EECE 571F: Deep Learning with Structures

Lecture 3: Graph Neural Networks
Message Passing Models

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University of British Columbia

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Course Scope

- Brief Intro to Deep Learning

- Geometric Deep Learning

  - Deep Learning Models for Sets and Sequences: Deep Sets & Transformers
  - Deep Learning Models for Graphs: Message Passing & Graph Convolution GNNs
  - Group Equivariant Deep Learning

- Probabilistic Deep Learning

  - Auto-regressive models, Large Language Models (LLMs)
  - Variational Auto-Encoders (VAEs) and Generative Adversarial Networks (GANs)
  - Energy based models (EBMs)
  - Diffusion/Score based models

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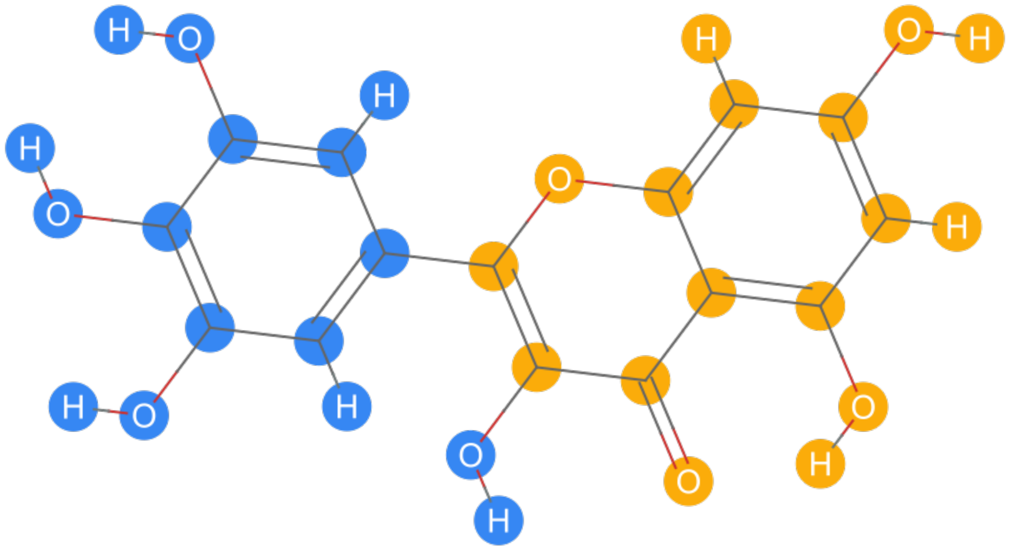
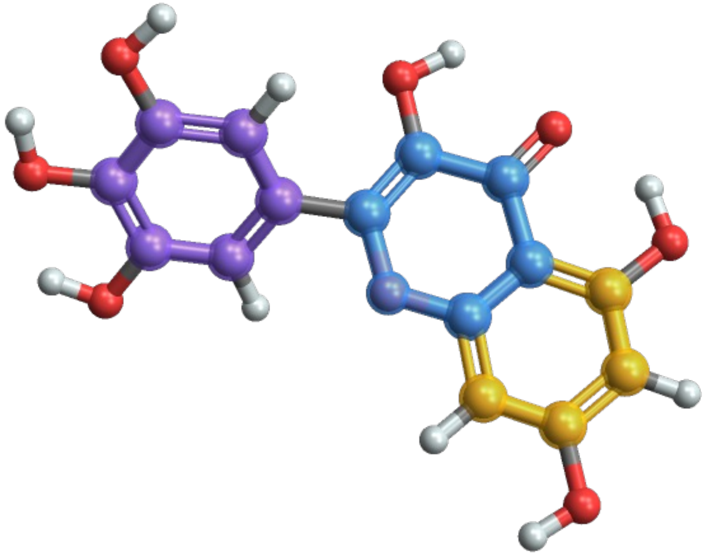
Motivating Applications of Graphs

- 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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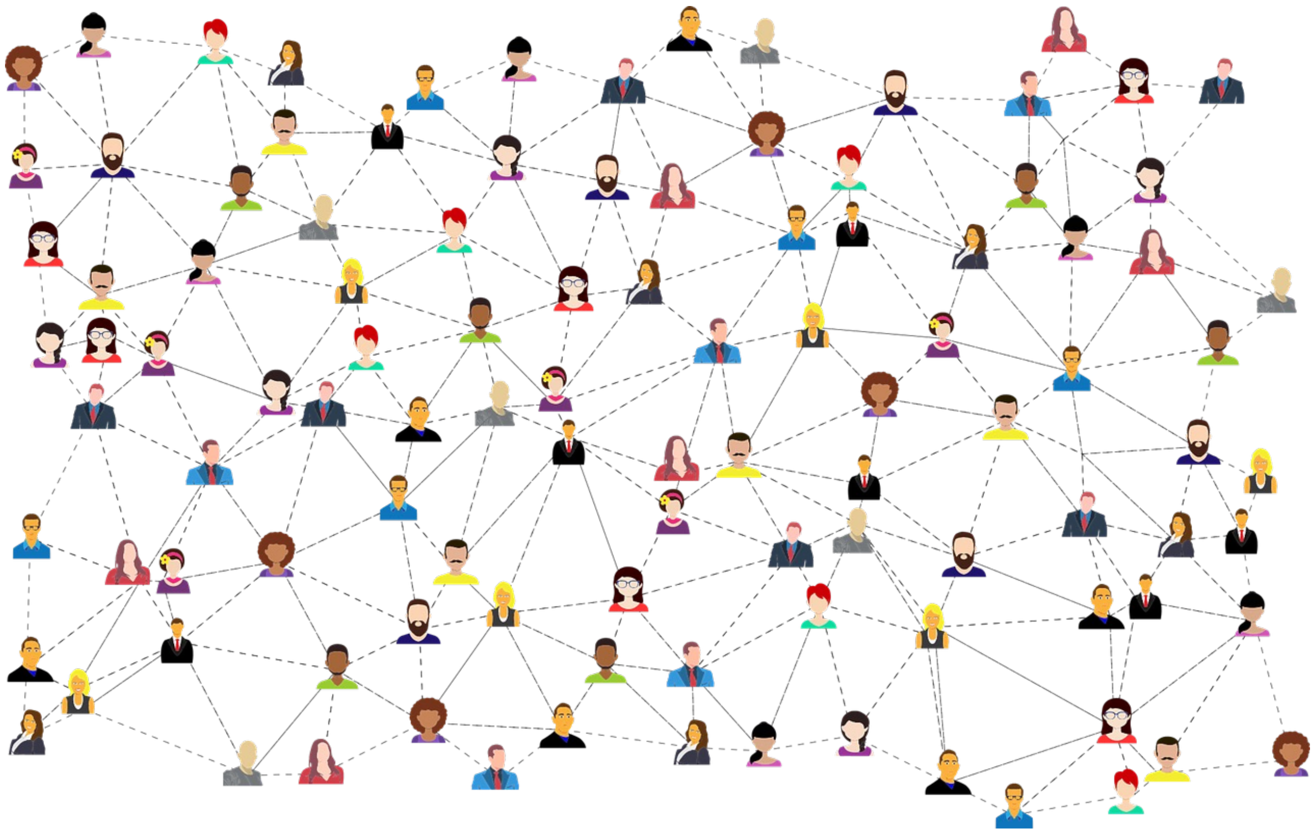
Motivating Applications of Graphs

- Social Networks

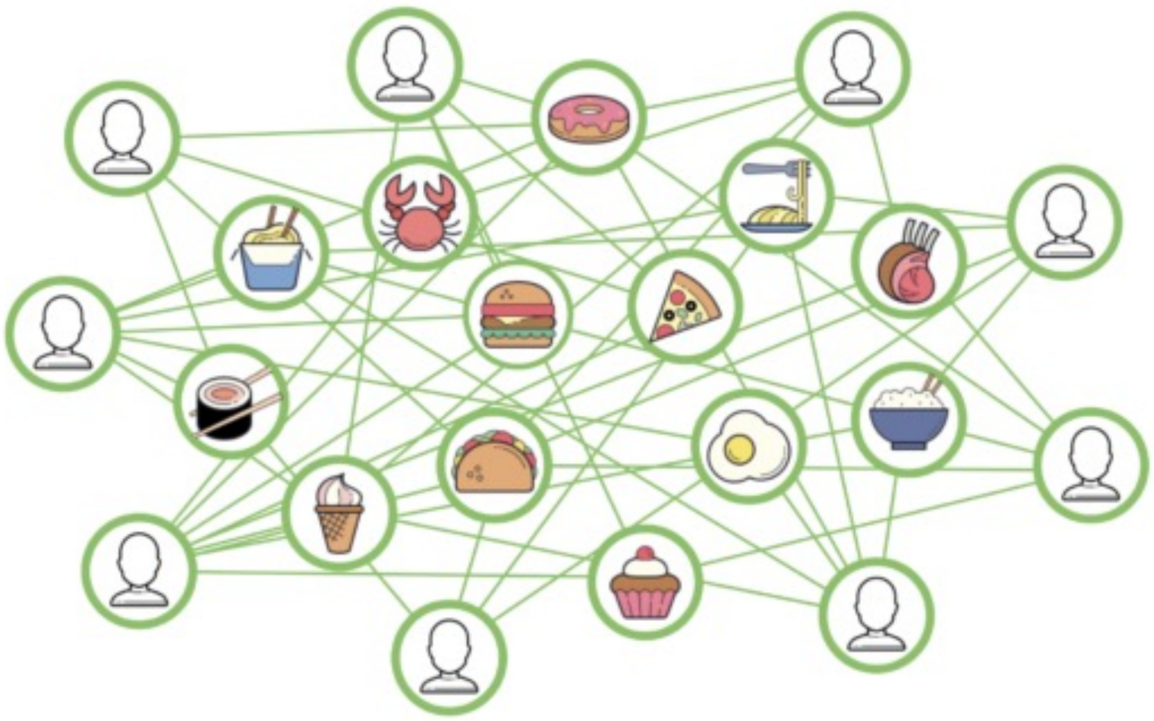


Link Prediction

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

- Network-based Recommendation

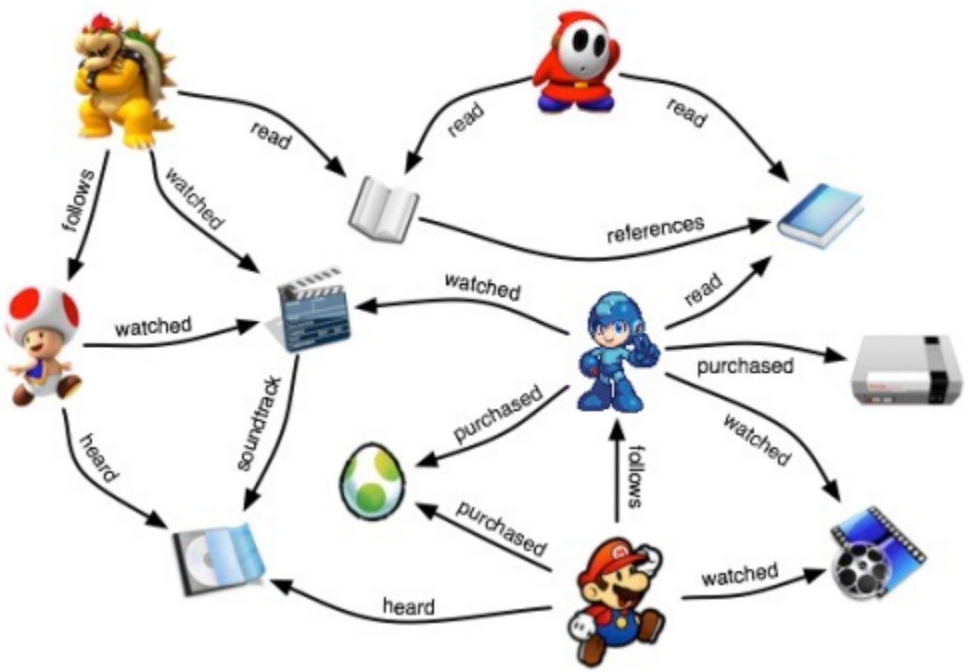


Image Credit: http://blog.soton.ac.uk/hive/2012/05/10/recommendation-system-of-hive/

Motivating Applications of Graphs

- Citation Networks

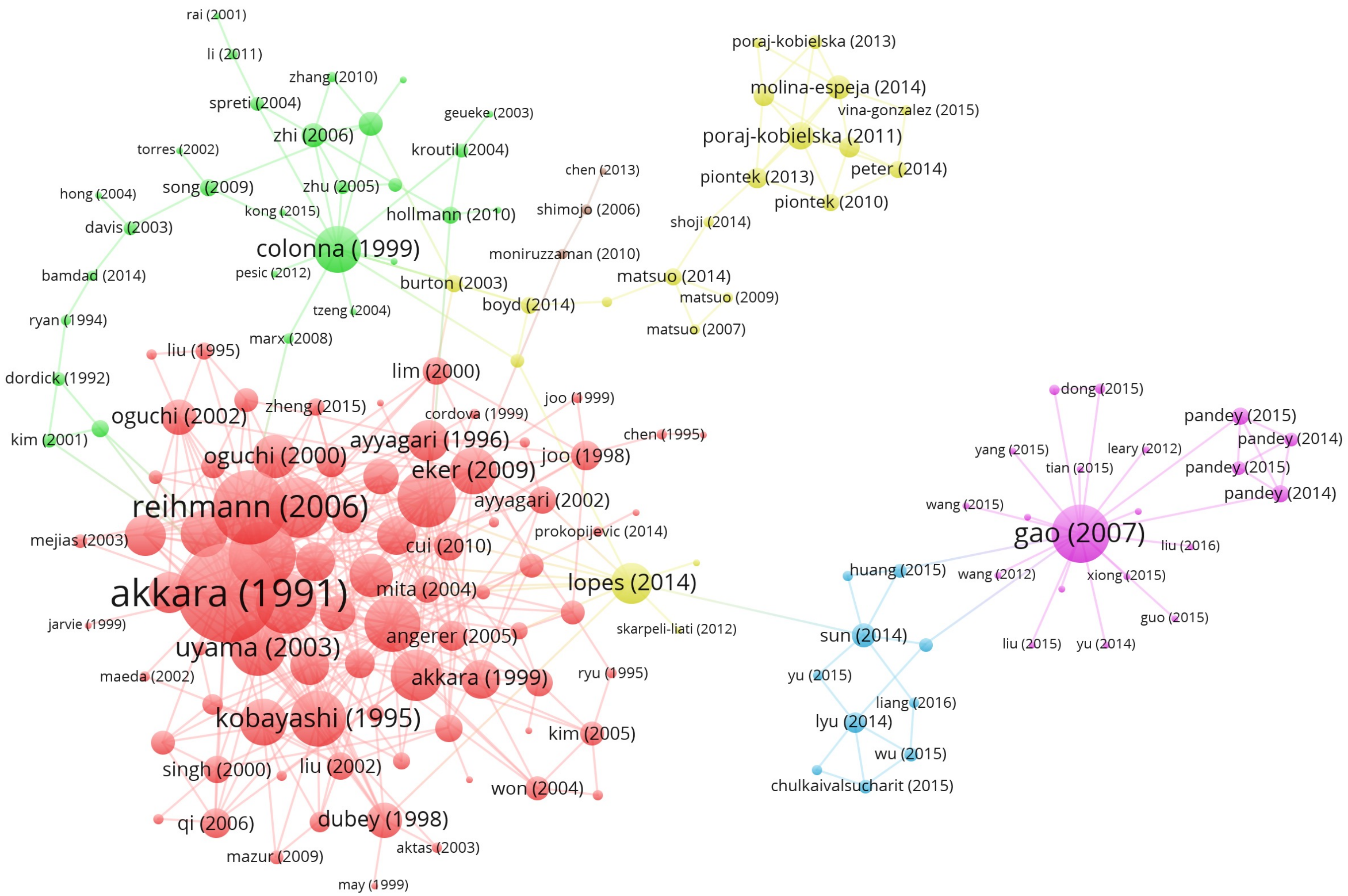
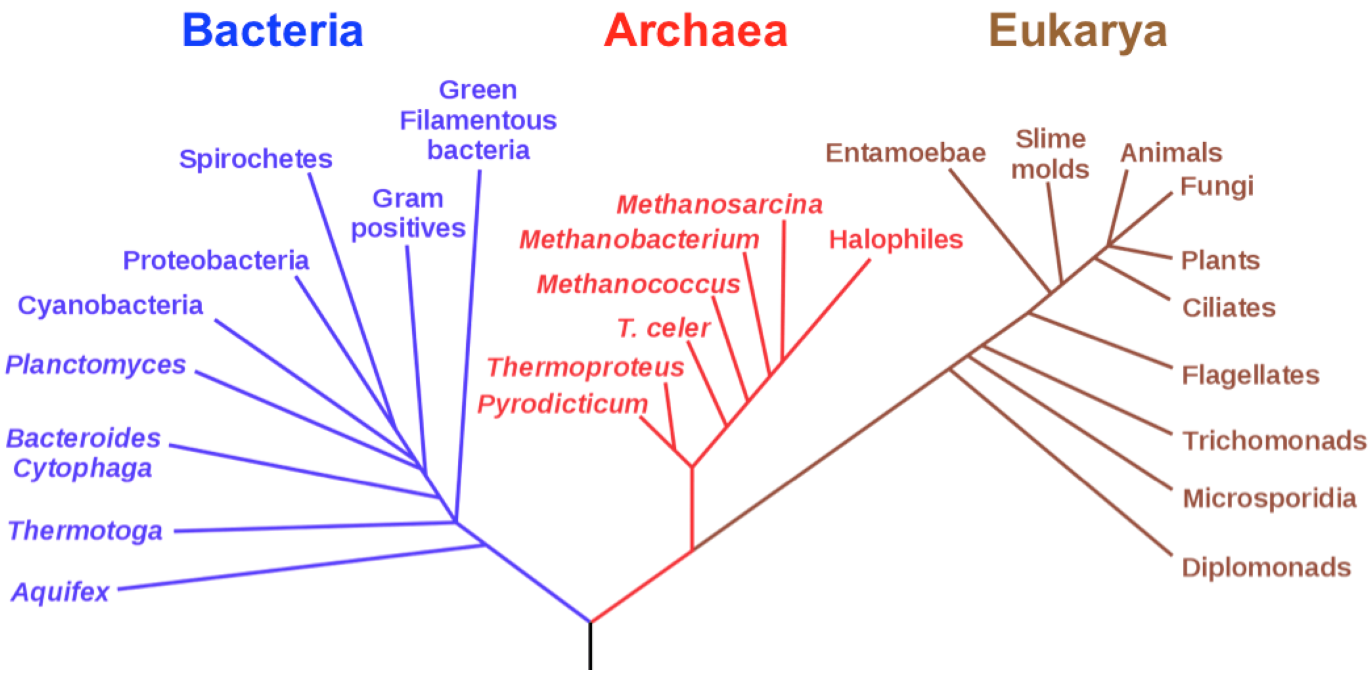


