EECE 571F: Advanced Topics in Deep Learning

Lecture 3: Graph Neural Networks I
Message Passing Models

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University of British Columbia

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Outline

- Motivating Applications

- Graph Neural Networks (GNNs)

  - Graph representations
  - Graph isomorphism & automorphism
  - Challenges of graph data
  - Graph Neural Networks (GNNs): history & basics
  - Message passing framework of GNNs
  - Instantiation of message passing
  - Relationship with Transformers

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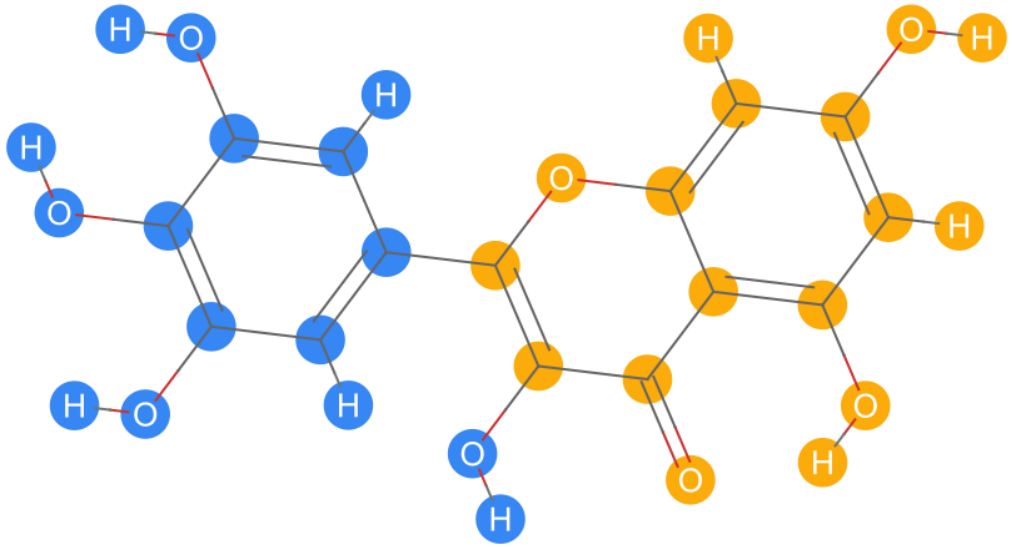
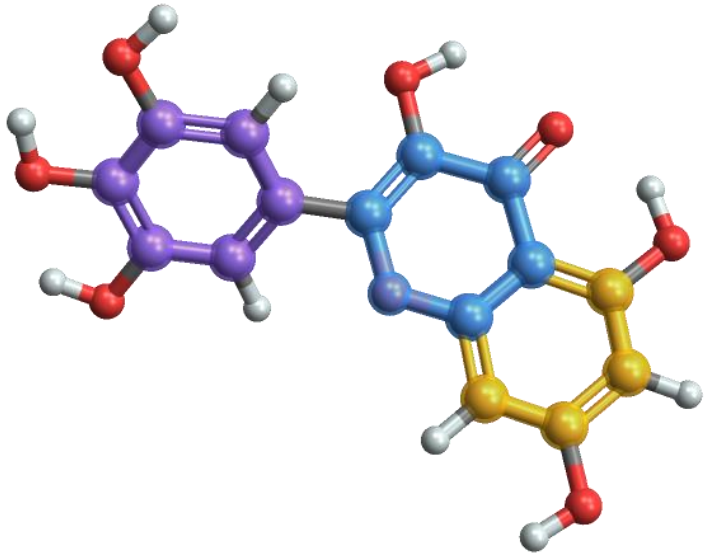
Motivating Applications of Graphs

- Molecules





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

Image Credit: https://www.wolfram.com/language/12/molecular-structure-and-computation/molecule-graphs.html.en?product=mathematica
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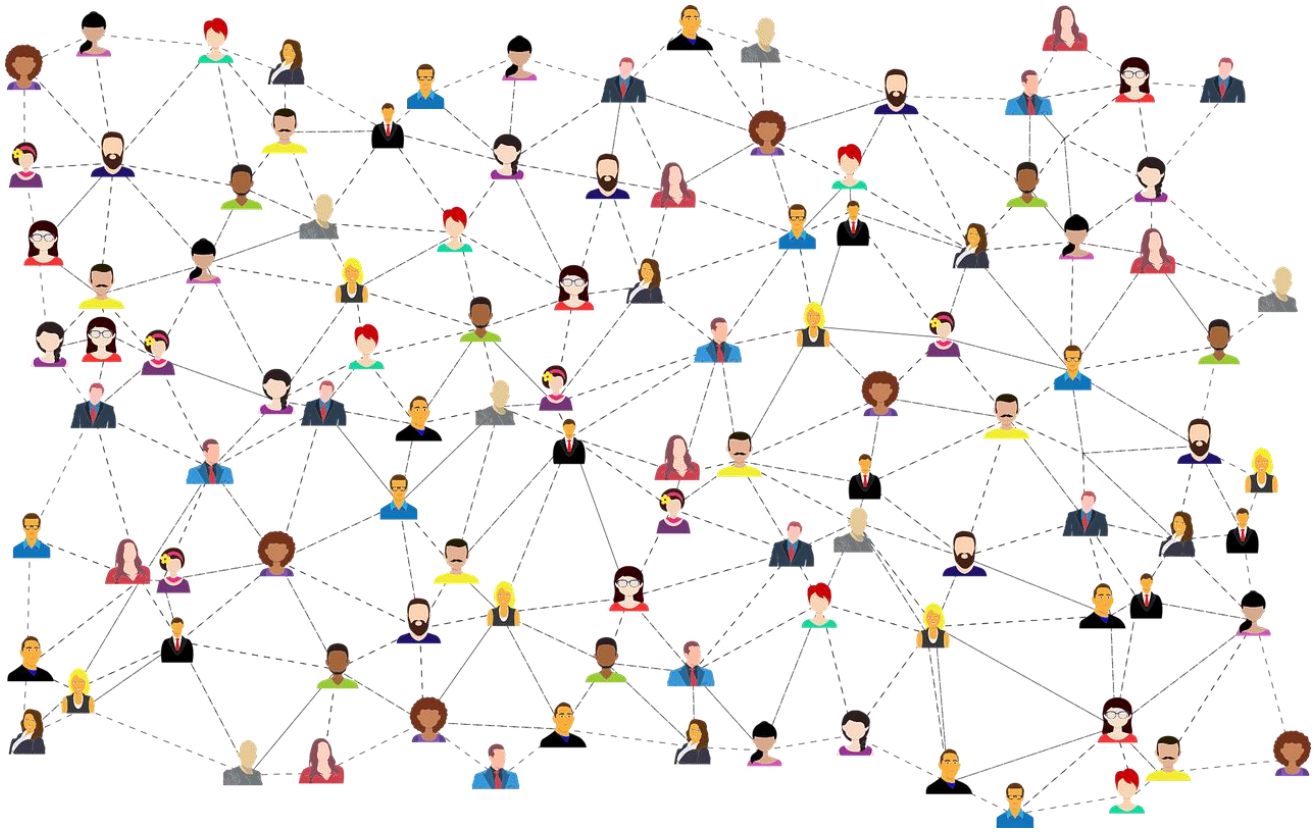
Motivating Applications of Graphs

- Social Networks

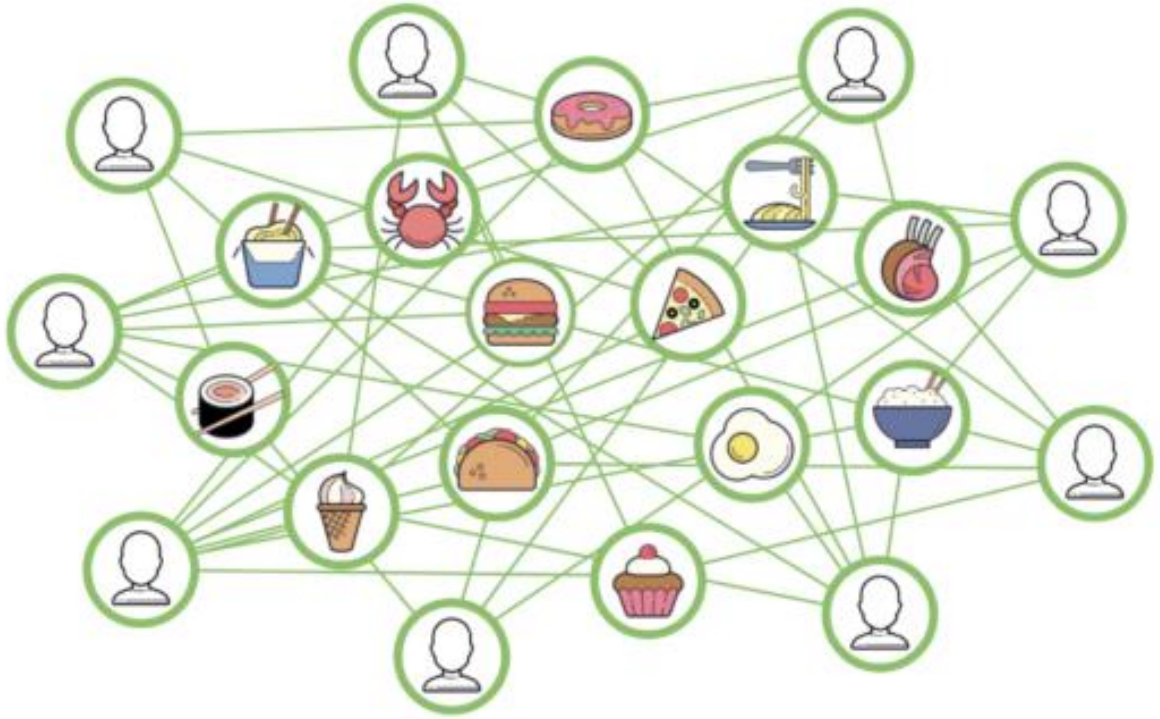


Link Prediction

Image Credit: https://www.euroscientist.com/imagine-a-social-network-like-facebook-with-no-facebook/

Motivating Applications of Graphs

- Network-based Recommendations



Food Discovery

Image Credit: https://eng.uber.com/uber-eats-graph-learning/

Motivating Applications of Graphs

- Citation Networks

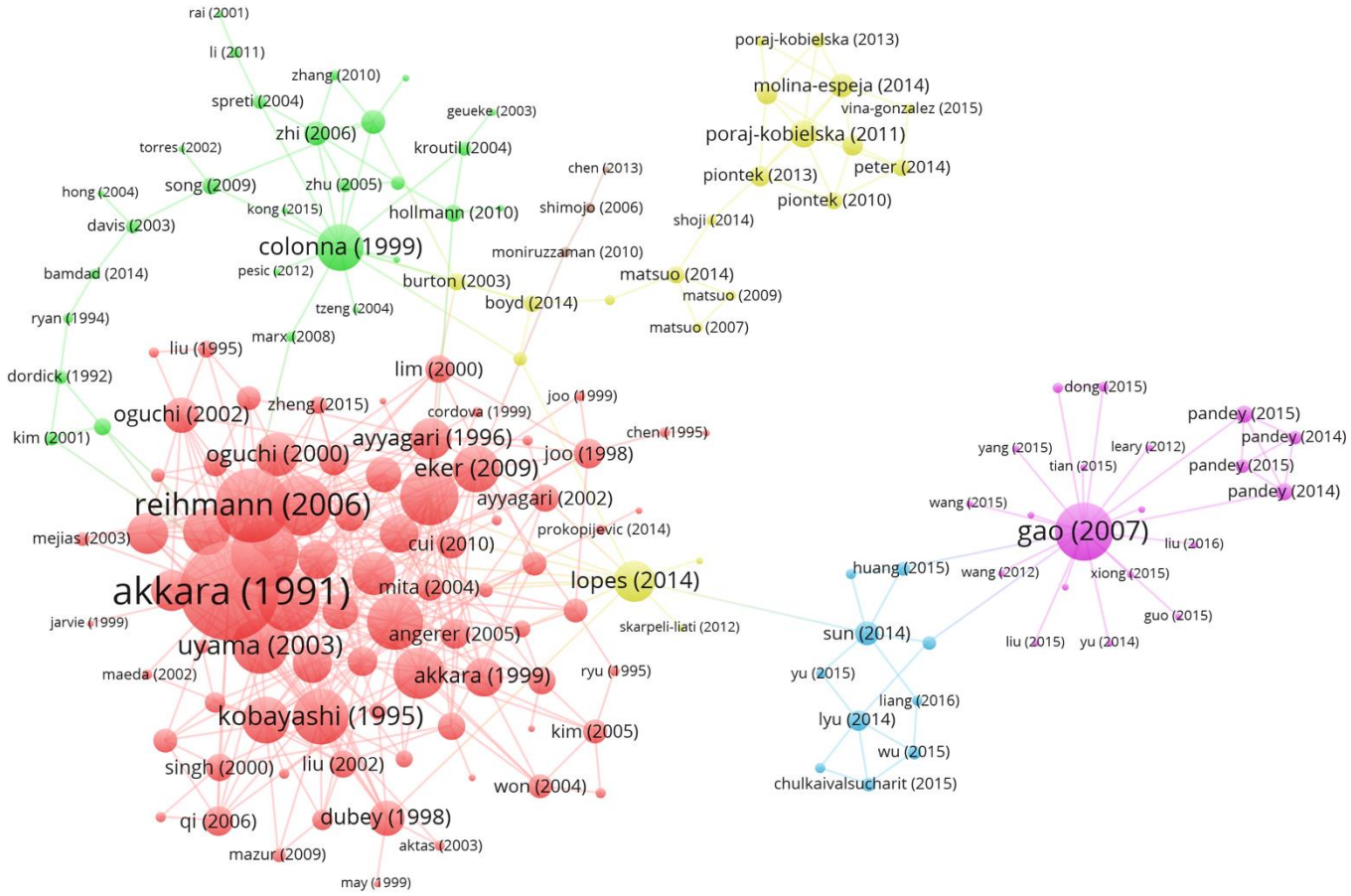
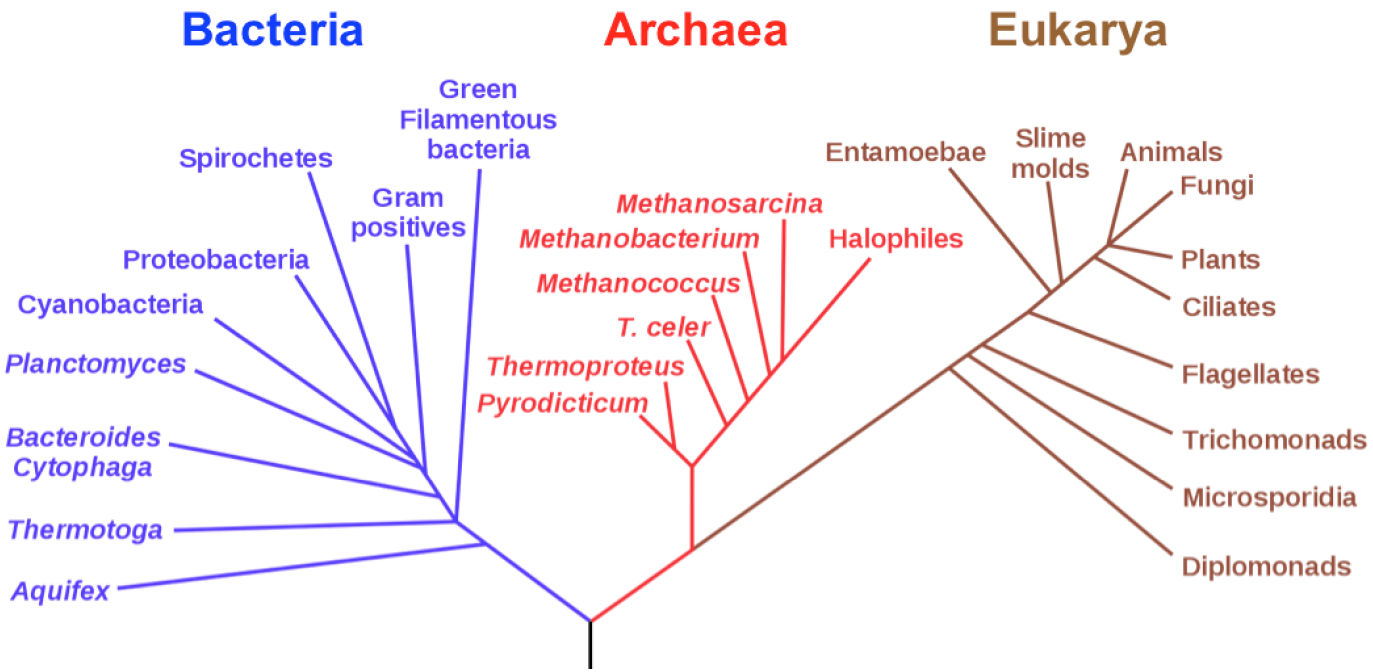


