Introduction to Graph Neural Networks

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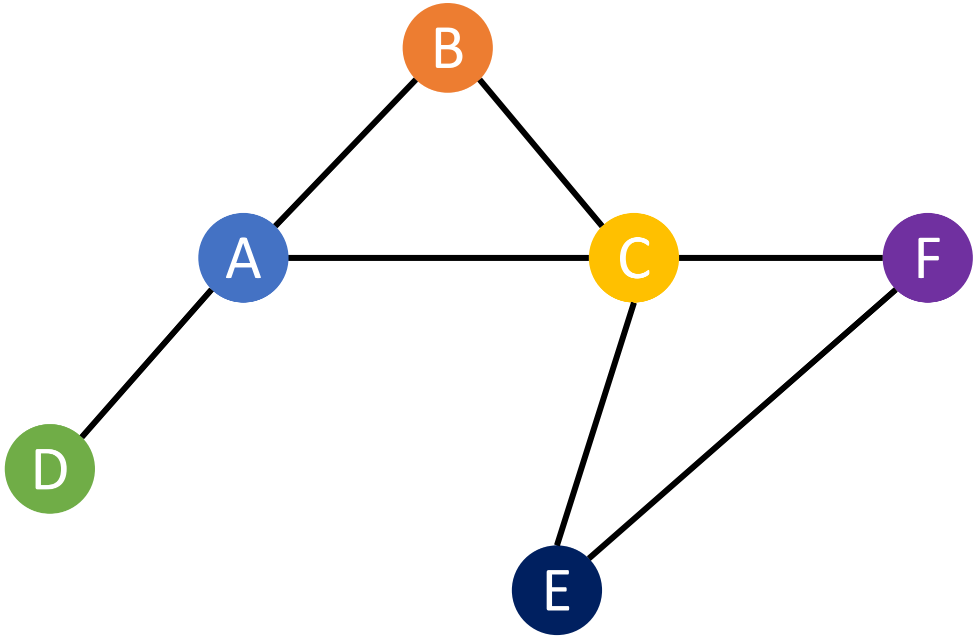
Computer Science Department

Carnegie Mellon University

Talk objectives

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

What is a graph?

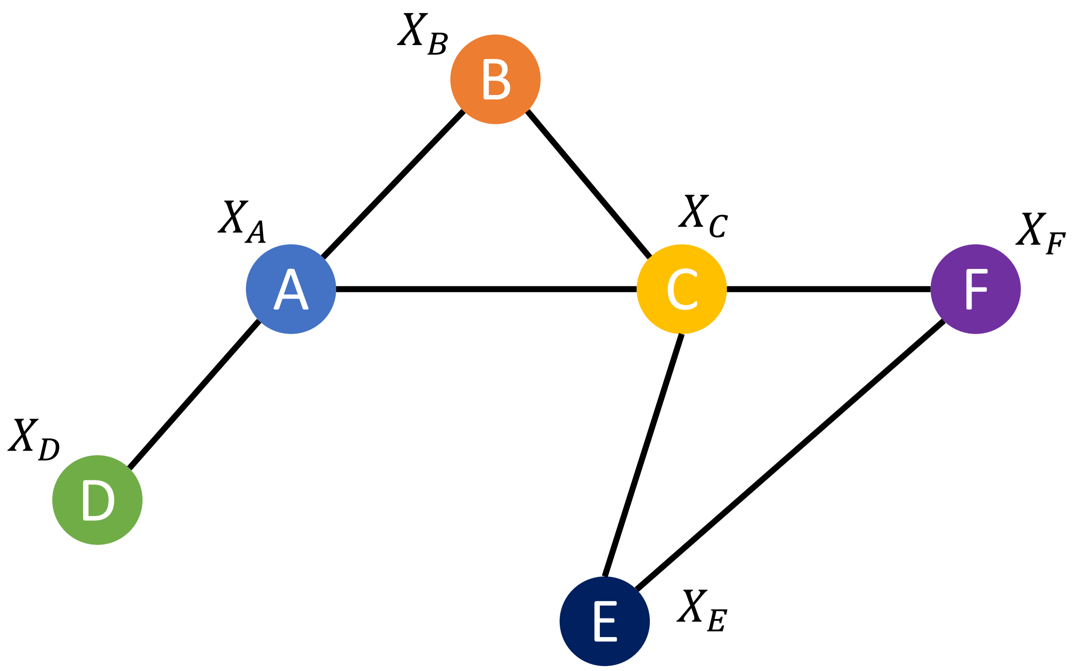


A graph is composed of
- **Nodes** (also called vertices)
- **Edges** connecting a pair of nodes

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)
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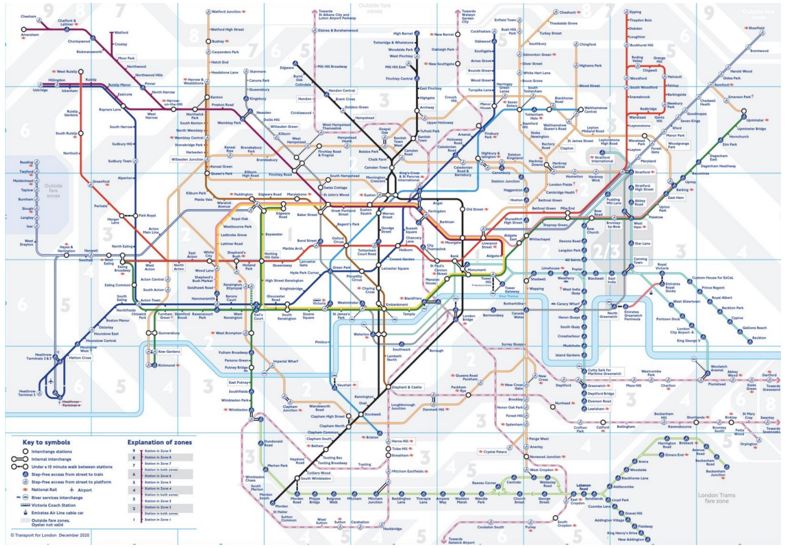
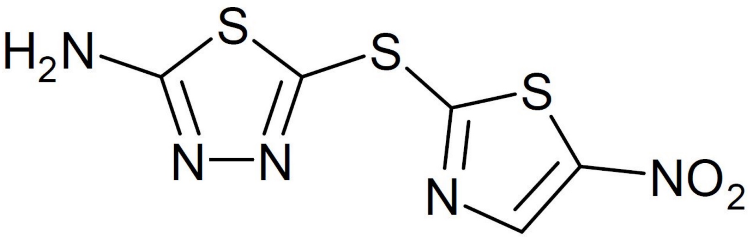
presented in an **adjacency matrix**

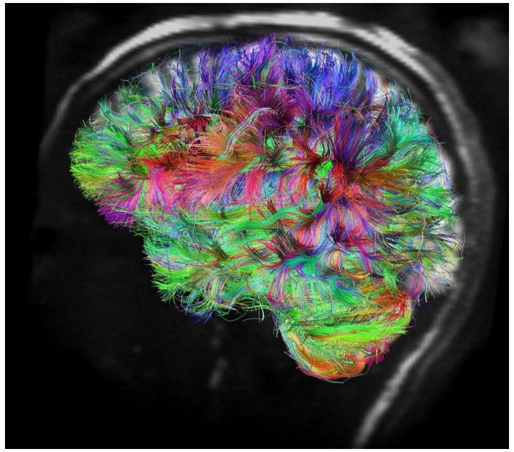
Nodes can have **feature vectors**

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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ıral Network

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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

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September 24, 2020 | Zack Savitsky

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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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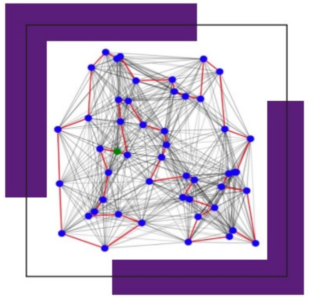


Patterns

CellPress OPEN ACCESS

Opinion

Neural algorithmic reasoning

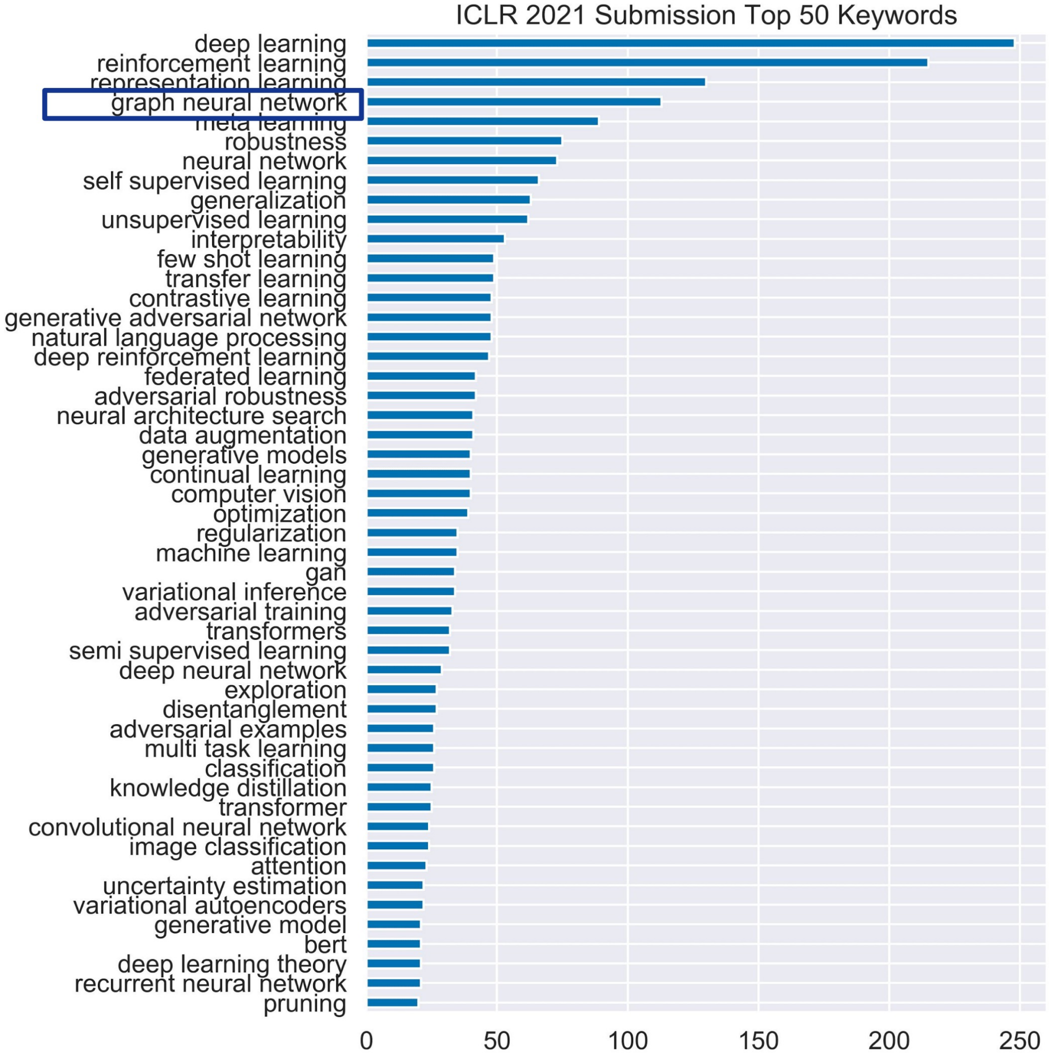
Petar Veličković[1,*] and Charles Blundell[1]
[1]DeepMind, London, Greater London, UK
*Correspondence: petarv@google.com

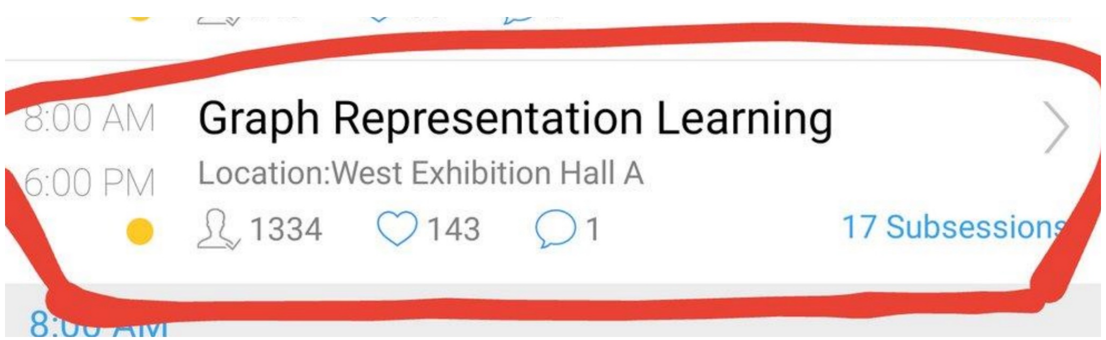
https://doi.org/10.1016/j.patter.2021.100273

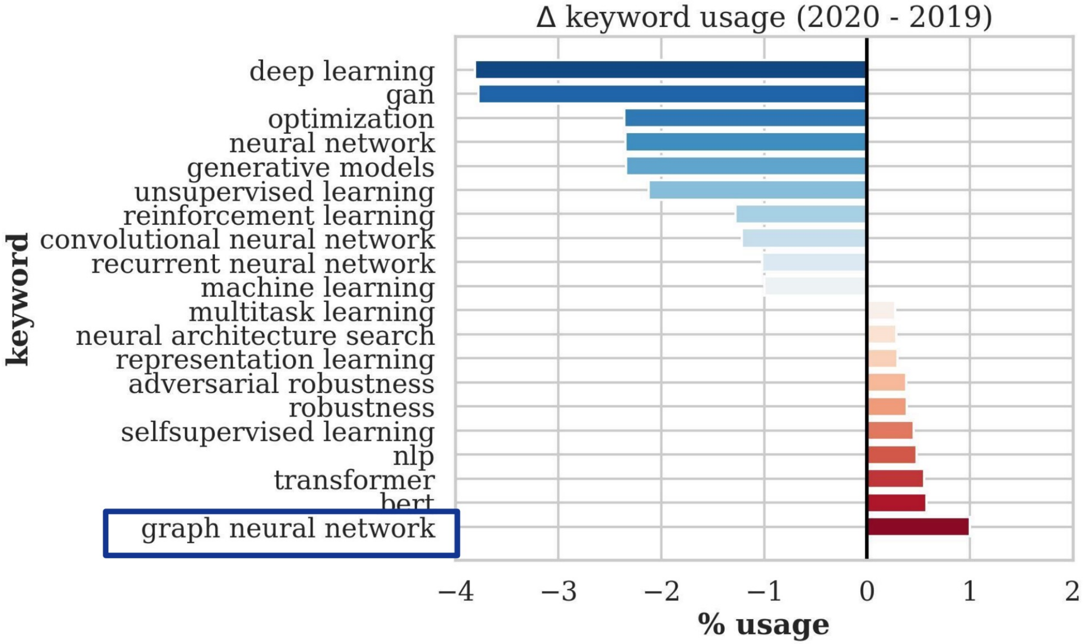
We present neural algorithmic reasoning—the art of building neural networks that are able to execute algorithmic computation—and provide our opinion on its transformative potential for running classical algorithms on inputs previously considered inaccessible to them.

(slide: P. Veličković)

A very hot research topic

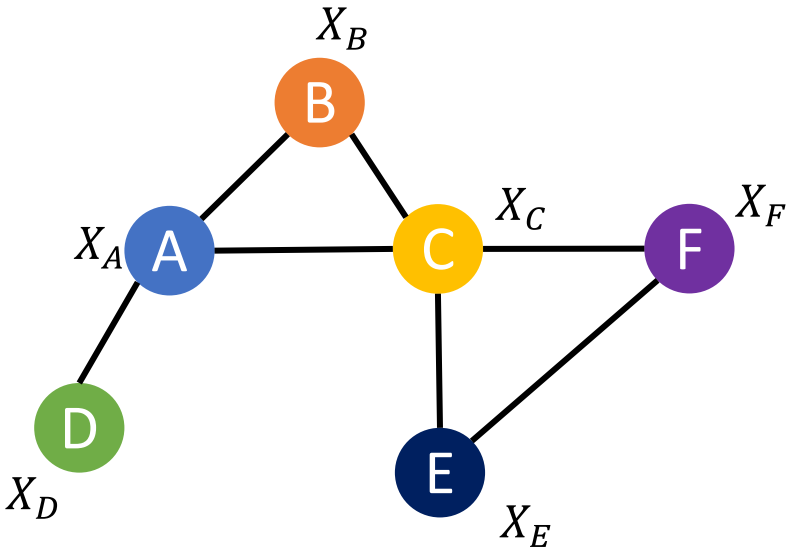






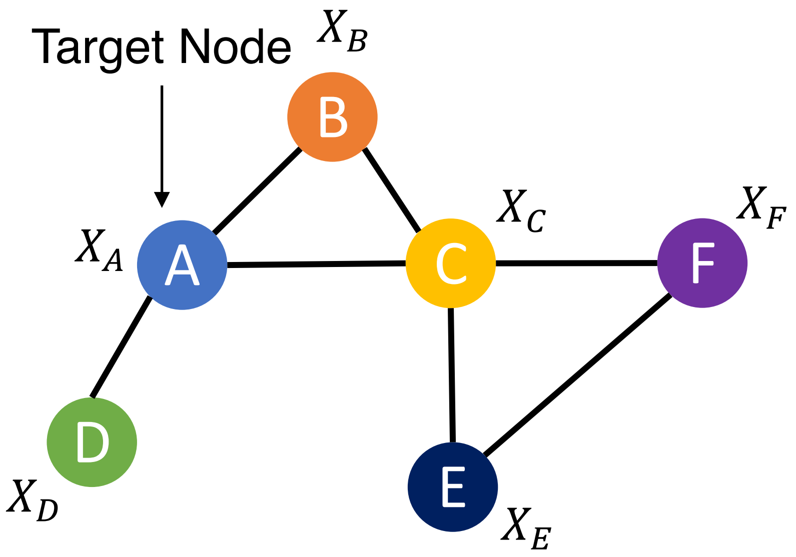
What is Graph Neural Network?

Problem definition



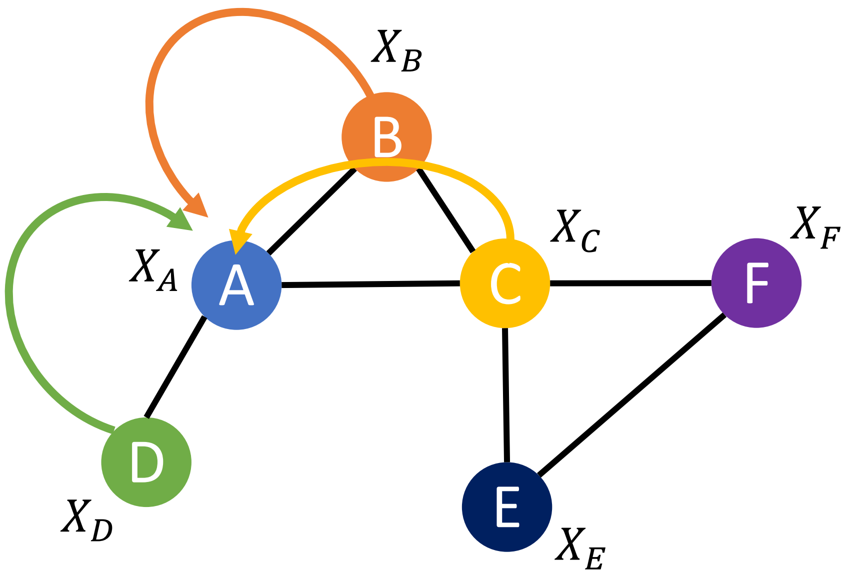
- **Given**
  - A graph
  - Node attributes
  - (part of nodes are labeled)
- **Find**
  - Node embeddings
- **Predict**
  - Labels for the remaining nodes

Graph Neural Networks



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

Graph Neural Networks



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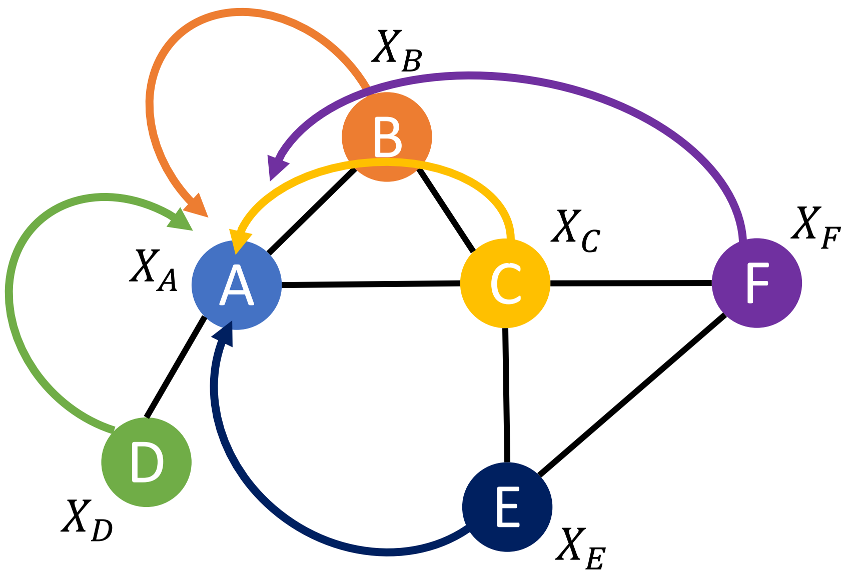
Graph Neural Networks



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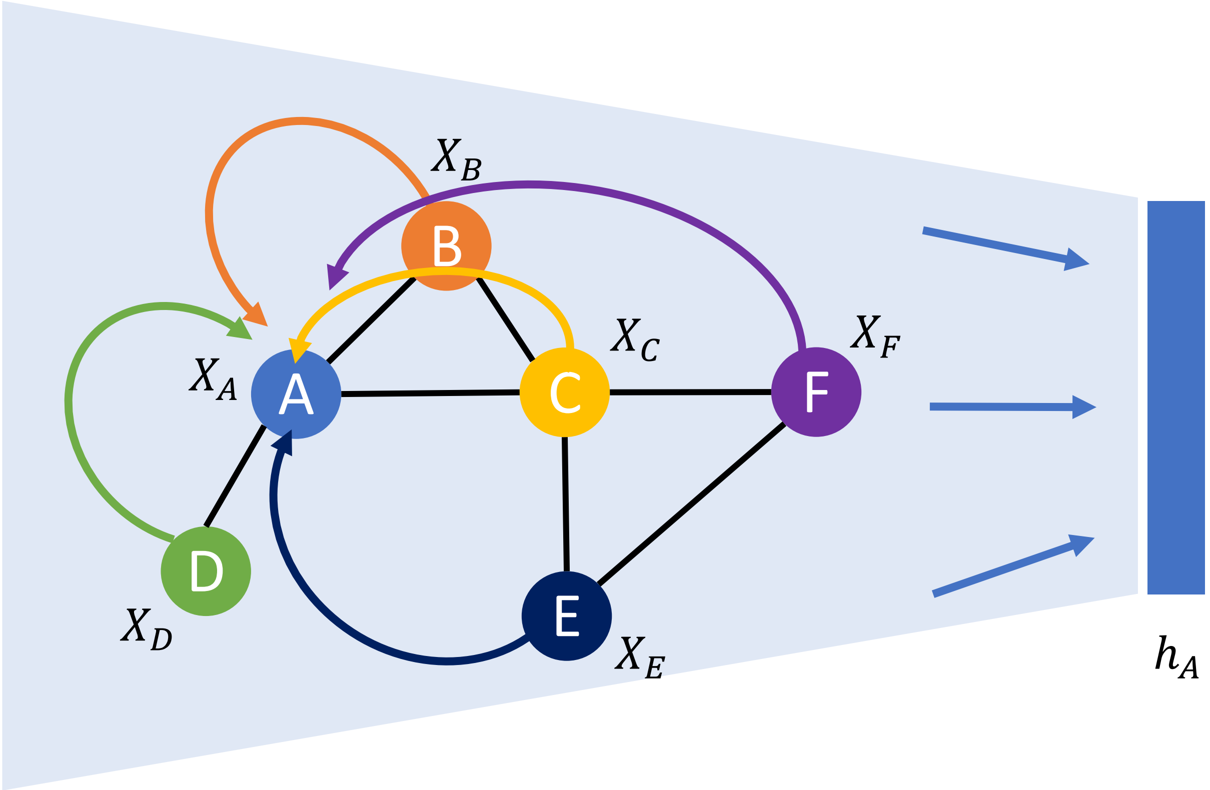
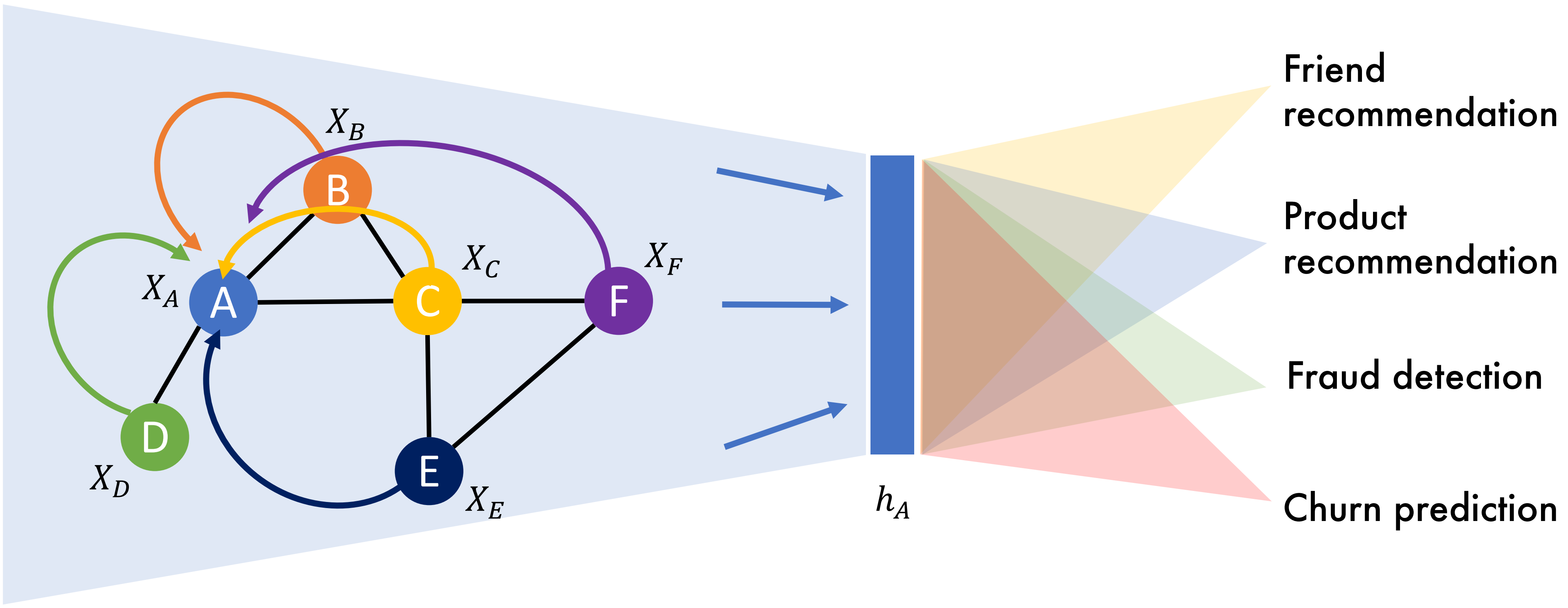
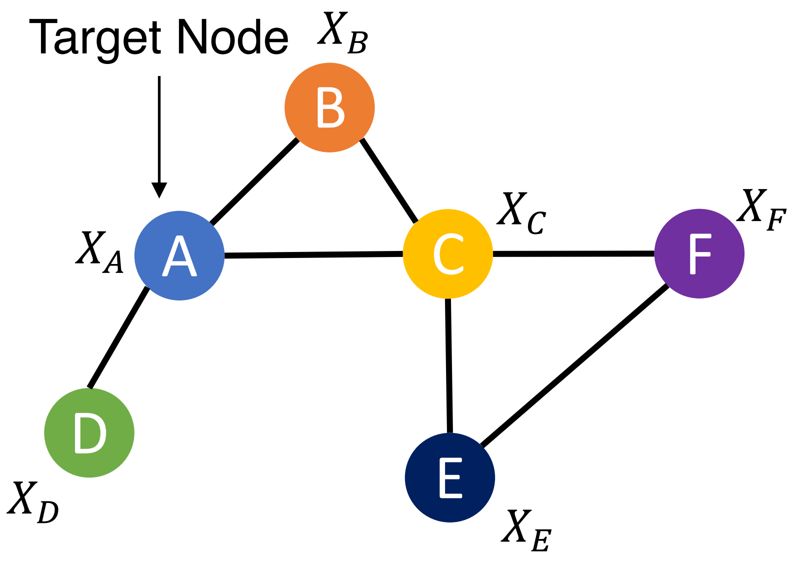
Graph Neural Networks