Image Credit: https://www.tudelft.nl/en/library/research-analytics/case-12-citation-networks-2

Motivating Applications of Graphs

- Phylogenetic Tree

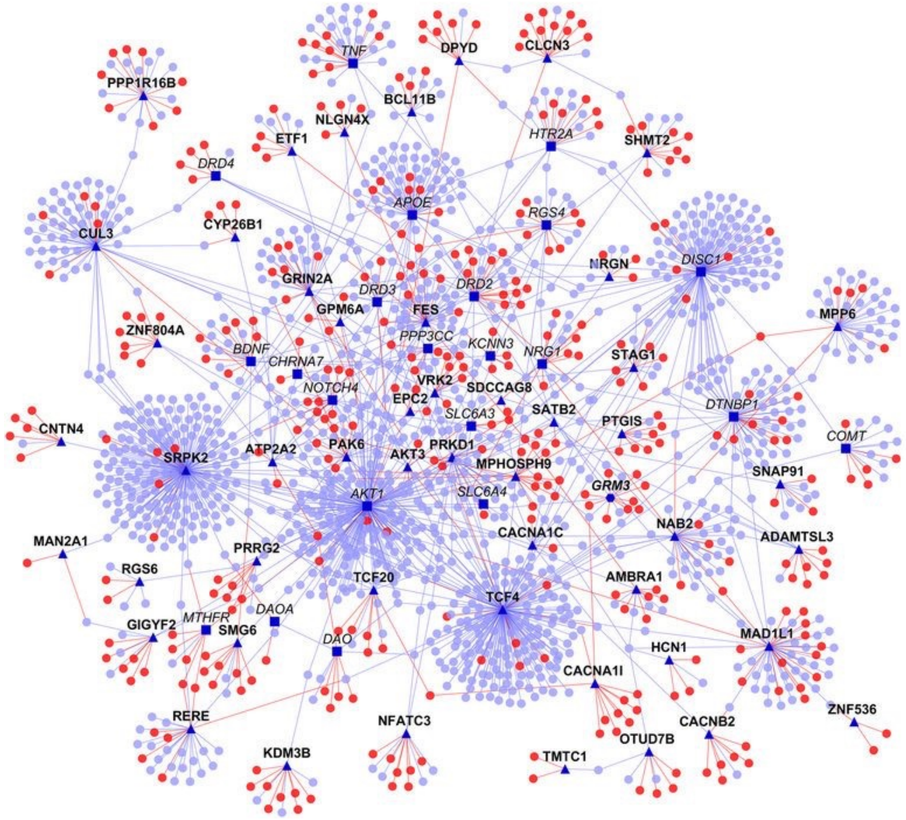


A phylogenetic tree based on rRNA genes showing the three life domains

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

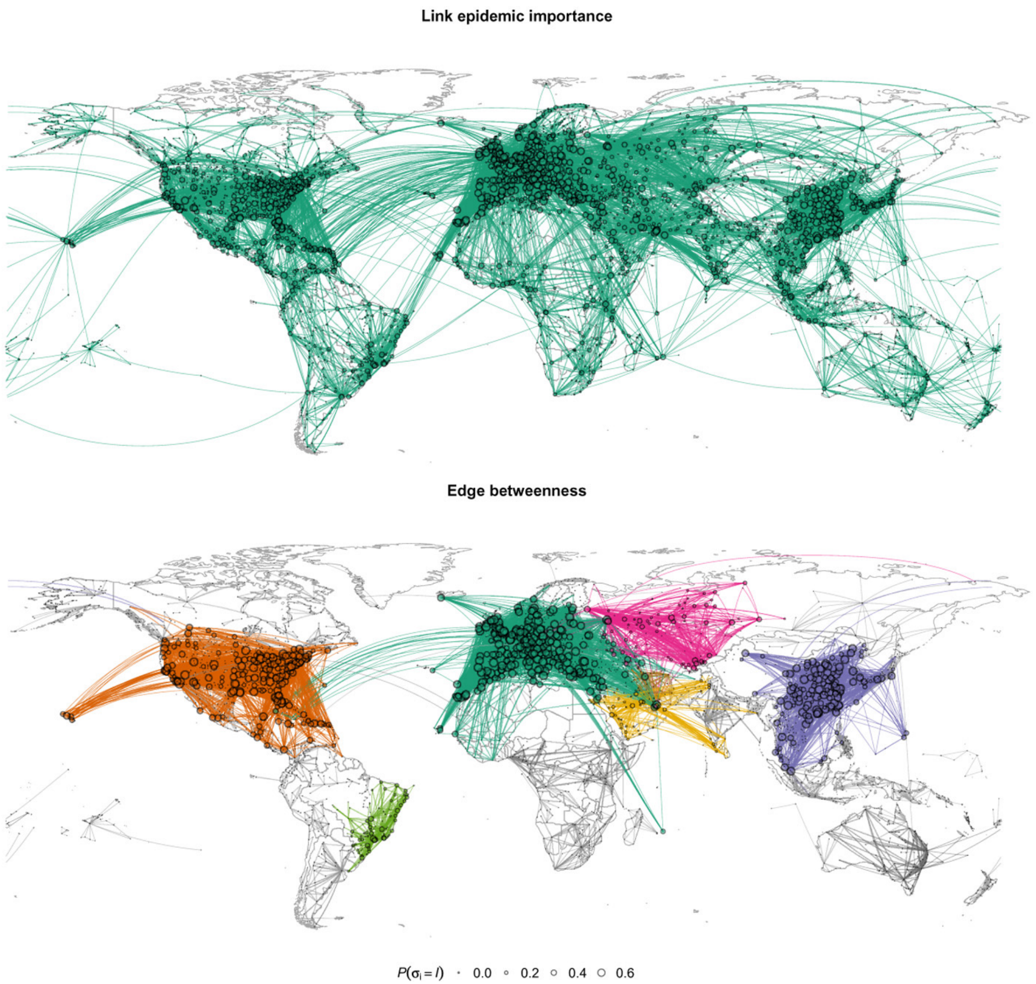


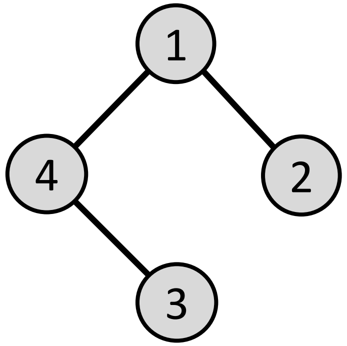
Image Credit: https://www.science.org/doi/10.1126/sciadv.aau4212

Deep Learning for Graphs

Graph Representations

- Connectivity

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

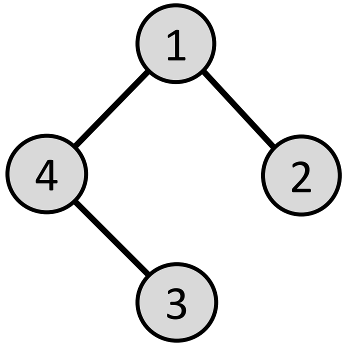


V = {1,2,3,4}, E = {(1,2), (1,4), (4,3)}

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)
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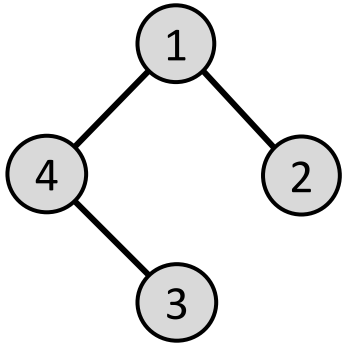
- Feature
    1. Node Feature: X
    2. Edge Feature
    3. Graph Feature



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Deep Learning for Graphs

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  1. Adjacency List: G = (V, E)
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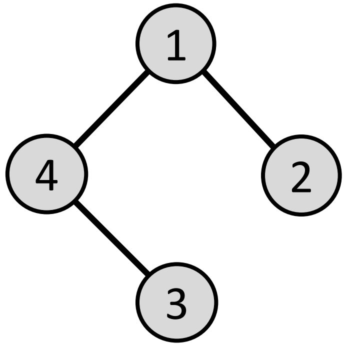
Graph Data = (A, X)



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Deep Learning for Graphs

Permutation

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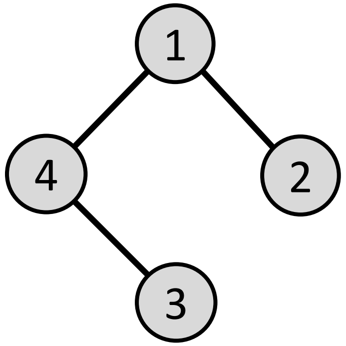

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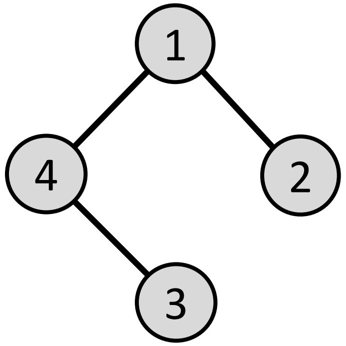

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Original Adj Matrix

Deep Learning for Graphs

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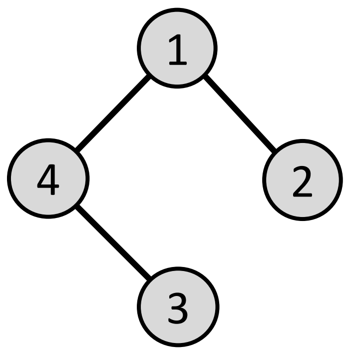

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Permute Rows

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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
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Transposed Permutation Matrix

Deep Learning for Graphs

Permutation

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

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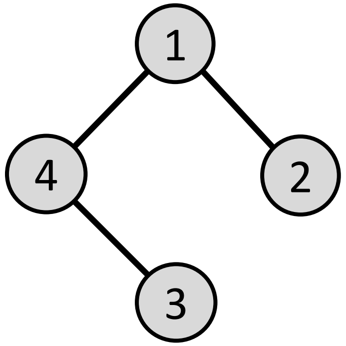

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Transposed Permutation Matrix

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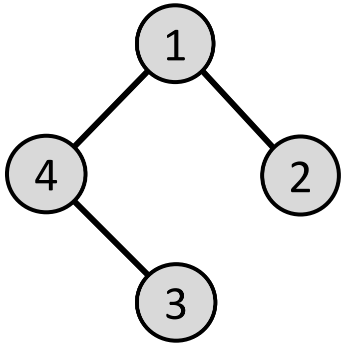

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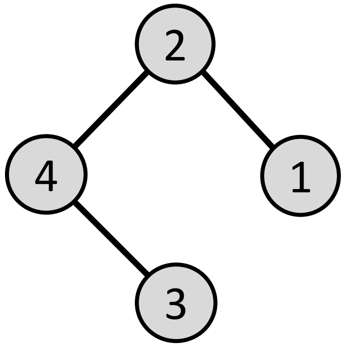

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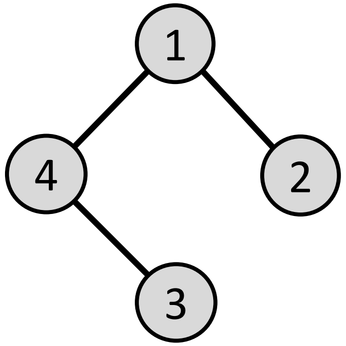

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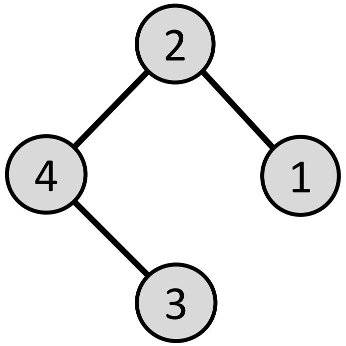
V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

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 for Graphs

Permutation

V = [1,2,3,4] => V’ = [4,3,2,1]

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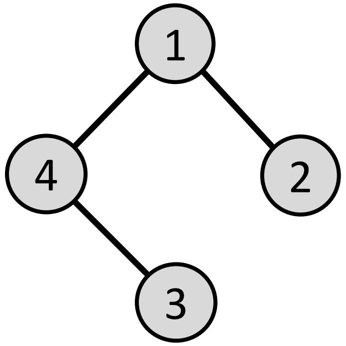

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Deep Learning for Graphs

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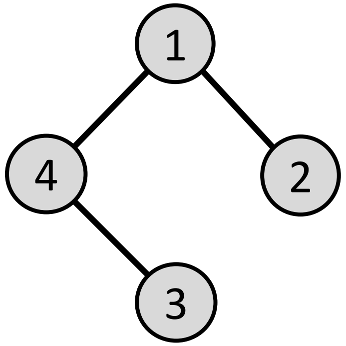

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Original Adj Matrix

Deep Learning for Graphs

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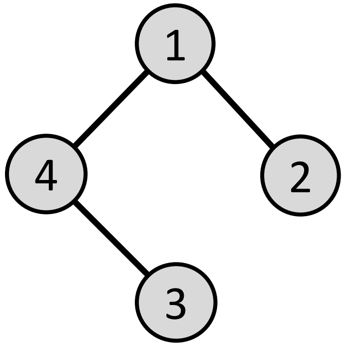

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Permute Rows

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Permutation Matrix

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Original Adj Matrix

Permute Columns

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Transposed Permutation Matrix

Deep Learning for Graphs

Permutation

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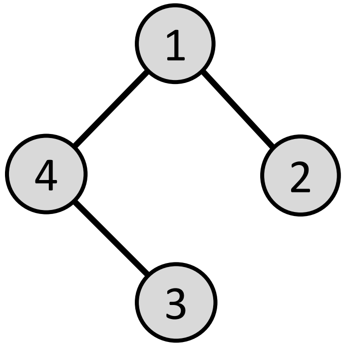

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Deep Learning for Graphs

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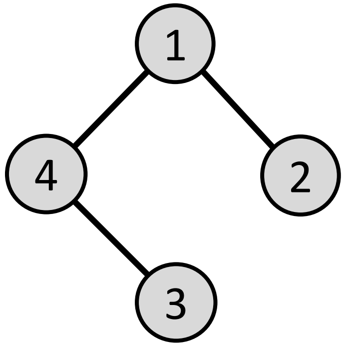