Image Credit: https://www.tudelft.nl/en/library/research-analytics/case-12-citation-networks-2

Motivating Applications of Graphs

- Phylogenetic Tree

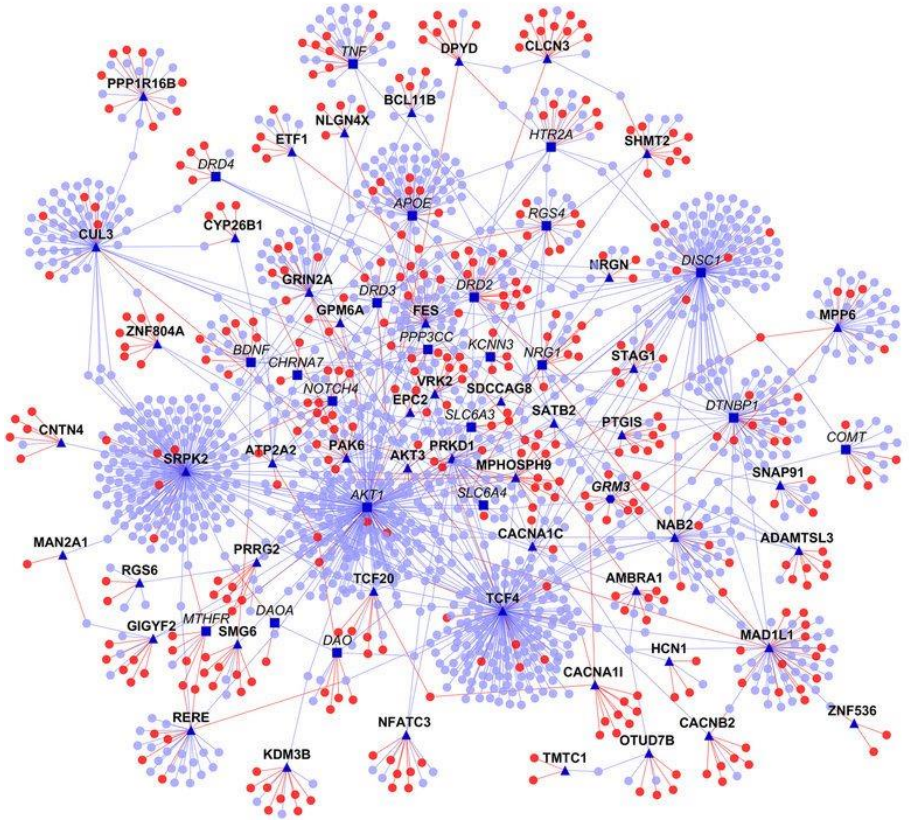


A phylogenetic tree based on rRNA genes showing the three life domains

Image Credit: https://en.wikipedia.org/wiki/Phylogenetic_tree

Motivating Applications of Graphs

- Protein-Protein Interactions (PPIs)



Schizophrenia PPI

Image Credit: https://en.wikipedia.org/wiki/Protein%E2%80%93protein_interaction

Motivating Applications of Graphs

- Epidemic Networks

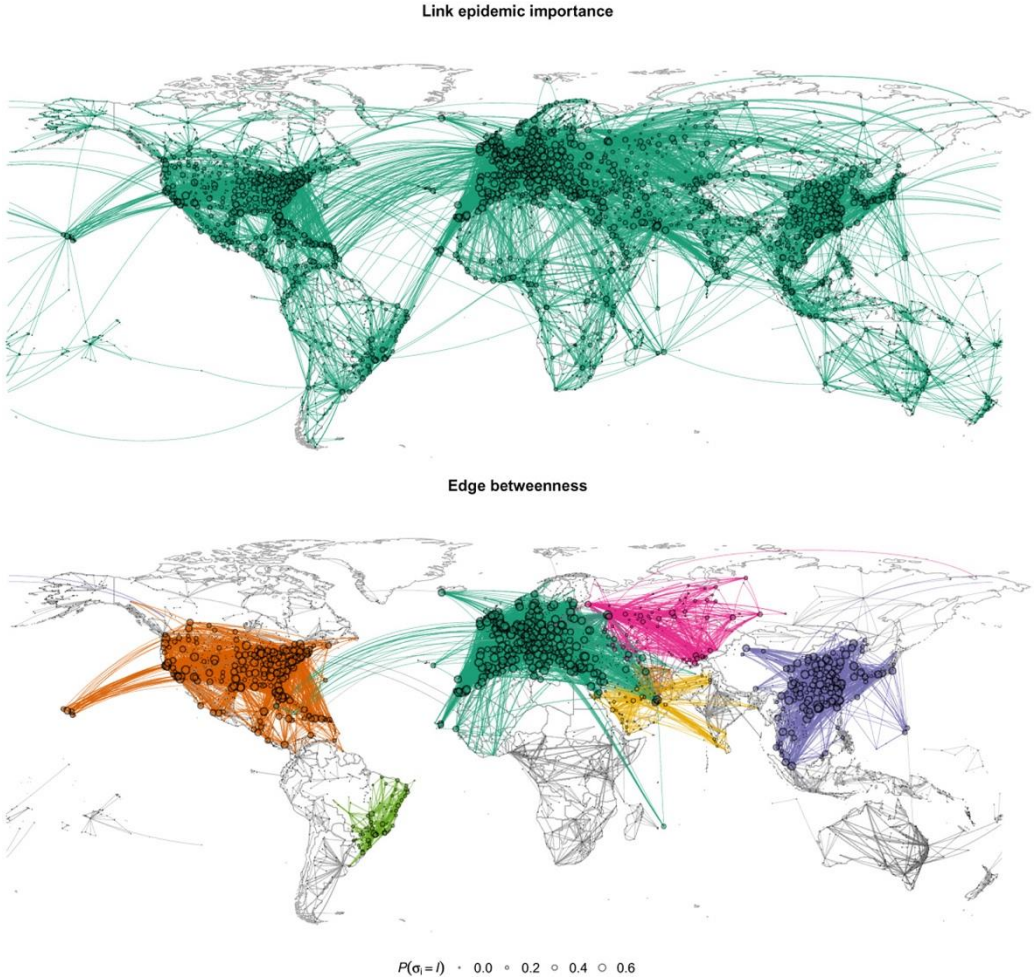


Image Credit: https://www.science.org/doi/10.1126/sciadv.aau4212

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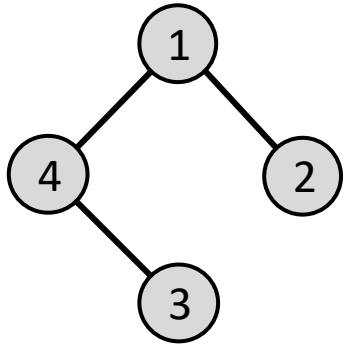
Deep Learning for Graphs

Graph Representations

- Connectivity

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

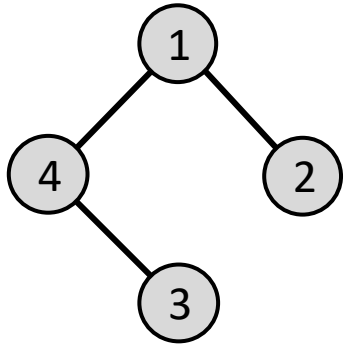


V = {1,2,3,4}, E = {(1,2), (1,4), (4,3)}

Deep Learning for Graphs

Graph Representations

- Connectivity
    1. Adjacency List: G = (V, E)
    2. Adjacency Matrix: A (sometimes we have weights)



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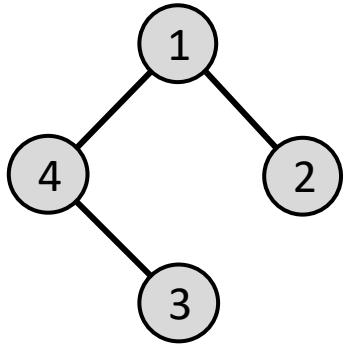
Deep Learning for Graphs

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 for Graphs

Graph Representations

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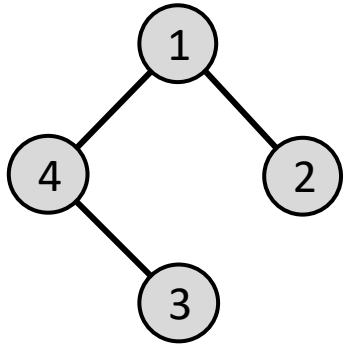
    3. Graph Feature

Graph Data = (A, X)



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Deep Learning for Graphs

Permutation

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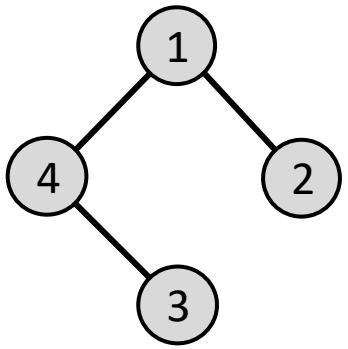

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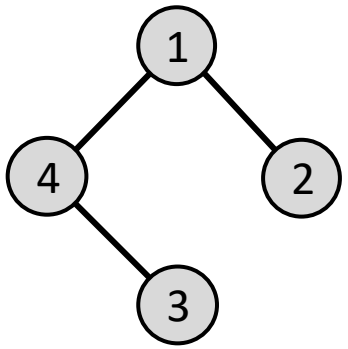

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Original Adj Matrix

Deep Learning for Graphs

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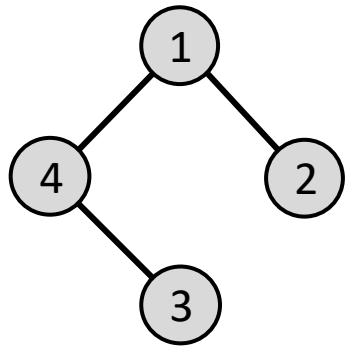

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V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

Permute Rows

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

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
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Transposed Permutation Matrix

Deep Learning for Graphs

Permutation

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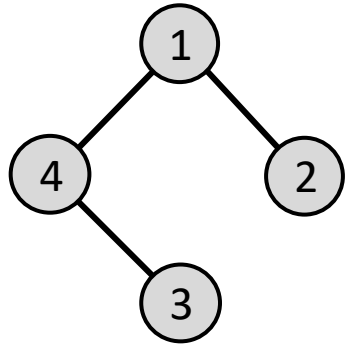

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Original Adj Matrix

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Transposed Permutation Matrix

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Permuted Adj Matrix

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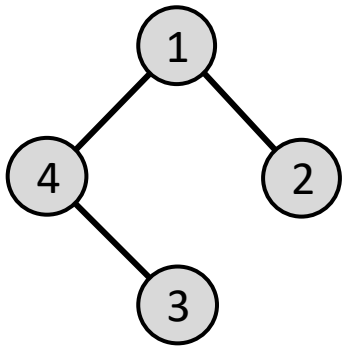

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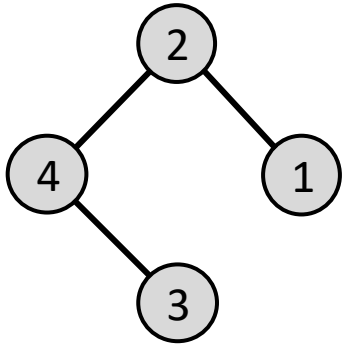

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V' = [2,1,3,4], E' = [(2,1), (2,4), (4,3)]

Deep Learning for Graphs

Permutation

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

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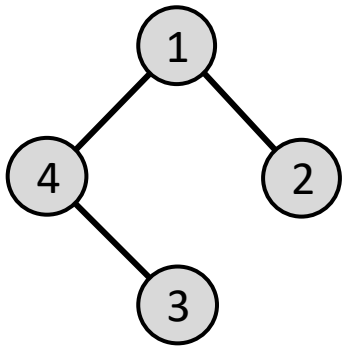

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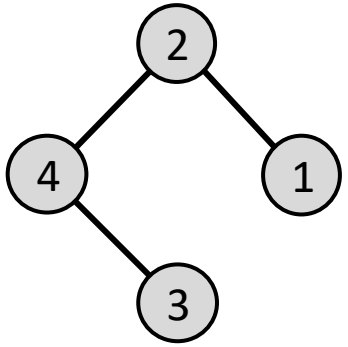
V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

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 for Graphs

Permutation

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

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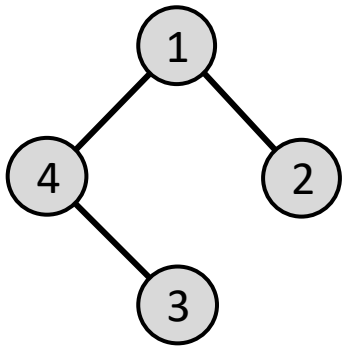

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Deep Learning for Graphs

Permutation

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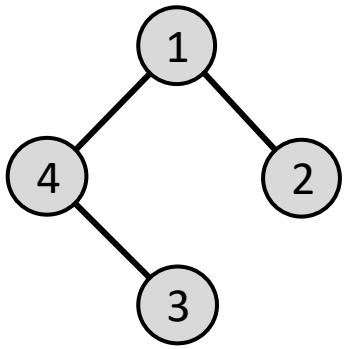

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Original Adj Matrix

Deep Learning for Graphs

Permutation

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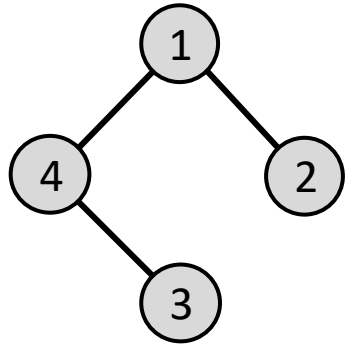

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V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

Permute Rows

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

Permutation Matrix

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

Permute Columns

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

Deep Learning for Graphs

Permutation

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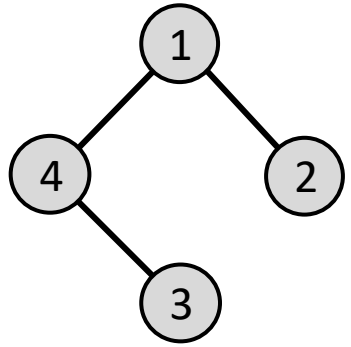

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Permutation Matrix

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Original Adj Matrix

Permute Columns

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Transposed Permutation Matrix

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Permuted Adj Matrix

Deep Learning for Graphs

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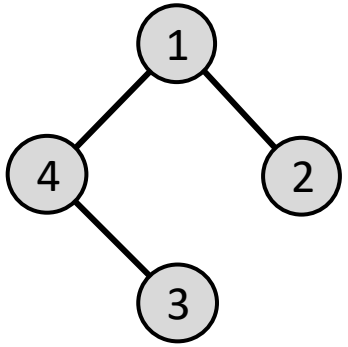

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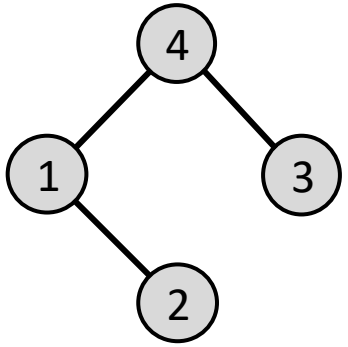

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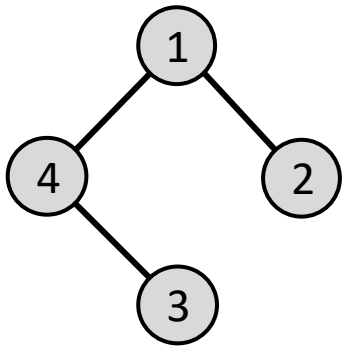

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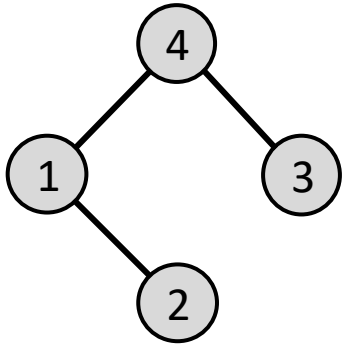
Graph Automorphism:

*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.*

$$PAP^{\top} = A$$



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

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

Deep Learning for 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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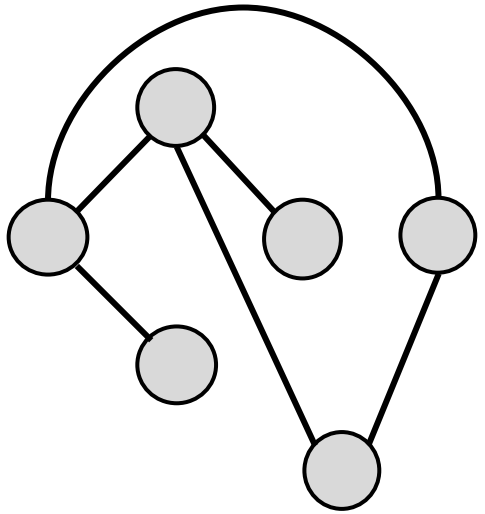
Deep Learning for Graphs

Key Challenges:

- **Unordered Neighbors**



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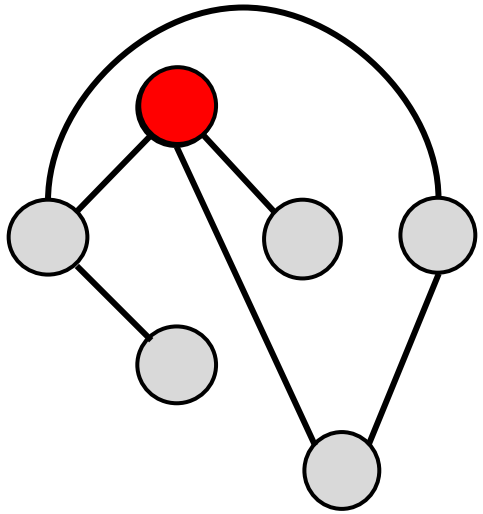

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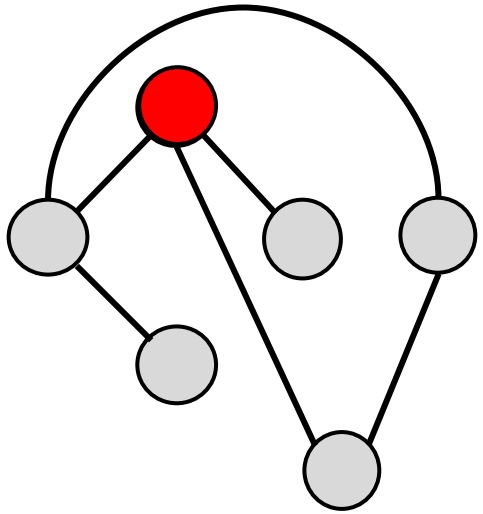

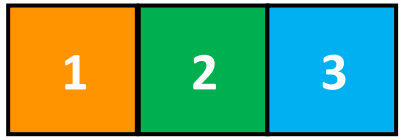

Deep Learning for Graphs

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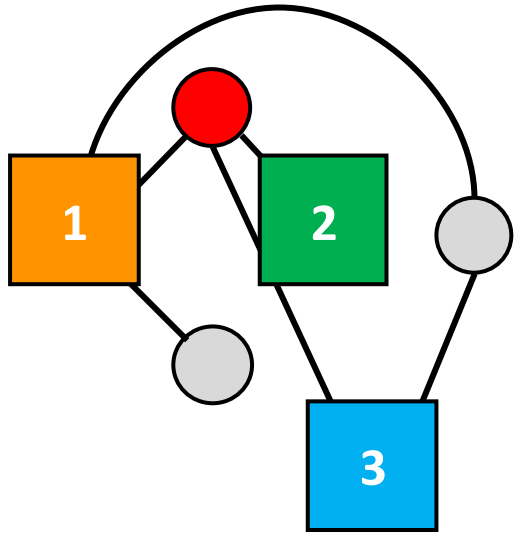

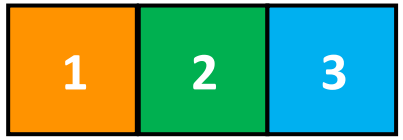

Option 1

Deep Learning for Graphs

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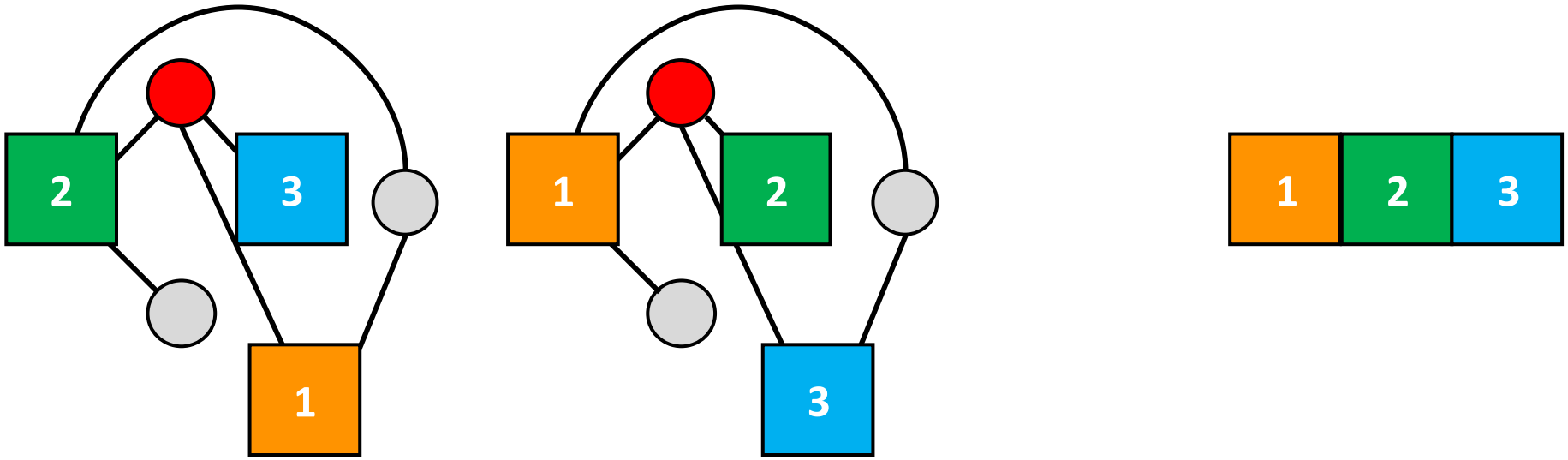
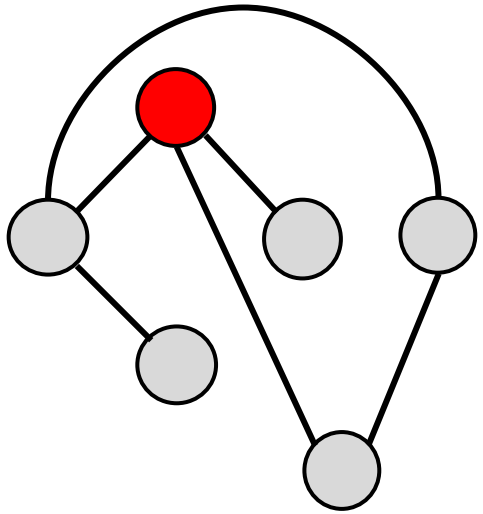


Option 2 Option 1

Deep Learning for Graphs

Key Challenges:

- Unordered Neighbors
- **Varying Neighborhood Sizes**



Deep Learning for Graphs

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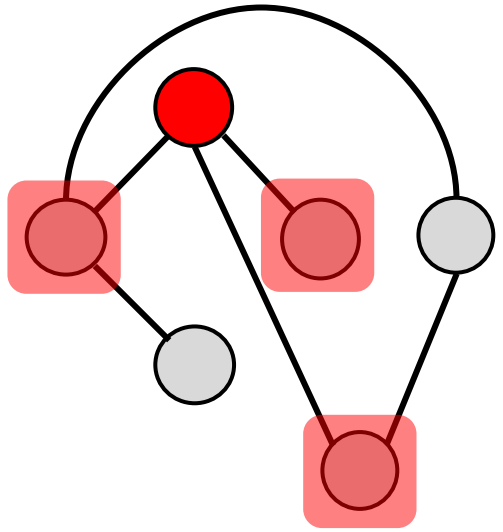

Deep Learning for Graphs

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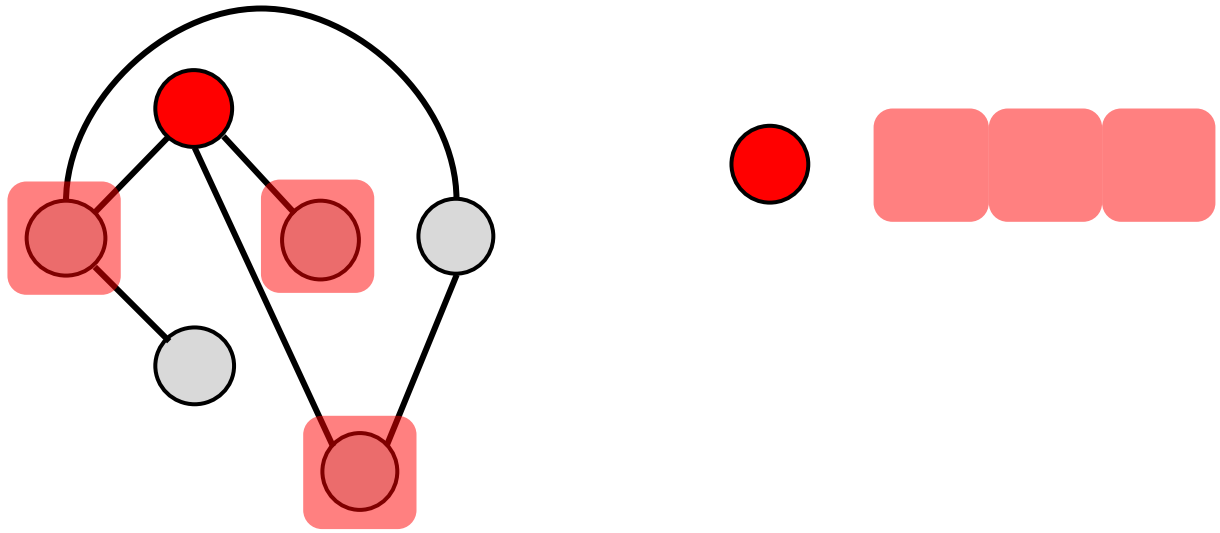

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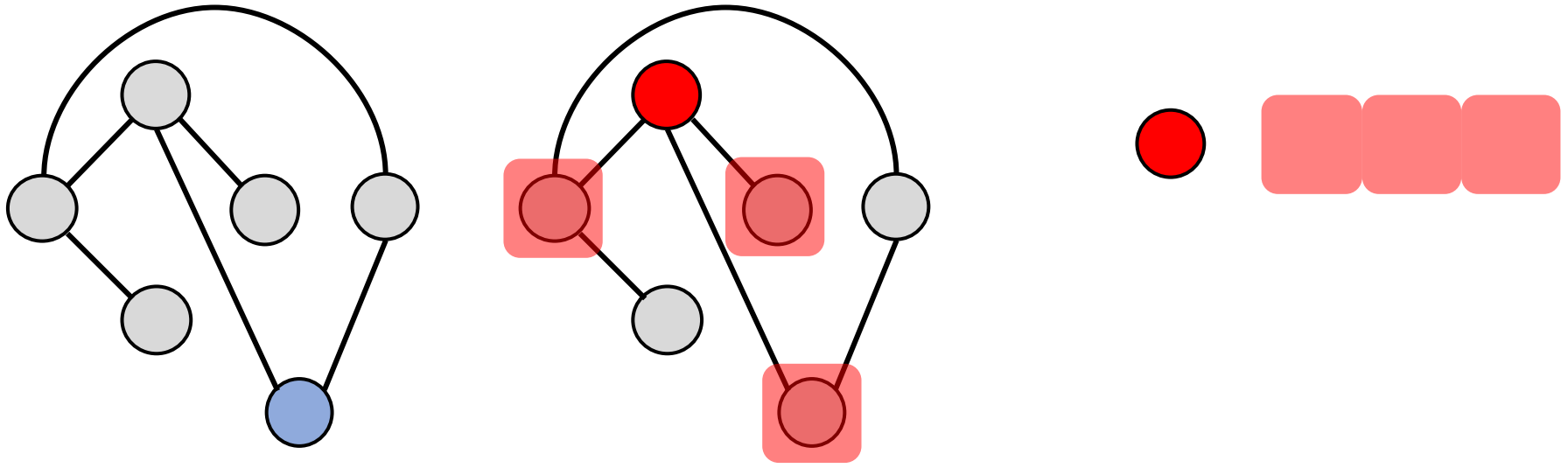

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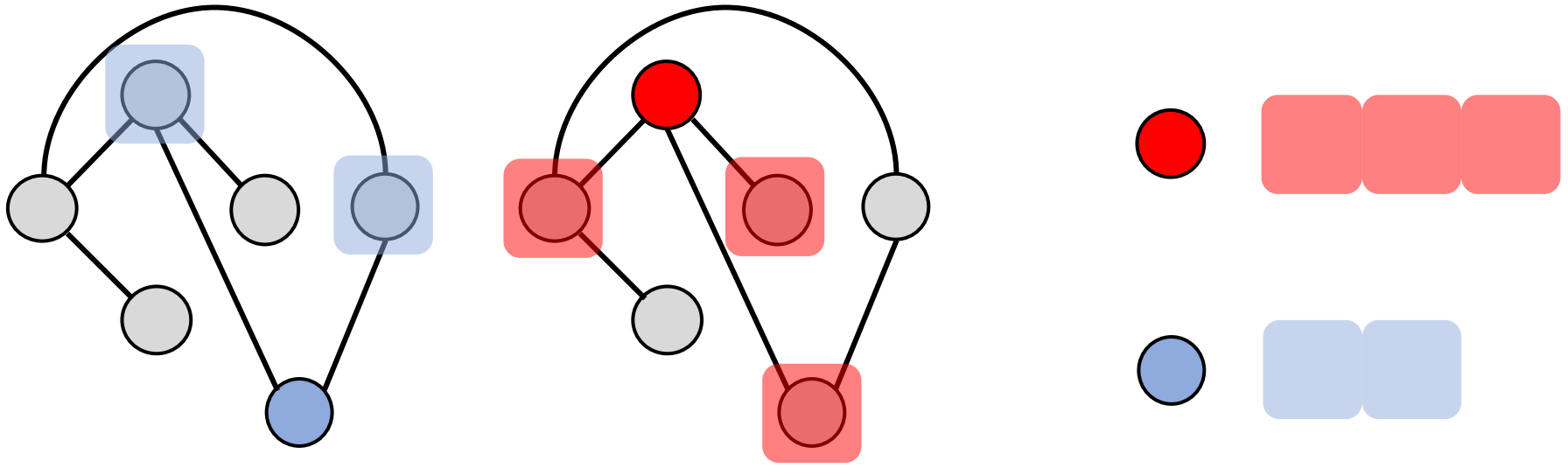

Deep Learning for Graphs

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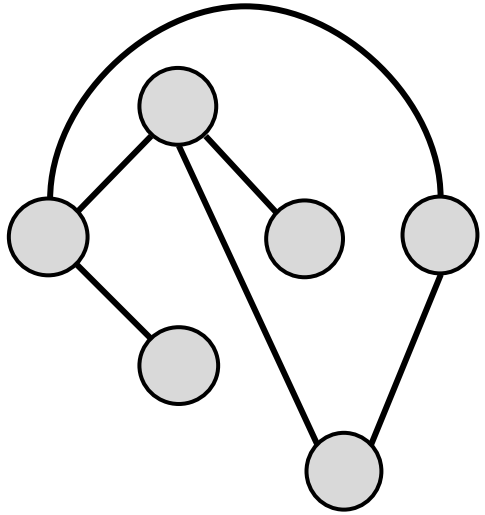

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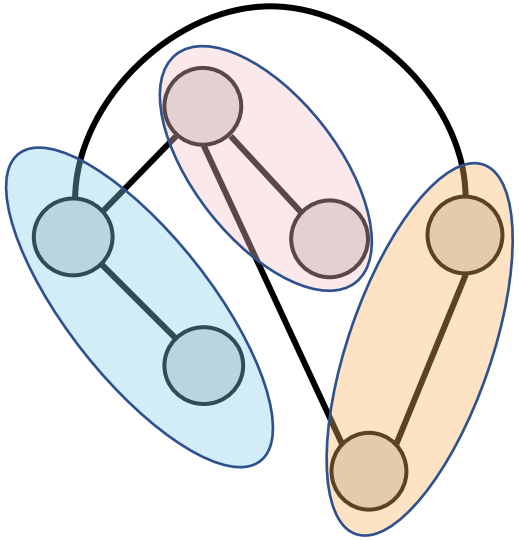