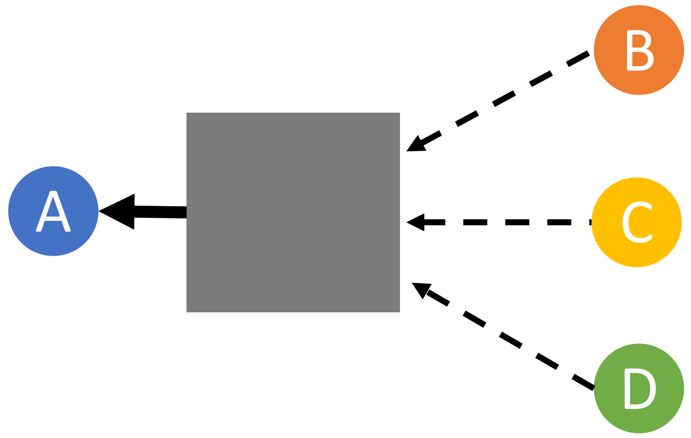


Graph Neural Networks



Graph Neural Networks





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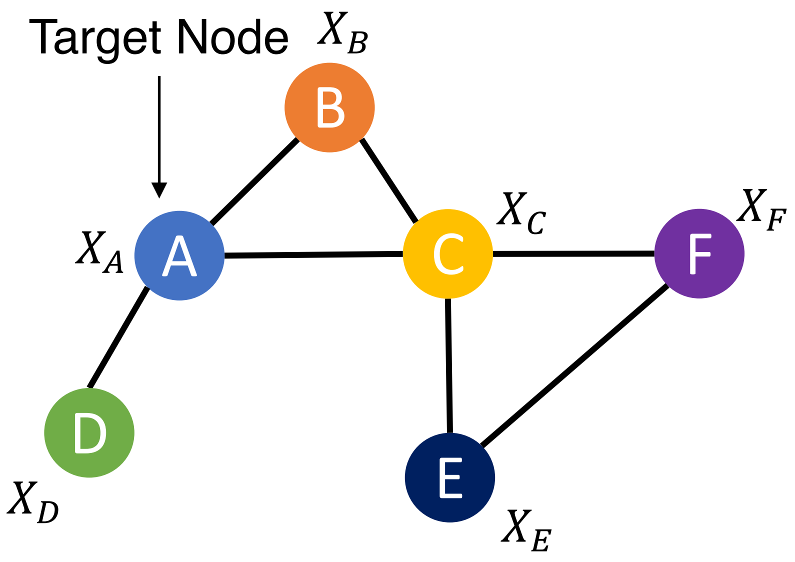

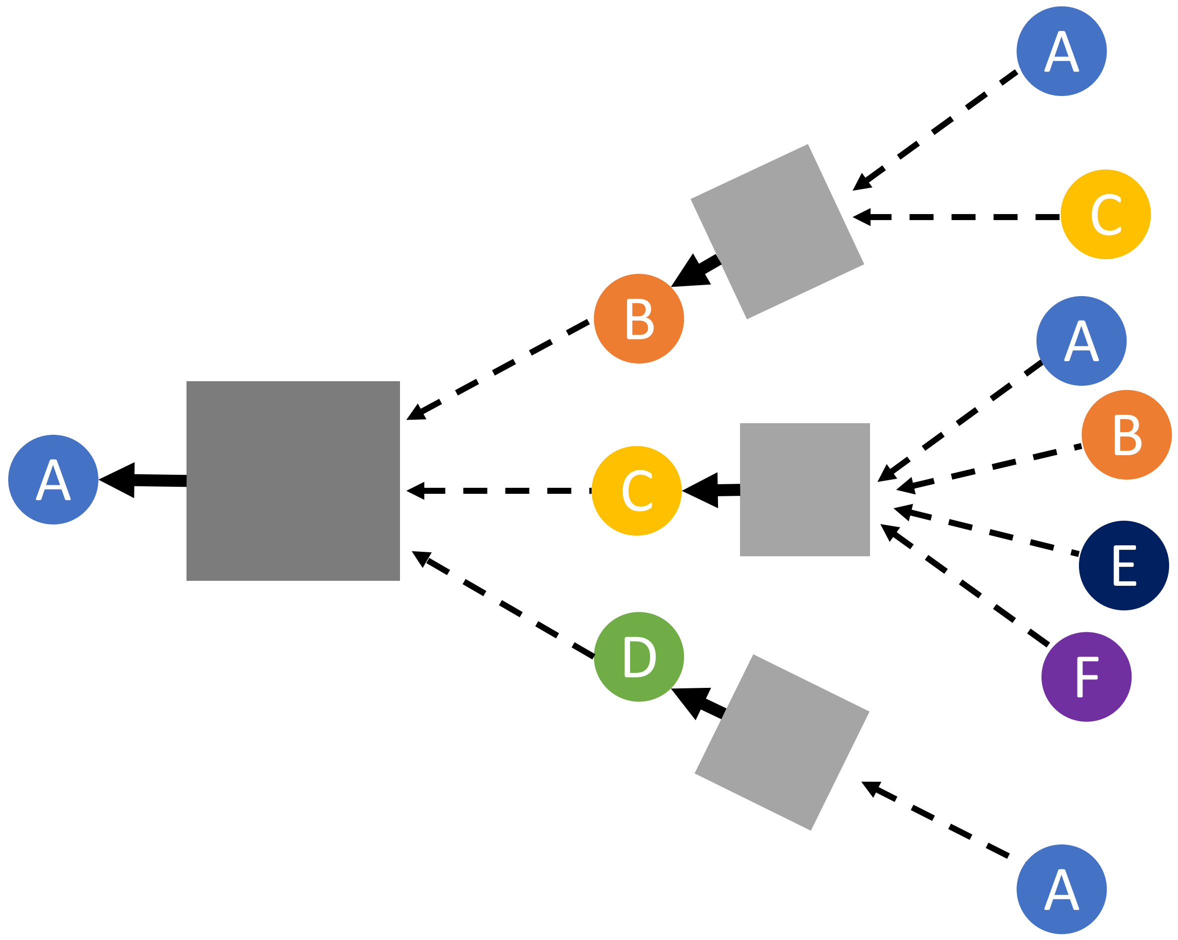

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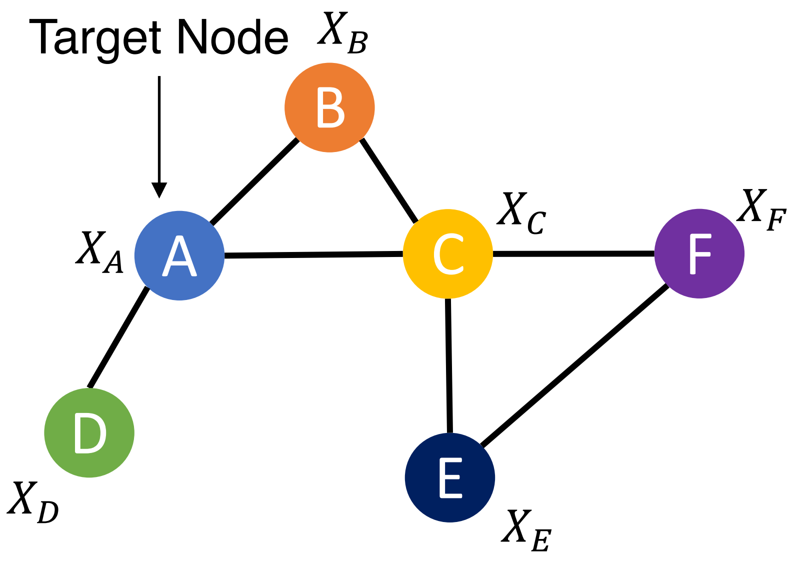

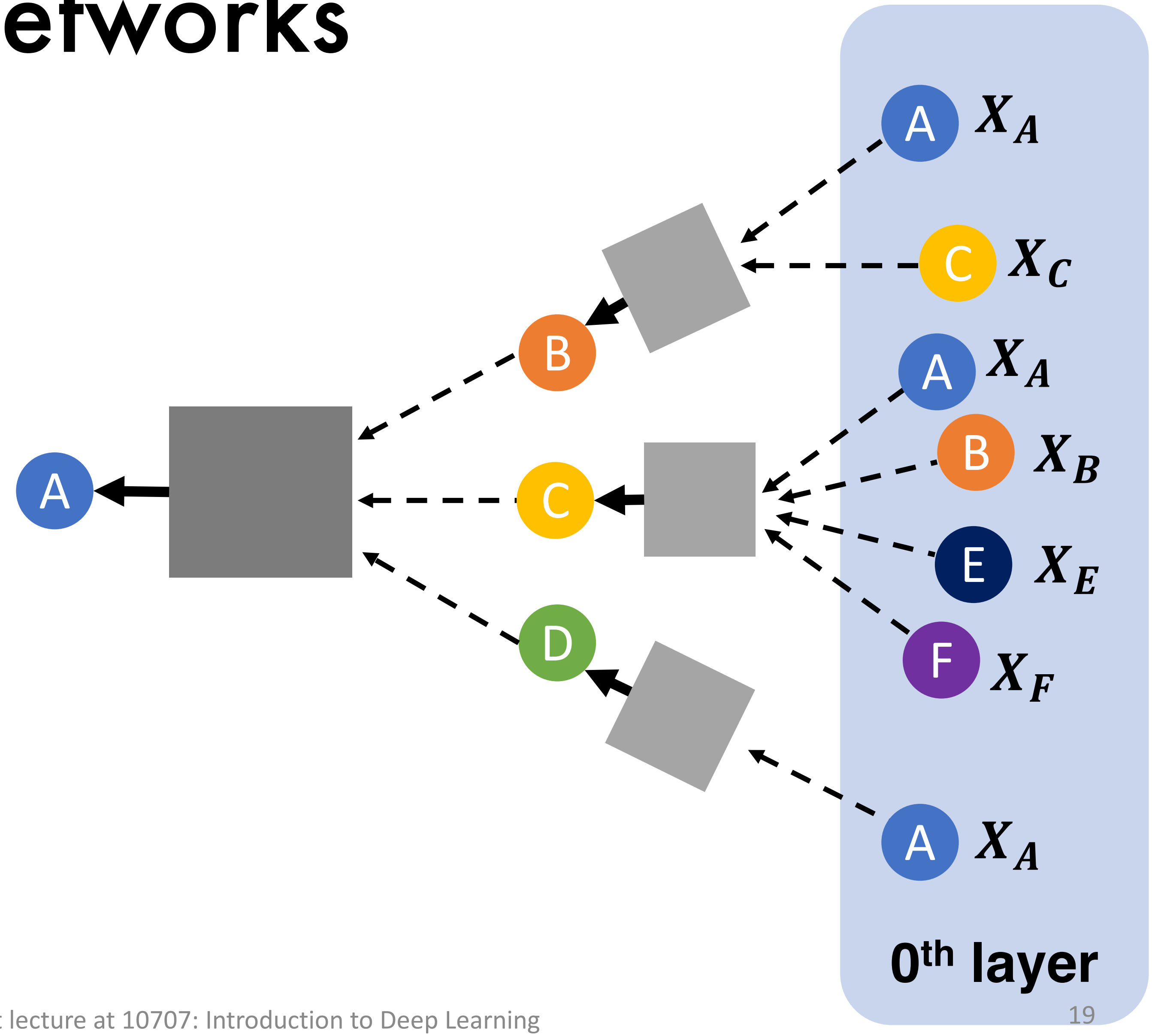

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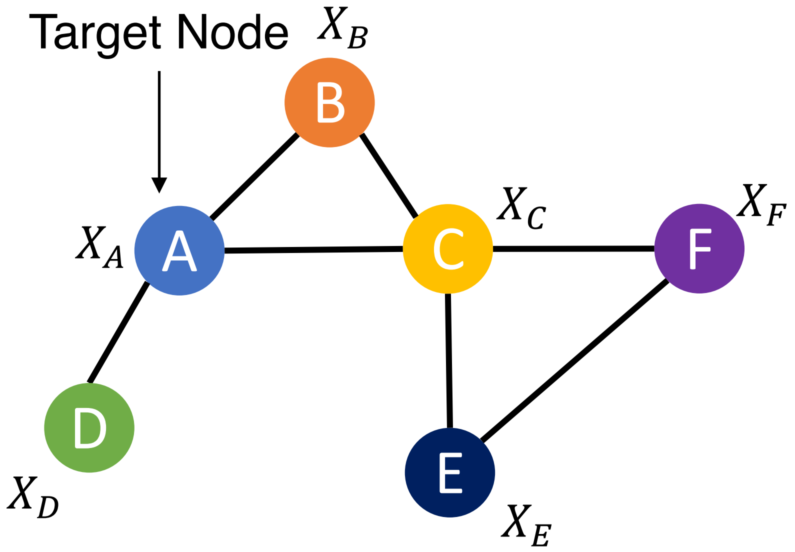

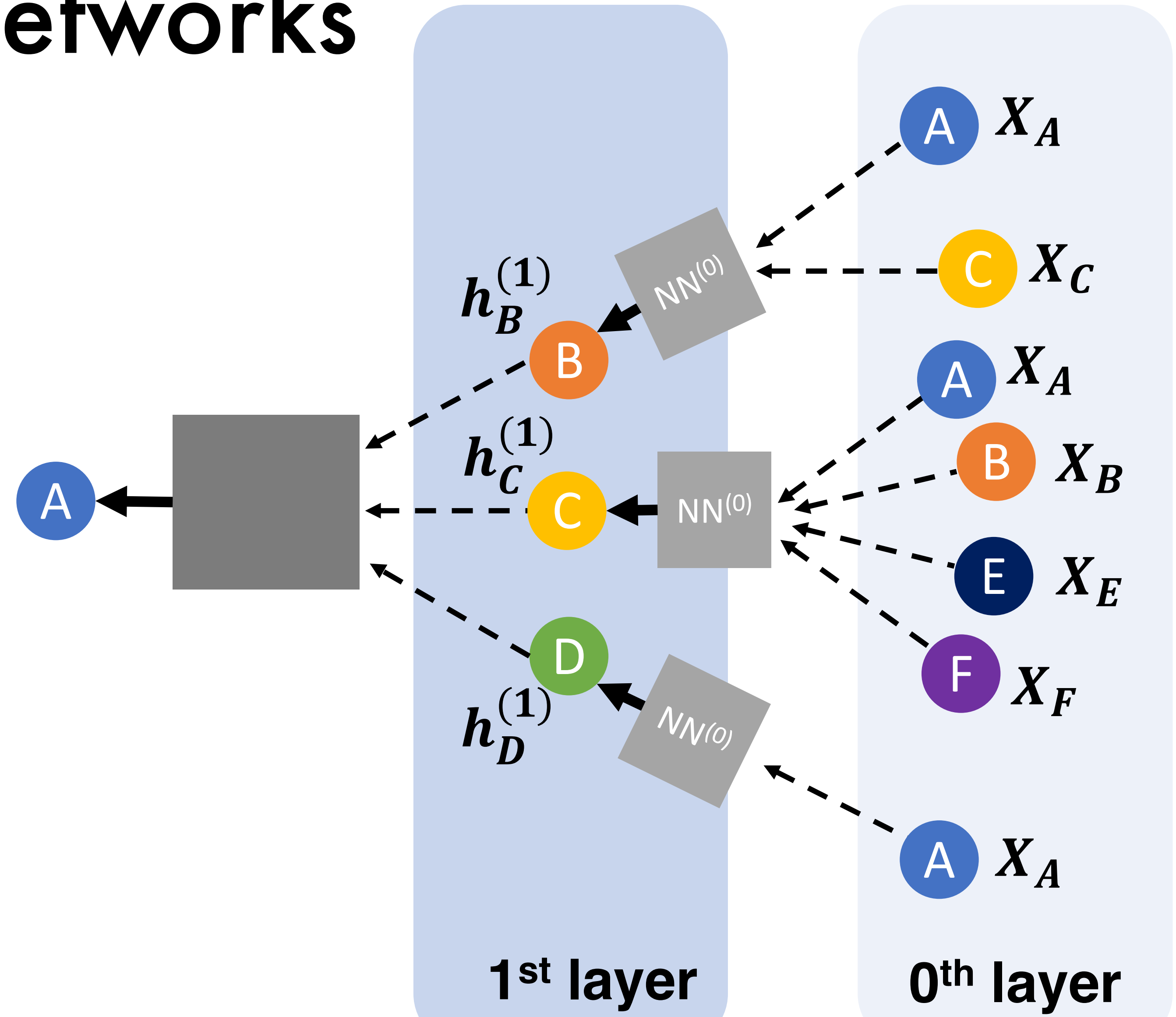

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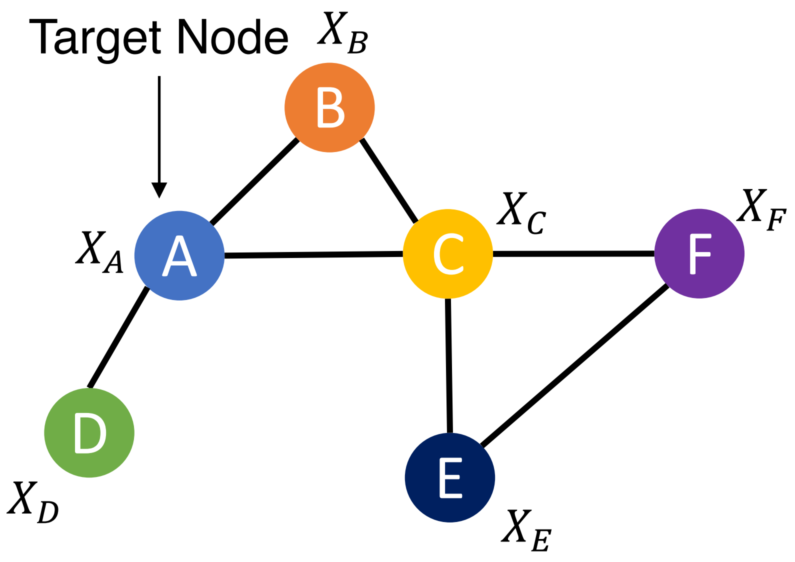
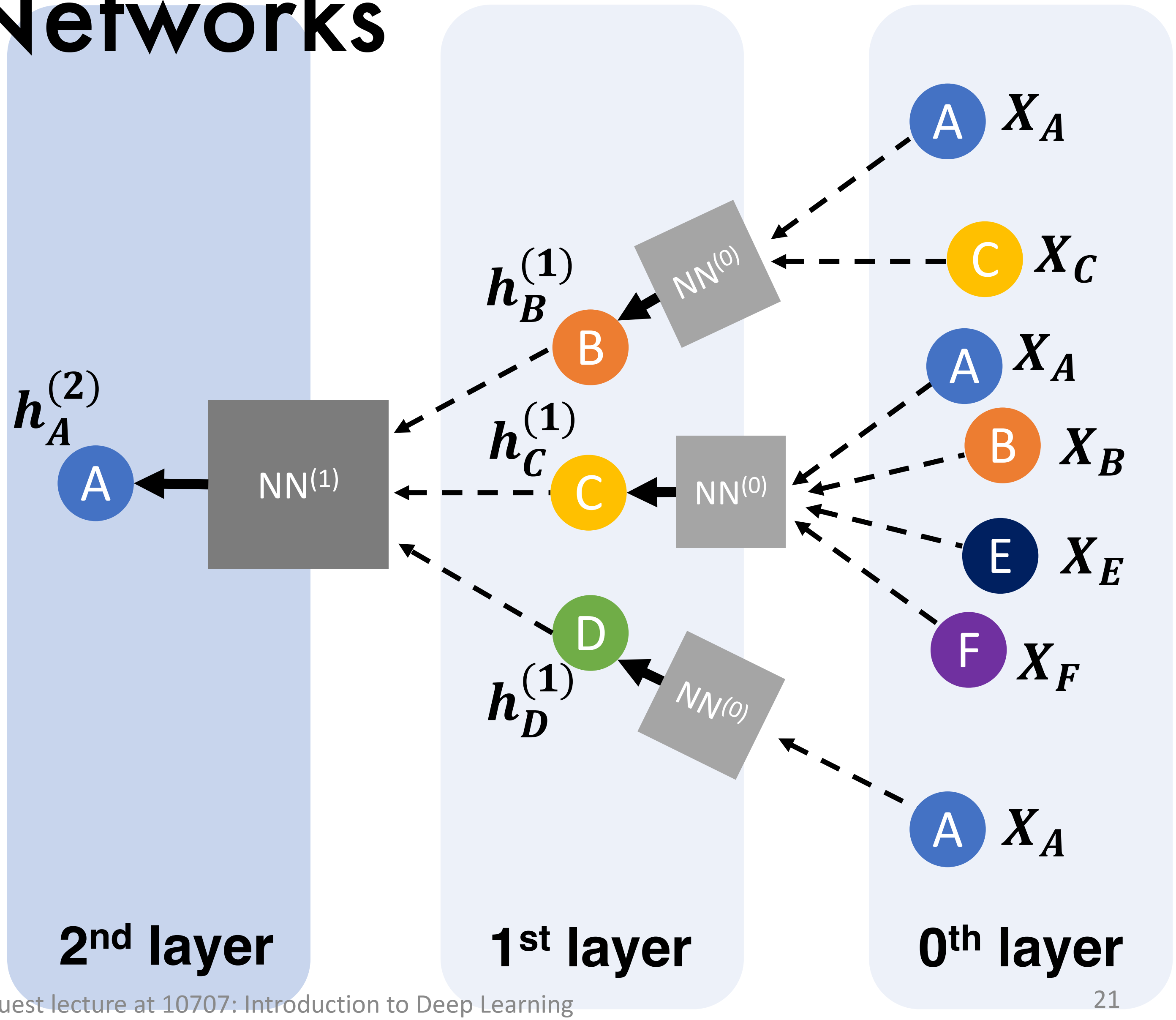


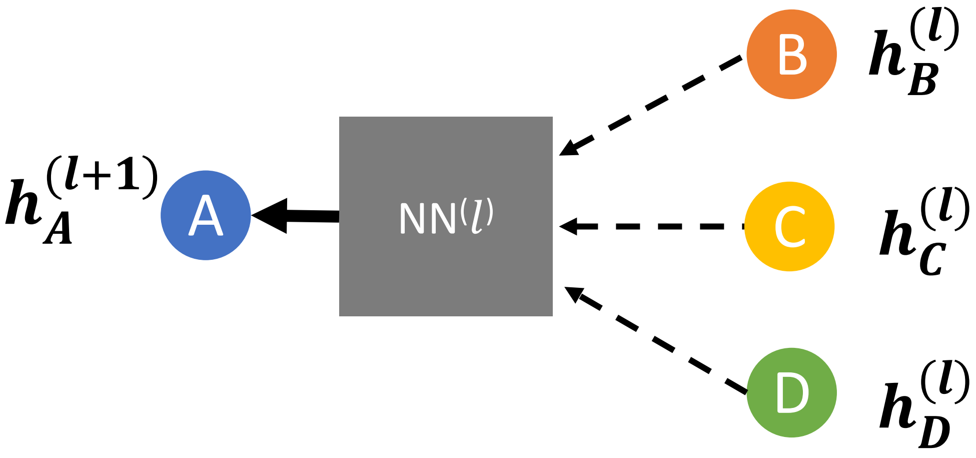


Graph Neural Networks

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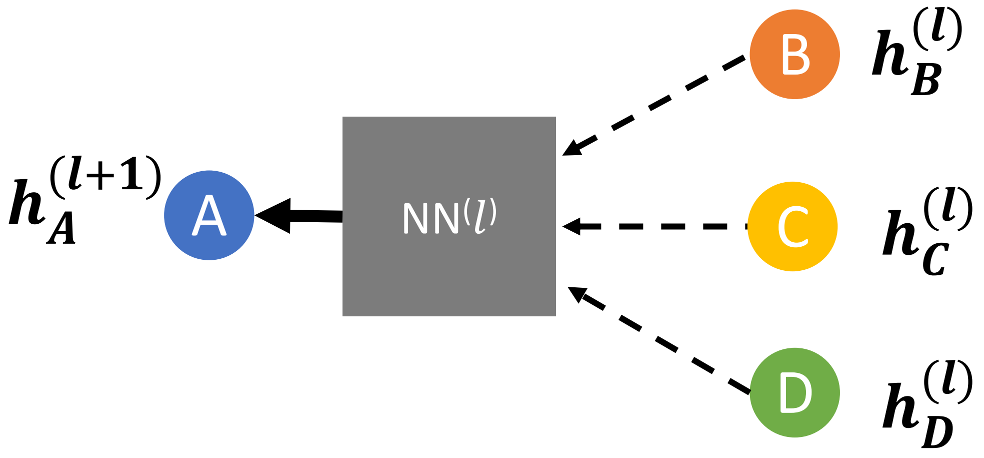
$$= \boldsymbol{f}^{(l)}\left(h_A^{(l)}, h_B^{(l)} h_C^{(l)} h_D^{(l)}\right)$$