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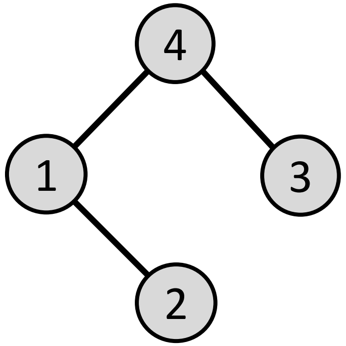

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Deep Learning for Graphs

Permutation

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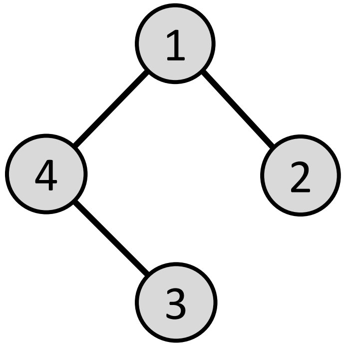

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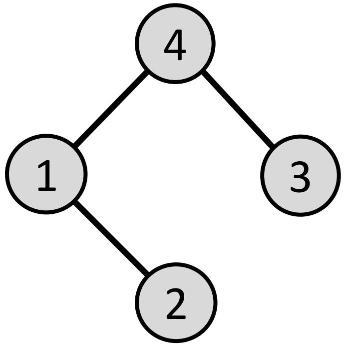
Graph Automorphism:

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 for Graphs

Permutation Invariance & Equivariance

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

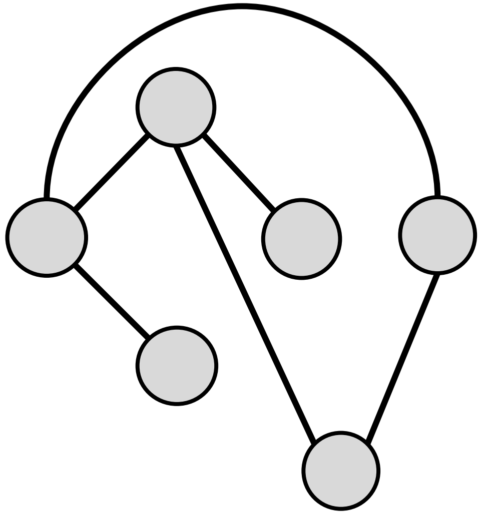
Invariance: $$f(PAP^\top, PX) = f(A, X)$$

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

Deep Learning for Graphs

Key Challenges:

- **Unordered Neighbors**



Deep Learning for Graphs

Key Challenges:

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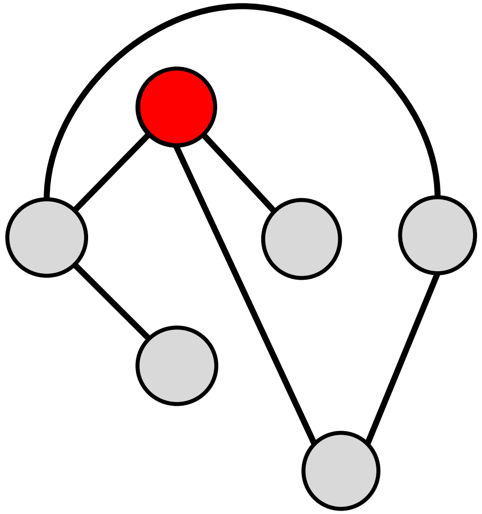
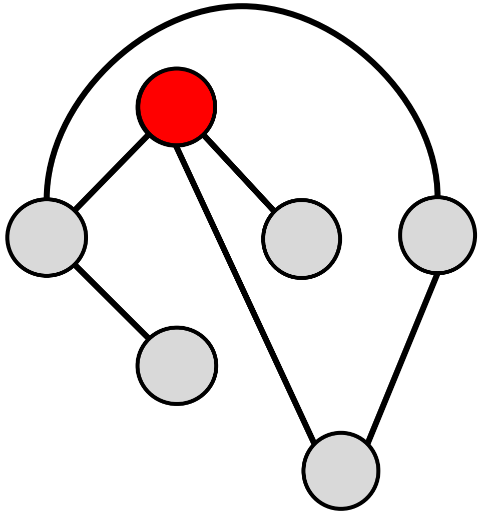
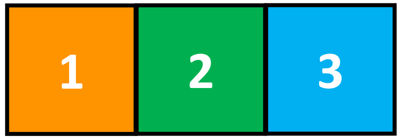


Deep Learning for Graphs

Key Challenges:

- **Unordered Neighbors**





Deep Learning for Graphs

Key Challenges:

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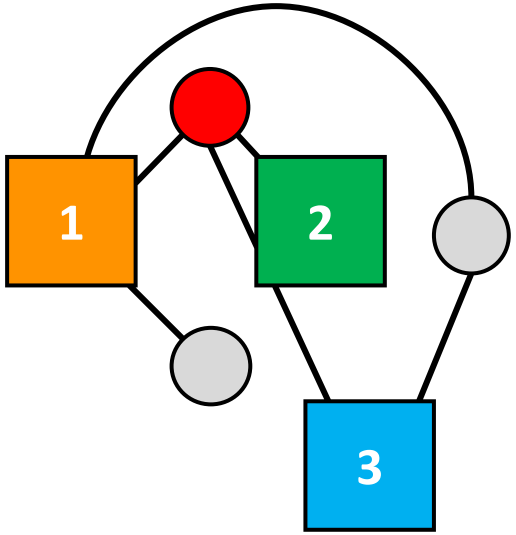
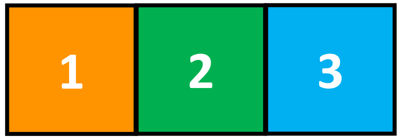


Option 1



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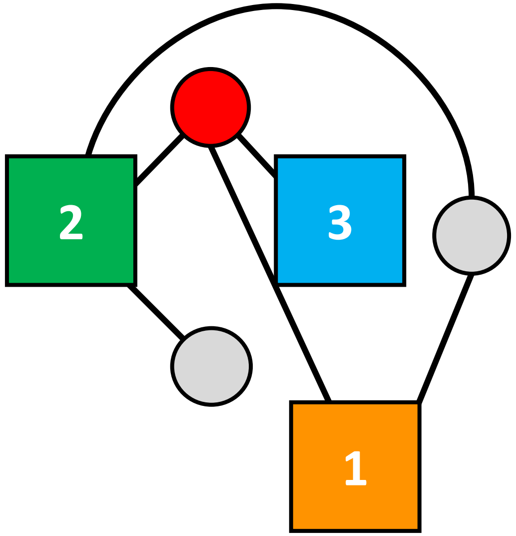
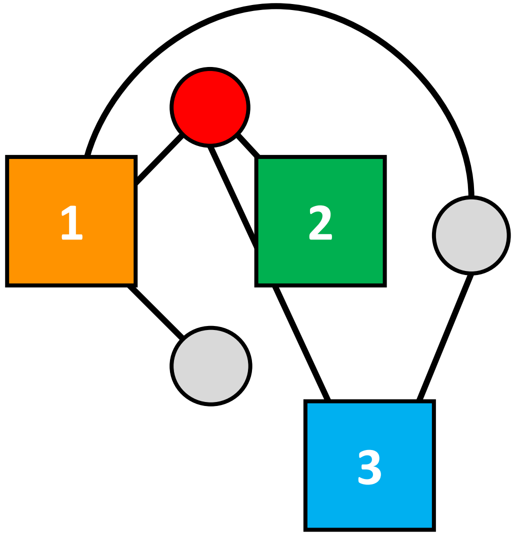


Option 2



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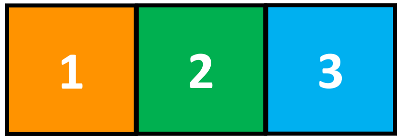

Deep Learning for Graphs

Key Challenges:

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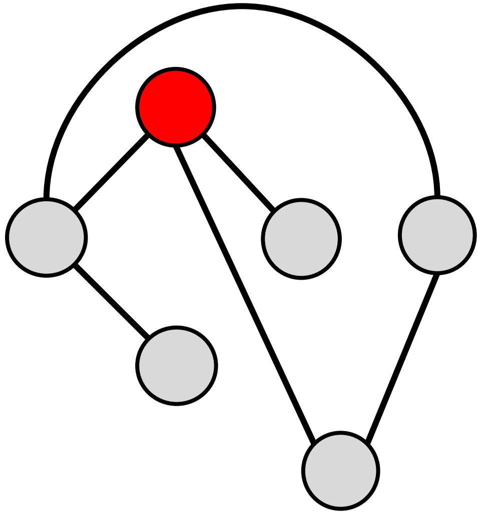

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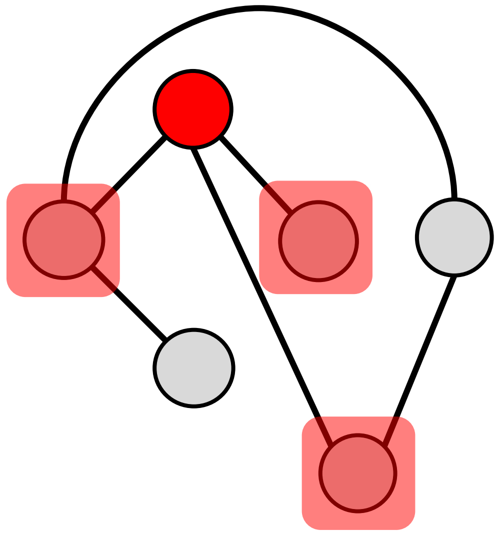

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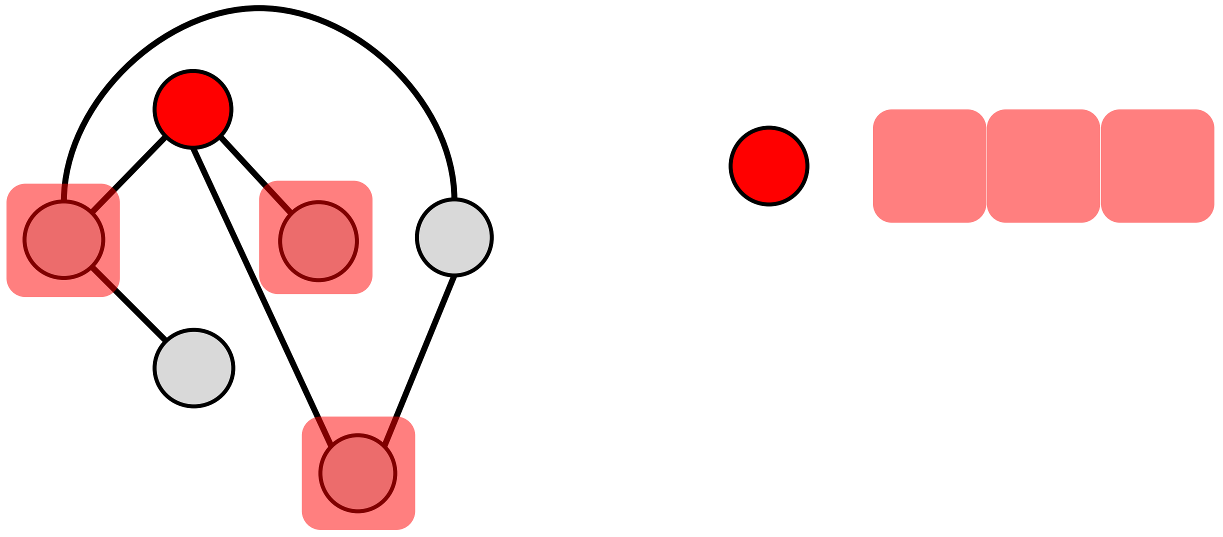

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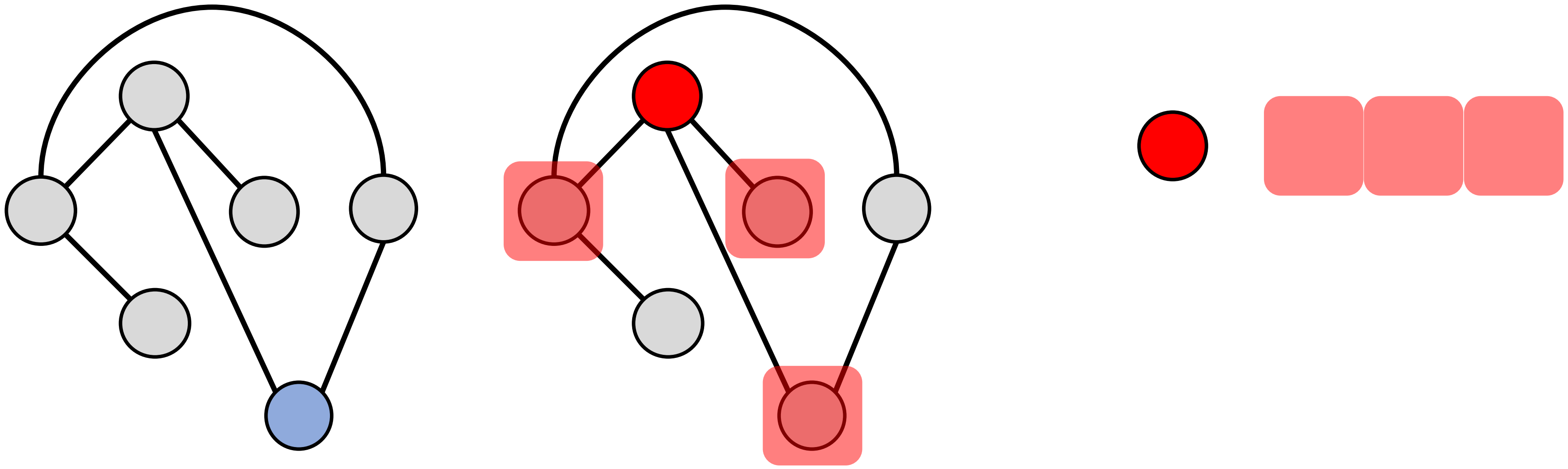

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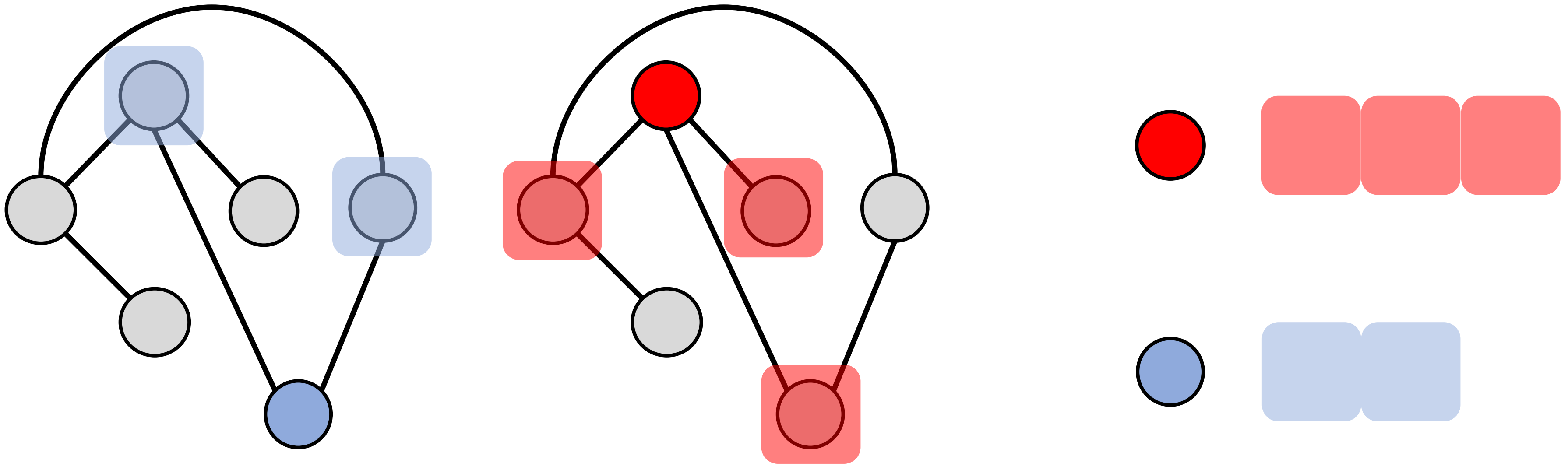

Deep Learning for Graphs

Key Challenges:

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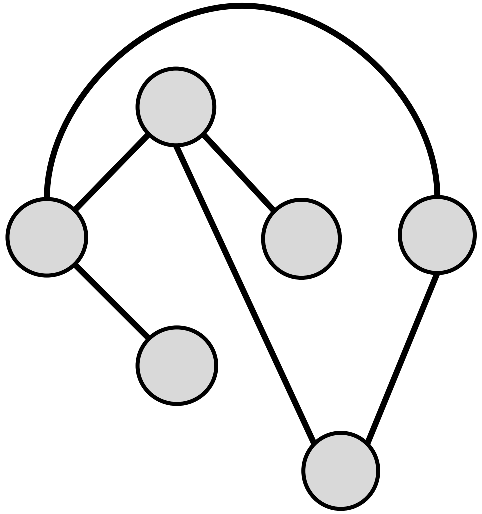

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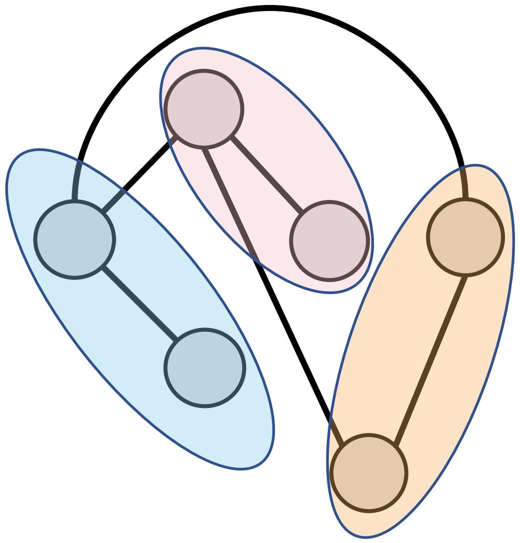

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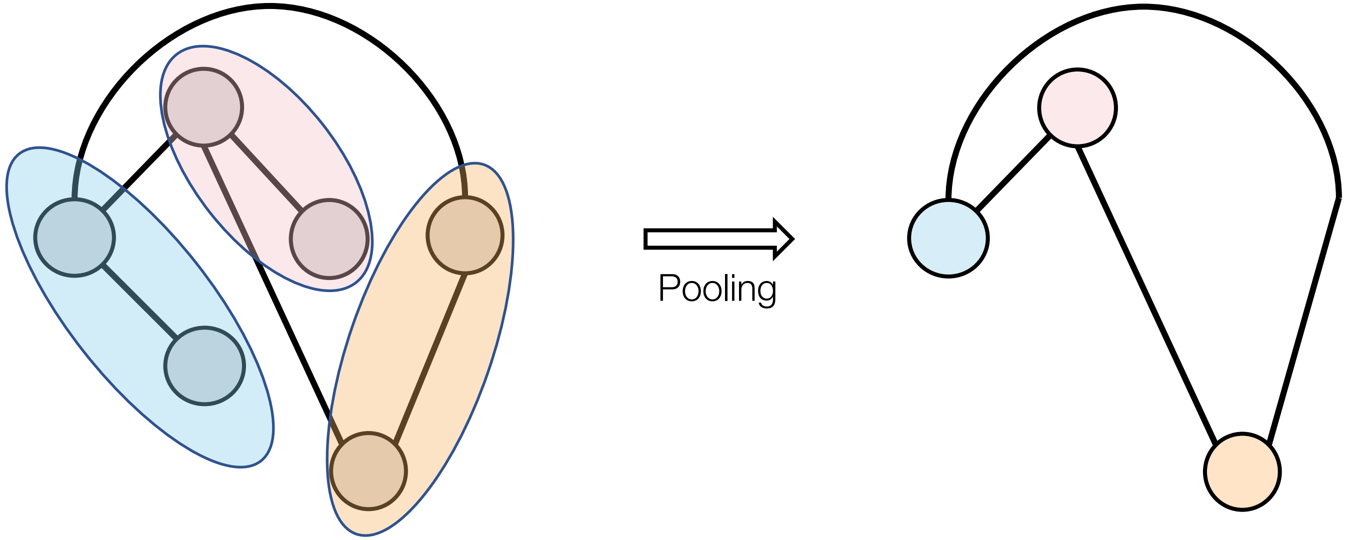

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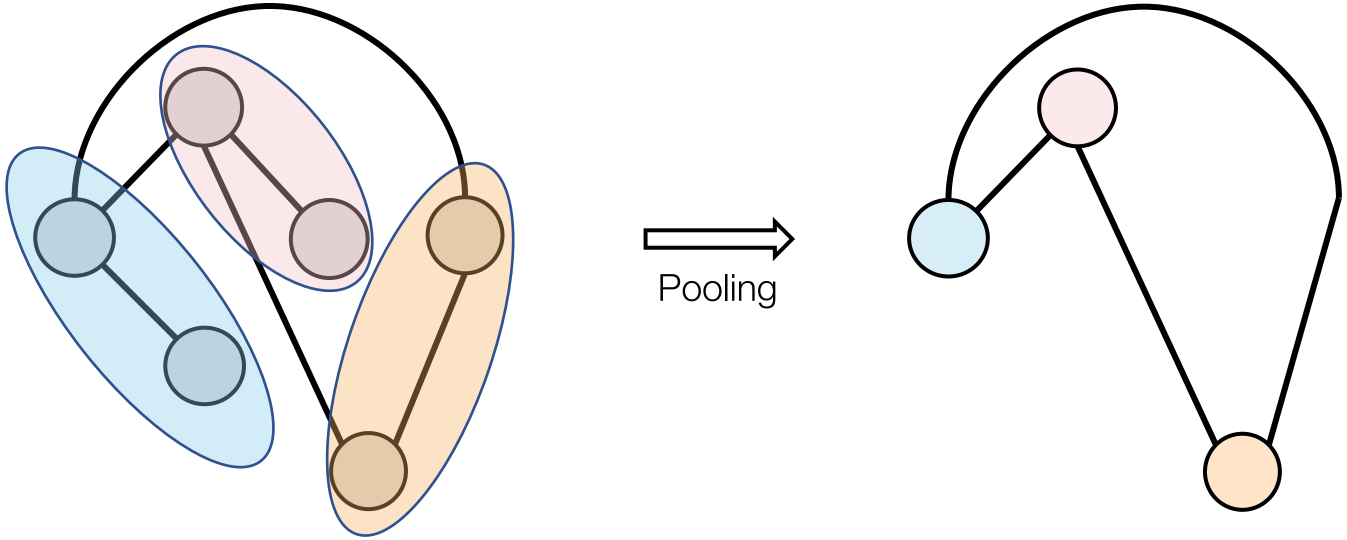

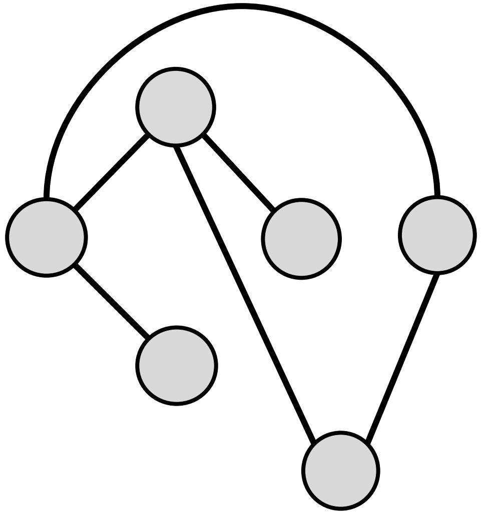

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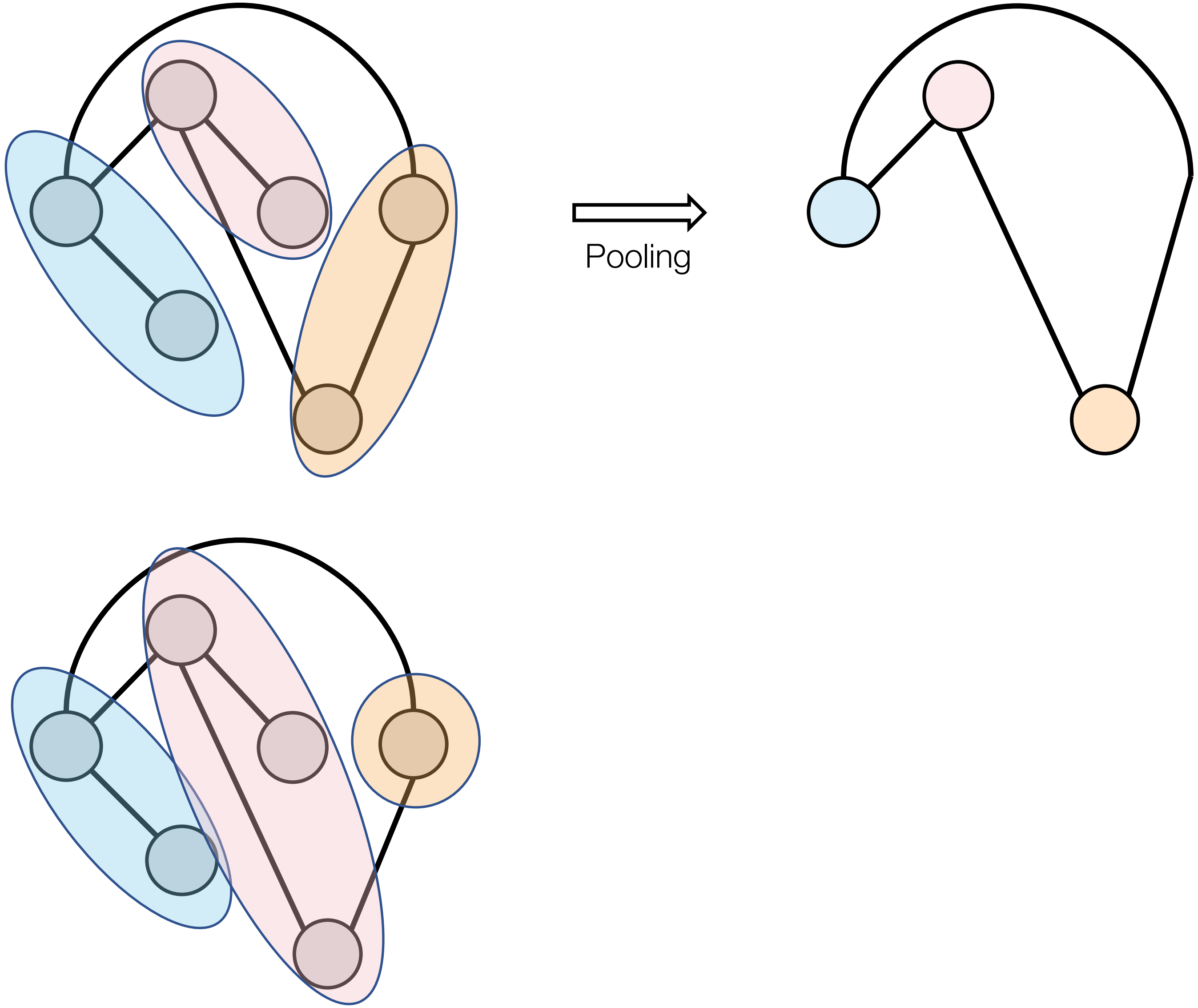

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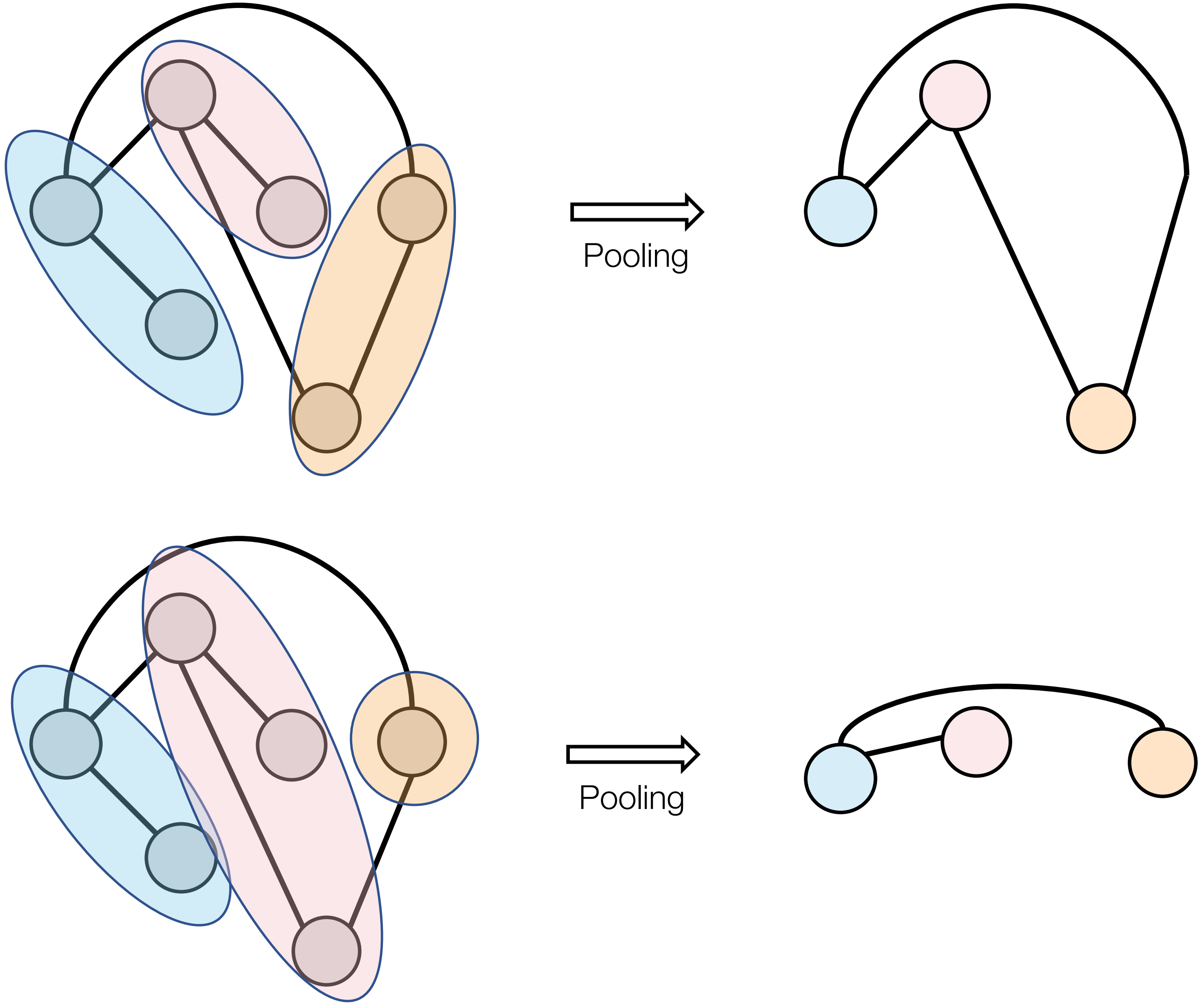

Deep Learning for Graphs

Graph Neural Networks (GNNs)

- Neural networks that can process general graph structured data

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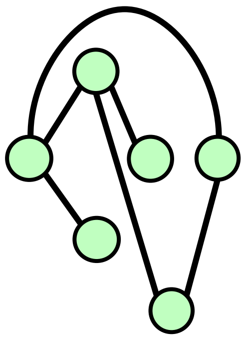
- GNNs have been independently studied in signal processing community under **Graph Signal Processing**
- The study of GNNs and other related models are also called **Geometric Deep Learning**

Graph Neural Networks (GNNs)



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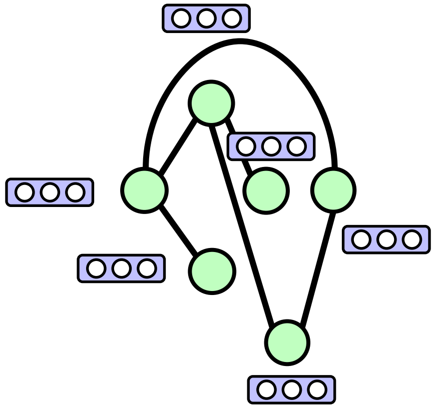
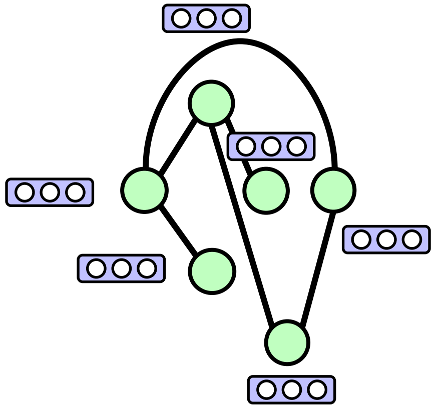