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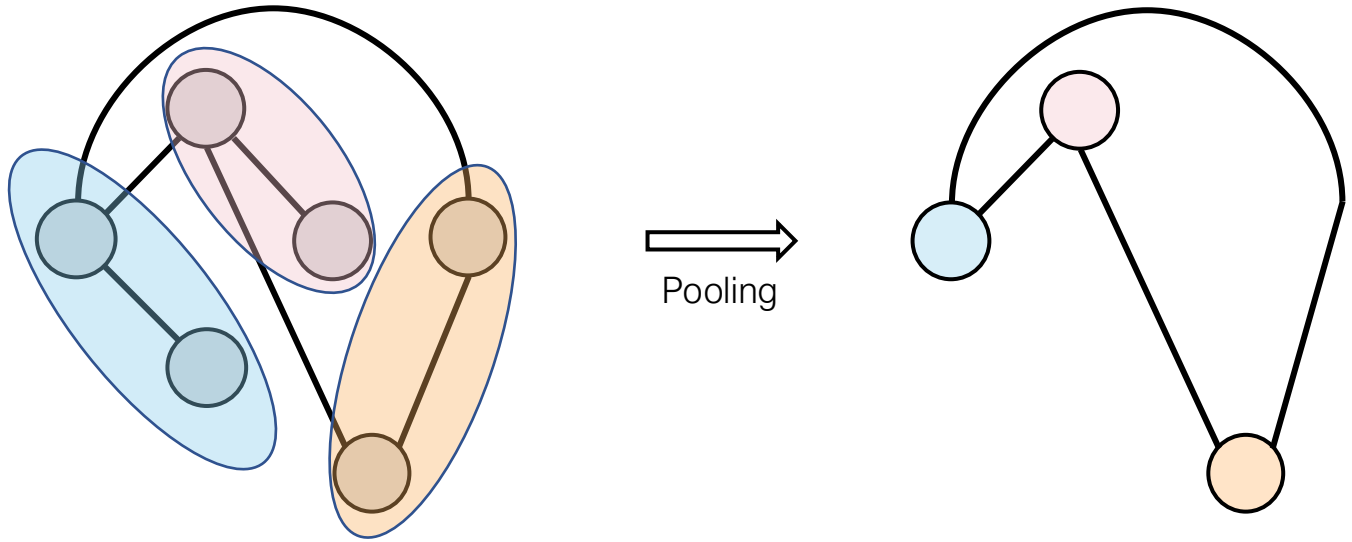

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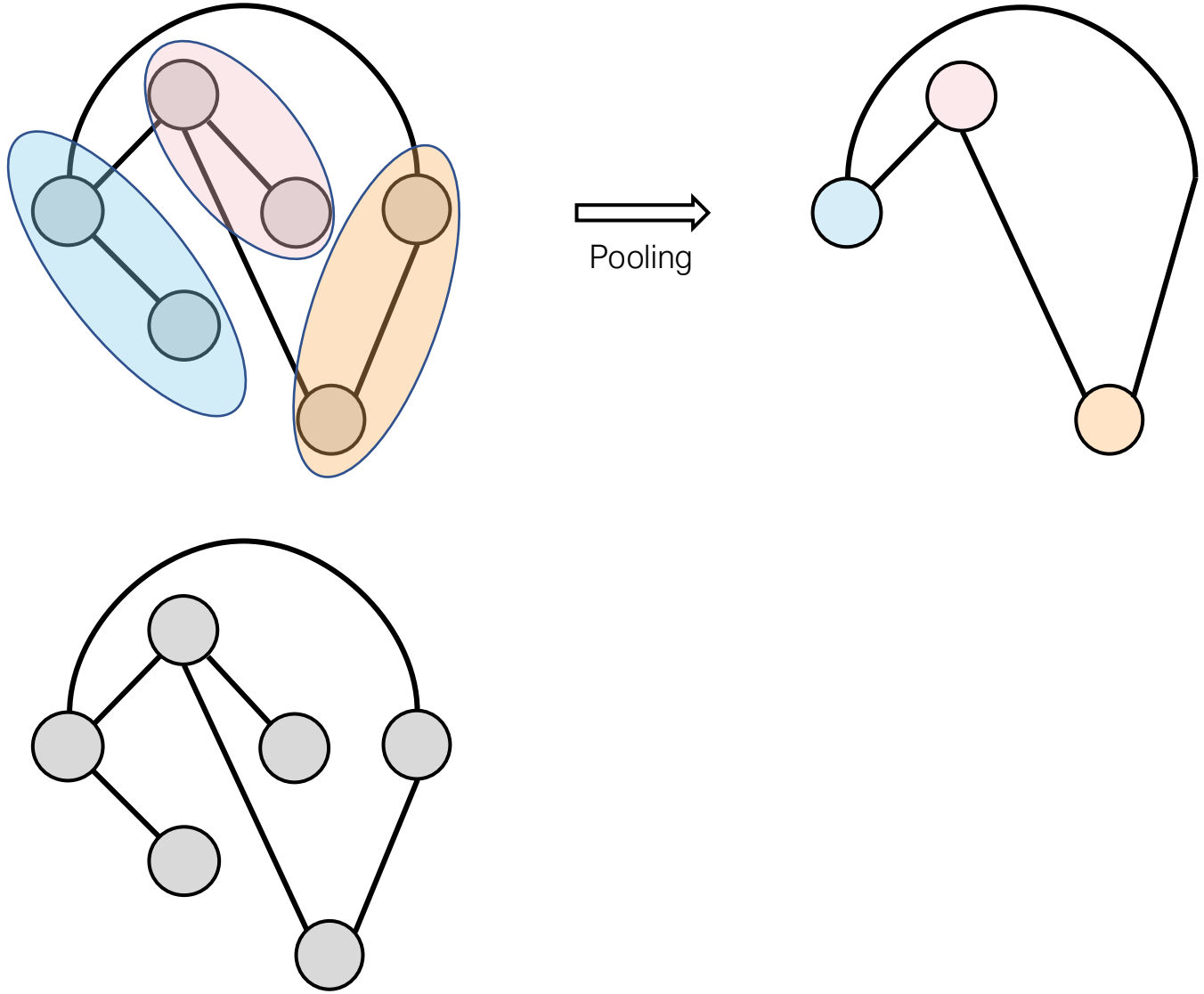

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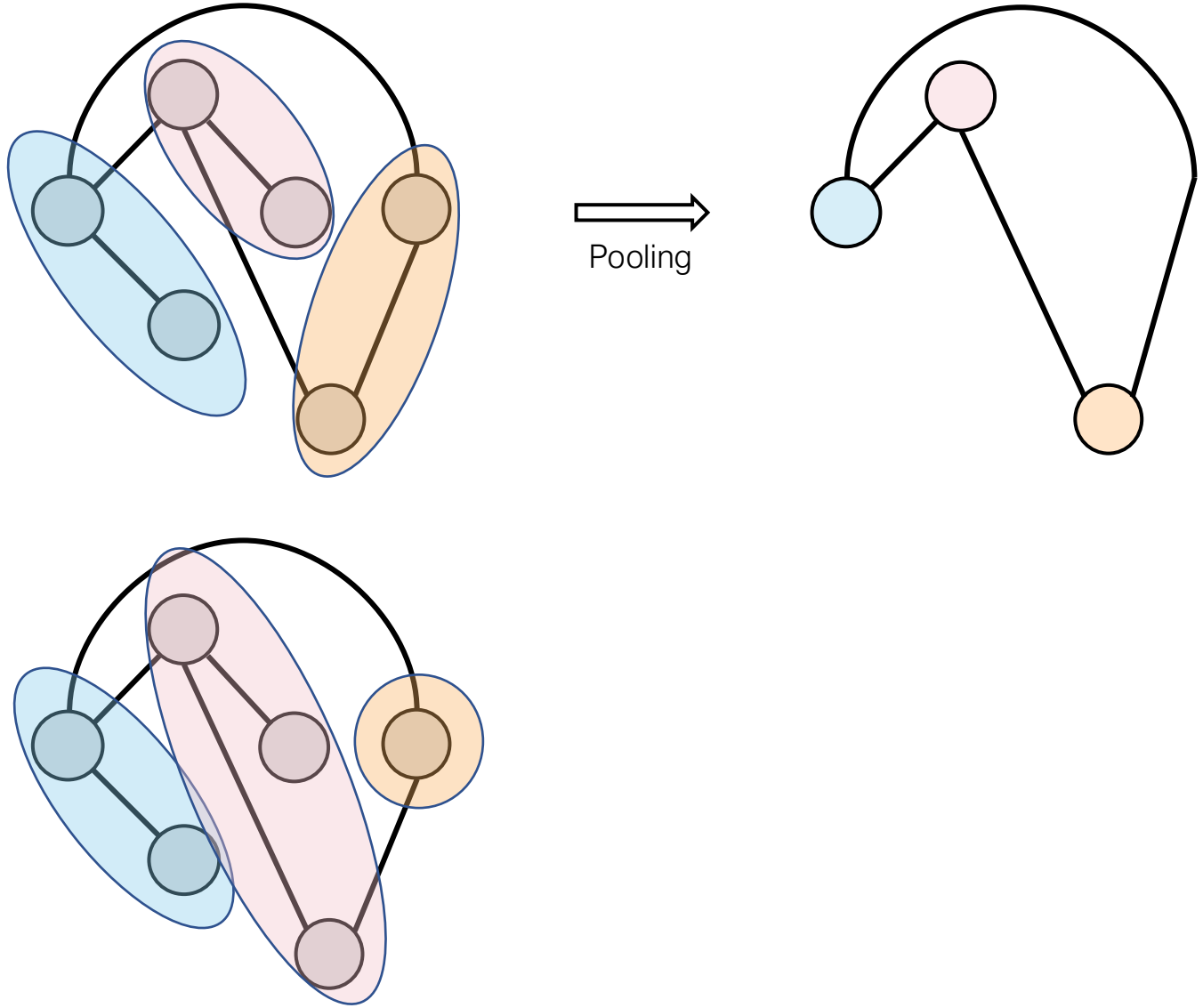

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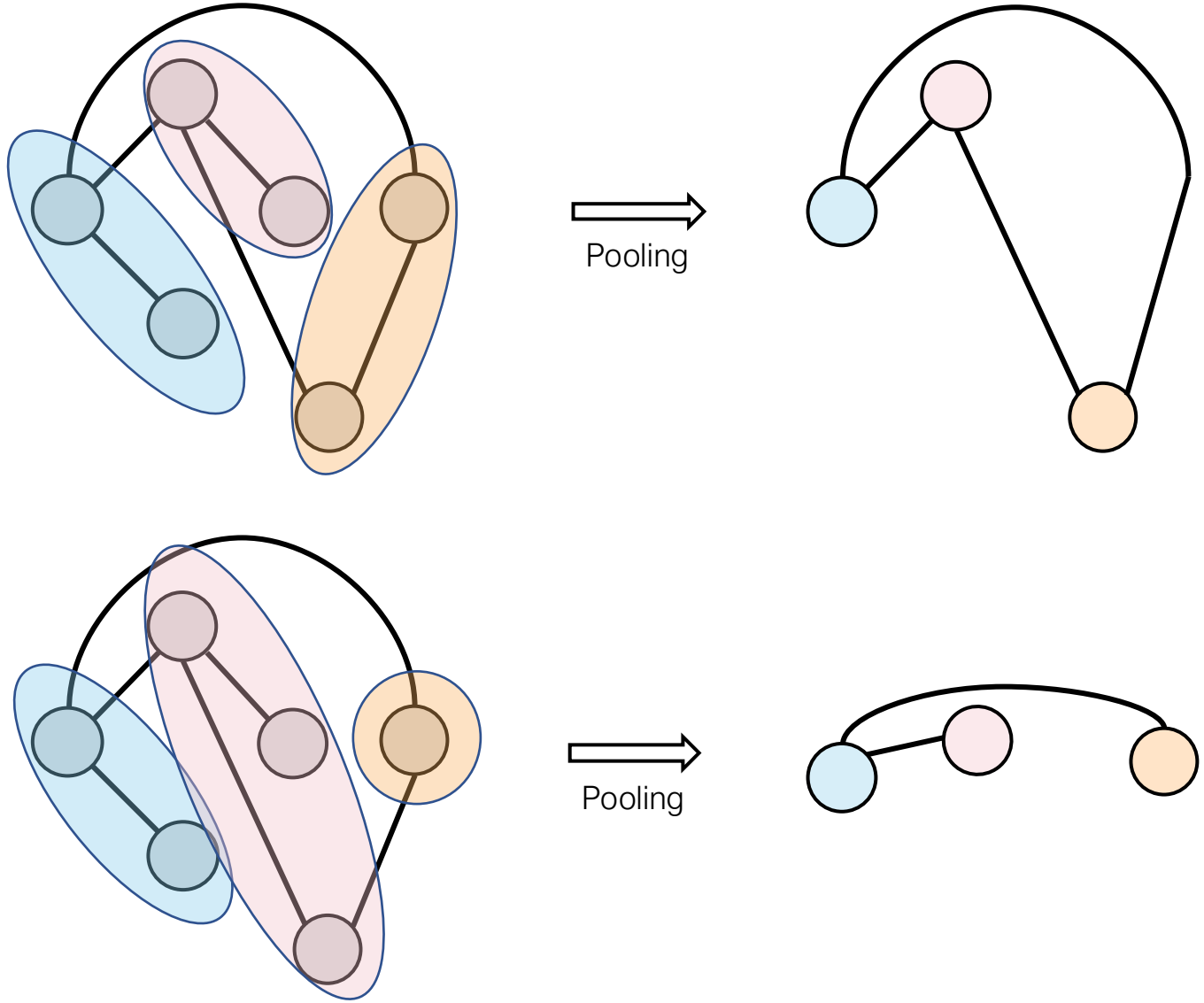

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Deep Learning for Graphs

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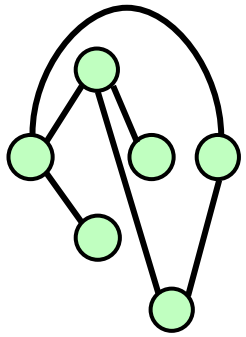

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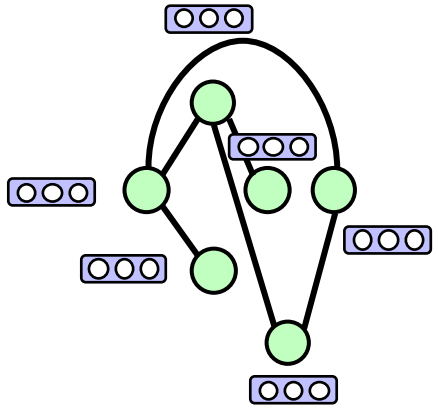
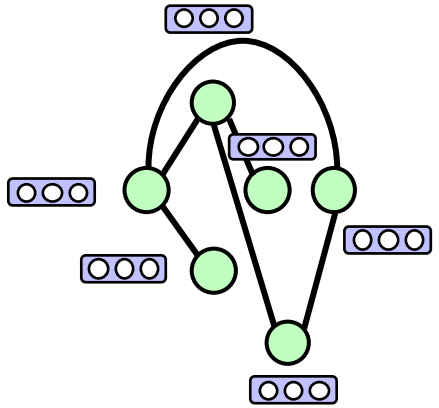


Input Encoding

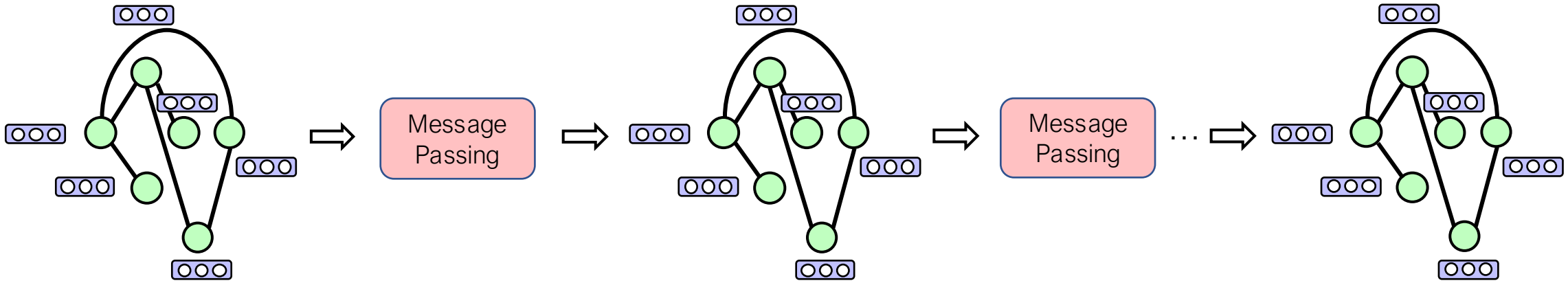
Graph Neural Networks (GNNs)