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

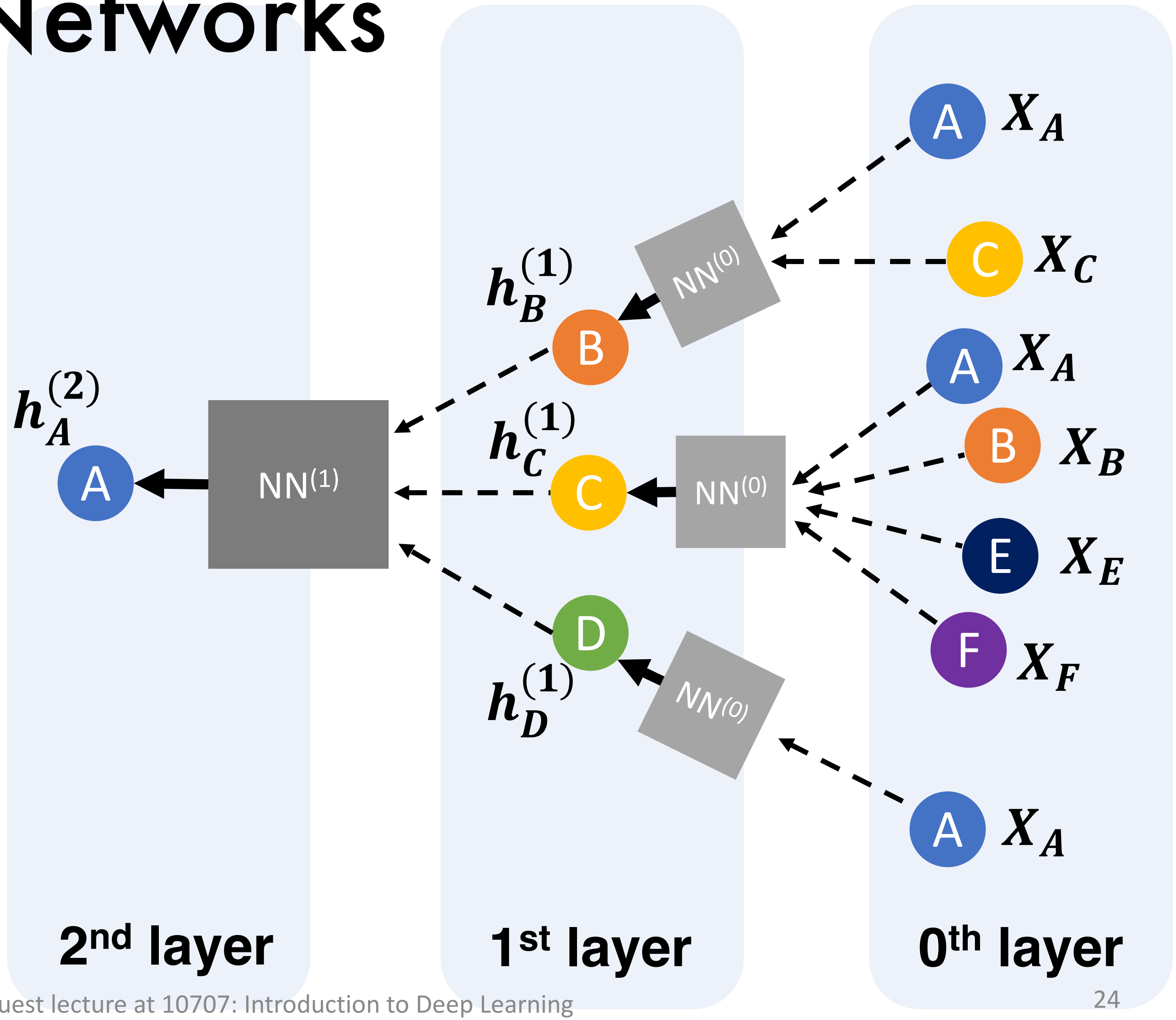
In each layer l ,
for each target node v :

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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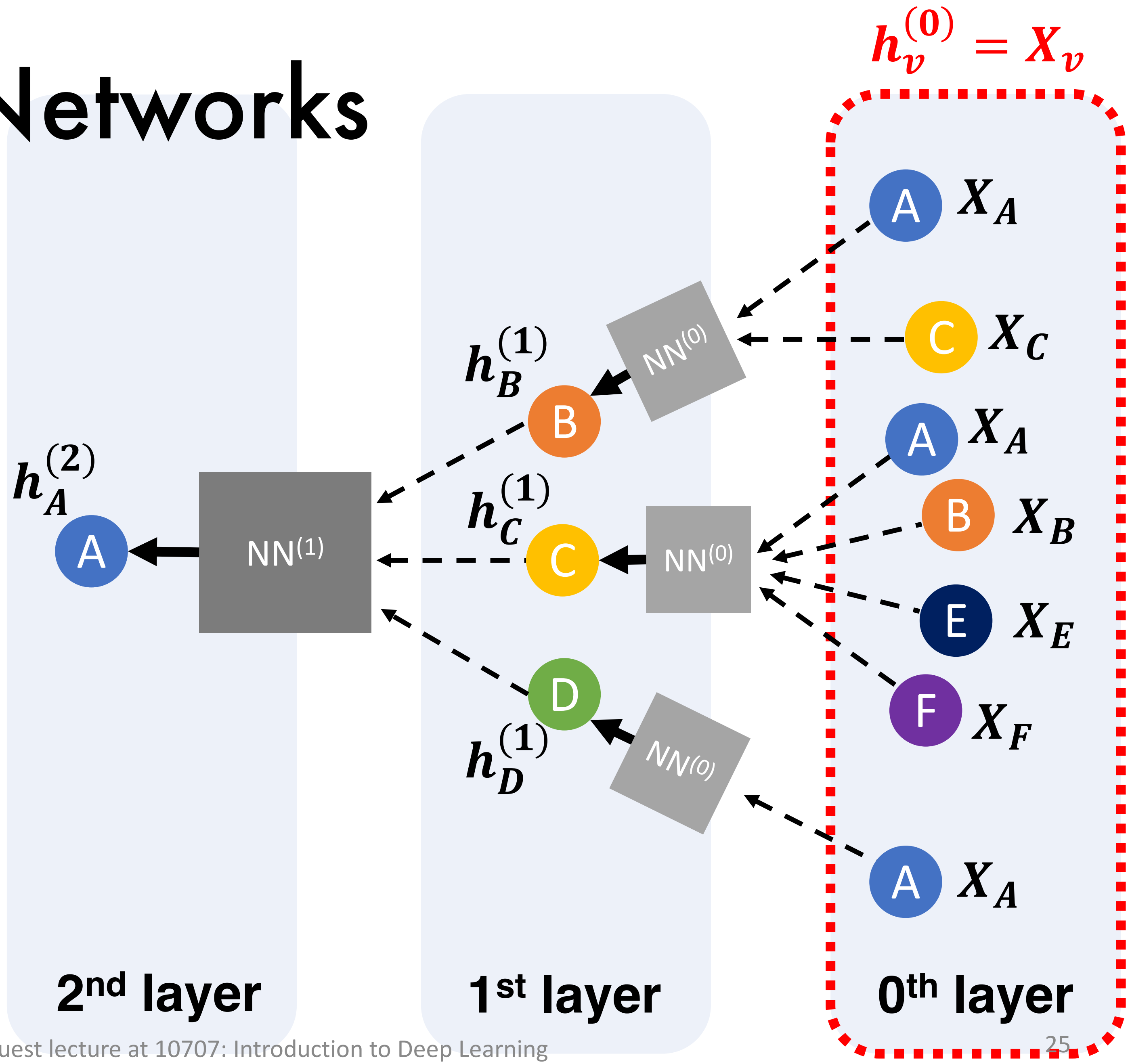

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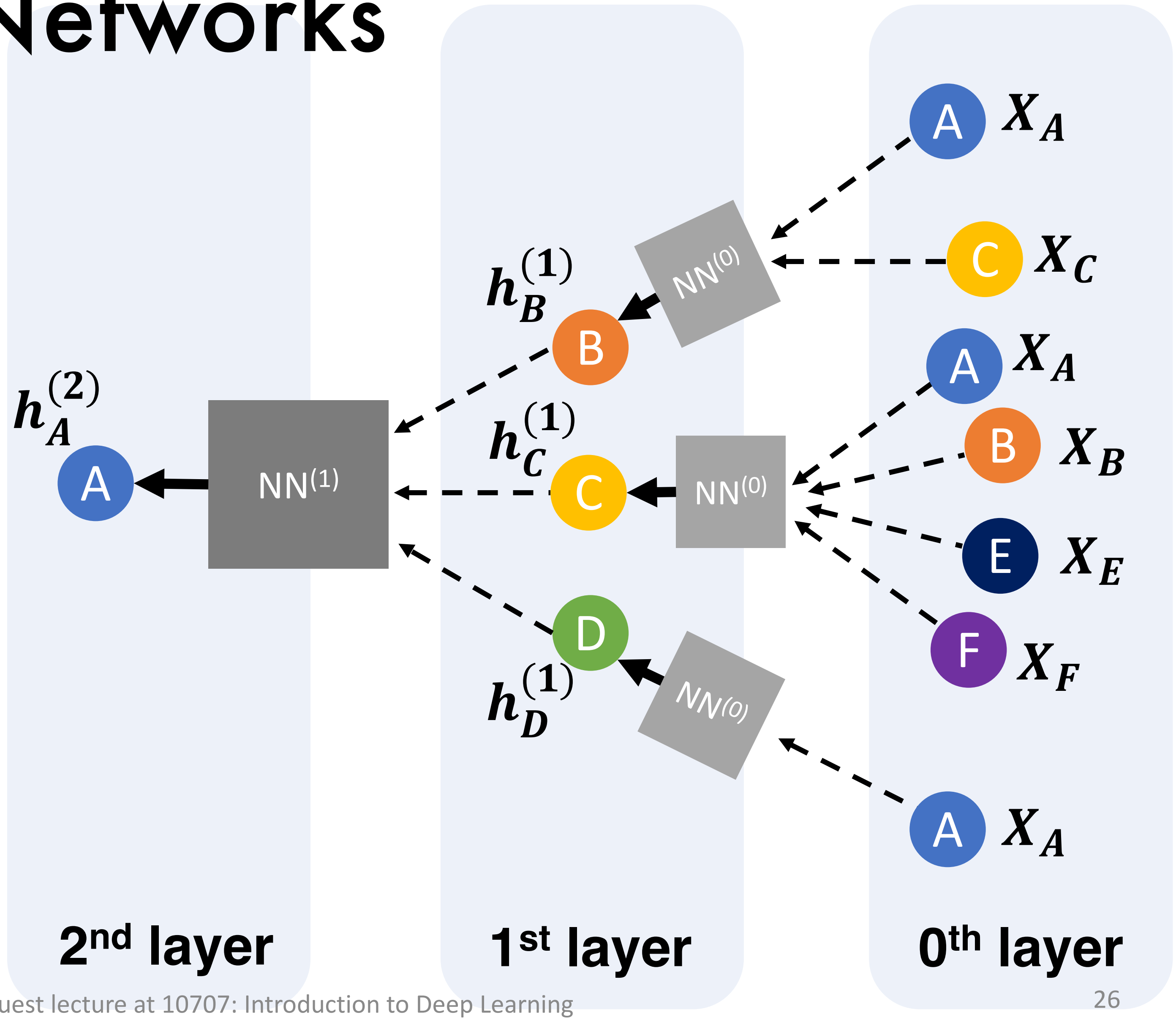


Graph Neural Networks

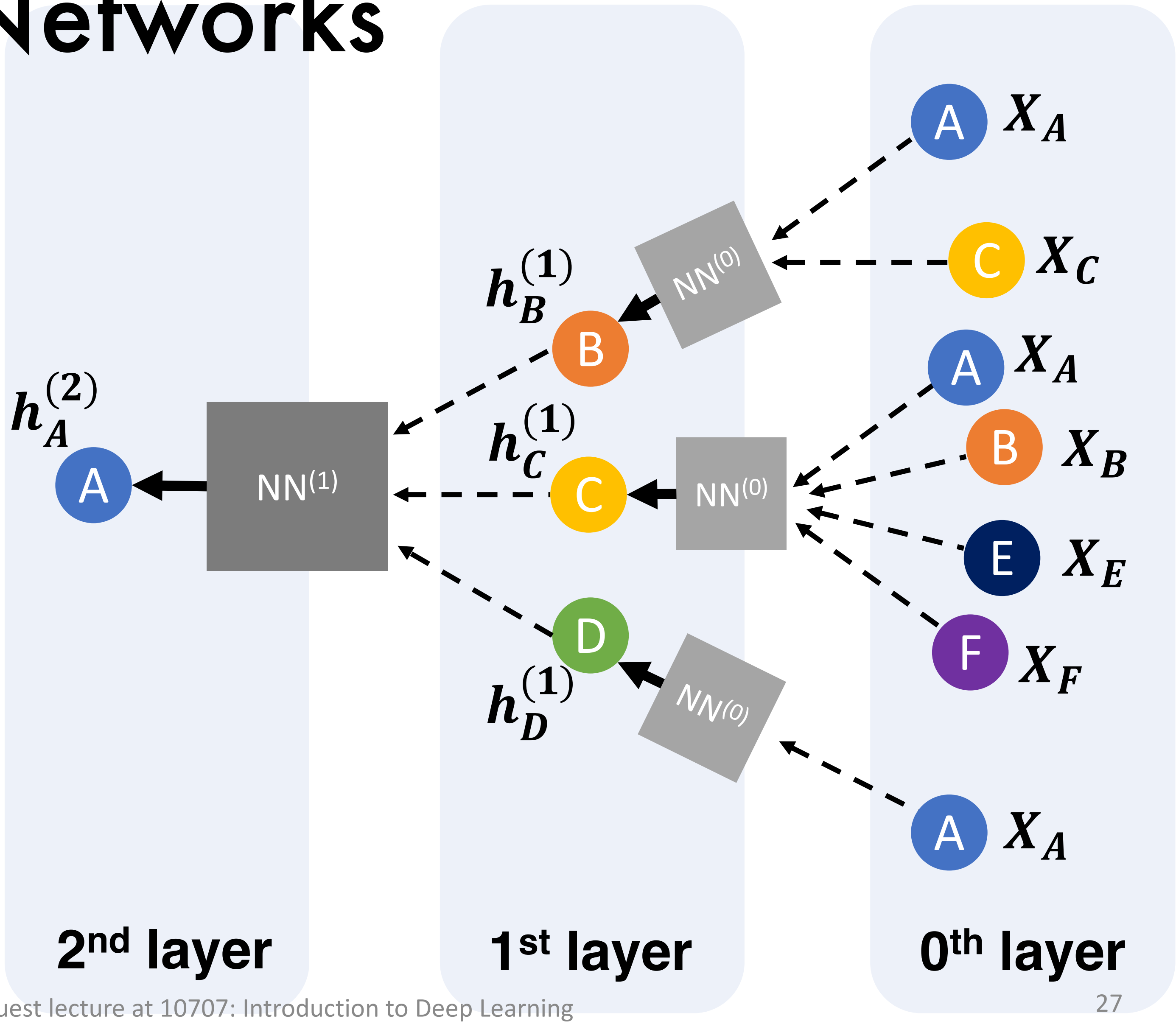
Graph Convolutional Networks[1]

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

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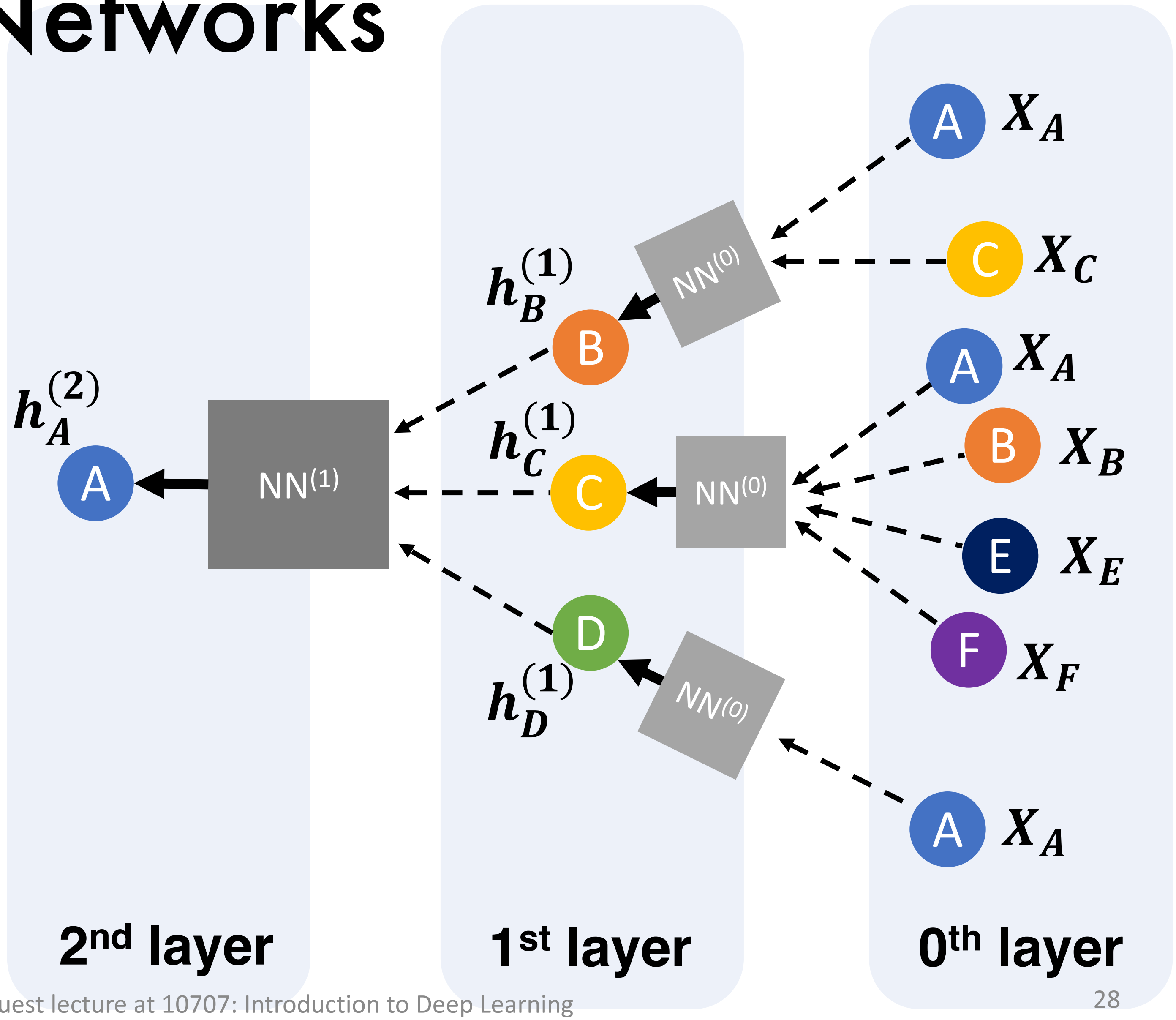
2. Transform messages

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



[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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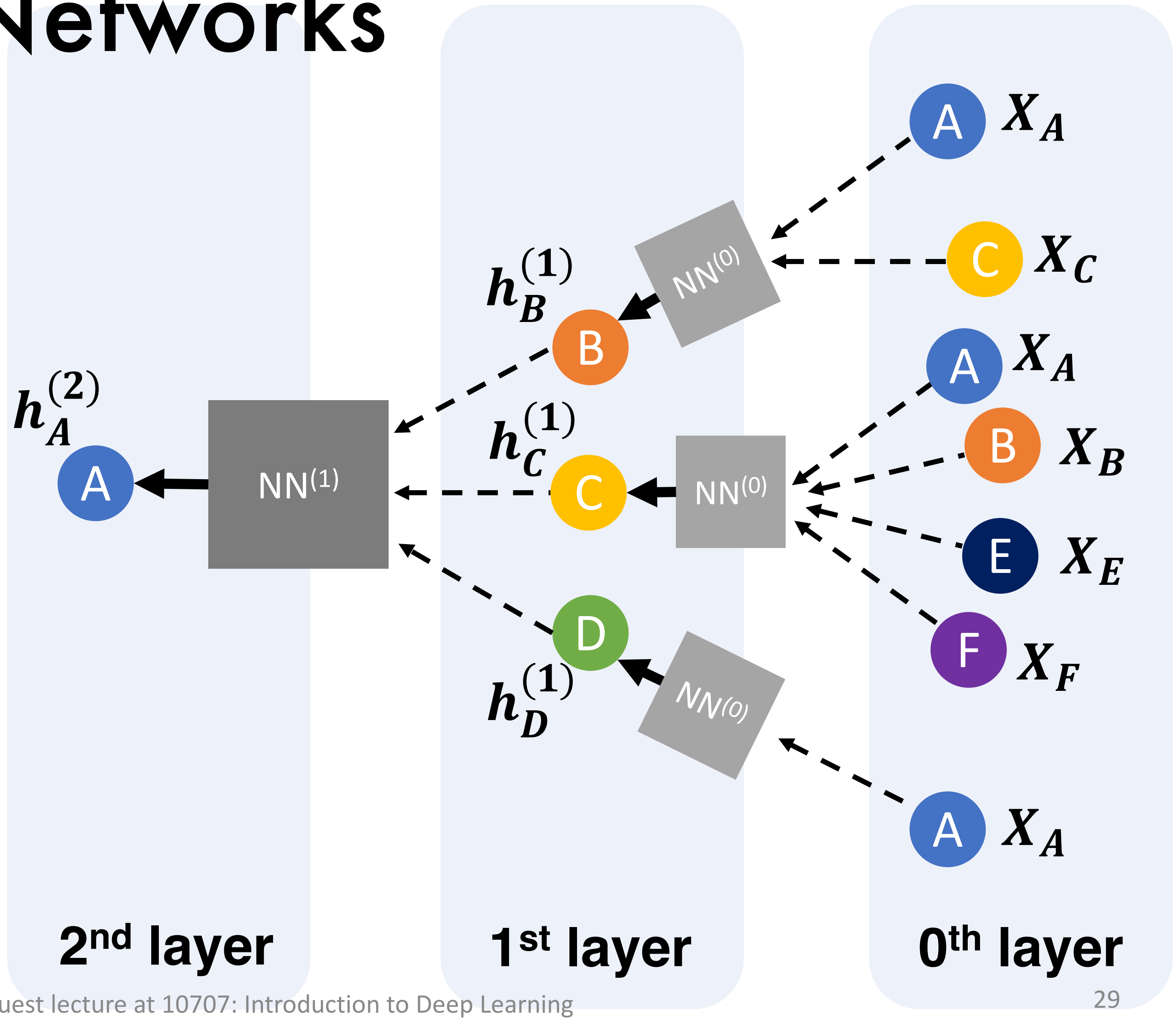
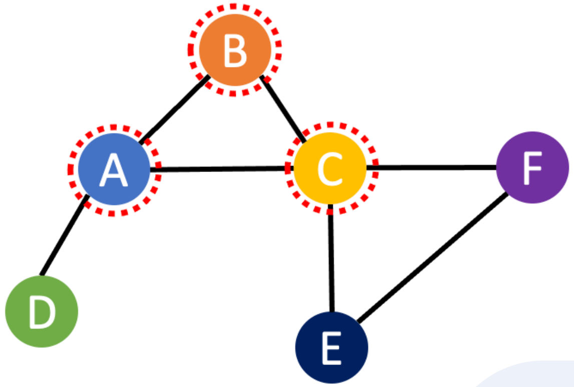
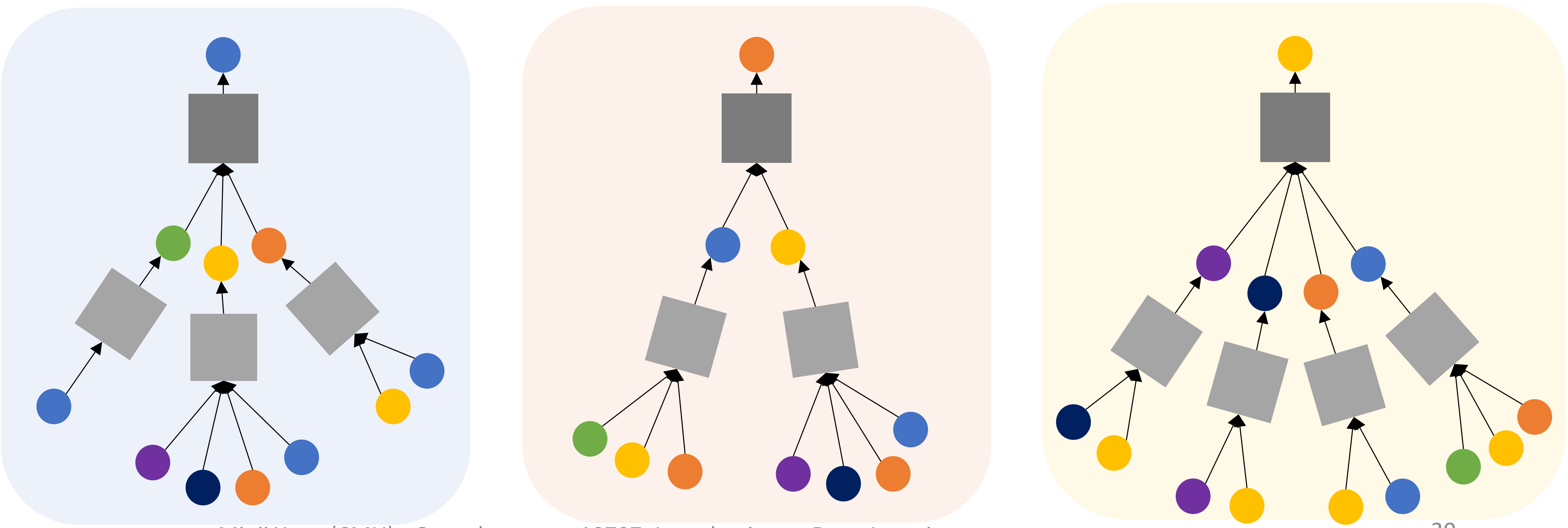


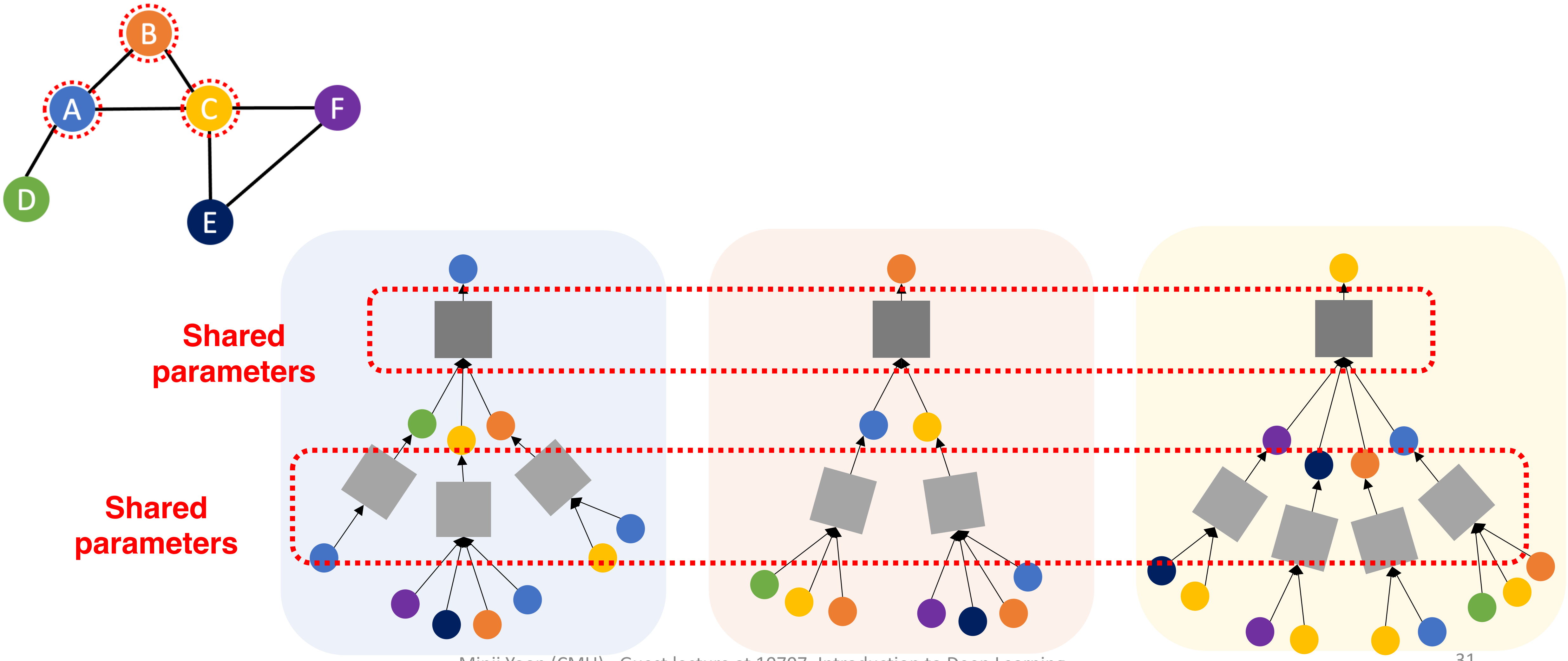
[3] Wu, Felix, et al. "Simplifying graph convolutional networks."

