CPEN 455: Deep Learning

Lecture 7: Graph Neural Networks

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University of British Columbia

Winter, Term 2, 2024

Outline

- Applications of Graphs
- Background
- Challenges of Deep Learning on Graphs
- GNNs
  - Overview
  - Message Passing
  - Message Passing Architectures
  - Readout
- Implementation
- Relationship w. Transformers

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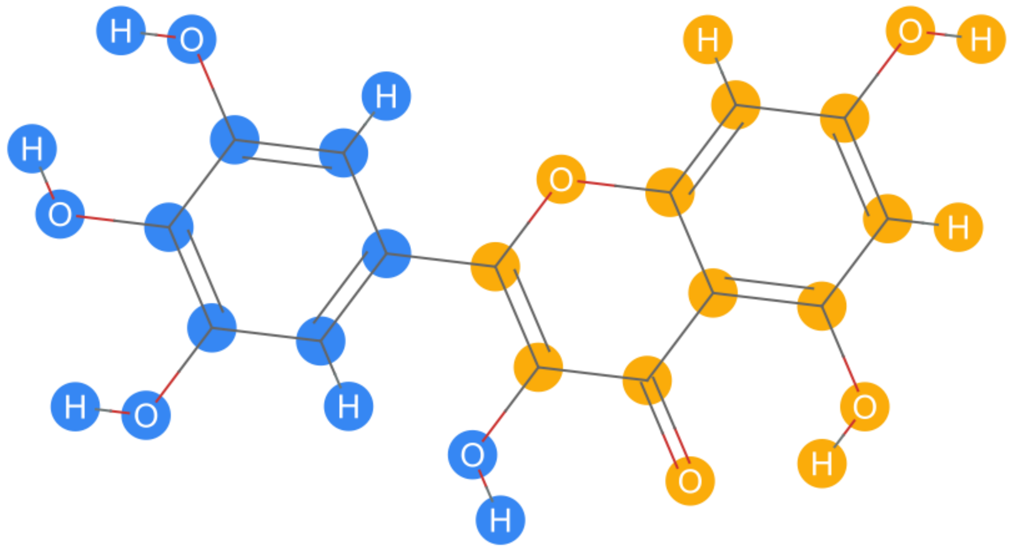
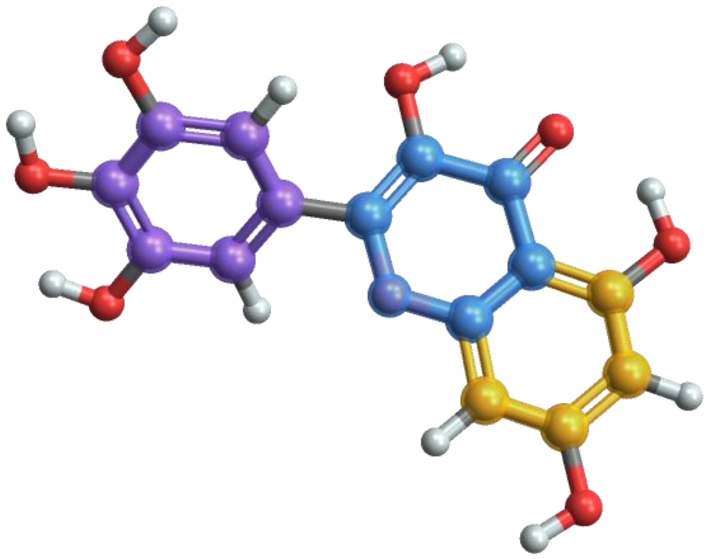
Motivating Applications of Graphs

- Molecules



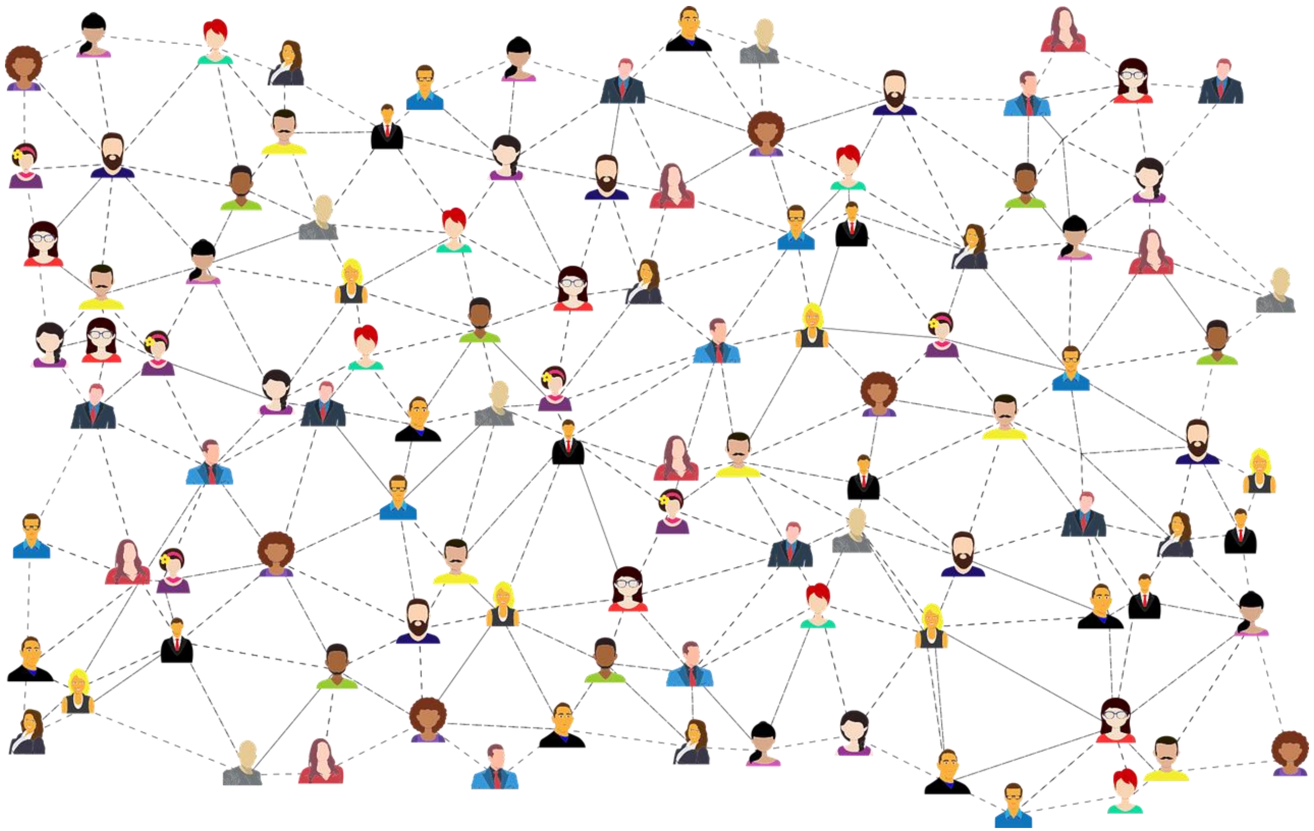


- Multi-edges exist
- Nodes have types
- Edges have types

Image Credit: [1]

Motivating Applications of Graphs

- Social Networks

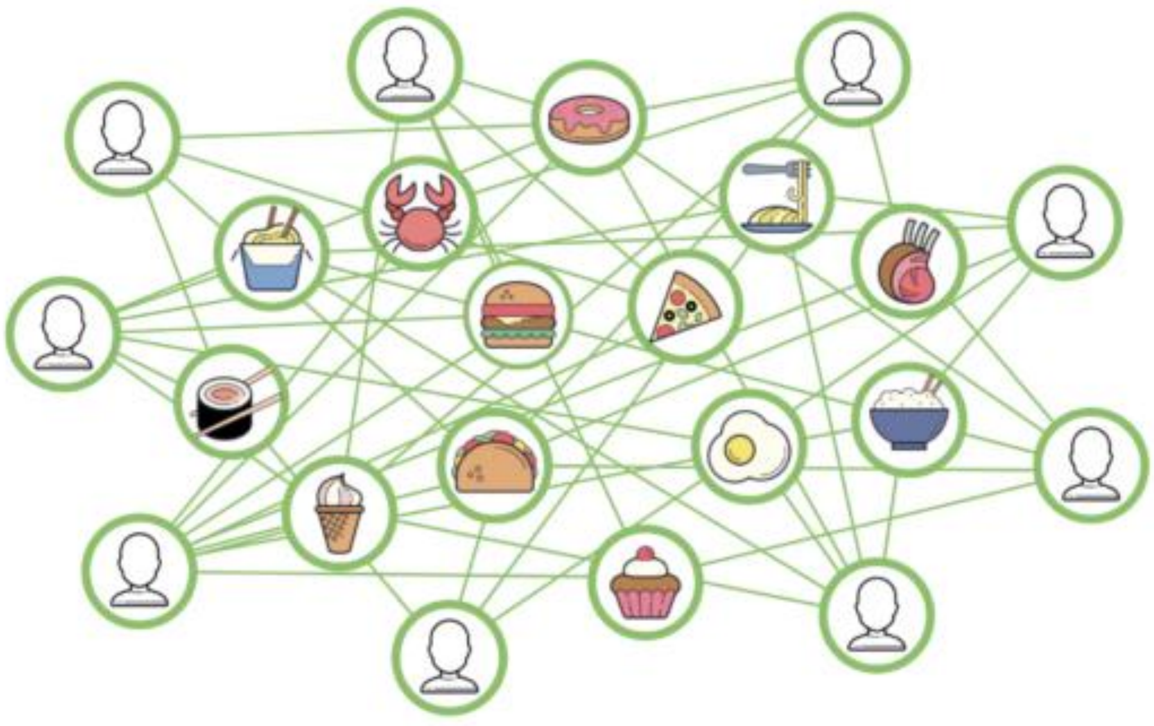


Link Prediction

Image Credit: [2]

Motivating Applications of Graphs

- Network-based Recommendations



Food Discovery

Image Credit: [3]

Motivating Applications of Graphs

- Citation Networks

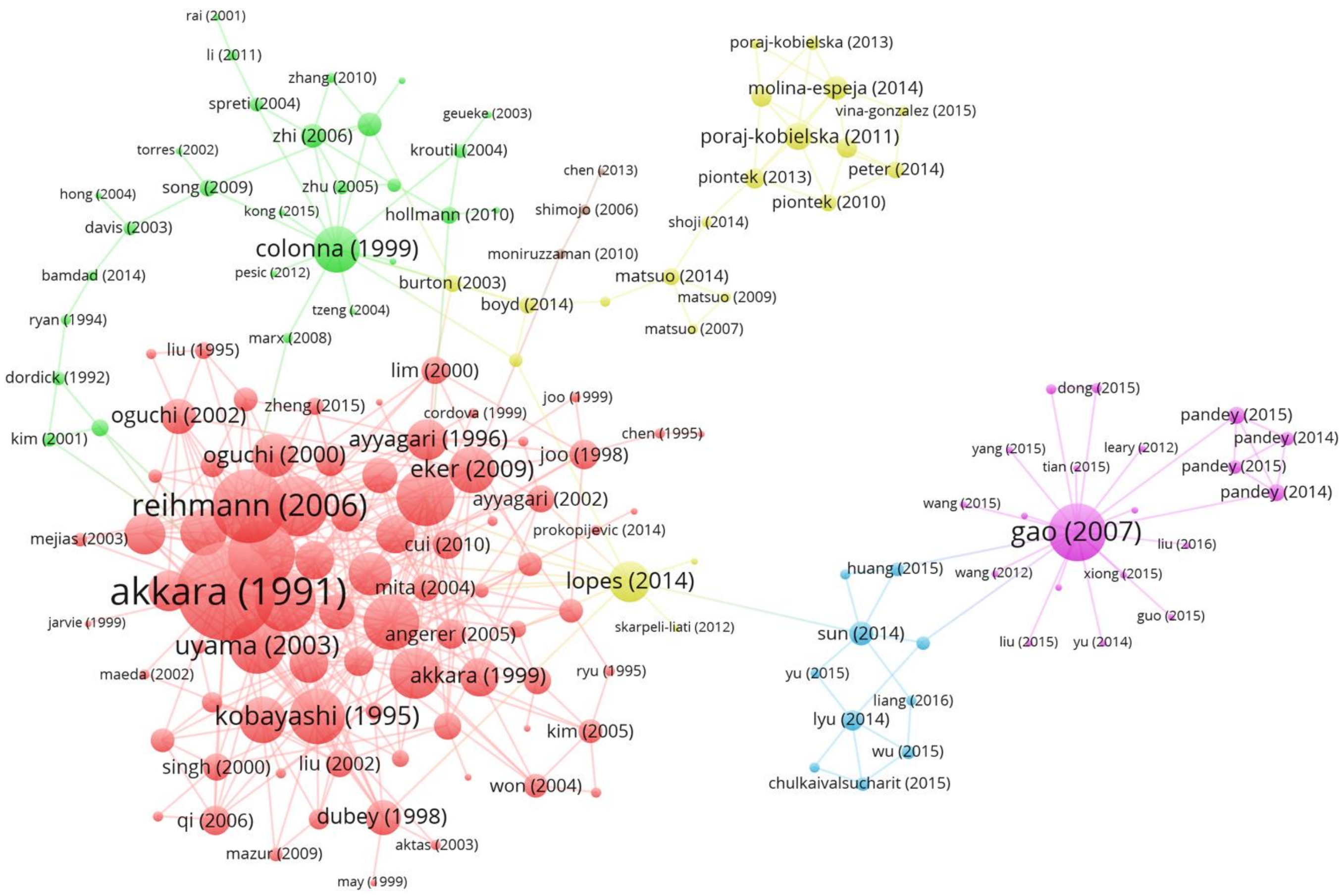
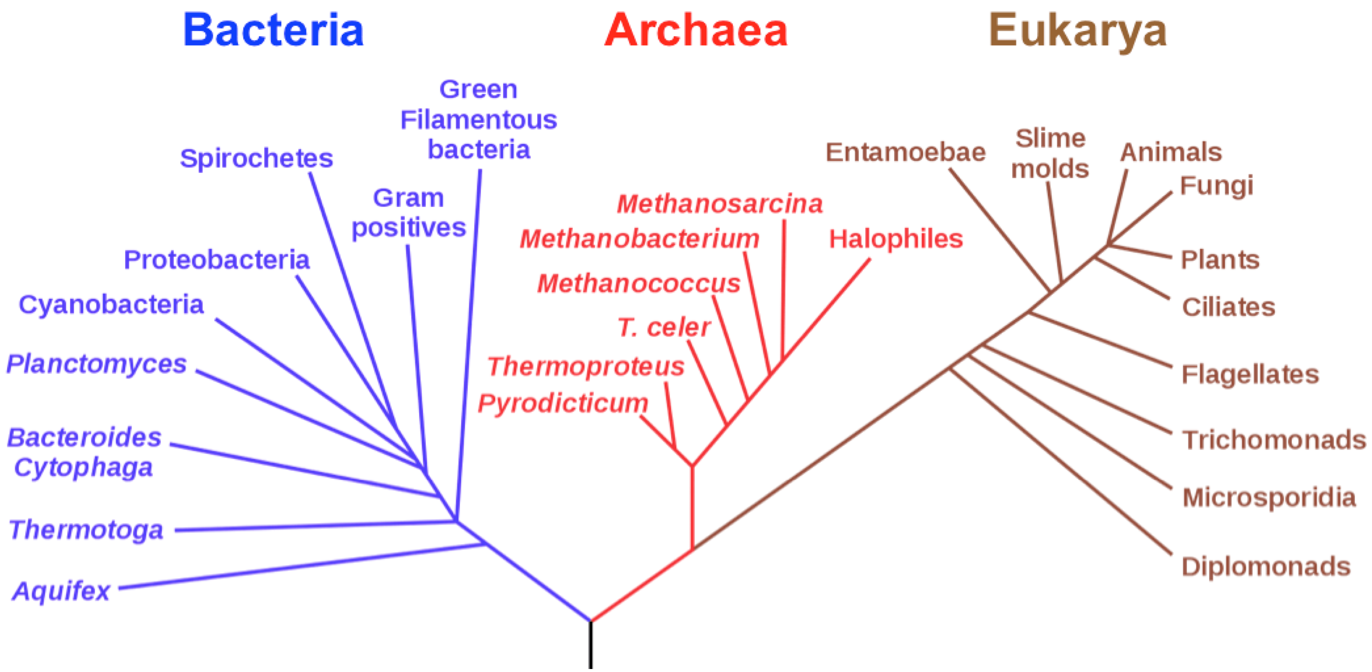


Image Credit: [4]

