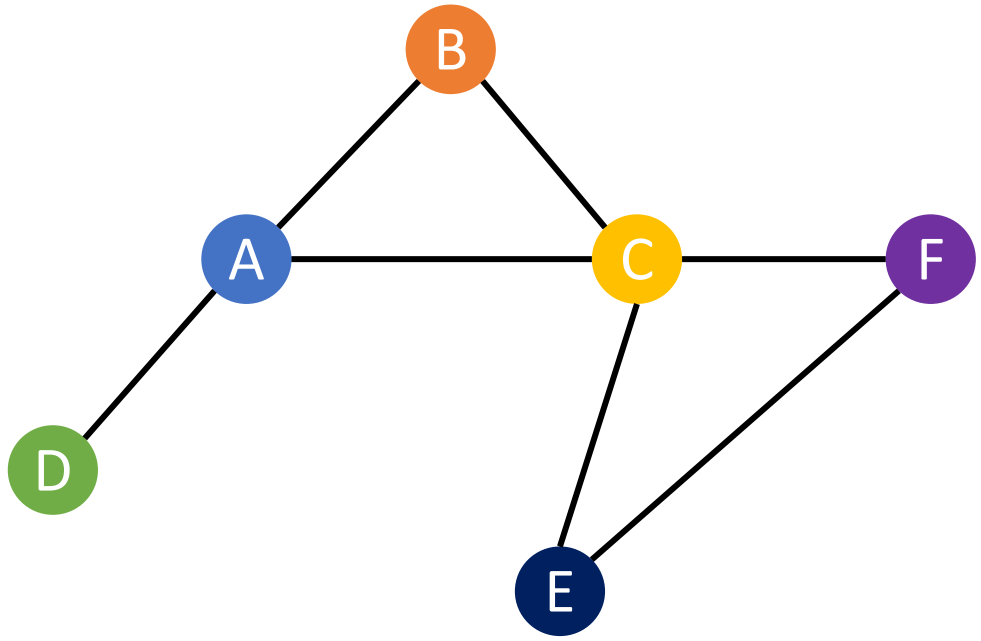
Introduction to Graph Deep Learning

Minji Yoon
Computer Science Department
Carnegie Mellon University

Talk objectives

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

What is a graph?

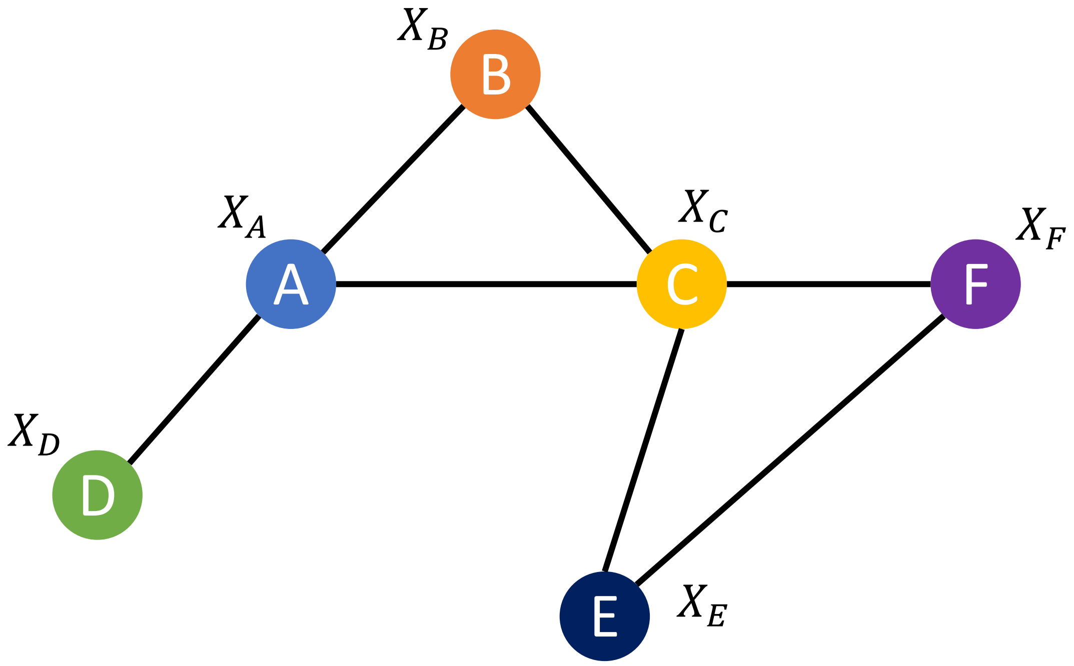


A graph is composed of
- **Nodes** (also called vertices)
- **Edges** connecting a pair of nodes

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

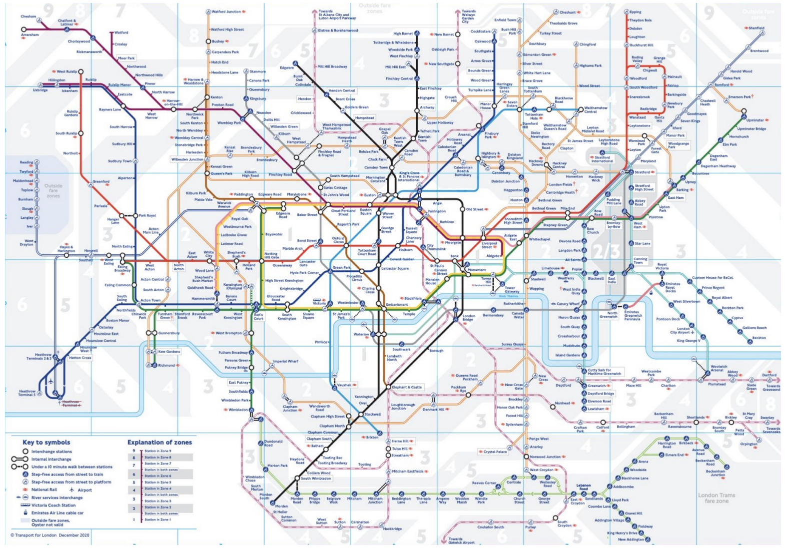
- **Nodes** (also called vertices)
- **Edges** connecting a pair of nodes

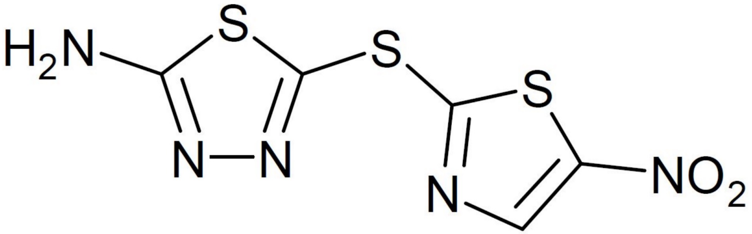
presented in an **adjacency matrix**

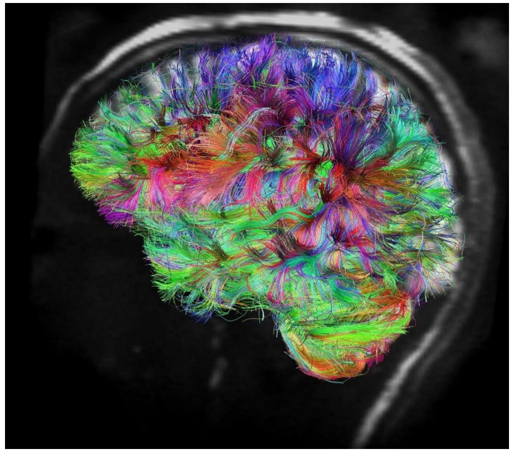
Nodes can have **feature vectors**

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

Graphs are everywhere







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ı to image search uses images returned by traditional search
des in a graph neural network through which similarity signals are
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Hanrui Wang[1], Kuan Wang[1], Jiacheng Yang[1], Linxiao Shen[2], Nan Sun[2], Hae-Seung Lee[1], Song Han[1]

[1]Massachusetts Institute of Technology

[2]UT Austin

HAN LAB Hardware, AI and Neural-nets

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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.

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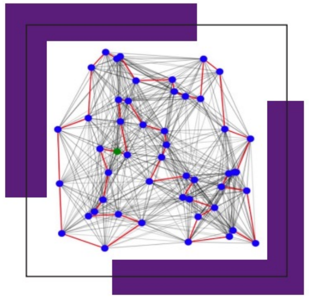


Patterns

CellPress OPEN ACCESS

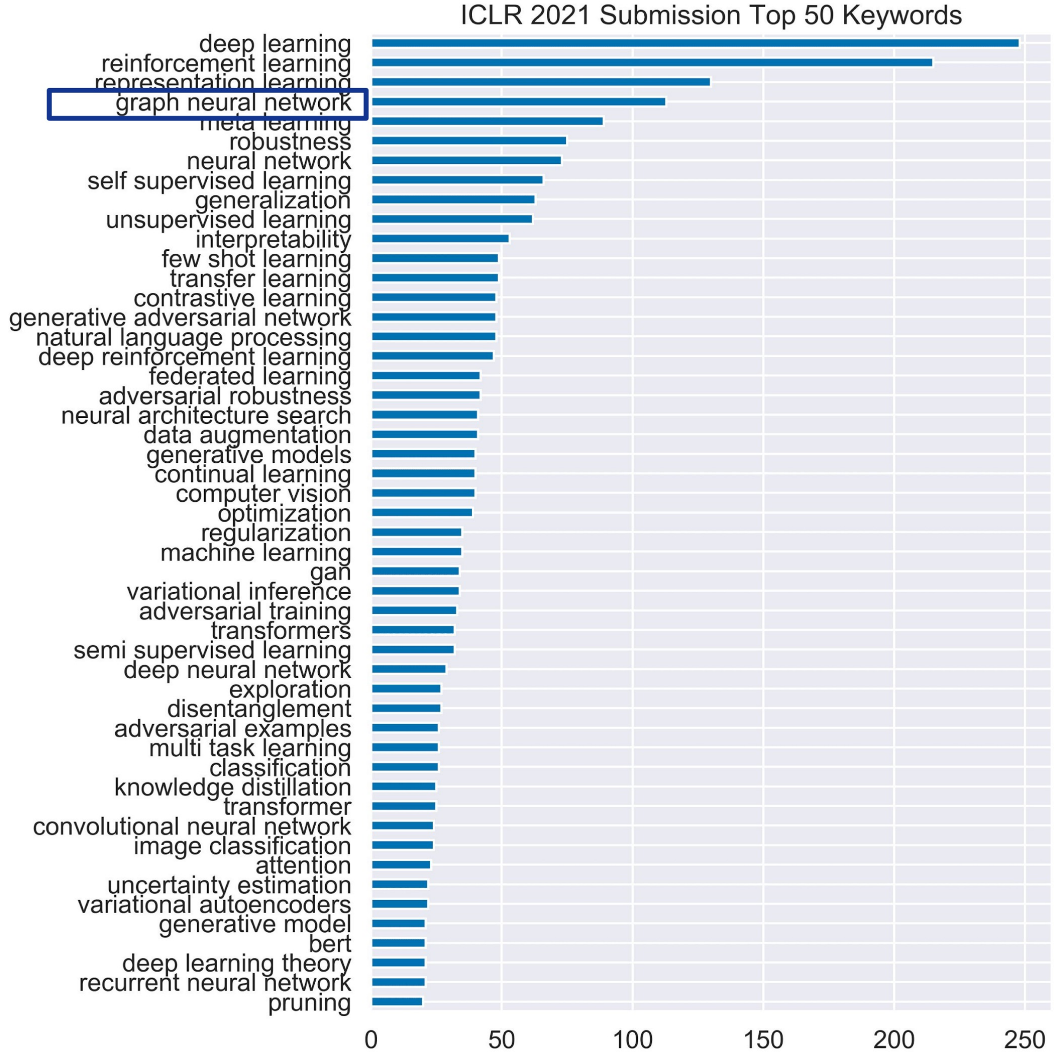
Opinion

Neural algorithmic reasoning

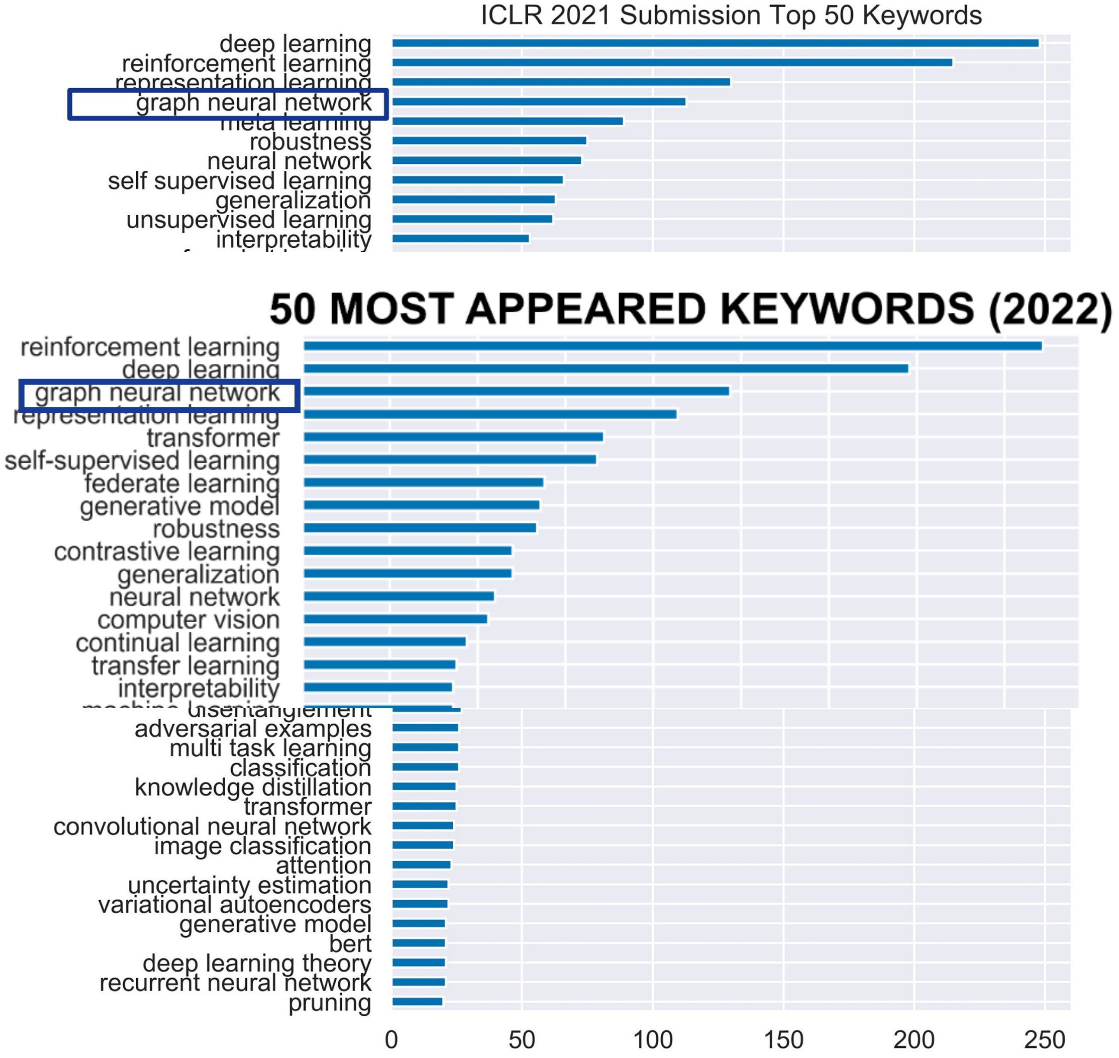
Petar Veličković[1,*] and Charles Blundell[1]
[1]DeepMind, London, Greater London, UK
*Correspondence: petarv@google.com
https://doi.org/10.1016/j.patter.2021.100273

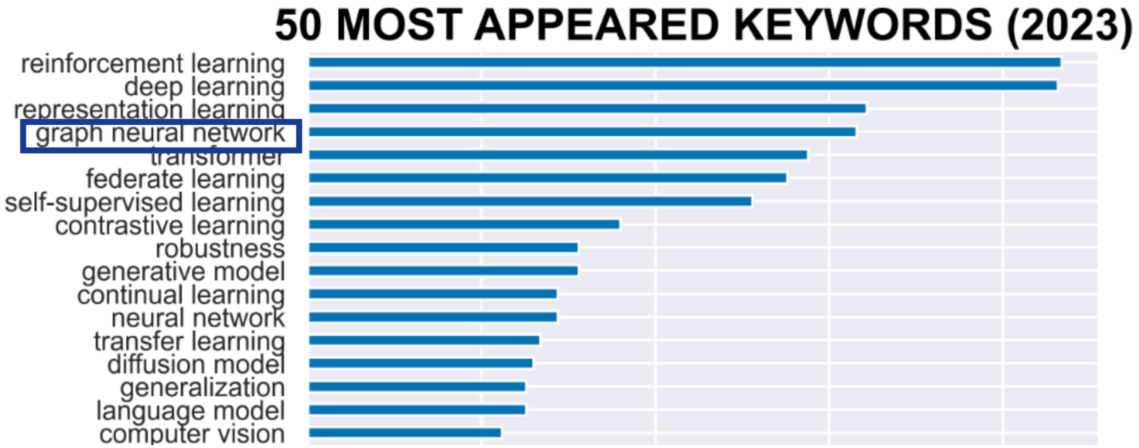
We present neural algorithmic reasoning—the art of building neural networks that are able to execute algorithmic computation—and provide our opinion on its transformative potential for running classical algorithms on inputs previously considered inaccessible to them.

Popular research topic



Popular research topic





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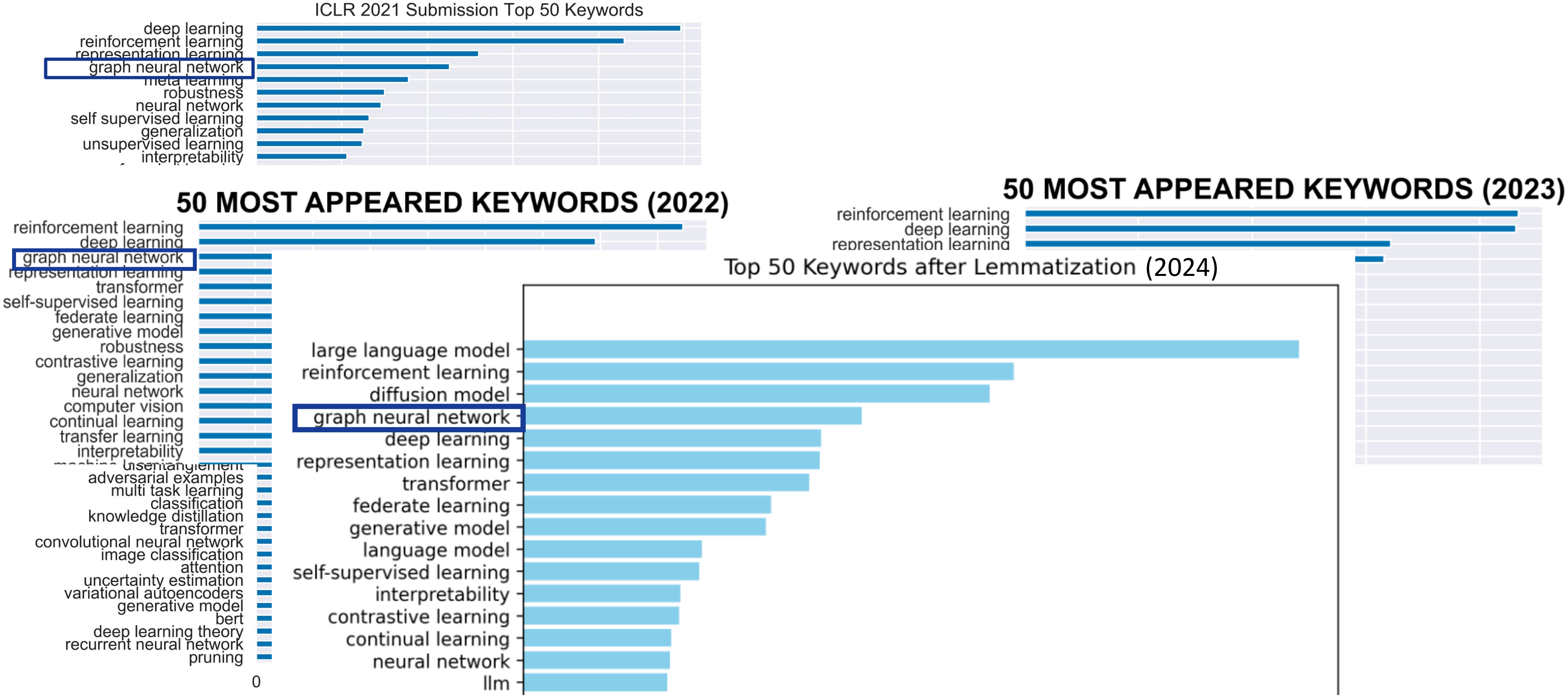
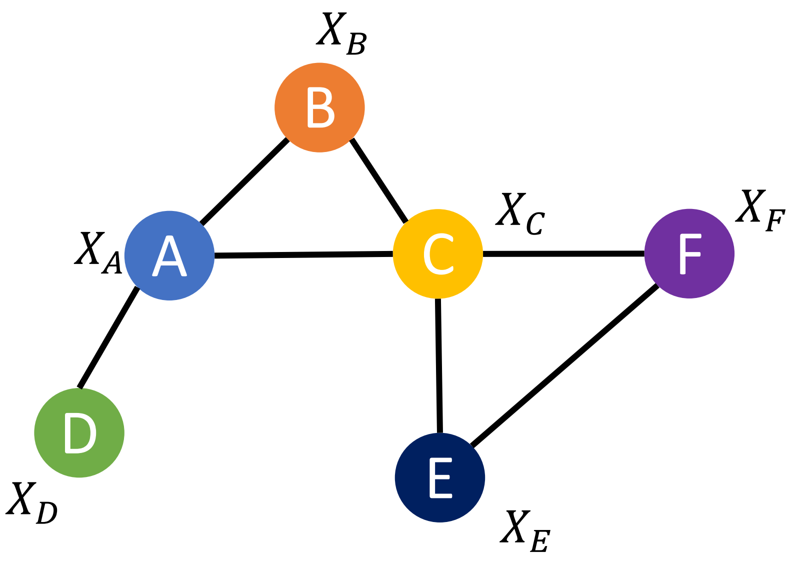


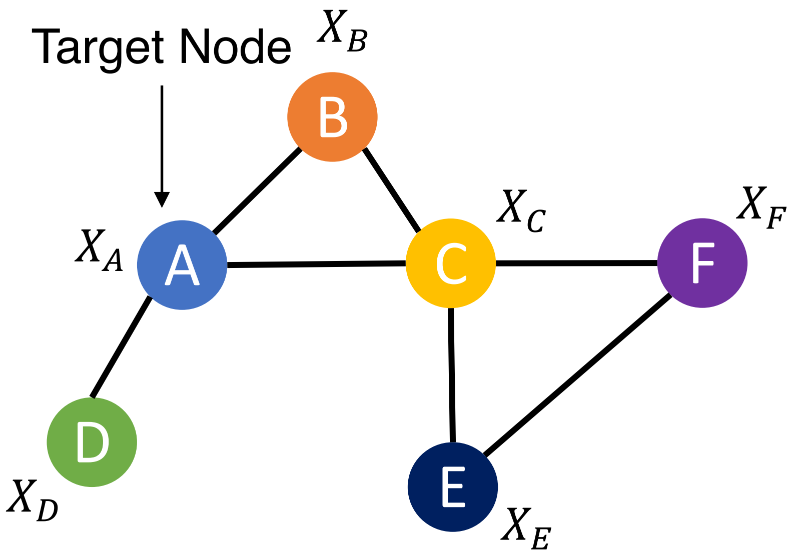
What is Graph Neural Network?