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*

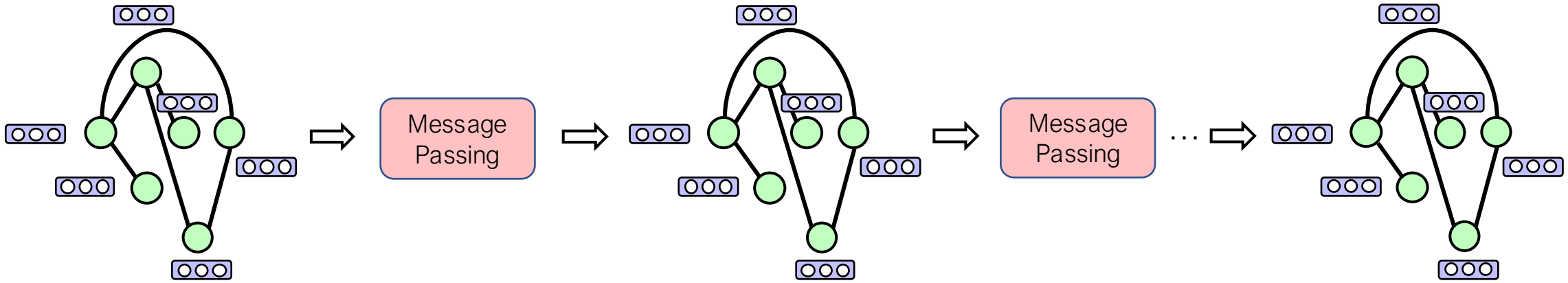
Graph Neural Networks (GNNs)



Input Encoding

Message Passing Layers/Steps

Graph Neural Networks (GNNs)

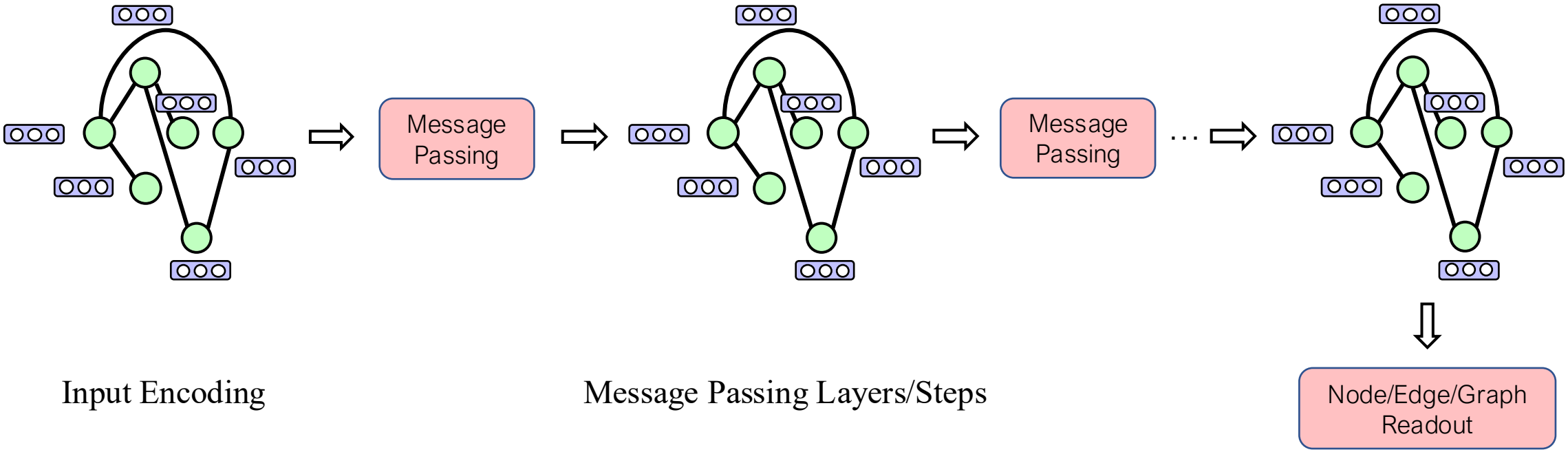


Input Encoding

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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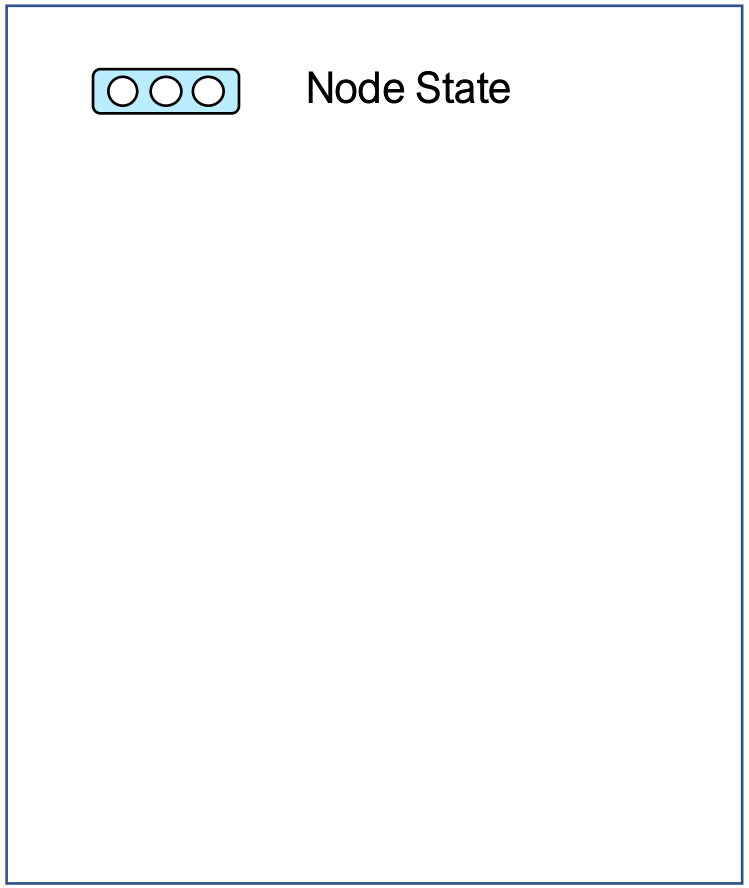
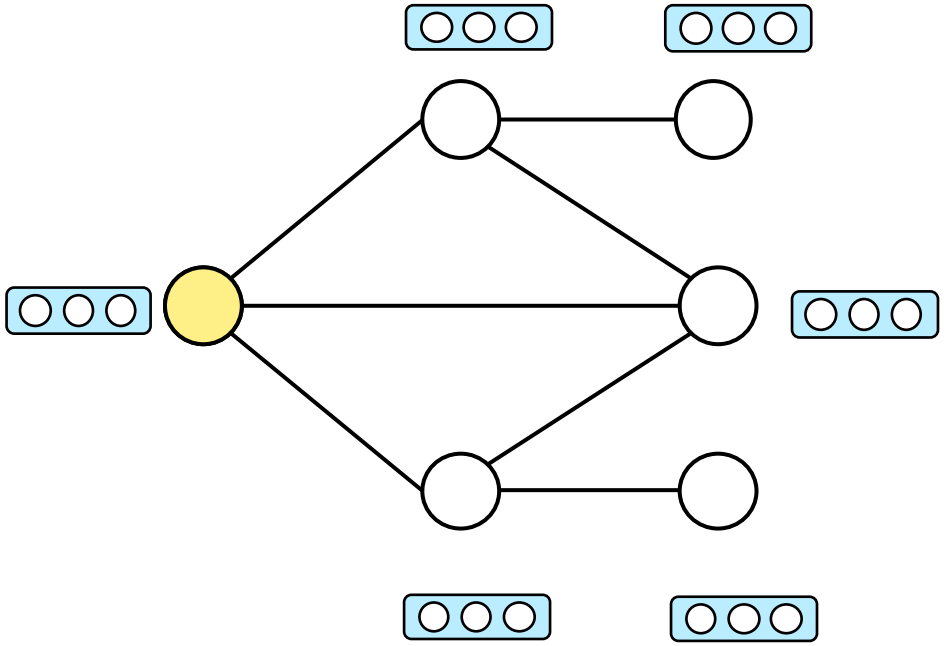
Message Passing in GNNs

$\mathbf{h}_i^t$



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



Message Passing in GNNs

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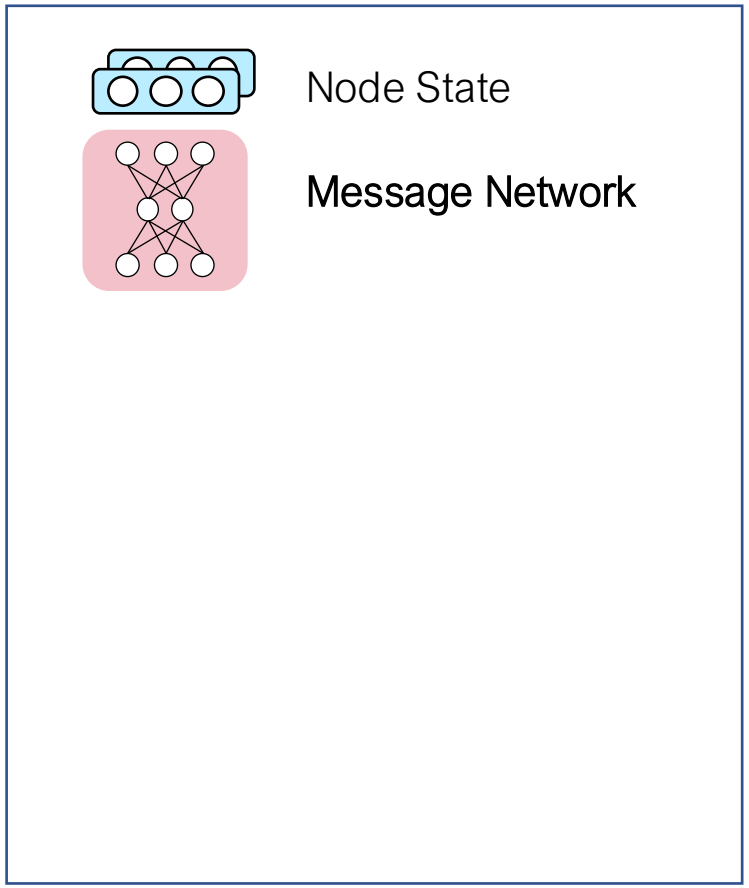

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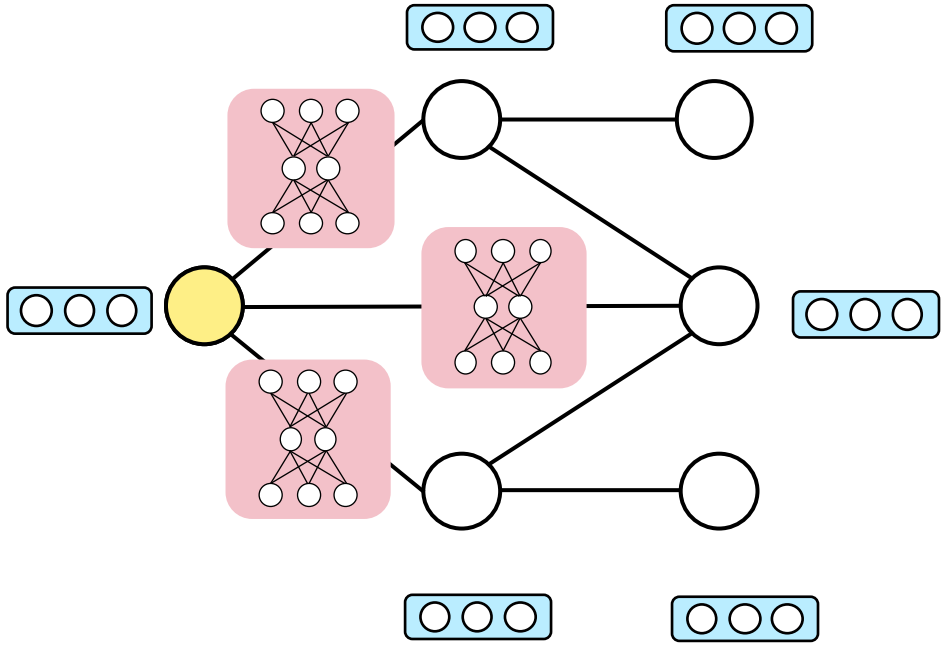

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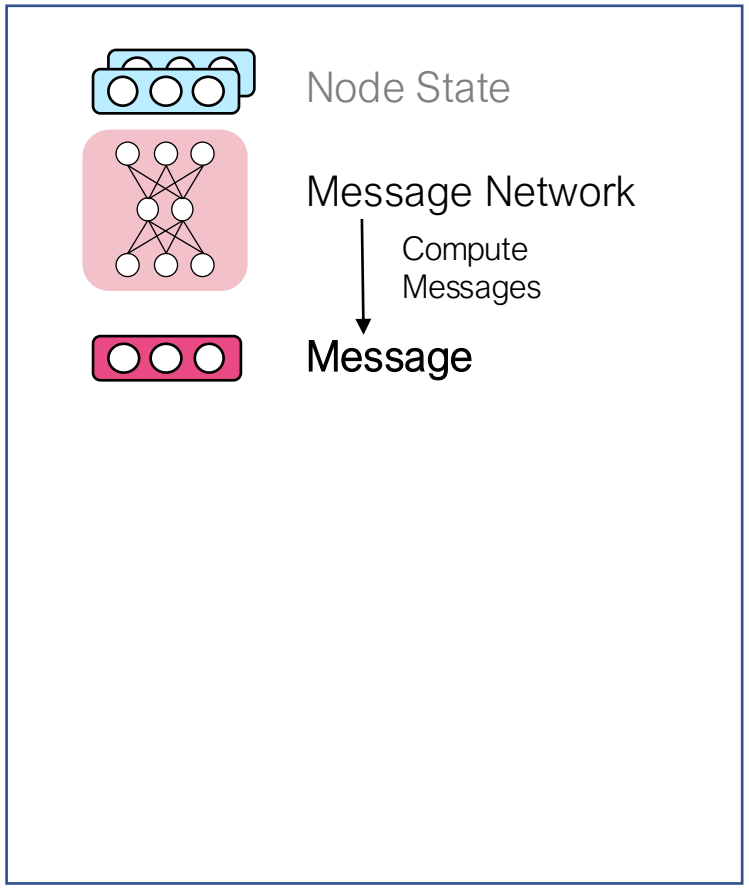
$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$



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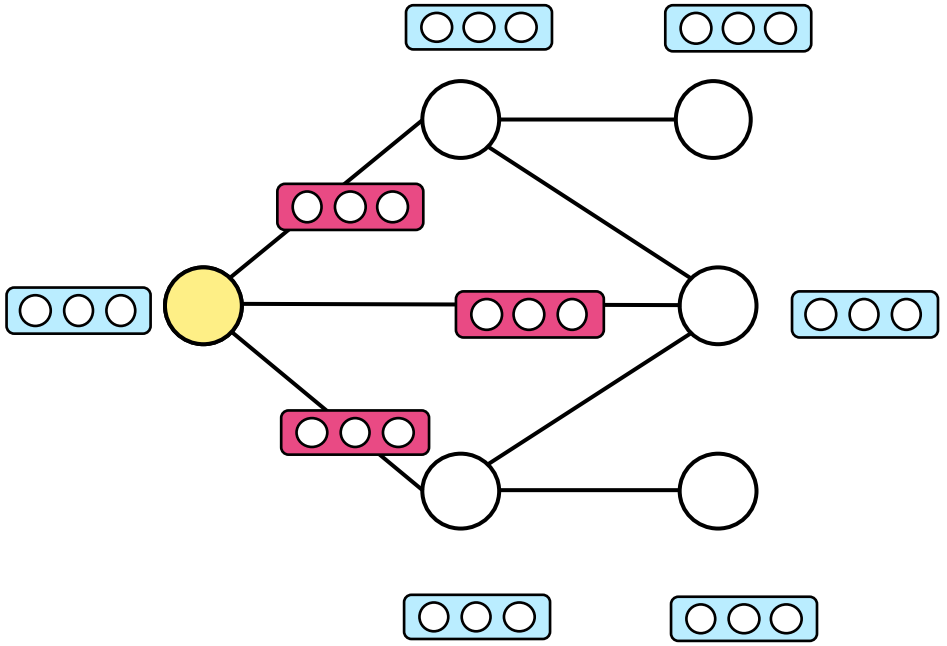