Motivating Applications of Graphs

- Phylogenetic Tree

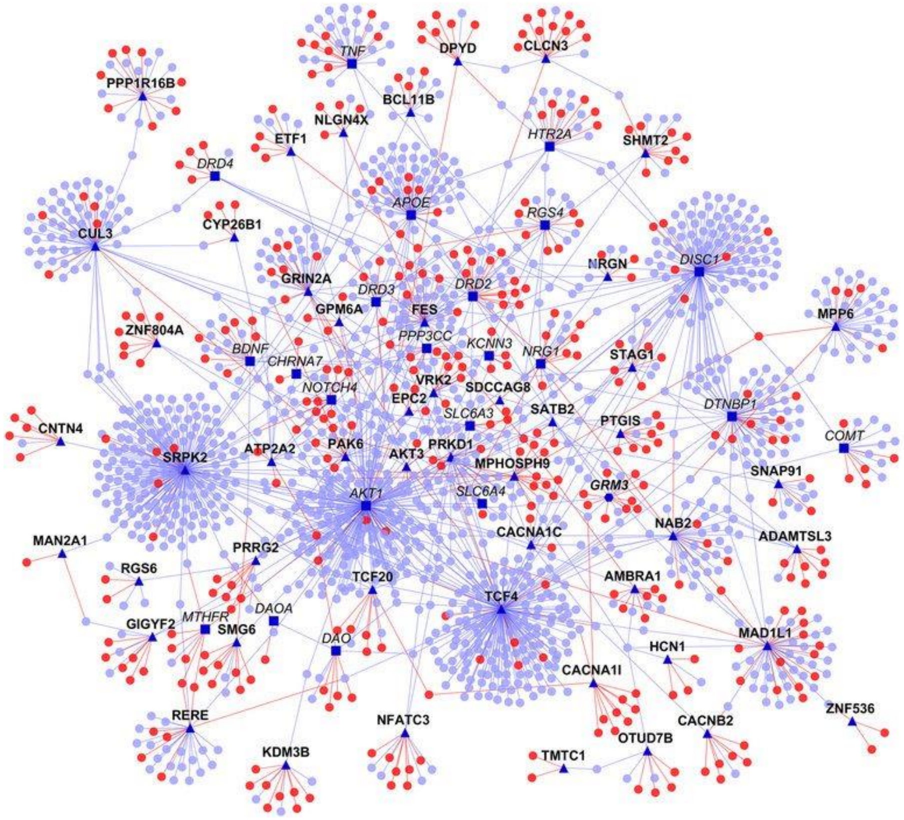


A phylogenetic tree based on rRNA genes showing the three life domains

Image Credit: [5]

Motivating Applications of Graphs

- Protein-Protein Interactions (PPIs)



Schizophrenia PPI

Image Credit: [6]

Motivating Applications of Graphs

- Epidemic Networks

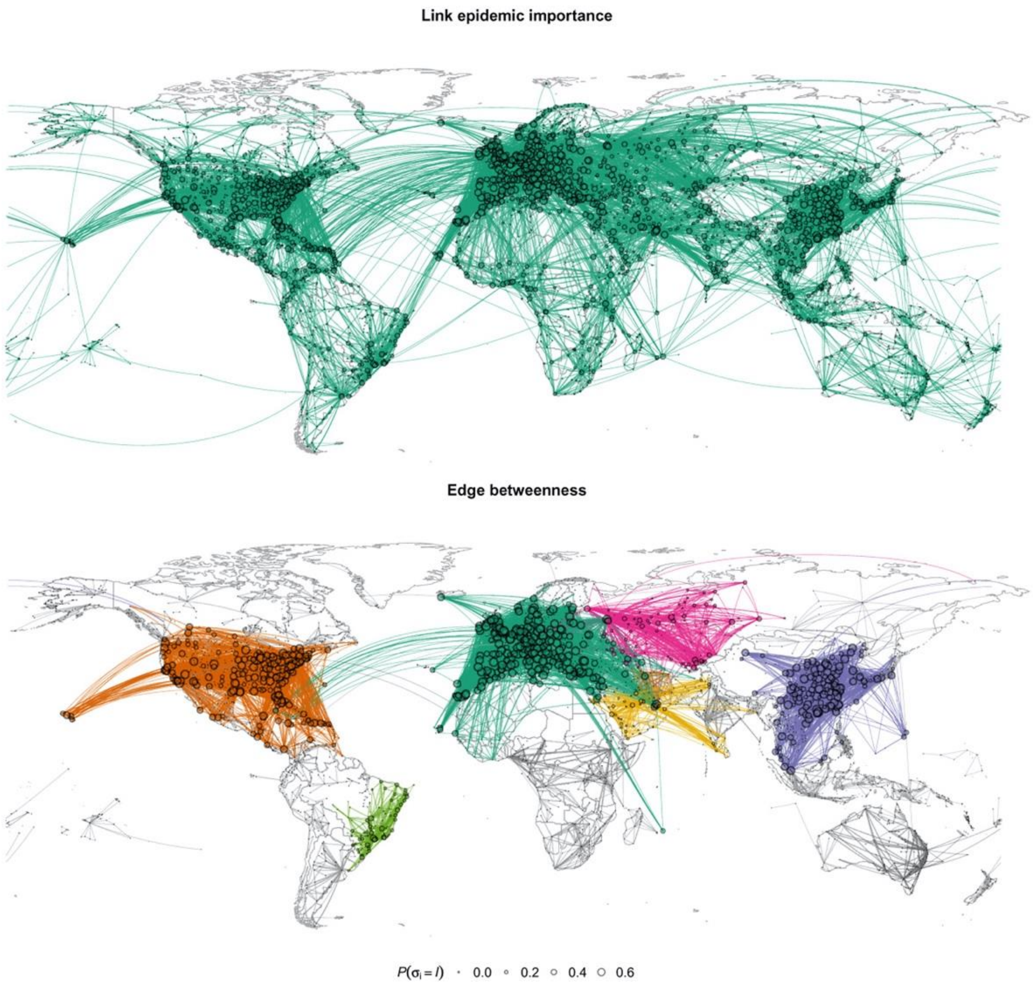


Image Credit: [7]

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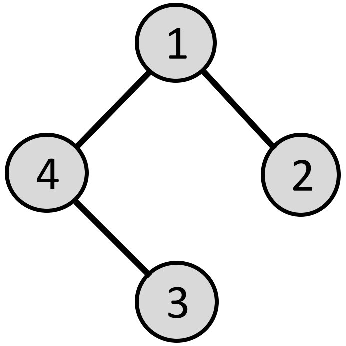
Deep Learning on Graphs

Graph Representations

- Connectivity

    1. Adjacency List: G = (V, E)



V = {1,2,3,4}, E = {(1,2), (1,4), (4,3)}

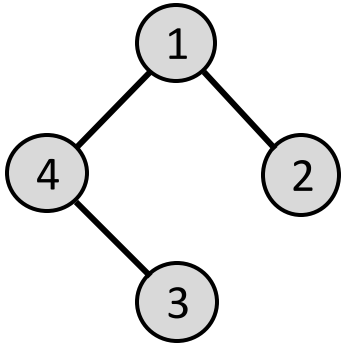
Deep Learning on Graphs

Graph Representations

- Connectivity

  1. Adjacency List: G = (V, E)

  2. Adjacency Matrix: A (sometimes we have weights)



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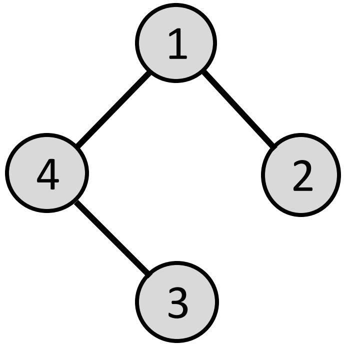
Deep Learning on Graphs

Graph Representations

- Connectivity
    1. Adjacency List: G = (V, E)
    2. Adjacency Matrix: A (sometimes we have weights)
- Feature
    1. Node Feature: X
    2. Edge Feature
    3. Graph Feature



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Deep Learning on Graphs

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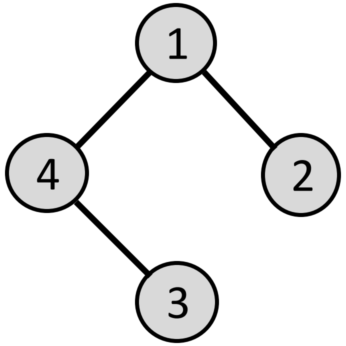
Graph Data = (A, X)



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Deep Learning on Graphs

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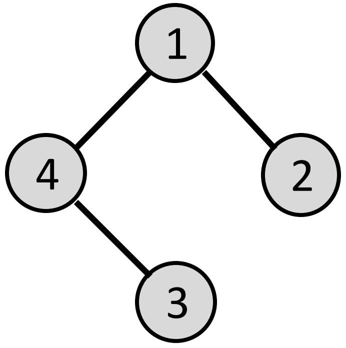

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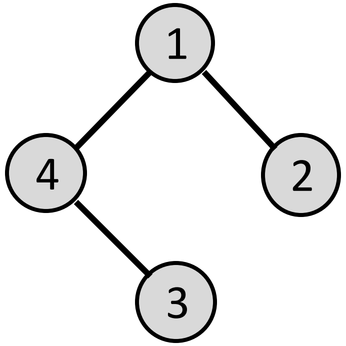

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Original Adj Matrix

Deep Learning on Graphs

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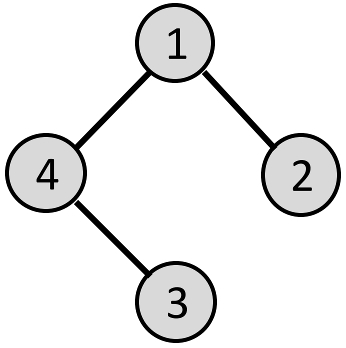

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V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

Permute Rows

	1	2	3	4
1	0	1	0	0
2	1	0	0	0
3	0	0	1	0
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Permutation Matrix

	1	2	3	4
1	0	1	0	1
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Original Adj Matrix

Permute Columns

	1	2	3	4
1	0	1	0	0
2	1	0	0	0
3	0	0	1	0
4	0	0	0	1

Transposed Permutation Matrix

Deep Learning on Graphs

Permutation

V = [1,2,3,4] => V' = [2,1,3,4]

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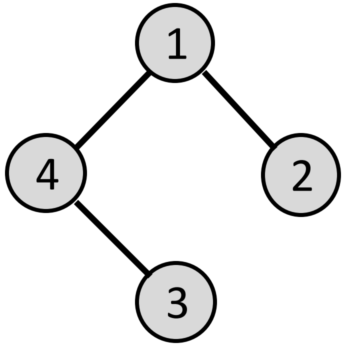

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Permutation Matrix

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Original Adj Matrix

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Transposed Permutation Matrix

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Permuted Adj Matrix

Deep Learning on Graphs

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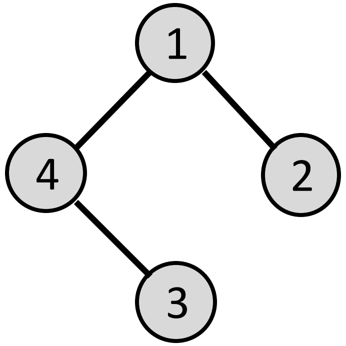

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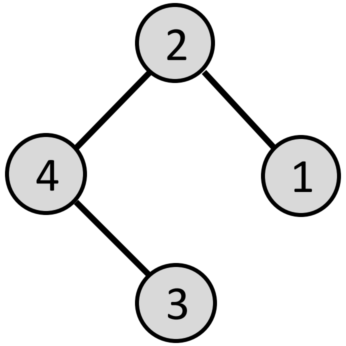

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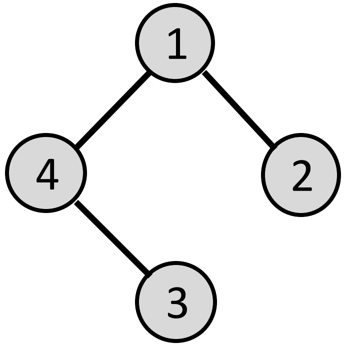

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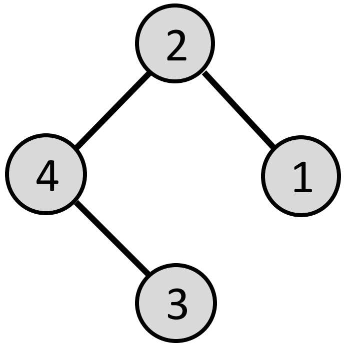
V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

Graph Isomorphism:

A bijection f between the vertex sets of G1 and G2 such that any two vertices u and v of G1 are adjacent ***iff*** *f(u) and f(v) are adjacent in G2.*

$$PA_1P^\top = A_2$$



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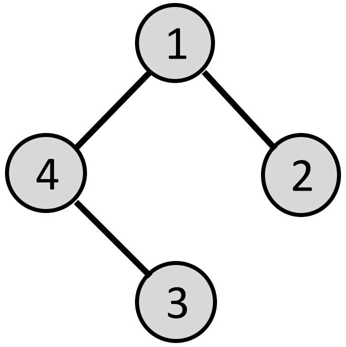
V' = [2,1,3,4], E' = [(2,1), (2,4), (4,3)]

Deep Learning on Graphs

Permutation

V = [1,2,3,4] => V’ = [4,3,2,1]

E = [(1,2), (1,4), (4,3)] => E’ = [(4,3), (4,1), (1,2)]



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Deep Learning on Graphs

Permutation

V = [1,2,3,4] => V’ = [4,3,2,1]

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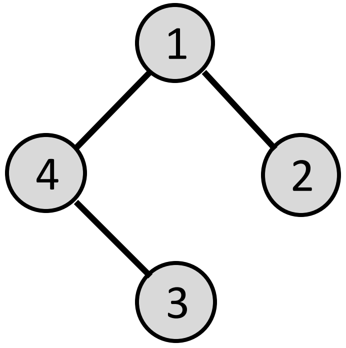

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Original Adj Matrix

Deep Learning on Graphs

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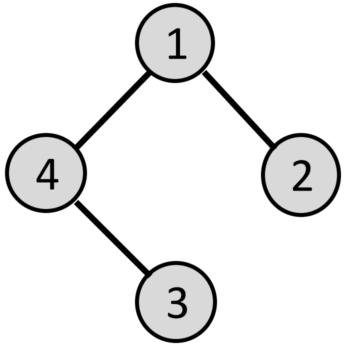

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Permutation Matrix

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Original Adj Matrix

Permute Columns

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Transposed Permutation Matrix

Deep Learning on Graphs

Permutation

V = [1,2,3,4] => V' = [4,3,2,1]

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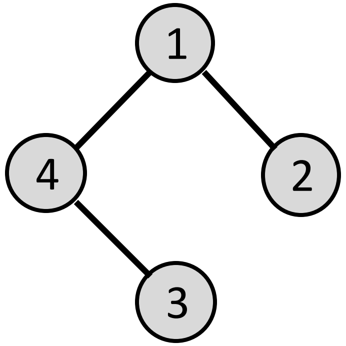

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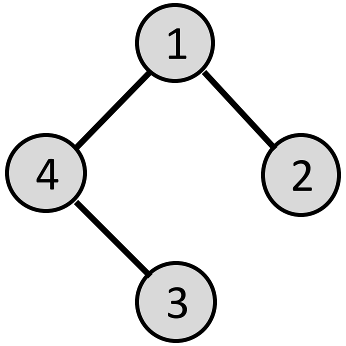

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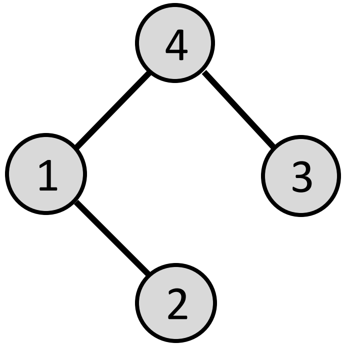

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Deep Learning on Graphs

Permutation

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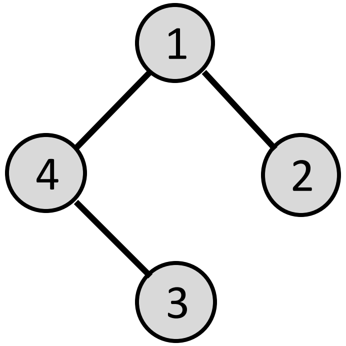

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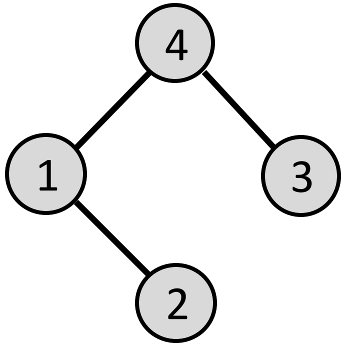
Graph Automorphism:

A permutation σ of the vertex set V, such that the pair of vertices (u,v) form an edge ***iff*** *the pair (σ(u),σ(v)) also form an edge.*

$$PAP^\top = A$$



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Deep Learning on Graphs

Permutation Invariance & Equivariance

Graph Data (A, X), Model $f(A, X)$

Invariance: $$f(PAP^\top, PX) = f(A, X)$$

Equivariance: $$f(PAP^\top, PX) = Pf(A, X)$$

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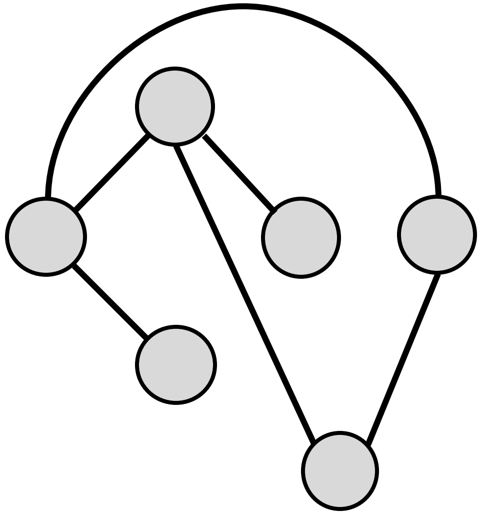
Deep Learning on Graphs