Problem definition



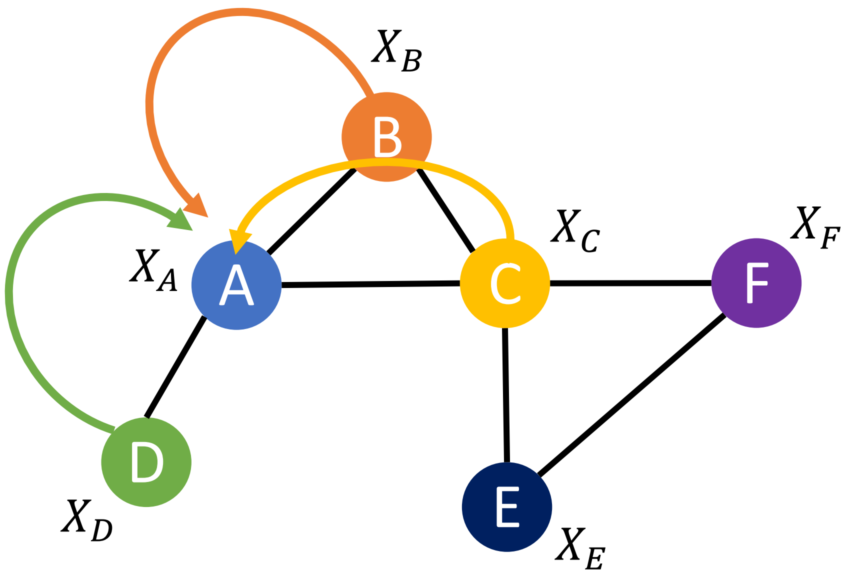
- **Given**
  - A graph
  - Node attributes
  - (part of nodes are labeled)
- **Find**
  - Node embeddings
- **Predict**
  - Labels for the remaining nodes

Graph Neural Networks



"Homophily: connected nodes are related/informative/similar"

Graph Neural Networks



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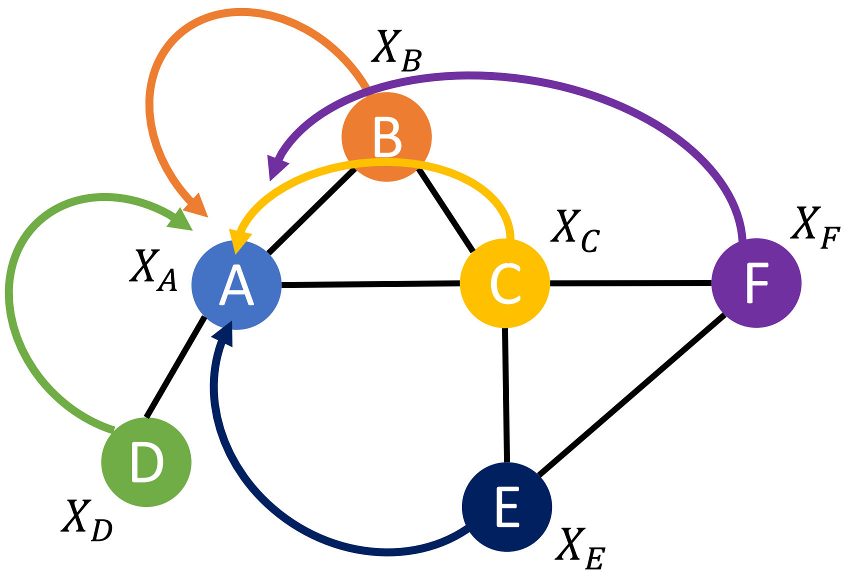
Graph Neural Networks



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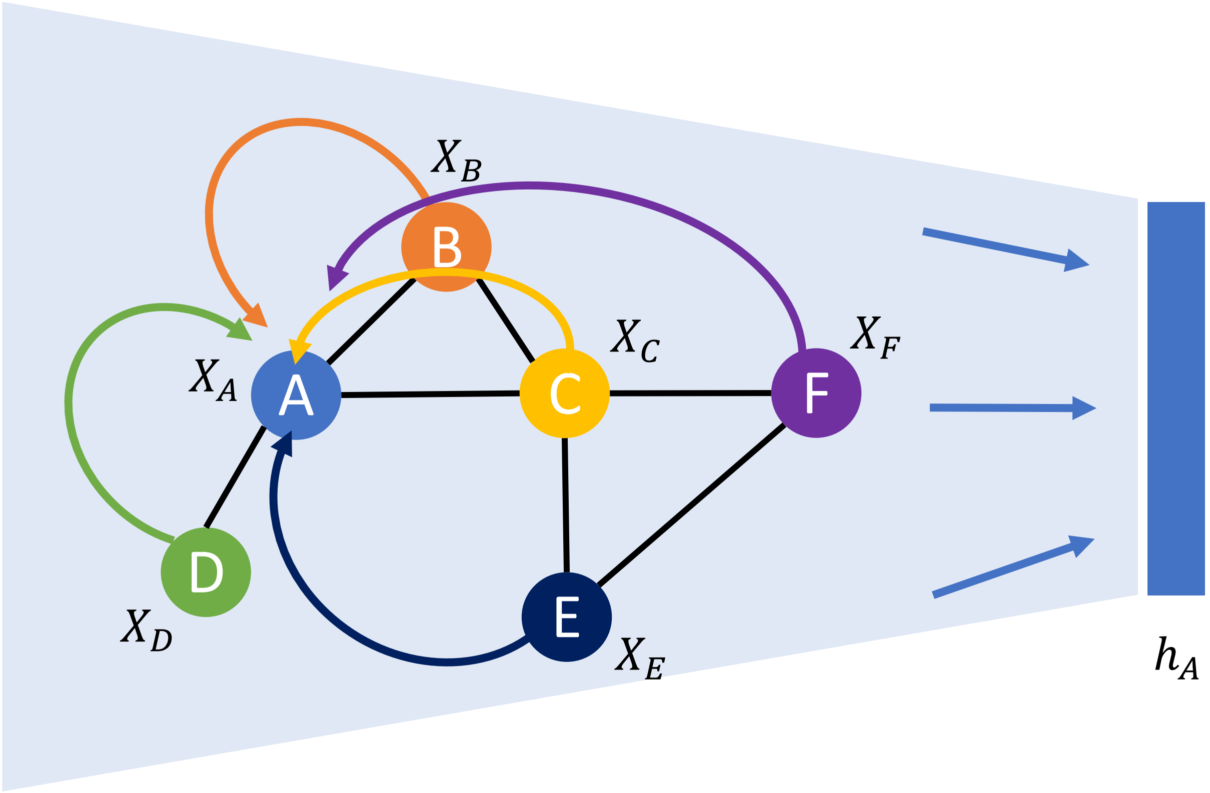
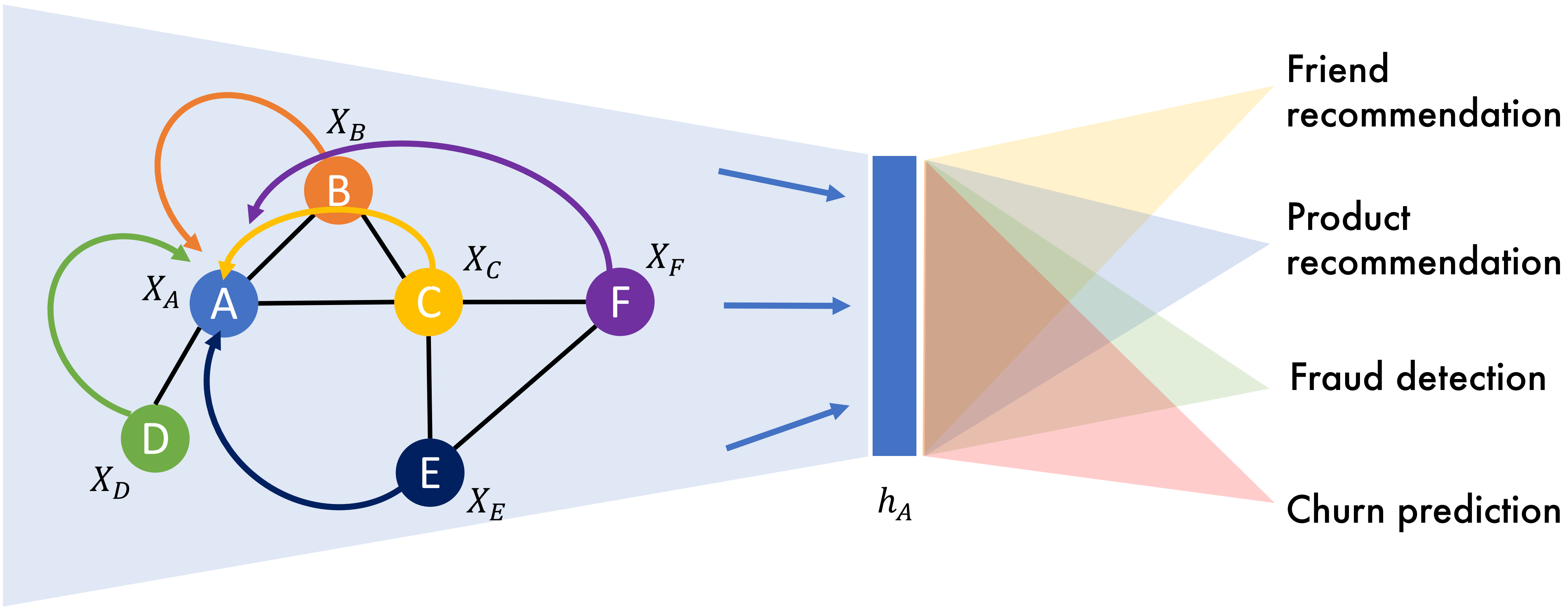
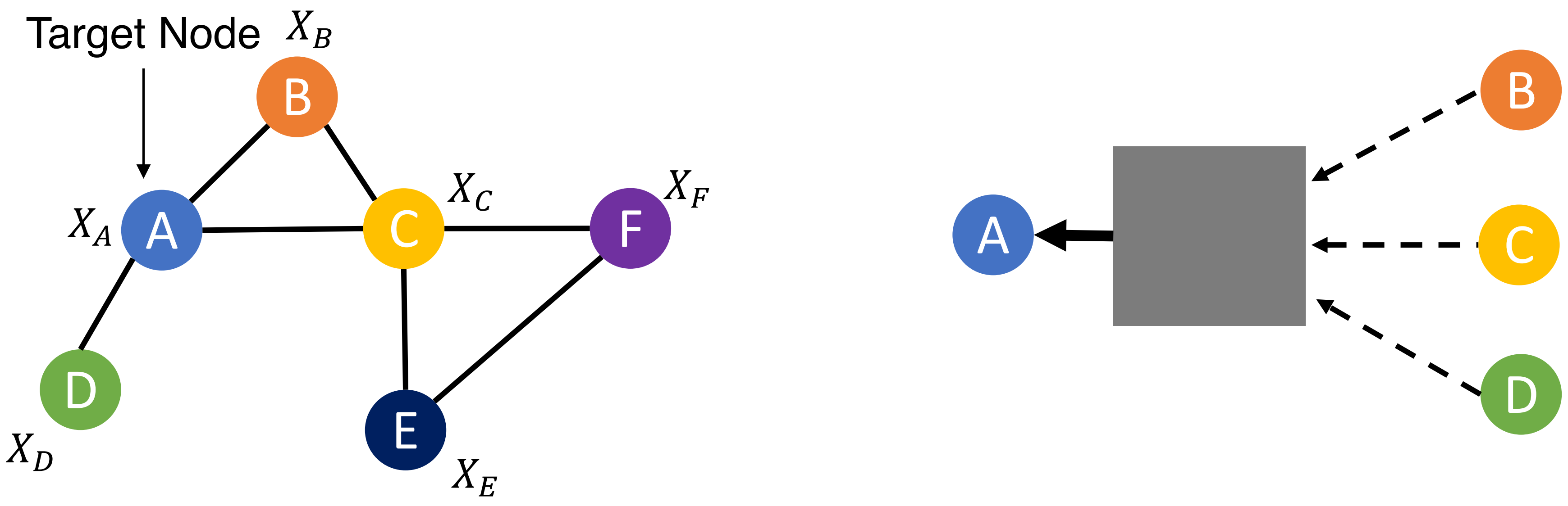
Graph Neural Networks



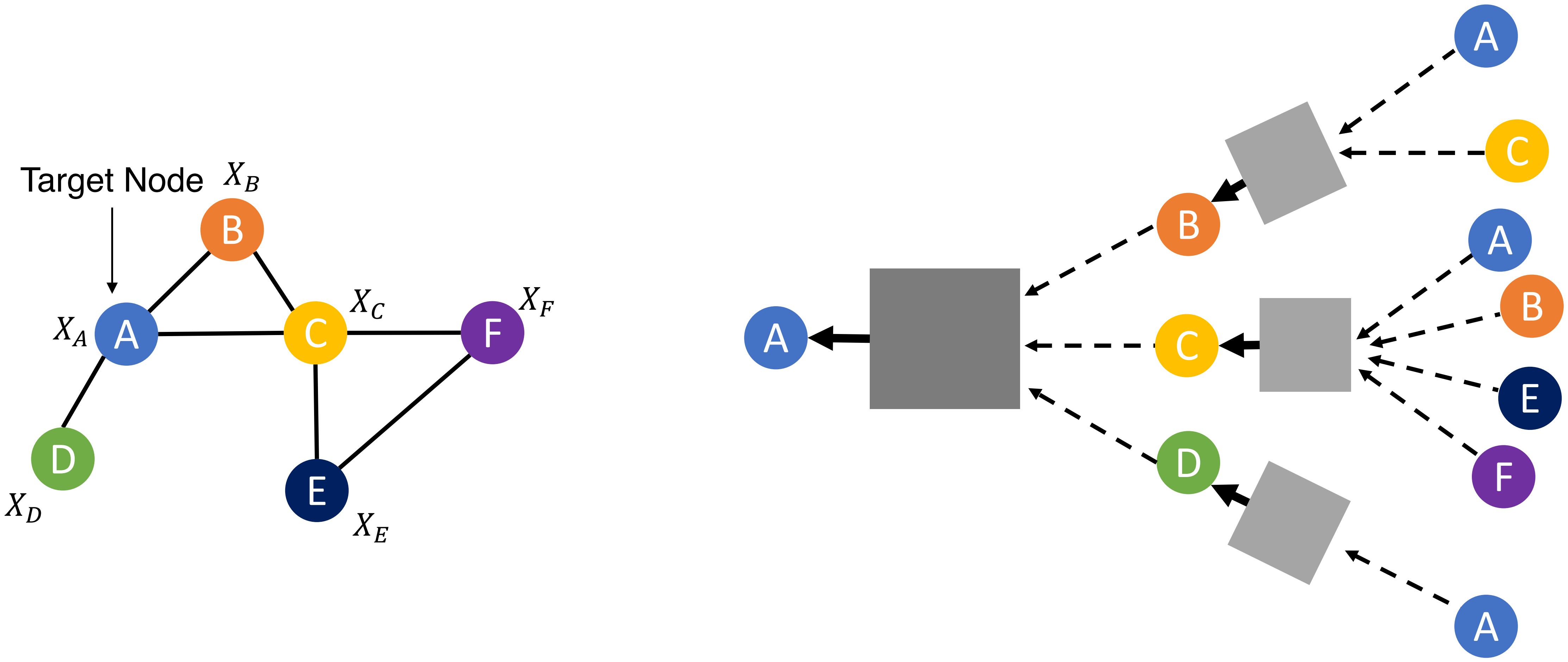
Graph Neural Networks



Graph Neural Networks



Graph Neural Networks



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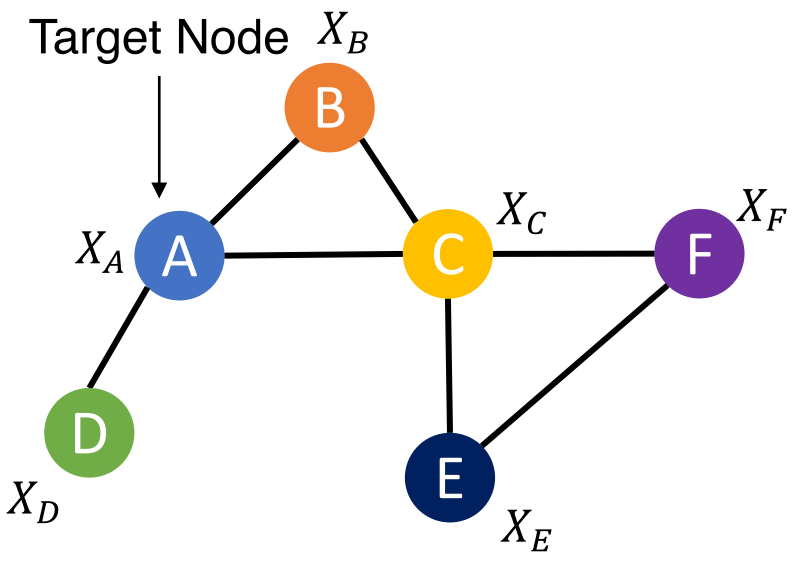

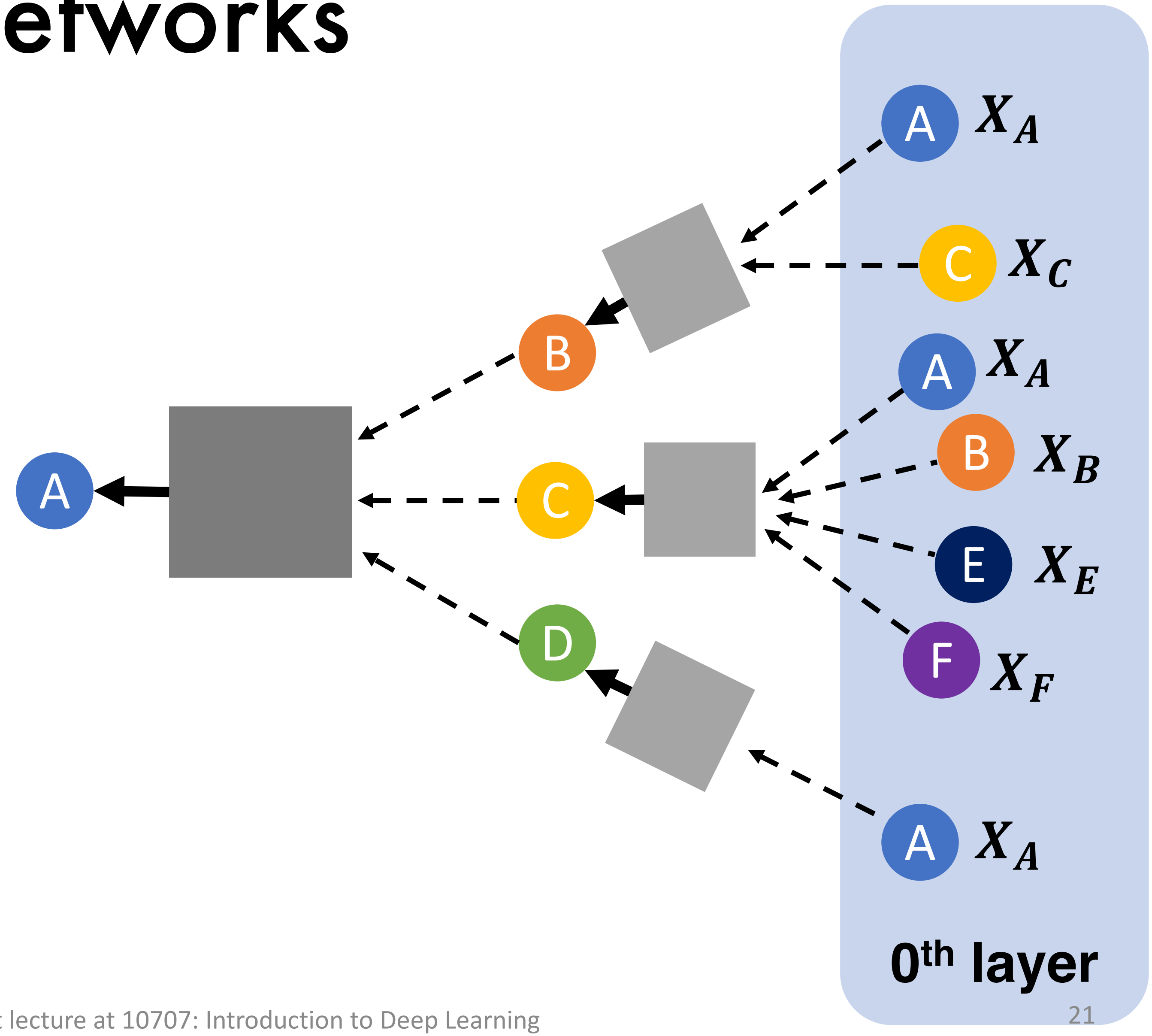

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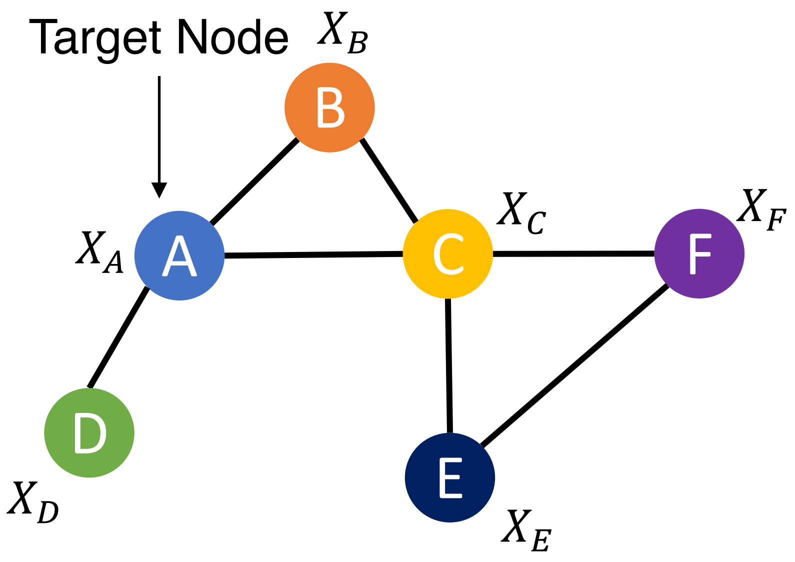
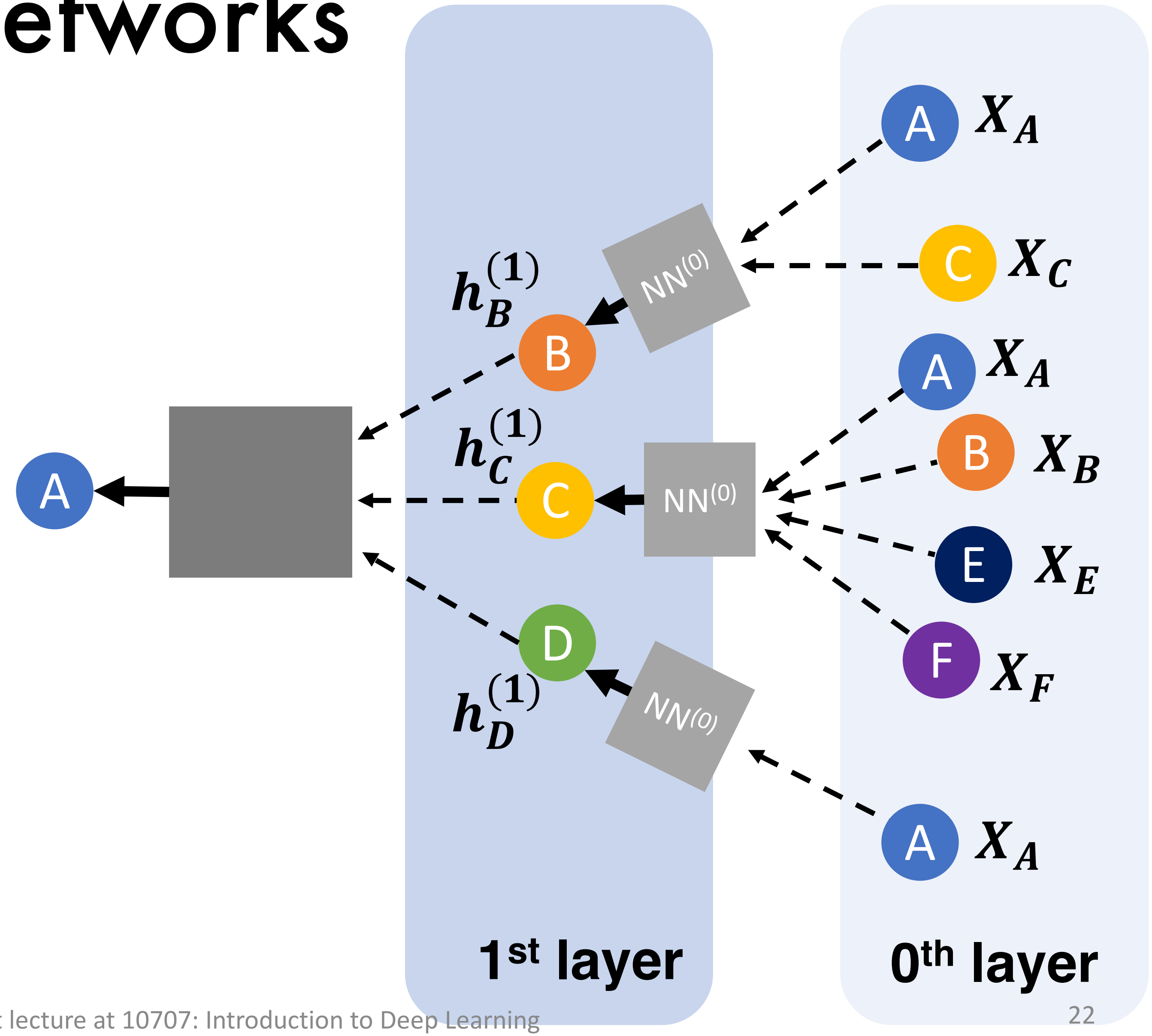
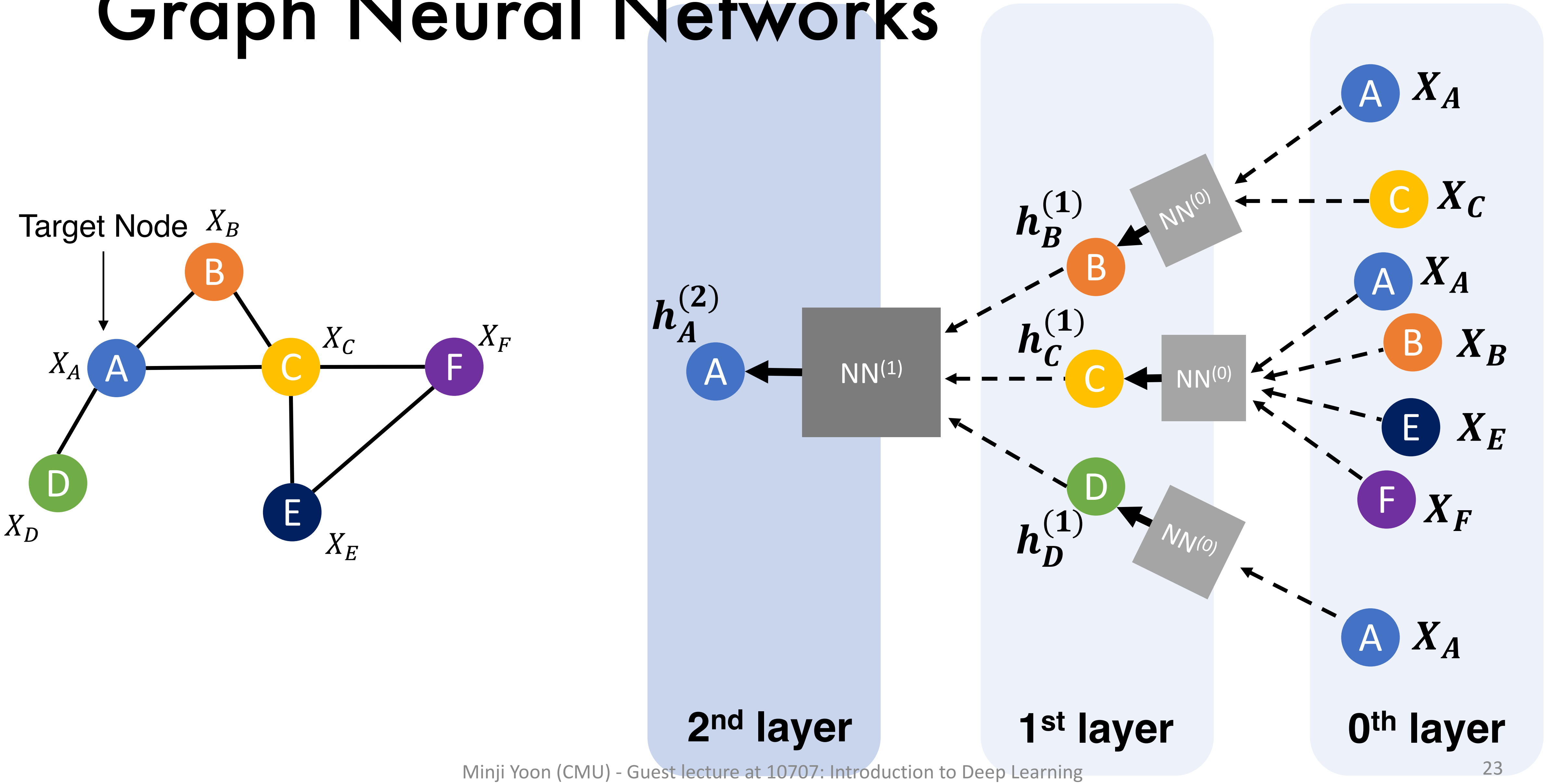




Graph Neural Networks

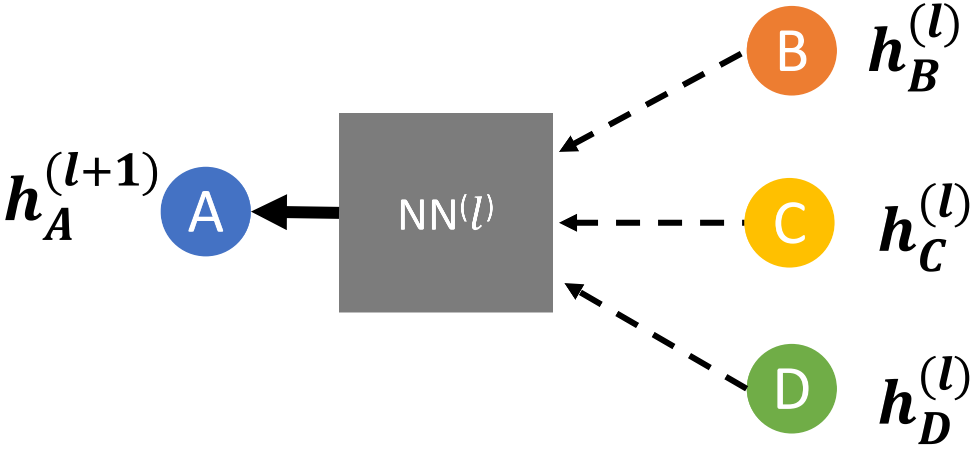


Graph Neural Networks

1. **Aggregate messages from neighbors**

$h_v^{(l)}$: node embedding of v at l-th layer
$\mathcal{N}(v)$: neighboring nodes of v
$\boldsymbol{f}^{(l)}$: aggregation function at l-th layer
$m_v^{(l)}$: message vector of v at l-th layer