Computation graphs



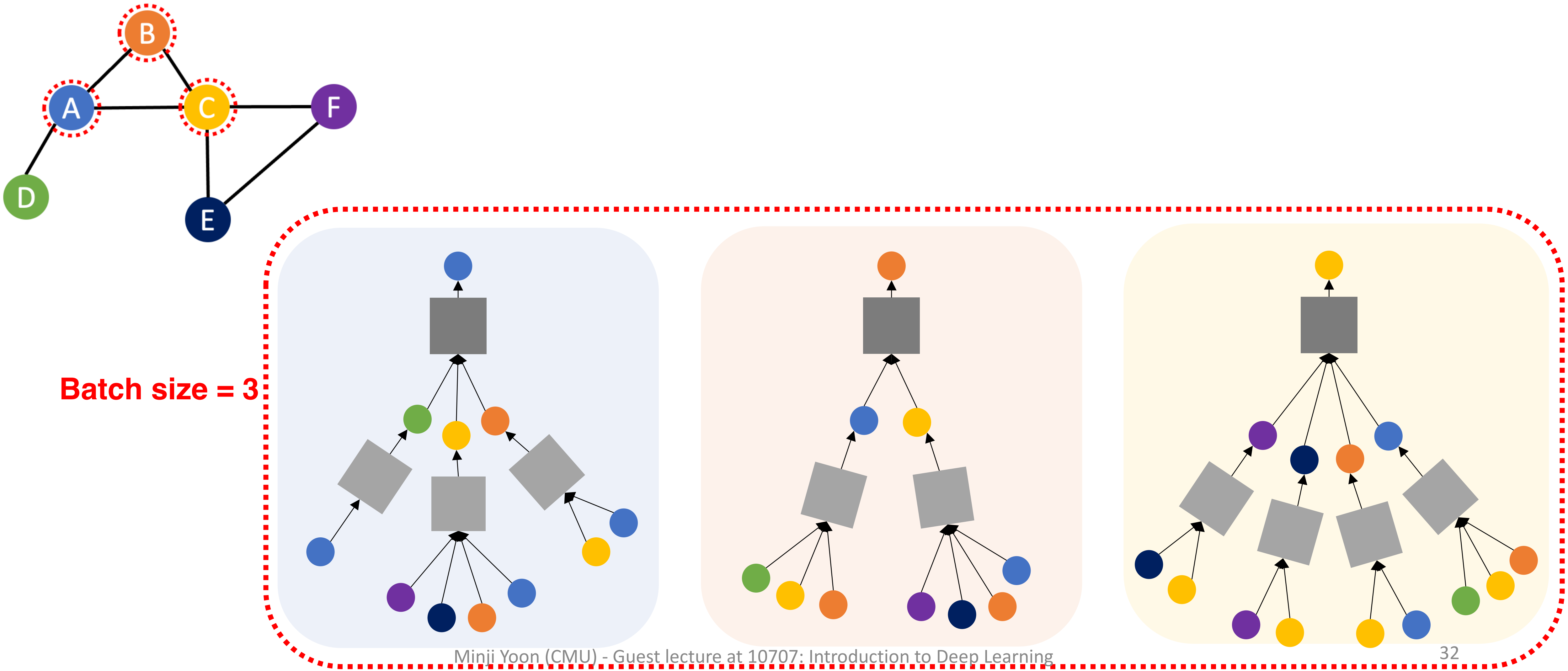


Computation graphs



Batch execution

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



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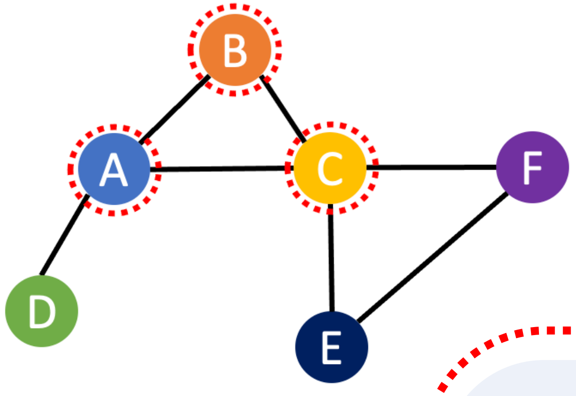
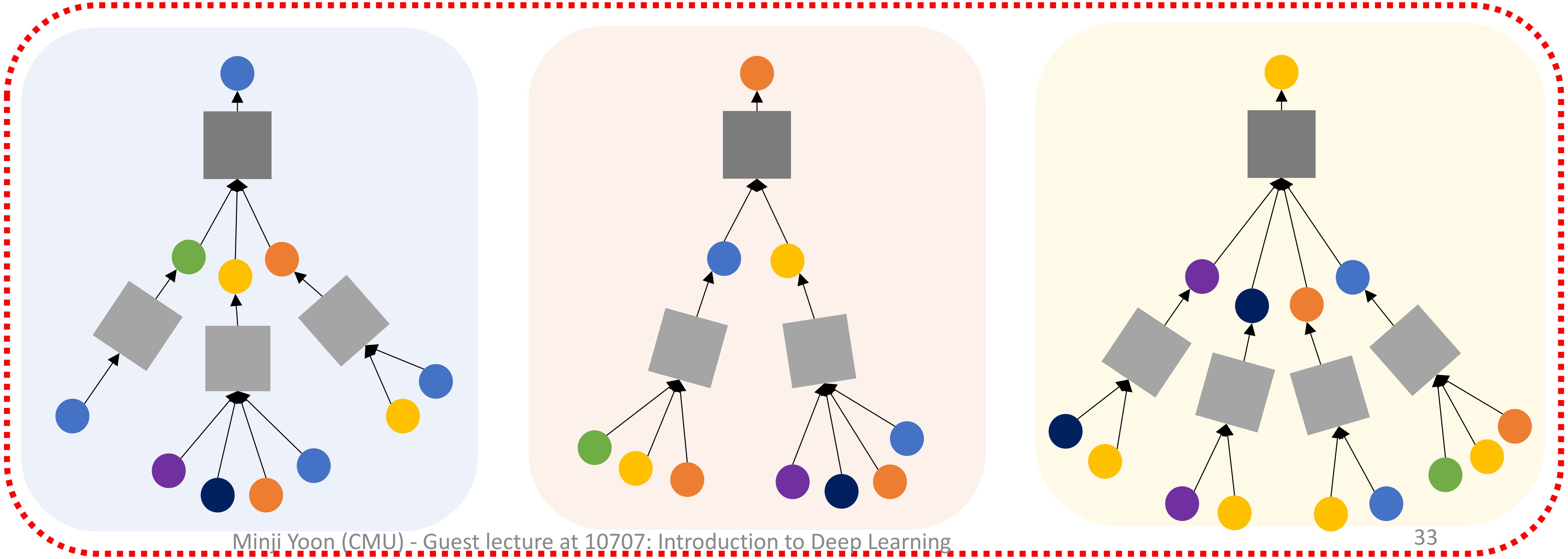
$$\boldsymbol{H}^{(l)} = \sigma(\widetilde{(\boldsymbol{A}+\boldsymbol{I})}\boldsymbol{H}^{(l-1)}\boldsymbol{W}^{(l)})$$

Node embedding matrix

(row-normalized) **Adjacency matrix**



Batch size = 3



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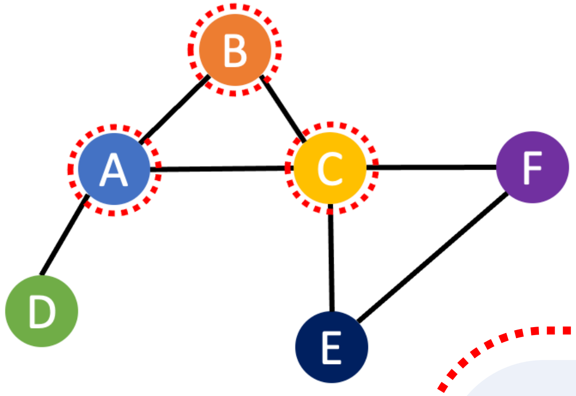
Fixed **Trainable**



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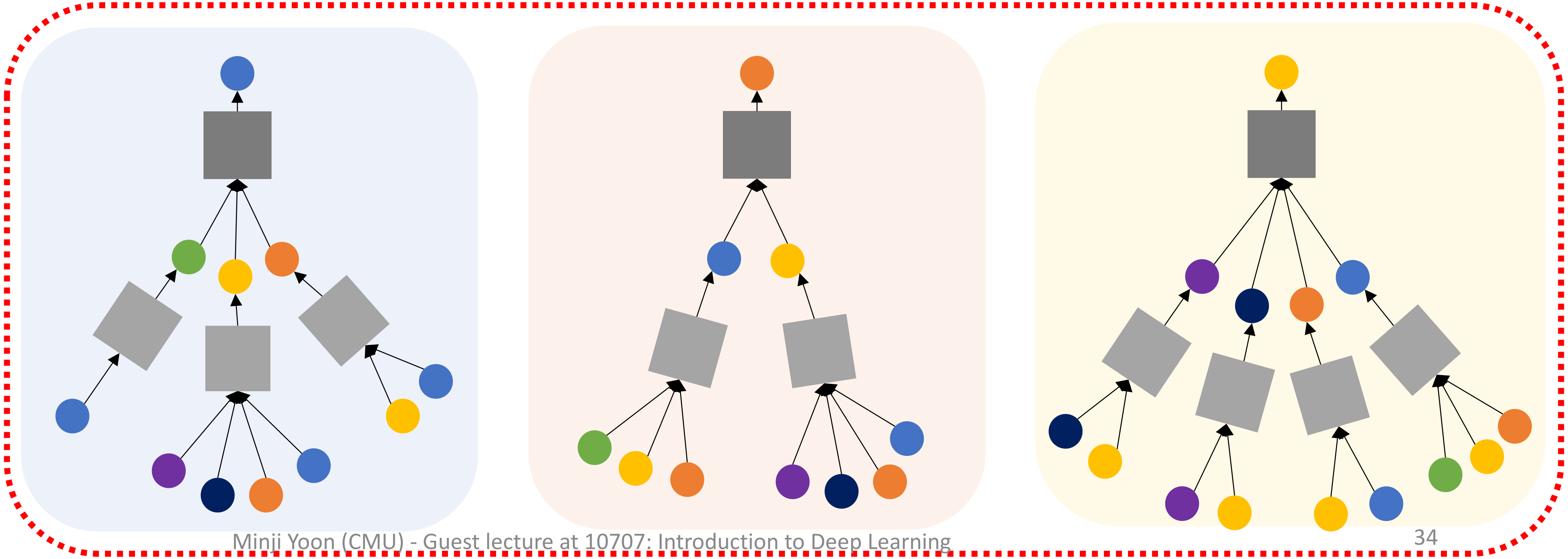
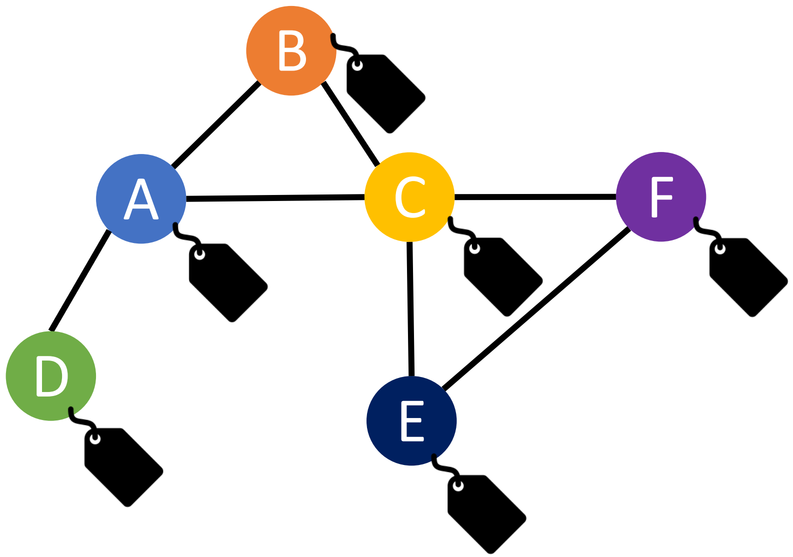


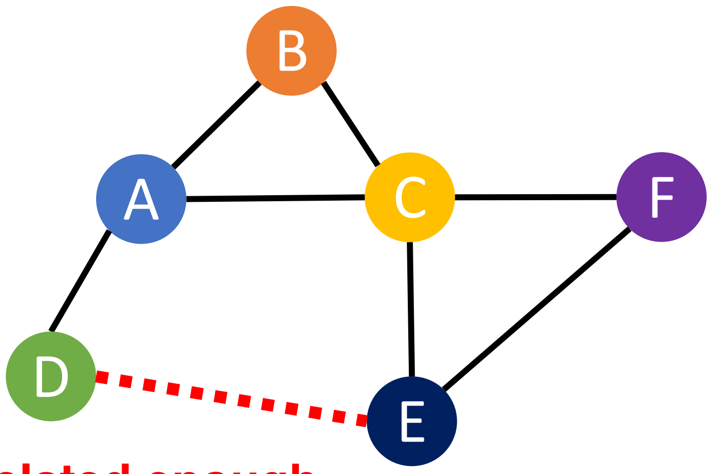
Downstream tasks

- Node-level prediction



Downstream tasks

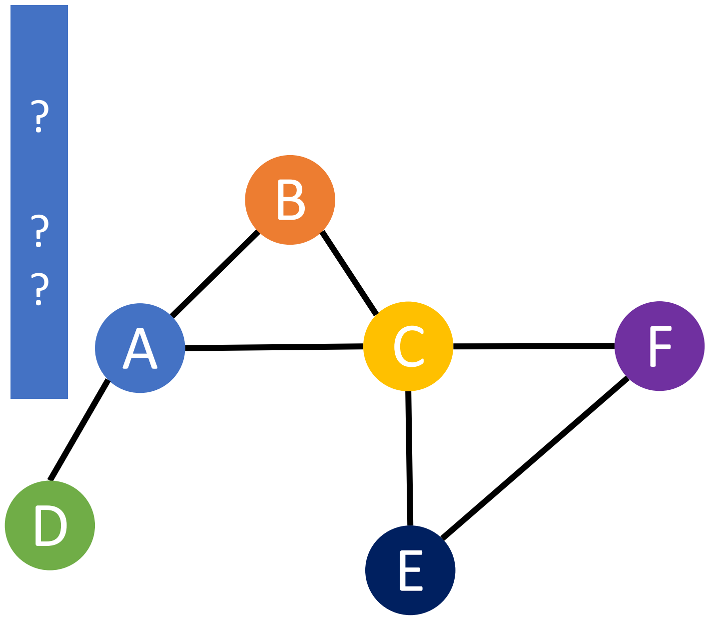
- Node-level prediction
- Edge-level prediction



D and E are related enough to be connected?

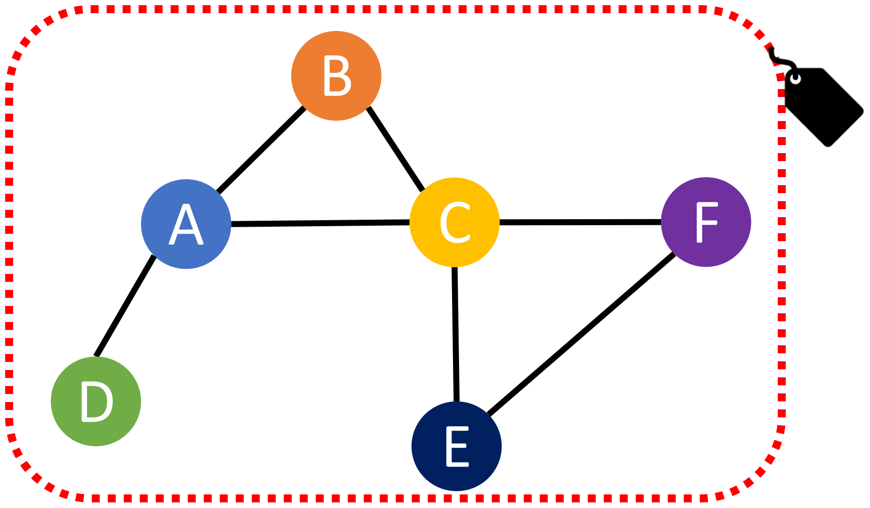
Downstream tasks

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



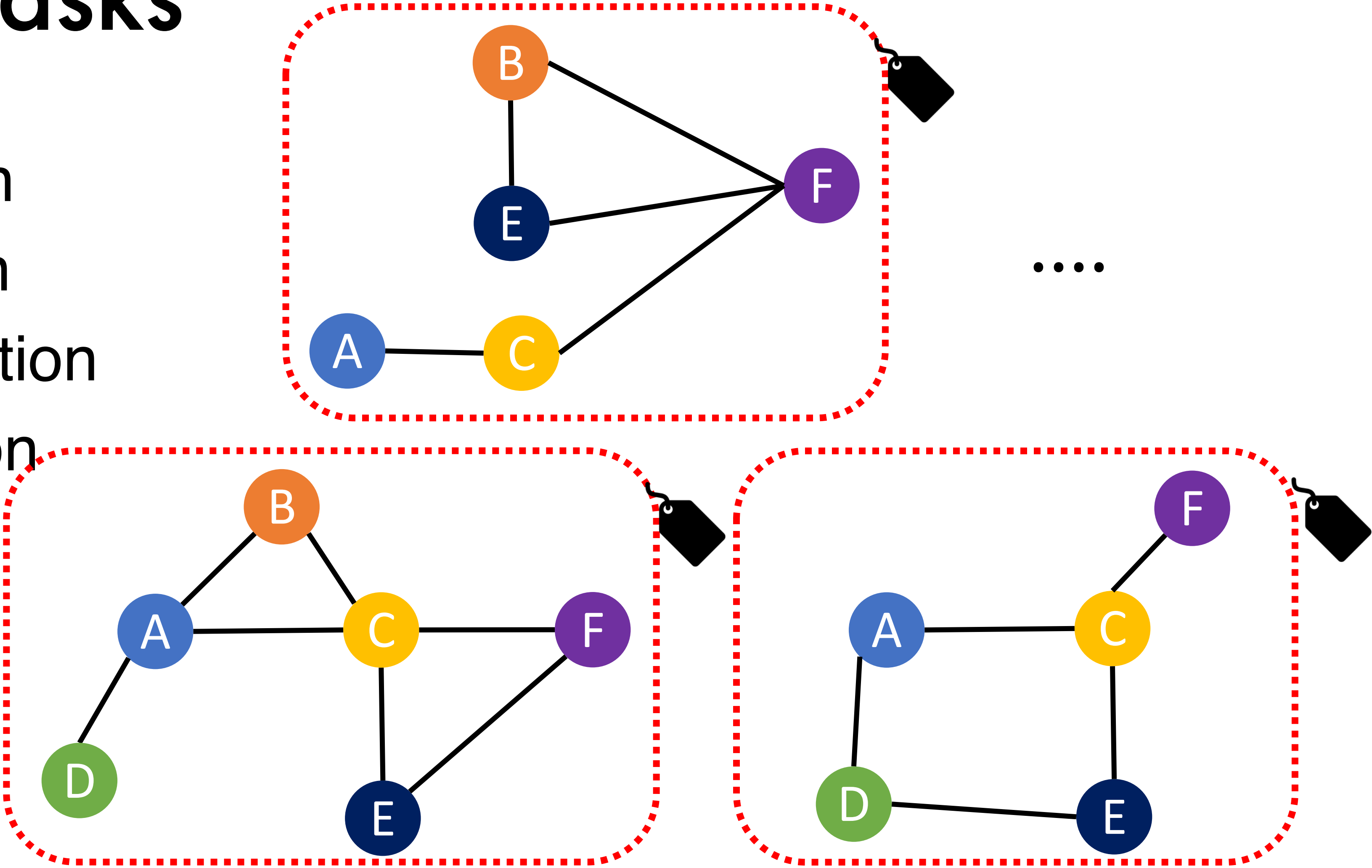
Downstream tasks

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



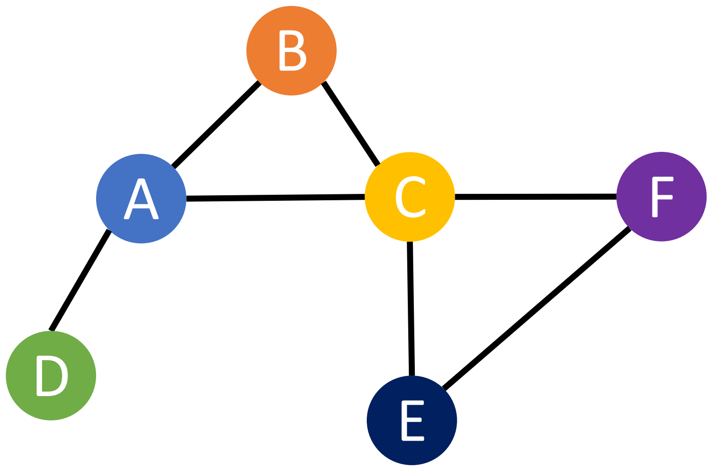
Downstream tasks

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

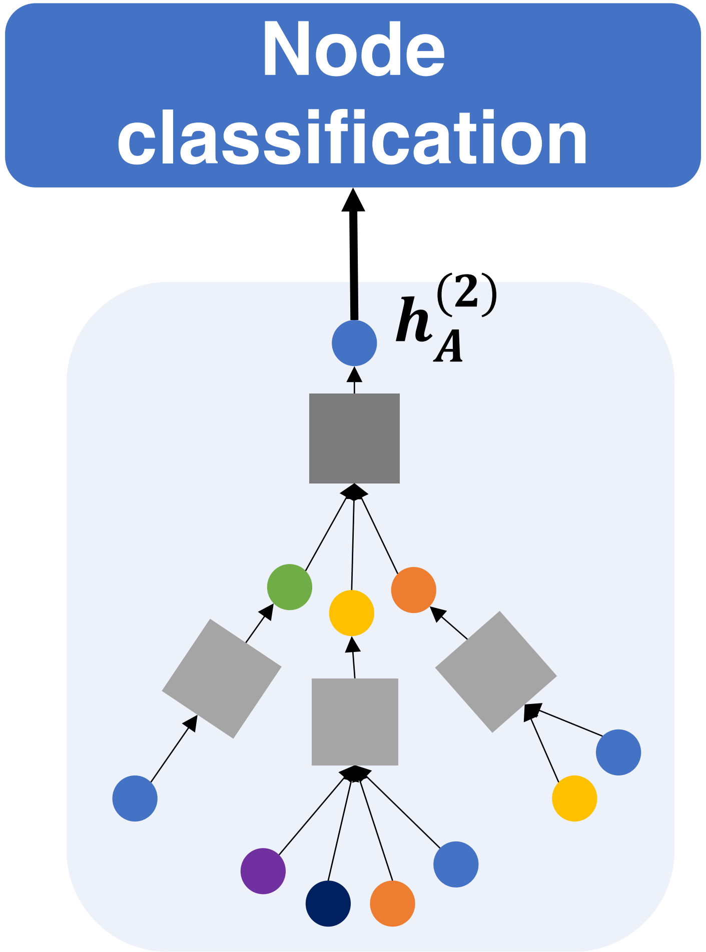


Downstream tasks

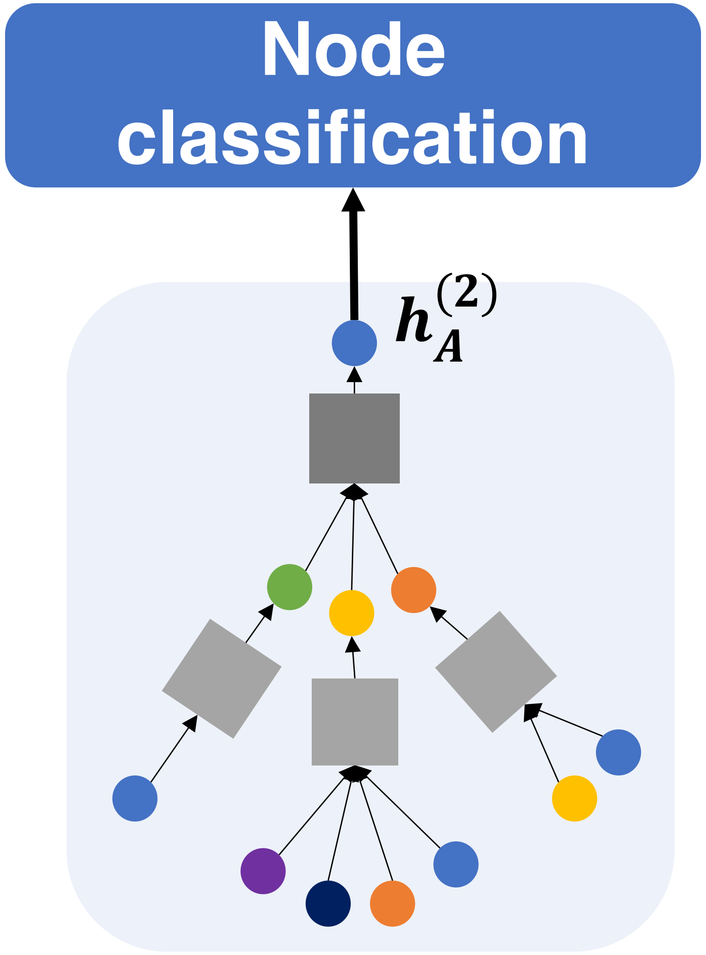
- **Node-level prediction**
- Edge-level prediction
- Attribute-level prediction
- **Graph-level prediction**