Key Challenges:

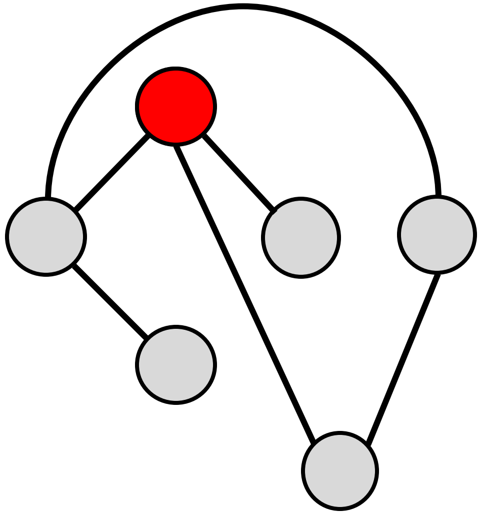
- **Unordered Neighbors**



Deep Learning on Graphs

Key Challenges:

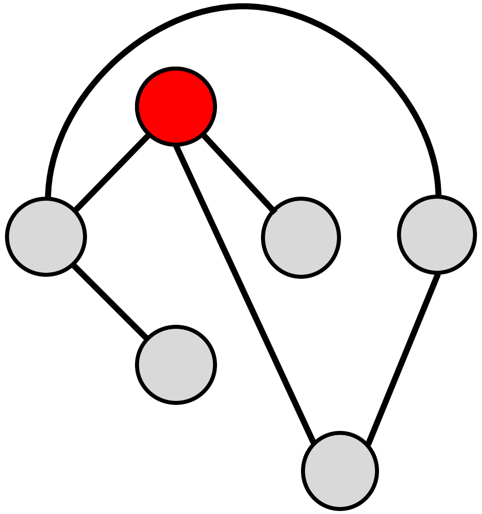
- **Unordered Neighbors**

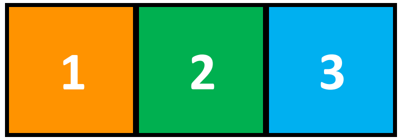


Deep Learning on Graphs

Key Challenges:

- **Unordered Neighbors**





Deep Learning on Graphs

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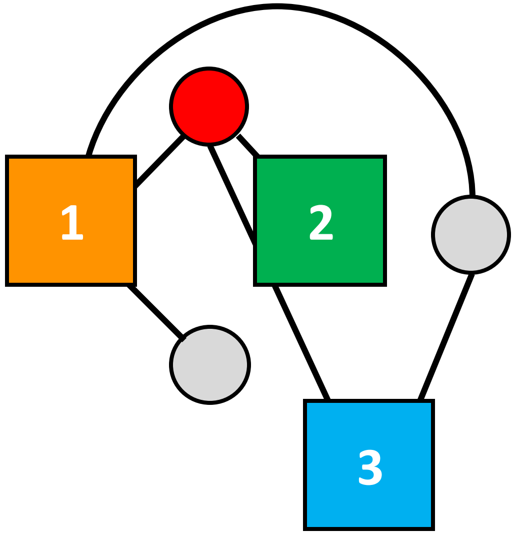
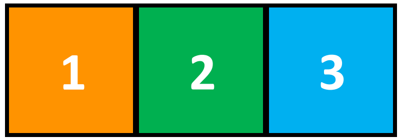


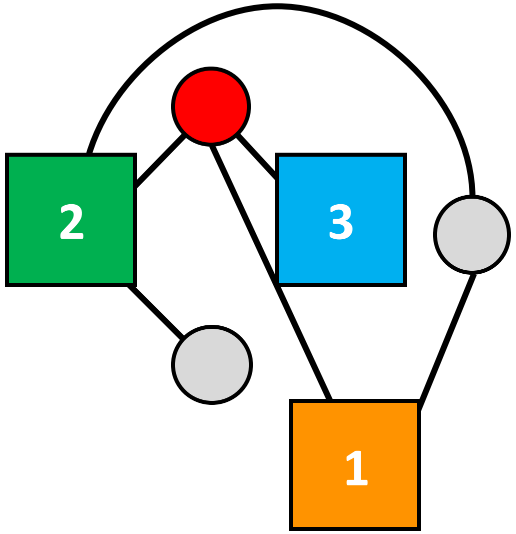
Option 1



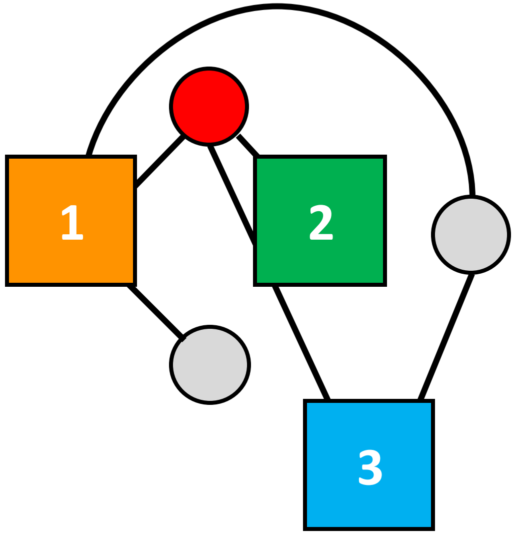
Deep Learning on Graphs

Key Challenges:

- **Unordered Neighbors**



Option 2



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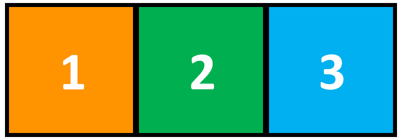
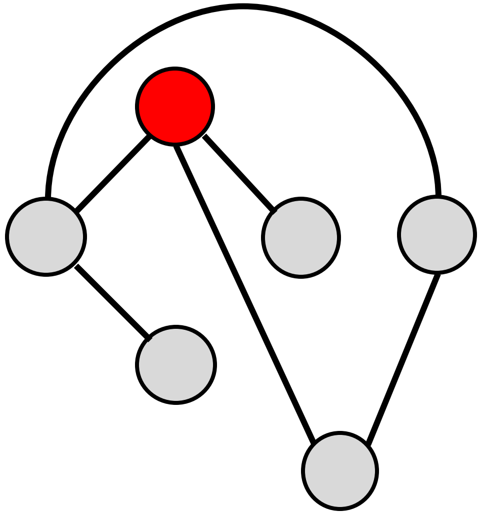


Deep Learning on Graphs

Key Challenges:

- Unordered Neighbors
- **Varying Neighborhood Sizes**



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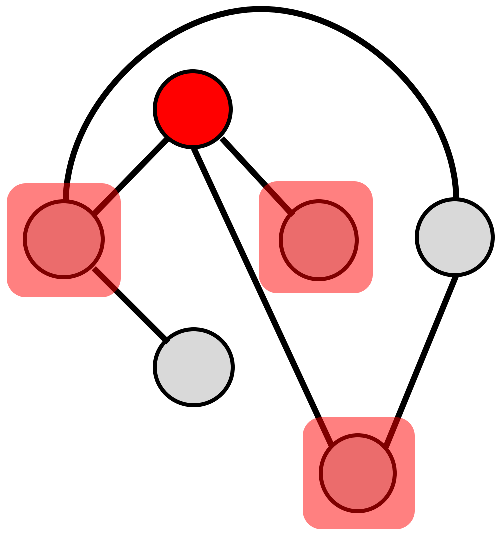

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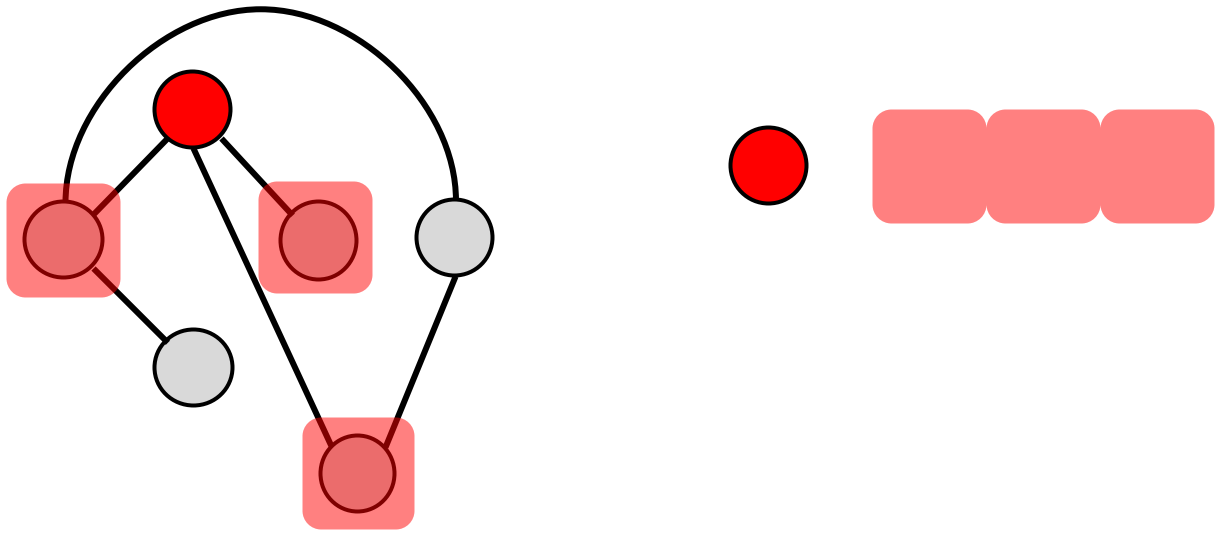

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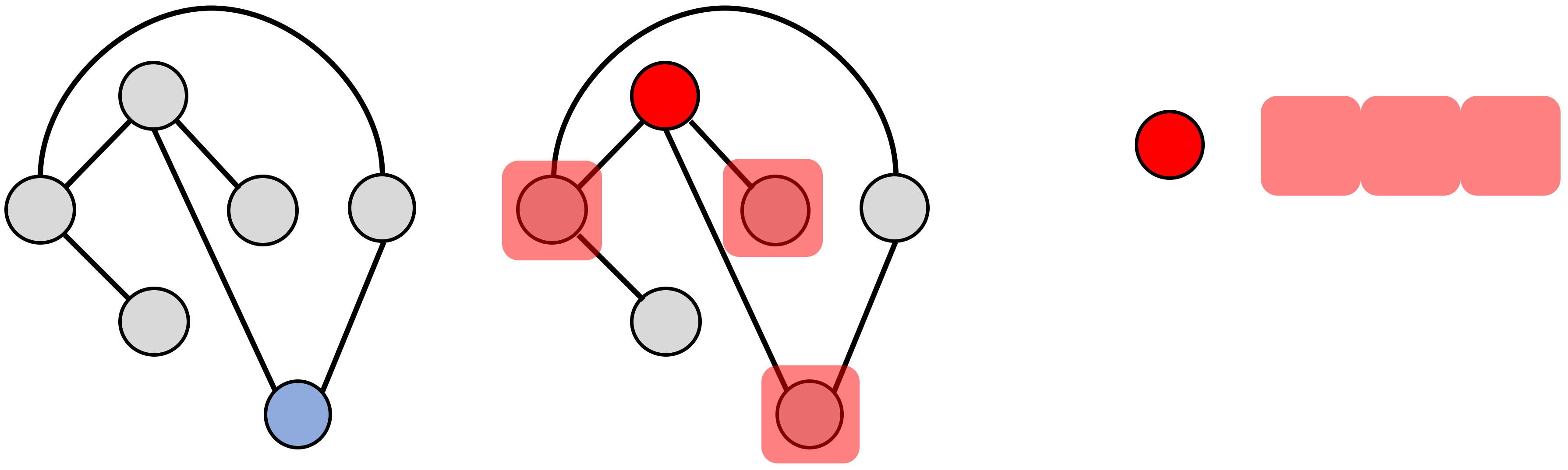

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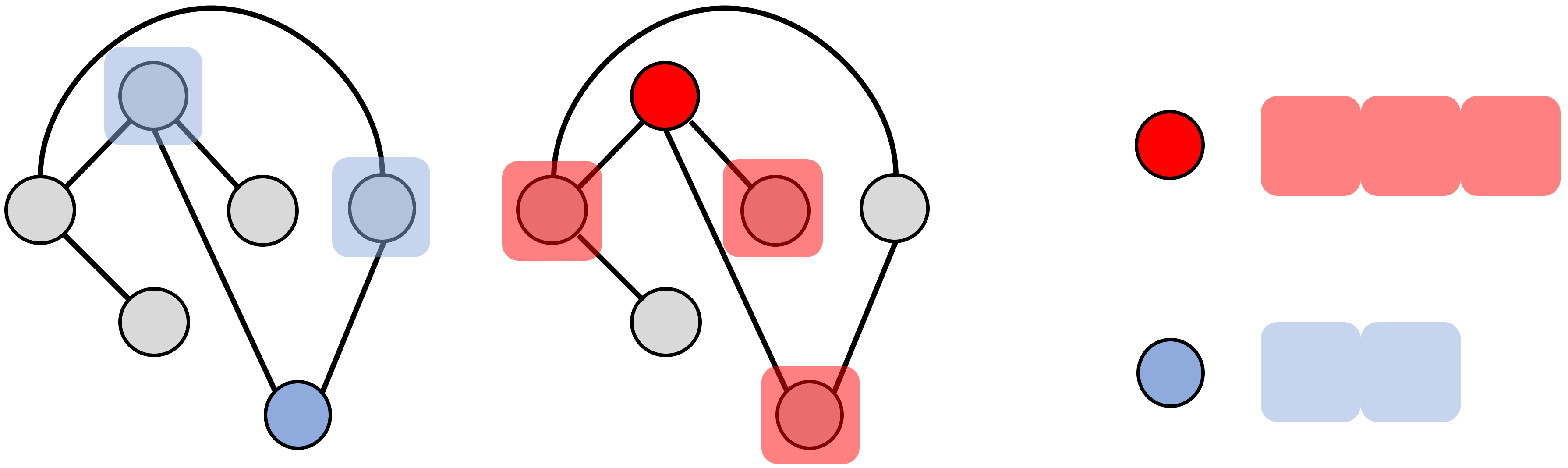

Deep Learning on Graphs

Key Challenges:

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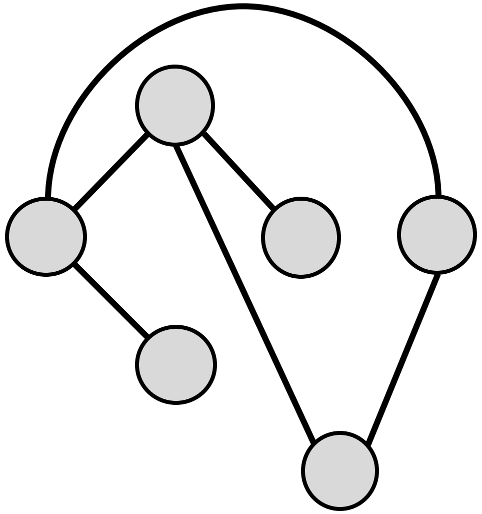

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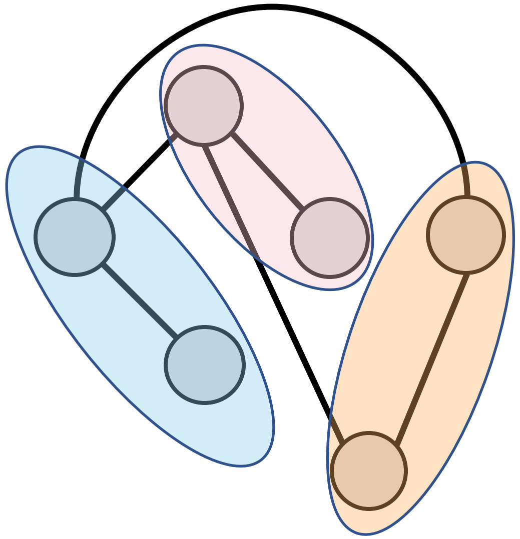

