Authors

Jonathan M. Stokes, Kevin Yang, Kyle Swanson, ..., Tommi S. Jaakkola, Regina Barzilay, James J. Collins

### Correspondence

regina@csail.mit.edu (R.B.), jimjc@mit.edu (J.J.C.)



Sign in

News

Sport

Reel

Worklife

Travel

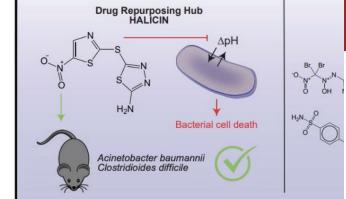
Future

## NEWS

Home | Video | World | UK | Business | Tech | Science | Stories | Entertainment & Arts

BBC WORKLIFE

Our new guide  
for getting ahead



nature

Subscribe

NEWS · 20 FEBRUARY 2020

## Powerful antibiotics discovered using AI

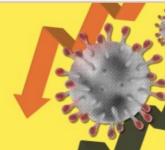
Machine learning spots molecules that work even against ‘untreatable’ strains of bacteria.

FINANCIAL TIMES

COMPANIES TECH MARKETS GRAPHICS OPINION WORK & CAREERS LIFE & ARTS HOW TO SPEND IT

### CORONAVIRUS BUSINESS UPDATE

Get 30 days' complimentary access to our Coronavirus Business Update newsletter



### intelligence

#### Robotics



‘Death of the office’ homeworking claims exaggerated



Anti-social robots have increased social distancing

### Artificial intelligence

+ Add to myFT

## AI discovers antibiotics to treat drug-resistant diseases

Machine learning uncovers potent new drug able to kill 35 powerful bacteria

## Scientists discover powerful antibiotic using AI

21 February 2020

Share

[29] Jonathan M. Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

# Still many open problems..

- And many more chances to do groundbreaking research
- (ex) other graph formats
  - 3-dimensional graphs
  - Temporal graphs
  - ....

# Thank you!

Questions?

[minjiy@cs.cmu.edu](mailto:minjiy@cs.cmu.edu) | <https://minjiyon.xyz>