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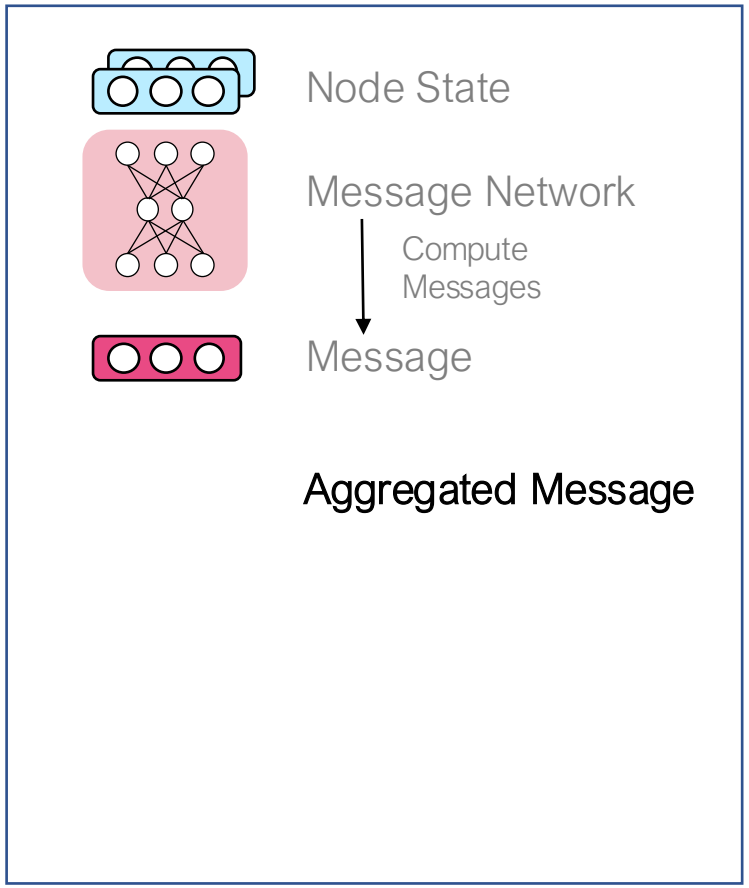

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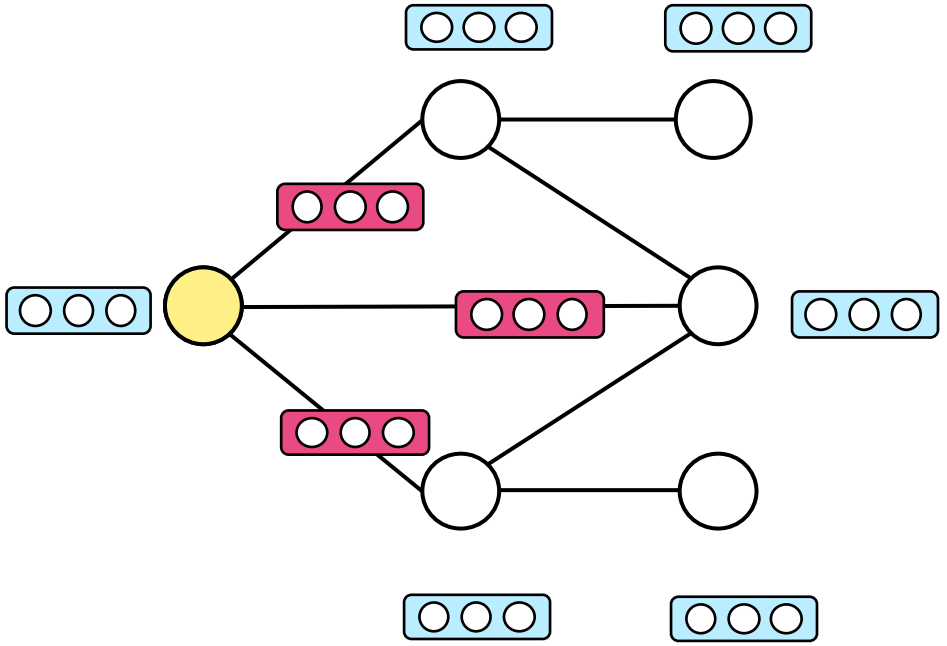

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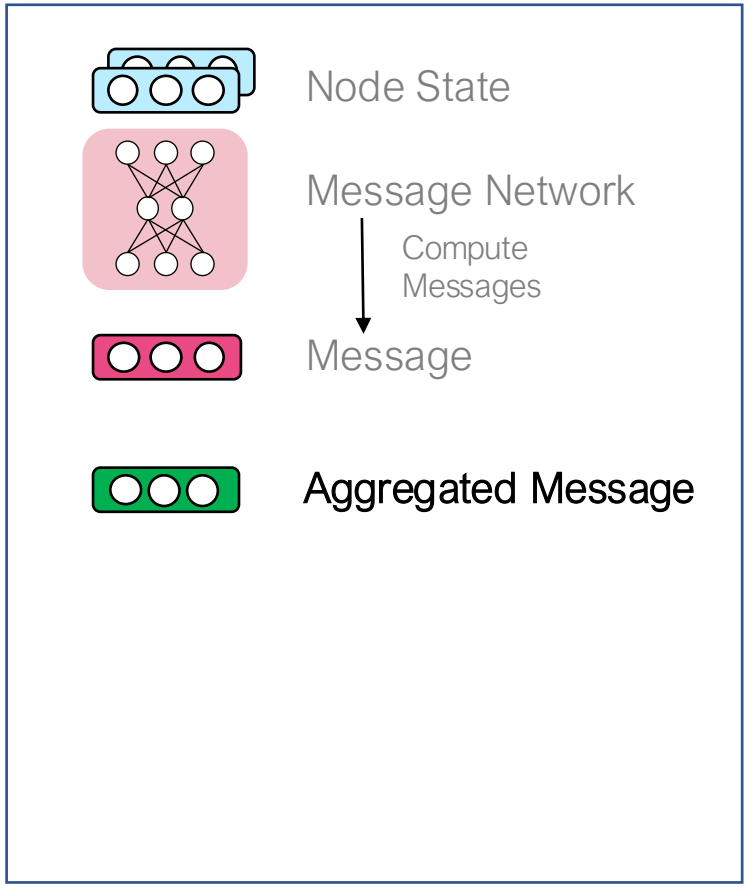

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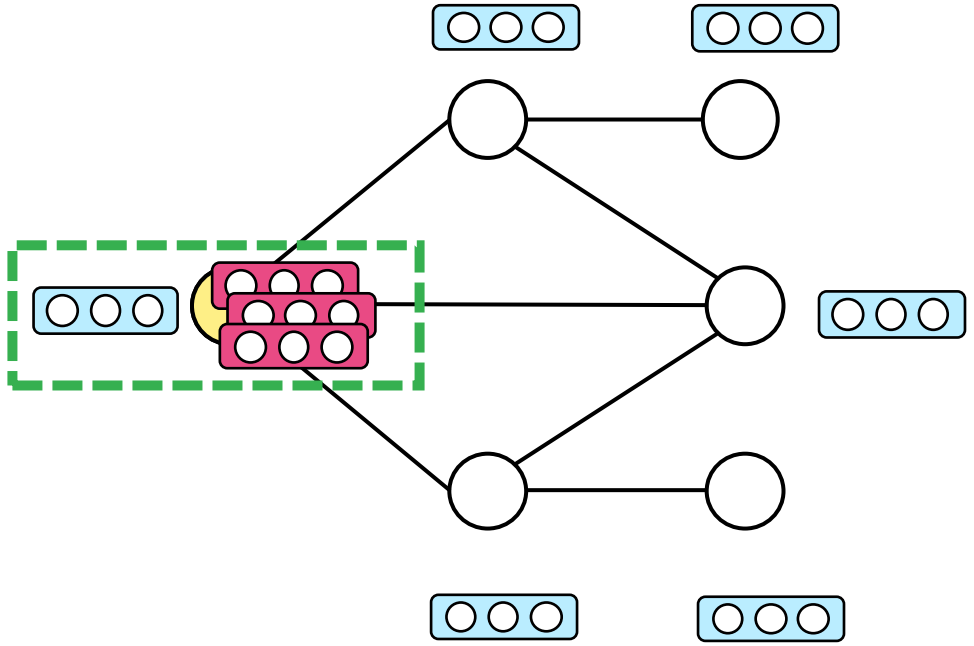

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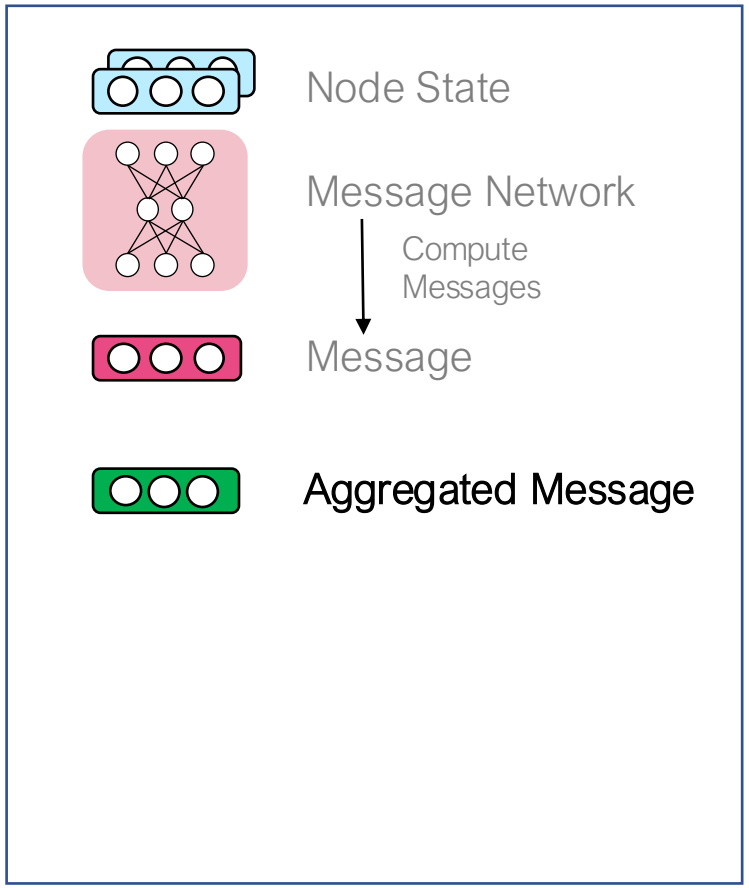

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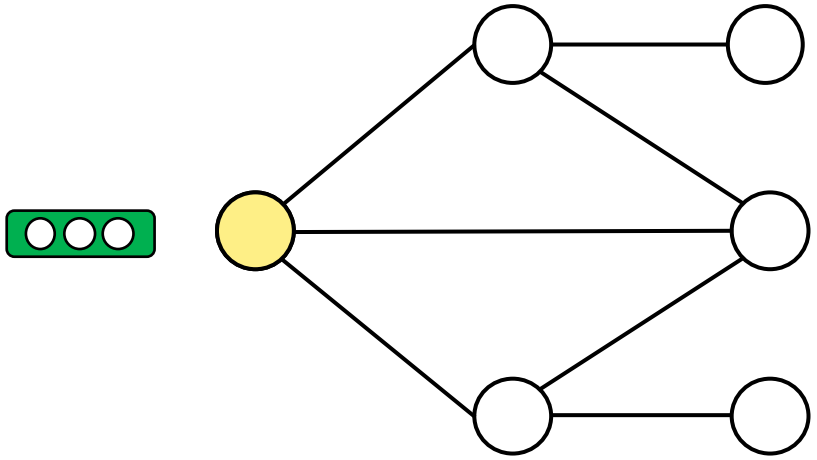

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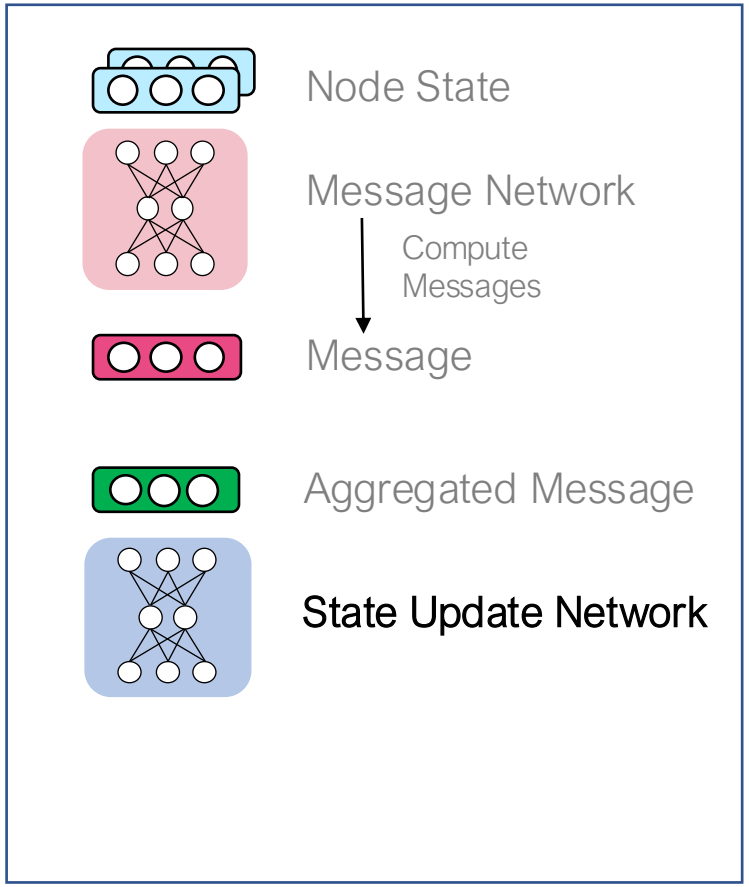

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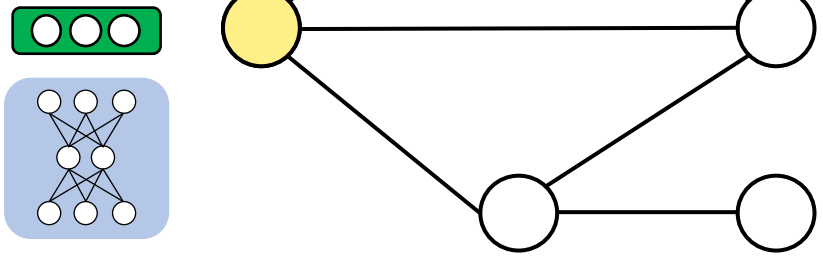

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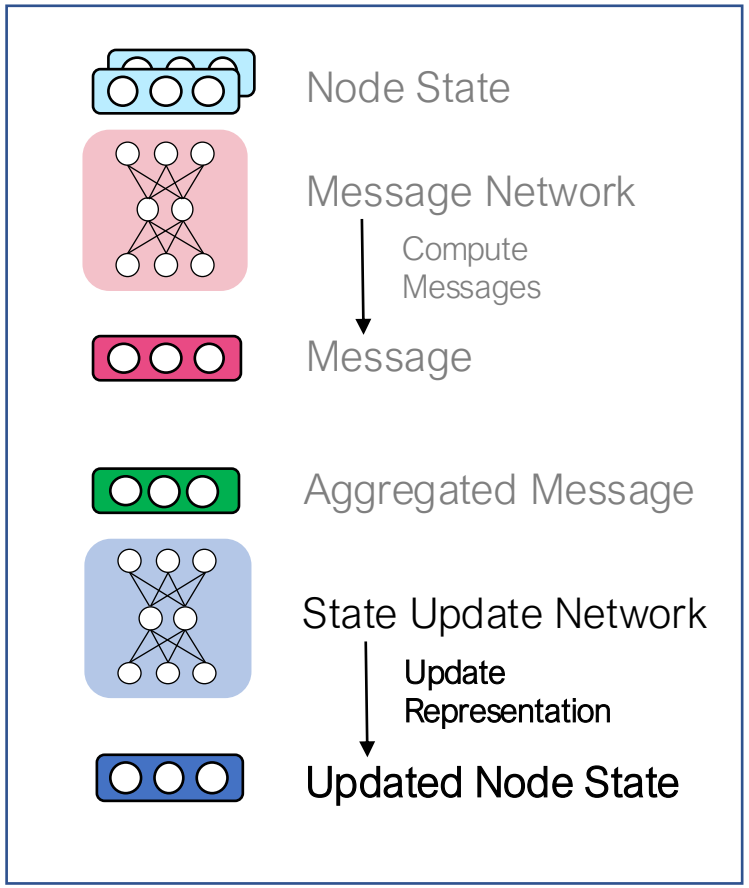
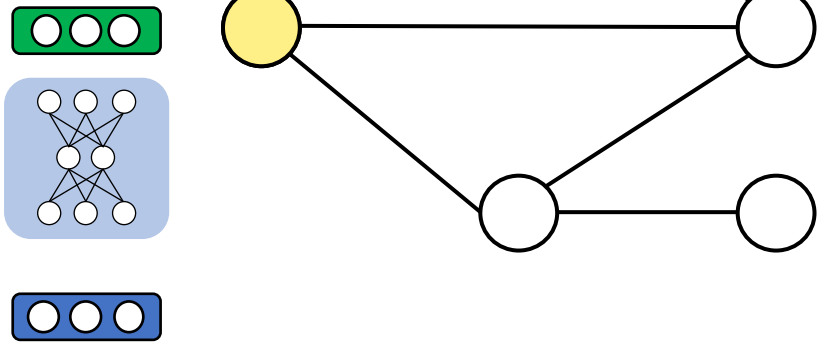