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



Neighbors of node A
$\mathcal{N}(A) = \{B, C, D\}$

Graph Neural Networks

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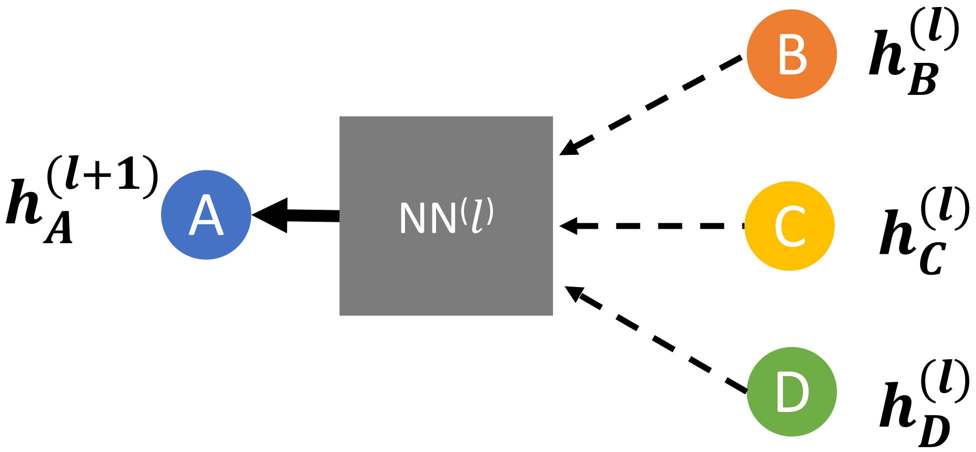
$$= \boldsymbol{f}^{(l)}\left(h_A^{(l)}, h_B^{(l)} h_C^{(l)} h_D^{(l)}\right)$$

2. Transform messages

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

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



Neighbors of node A
$\mathcal{N}(A) = \{B, C, D\}$

Graph Neural Networks

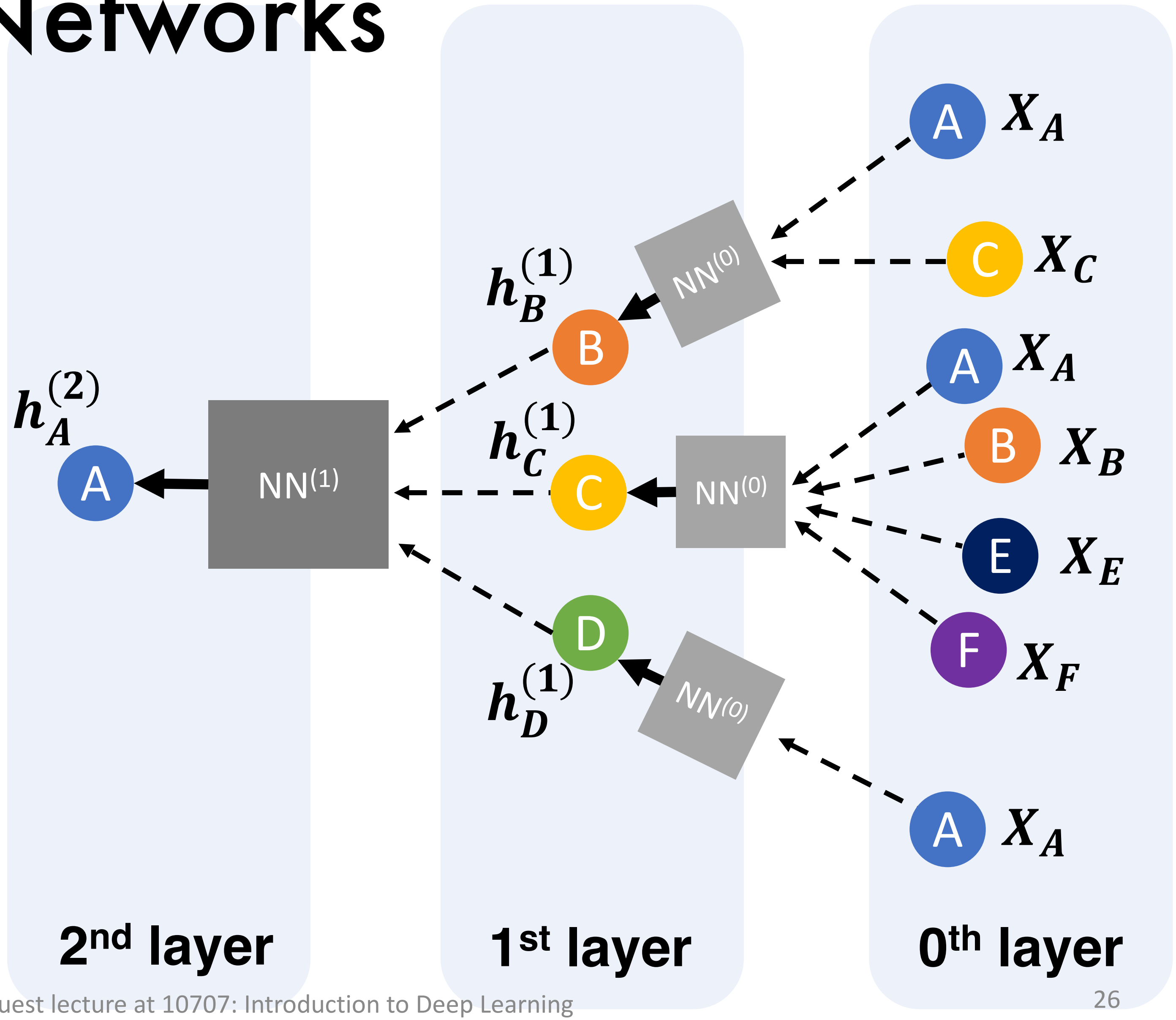
In each layer l ,
for each target node v :

1. Aggregate messages

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

2. Transform messages

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



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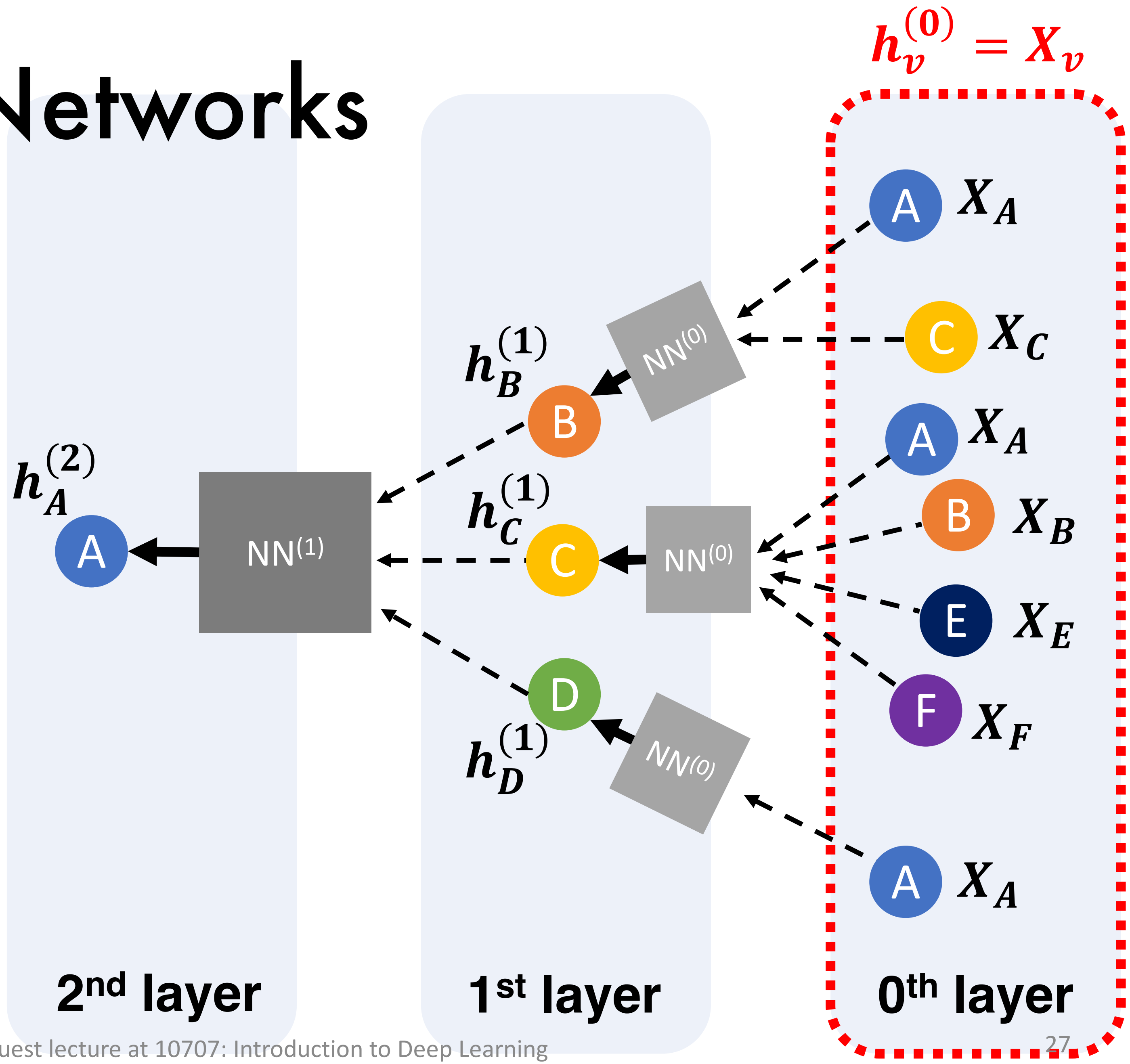

Graph Neural Networks

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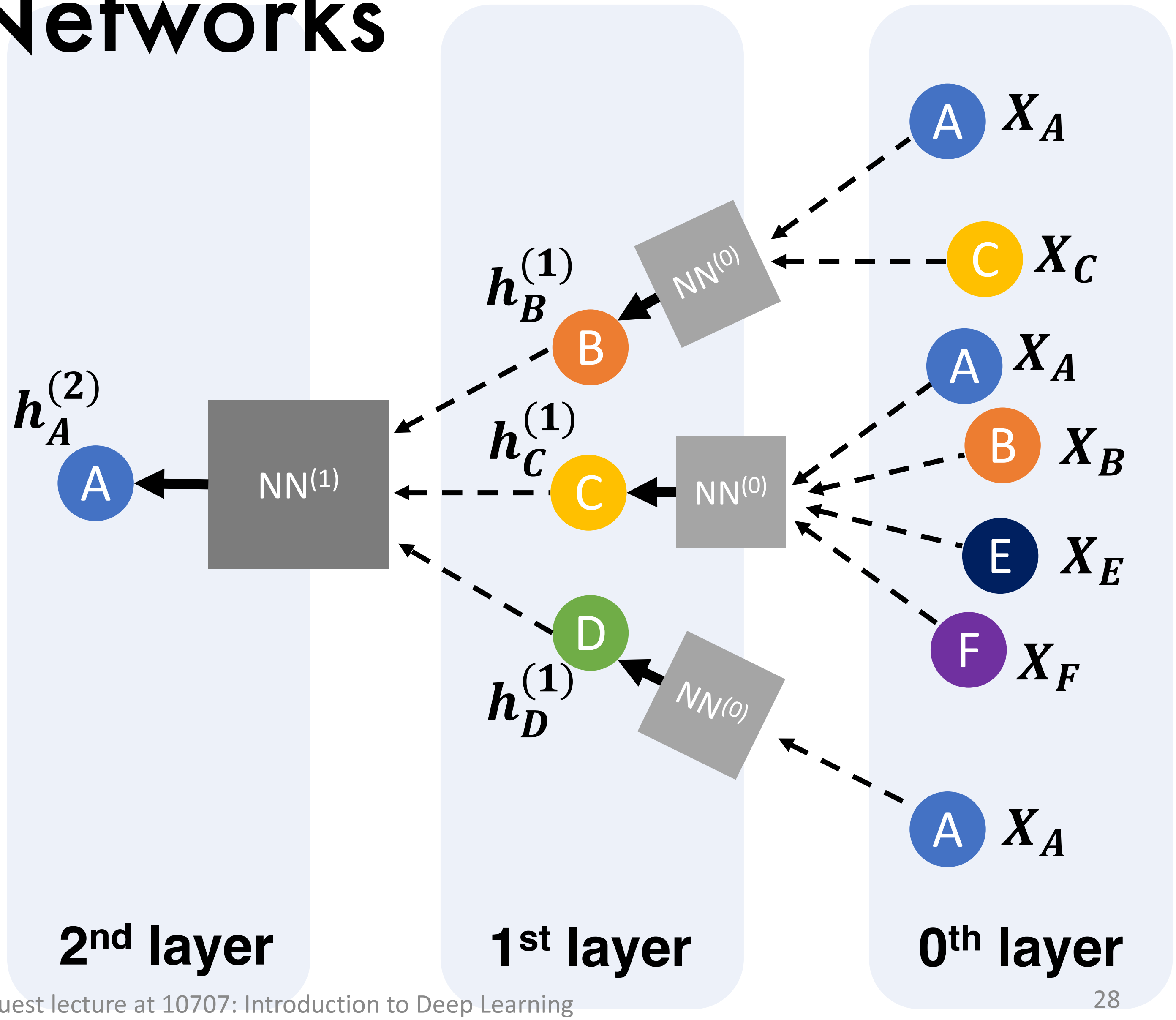


Graph Neural Networks

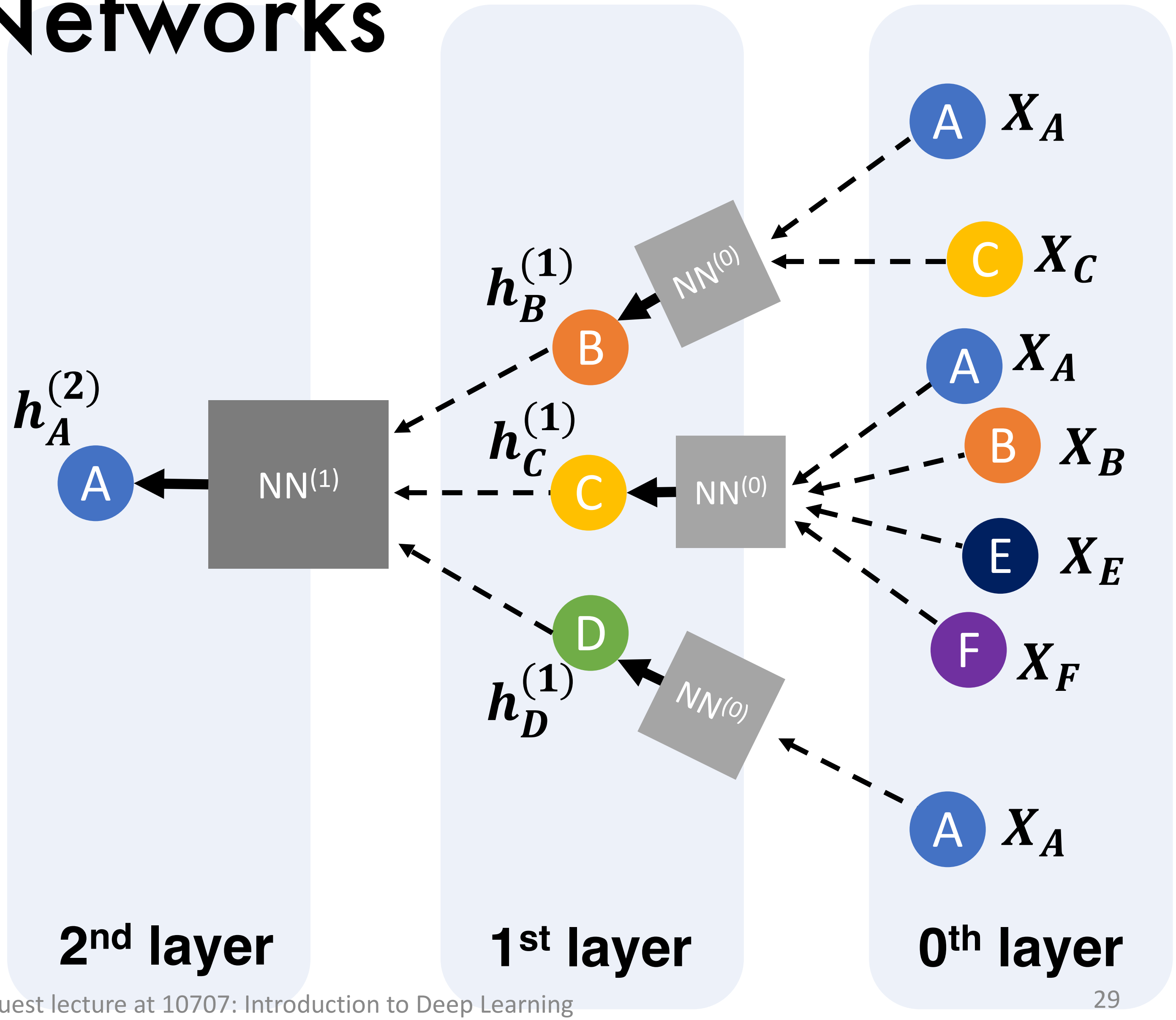
Graph Convolutional Networks[1]

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

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



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

Graph Neural Networks

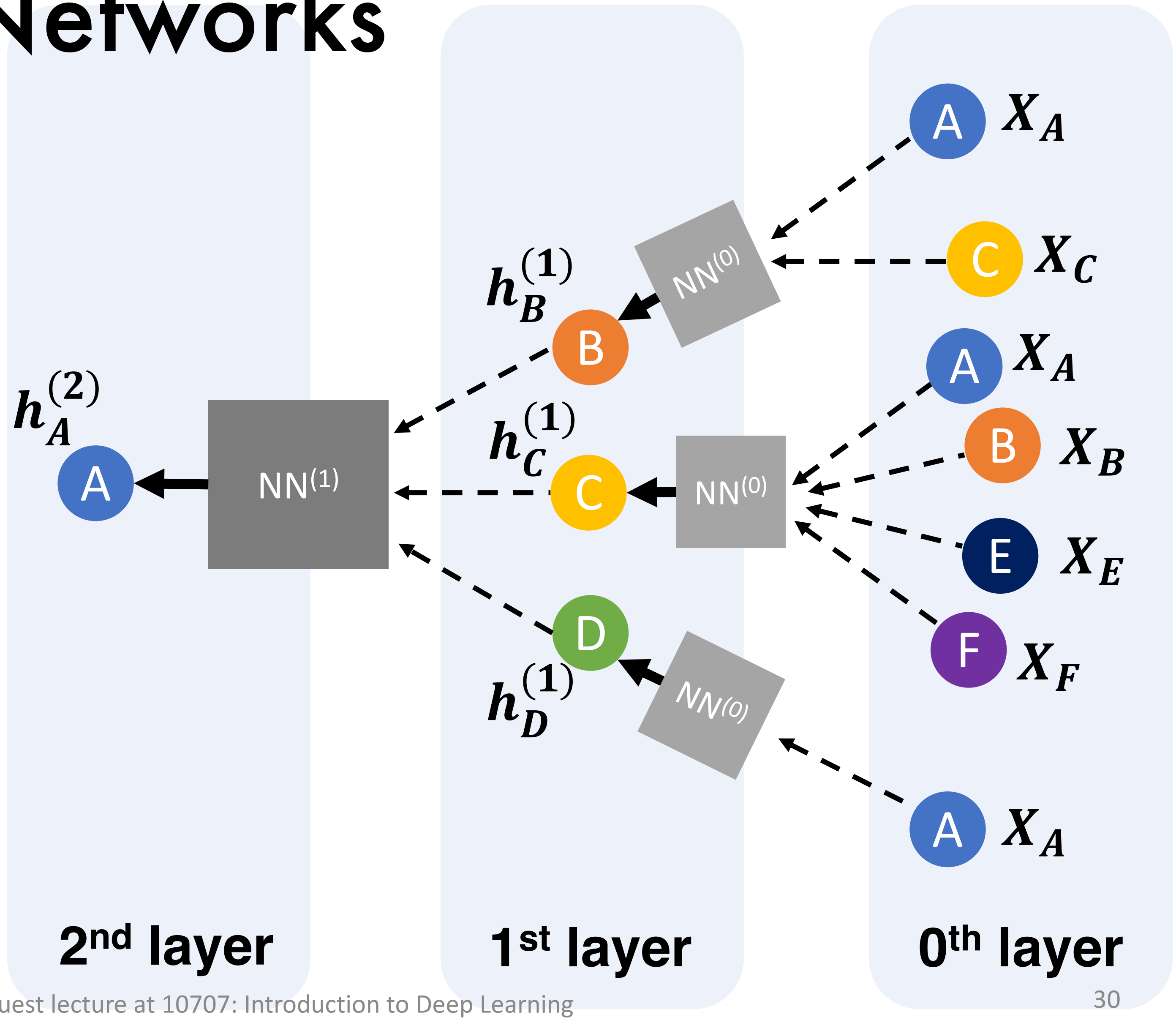
Graph Isomorphism Networks[2]

1. Aggregate messages

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

2. Transform messages

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



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

Graph Neural Networks

Simplified GCN[3]

1. Aggregate messages

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

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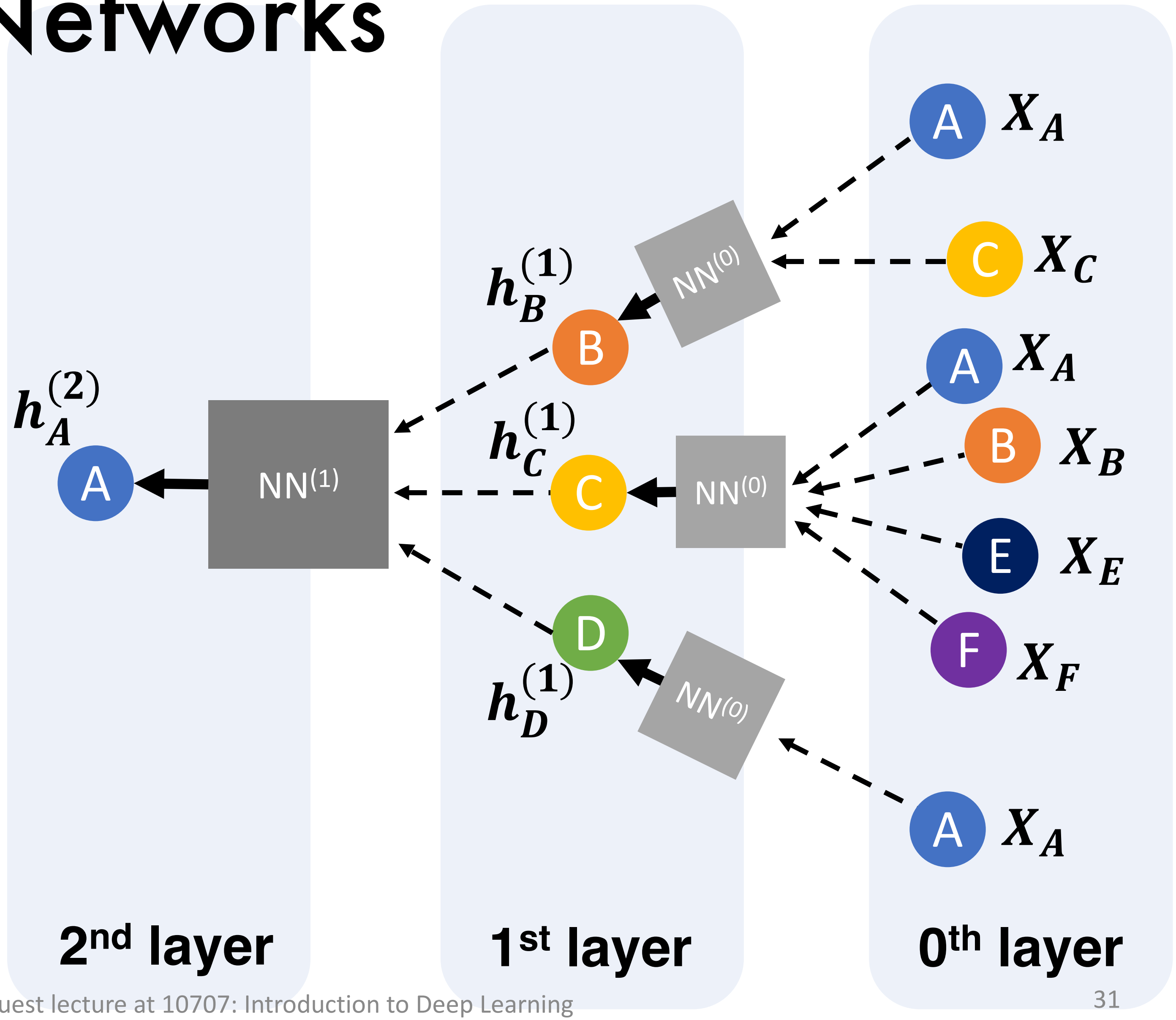
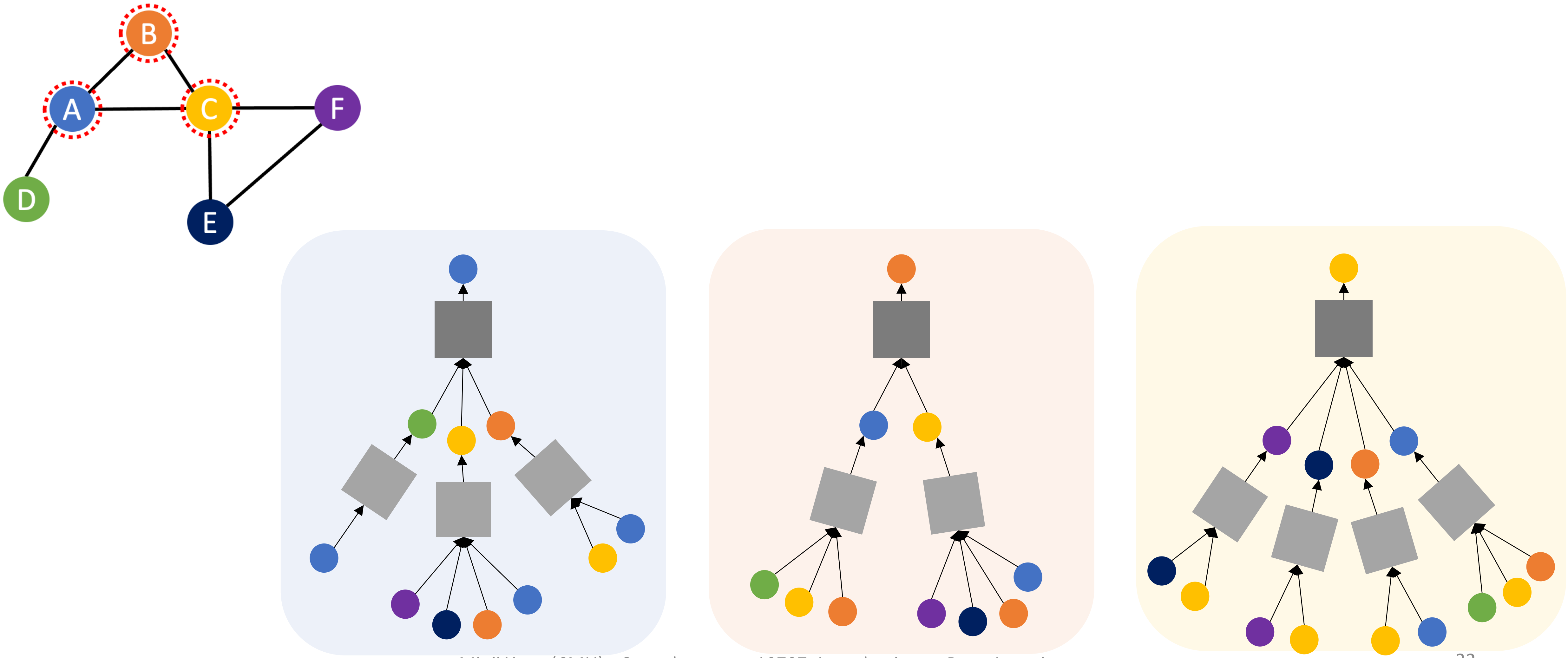
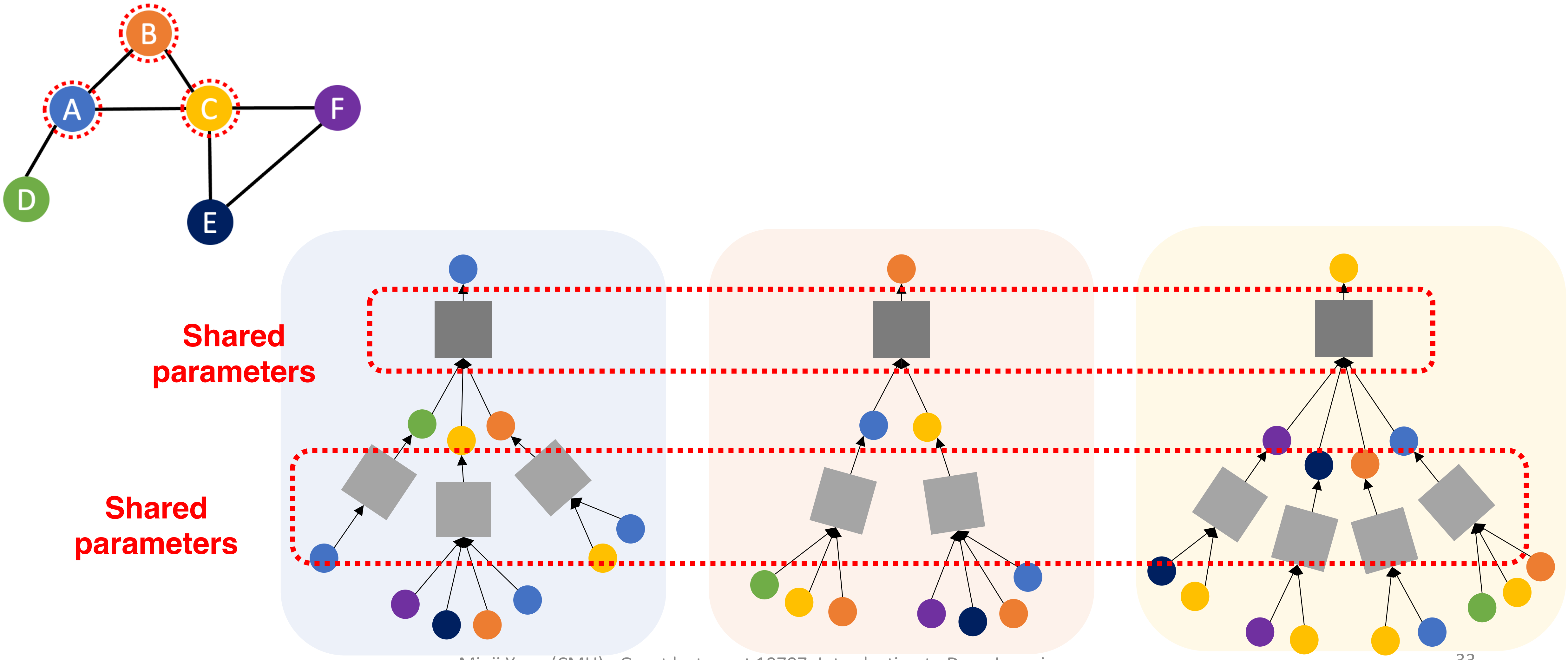


[3] Wu, Felix, et al. "Simplifying graph convolutional networks."