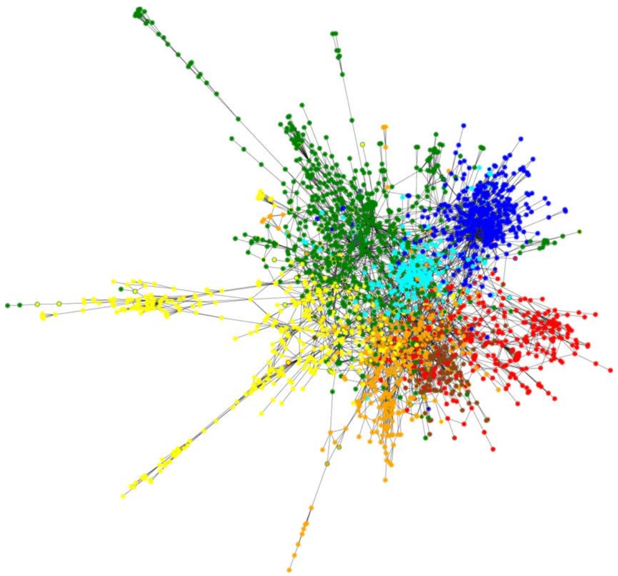


Node-level prediction tasks



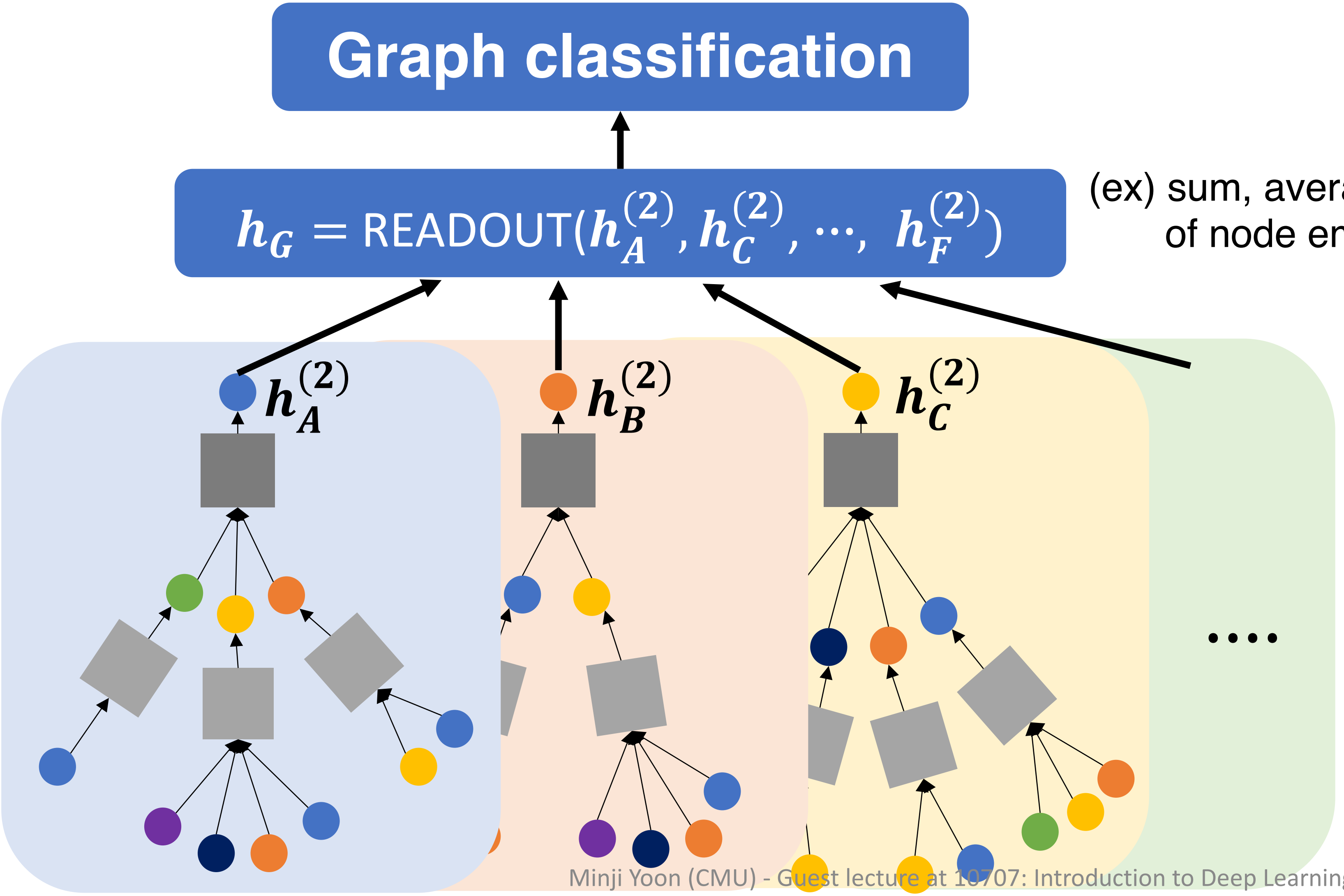
Node-level prediction tasks





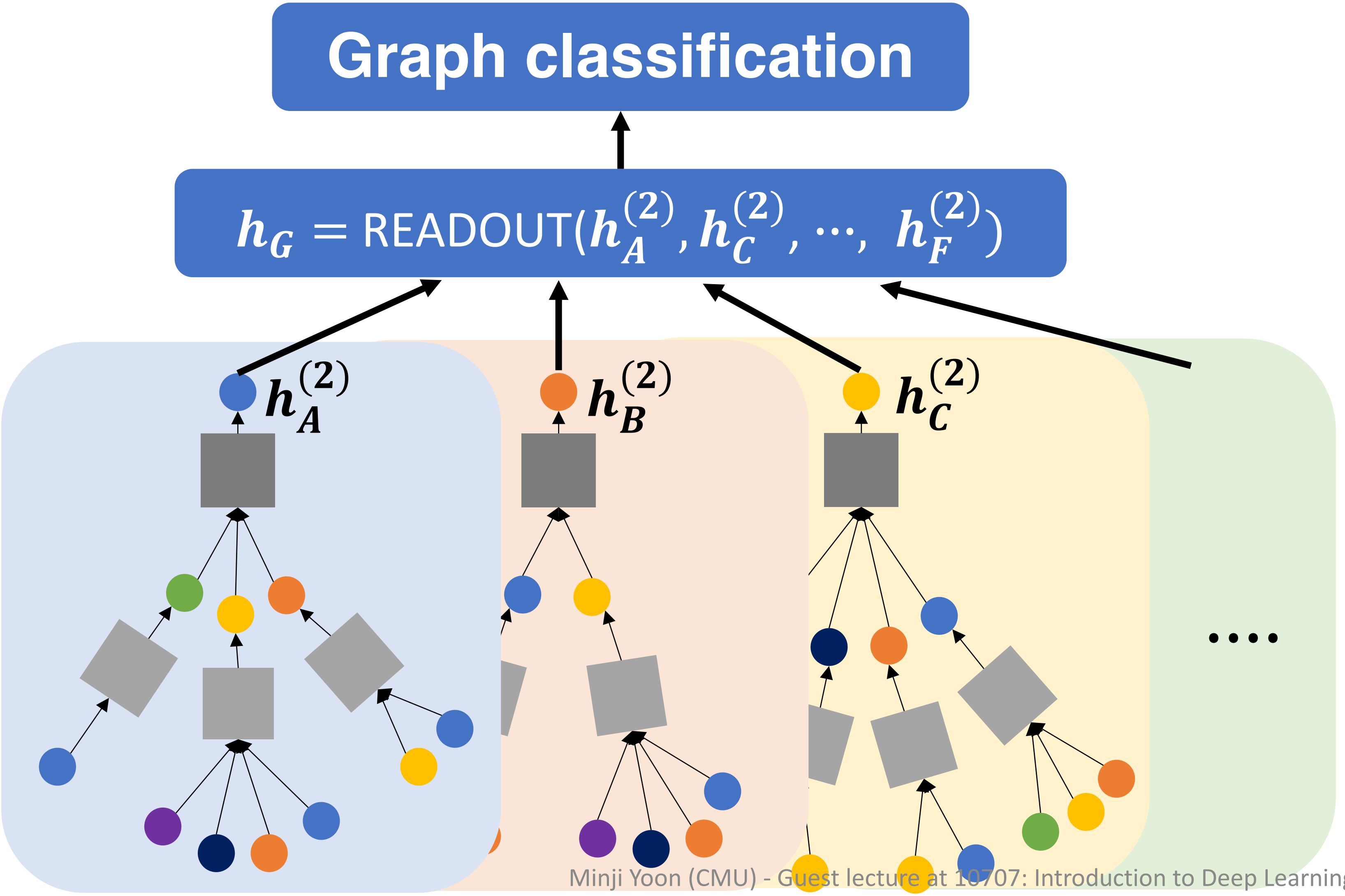
- Classify **papers** into topics on **citation networks**
- Cluster **posts** into subgroups on **Reddit networks**
- Classify **products** into categories on **Amazon co-purchase graphs**

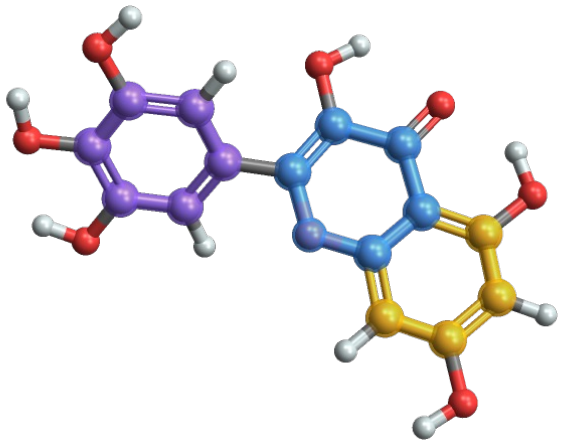
Graph-level prediction tasks



(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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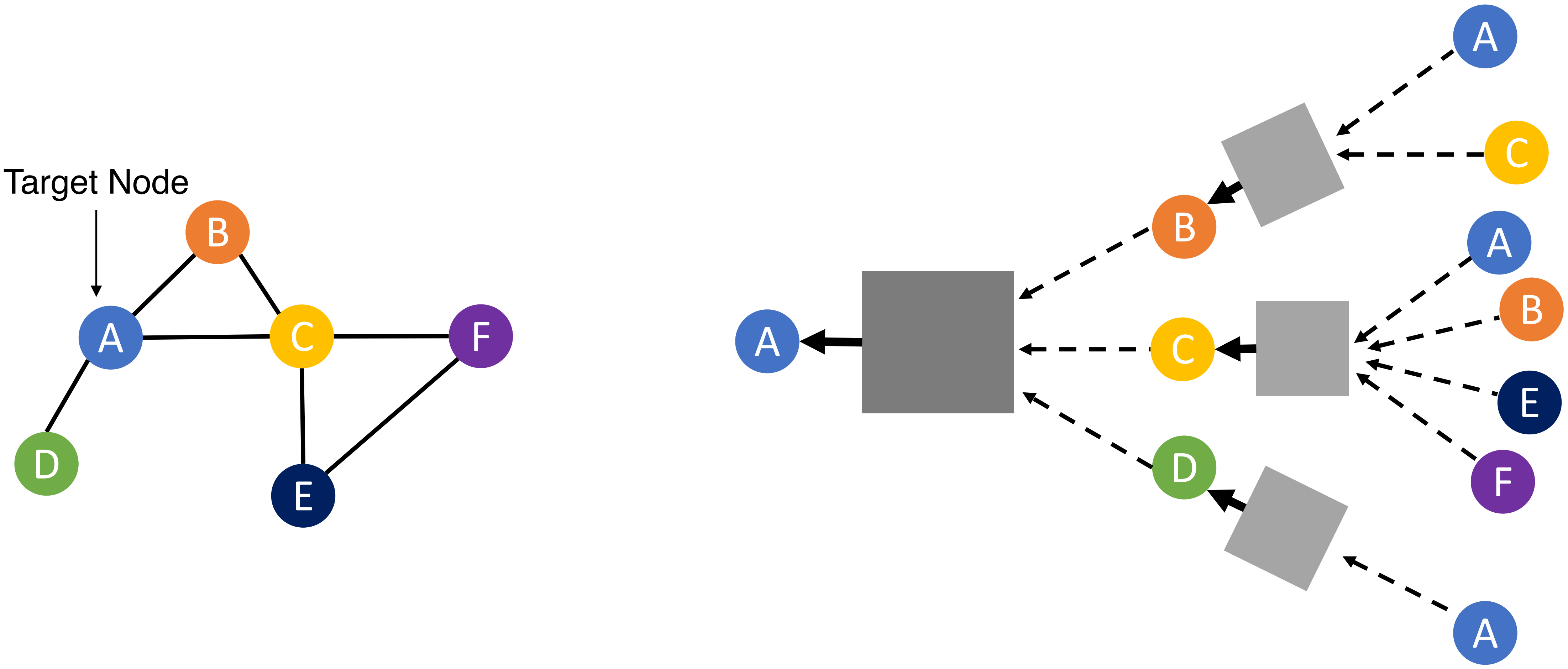
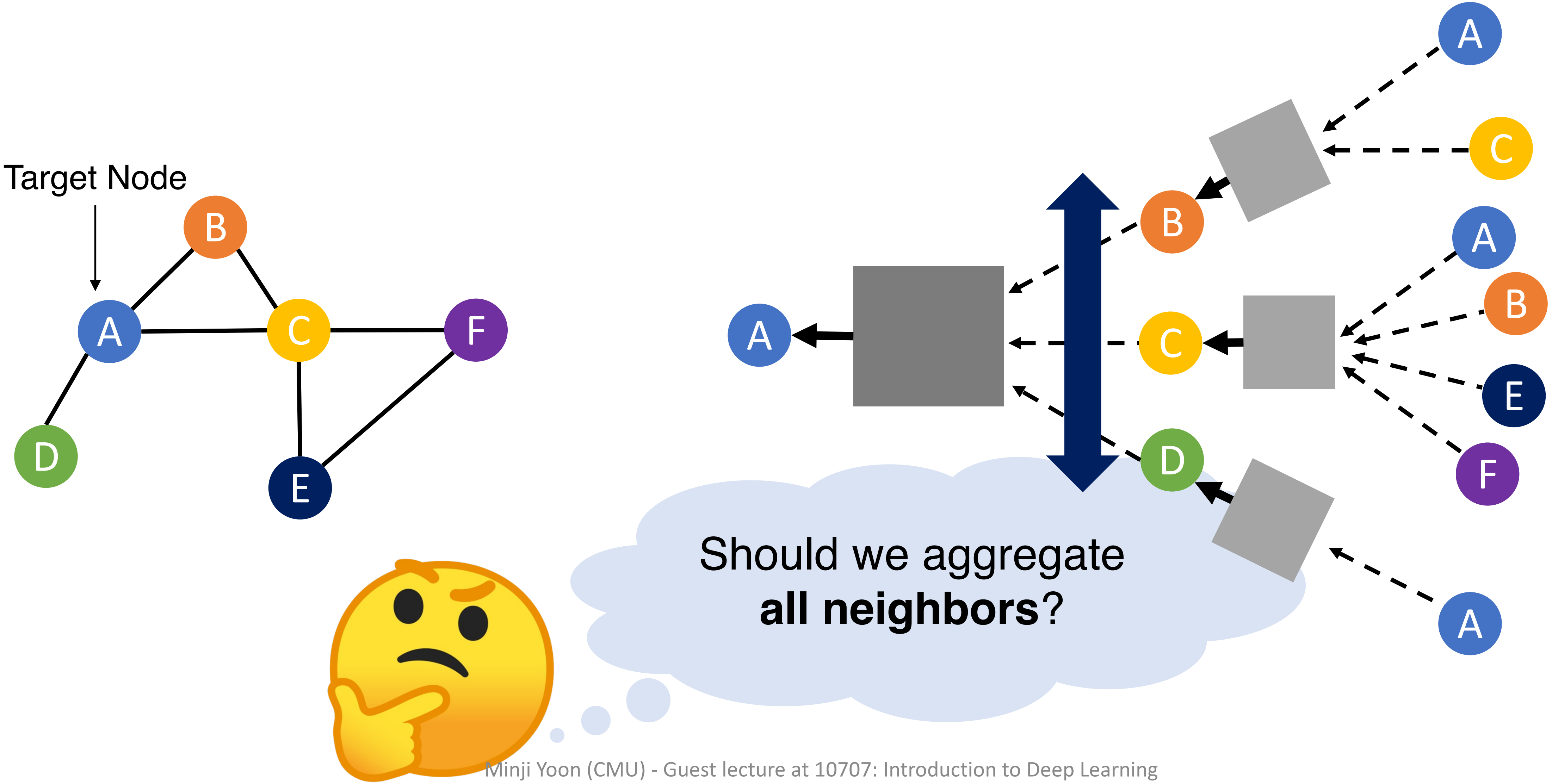
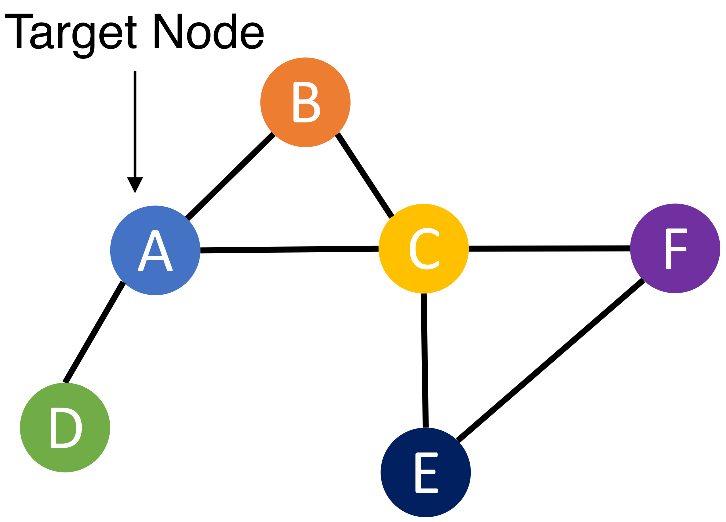
Graph Neural Networks