(t+1)-th message passing step/layer



Message Passing in GNNs

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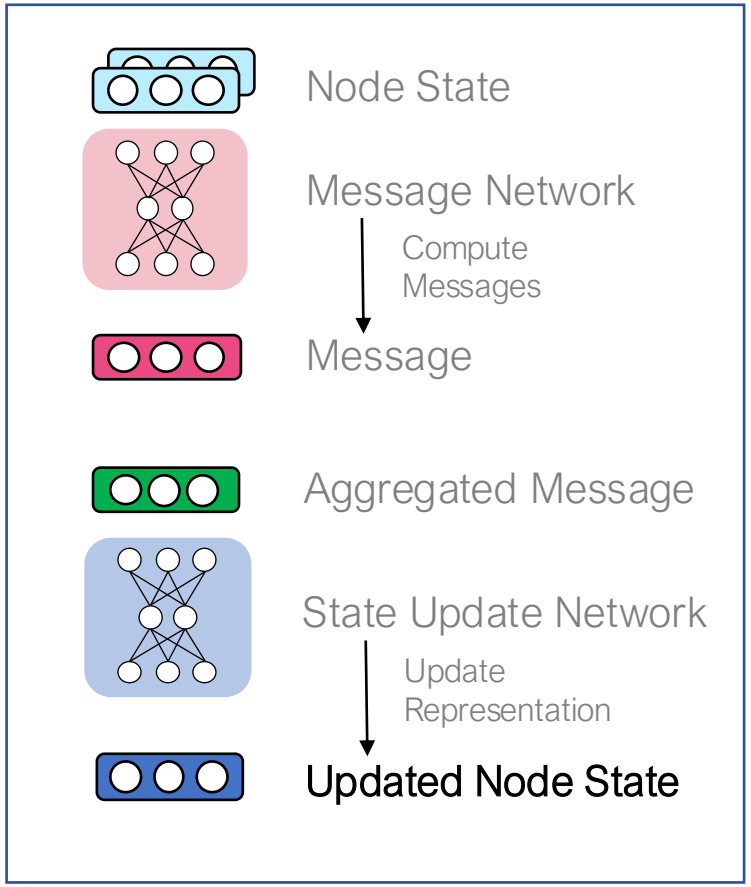

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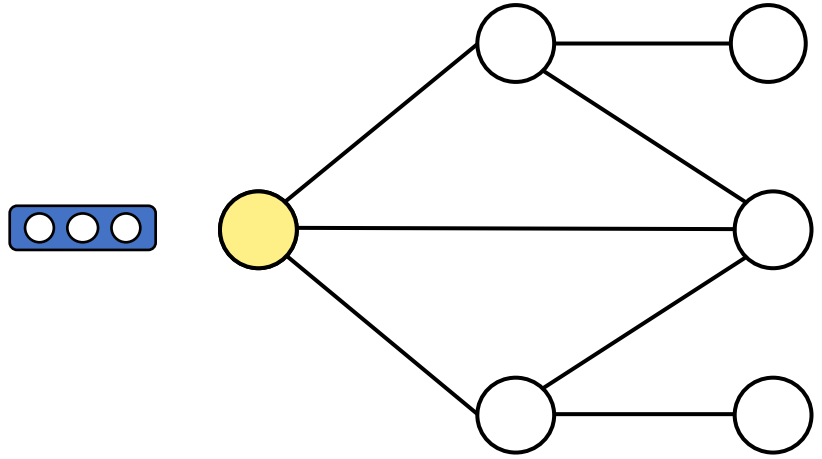

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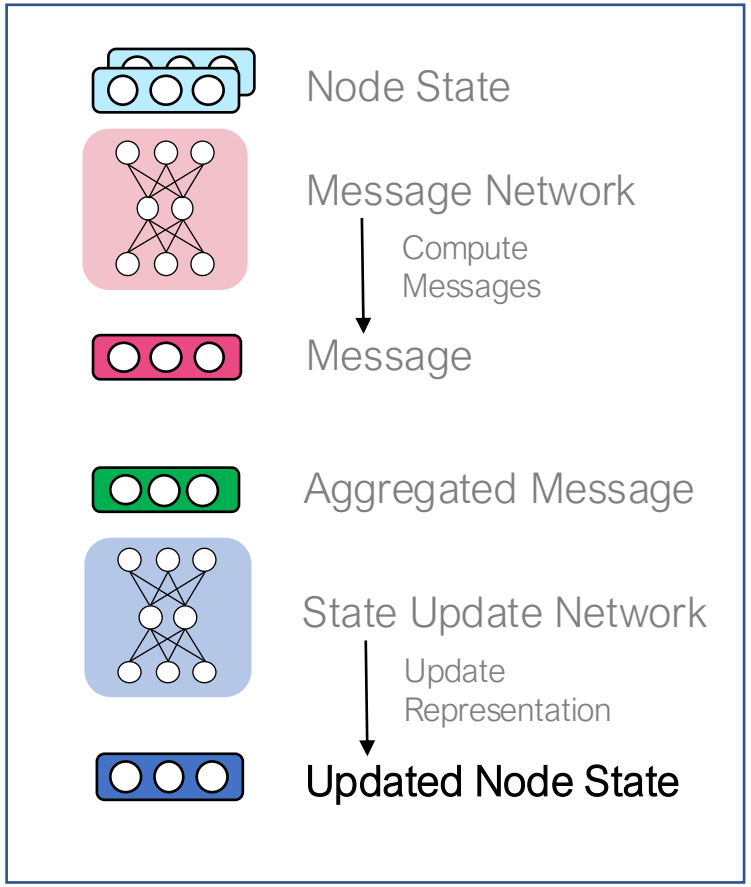

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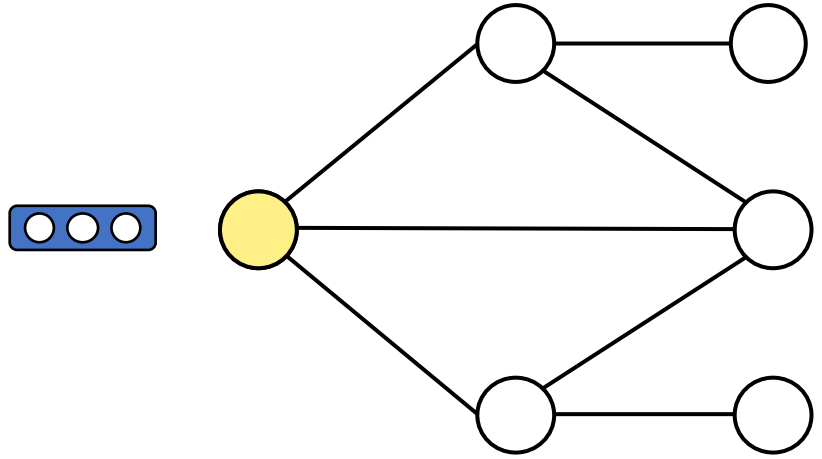

- Parallel Schedule!

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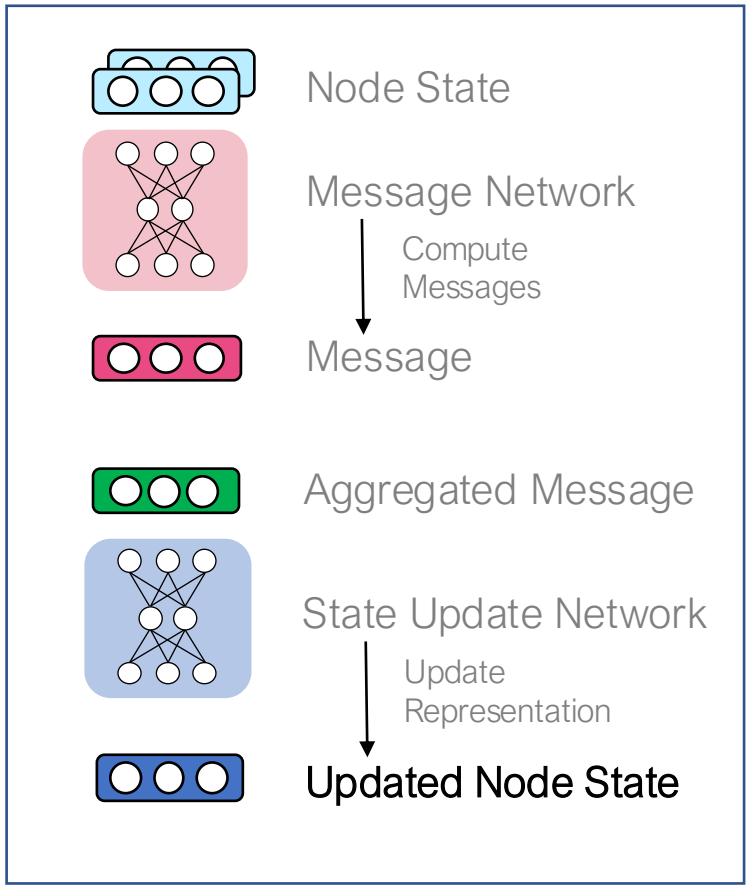

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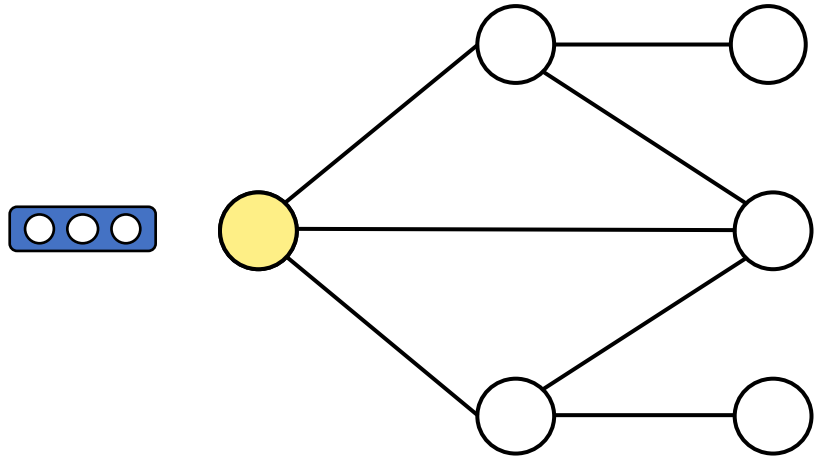

- Parallel Schedule!
- Other schedules [1] are possible and could improve performance in certain tasks!

[1] Liao, R., Brockschmidt, M., Tarlow, D., Gaunt, A.L., Urtasun, R. and Zemel, R., 2018. Graph partition neural networks for semi-supervised classification. arXiv preprint arXiv:1803.06272.

Outline

- Motivating Applications

- Graph Neural Networks (GNNs)

  - Graph representations
  - Graph isomorphism & automorphism
  - Challenges of graph data
  - Graph Neural Networks (GNNs): history & basics
  - Message passing framework of GNNs
  - **Instantiation of message passing**
  - Relationship with Transformers

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

2. Aggregate Messages

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Edge Feature

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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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2. Edge Readout

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

$$f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T) = \text{MLP}([\mathbf{h}_i^T, \mathbf{h}_j^T])$$

$$f_{\text{readout}}(\mathbf{h}_i^T, \mathbf{h}_j^T, e_{ij}) = \text{MLP}([\mathbf{h}_i^T, \mathbf{h}_j^T, e_{ij}])$$

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

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!*

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!*

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

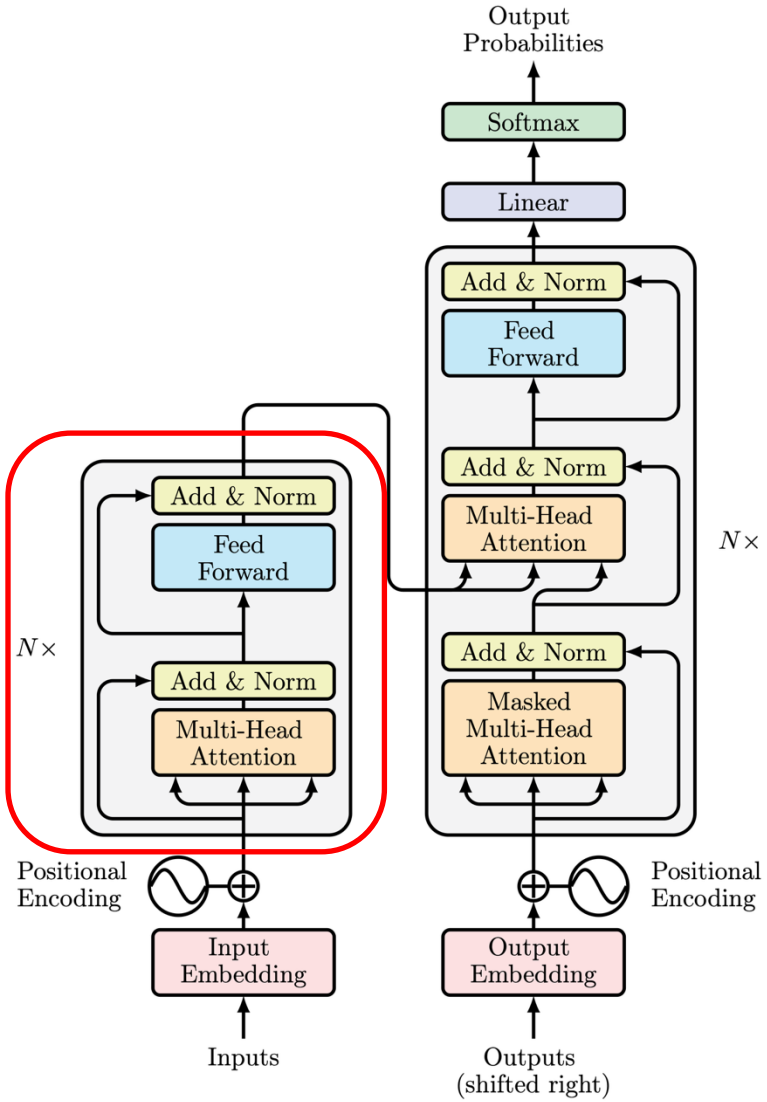
Outline

- Motivating Applications

- Graph Neural Networks (GNNs)

  - Graph representations
  - Graph isomorphism & automorphism
  - Challenges of graph data
  - Graph Neural Networks (GNNs): history & basics
  - Message passing framework of GNNs
  - Instantiation of message passing
  - **Relationship with Transformers**