Input Encoding

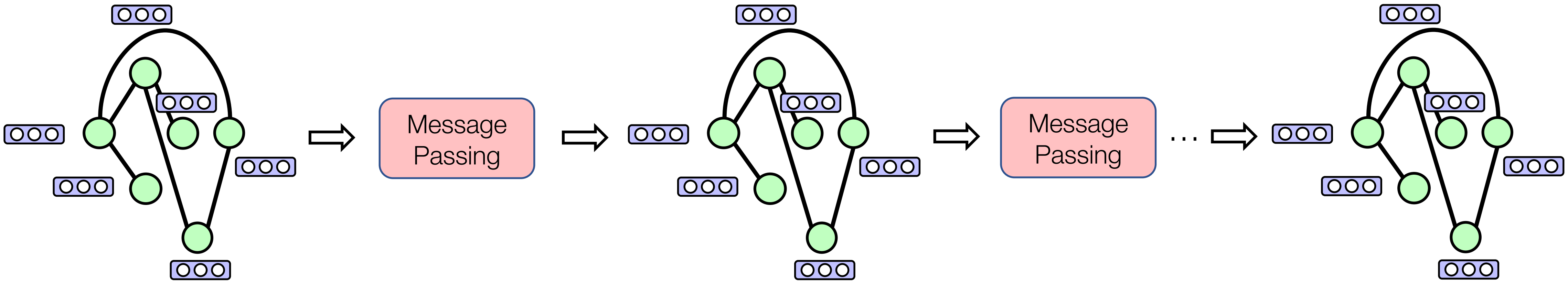
Graph Neural Networks (GNNs)



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*

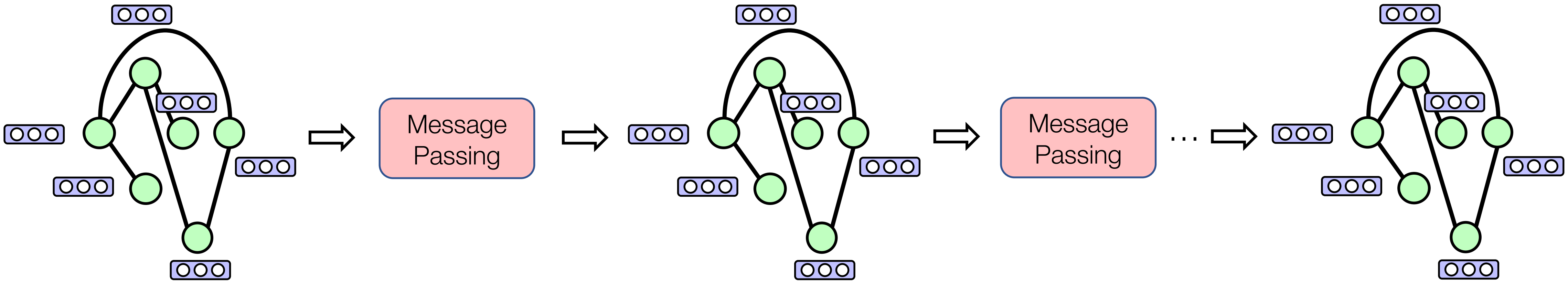
Graph Neural Networks (GNNs)



Input Encoding

Message Passing Layers/Steps

Graph Neural Networks (GNNs)

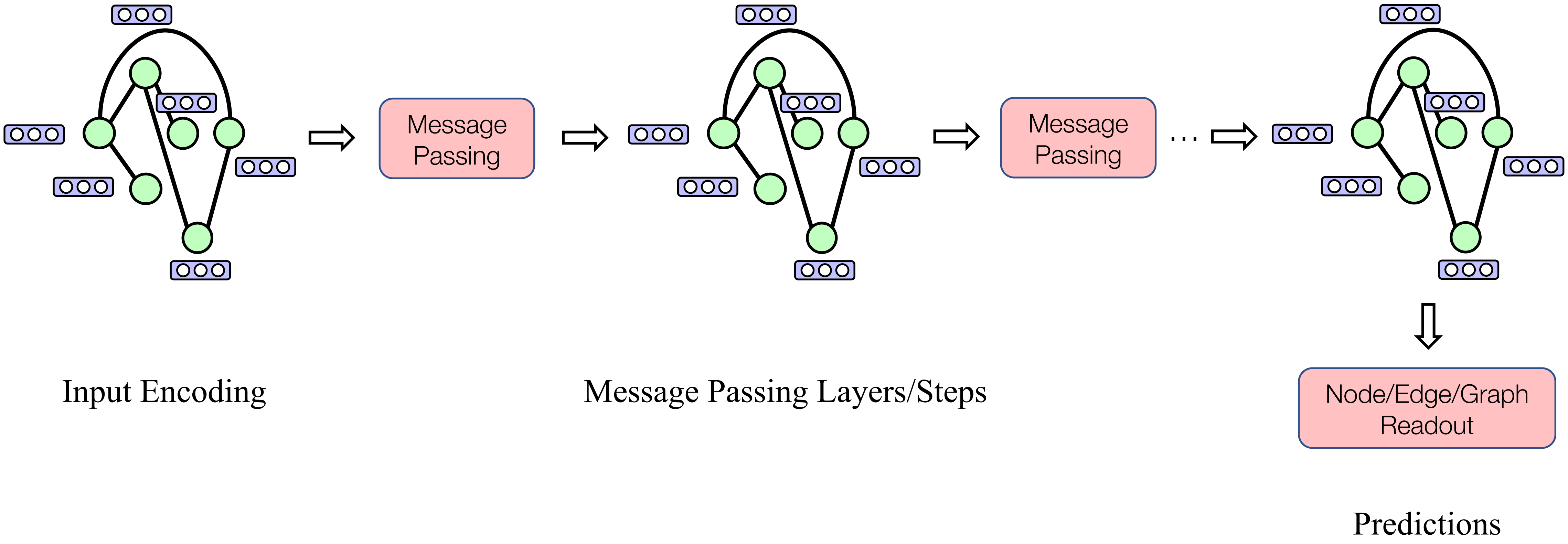


Input Encoding

Message Passing Layers/Steps

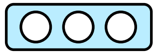
Steps: share message passing module (Recurrent Networks)
Layers: do not share message passing module (Feedforward Networks)

Graph Neural Networks (GNNs)

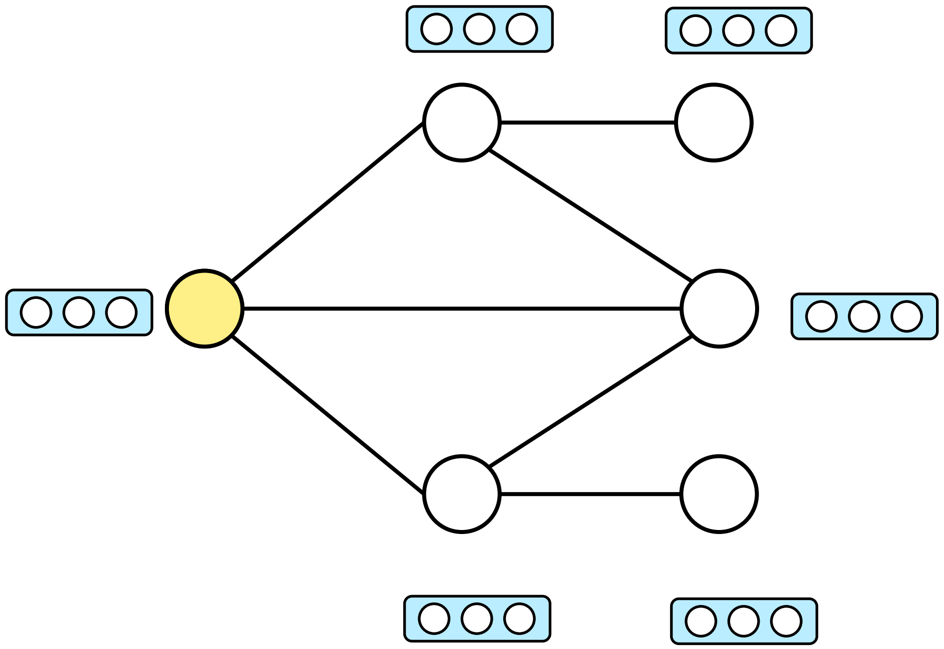


Message Passing in GNNs

$\mathbf{h}_i^t$

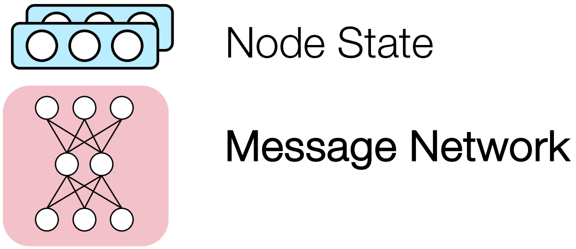
 Node State

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



Message Passing in GNNs

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



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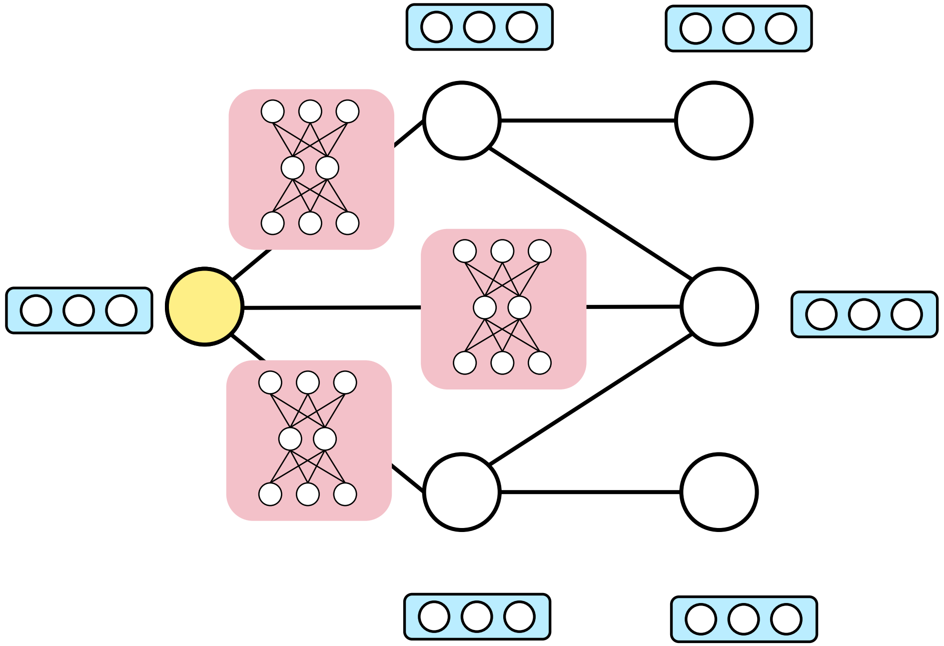
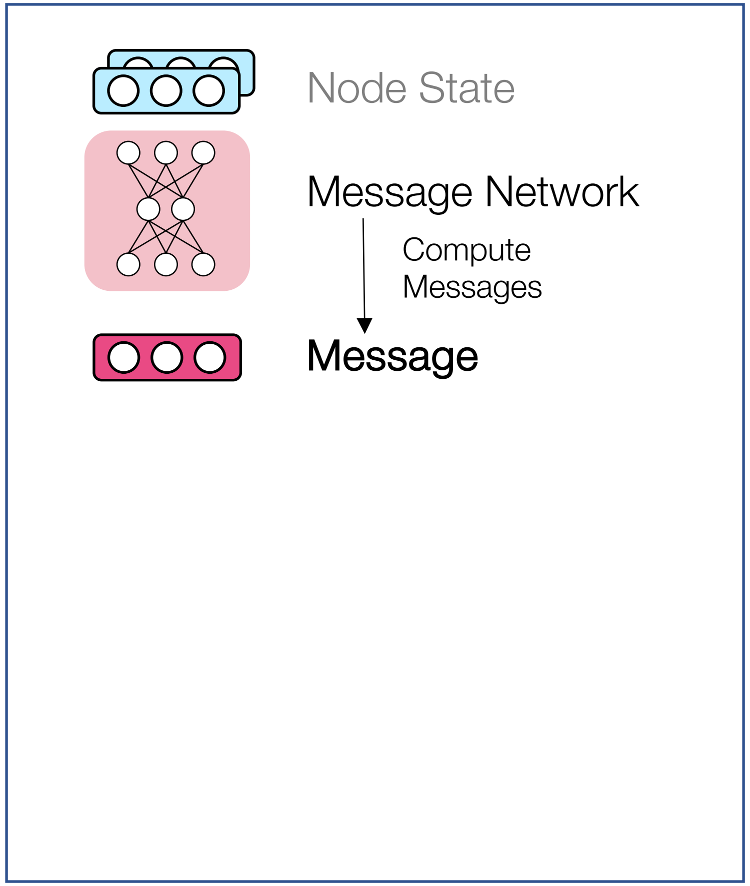


Message Passing in GNNs

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

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



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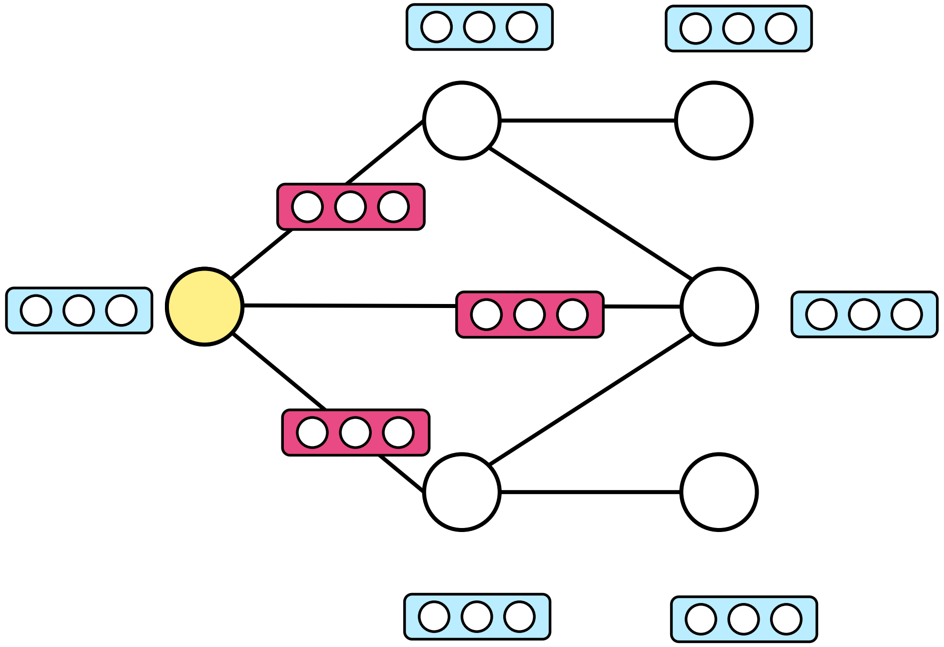

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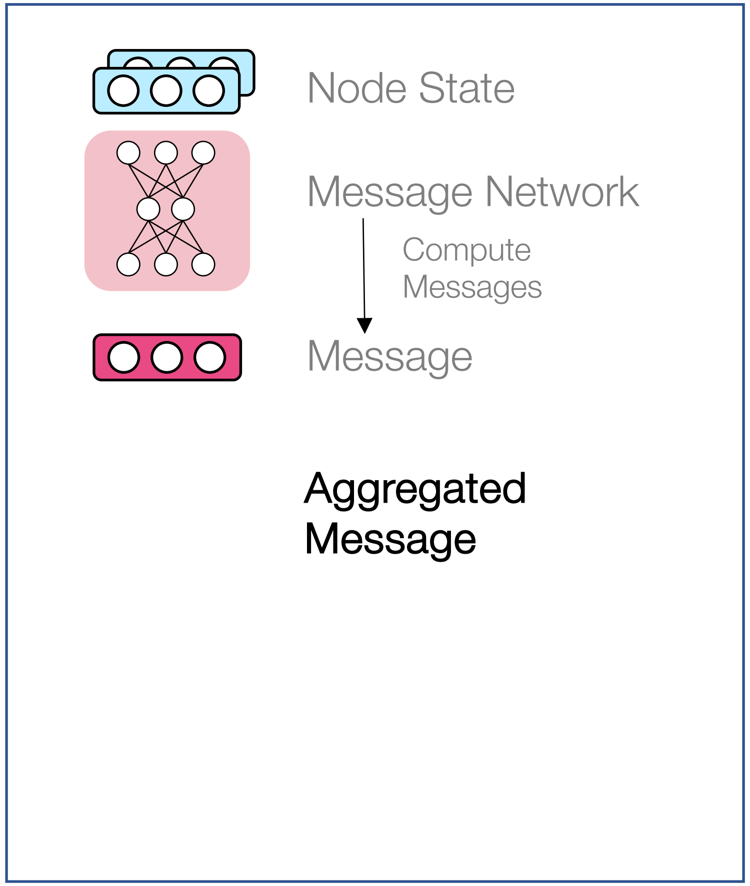