Computation graphs

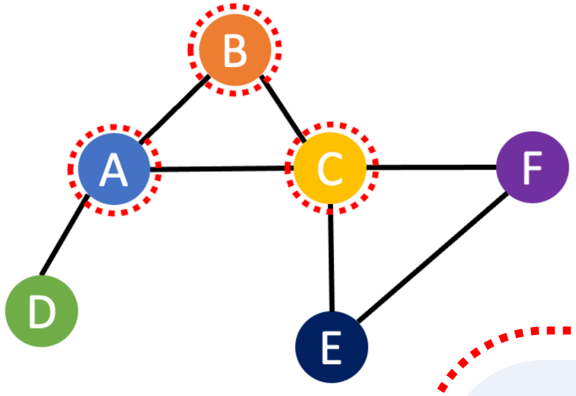


Computation graphs

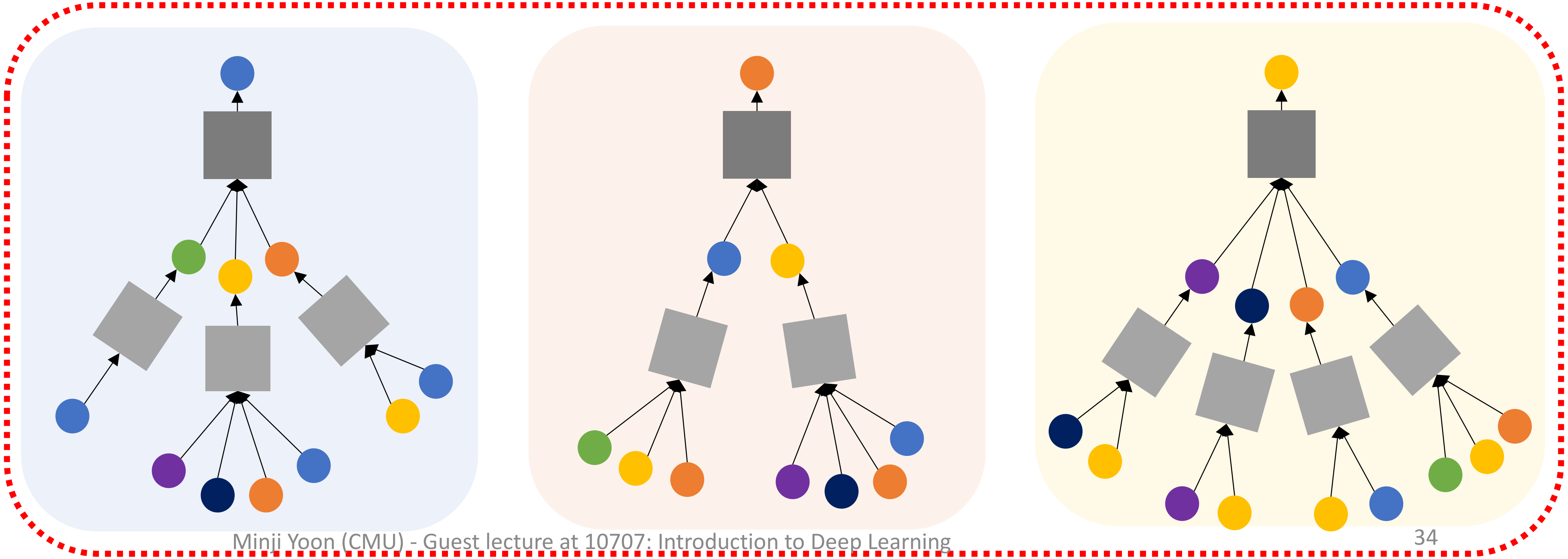


Batch execution

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



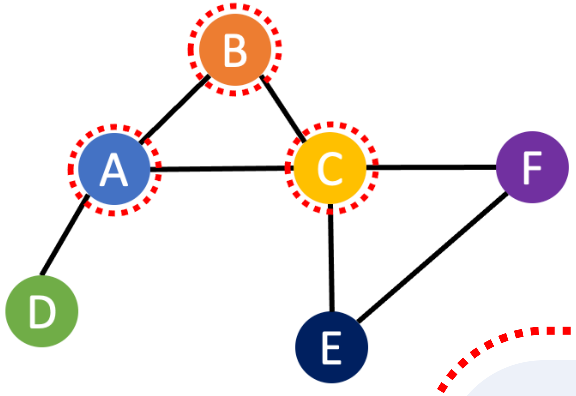
Batch size = 3



Batch execution

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

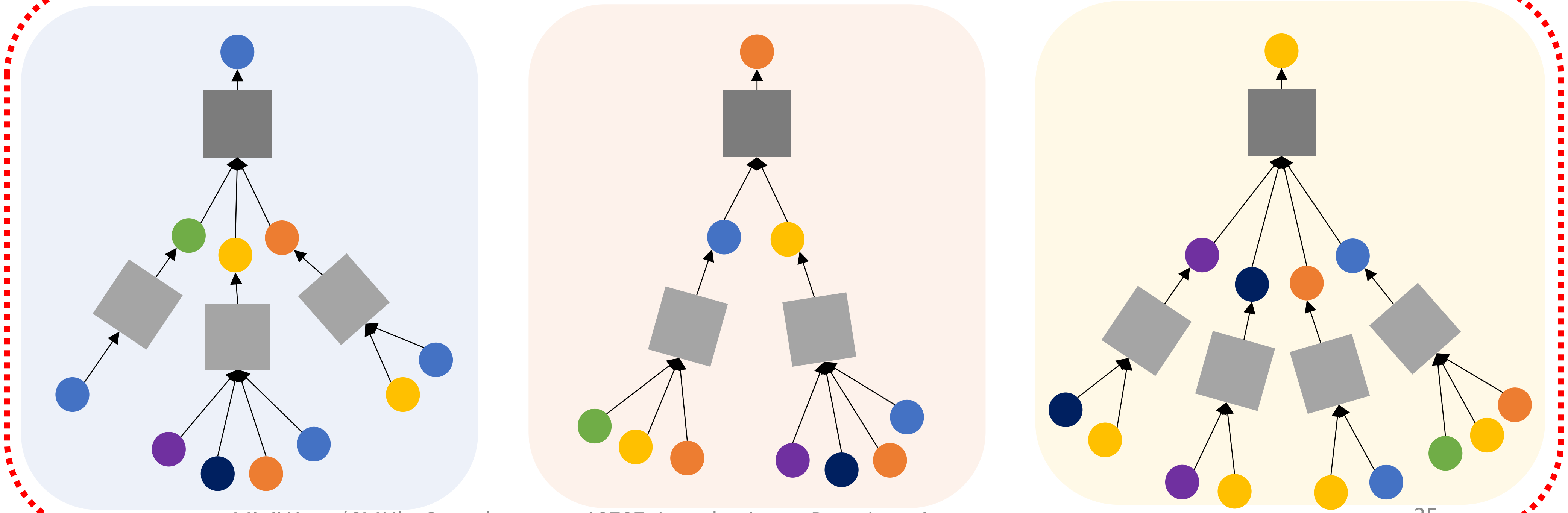
$$\boldsymbol{H}^{(l)} = \sigma(\widetilde{(\boldsymbol{A}+\boldsymbol{I})}\boldsymbol{H}^{(l-1)}\boldsymbol{W}^{(l)})$$



Node embedding matrix

(row-normalized) **Adjacency matrix**

Batch size = 3



Batch execution

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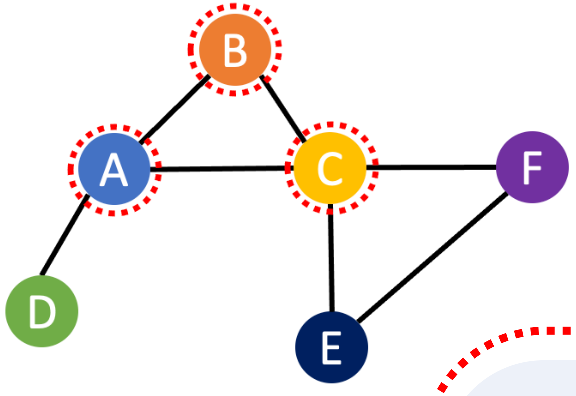
Fixed **Trainable**



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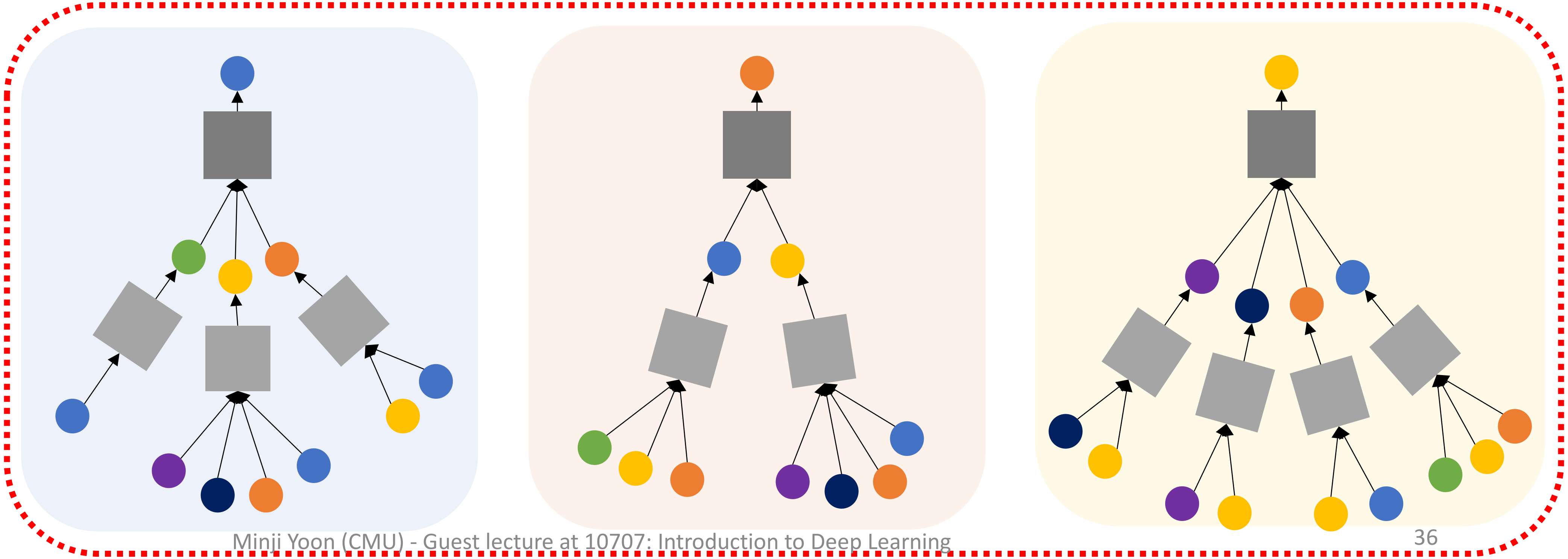
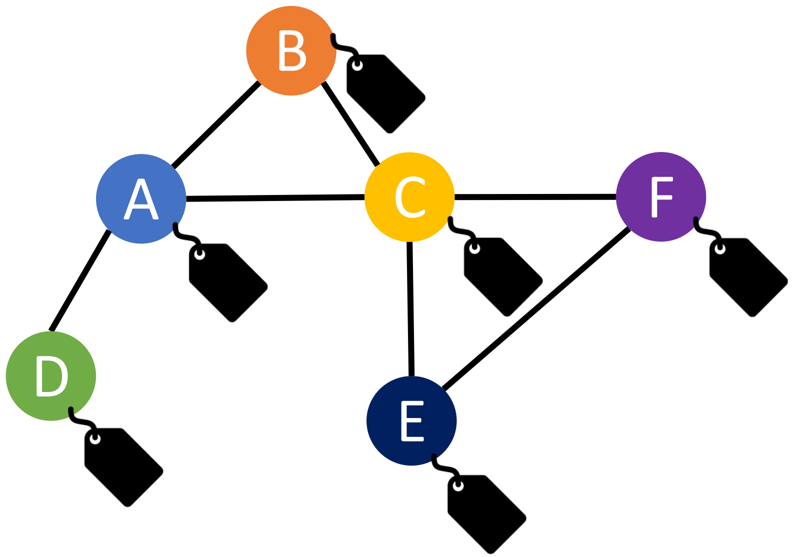


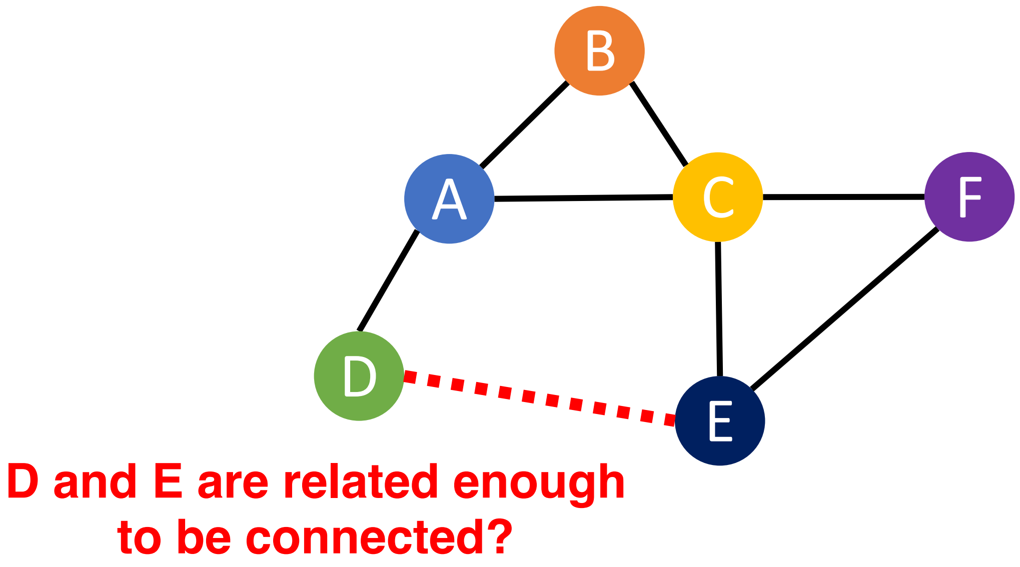
Downstream tasks

- Node-level prediction



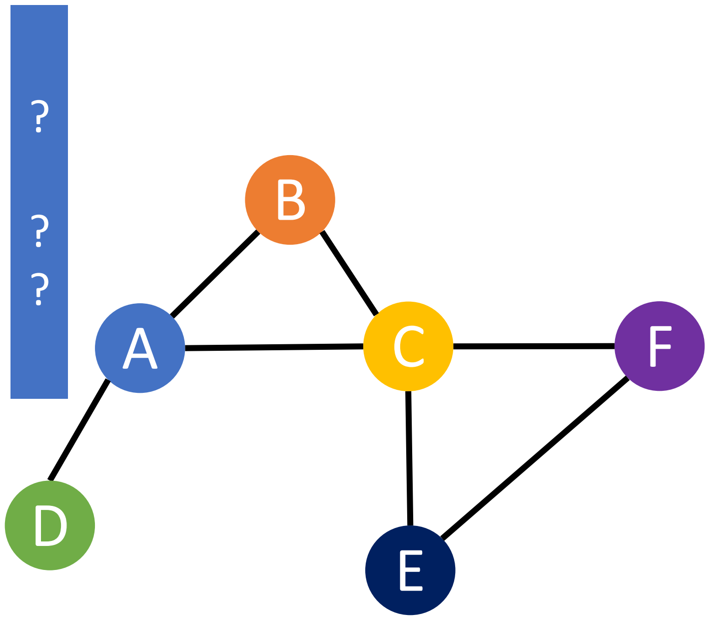
Downstream tasks

- Node-level prediction
- Edge-level prediction



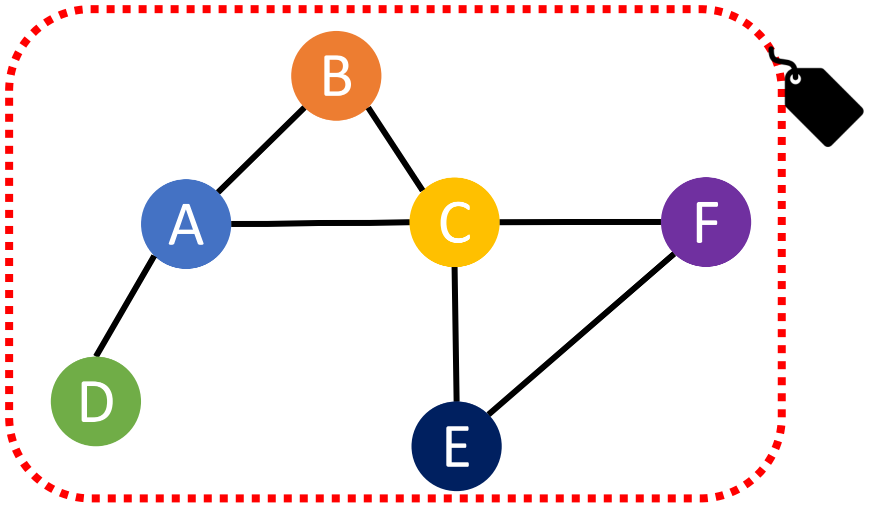
Downstream tasks

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



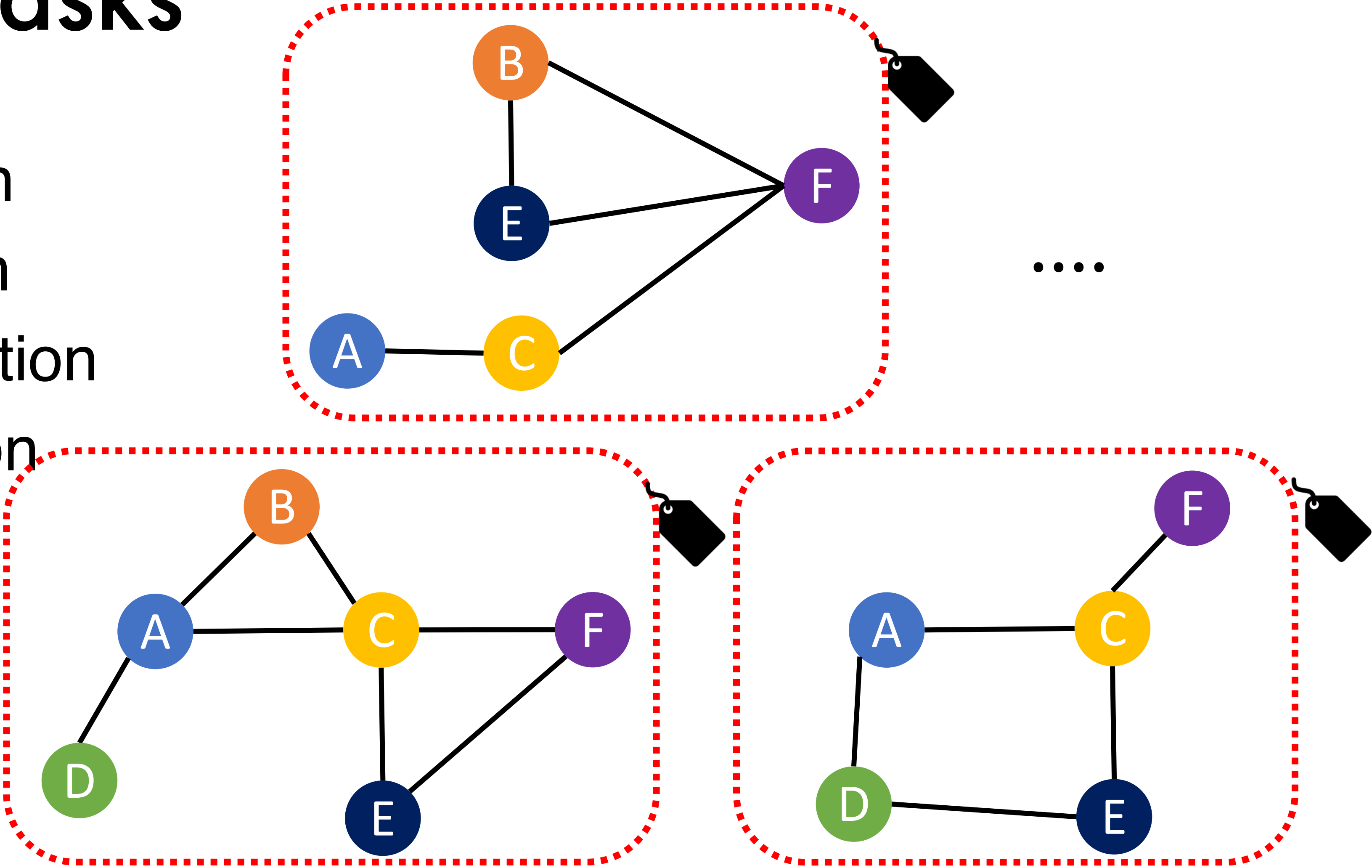
Downstream tasks

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



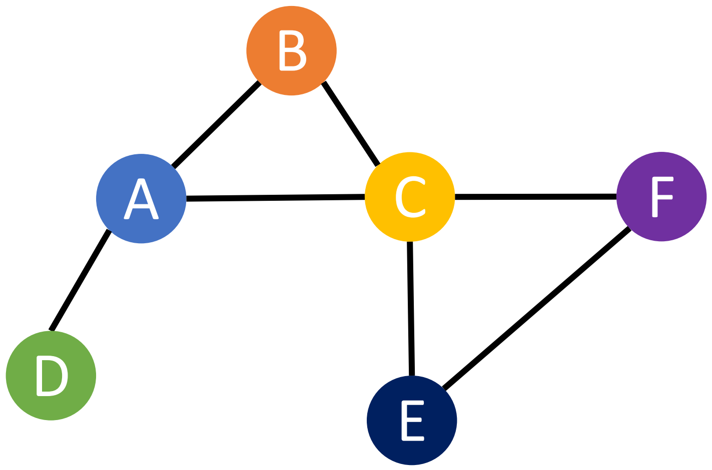
Downstream tasks

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

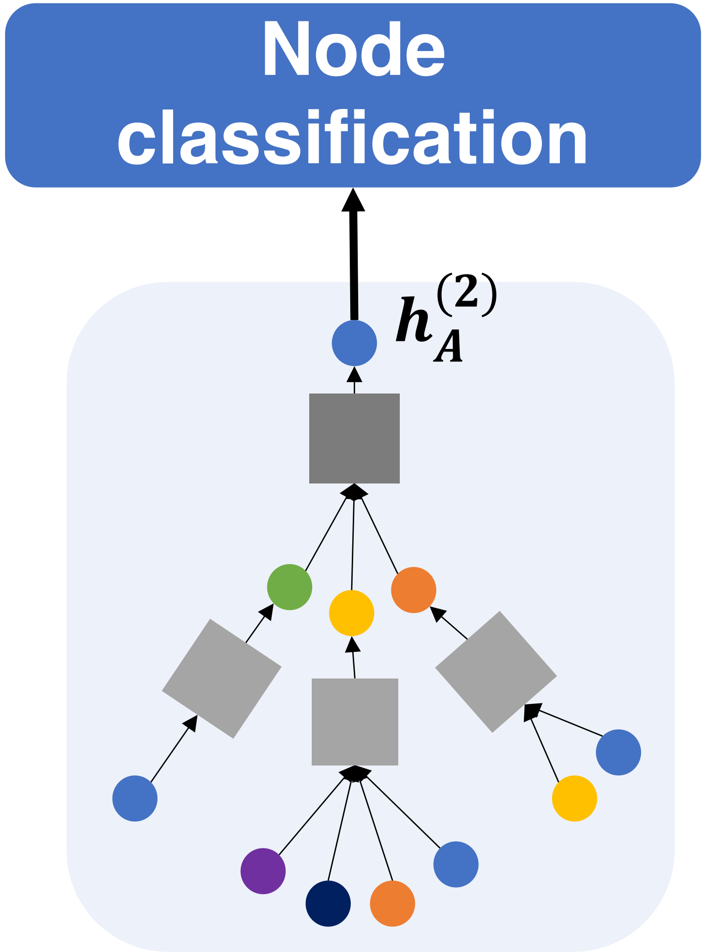


Downstream tasks

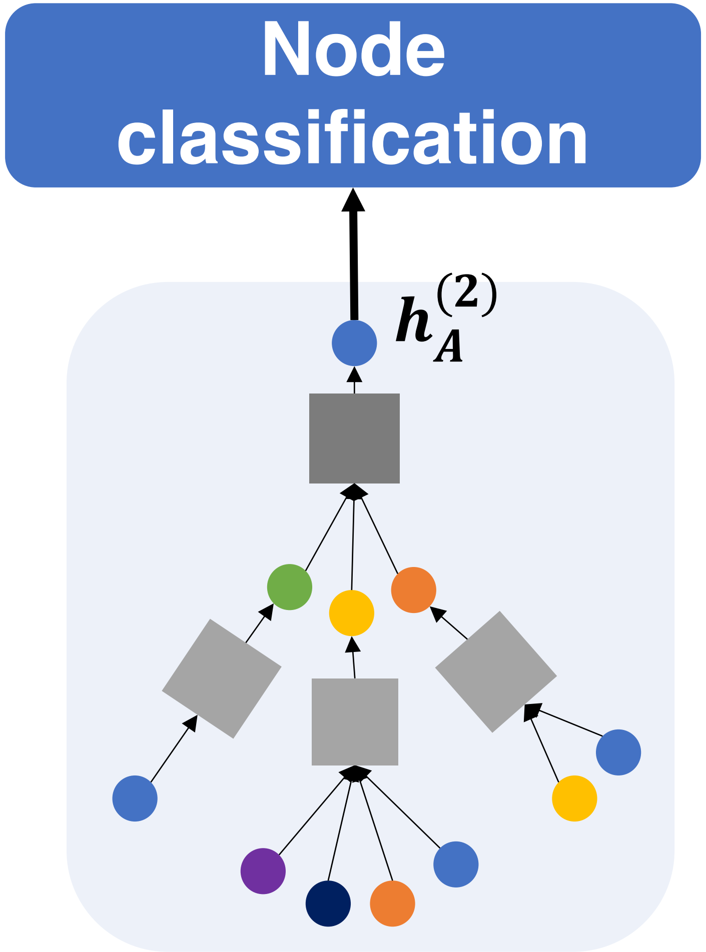
- **Node-level prediction**
- Edge-level prediction
- Attribute-level prediction
- **Graph-level prediction**