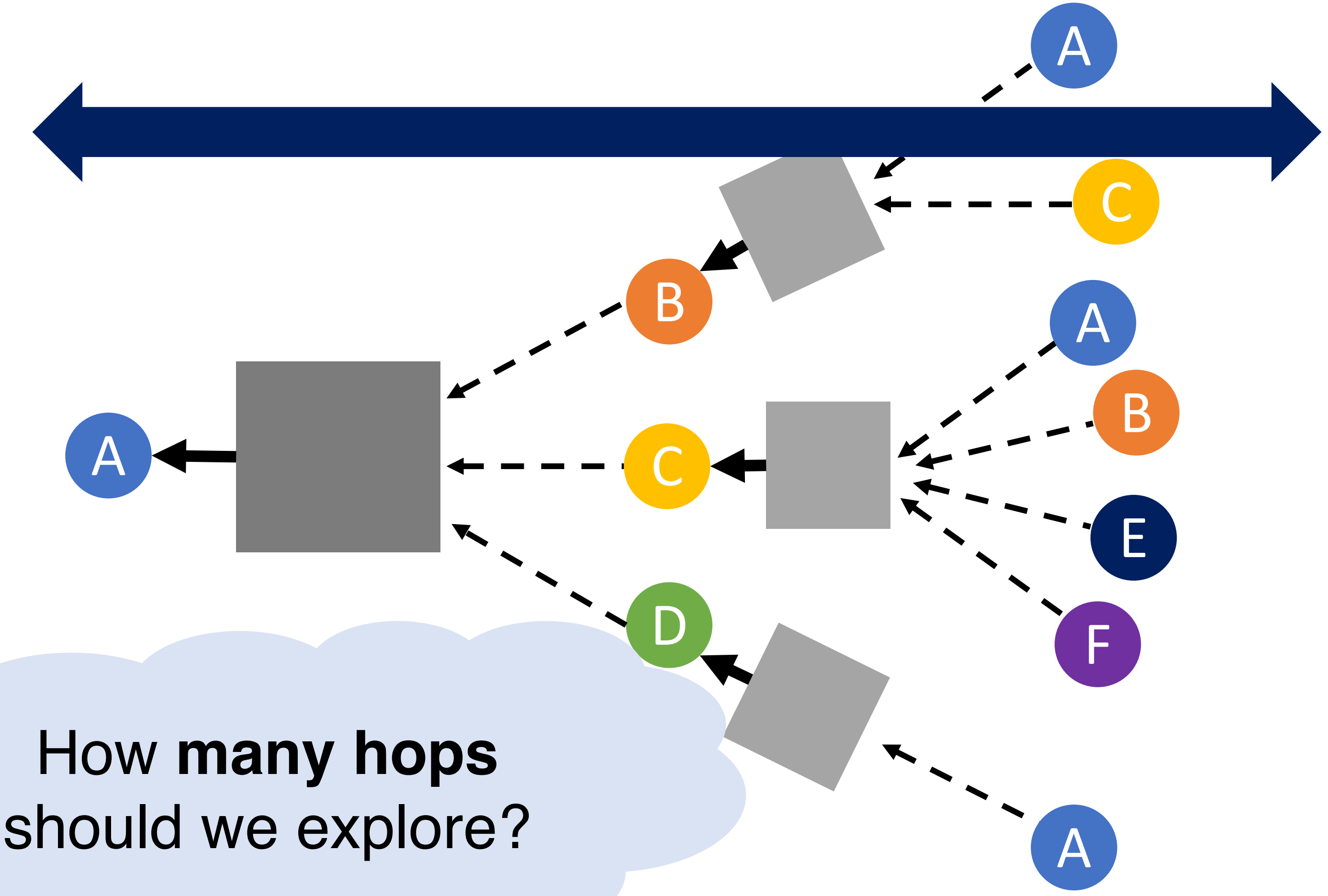


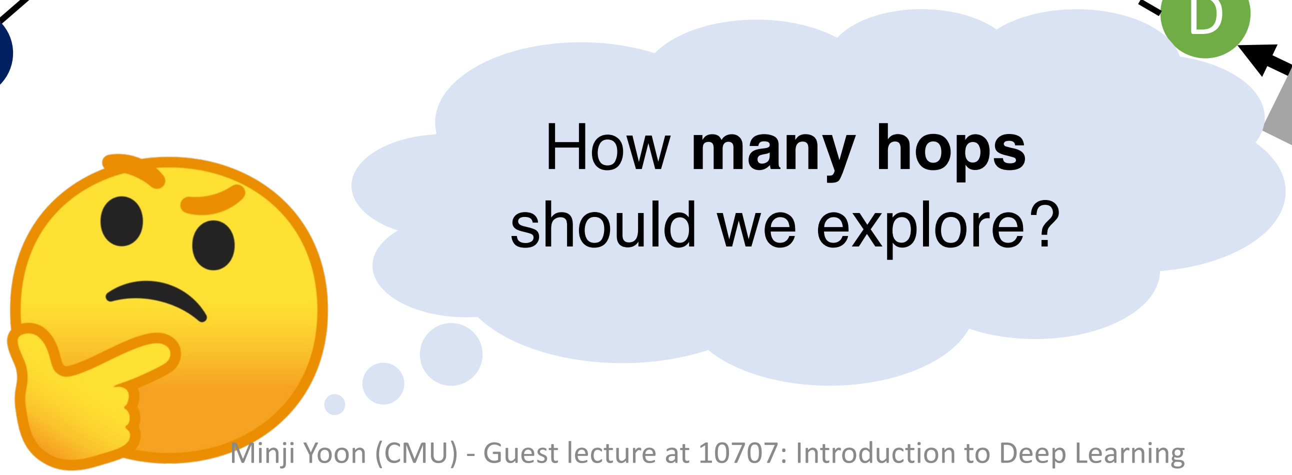
Graph Neural Networks - Width



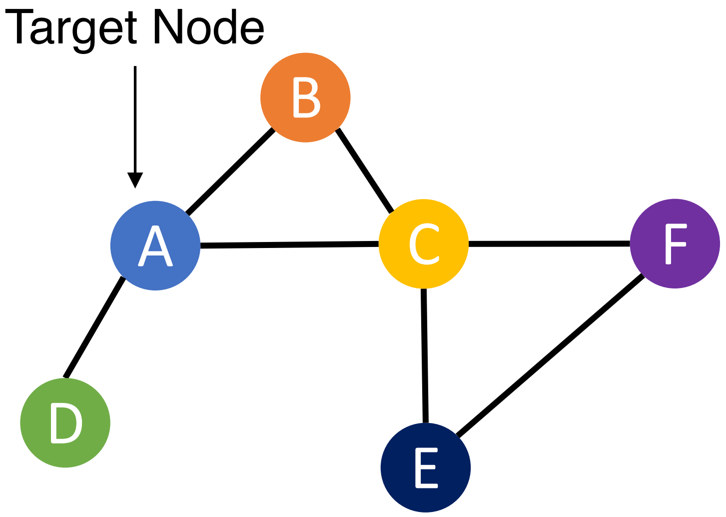
Graph Neural Networks - Depth

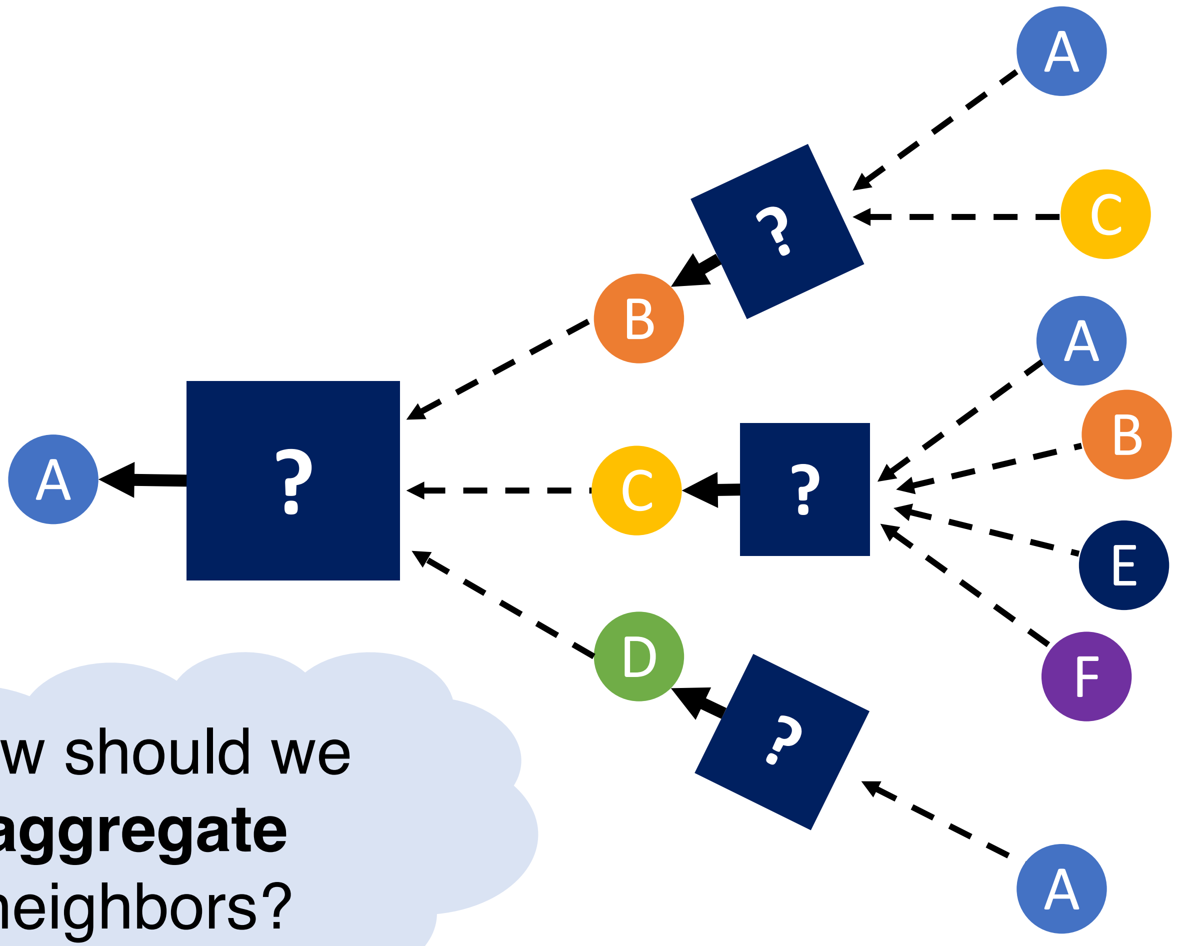






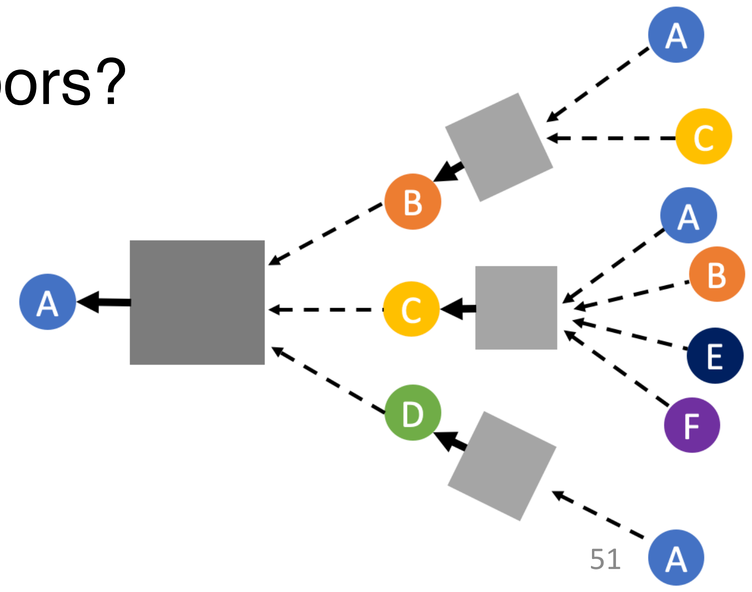
Graph Neural Networks - Aggregation





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

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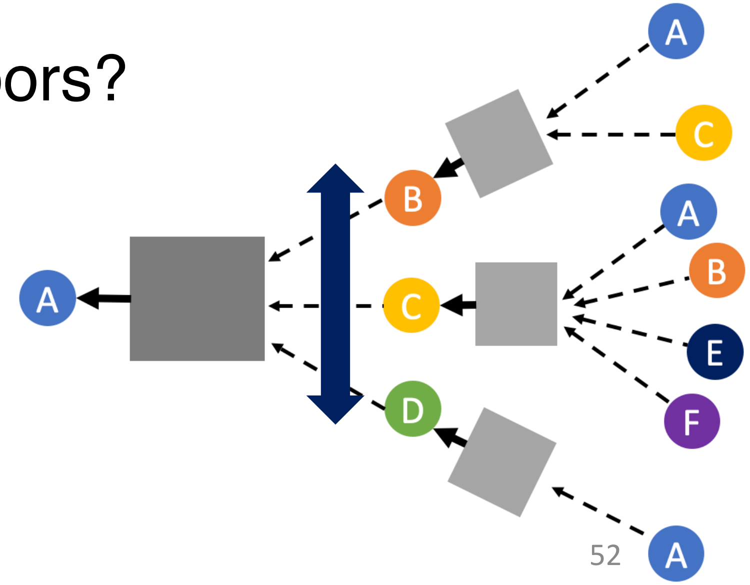
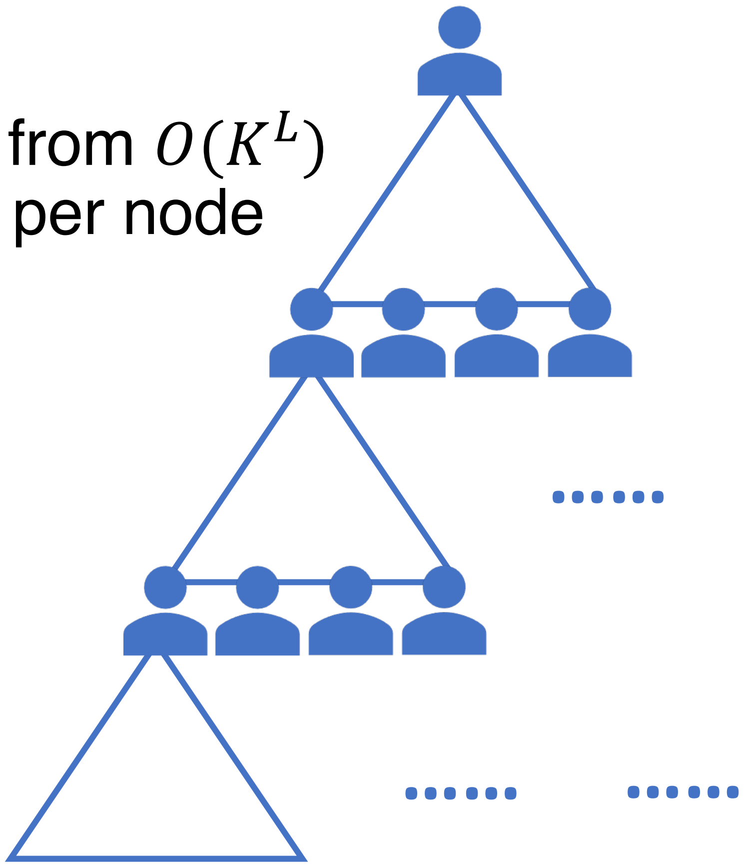


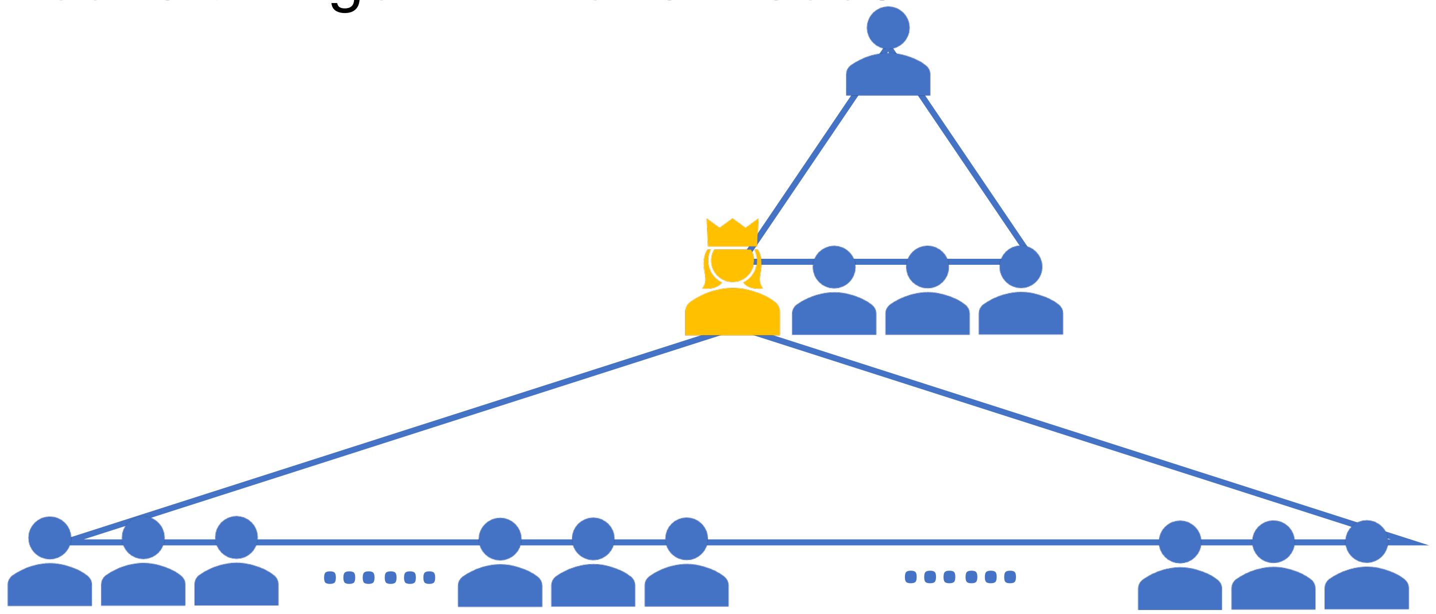
Aggregation Width in GNNs

- 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

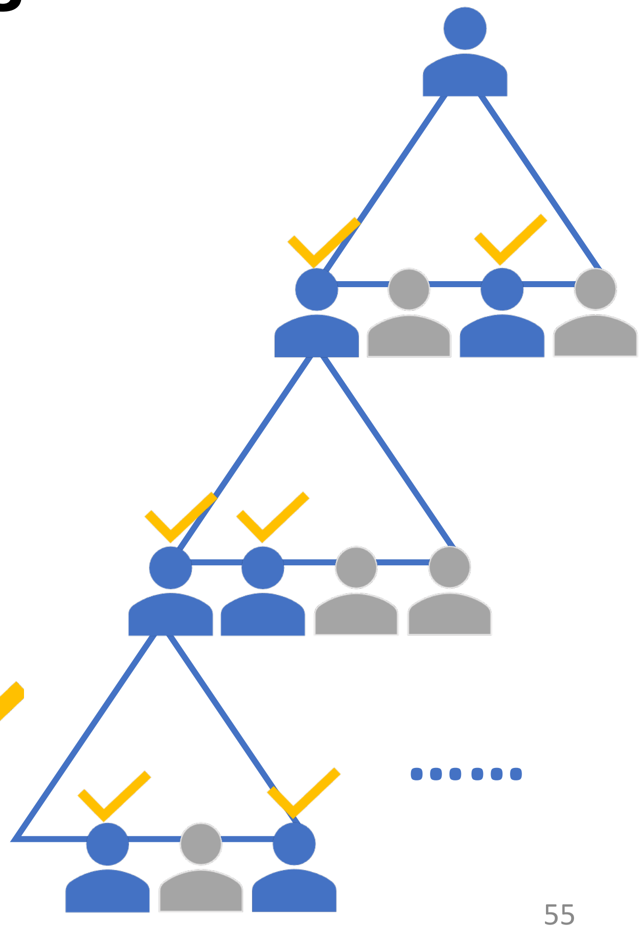
- If we aggregate all neighbors, GNNs have scalability issues
- Neighbor explosion
  - Hub nodes who are connected to a huge number of nodes



Aggregation Width in GNNs

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

Sample the 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]

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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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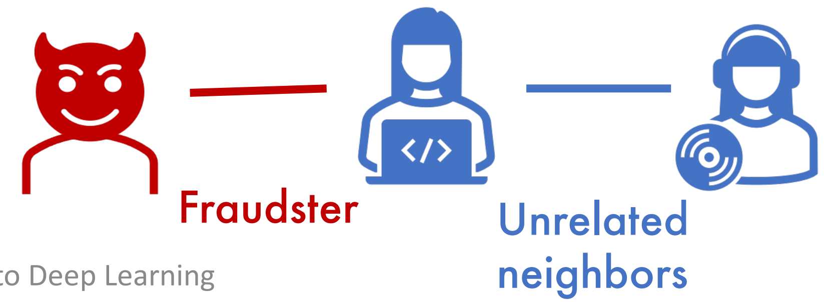
Real-world graphs are noisy!!



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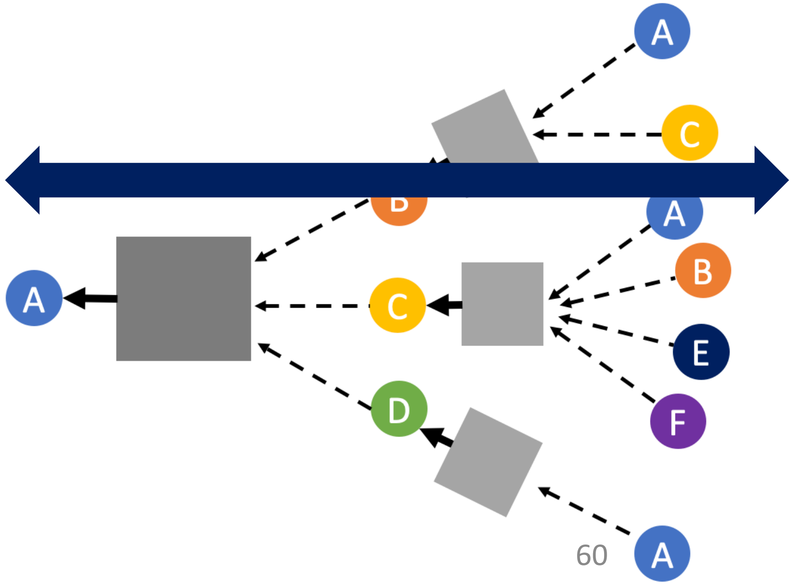
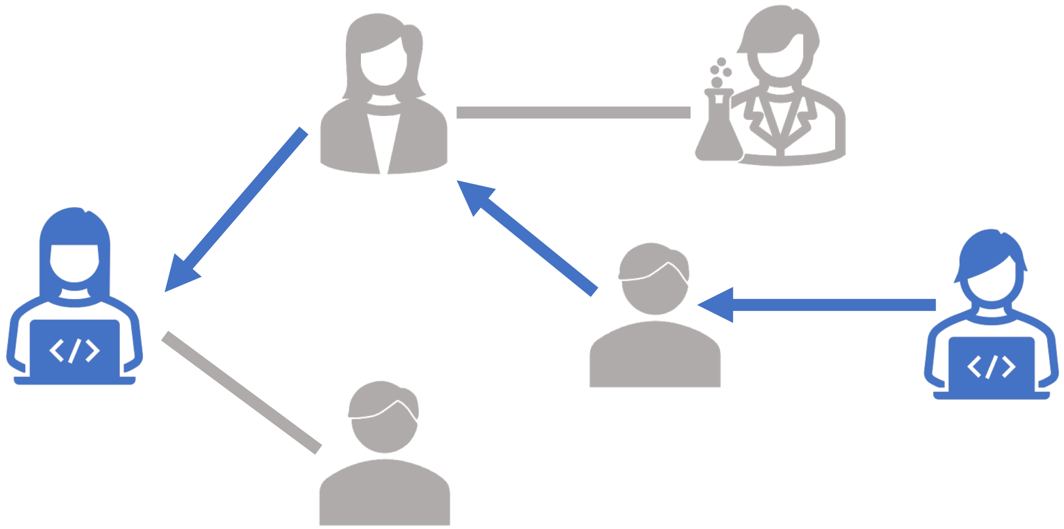


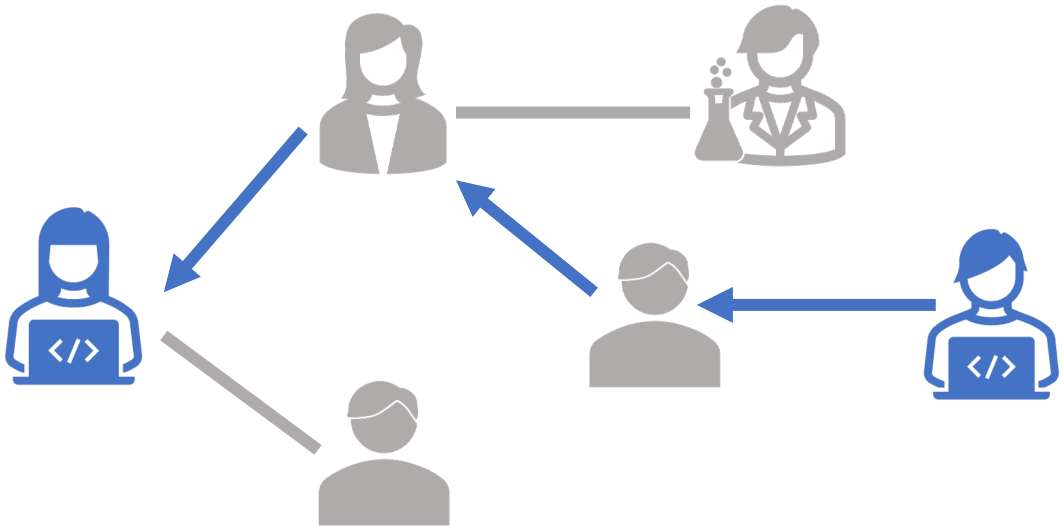
Aggregation Depth in GNNs

- 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?

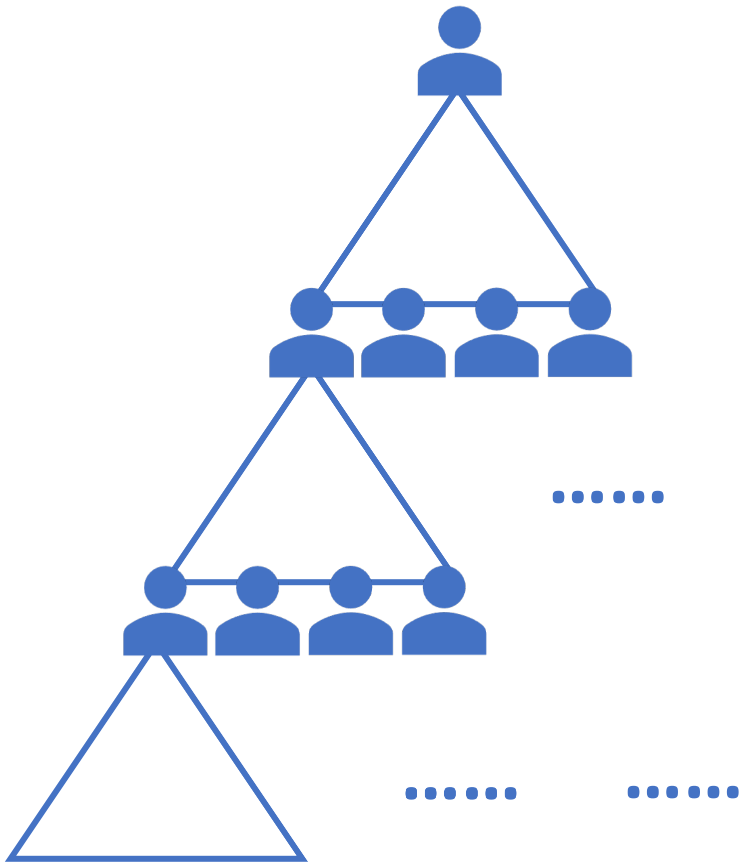


Aggregation Depth in GNNs

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

Aggregation Depth in GNNs

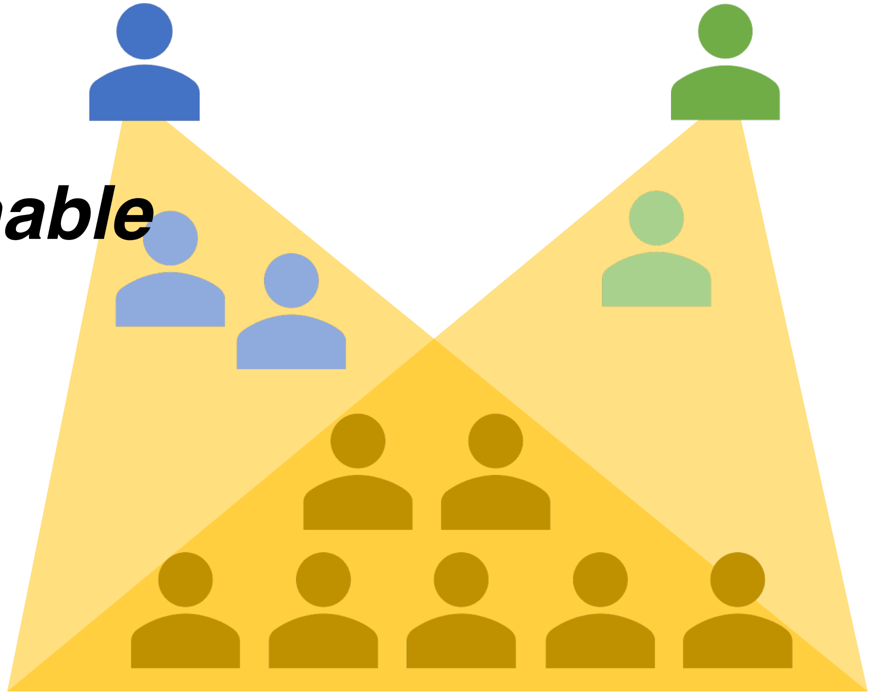
- When we increase the depth L more than this, GNNs face neighbor explosion $O(K^L)$
  - **Over-smoothing**
  - **Over-squashing**



Aggregation Depth in GNNs

Over-smoothing[10]

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

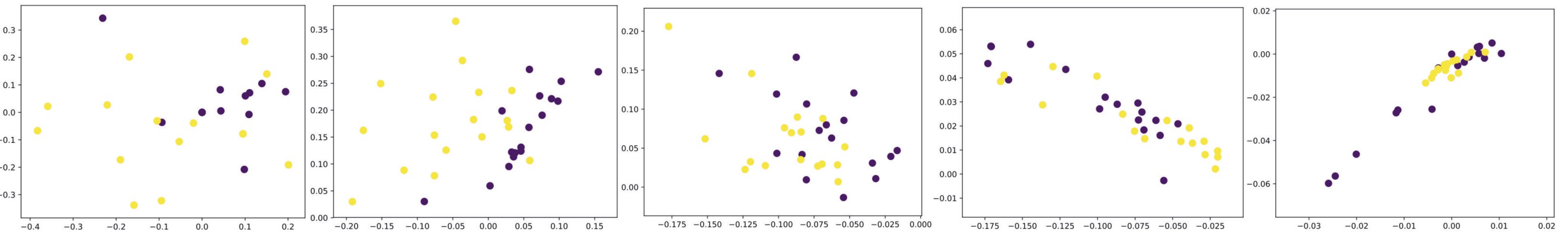


[10] Qimai Li, et al. "Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning"

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

Mitigate over-smoothing

PairNorm[11]