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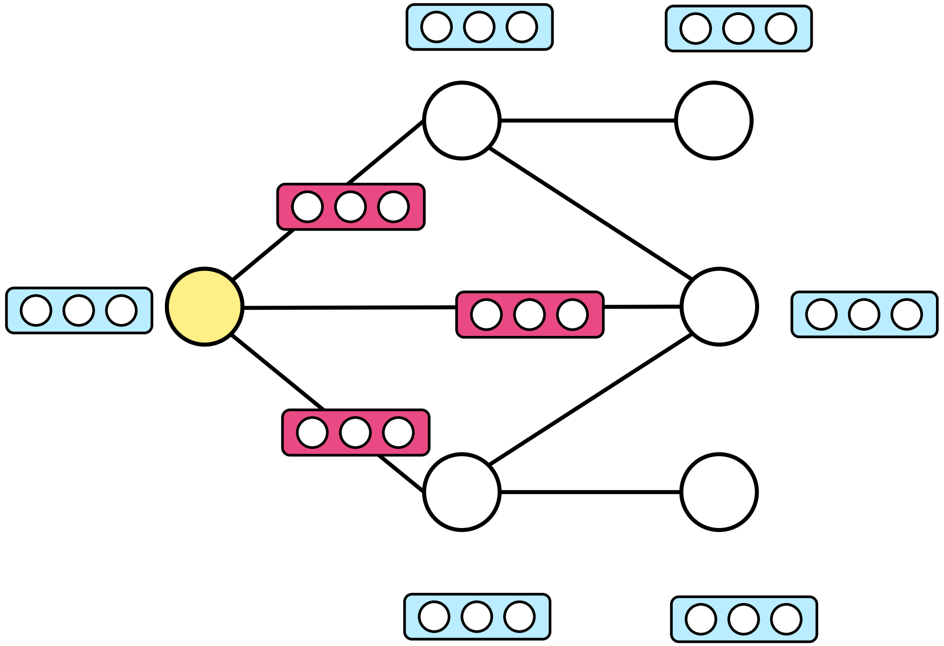

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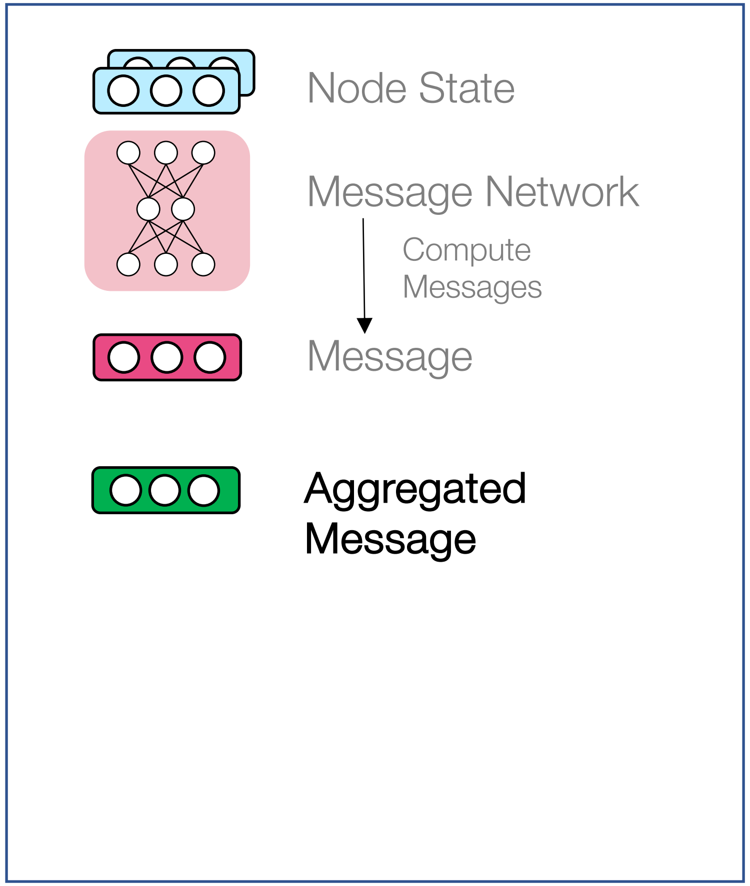

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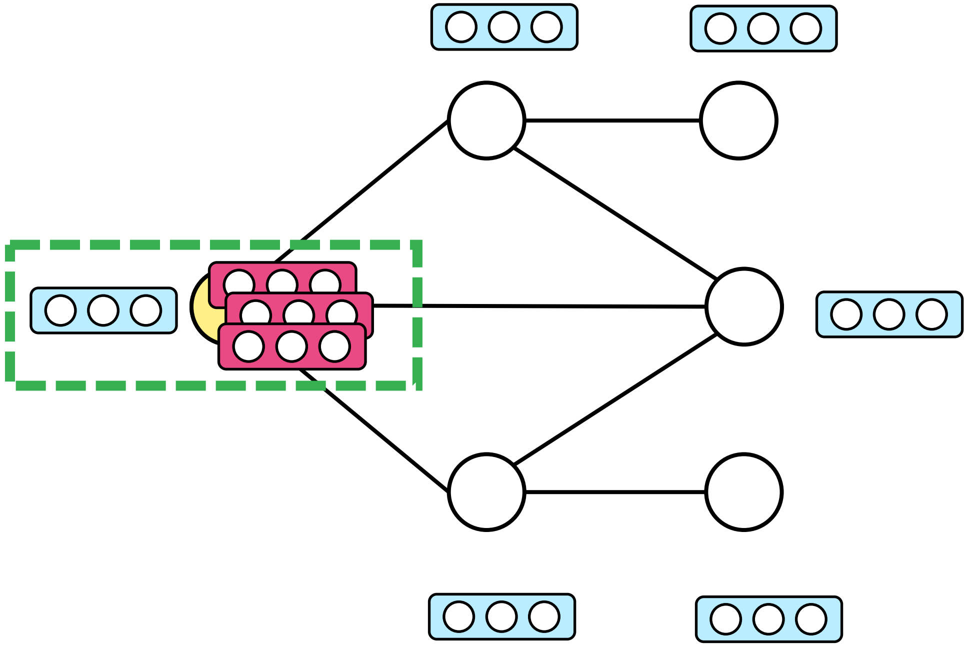

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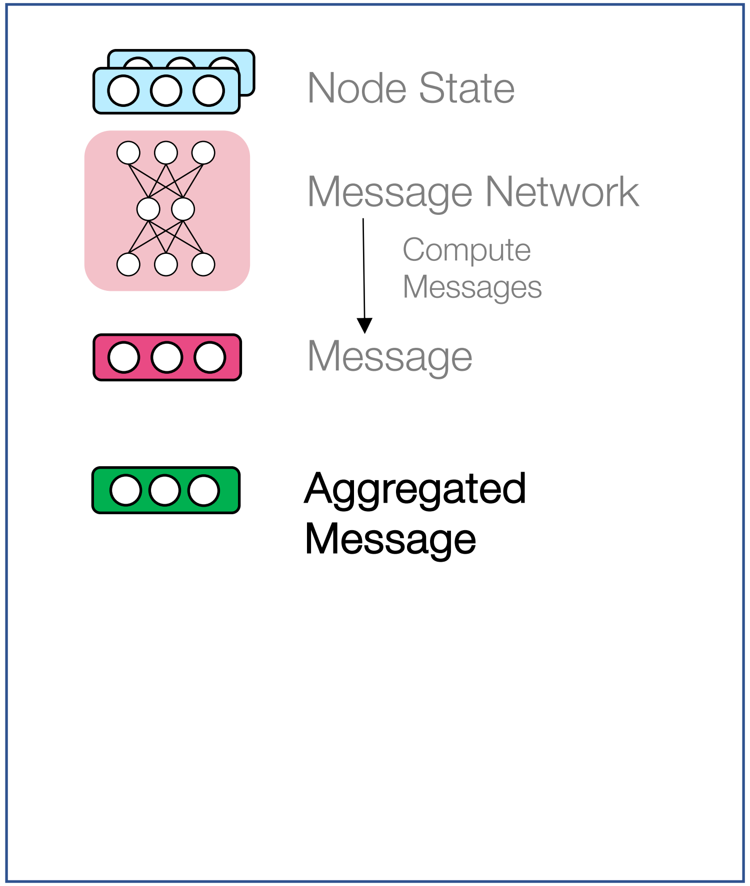

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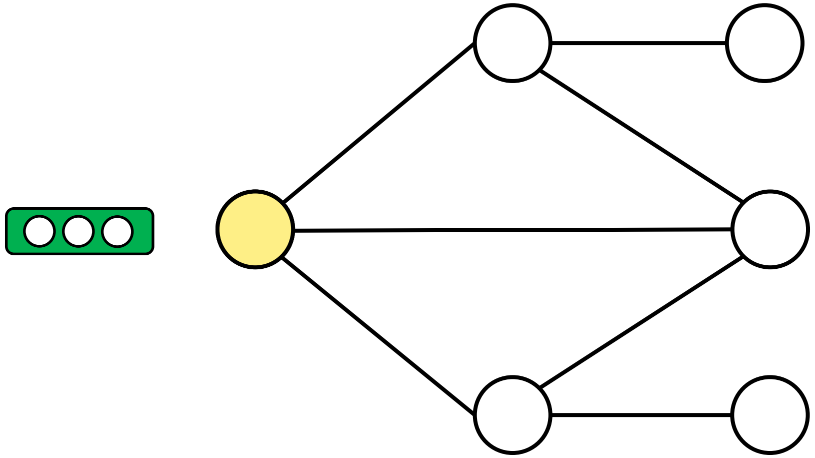

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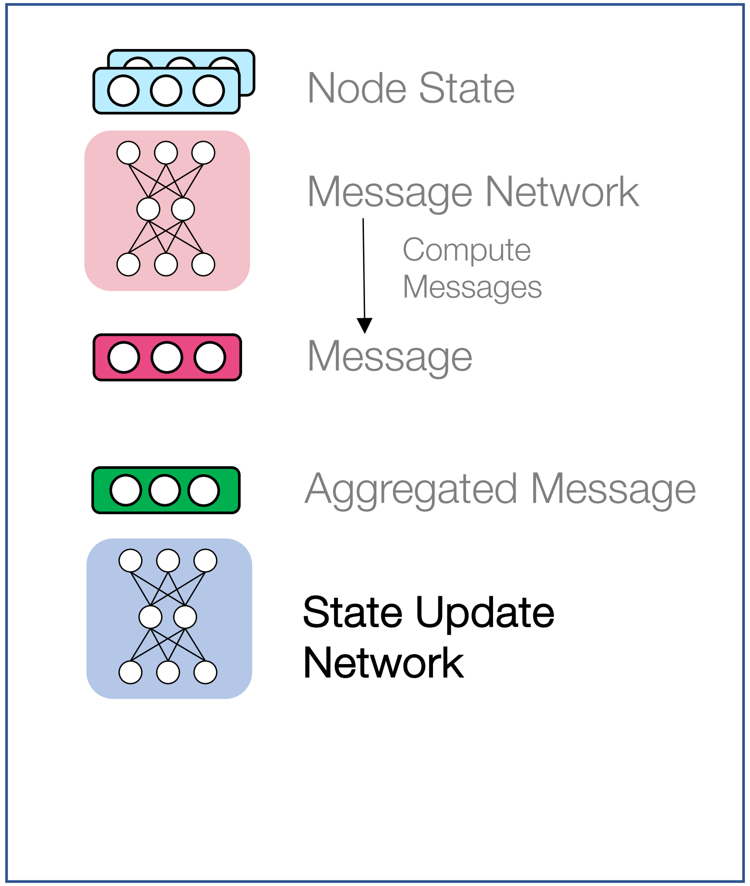

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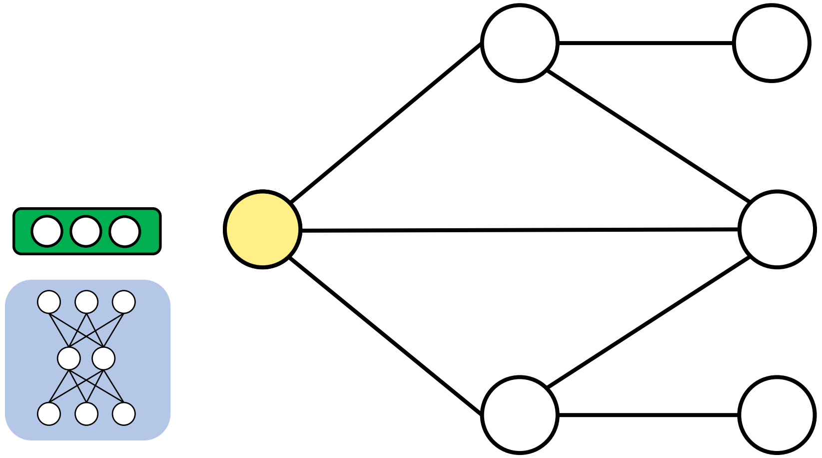

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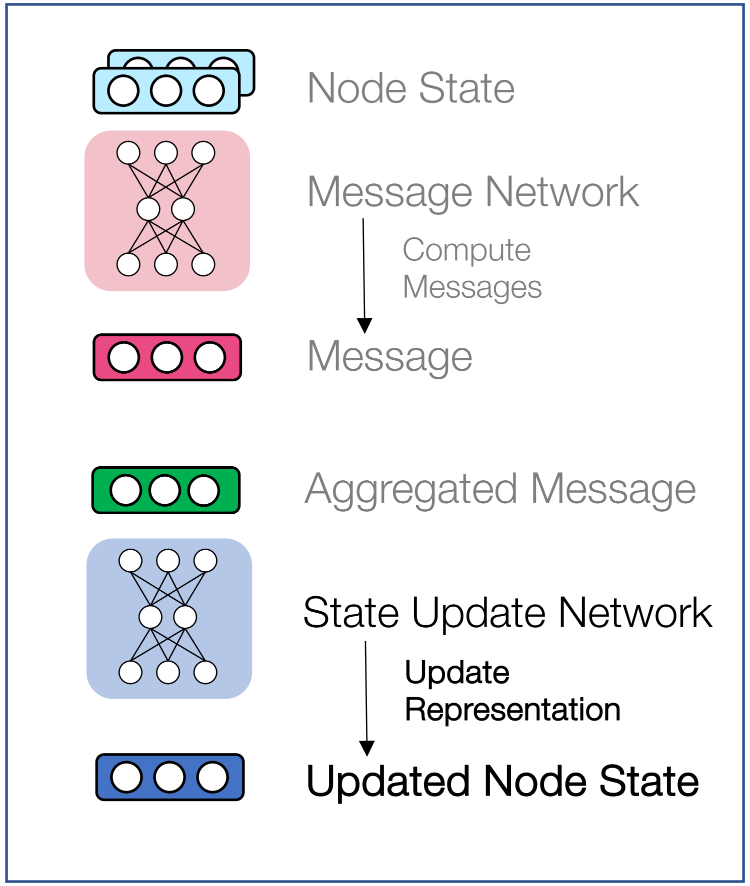

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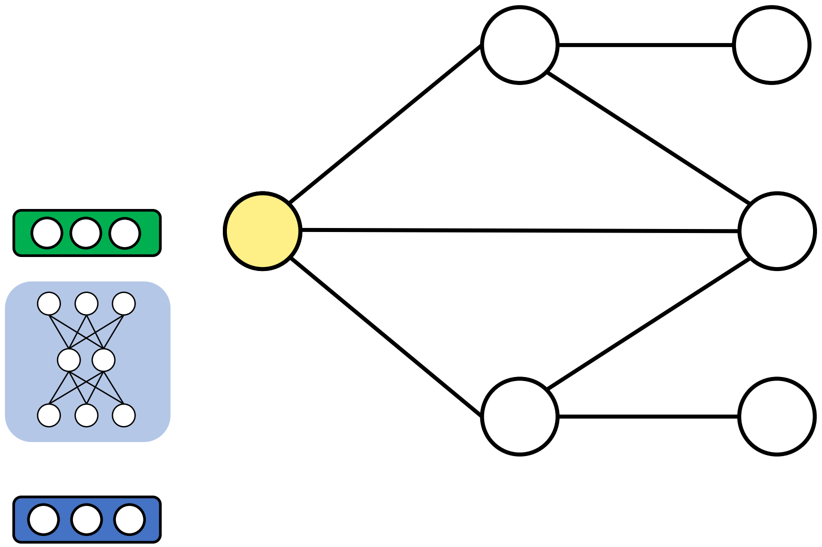