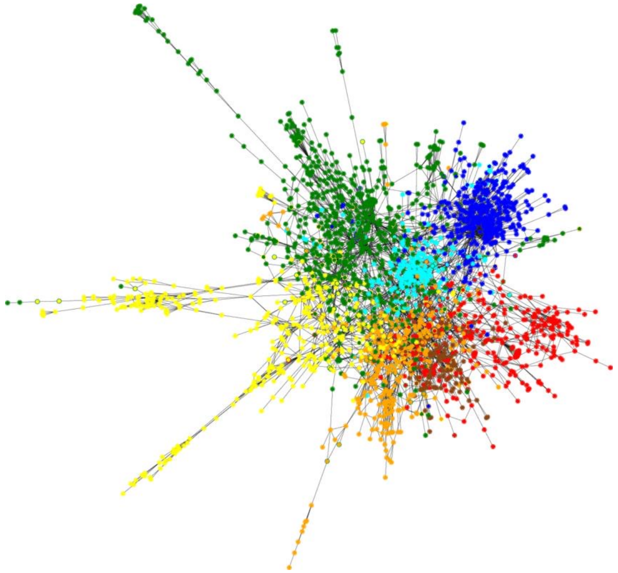


Node-level prediction tasks



Node-level prediction tasks





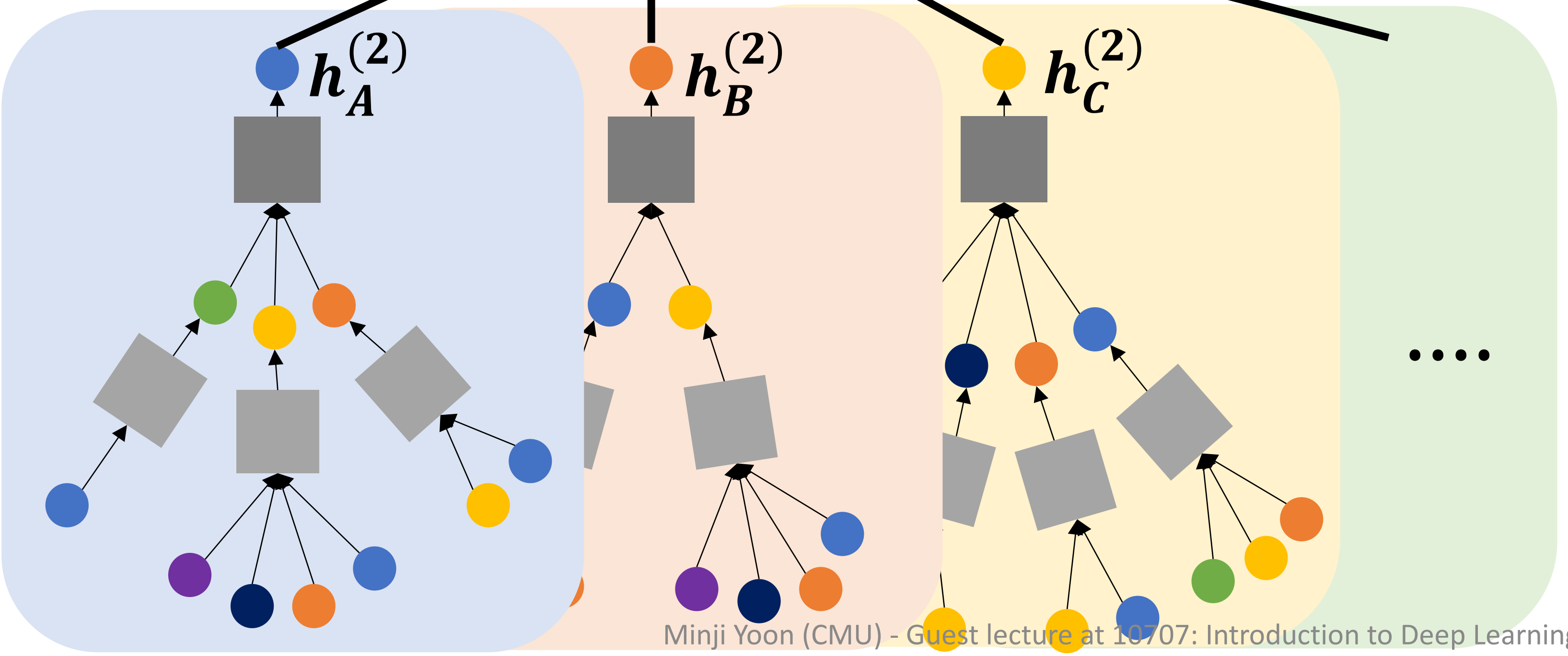
- Classify **papers** into topics on **citation networks**
- Cluster **posts** into subgroups on **Reddit networks**
- Classify **products** into categories on **Amazon co-purchase graphs**

Graph-level prediction tasks

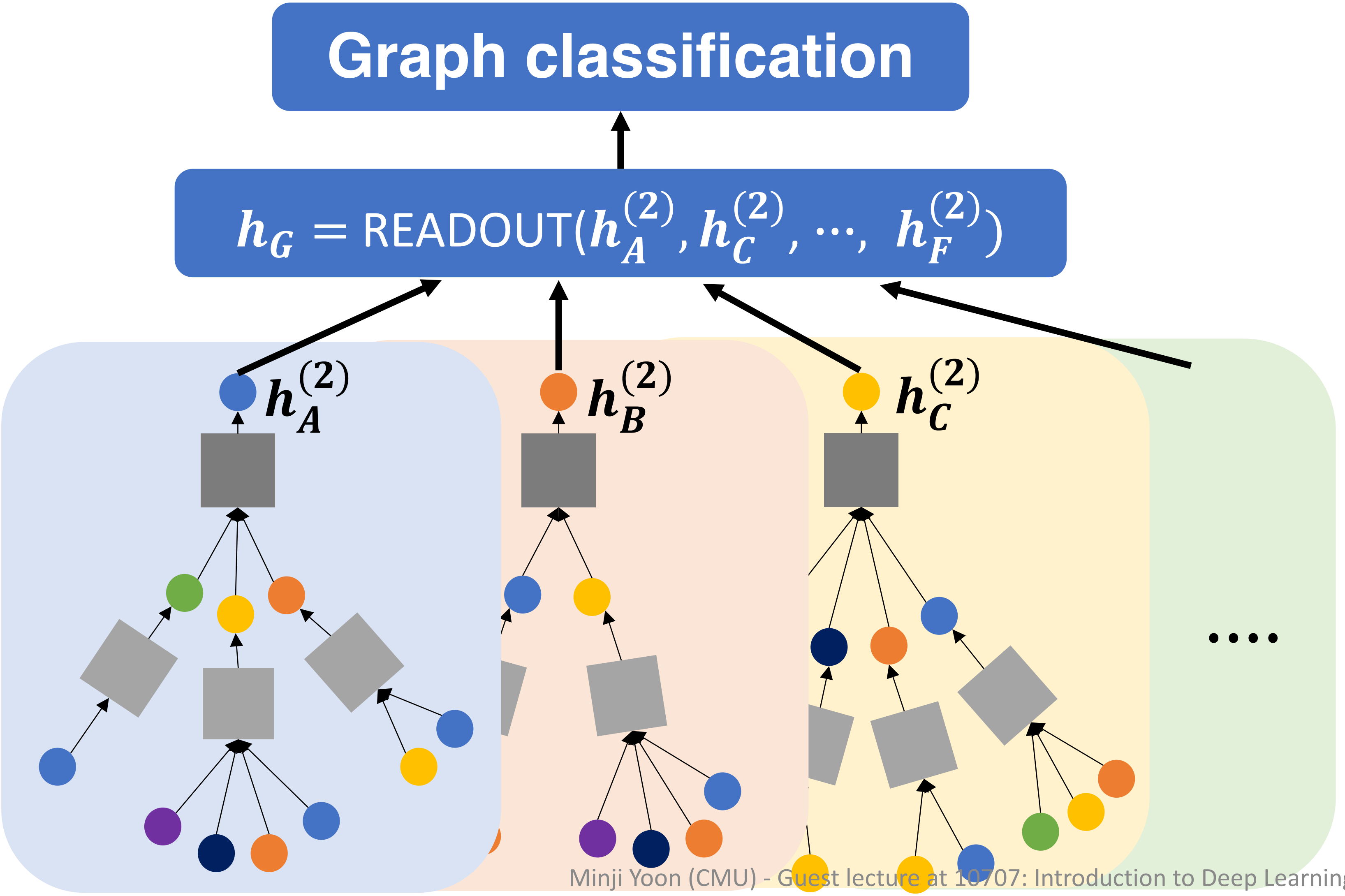
Graph classification

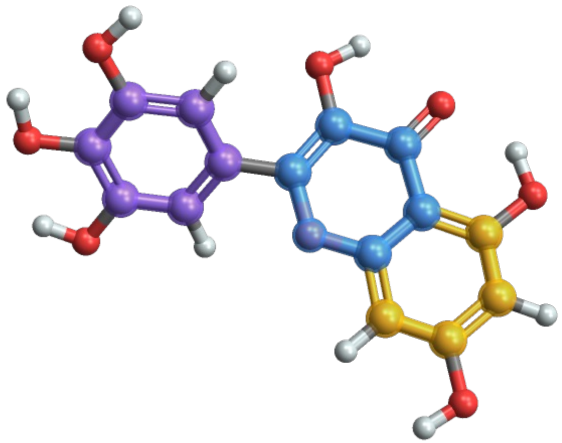
$$h_G = \text{READOUT}(h_A^{(2)}, h_C^{(2)}, \cdots, h_F^{(2)})$$

(ex) sum, average, min/max pooling of node embeddings



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..

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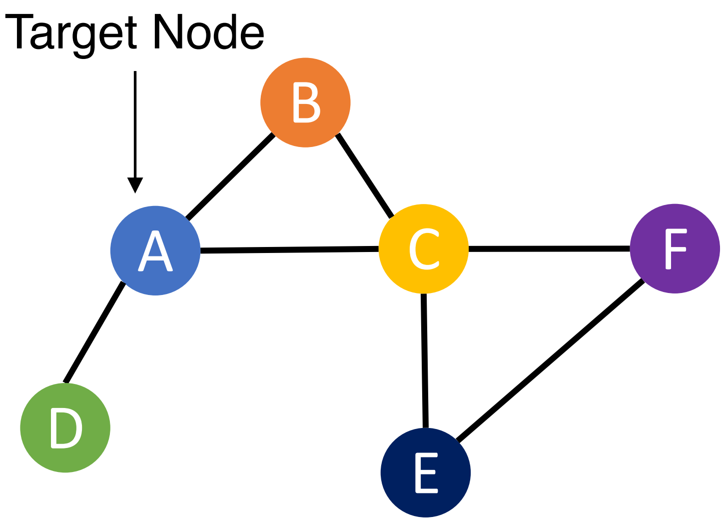
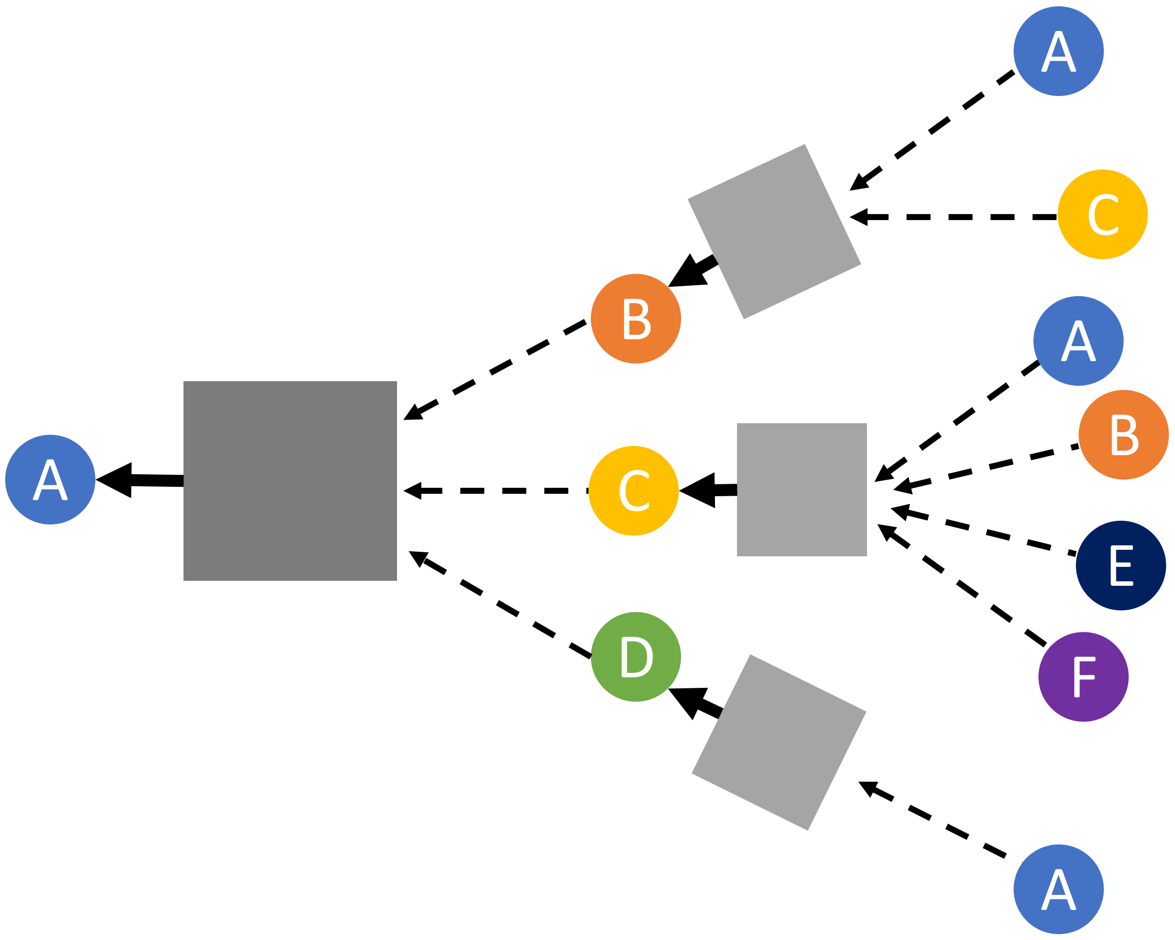
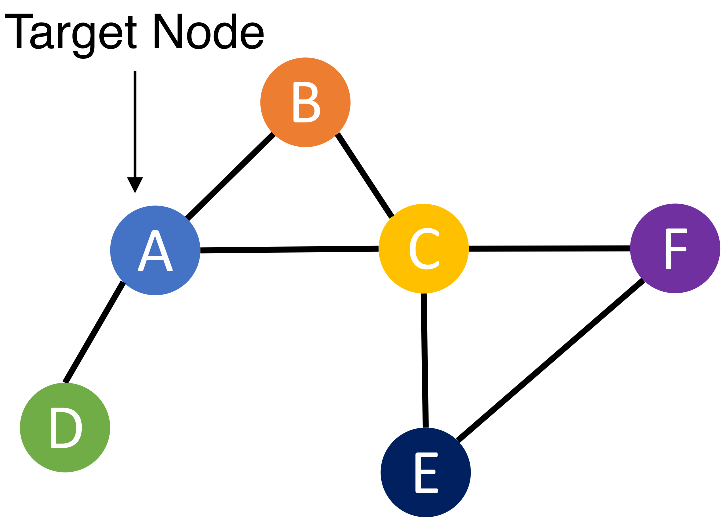
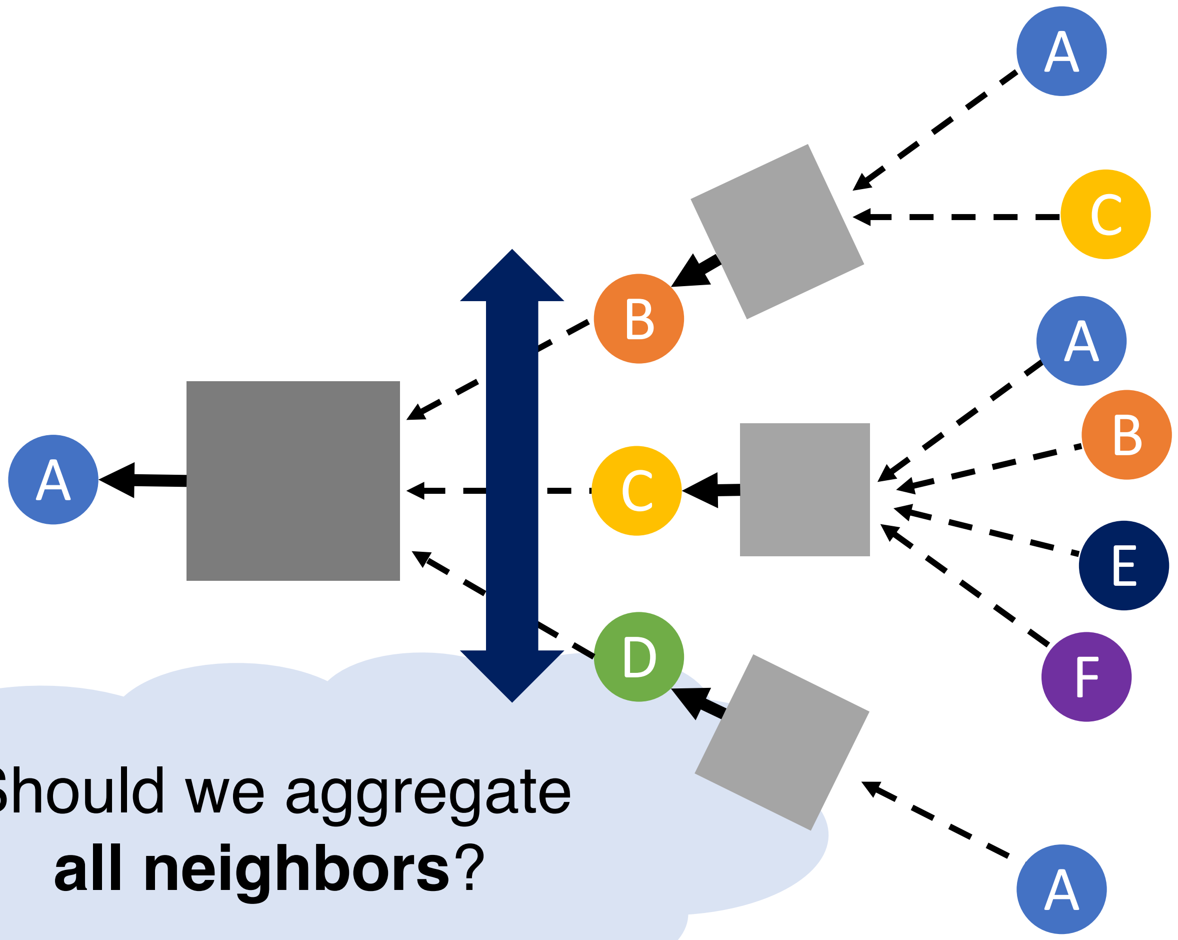
Graph Neural Networks





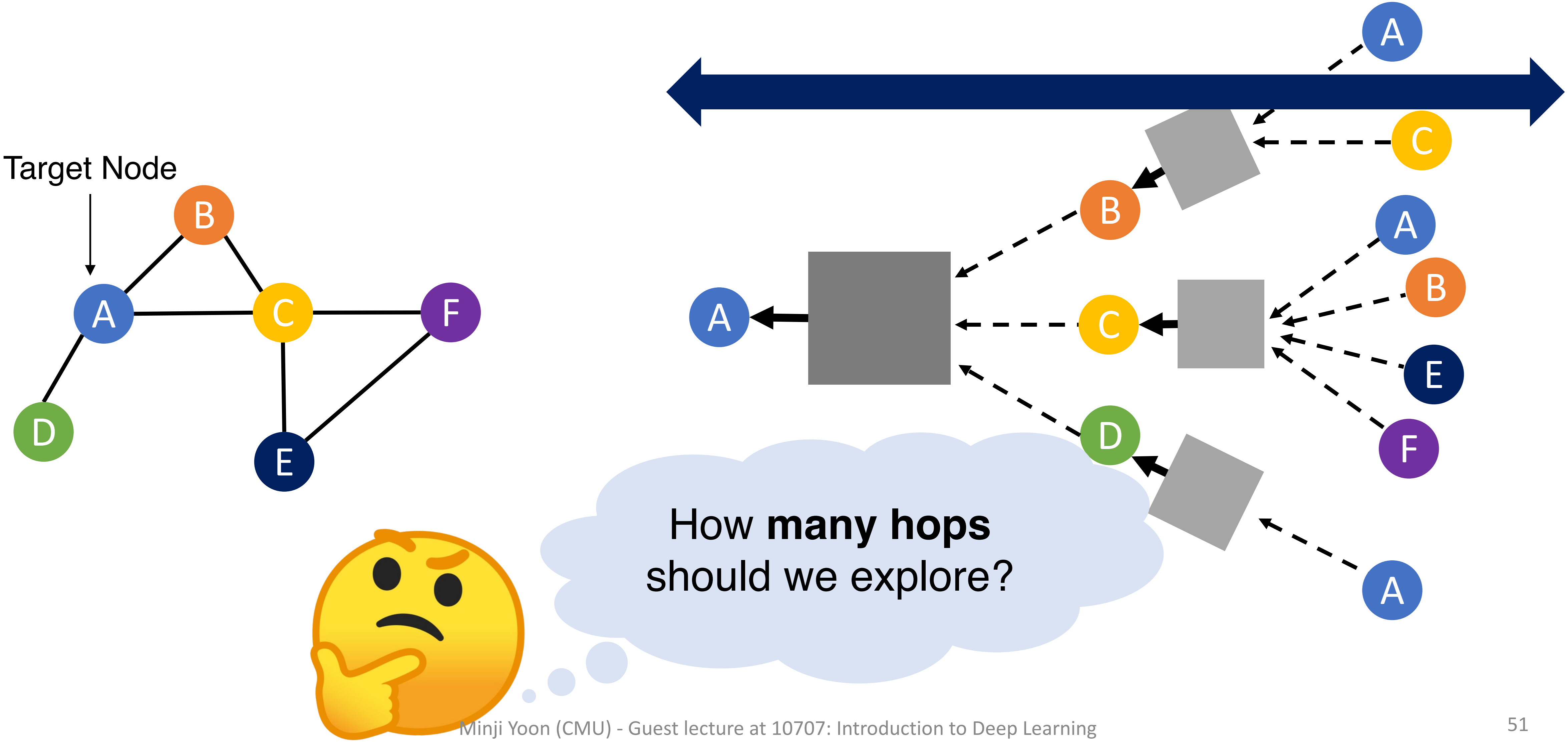
Graph Neural Networks - Width



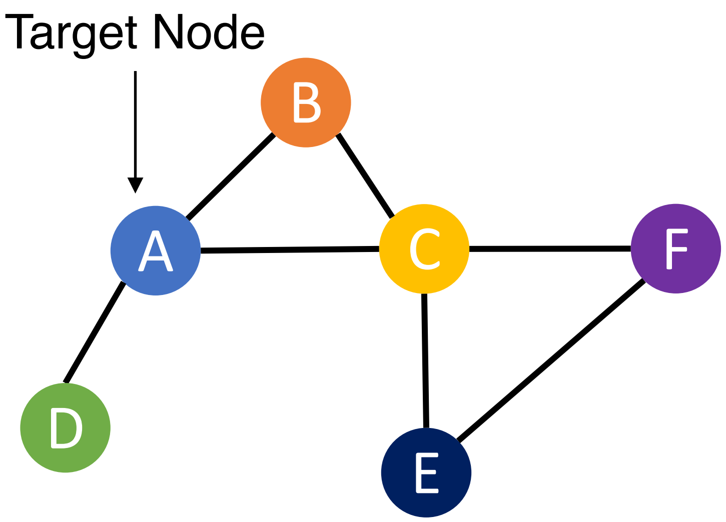


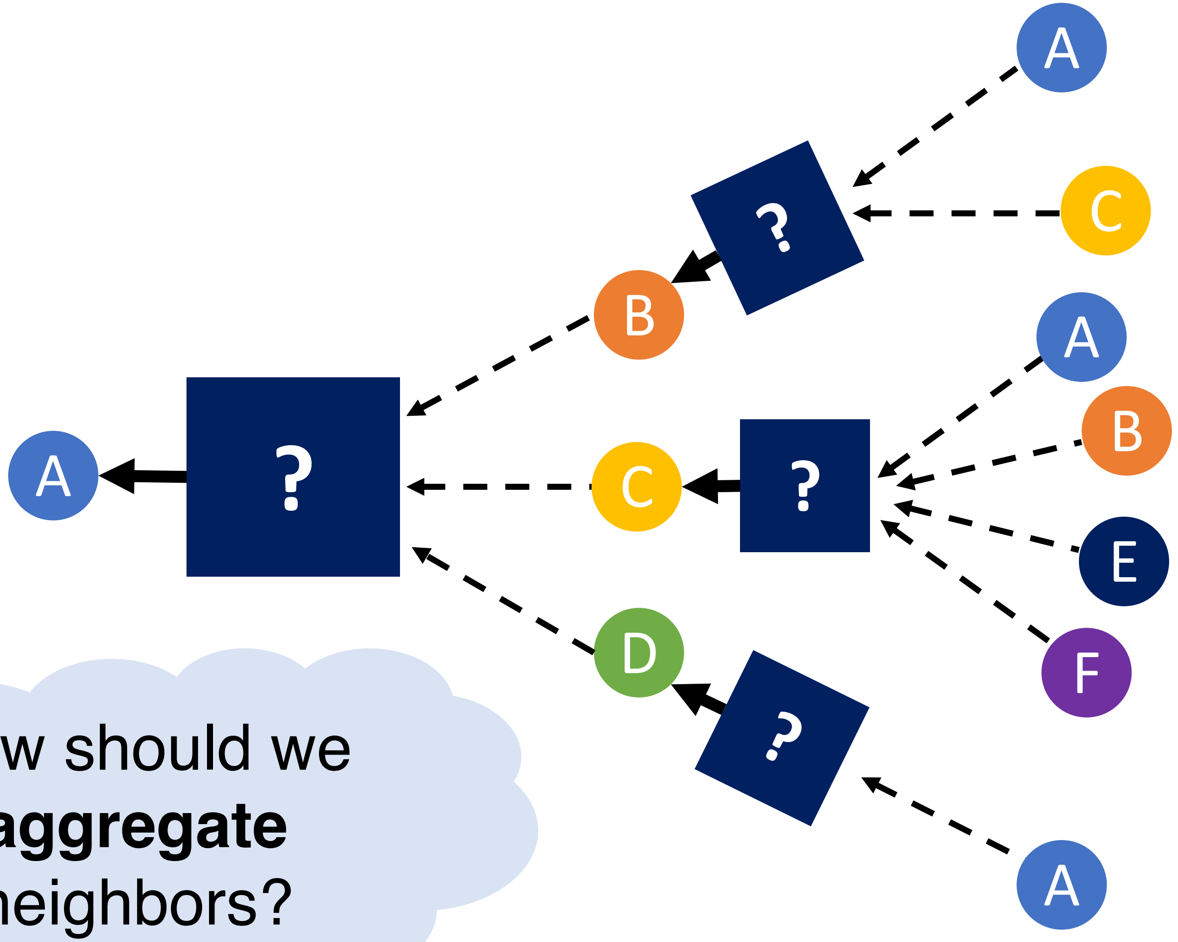
Should we aggregate **all neighbors**?