Relationships with Transformer



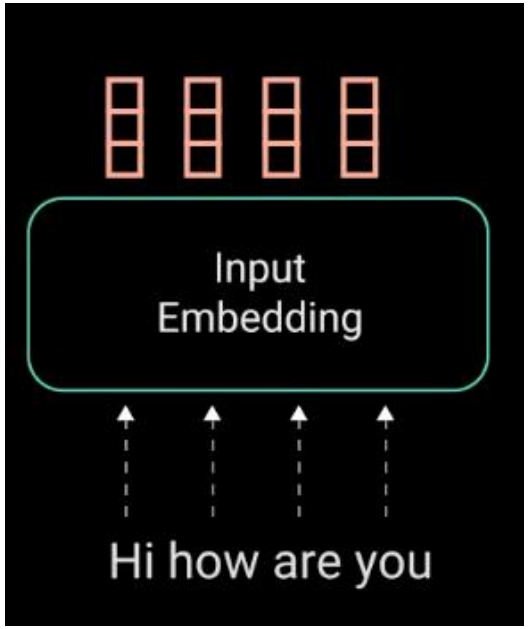
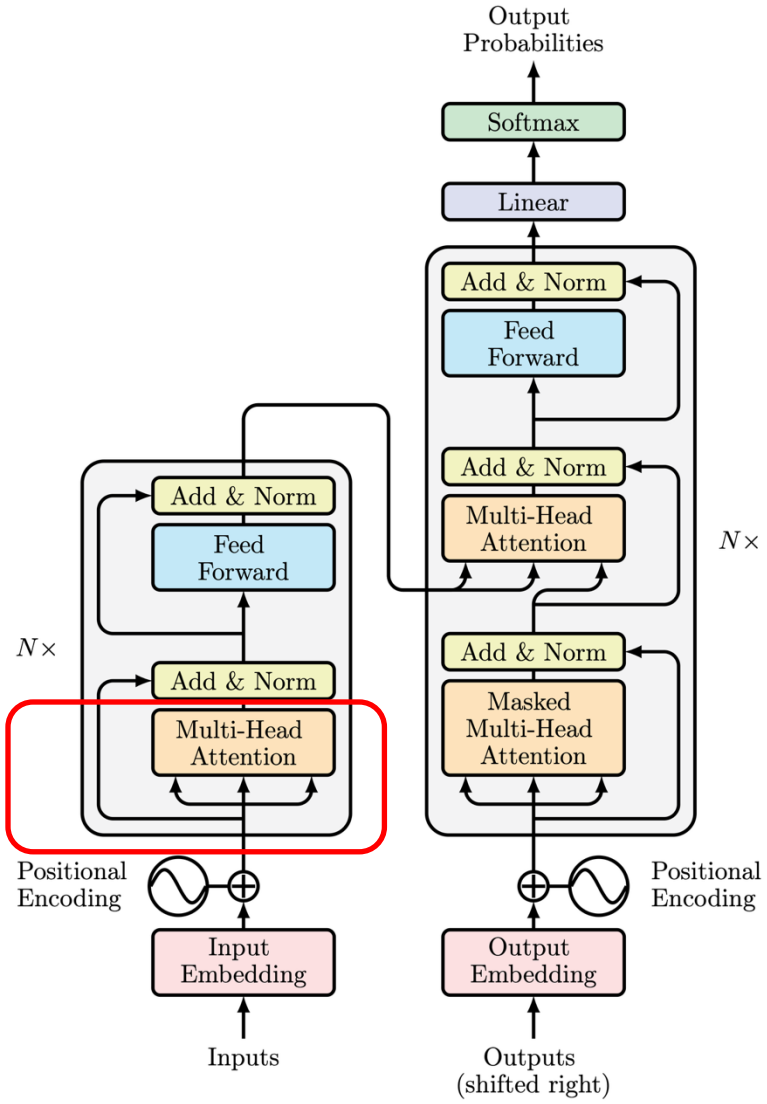
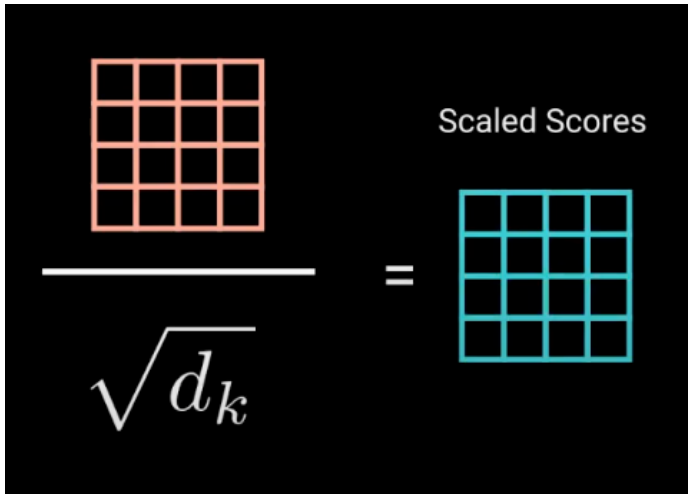
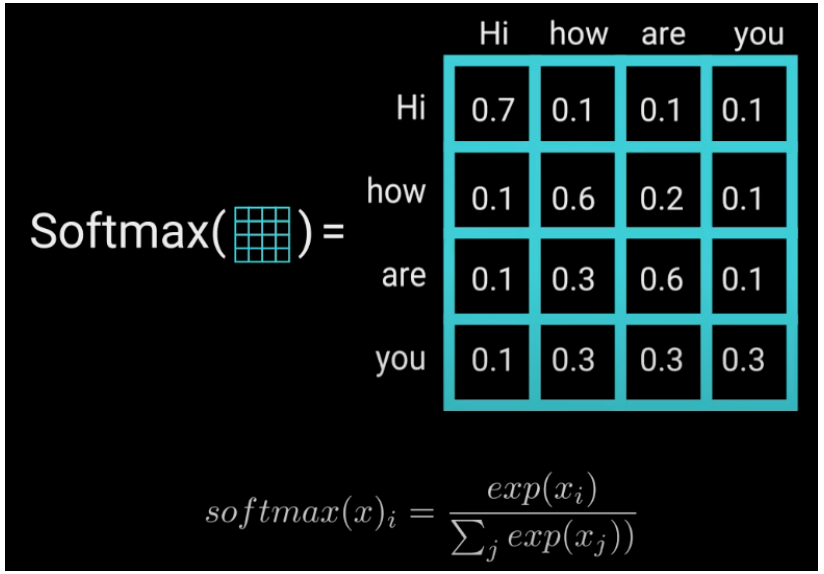


Image Credit: Vaswani, A., et al. Attention is all you need. NeurIPS 2017. https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Relationships with Transformer







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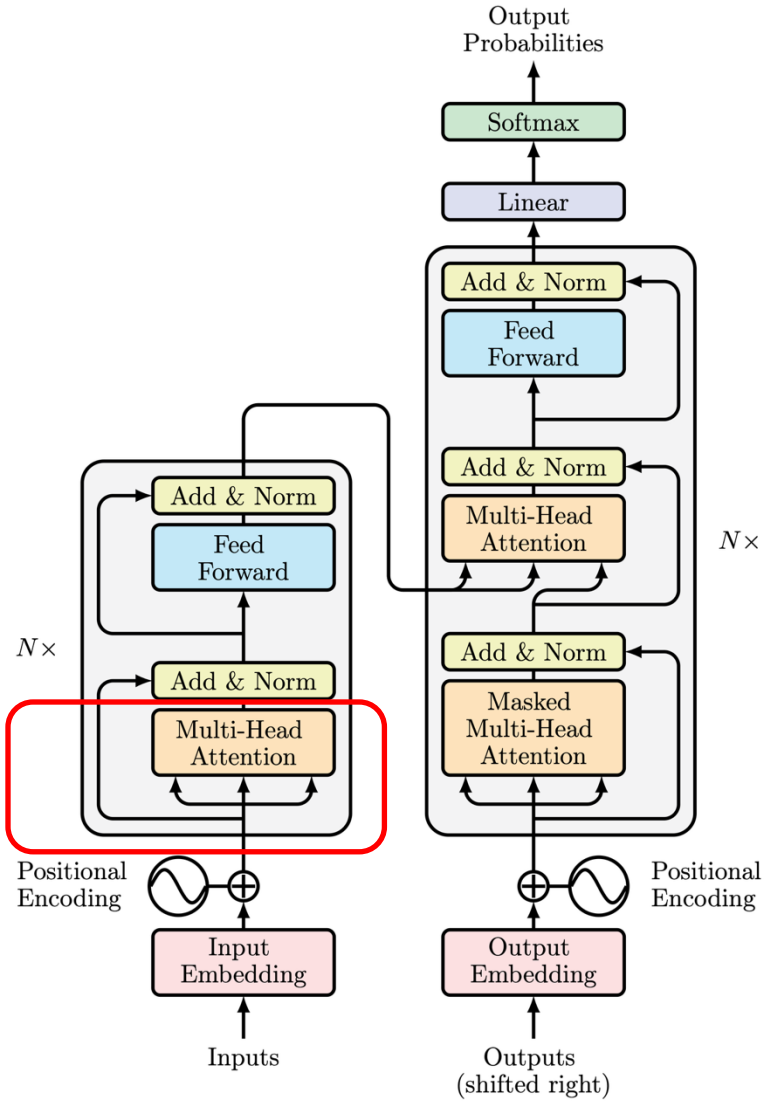
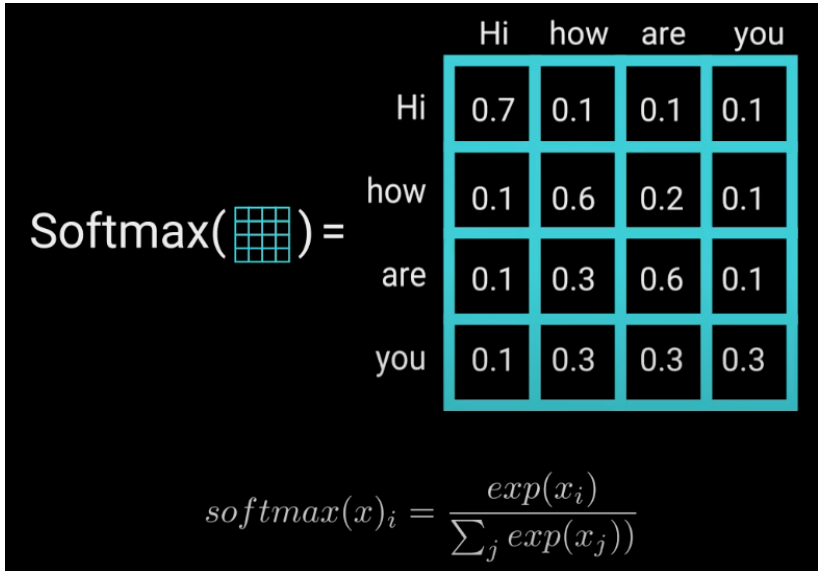


- Attention can be viewed as the weighted adjacency matrix of a fully connected graph!



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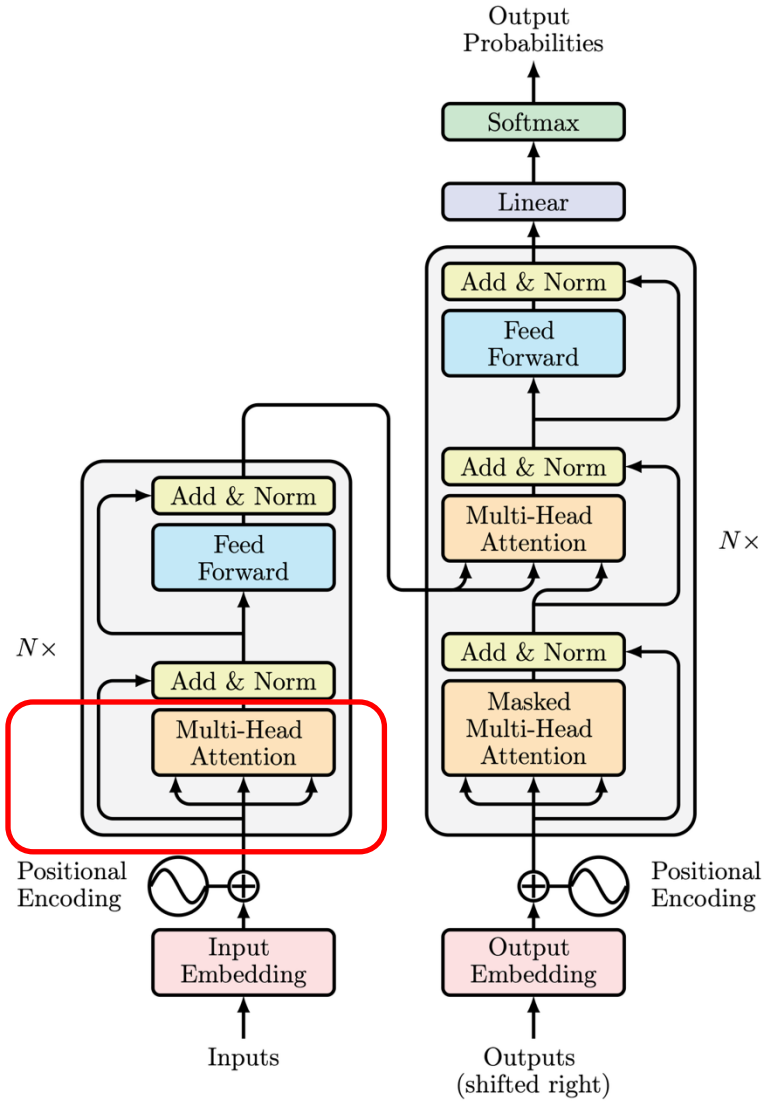
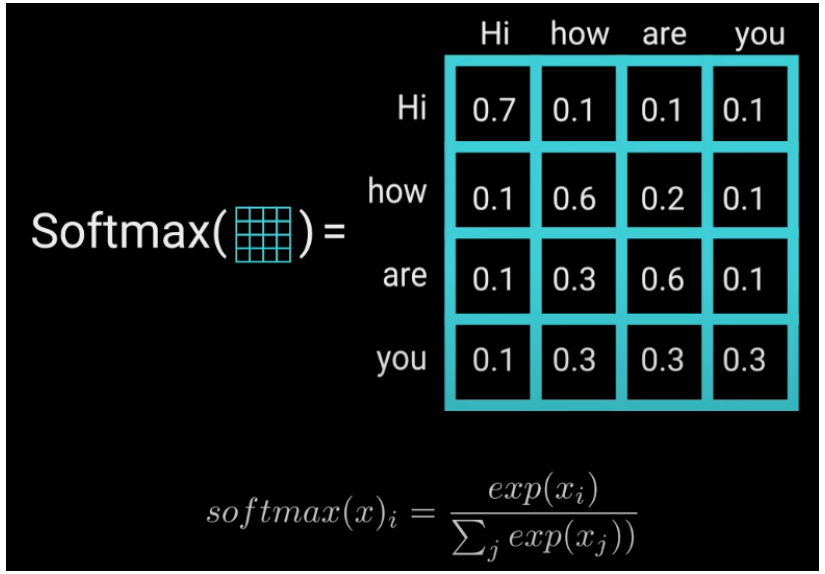
Relationships with Transformer



- 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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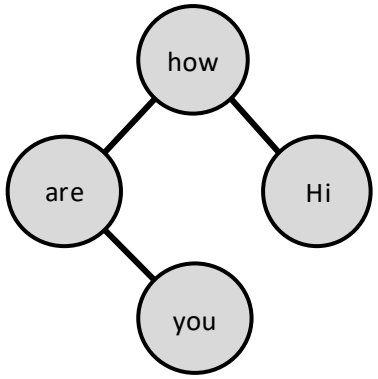
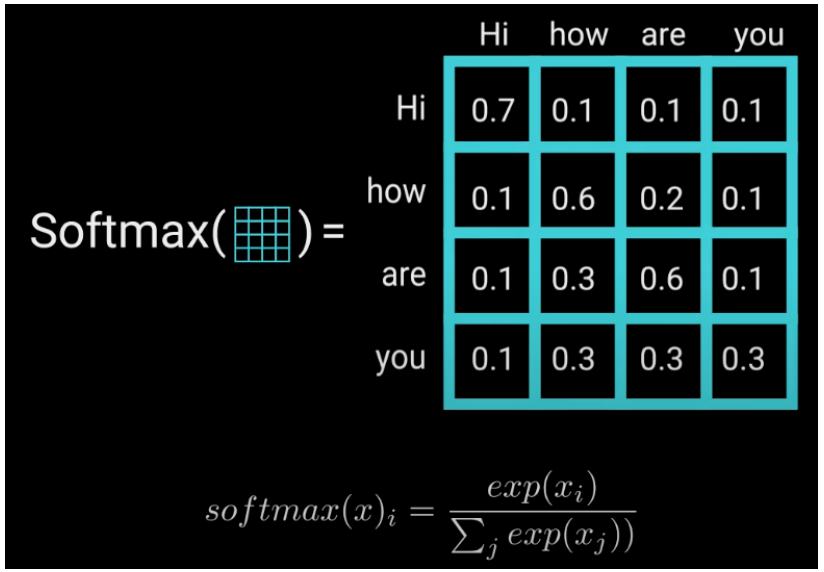
Encode Graph Structures in Transformers

- Apply the adjacency matrix as a mask to the attention and renormalize it, like Graph Attention Networks (GAT) [1]
- Encode connectivities/distances as bias of the attention [2]
- Systematic investigation of various designs for graph Transformers [3]



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



[1] Veličković, Petar, et al. "Graph attention networks." ICLR. 2018. [2] Ying, Chengxuan, et al. "Do transformers really perform badly for graph representation?." NeurIPS. 2021. [3] Rampášek, Ladislav, et al. "Recipe for a general, powerful, scalable graph transformer." NeurIPS. 2022.
Image Credit: https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Questions?