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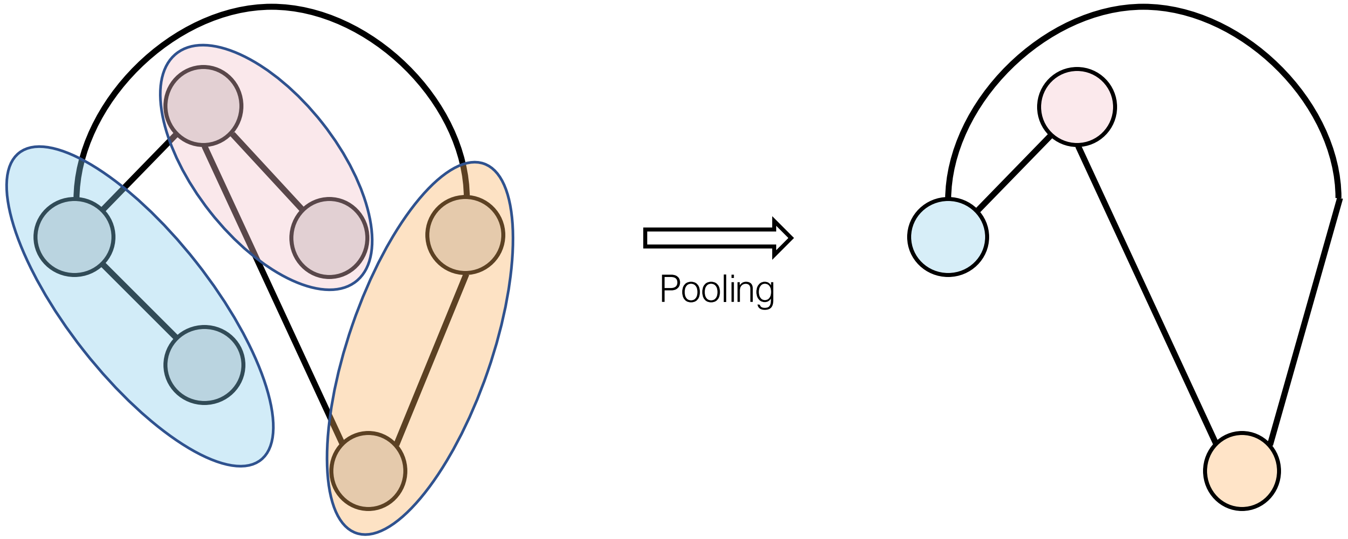

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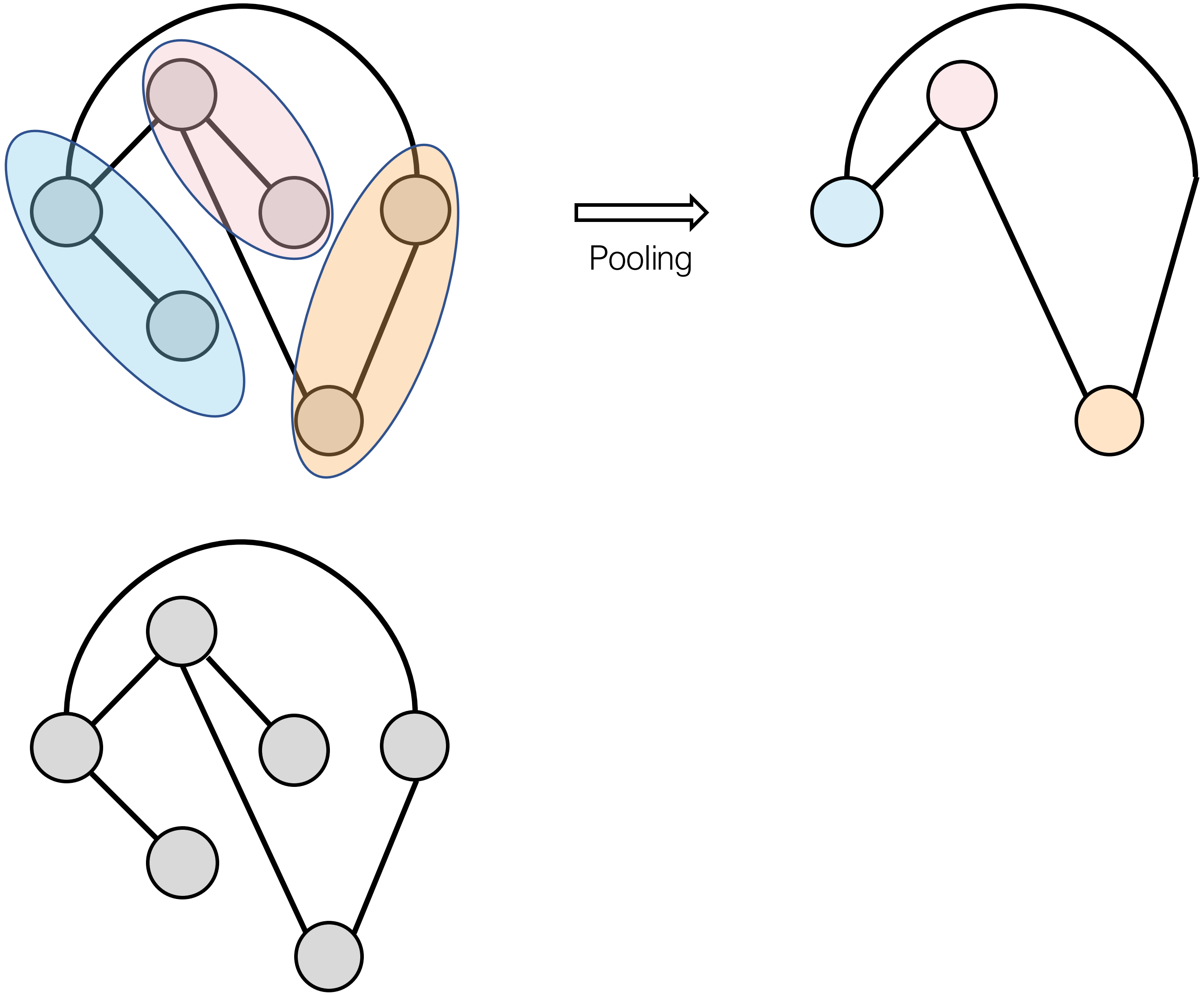

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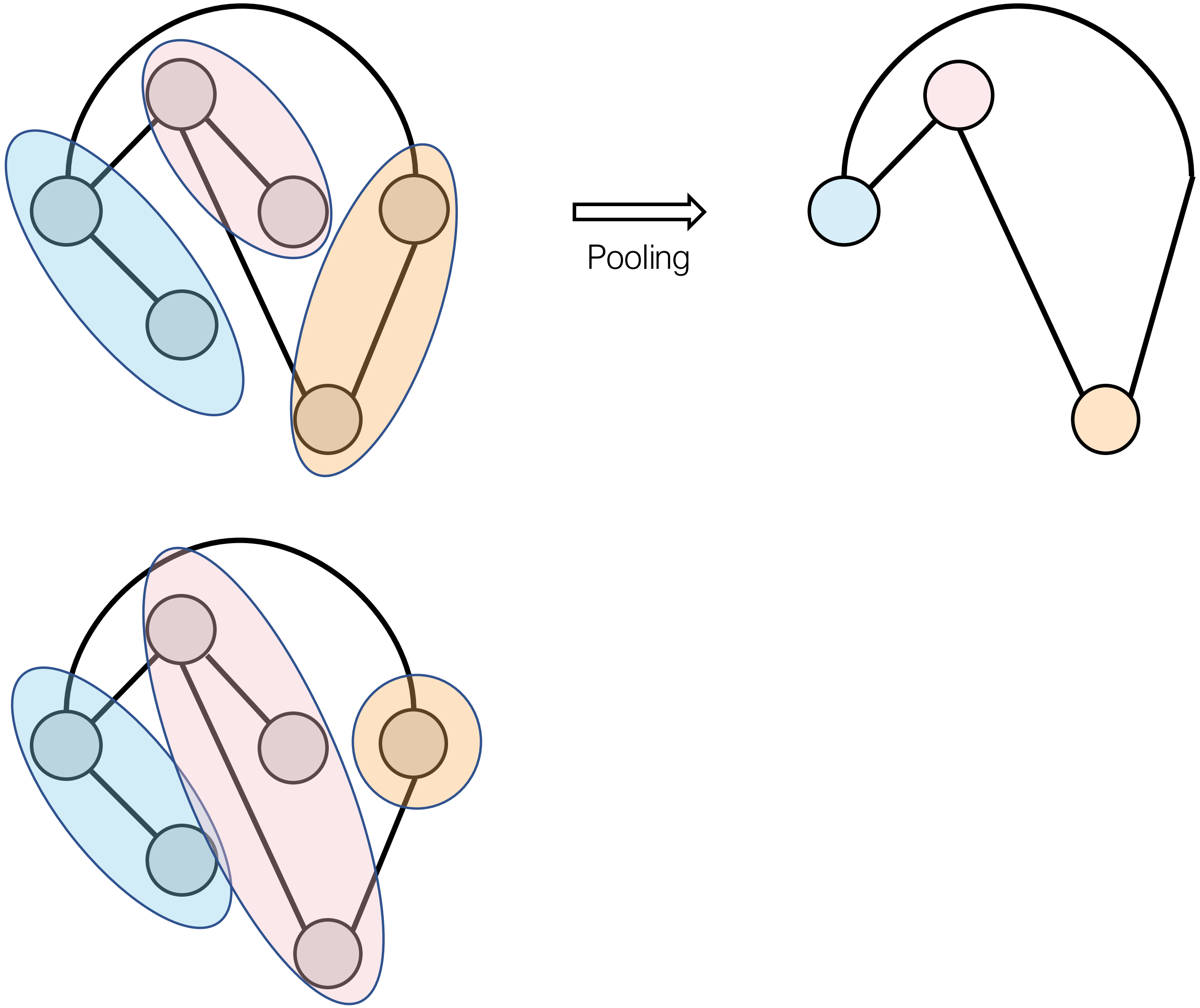

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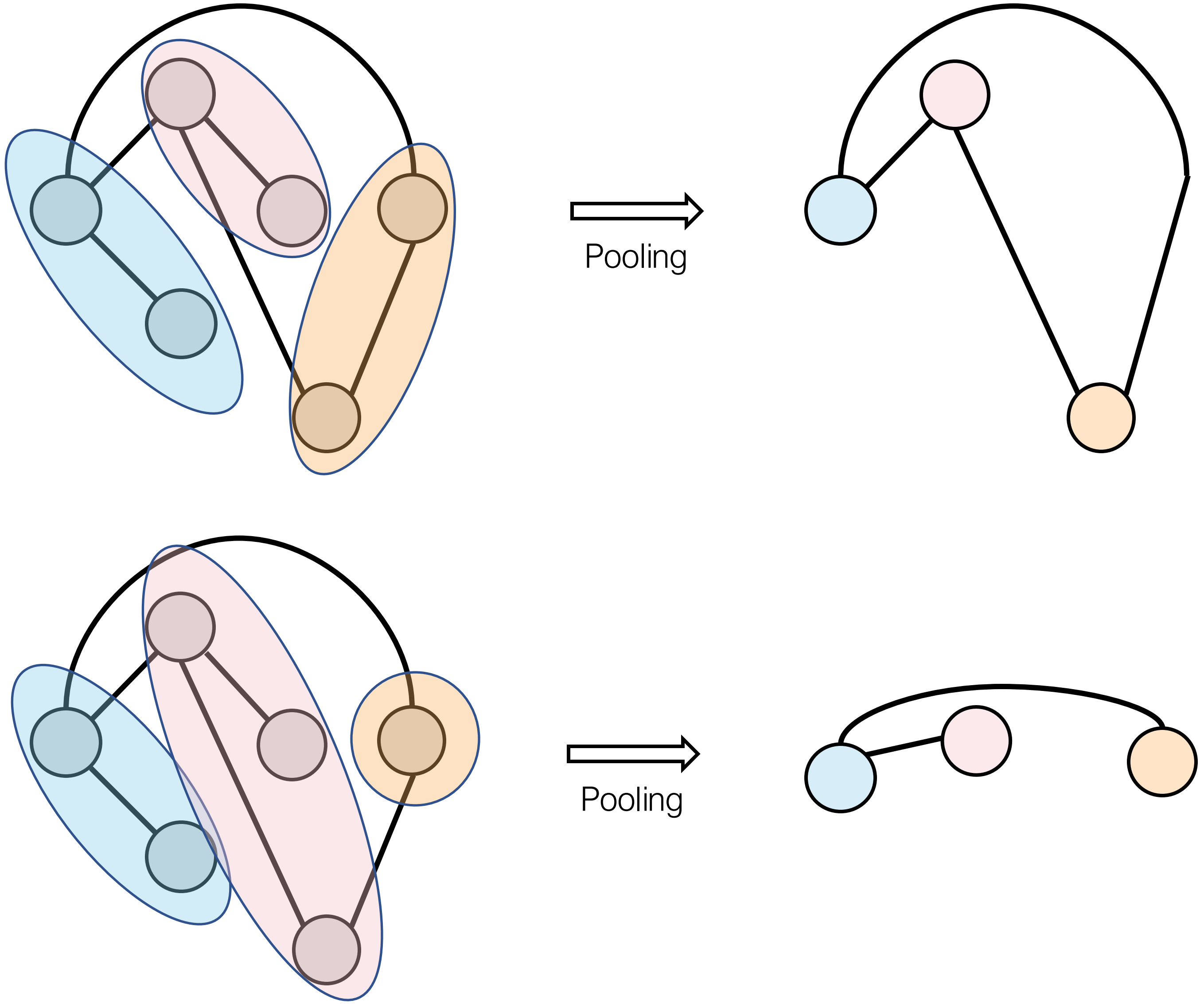

Outline

- Applications of Graphs
- Background
- Challenges of Deep Learning on Graphs
- GNNs
    - **Overview**
    - Message Passing
    - Message Passing Architectures
    - Readout
- Implementation
- Relationship w. Transformers

Deep Learning on Graphs

Graph Neural Networks (GNNs)

- Neural networks that can process general graph structured data

Deep Learning on Graphs

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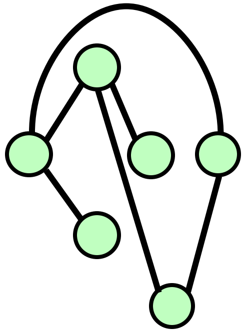
- Most of GNNs (if not all) can be incorporated by the **Message Passing** paradigm [11]
- GNNs have been independently studied in signal processing community under **Graph Signal Processing**
- The study of GNNs and other related models are also called **Geometric Deep Learning**

Graph Neural Networks (GNNs)



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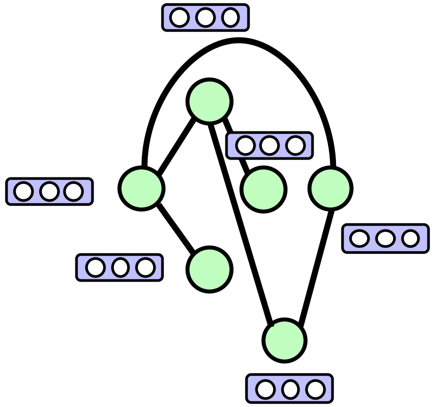
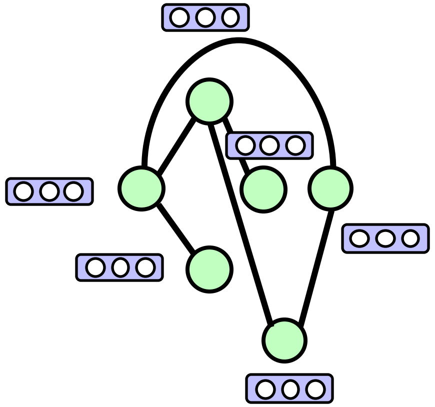


Input Encoding

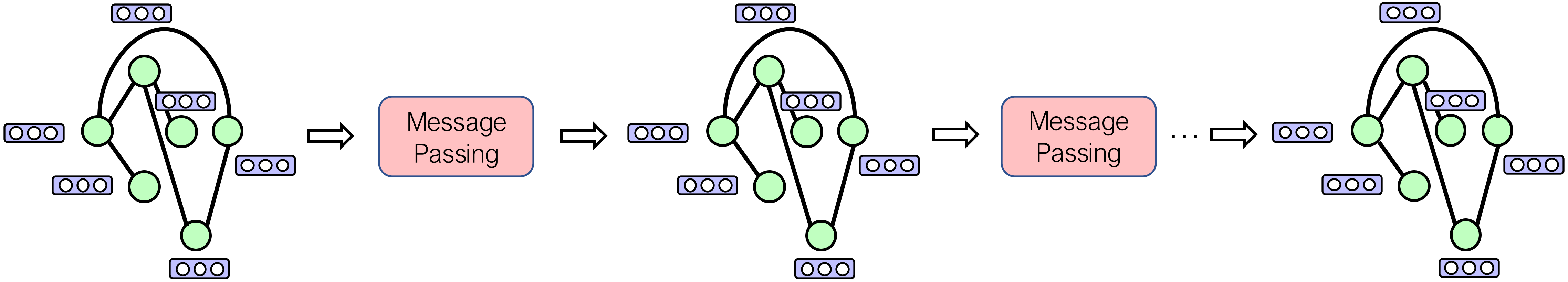
Graph Neural Networks (GNNs)



Input Encoding

1. Node Feature
   - *If it is unavailable, use 1-of-K, random, index/size encoding of node index)*
2. Edge Feature
   - *Feed it to message network*
3. Graph Feature
   - *Treat it as a super node in your graph*
   - *Feed graph feature to readout layer*