Graph Neural Networks - Depth



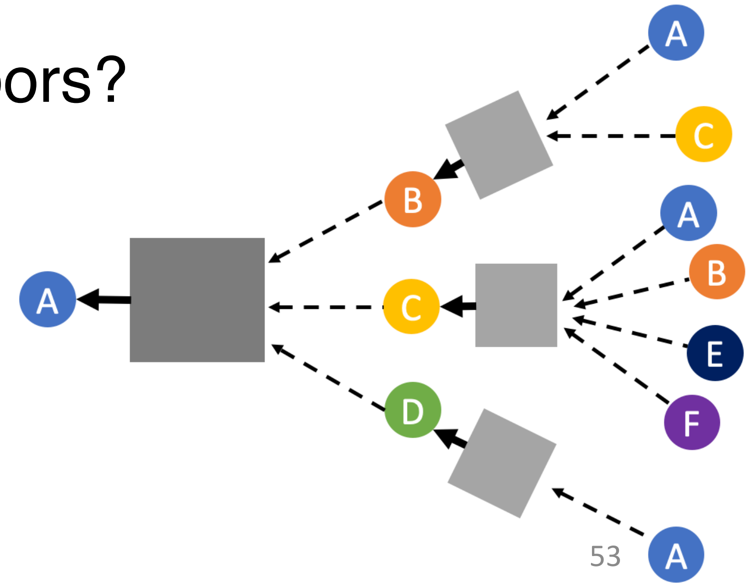
Graph Neural Networks - Aggregation





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?
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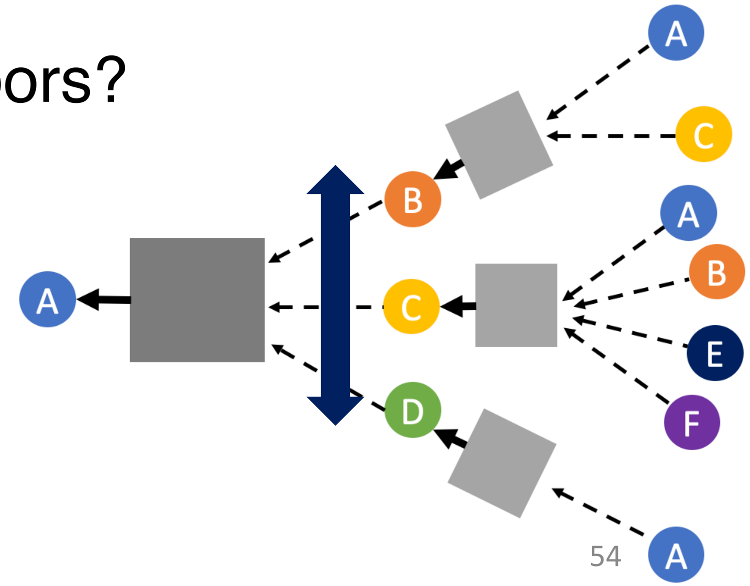
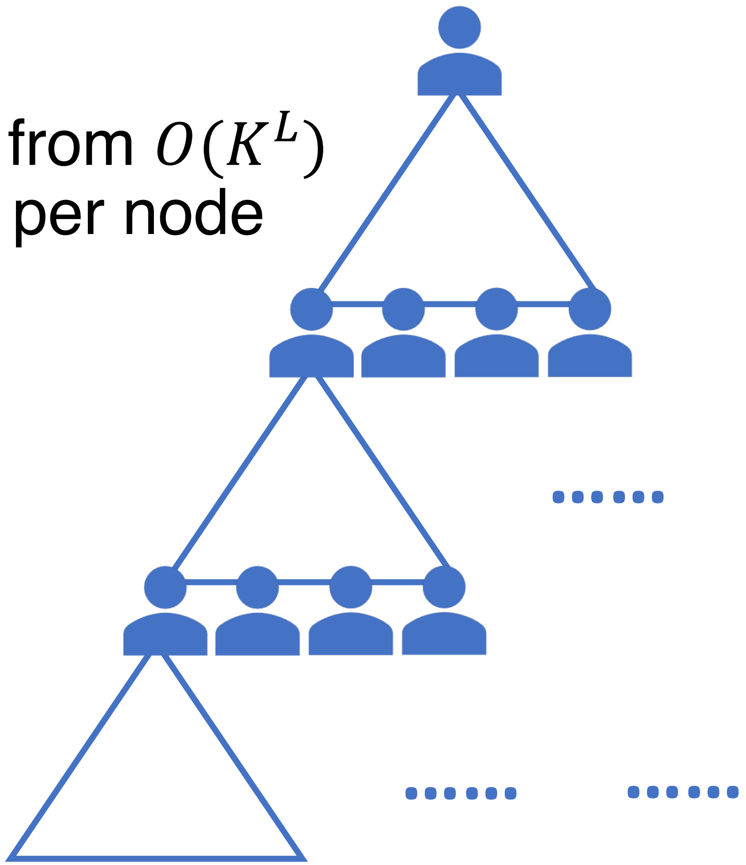


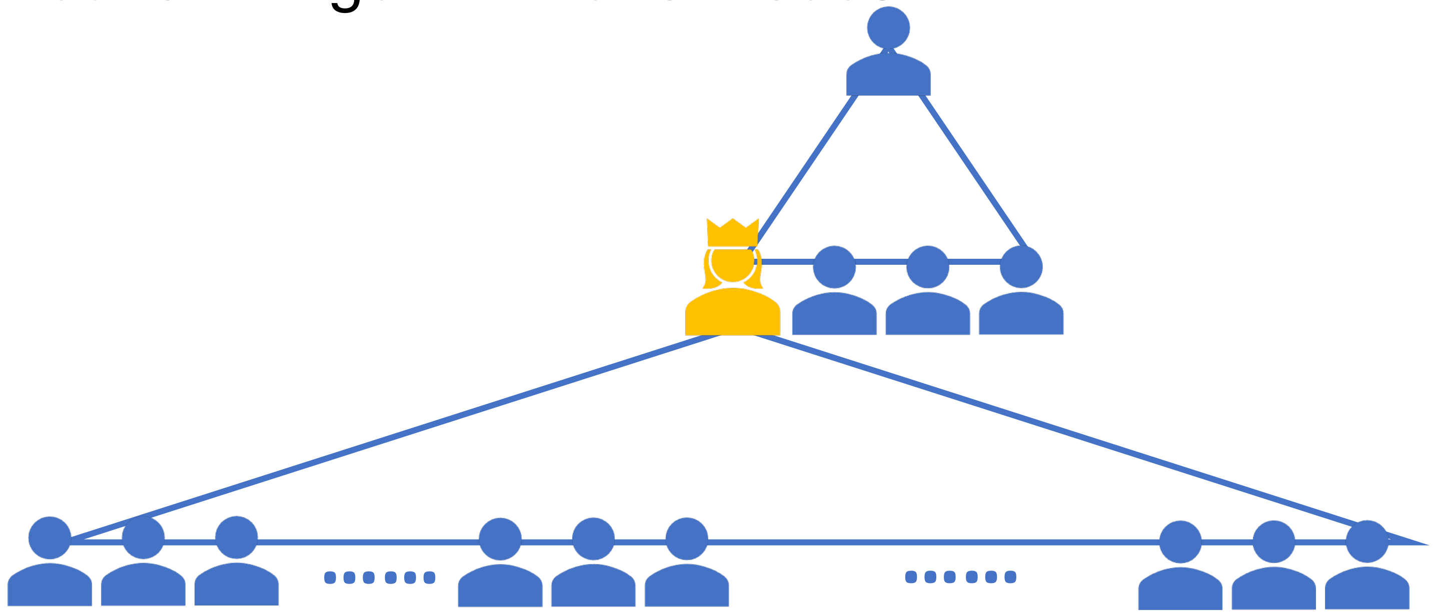
Aggregation Width in GNNs

- 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



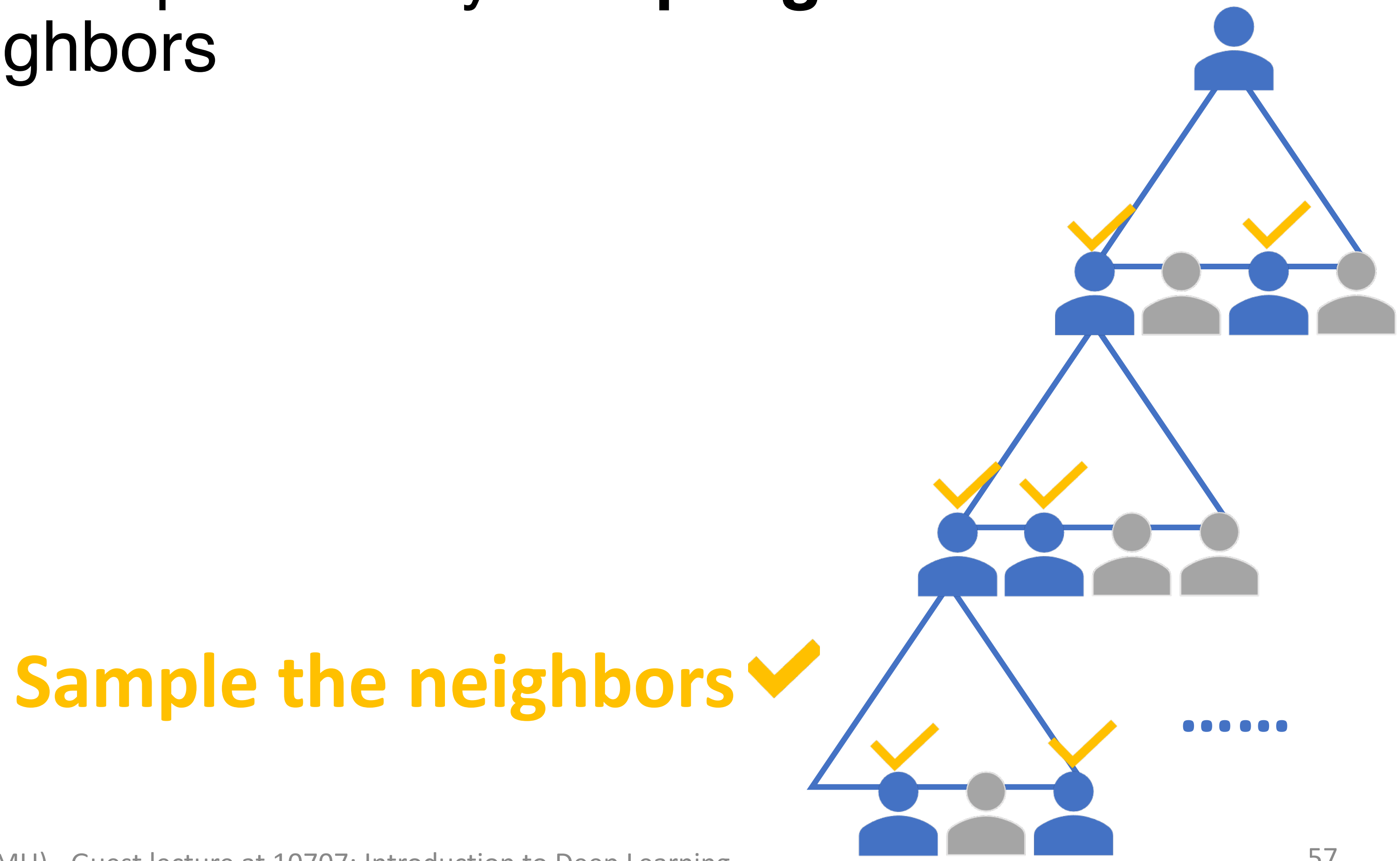
Aggregation Width in GNNs

- 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*[4]
- Importance sampling
  - Assign **different** sampling probabilities to all neighbors
  - *FastGCN*[5], *LADIES*[6], *AS-GCN*[7], *GCN-BS*[8], *PASS*[9]

[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*[5], *LADIES*[6], *AS-GCN*[7], *GCN-BS*[8]
- **Maximize GNN performance**
  - *PASS*[9]

[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”
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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	**0.821**	**0.715**	**0.858**	**0.757**	**0.855**	**0.884**	**0.934**

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

Aggregation Width in GNNs

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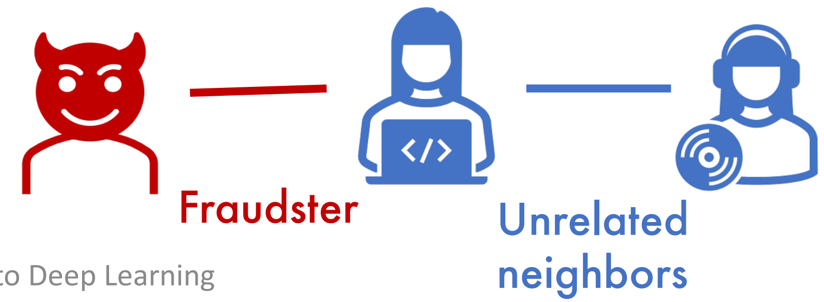
Real-world graphs are noisy!!



Graph Neural Network Architectures

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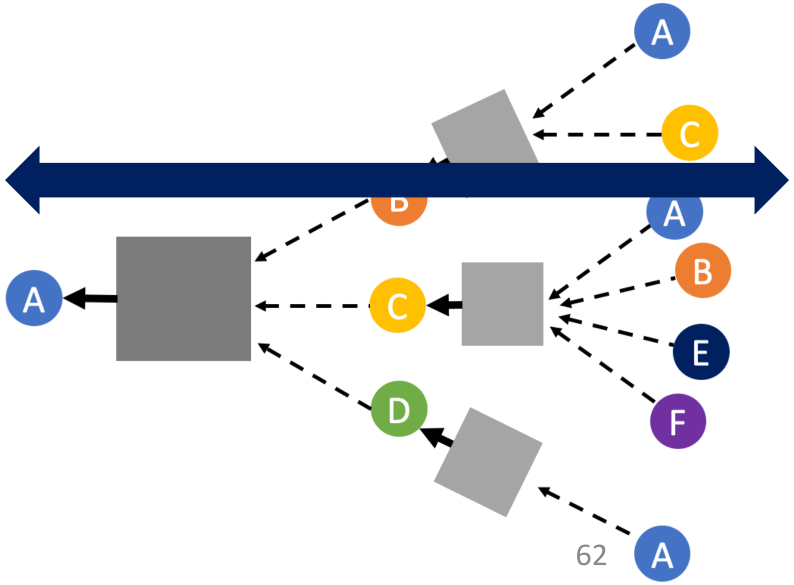
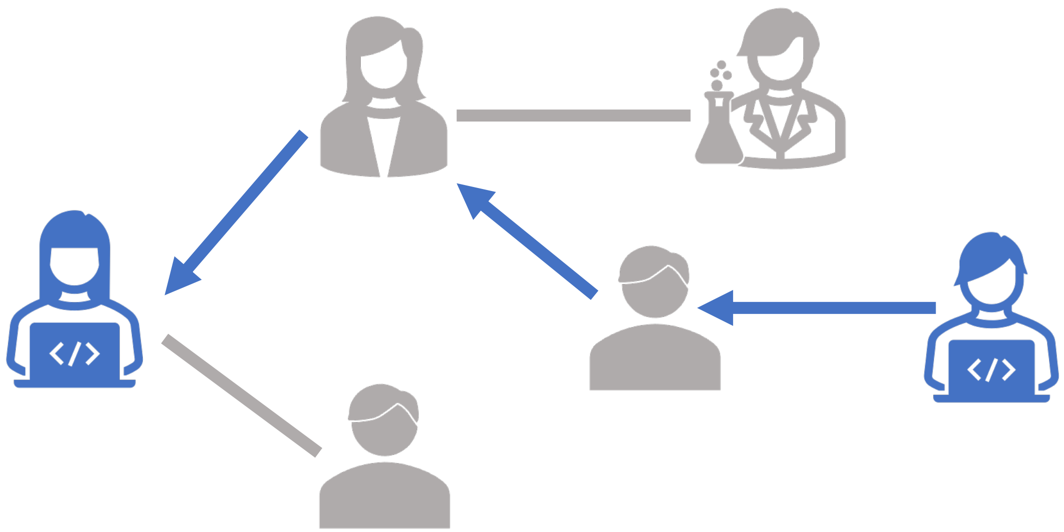


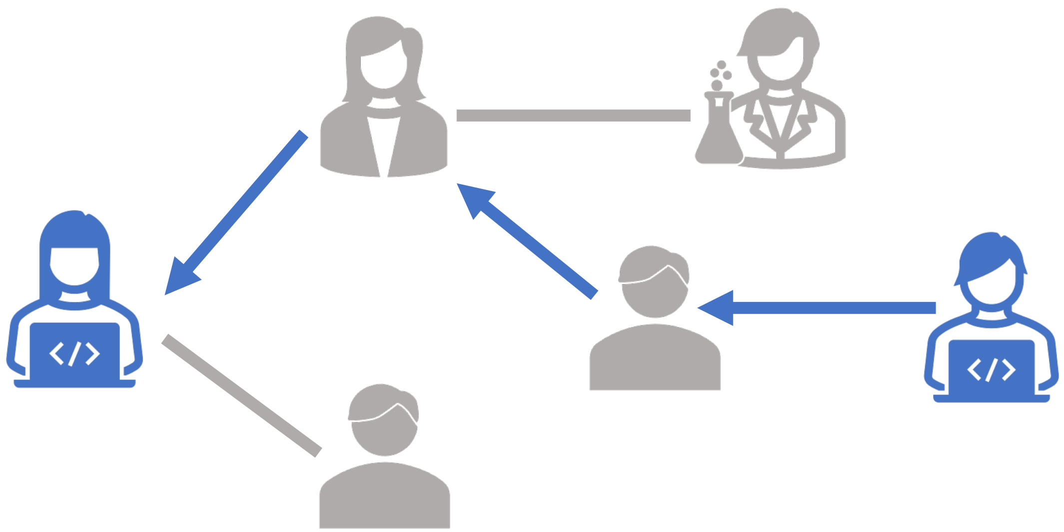
Aggregation Depth in GNNs

- 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?



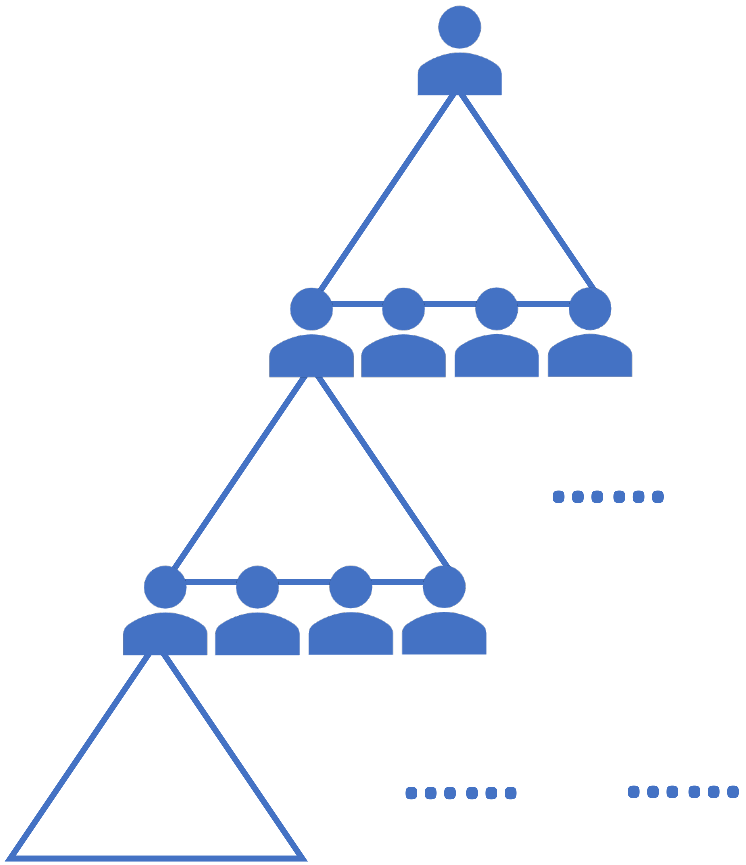
Aggregation Depth in GNNs

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

Wasn’t it Deeeep Learning?

Aggregation Depth in GNNs

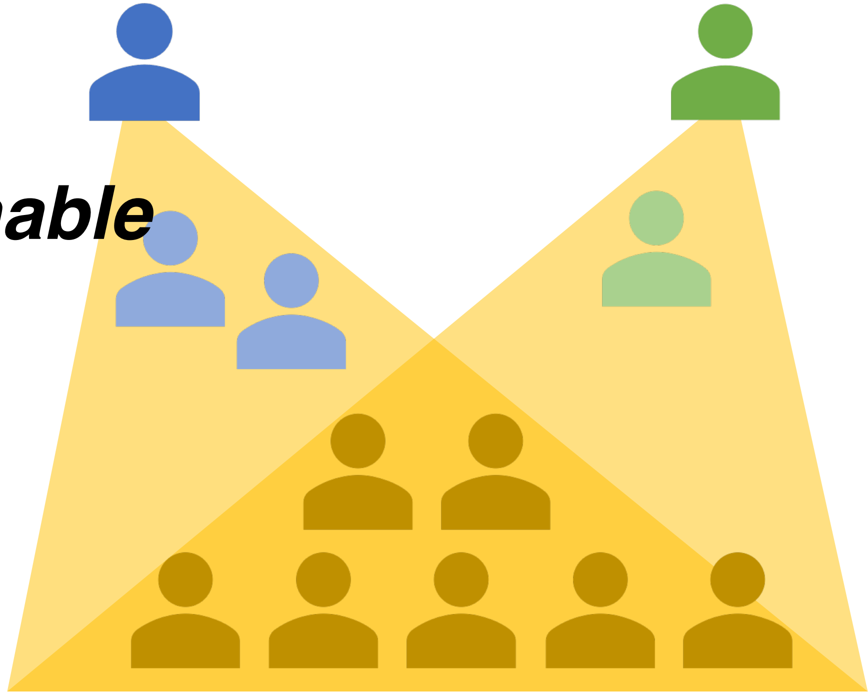
- When we increase the depth L more than this, GNNs face neighbor explosion $O(K^L)$
  - **Over-smoothing**
  - **Over-squashing**



Aggregation Depth in GNNs

Over-smoothing[10]

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

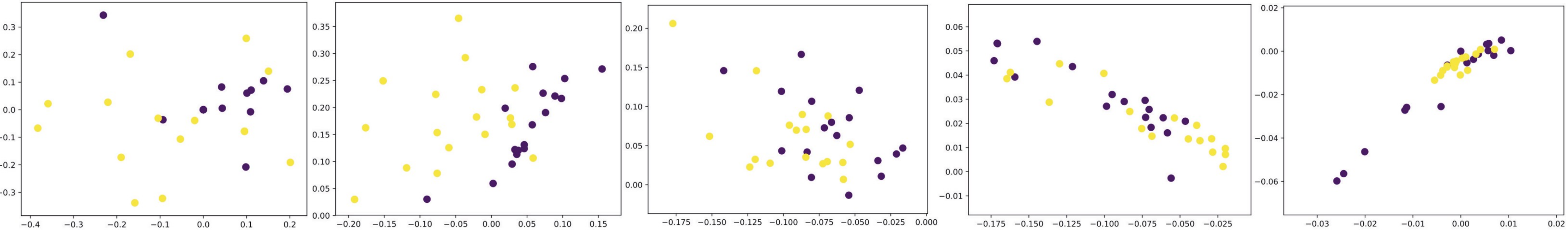


[10] Qimai Li, et al. "Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning"

Aggregation Depth in GNNs

Over-smoothing[10]

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



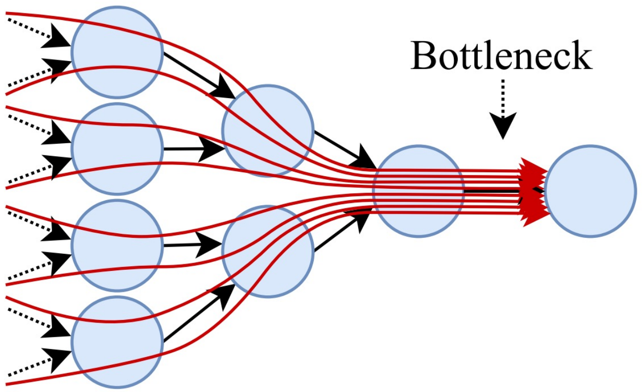
(a) 1-layer (b) 2-layer (c) 3-layer (d) 4-layer (e) 5-layer

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

Aggregation Depth in GNNs

Over-squashing[12]

- 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"