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

Connected pairs　　Disconnected pairs

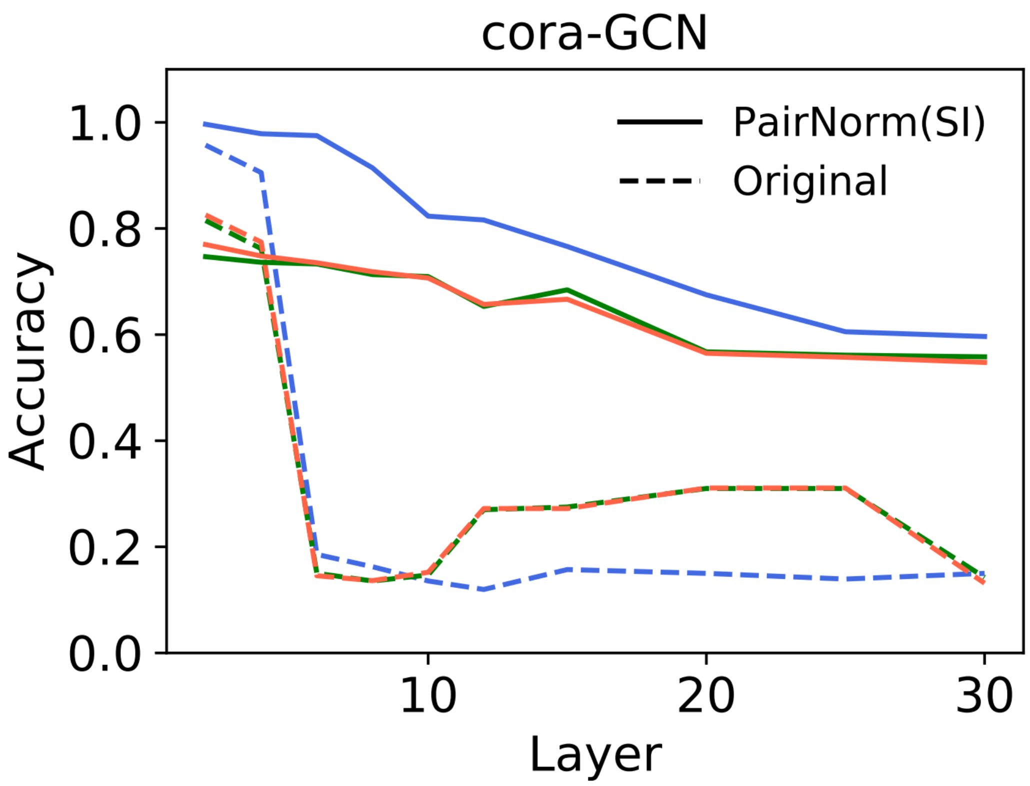
$$\mathrm{TPSD}(\dot{X}) = \sum_{(i,j)\in\mathcal{E}} ||\dot{x}_i - \dot{x}_j||_2^2 + \sum_{(i,j)\notin\mathcal{E}} ||\dot{x}_i - \dot{x}_j||_2^2 = \boldsymbol{C}$$

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

Aggregation Depth in GNNs

Mitigate over-smoothing

PairNorm[11]

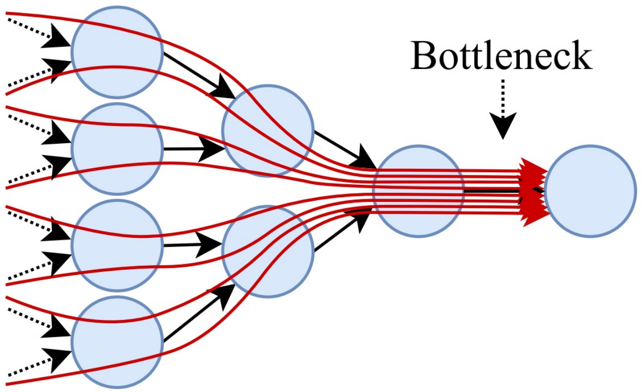


[11] Lingxiao Zhao, et al. "PAIRNORM: TACKLING OVERSMOOTHING IN GNNS"

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"

Aggregation Depth in GNNs

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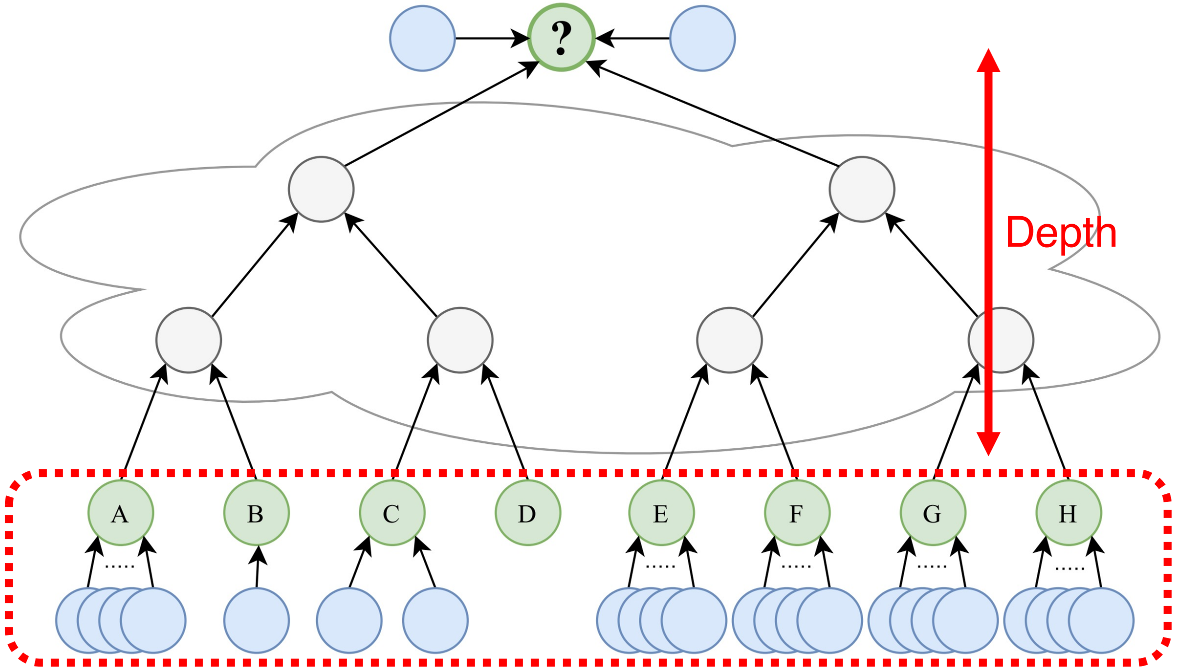

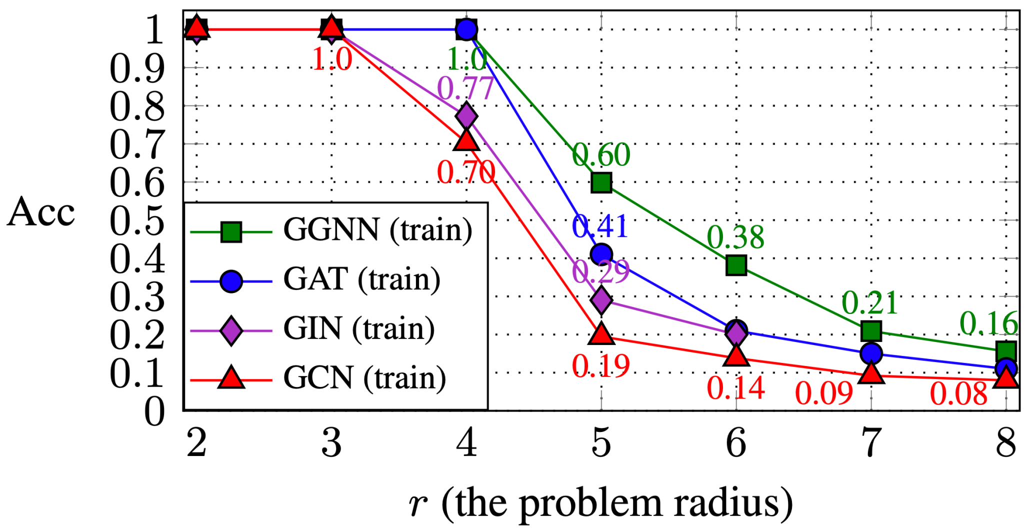

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Aggregation Depth in GNNs

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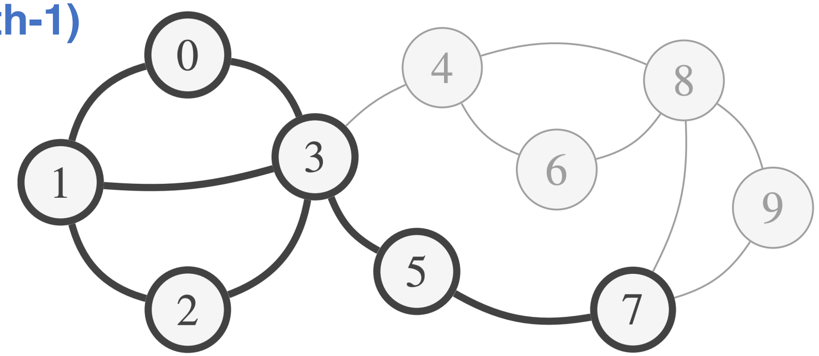
- **Depth-1**: neighborhood that each node aggregates information from
- **Depth-2**: number of layers in GNNs

Depth of neighborhood
(Depth-1)



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

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

Aggregation Depth in GNNs

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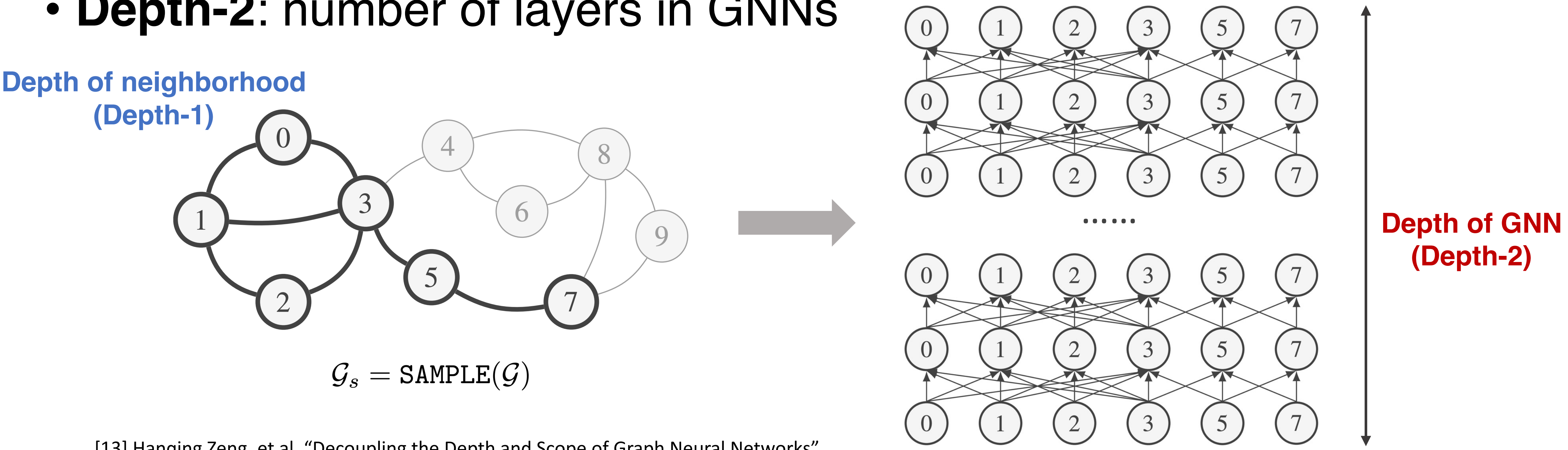

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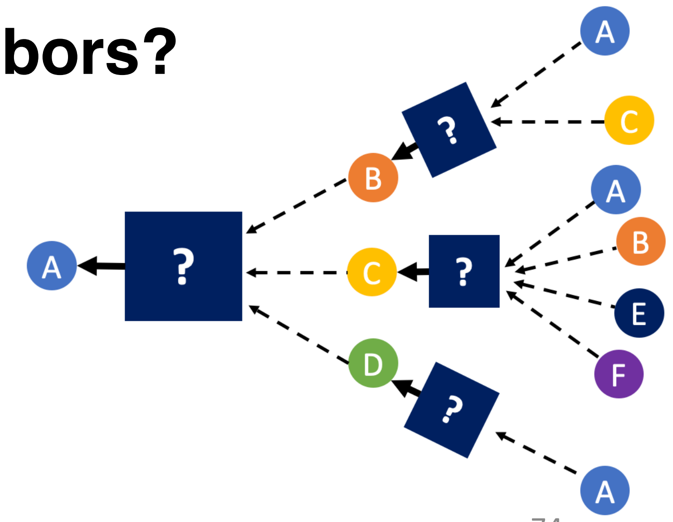


Aggregation strategy in GNNs

In each layer l :

Aggregate over neighbors

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

Transform messages

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

Aggregation strategy in GNNs

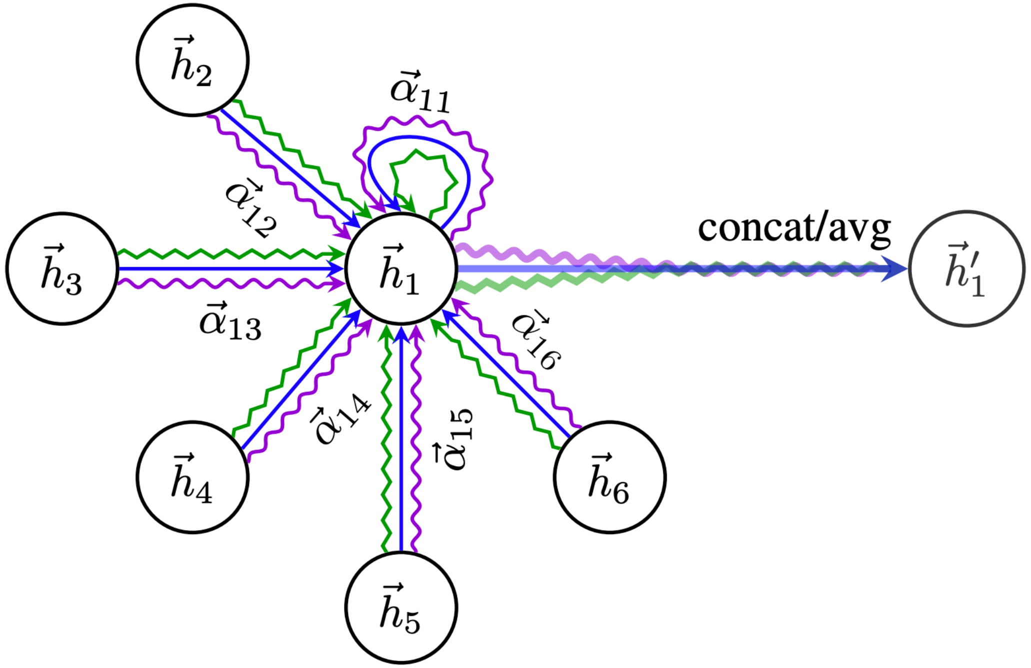
- GCN[1]
  - Average embeddings of neighboring nodes

[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

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

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?"

Aggregation strategy in GNNs

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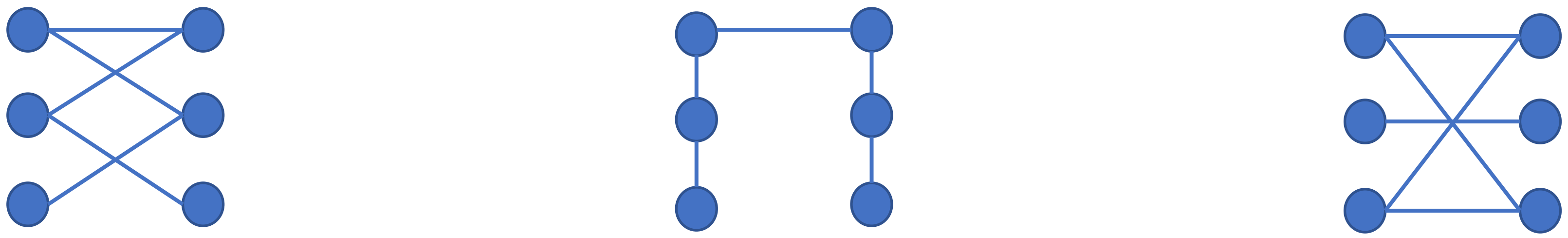

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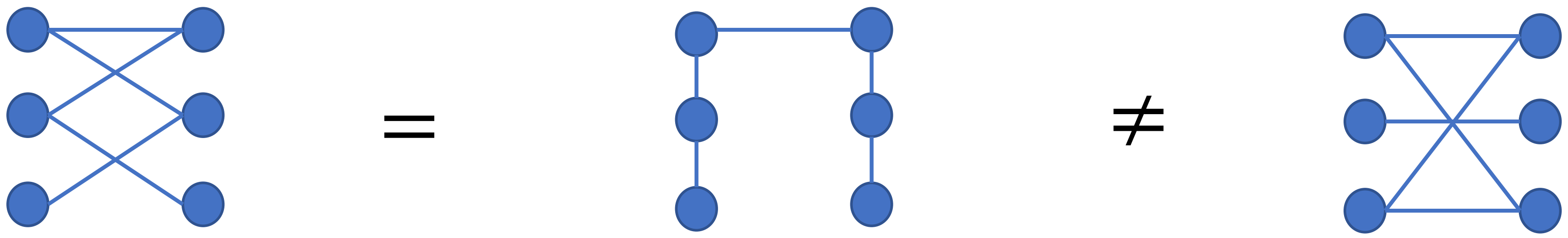

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Aggregation strategy in GNNs

- 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!!

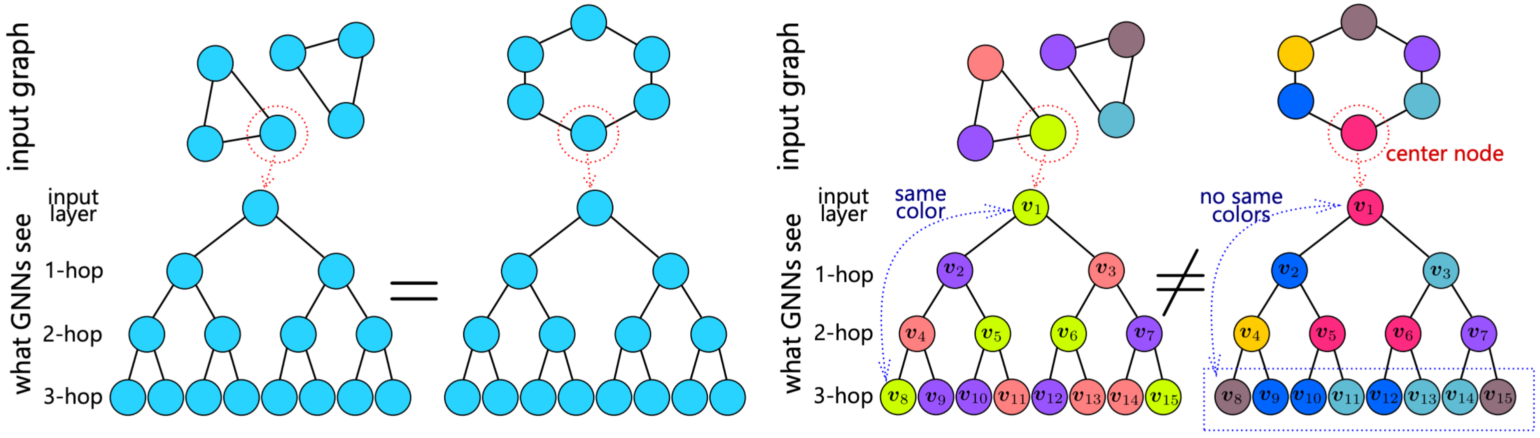
[2] Keyulu Xu., et al. "HOW POWERFUL ARE GRAPH NEURAL NETWORKS?"
[15] Boris Weisfeiler and AA Leman. "A reduction of a graph to a canonical form and an algebra arising during this reduction"

Aggregation strategy in GNNs

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

Aggregation strategy in GNNs

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

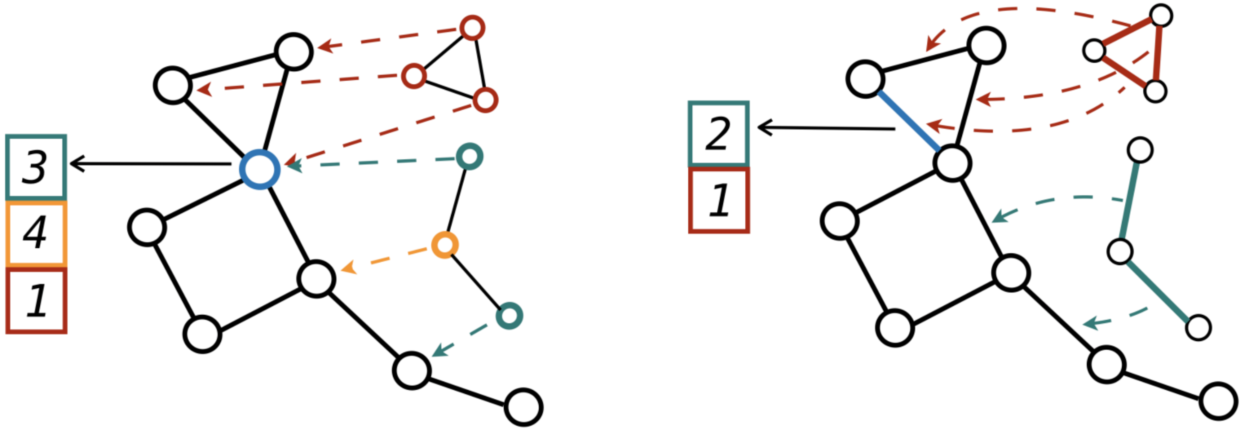


(a) Identical Features. (b) Random Features.

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

Aggregation strategy in GNNs

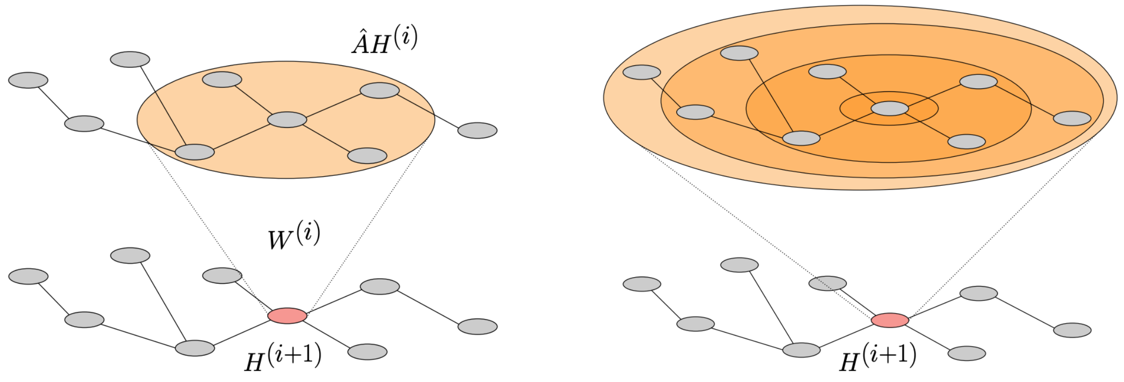
- Can we make more powerful GNNs?
- Augment nodes with handcrafted subgraph-based features[17]



[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[18]



$H^{(i+1)} = \sigma(\hat{A}H^{(i)}W^{(i)})$

(a) Traditional graph convolution.

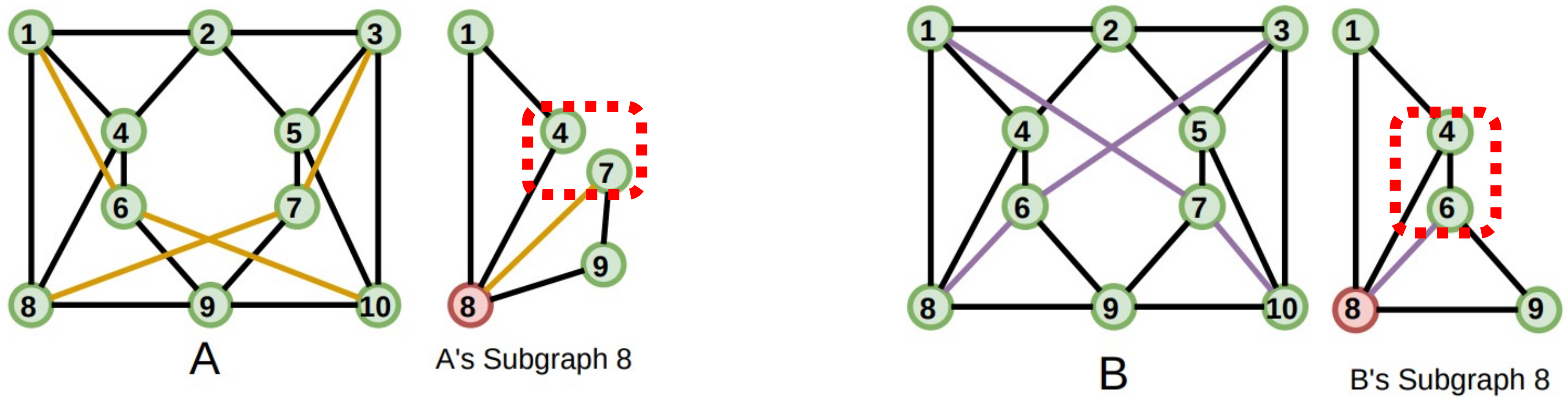
$H^{(i+1)} = \sigma\left(\hat{A}^0 H^{(i)} W_0^{(i)} \middle| \hat{A}^1 H^{(i)} W_1^{(i)} \middle| \dots\right)$

(b) Our mixed feature model.

[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[19]



[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.*

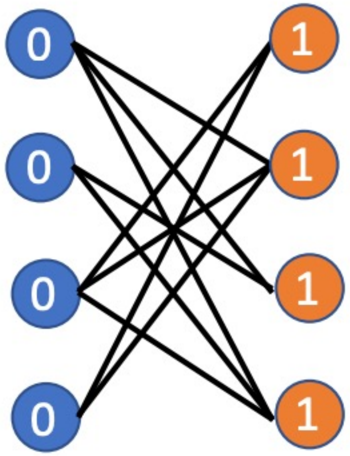
[20] Gabriele Corso, et al. "Principal Neighbourhood Aggregation for Graph Nets"

Aggregation strategy in GNNs

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

Aggregation strategy in GNNs

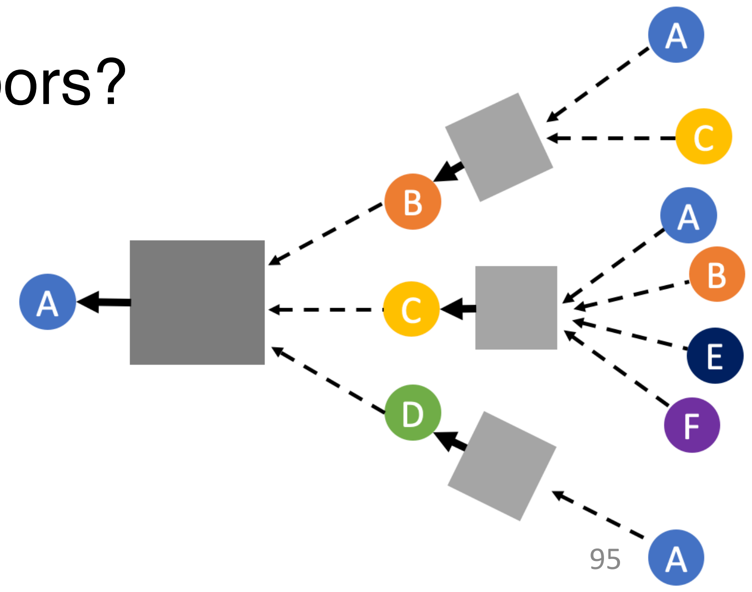
- Homophily assumption
  - Connected nodes are similar/related/informative
- How can we deal with **heterophilous networks**?[21,22]
  - Connected nodes have different class labels and dissimilar features



[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?"