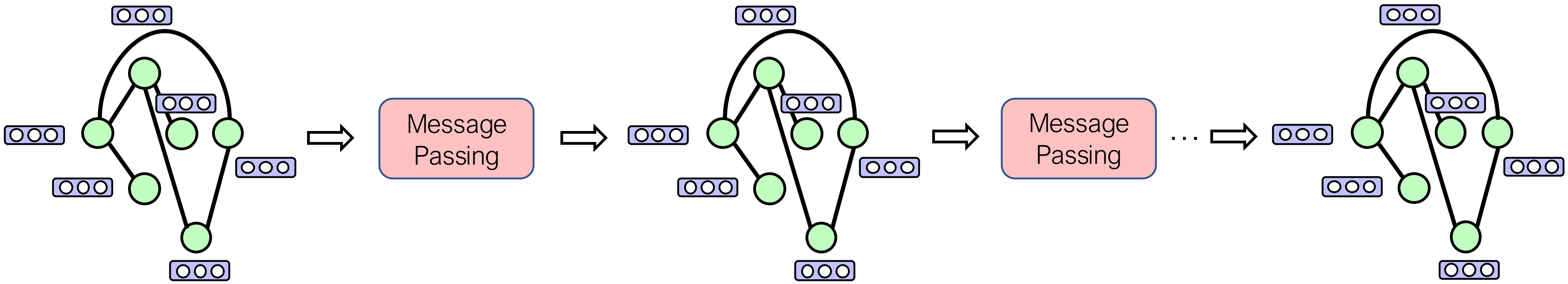
Graph Neural Networks (GNNs)



Input Encoding

Message Passing Layers/Steps

Graph Neural Networks (GNNs)

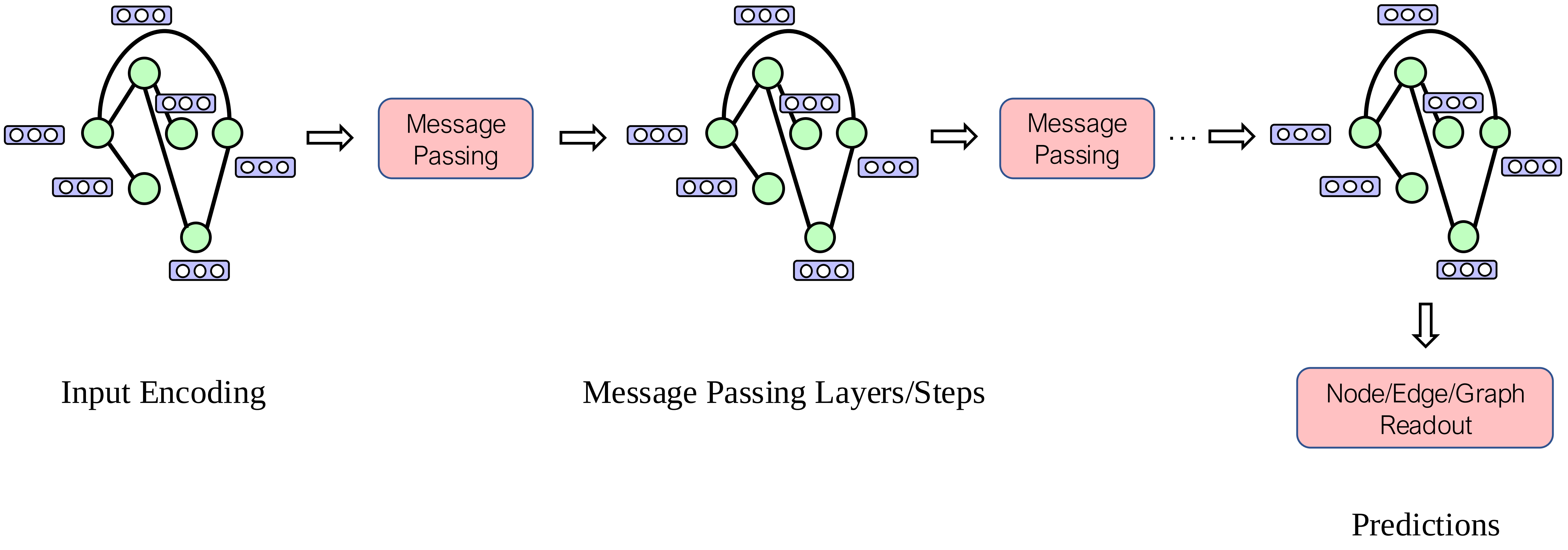


Input Encoding

Message Passing Layers/Steps

Steps: share message passing module (Recurrent Networks)
Layers: do not share message passing module (Feedforward Networks)

Graph Neural Networks (GNNs)



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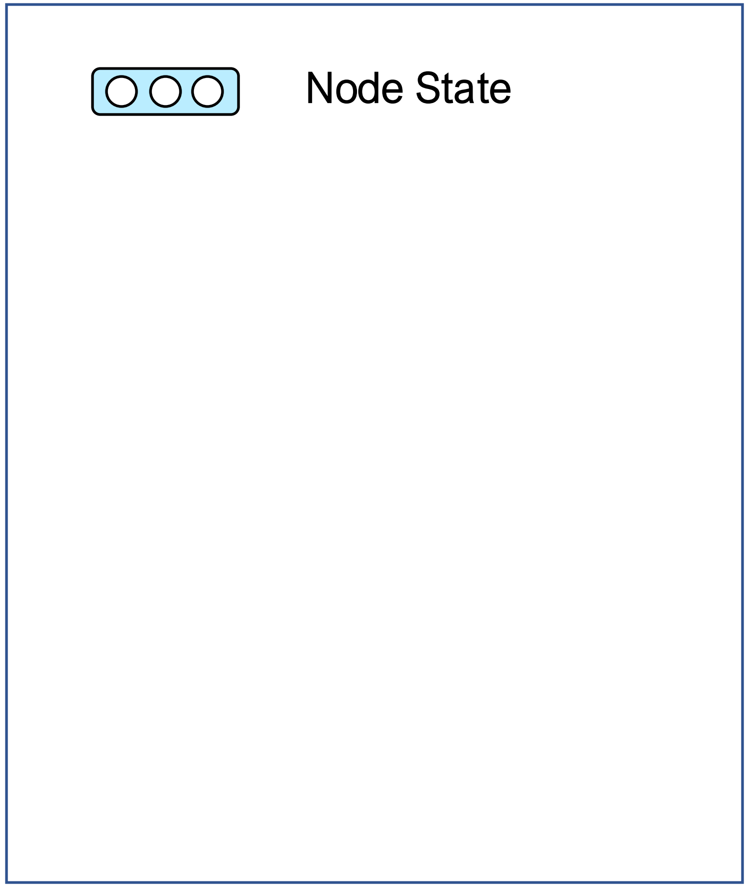
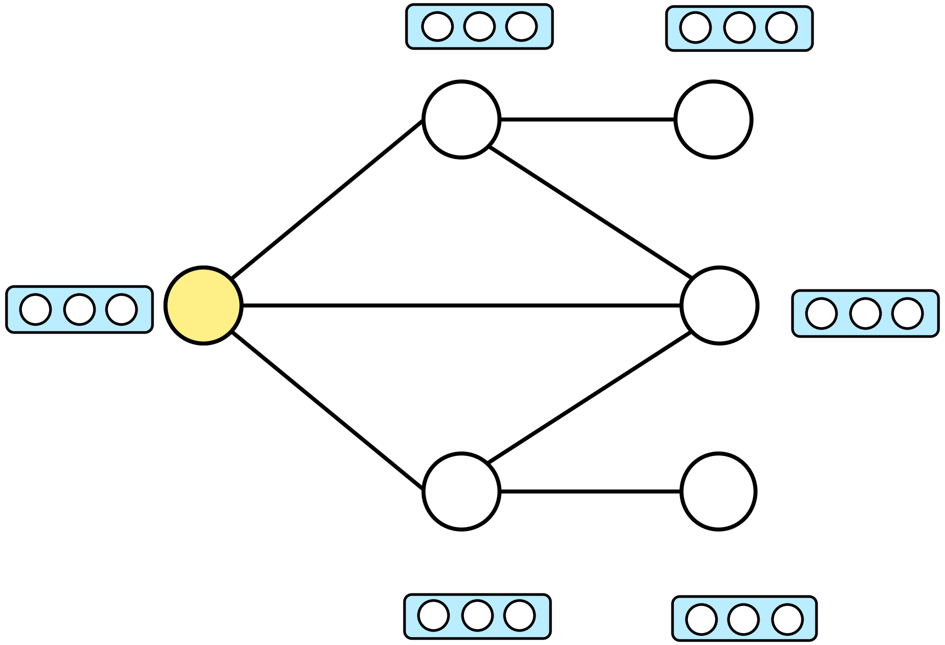
Message Passing in GNNs

$\mathbf{h}_i^t$

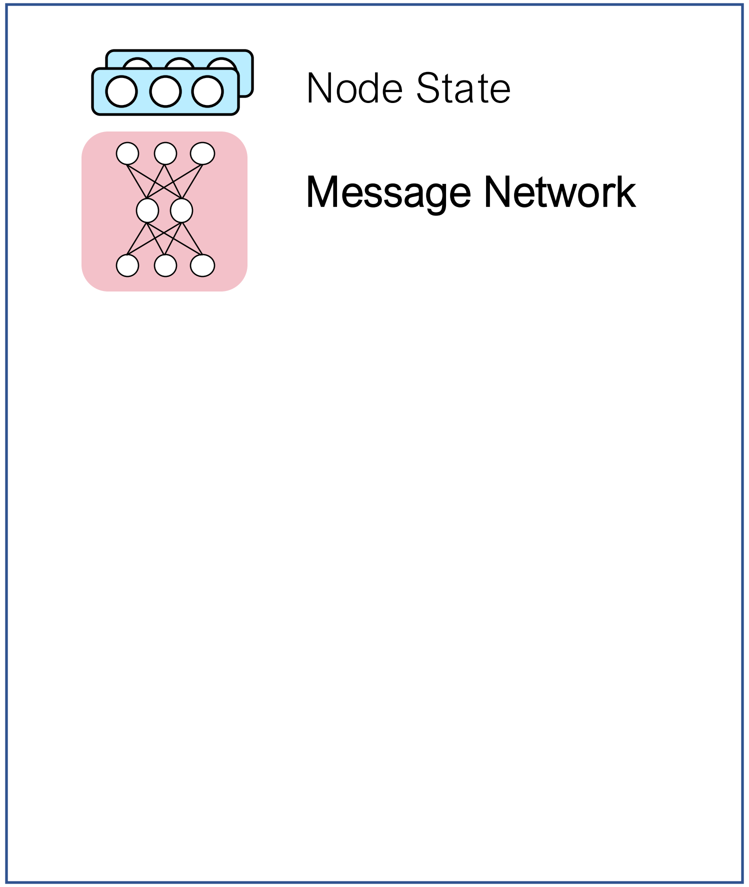


(t+1)-th message passing step/layer



Message Passing in GNNs

$\mathbf{h}_i^t \quad \mathbf{h}_j^t$



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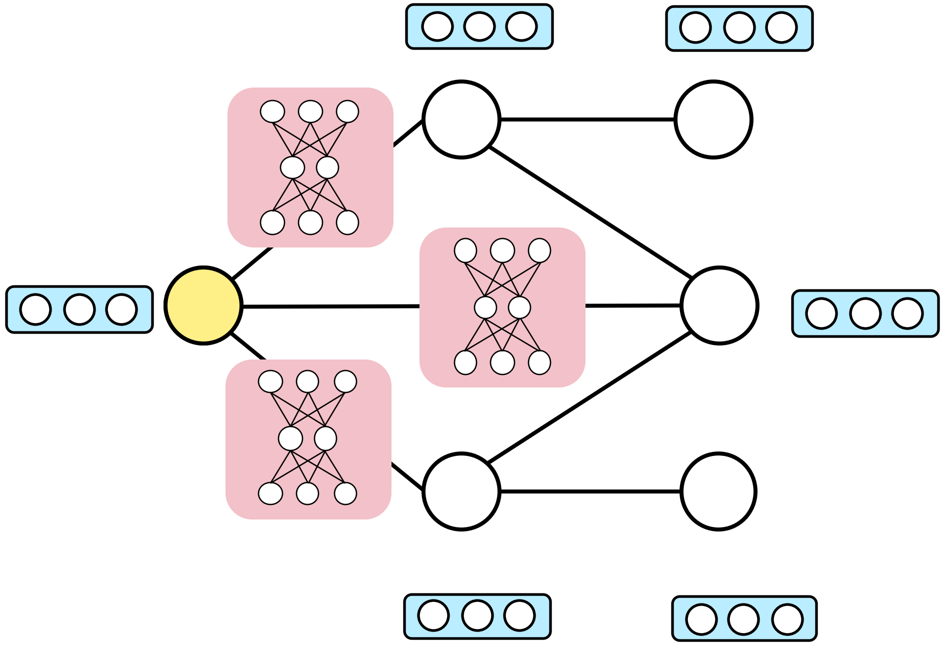

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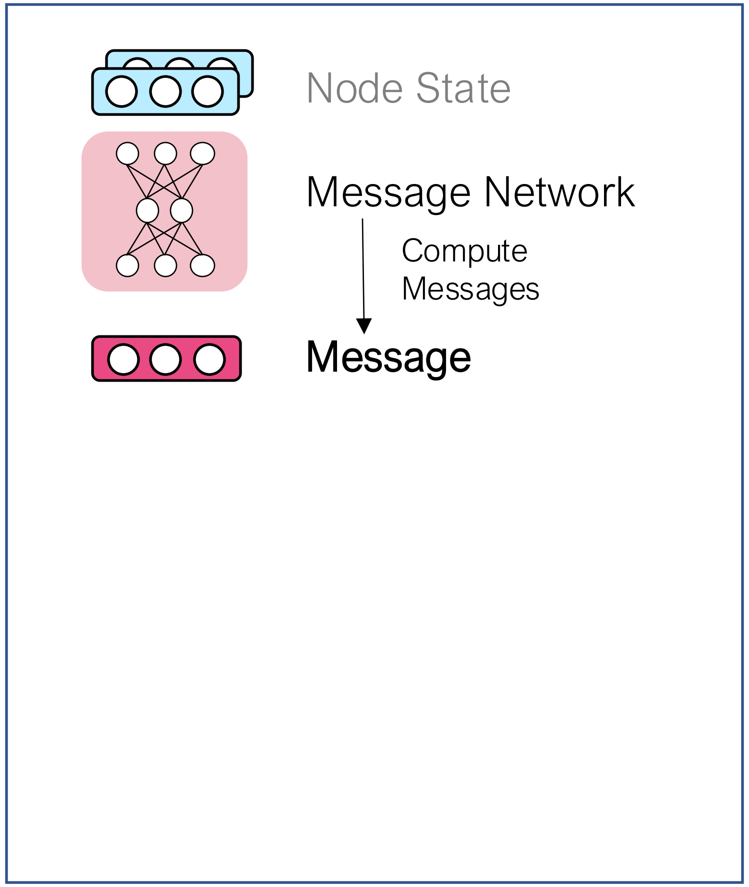

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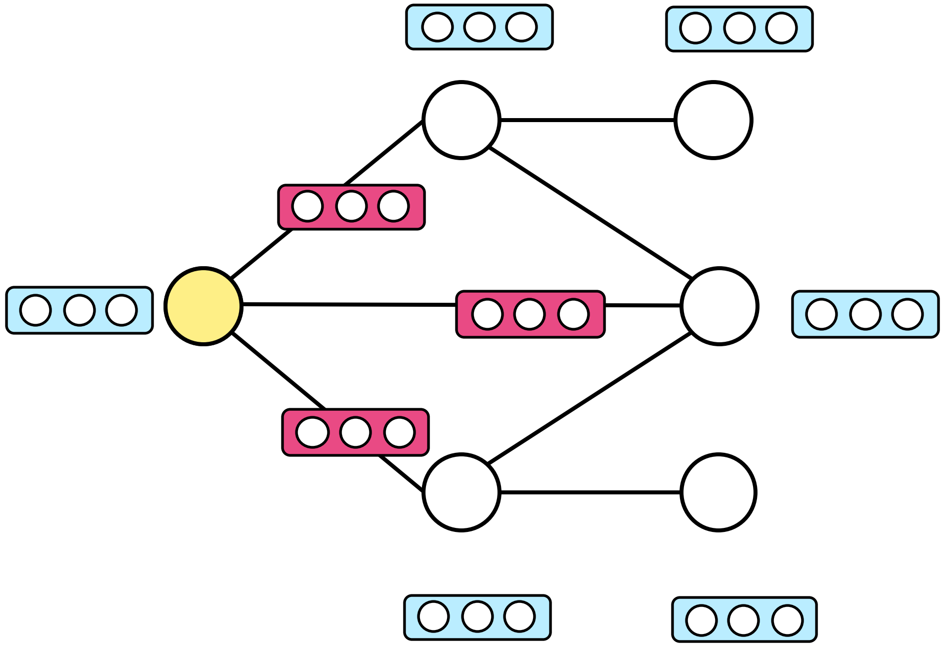