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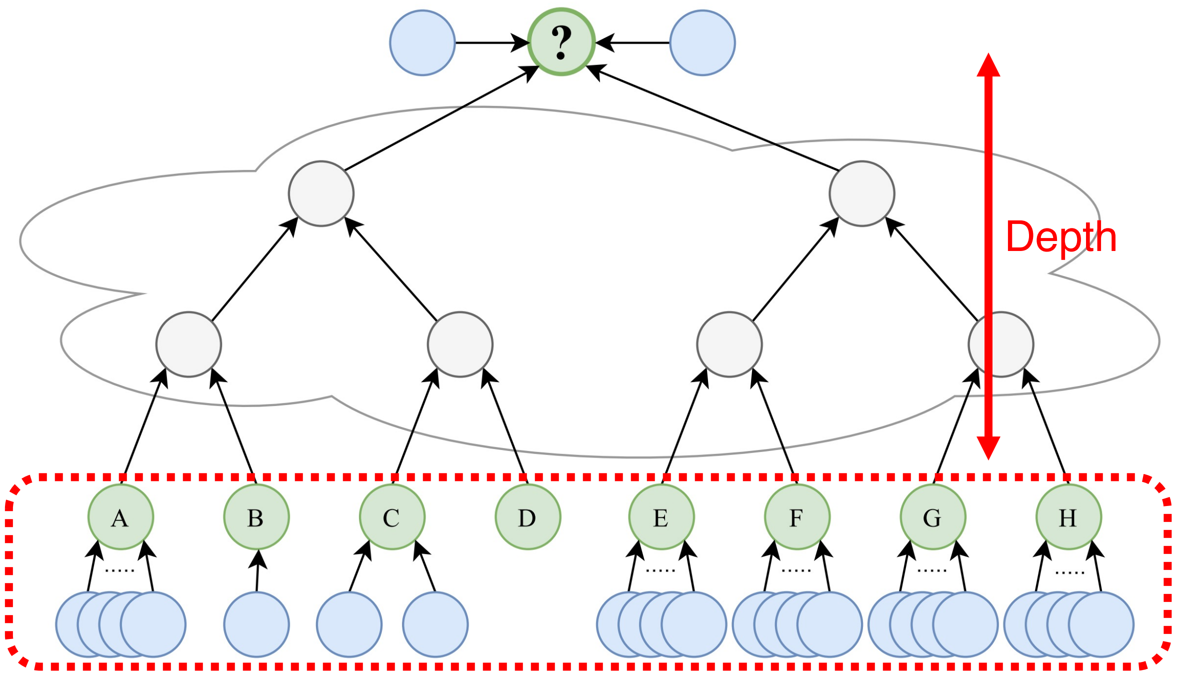

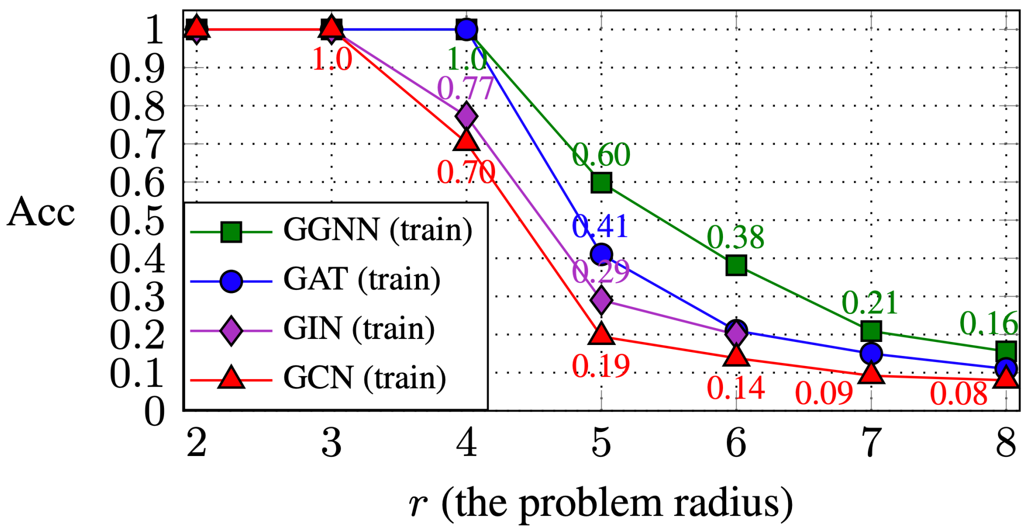

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Aggregation Depth in GNNs

Decoupling the two concepts of depths in GNNs[13]

- **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

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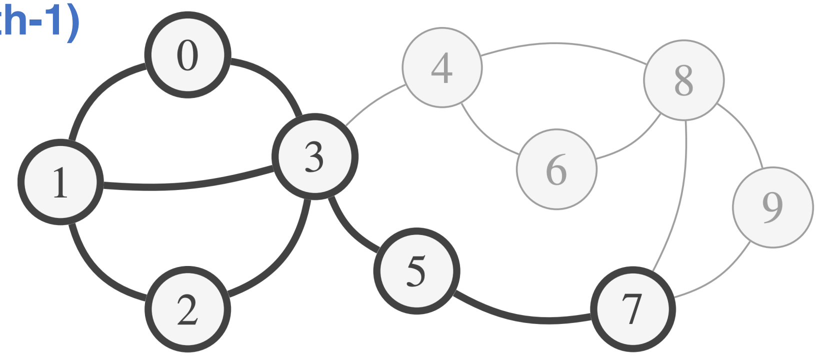
Depth of neighborhood
(Depth-1)



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

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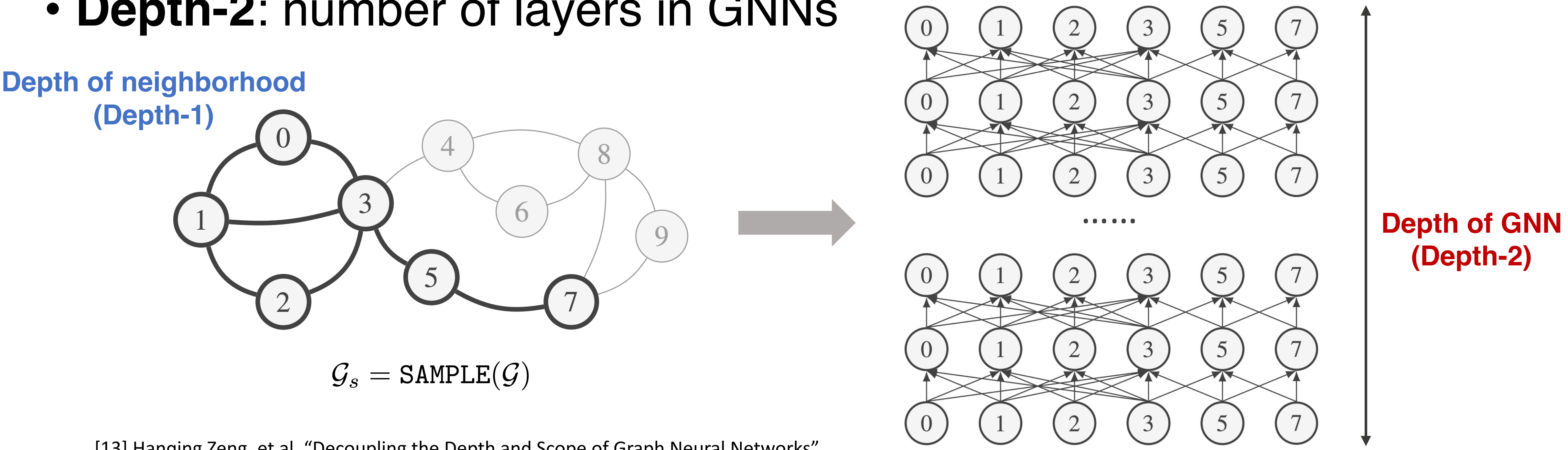

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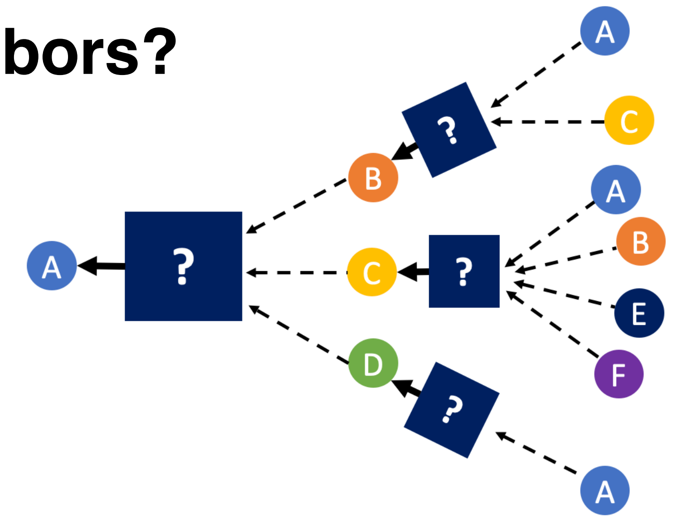


Aggregation strategy in GNNs

In each layer l :

Aggregate over neighbors

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

Transform messages

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

Aggregation strategy in GNNs

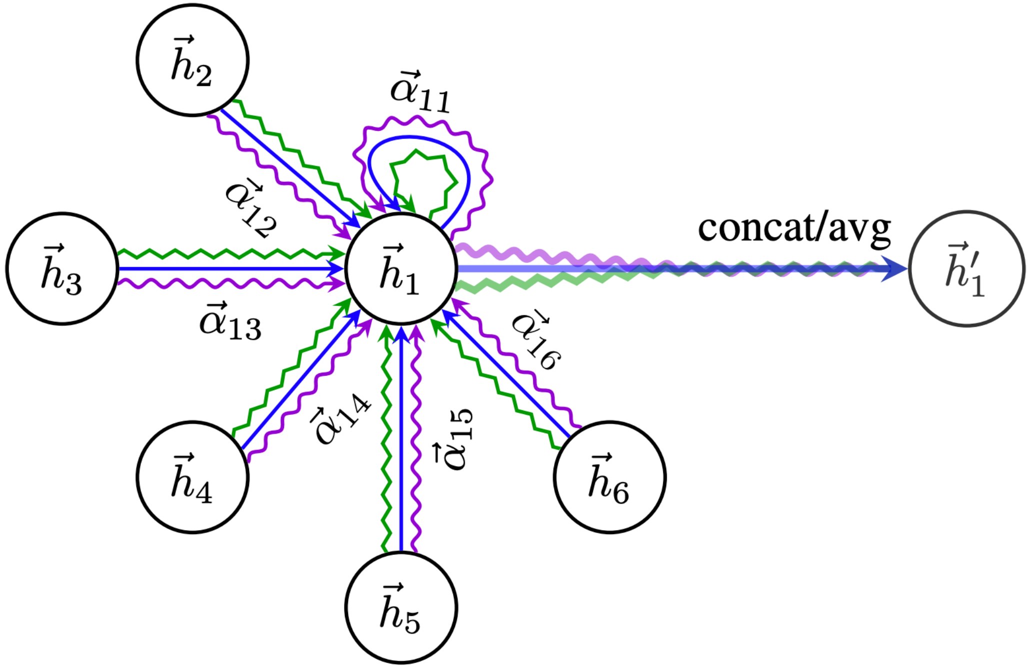
- GCN[1]
  - Average embeddings of neighboring nodes

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

Aggregation strategy in GNNs

- GAT[14]
  - 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."

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Core part of GNNs

Transform messages

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

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?[2]
- 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?”

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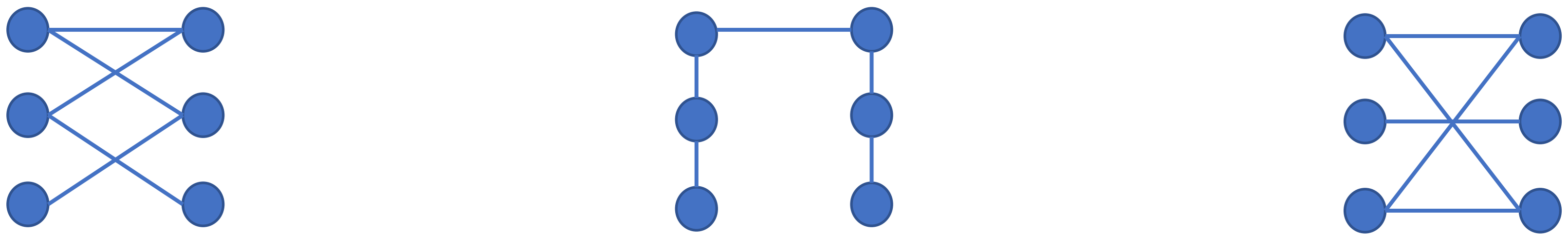

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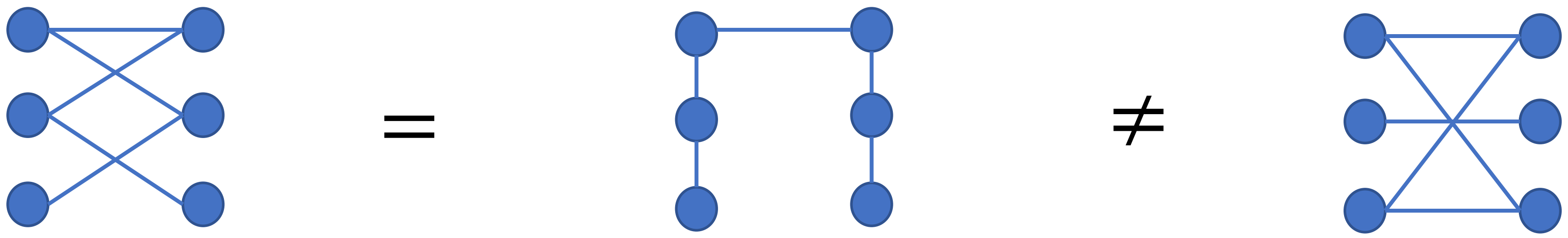

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Aggregation strategy in GNNs

- How powerful are Graph Neural Networks?[2]
  - Any aggregation-based GNN is at most as powerful as the **WL test**[15]
  - 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?[2]
  - Any aggregation-based GNN is at most as powerful as the **WL test**[15]
  - 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

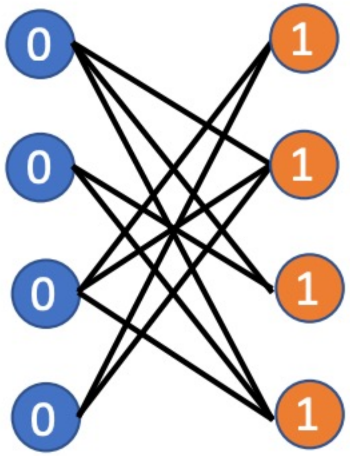
- Can we make more powerful GNNs?
    - Very active area, with many open problems

Aggregation strategy in GNNs

- 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**?[21,22]
  - 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?"

Aggregation strategy in GNNs

Improved accuracy after filtering datasets

- Heterophilous graph datasets have serious drawbacks[23]

	squirrel		
	accuracy on original dataset	accuracy on filtered dataset	ranks
ResNet	33.88 ± 1.79	36.55 ± 1.82	12 / 7
ResNet+SGC	34.36 ± 1.21	38.36 ± 1.97	11 / 5
ResNet+adj	65.46 ± 1.58	38.37 ± 1.99	2 / 4
GCN	39.06 ± 1.52	39.47 ± 1.47	6 / 2
SAGE	35.83 ± 1.32	36.09 ± 1.99	9 / 9
GAT	32.21 ± 1.63	35.62 ± 2.06	14 / 11
GAT-sep	35.72 ± 1.98	35.46 ± 3.10	10 / 13
GT	31.61 ± 1.10	36.30 ± 1.98	15 / 8
GT-sep	36.08 ± 1.58	36.66 ± 1.63	8 / 6
H_2GCN	29.45 ± 1.65	35.10 ± 1.15	17 / 15
CPGNN	30.91 ± 1.98	30.04 ± 2.03	16 / 16
GPR-GNN	33.39 ± 2.05	38.95 ± 1.99	13 / 3
FSGNN	68.93 ± 1.69	35.92 ± 1.32	1 / 10
GloGNN	61.21 ± 1.96	35.11 ± 1.24	3 / 14
FAGCN	47.63 ± 1.85	41.08 ± 2.27	4 / 1
GBK-GNN	37.06 ± 1.24	35.51 ± 1.65	7 / 12
JacobiConv	46.17 ± 4.34	29.71 ± 1.66	5 / 17

[23] Oleg Platonov., et al. "A critical look at the evaluation of GNNs under heterophily: are we really making progress?"

So far, we have talked about..

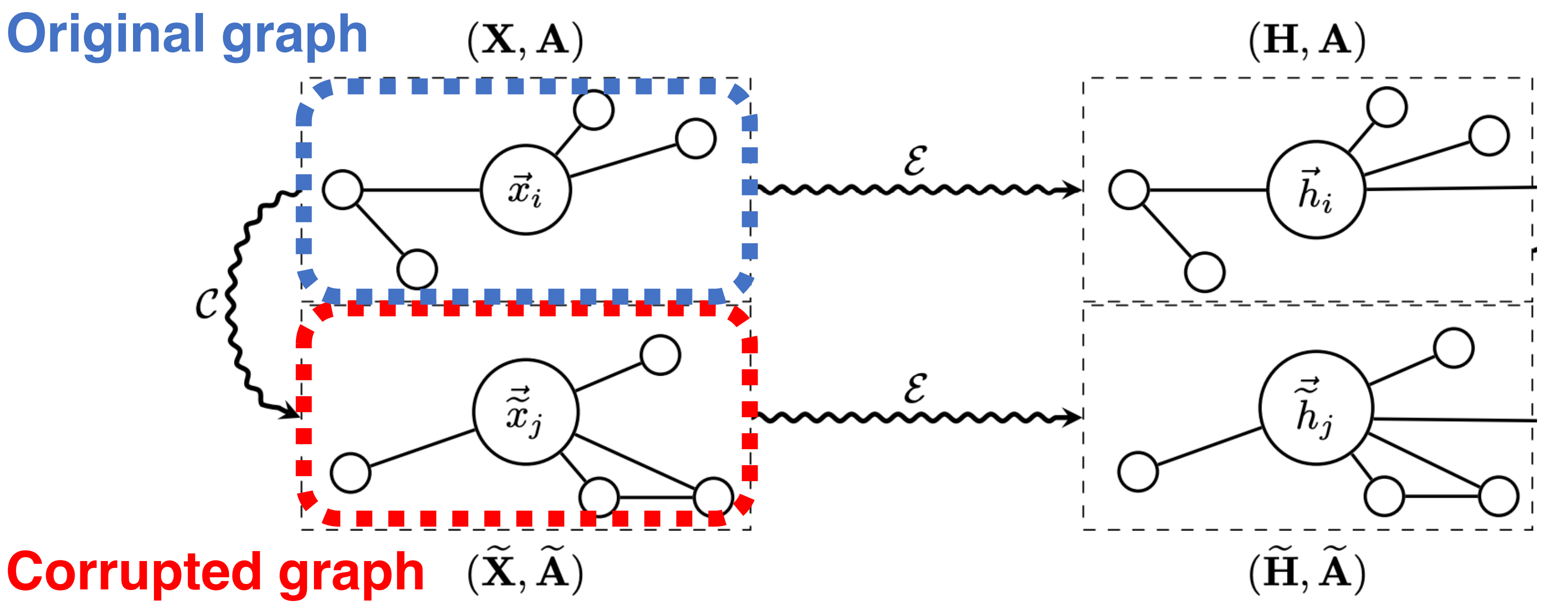
1. **Graph Neural Network**
   - Problem definition
   - Skeleton: aggregation, transformation operations
2. **Research questions in GNN architectures**
   - Width
   - Depth
   - Aggregation
3. **GNN training strategy**

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

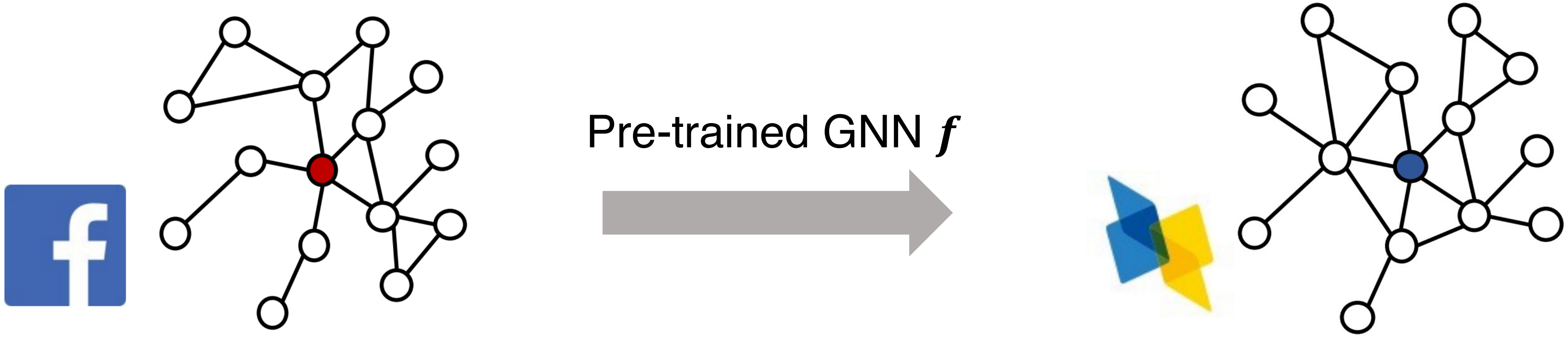
- Unsupervised learning[26]
  - Contrastive learning



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

How to train GNNs

- Transfer learning
  - Transfer a pre-trained GNN model between graphs[27]

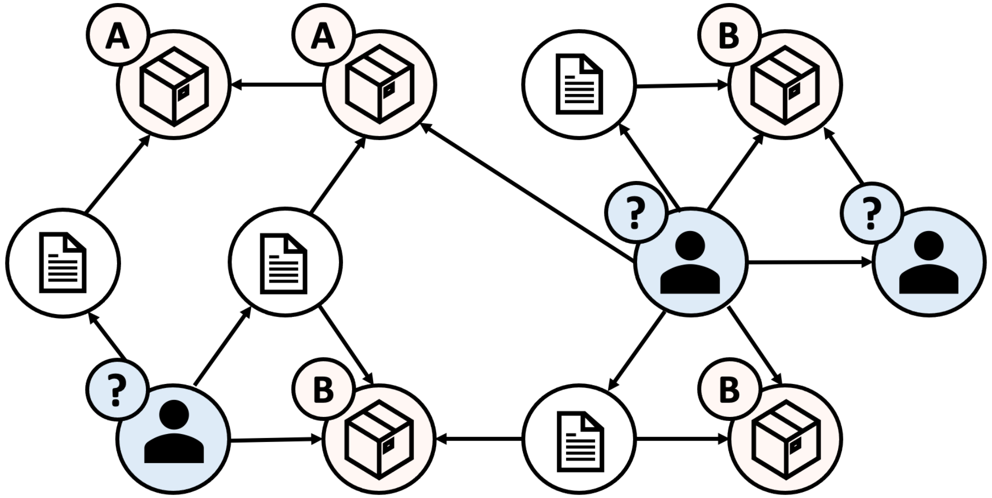


Facebook network **DBLP co-authorship network**

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

How to train GNNs

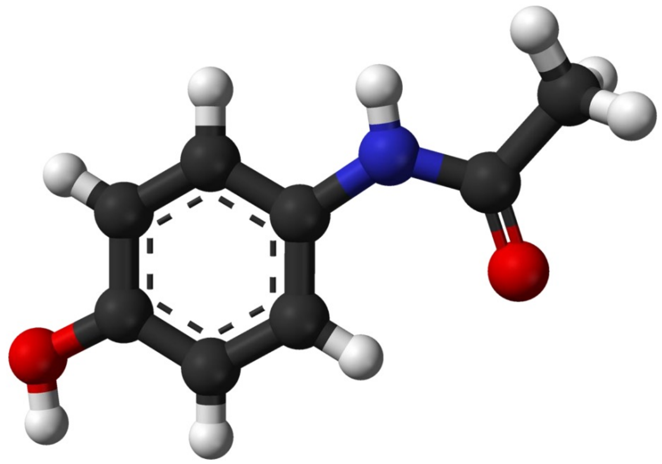
- Transfer learning
  - Transfer between different node types across a **heterogeneous graph**[28]

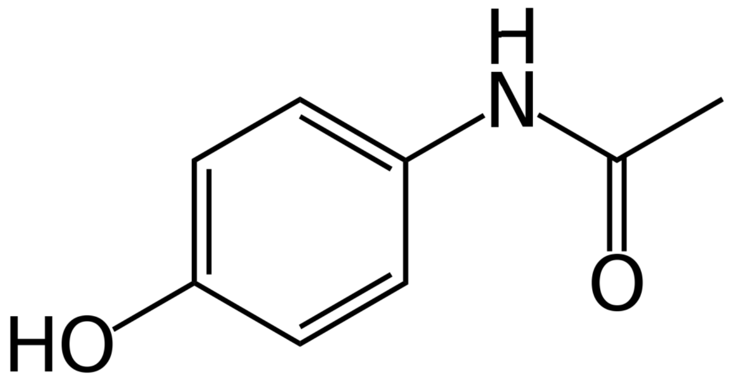


[28] Minji Yoon, et al. "Zero-shot Domain Adaptation of Heterogeneous Graphs via Knowledge Transfer Networks "

Impactful applications in science

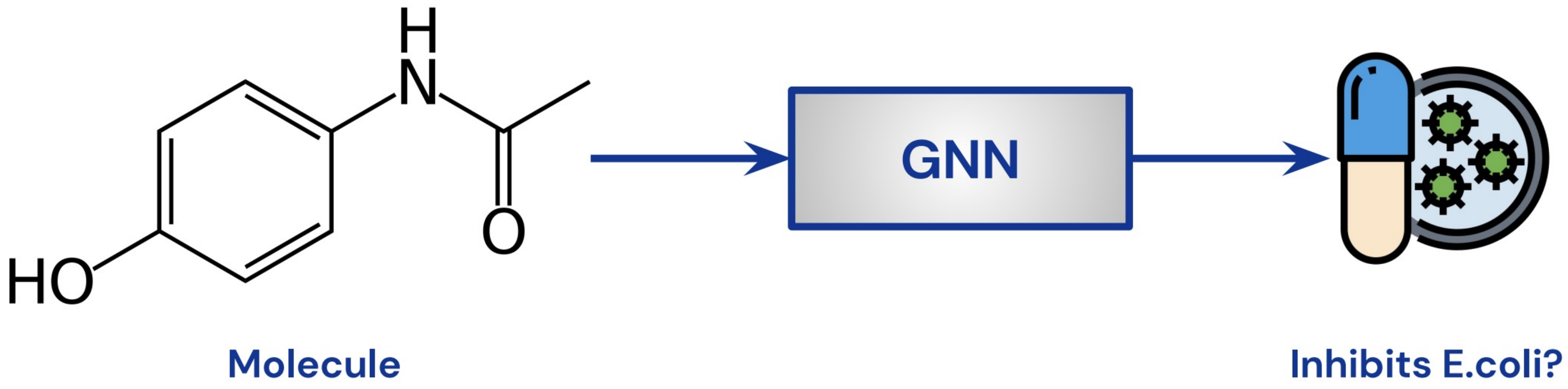
- GNNs for molecule classification
- Molecule
  - Node: atoms
  - Edge: bonds
  - Input features: atom type, charge, bond type





Impactful applications in science

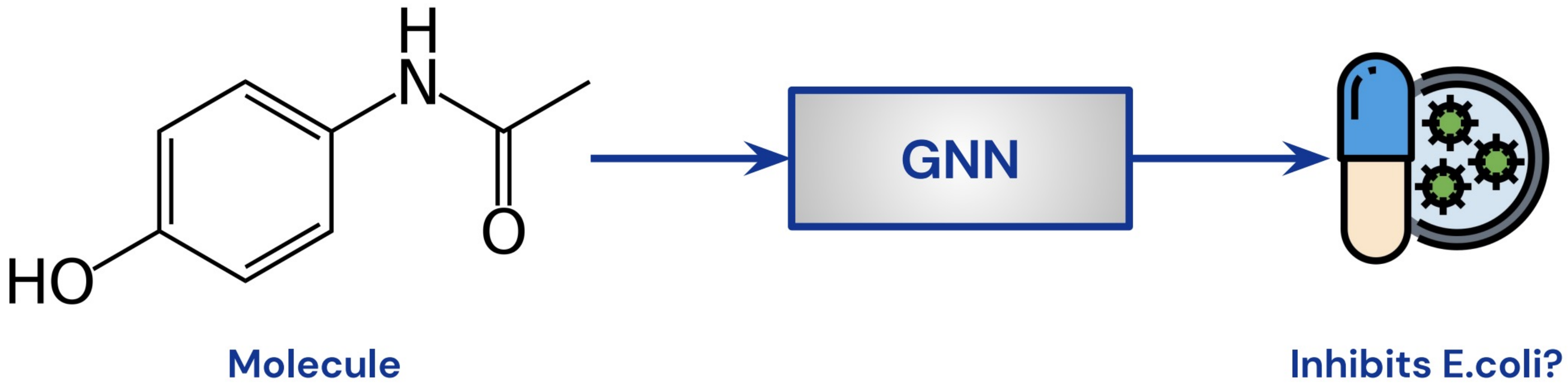
- Graph-level prediction: whether the molecule is a potent **drug**[29]
  - Binary classification on whether the drug will inhibit certain bacteria



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

Impactful applications in science

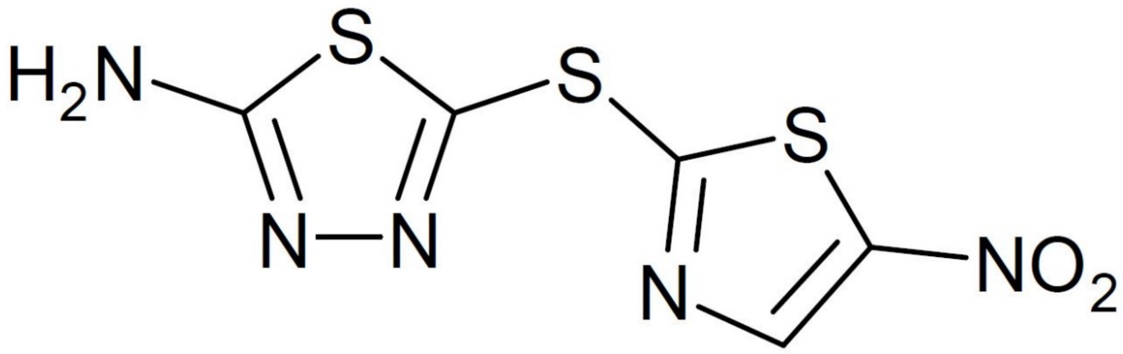
- Graph-level prediction: whether the molecule is a potent **drug**[29]
  - Execute on a large dataset of known candidate molecules
  - Select the ~ *top-100* candidates from the GNN model
  - Have chemists thoroughly investigate those



[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[29]



Halicin

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

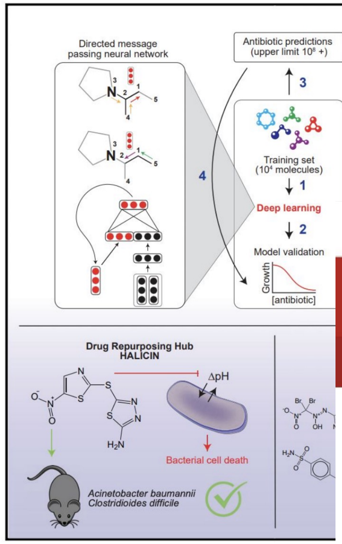
(slide: P. Veličković)

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.)