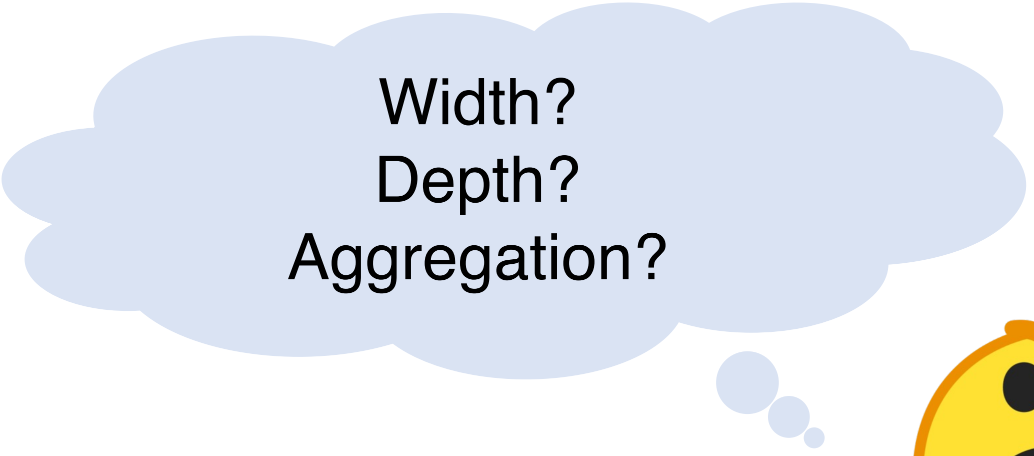
Graph Neural Network Architectures

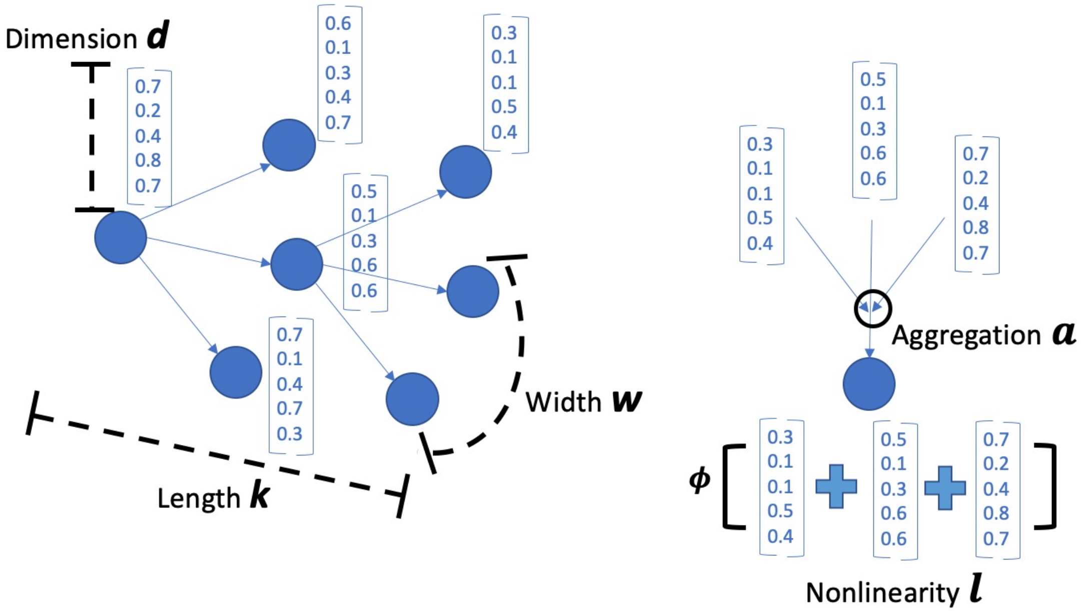
- Width
  - Which neighbors should we aggregate messages from?
- Depth
  - How many hops should we check?
- Aggregation
  - How should we aggregate messages from neighbors?



Neural Architecture Search for GNNs

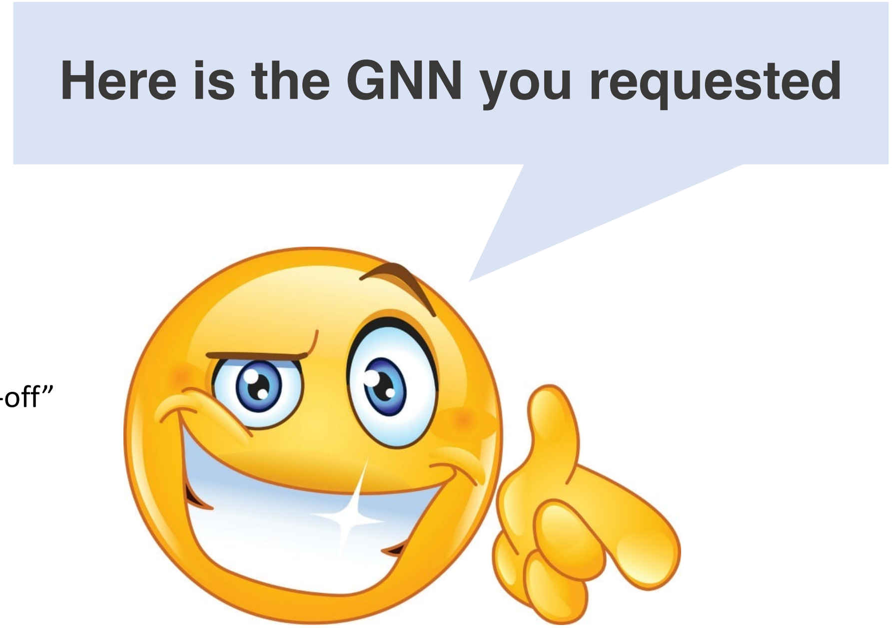
- Which *width, depth, and aggregation strategy* are proper for a given graph and task?





Neural Architecture Search for GNNs

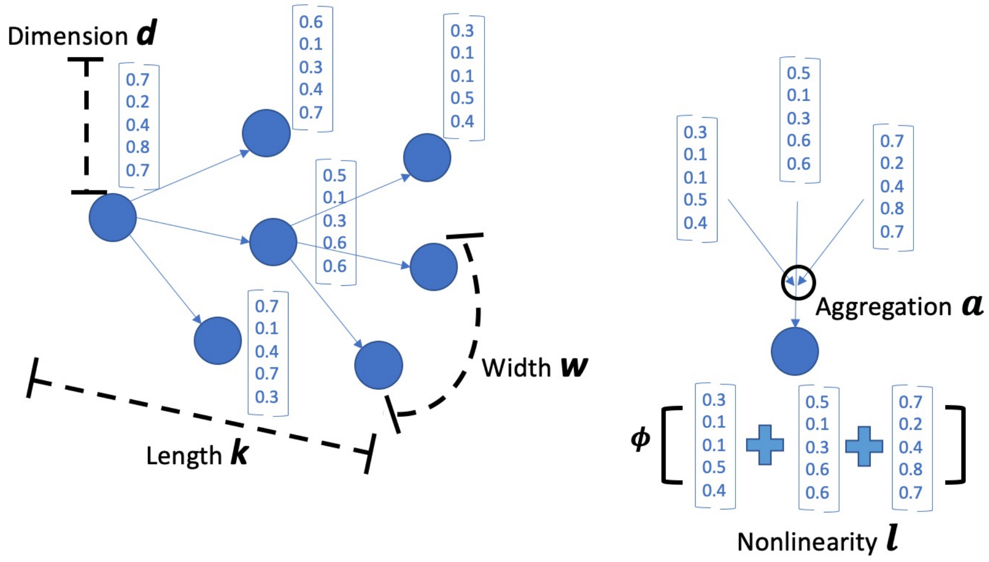
- Finding proper *width, depth, and aggregation strategy* for a given graph and task **automatically**[1,2,3]

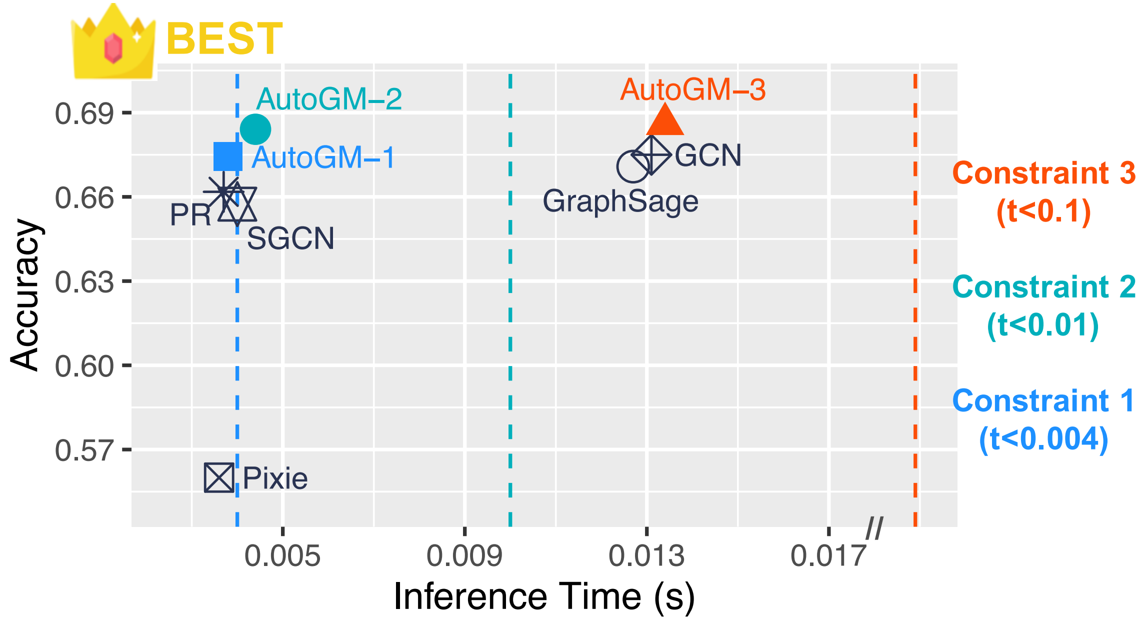


[23] Minji Yoon., et al. "Autonomous Graph Mining Algorithm Search with Best Speed/Accuracy Trade-off"
[24] Kaixiong Zhou, et al. "Auto-GNN: Neural Architecture Search of Graph Neural Networks"
[25] Yang Gao, et al. "GraphNAS: Graph Neural Architecture Search with Reinforcement Learning"

Neural Architecture Search for GNNs

- AutoGM[23]





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..

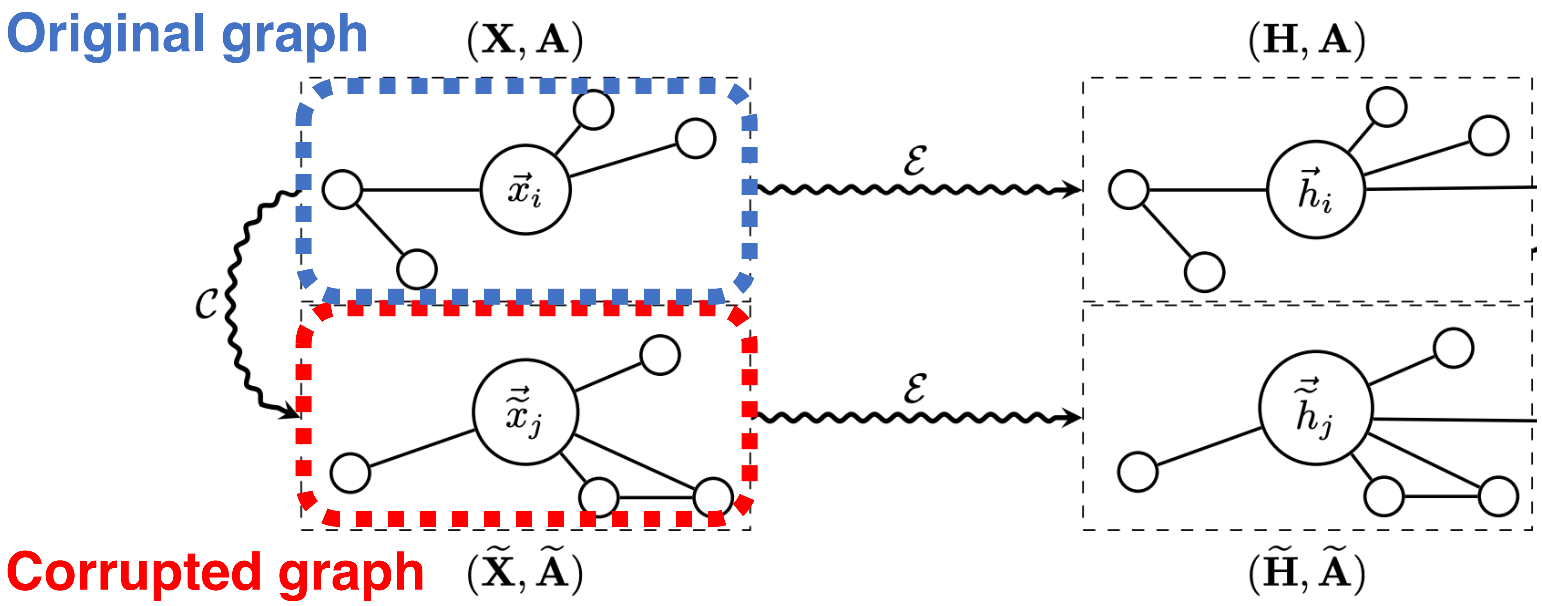
1. **Graph Neural Network**
   - Problem definition
   - Skeleton: aggregation, transformation operations
2. **Open research questions in GNN architectures**
   - Width
   - Depth
   - Aggregation
3. **GNN training strategy**

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

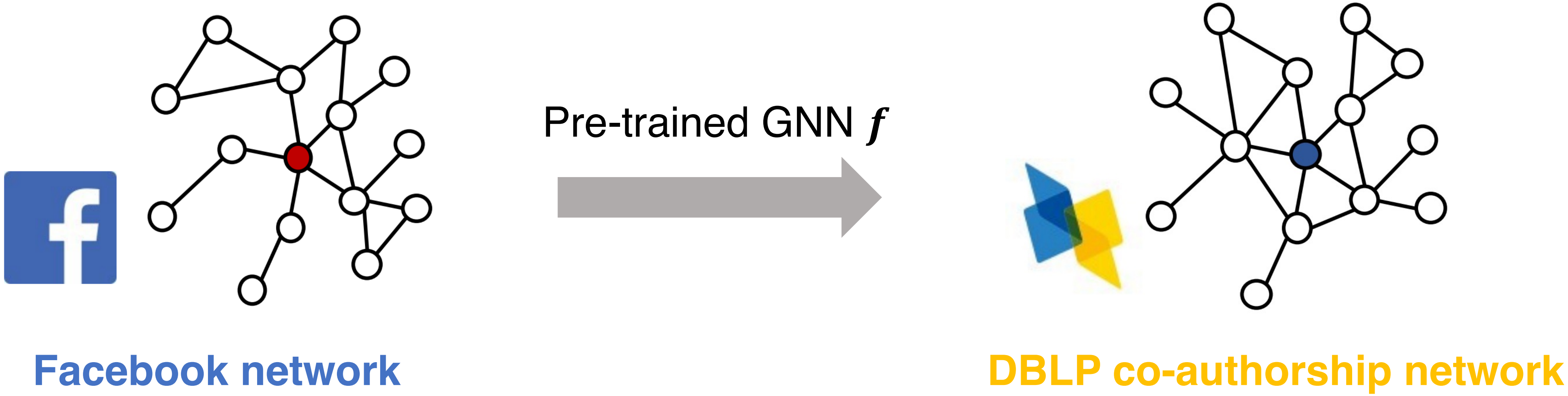
- Unsupervised learning[26]
  - Contrastive learning



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

How to train GNNs

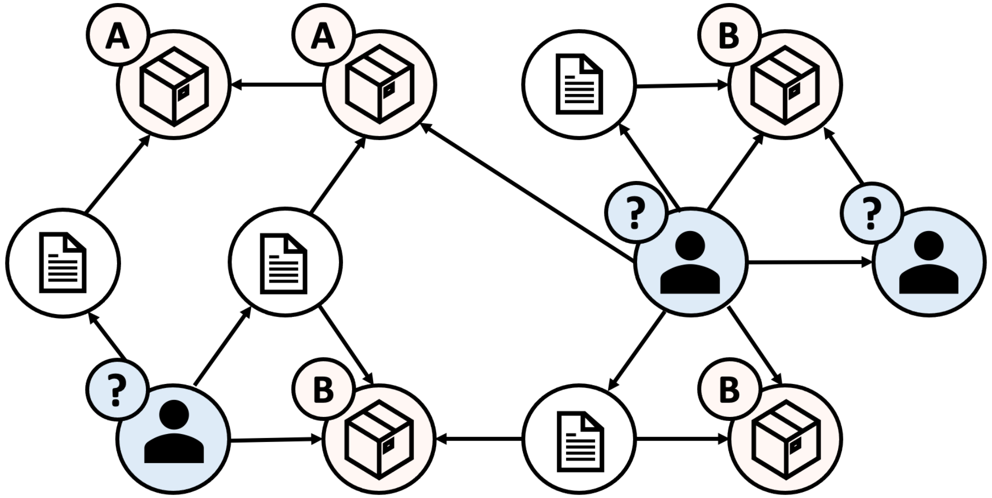
- Transfer learning
  - Transfer a pre-trained GNN model between graphs[27]



[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]



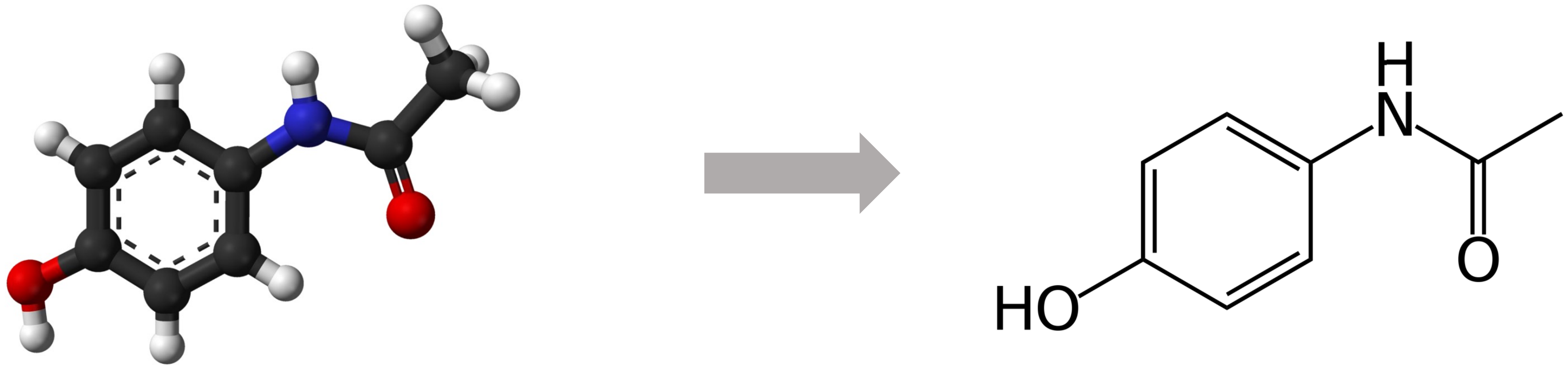
[28] Minji Yoon, et al. "Zero-shot Domain Adaptation of Heterogeneous Graphs via Knowledge Transfer Networks "

So far, we have talked about..

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

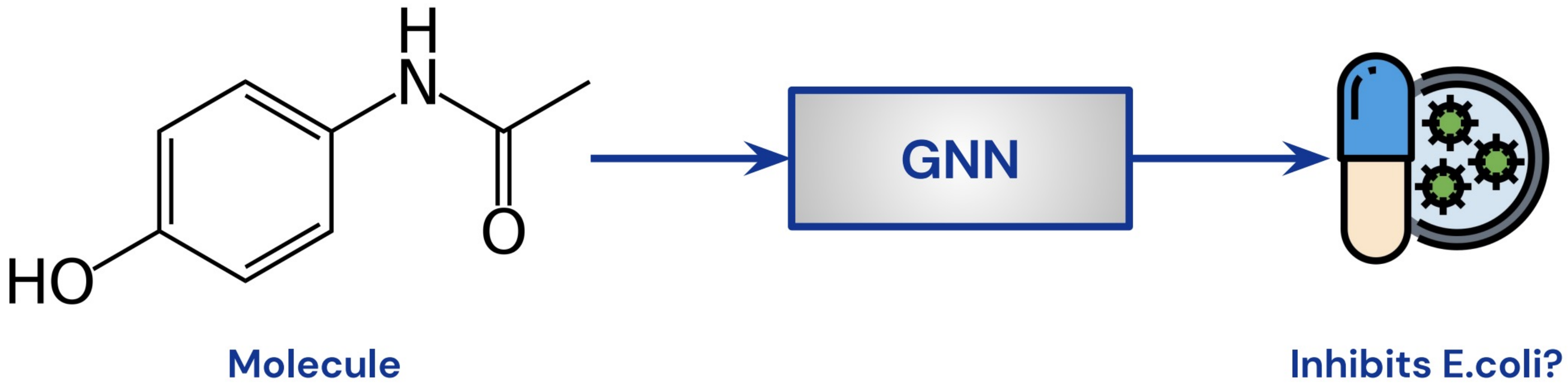
Impactful applications in science

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



Impactful applications in science

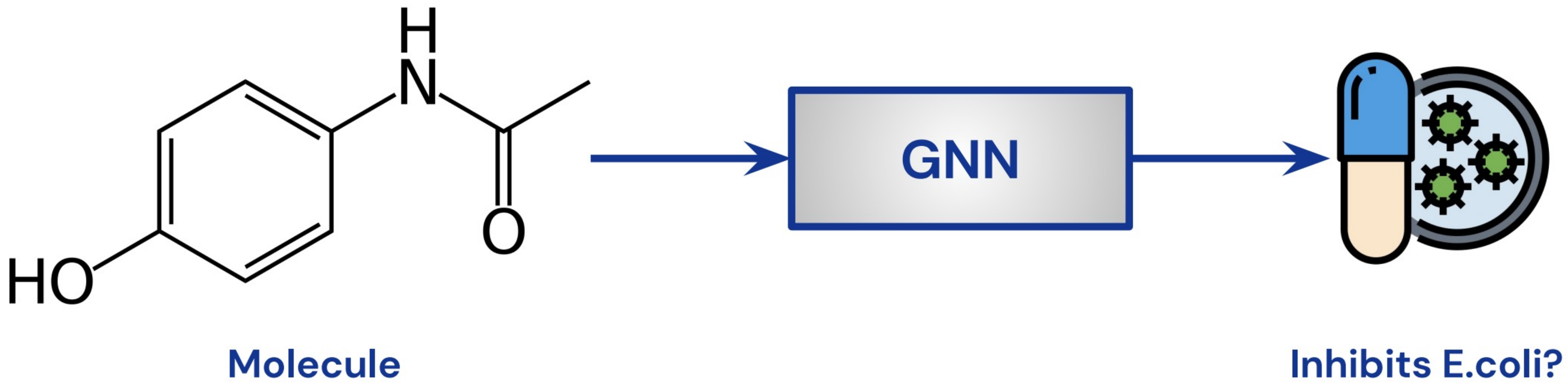
- Graph-level prediction: whether the molecule is a potent **drug**[29]
  - Binary classification on whether the drug will inhibit certain bacteria



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

Impactful applications in science

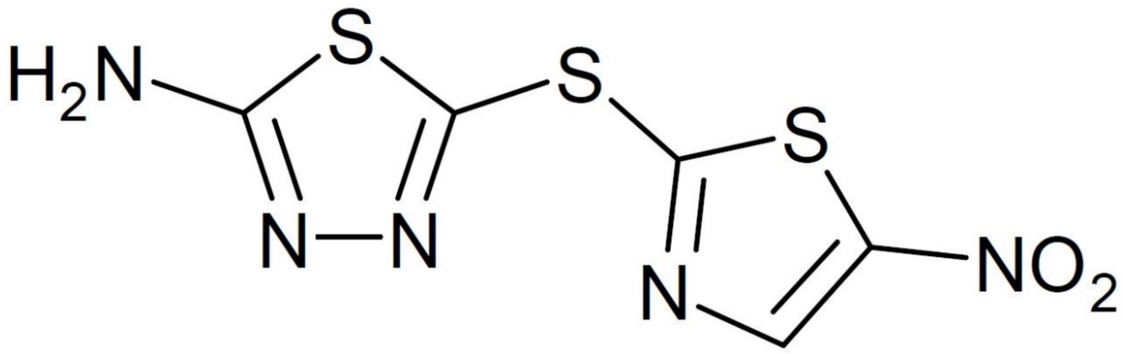
- Graph-level prediction: whether the molecule is a potent **drug**[29]
  - Execute on a large dataset of known candidate molecules
  - Select the ~ *top-100* candidates from the GNN model
  - Have chemists thoroughly investigate those



[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

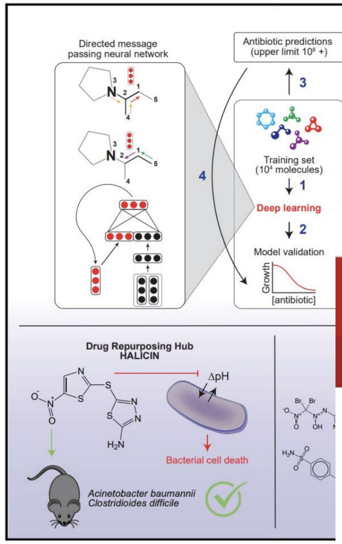
[29] Jonathan M.Stokes, et al. "A Deep Learning Approach to Antibiotic Discovery"

Impactful applications in science

Cell

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract



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AI discovers antibiotics to treat drug-resistant diseases

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

[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?

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