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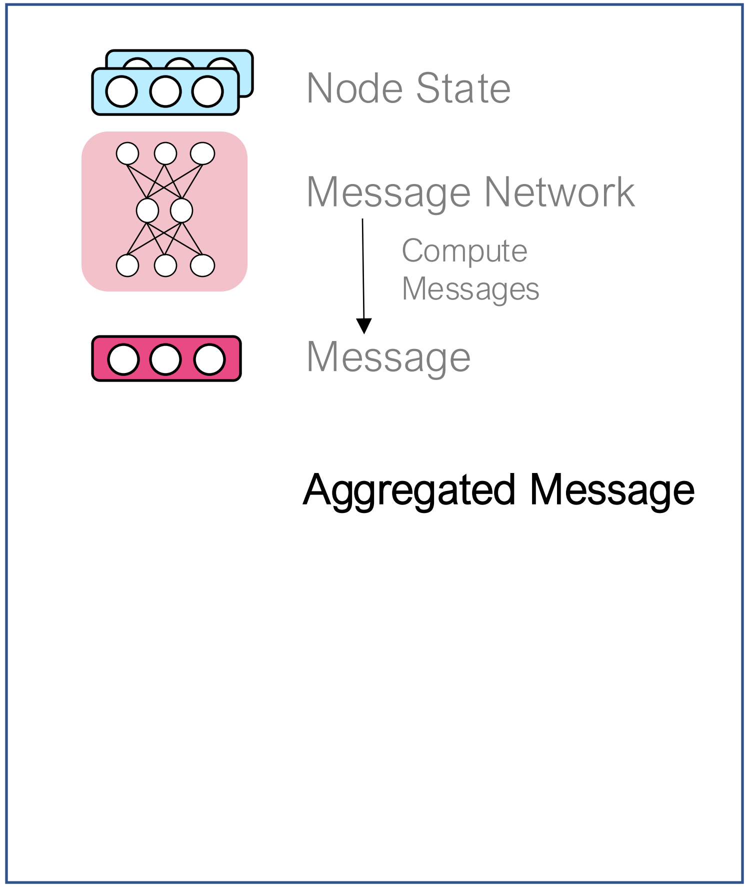

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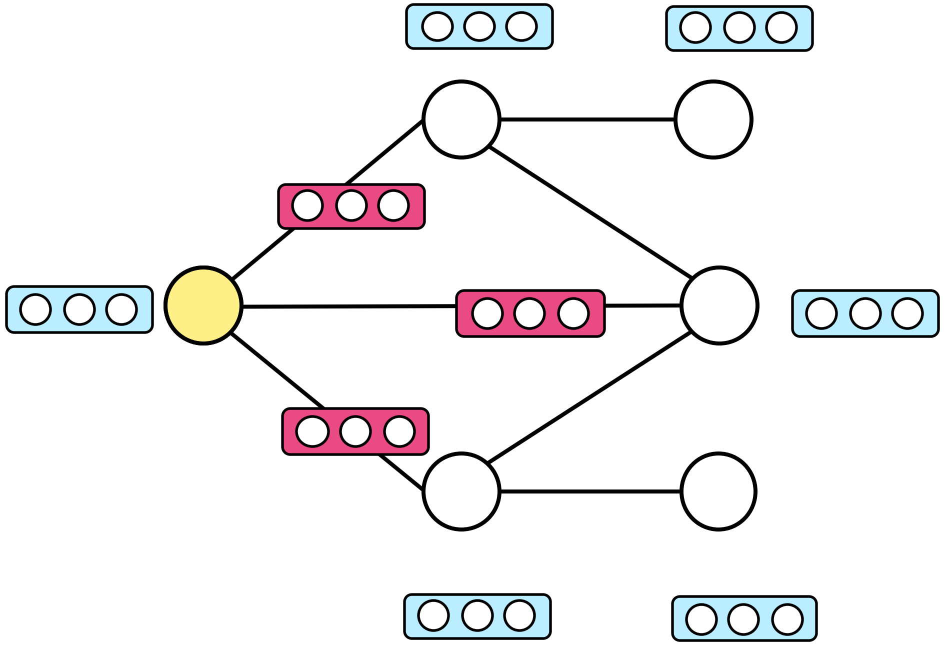

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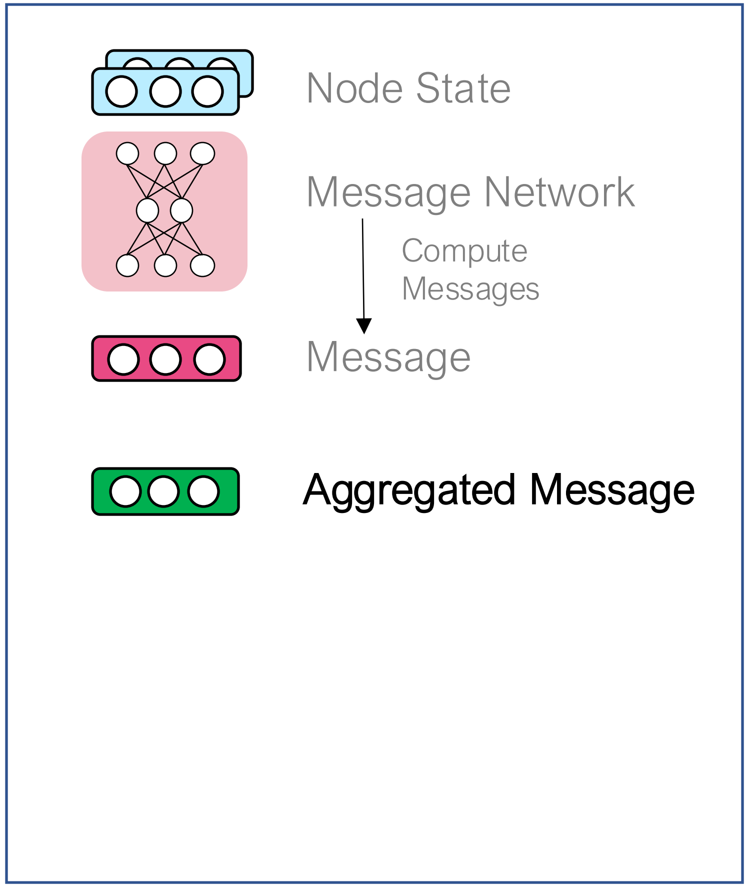

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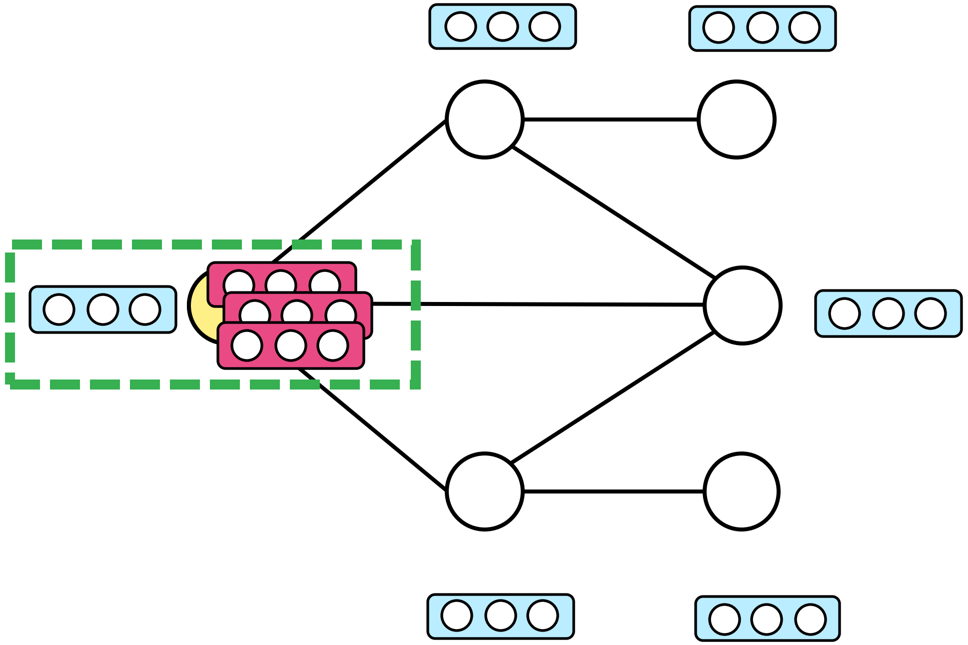

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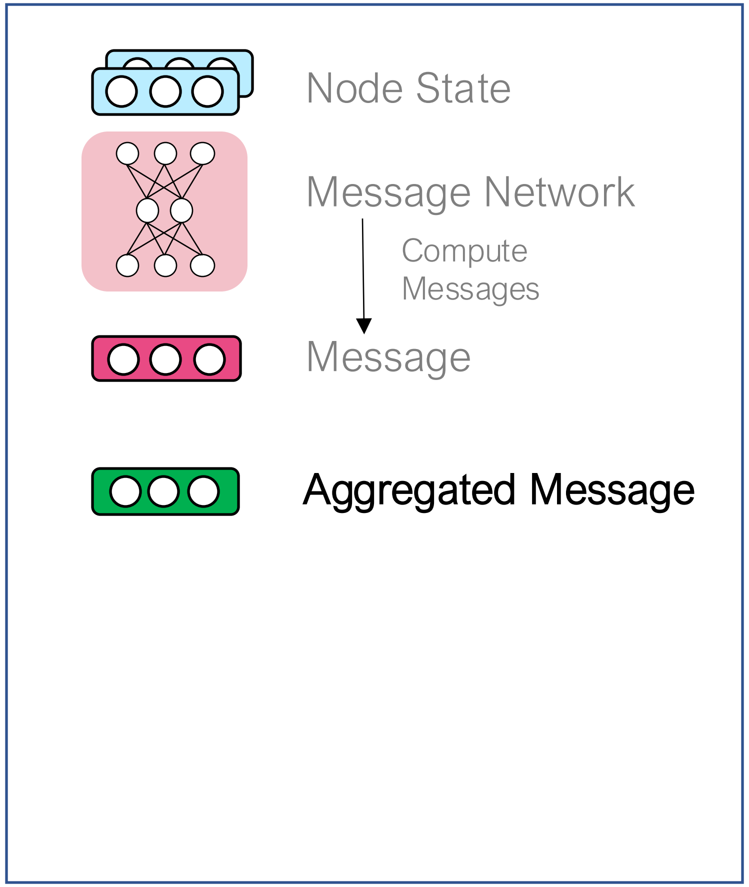

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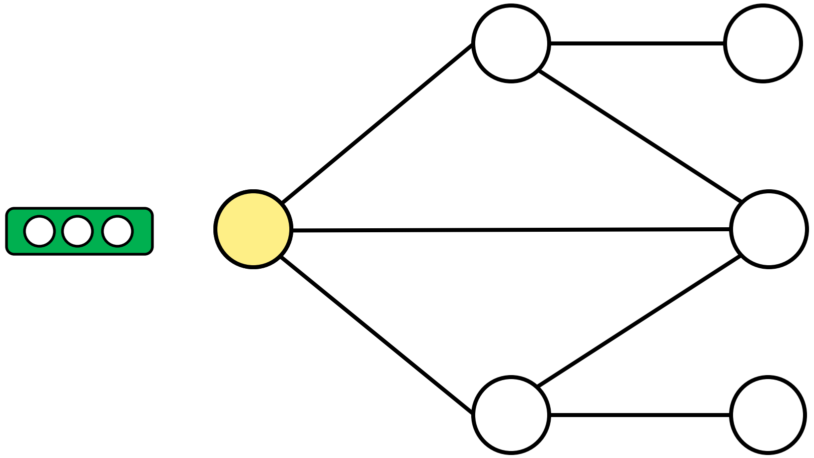

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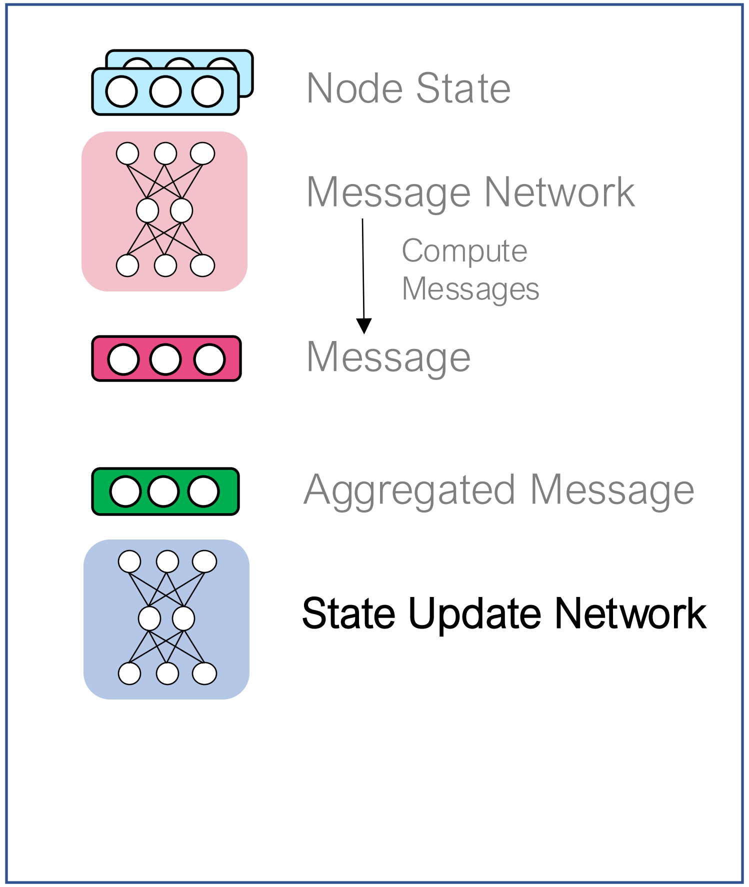

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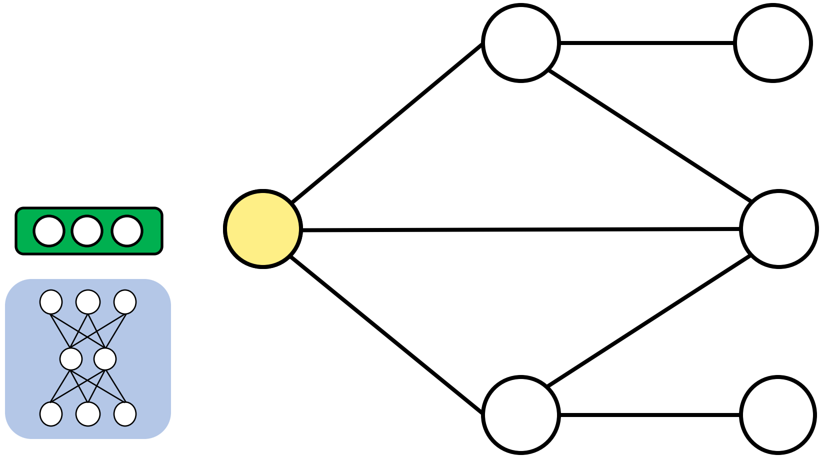

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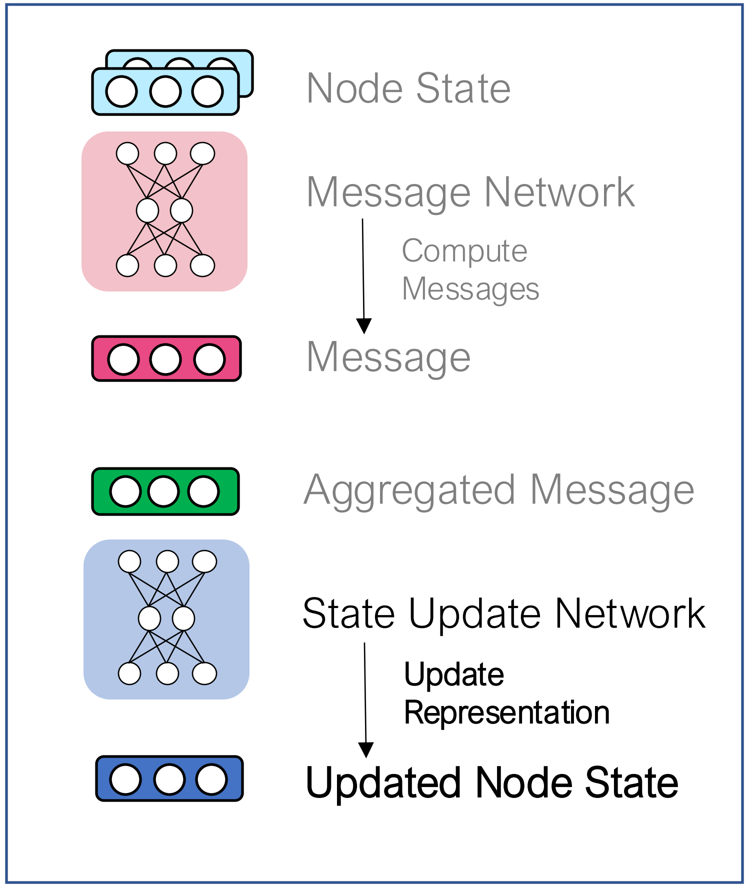