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

So far, we have talked about..

1. Graph Neural Network
2. Research questions in GNN architectures
3. GNN training strategy
4. Applications in science

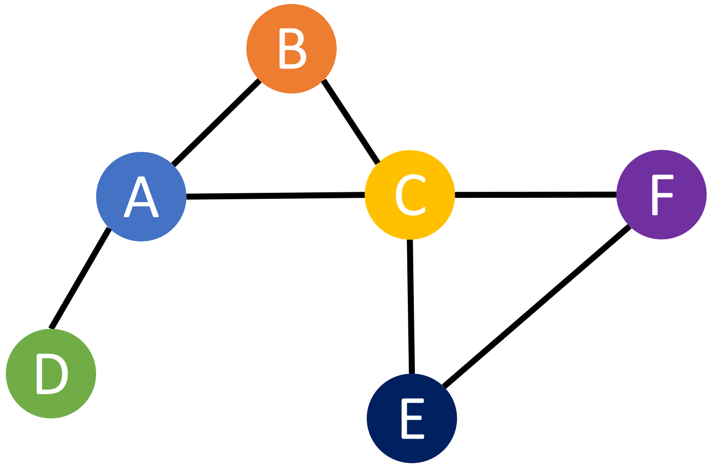
So far, we have talked about..

1. Graph Neural Network
2. Research questions in GNN architectures
3. GNN training strategy
4. Applications in science
5. **Recent Directions inspired by other disciplines**
   - **How to apply Transformers to graphs**
   - **How to utilize Large Language Models (LLMs) for graph tasks**

Advanced

Graph Transformer

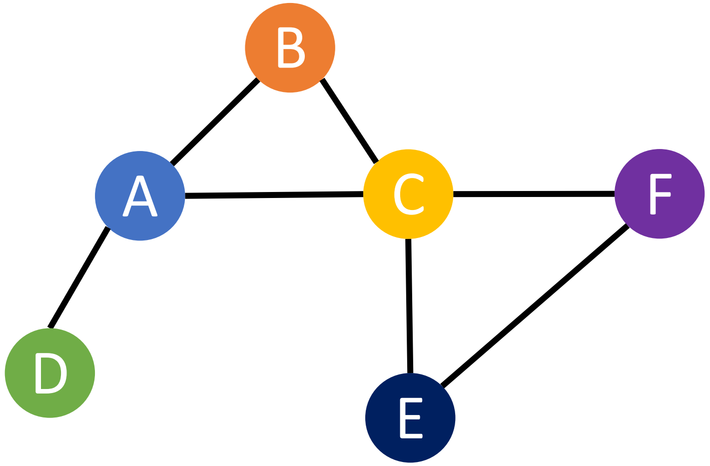
- Limitations of GNN
- Hard-coded structural inductive bias
  - Limited expressiveness (WL-test)
  - Oversmoothing
  - Oversquashing



Graph Transformer

- Aggregate from all nodes in a graph regardless of their connectivity

… Are we going to throw away the graph information?



Graph Transformer

- Graphormer[27]

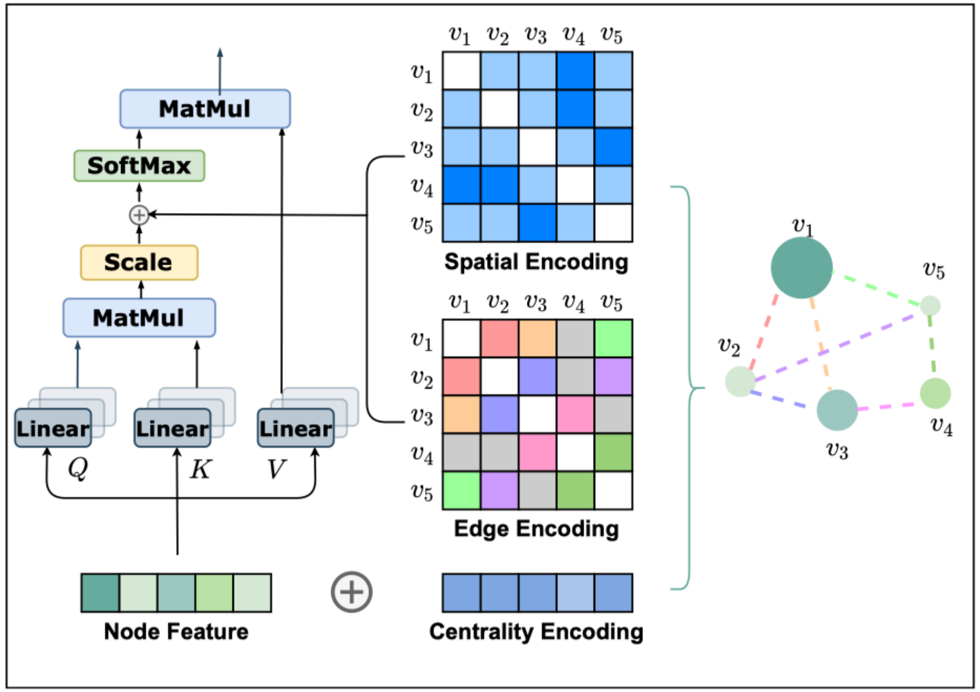
Degree information

$$h_i^{(0)} = x_i + \boxed{z^-_{\deg^-(v_i)} + z^+_{\deg^+(v_i)}}$$

$$A_{ij} = \frac{(h_i W_Q)(h_j W_K)^T}{\sqrt{d}} + \boxed{b_{\phi(v_i,v_j)} + c_{ij},} \text{ where } c_{ij} = \frac{1}{N}\sum_{n=1}^{N} x_{e_n}(w_n^E)^T$$

Spatial distance information

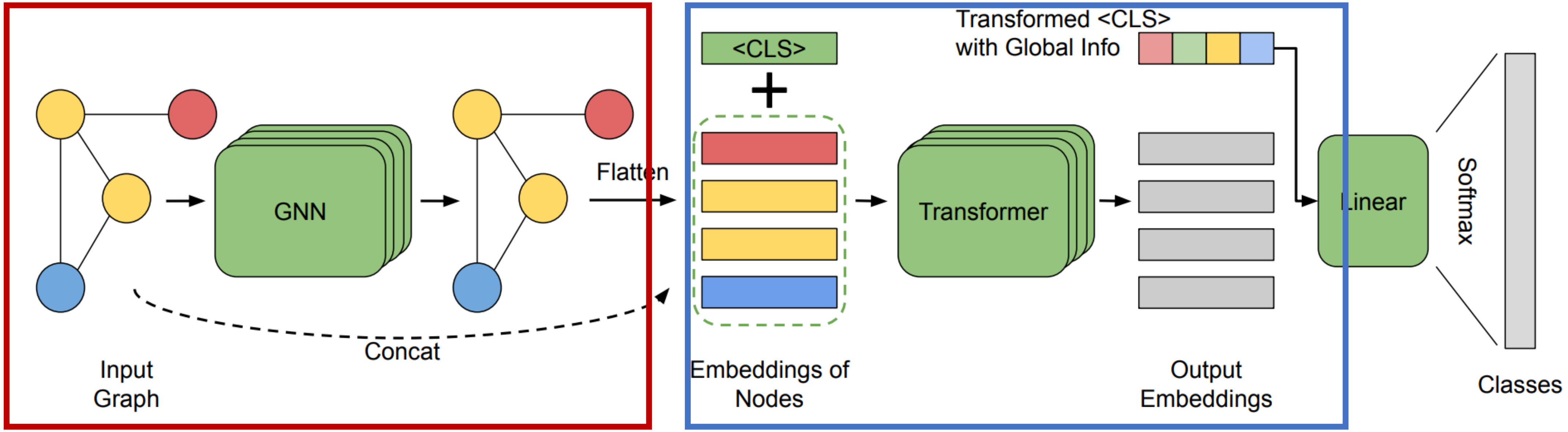
Edge attribute information



[27] Chengxuan Ying, et al. "Do Transformers Really Perform Bad for Graph Representation?"

Graph Transformer

- GraphTrans[28]



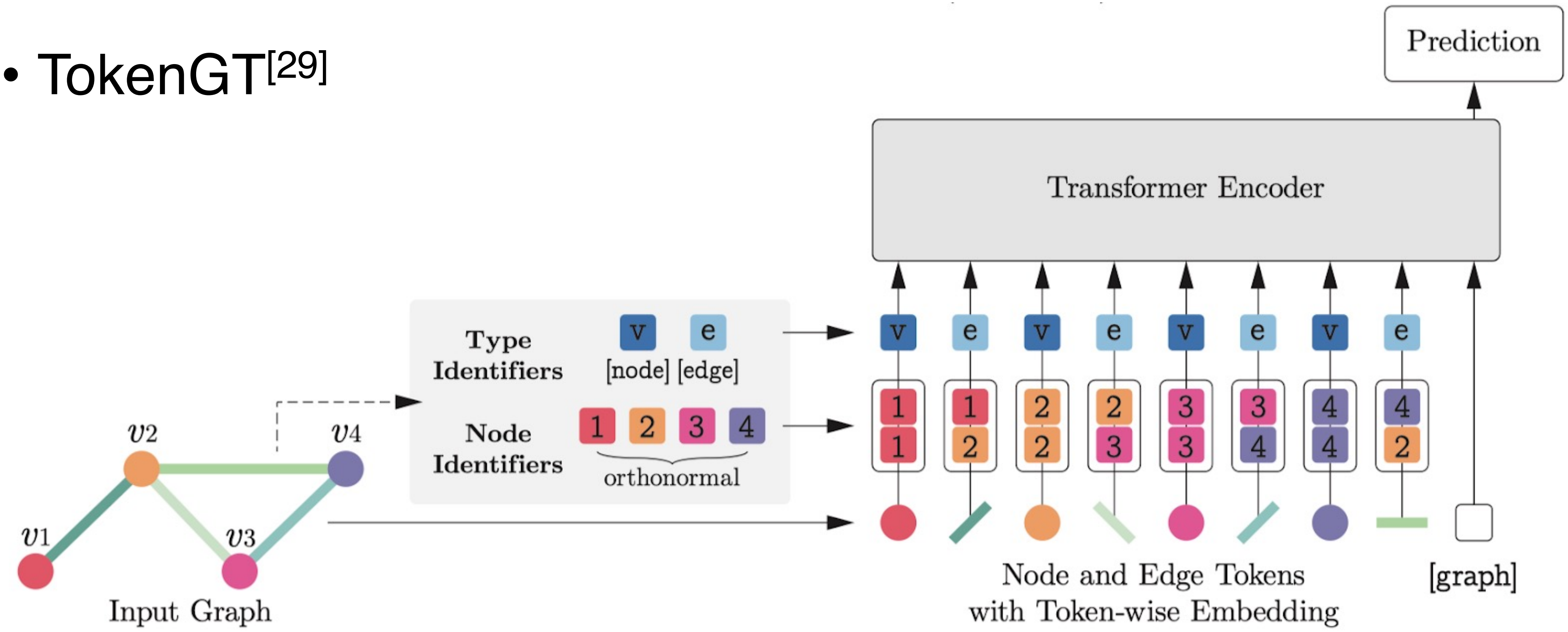
Local information

Global information

[28] Zhanghao Wu, et al. "Representing Long-Range Context for Graph Neural Networks with Global Attention"

Graph Transformer

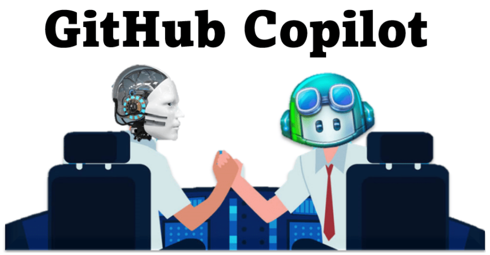
- TokenGT[29]

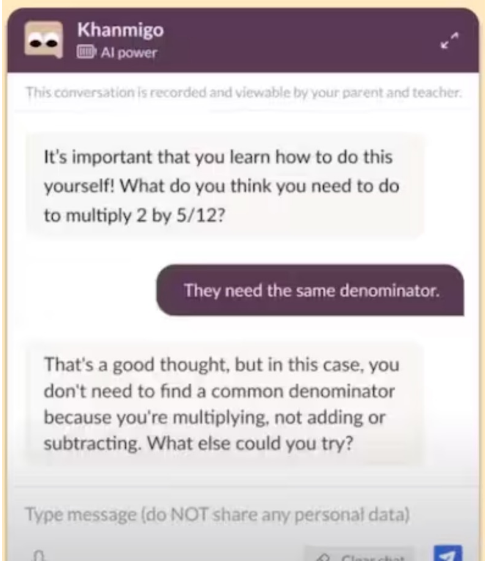


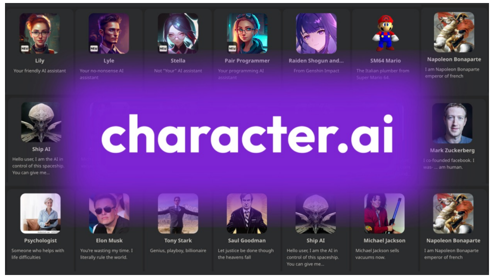
[29] Jinwoo Kim, et al. "Pure Transformers are Powerful Graph Learners"

LLM + GNN

- Large Language Model (LLM)
- ”Inflection point in AI”, “Dawn of Artificial General Intelligence”







Rowan Cheung @rowancheung · Follow

I just watched GPT-4 turn a hand-drawn sketch into a functional website.

This is insane.

Ammaar Reshi @ammaar · Follow

Can GPT-4 code an entire game for you? Yes, yes it can.

Pietro Schirano @skirano · Follow

I don't care that it's not AGI, GPT-4 is an incredible and transformative technology.

I recreated the game of Pong in under 60 seconds.
It was my first try.

Dan Shipper @danshipper · Follow

GPT-4 does drug discovery.

Give it a currently available drug and it can:

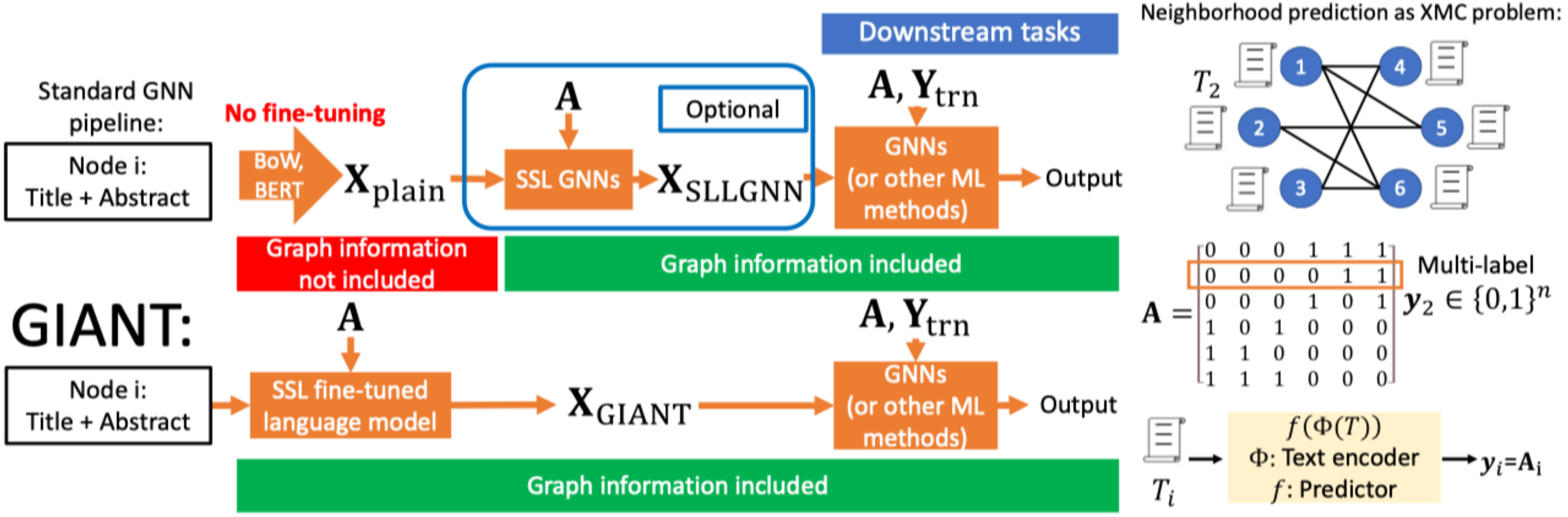
LLM + GNN

- Large Language Model (LLM)
- ”Inflection point in AI”, “Dawn of Artificial General Intelligence”

Can we improve GNN
using LLMs?

LLM + GNN

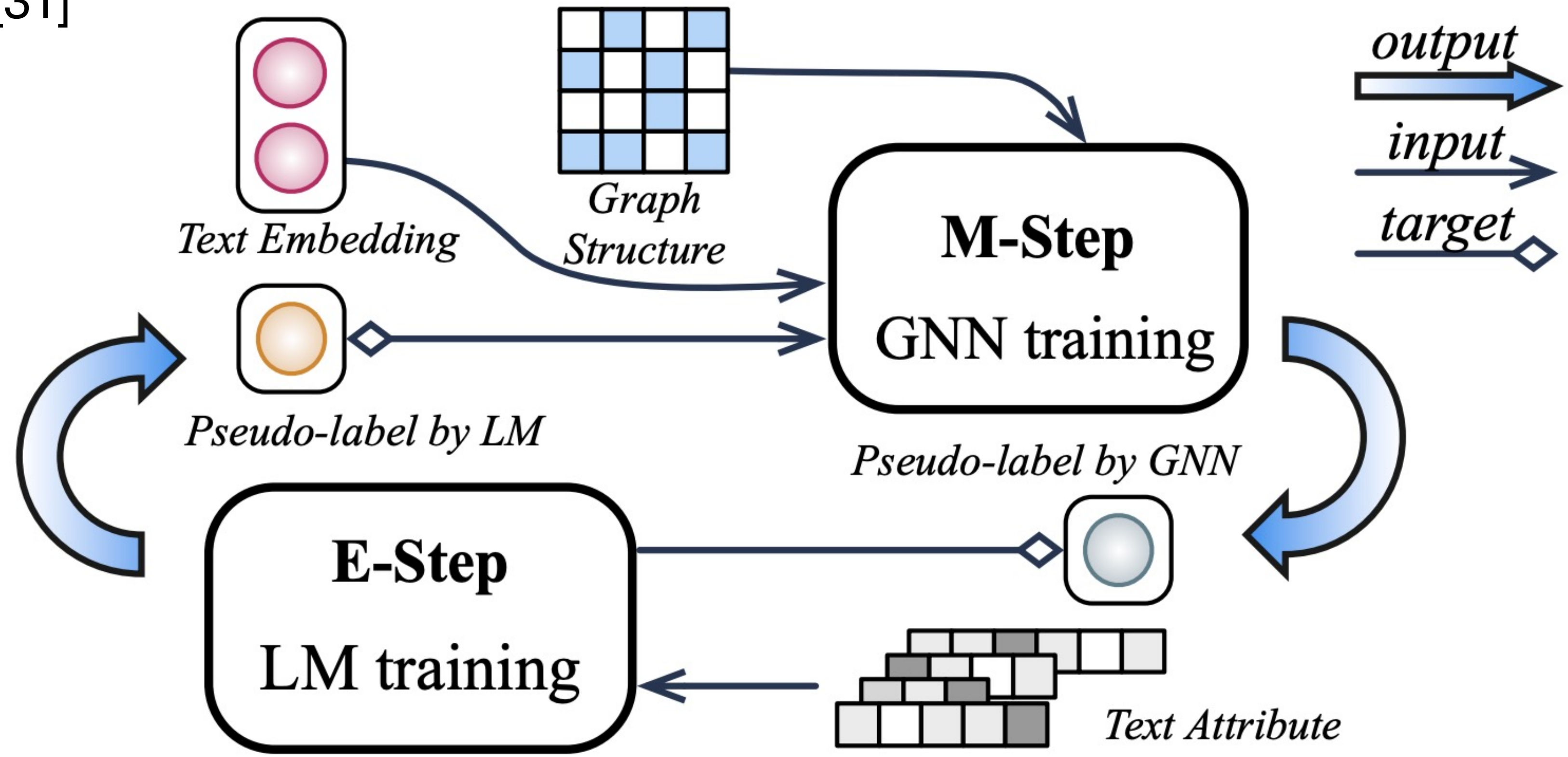
- GIANT[30]



[30] Eli Chien, et al. "Node Feature Extraction by Self-Supervised Multi-scale Neighborhood Prediction"

LLM + GNN

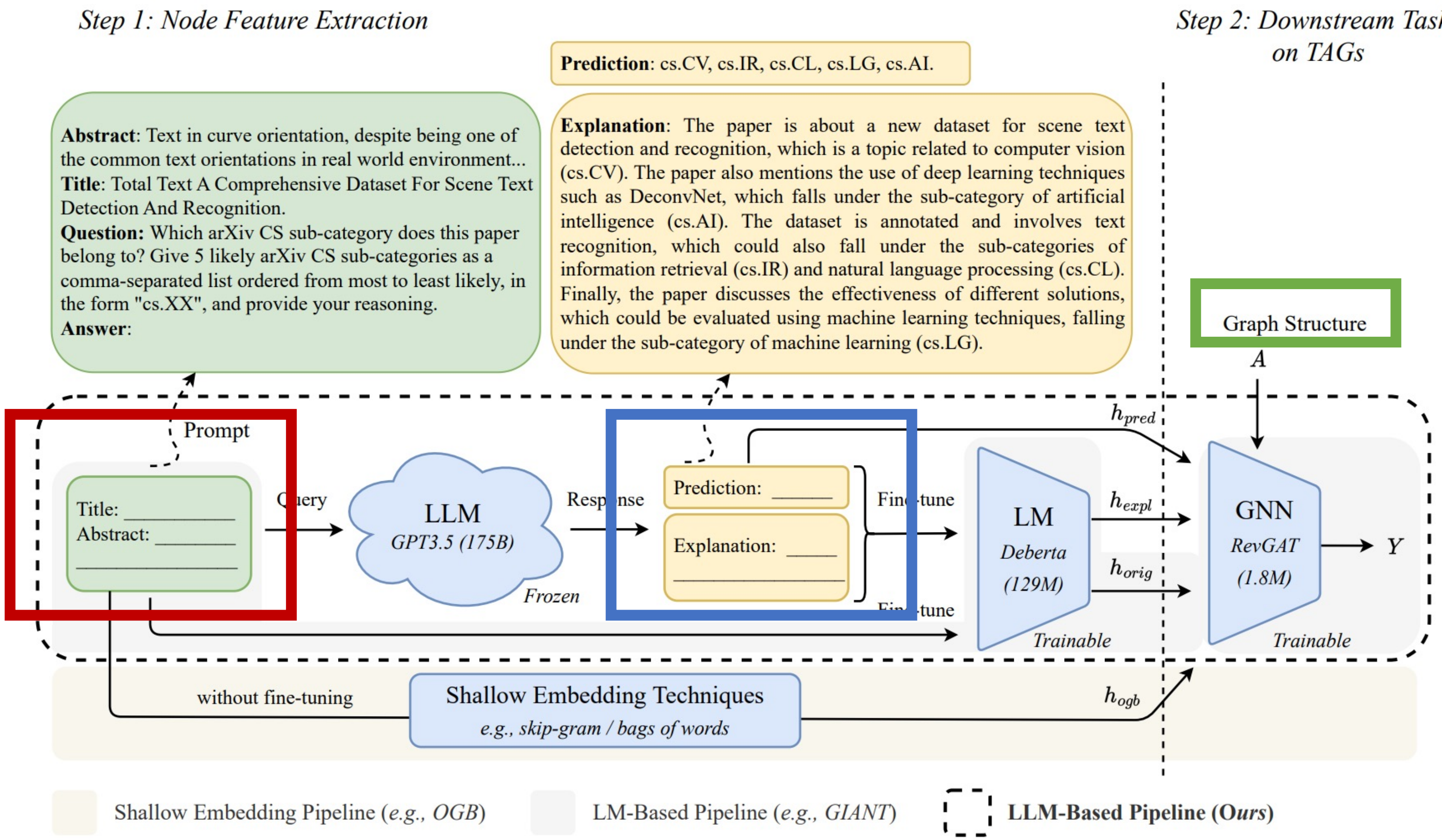
- GLEM[31]



[31] Jianan Zhao, et al. "Learning on Large-scale Text-attributed Graphs via Variational Inference"

LLM + GNN

- TAPE[32]



[32] Xiaoxin He, et al. "Harnessing Explanations: LLM-to-LM Interpreter for Enhanced Text-Attributed Graph Representation Learning"

Still many open problems..

- And many more chances to do groundbreaking research
- Diverse types of graphs
  - 3-dimensional graphs
  - Temporal graphs
  - Multimodal graphs
- Diverse types of architecture
  - Graph Convolution Networks
  - Graph Transformers
  - LLMs

Thank you!

Questions?

minjiy@cs.cmu.edu | https://www.minjiyoon.xyz