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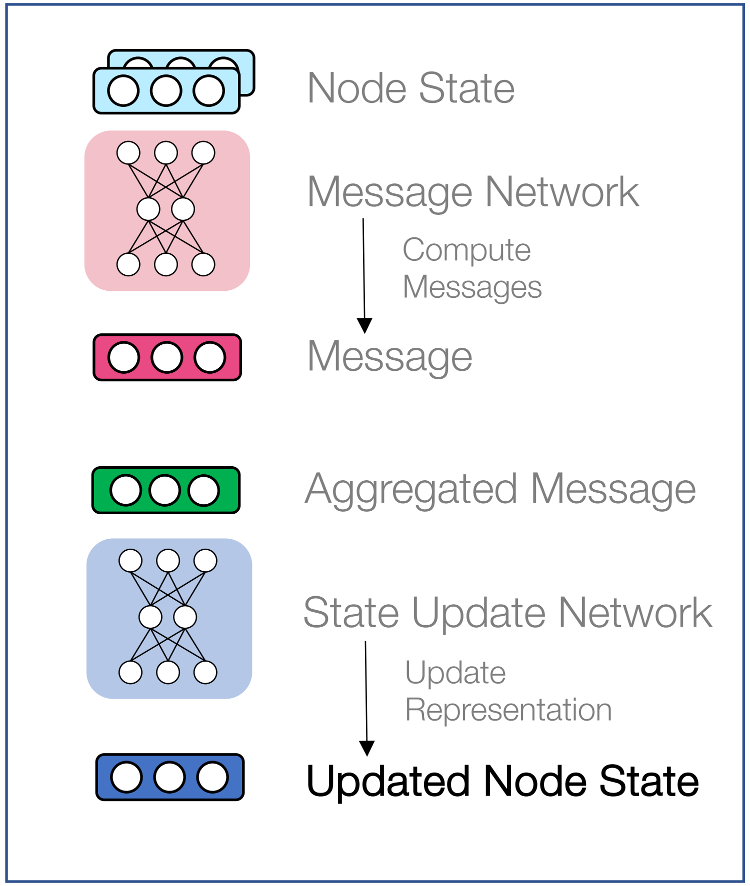

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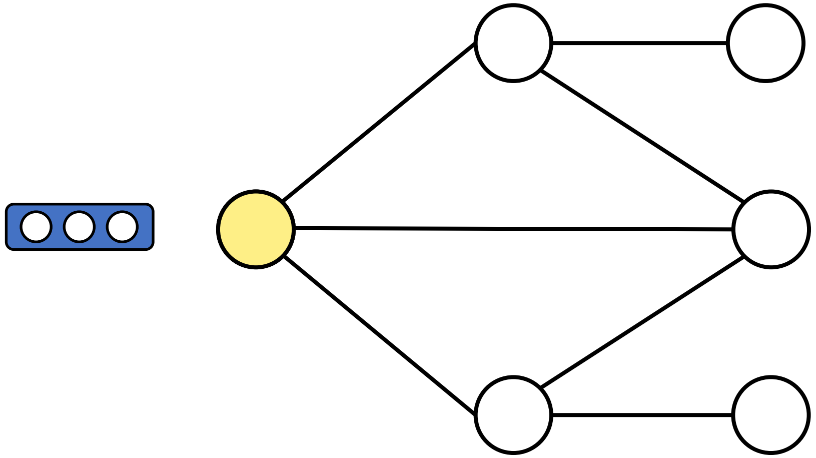

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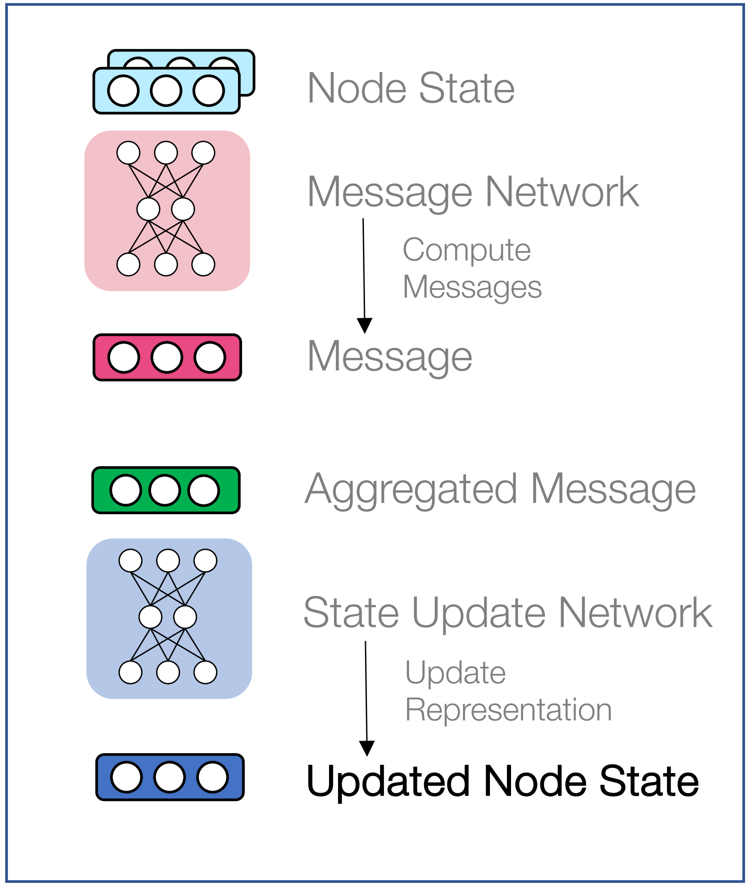

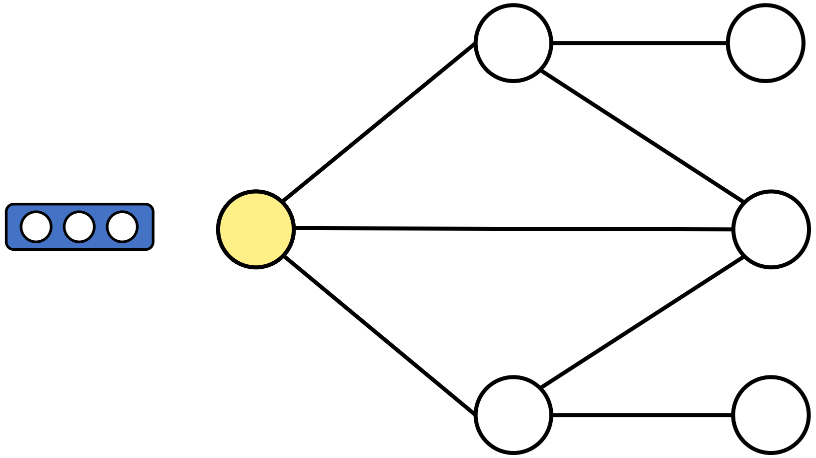

- Parallel Schedule!

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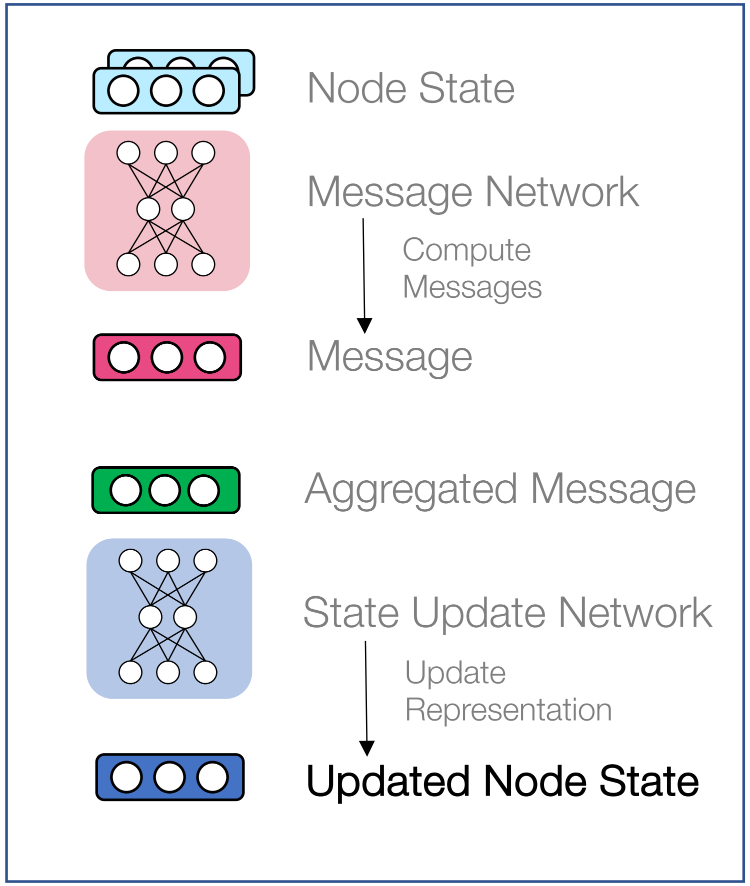

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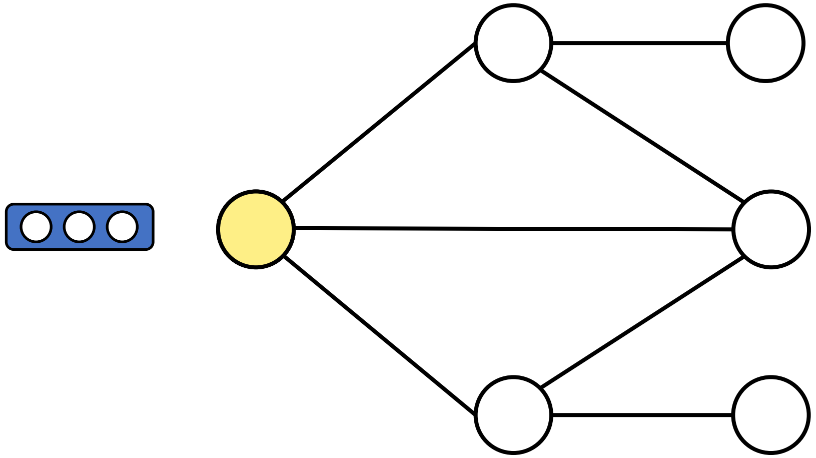

- Parallel Schedule!
- Other schedules [8] are possible and could improve performance in certain tasks!

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

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

3. Update Node Representations

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

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

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [4]

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Edge Feature

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Instantiations:

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

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{GRU}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$ [4,7]

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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**

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

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

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2. **Edge Readout**

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Edge Feature

Readout in GNNs

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Edge Feature

3. **Graph Readout**

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

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

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

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!*

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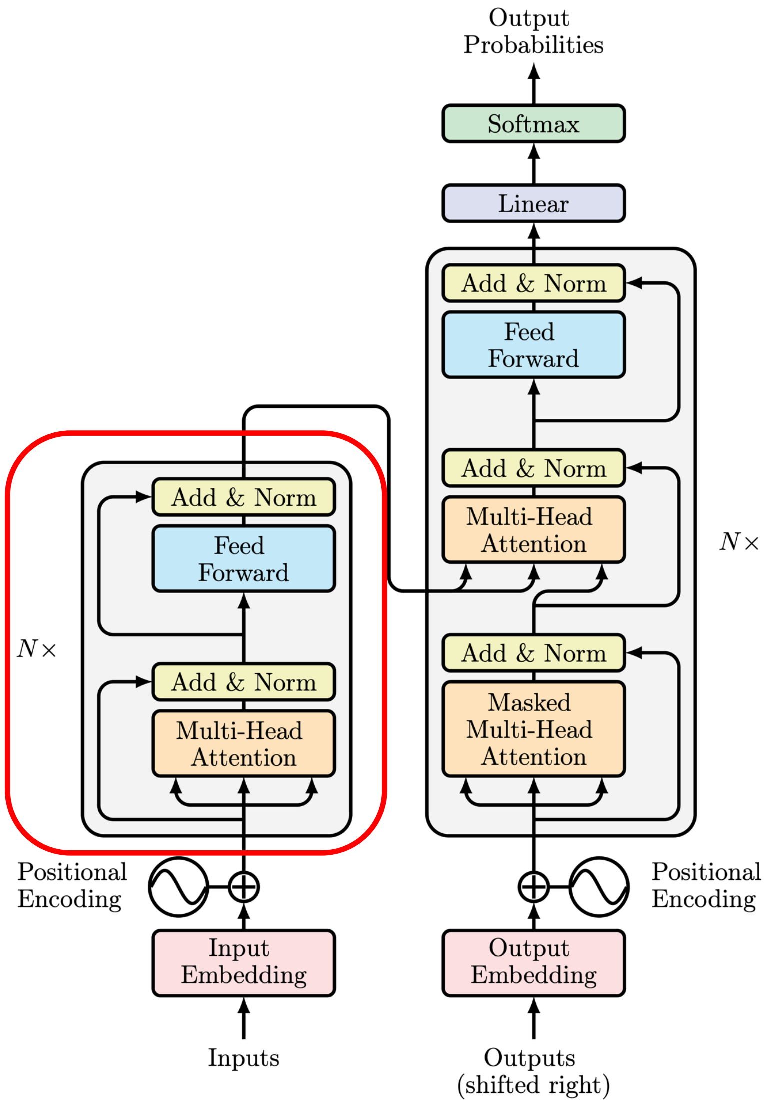
1. *Although graph could be very sparse, we should maximally exploit dense operators since they are efficient on GPUs!*

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

Relationships with Transformer



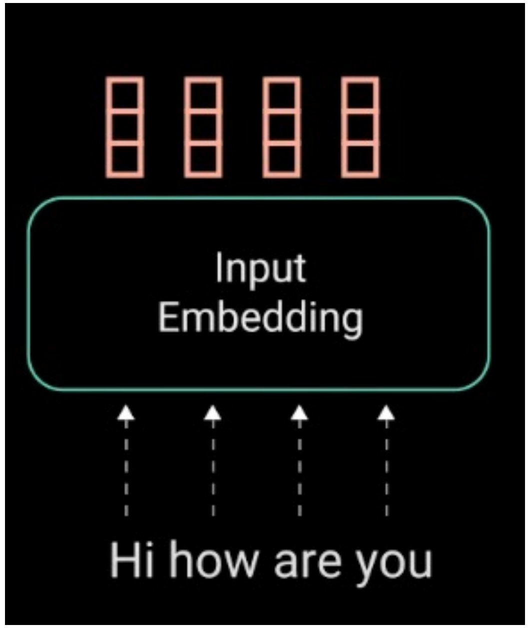


Image Credit: [9] & https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

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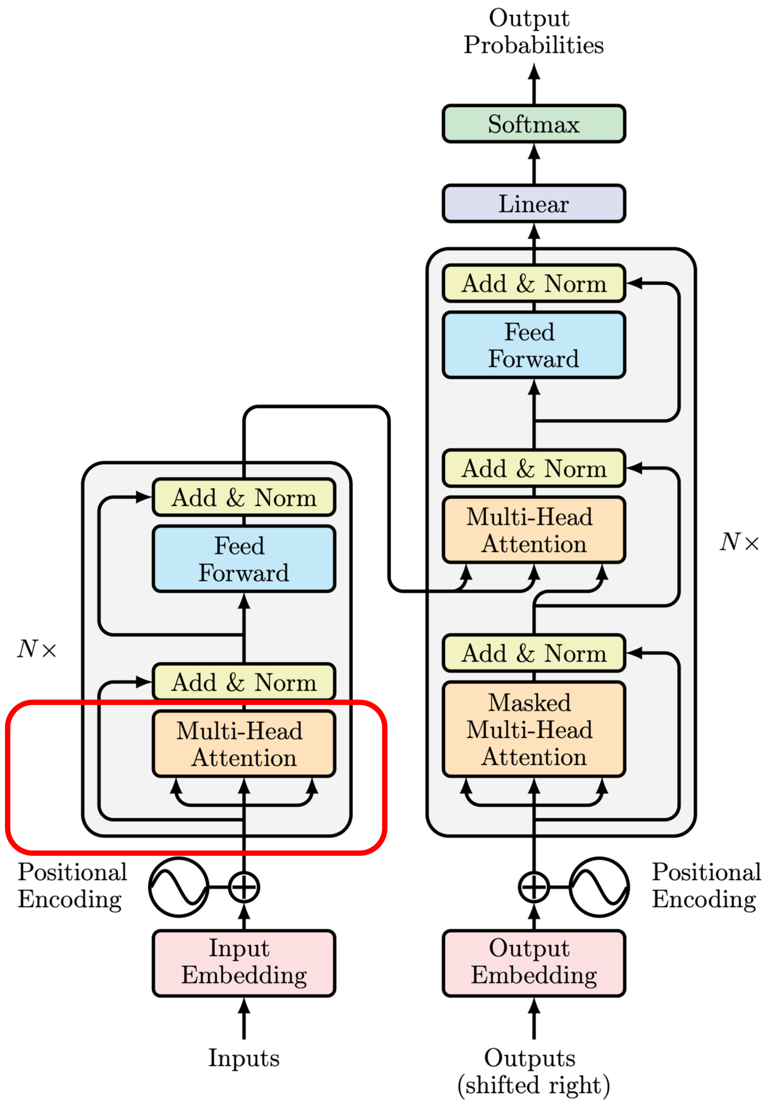