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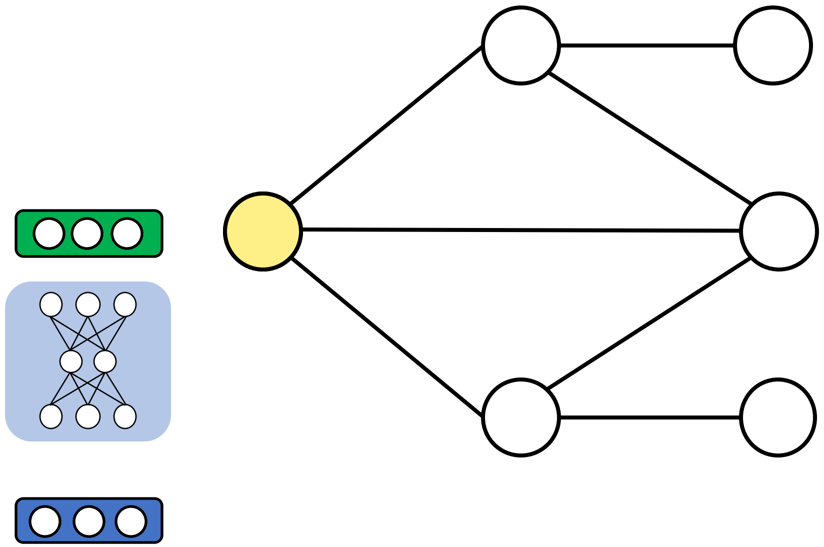

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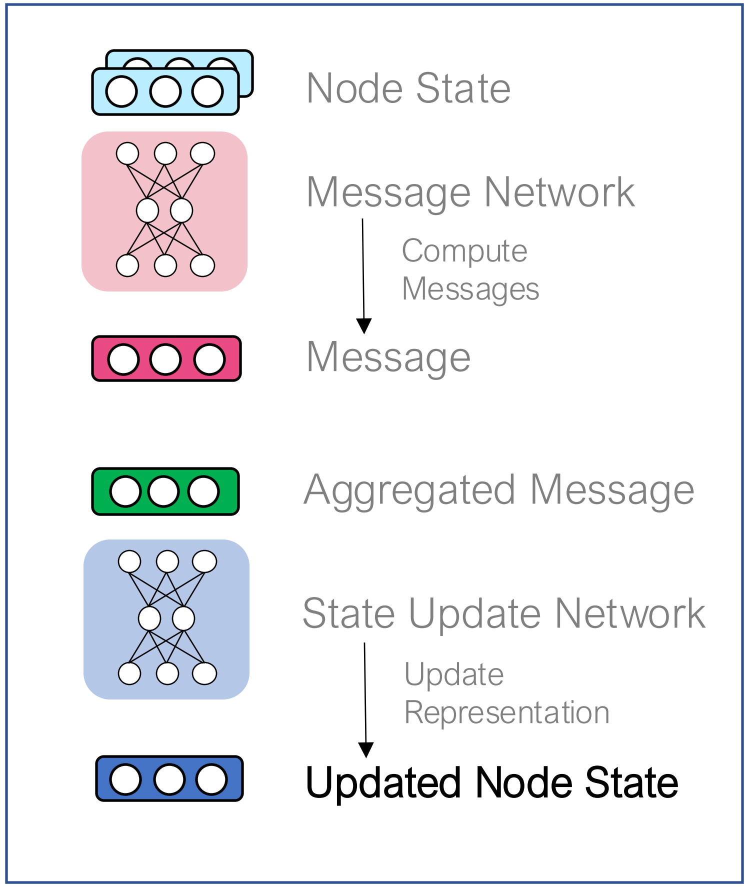

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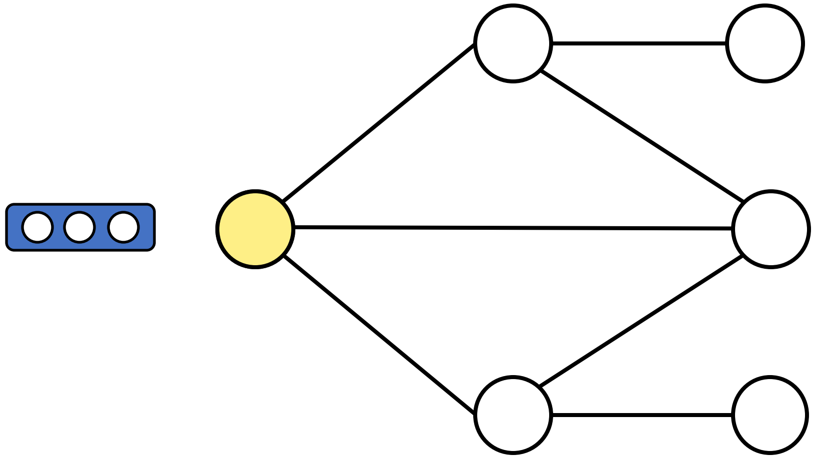

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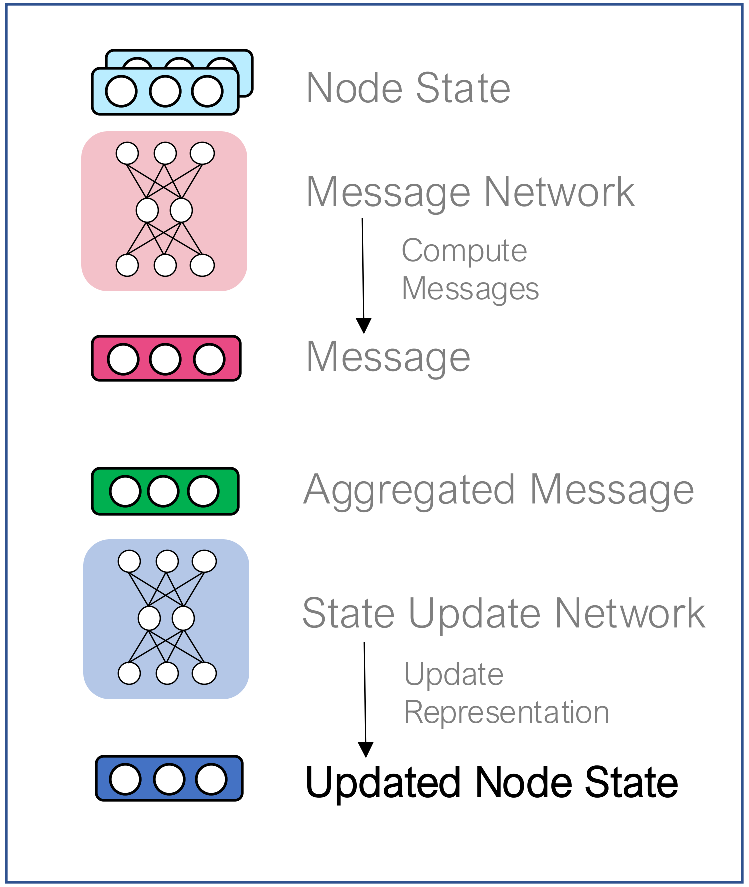

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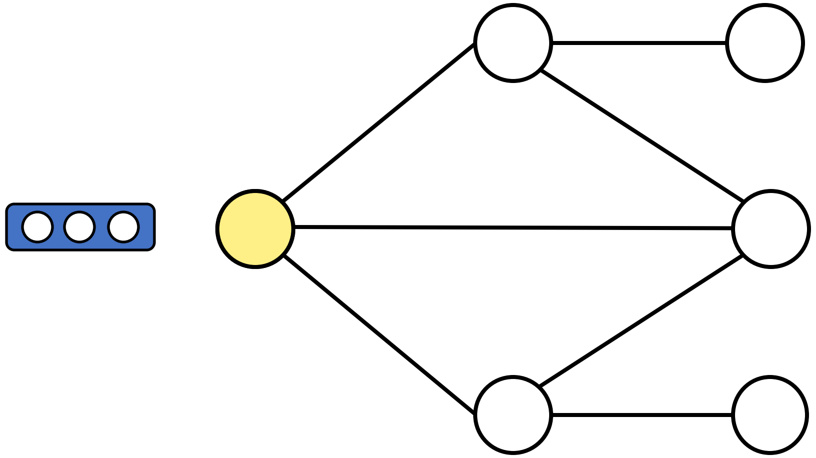

- Parallel Schedule!

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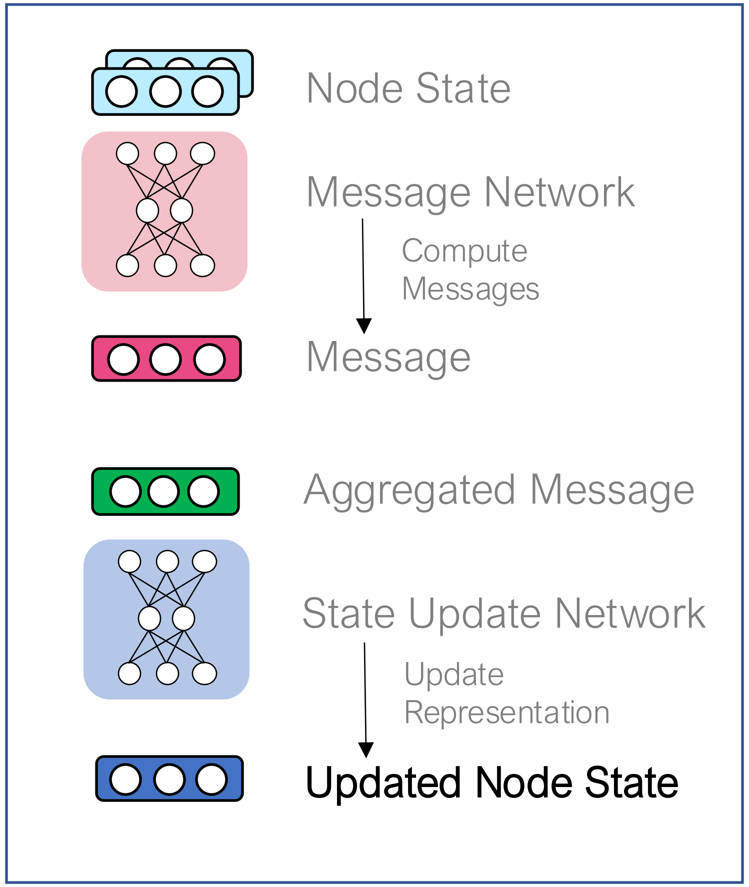

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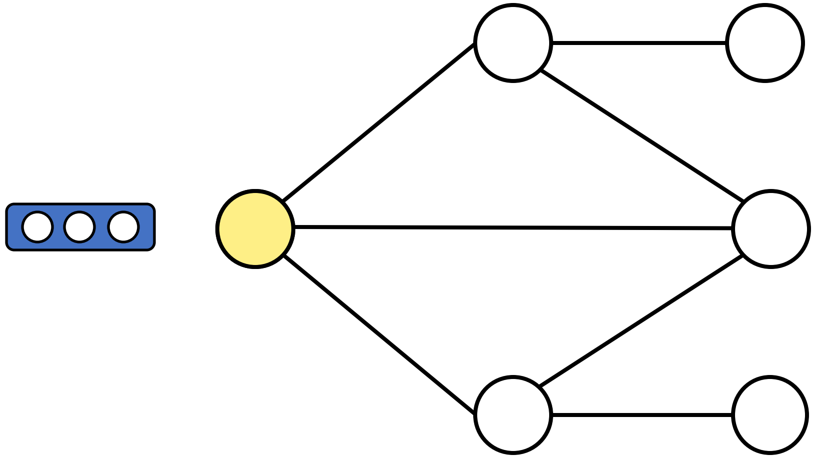

- Parallel Schedule!
- Other schedules [12] are possible and could improve performance in certain tasks!

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Message Passing in GNNs

Instantiations:

1. Compute Messages

$$\mathbf{m}_{ji}^{t} = f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

2. Aggregate Messages

$$\bar{\mathbf{m}}_i^t = f_{\mathrm{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right)$$

3. Update Node Representations

$$\mathbf{h}_i^{t+1} = f_{\mathrm{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$

Message Passing in GNNs

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$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [11]

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Edge Feature

Message Passing in GNNs

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Message Passing in GNNs

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Outline

- Applications of Graphs
- Background
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- GNNs
    - Overview
    - Message Passing
    - Message Passing Architectures
    - **Readout**
- Implementation
- Relationship w. Transformers

Readout in GNNs

Instantiations:

1. Node Readout

$$\mathbf{y}_i = f_{\text{readout}}(\mathbf{h}_i^T)$$

2. Edge Readout

$$\mathbf{y}_{ij} = f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T)$$

3. Graph Readout

$$\mathbf{y} = f_{\text{readout}}(\{\mathbf{h}_i^T\})$$

Readout in GNNs

Instantiations:

1. **Node Readout**

$$\mathbf{y}_i = f_{\text{readout}}(\mathbf{h}_i^T) \qquad f_{\text{readout}}(\mathbf{h}_i^T) = \text{MLP}(\mathbf{h}_i^T)$$

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Edge Feature

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Edge Feature

3. Graph Readout

$$\mathbf{y} = f_{\text{readout}}(\{\mathbf{h}_i^T\})$$

$$f_{\text{readout}}(\{\mathbf{h}_i^T\}) = \sum_i \sigma(\text{MLP}_1(\mathbf{h}_i^T))\text{MLP}_2(\mathbf{h}_i^T)$$

$$f_{\text{readout}}(\{\mathbf{h}_i^T\}, \mathbf{g}) = \sum_i \sigma(\text{MLP}_1(\mathbf{h}_i^T, \mathbf{g}))\text{MLP}_2(\mathbf{h}_i^T, \mathbf{g})$$

Graph Feature

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Implementations

1. *Although graph could be very sparse, we should maximally exploit dense operators since they are efficient on GPUs!*

2. *Parallel message passing is very GPU friendly!*

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Tips:

- Use adjacency list representation
- Compute messages for all edges in parallel
- Compute aggregations for all nodes in parallel
- Compute updates for all nodes in parallel

Outline

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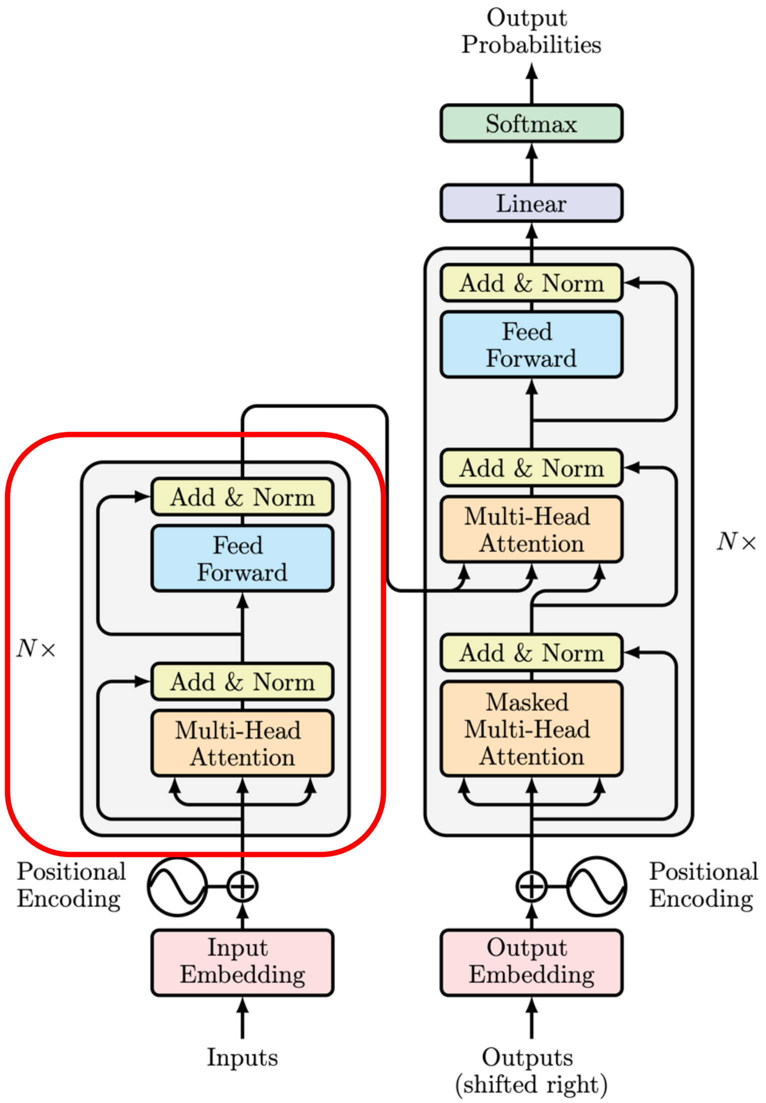
- **Relationship w. Transformers**

Relationships with Transformer



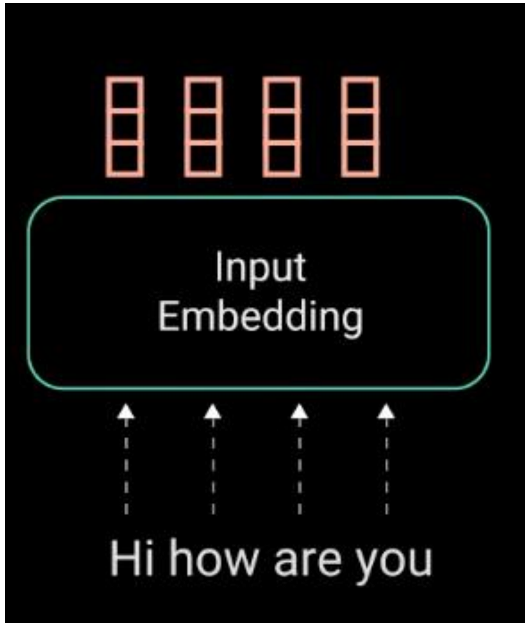
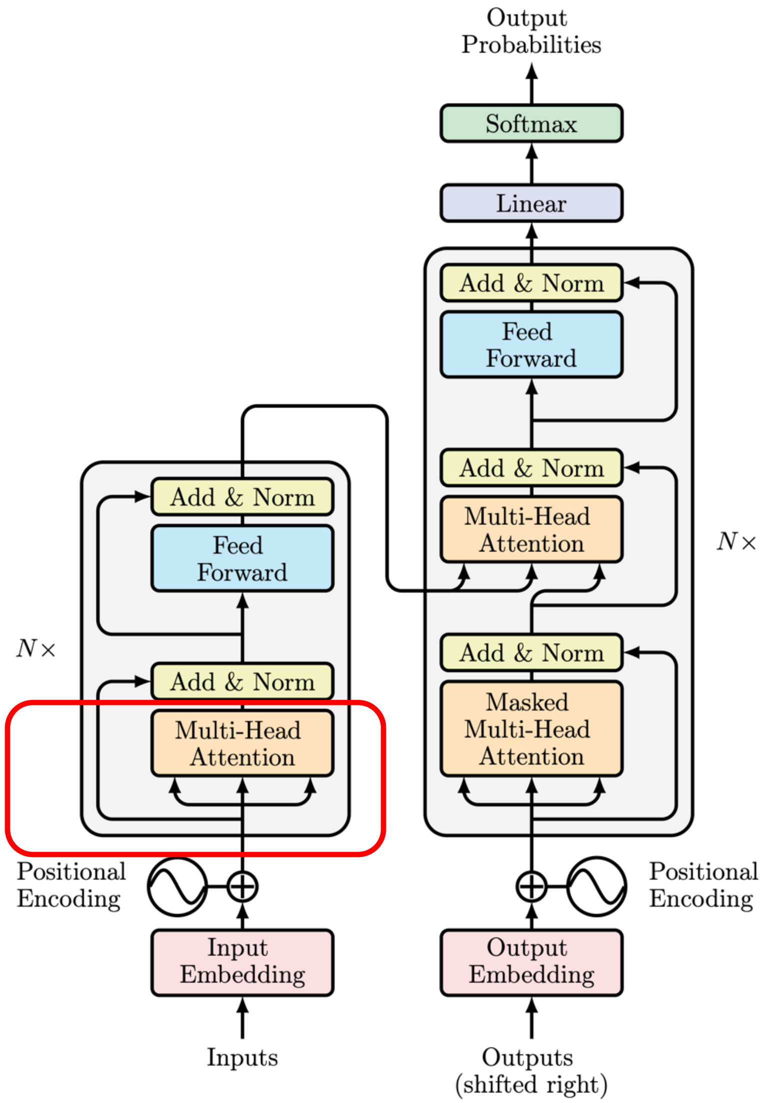
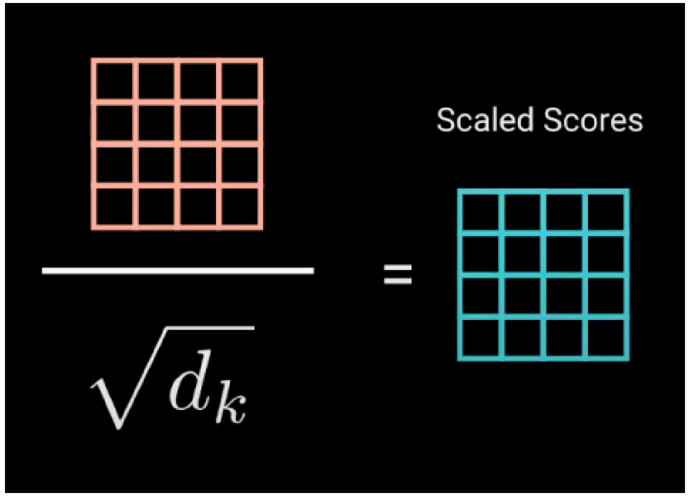
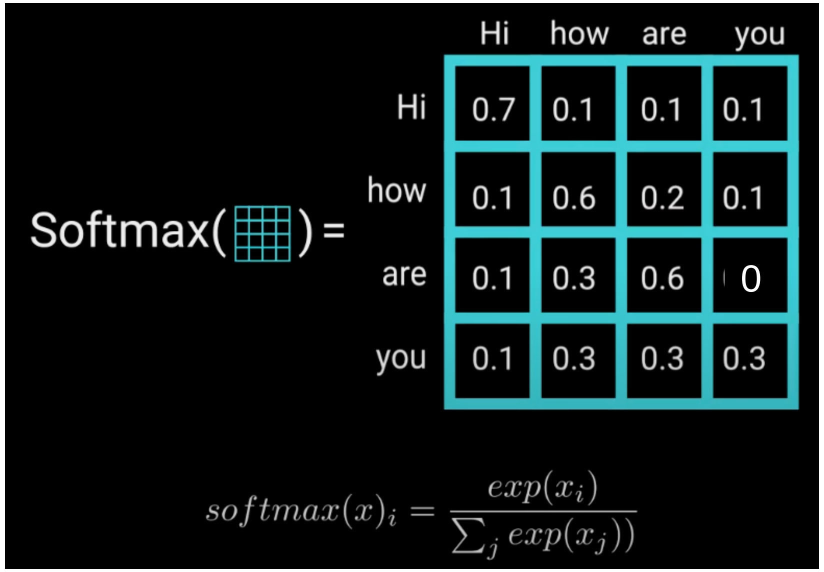


Image Credit: [16, 17]

Relationships with Transformer







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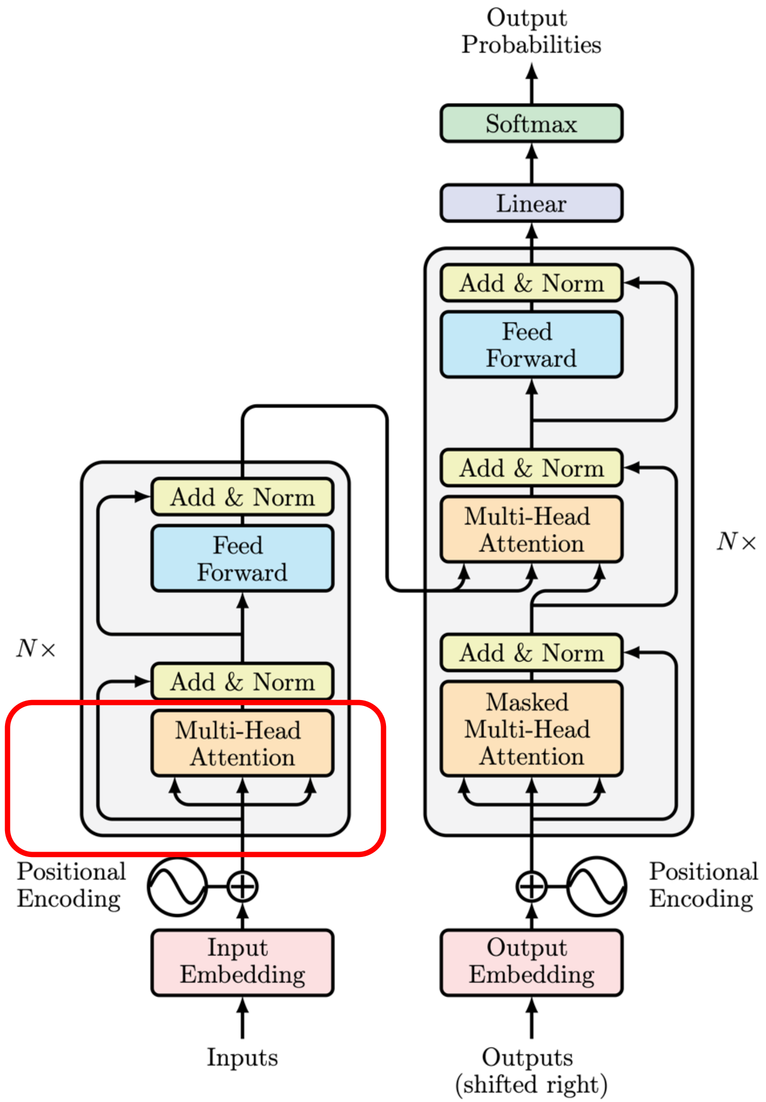
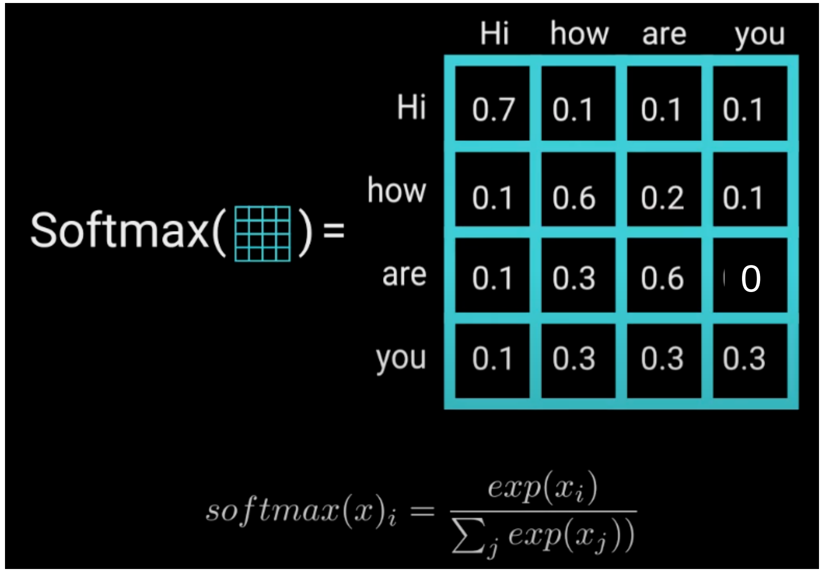


- Attention can be viewed as the weighted adjacency matrix of a fully connected graph!



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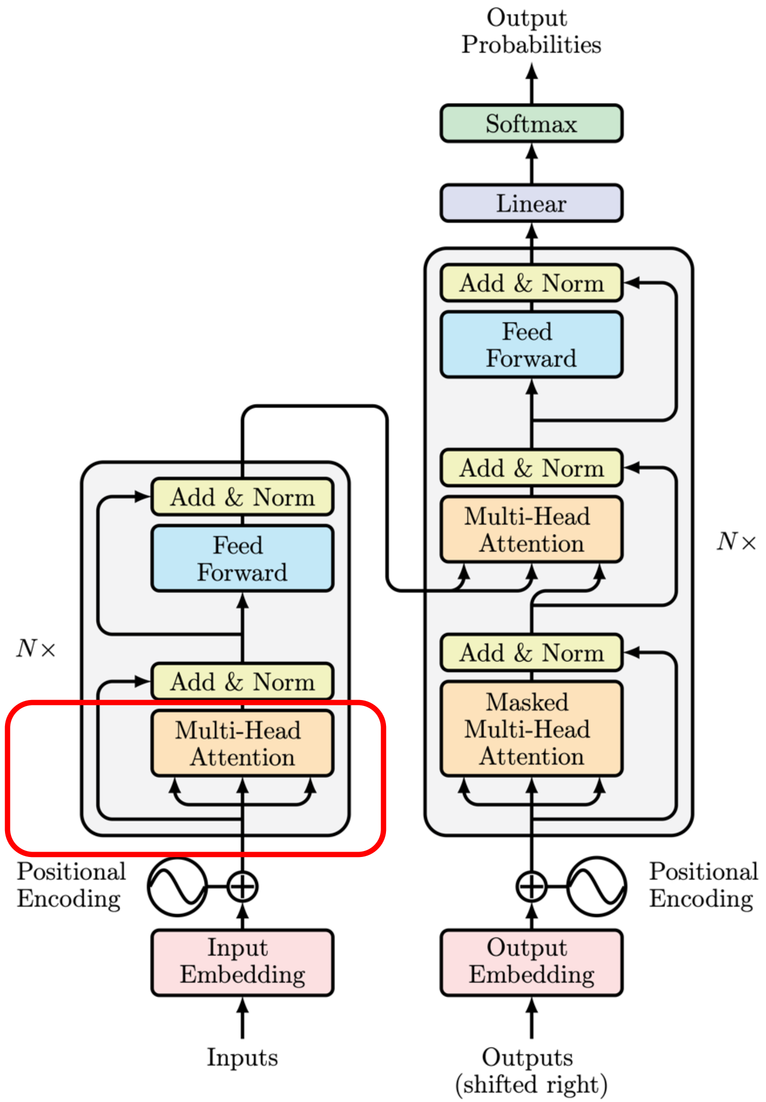
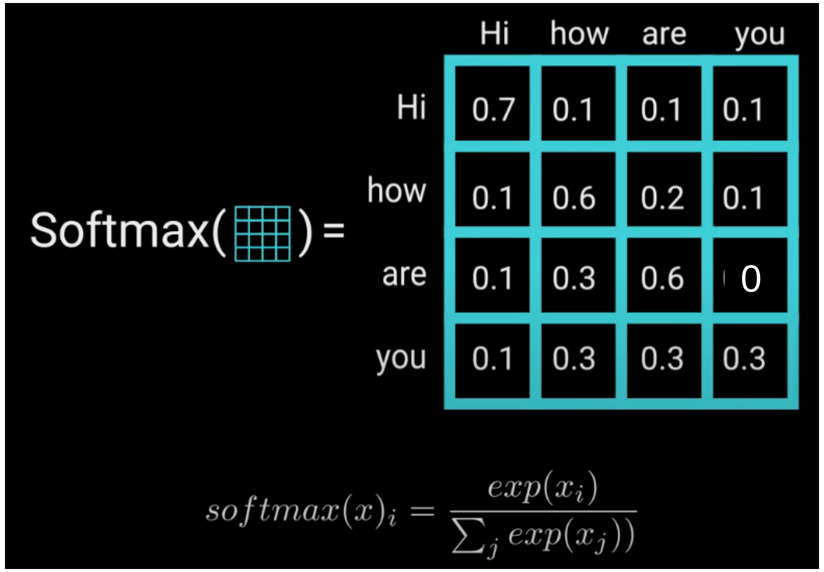


- Attention can be viewed as the weighted adjacency matrix of a fully connected graph!
- Transformers (esp. encoder) can be viewed as GNNs applied to fully connected graphs!



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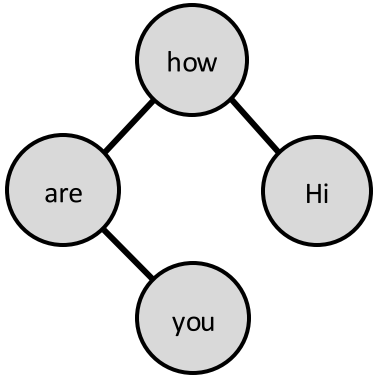
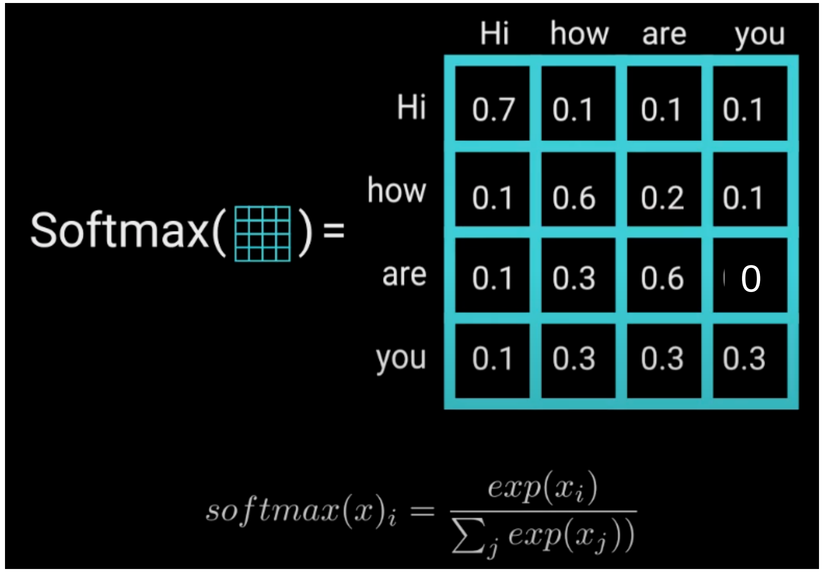
Encode Graph Structures in Transformers

- Apply the adjacency matrix as a mask to the attention and renormalize it, like Graph Attention Networks (GAT) [18]
- Encode connectivities/distances as bias of the attention [19]



	Hi	how	are	you
Hi	0	1	0	1
how	1	0	0	0
are	0	0	0	1
you	1	0	1	0



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Questions?