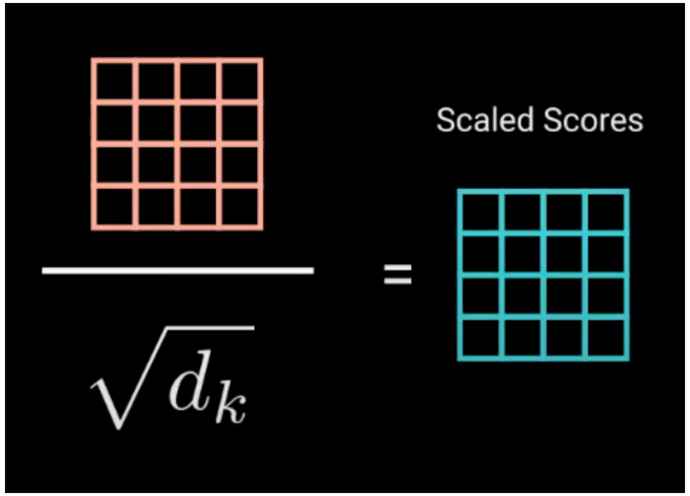

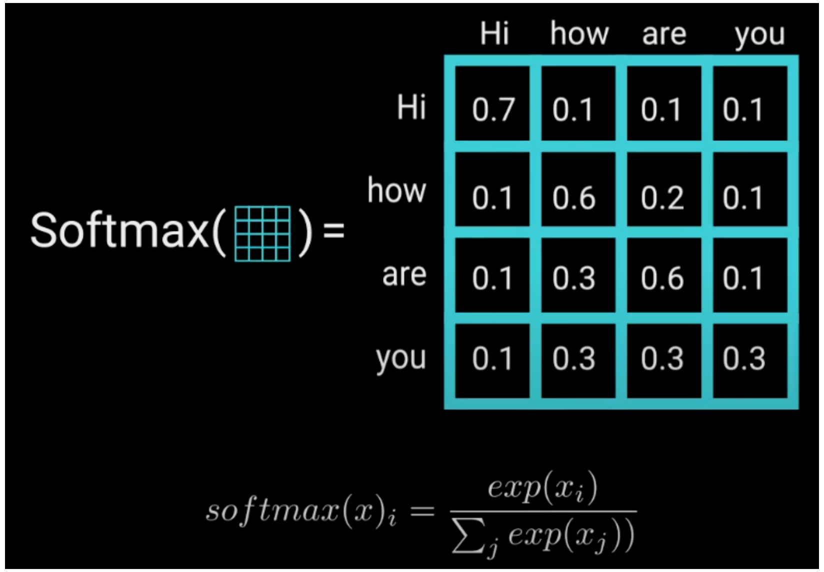

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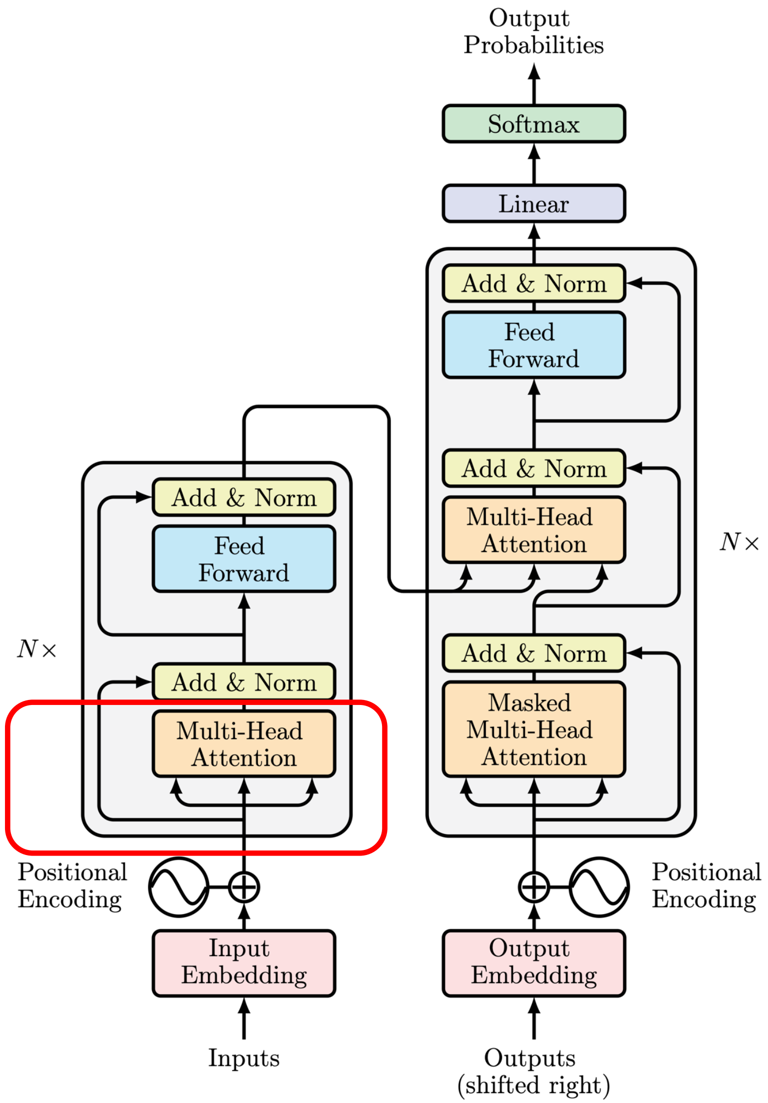
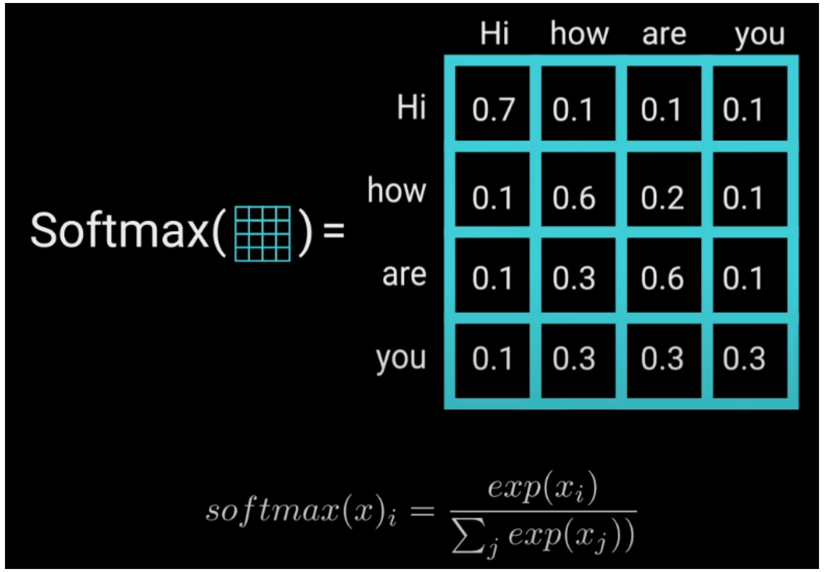


- Attention can be viewed as the weighted adjacency matrix of a fully connected graph!



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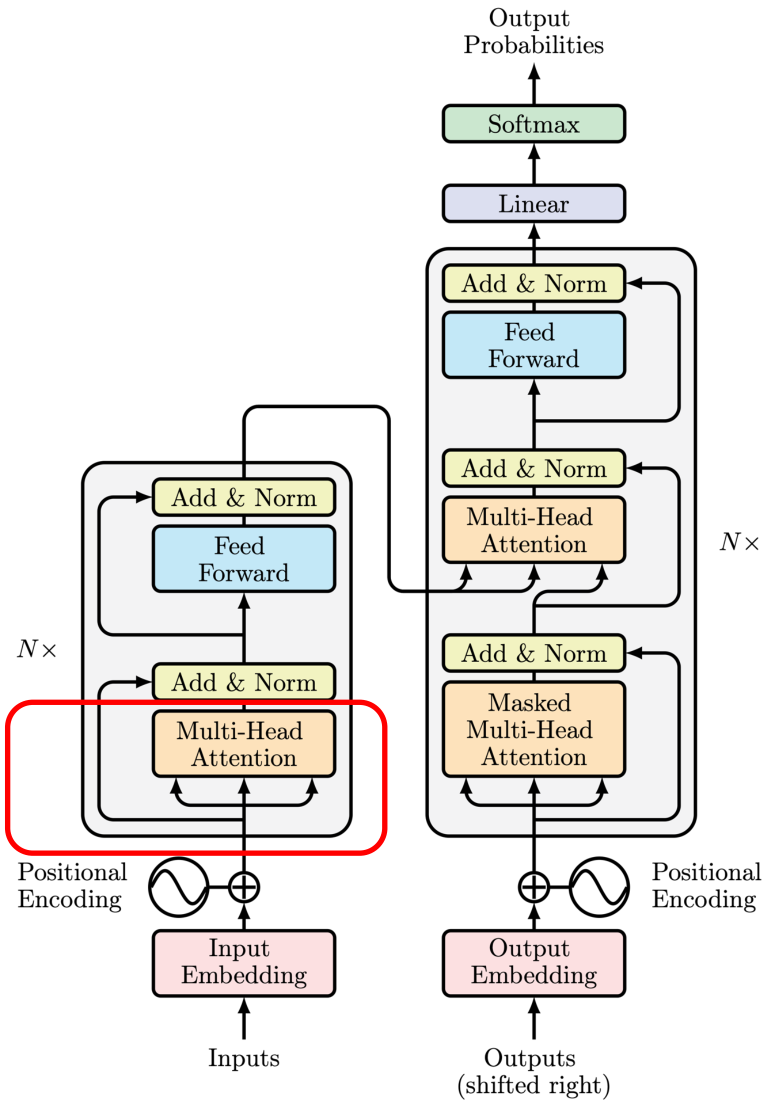
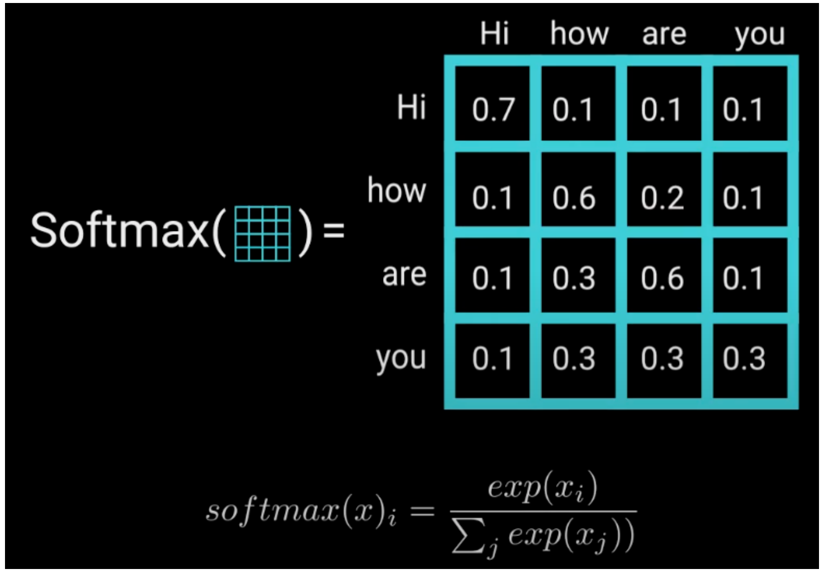


- Attention can be viewed as the weighted adjacency matrix of a fully connected graph!
- Transformers (esp. encoder) can be viewed as GNNs applied to fully connected graphs!



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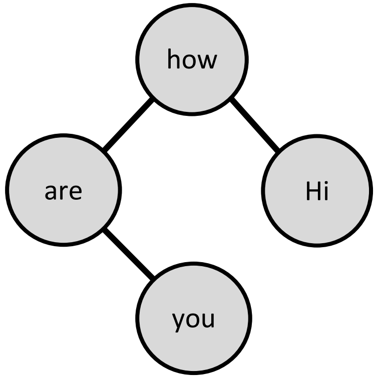
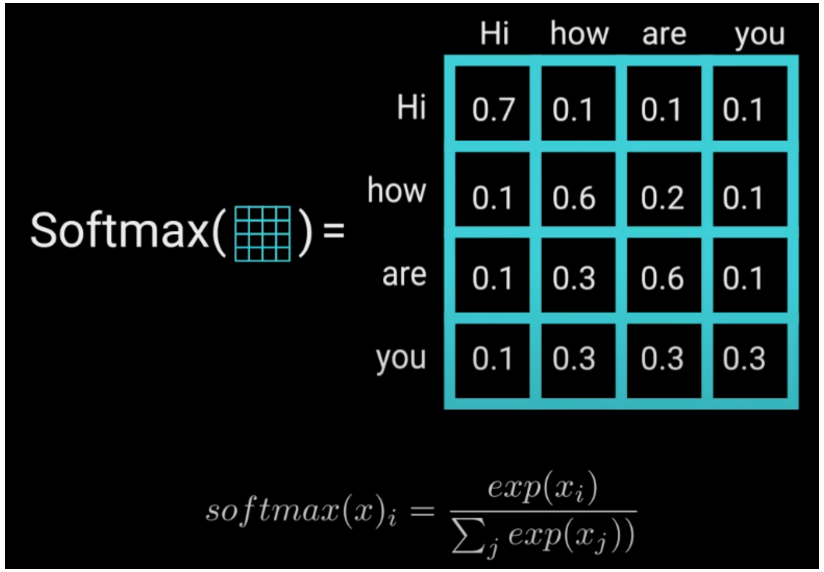
Encode Graph Structures in Transformers

- Apply the adjacency matrix as a mask to the attention and renormalize it, like Graph Attention Networks (GAT) [10]
- Encode connectivities/distances as bias of the attention [11]



	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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References

[1] Scarselli, F., Gori, M., Tsoi, A.C., Hagenbuchner, M. and Monfardini, G., 2008. The graph neural network model. IEEE transactions on neural networks, 20(1), pp.61-80.

[2] Goller, C. and Kuchler, A., 1996, June. Learning task-dependent distributed representations by backpropagation through structure. In Proceedings of International Conference on Neural Networks (ICNN'96) (Vol. 1, pp. 347-352). IEEE.

[3] Ackley, D.H., Hinton, G.E. and Sejnowski, T.J., 1985. A learning algorithm for Boltzmann machines. Cognitive science, 9(1), pp.147-169.

[4] Gilmer, J., Schoenholz, S.S., Riley, P.F., Vinyals, O. and Dahl, G.E., 2017, July. Neural message passing for quantum chemistry. In International conference on machine learning (pp. 1263-1272). PMLR.

[5] Morris, C., Ritzert, M., Fey, M., Hamilton, W.L., Lenssen, J.E., Rattan, G. and Grohe, M., 2019, July. Weisfeiler and leman go neural: Higher-order graph neural networks. In Proceedings of the AAAI Conference on Artificial Intelligence (Vol. 33, No. 01, pp. 4602-4609).

[6] Hamilton, W.L., Ying, R. and Leskovec, J., 2017, December. Inductive representation learning on large graphs. In Proceedings of the 31st International Conference on Neural Information Processing Systems (pp. 1025-1035).

[7] Li, Y., Tarlow, D., Brockschmidt, M. and Zemel, R., 2015. Gated graph sequence neural networks. arXiv preprint arXiv:1511.05493.

[8] 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.

References

[9] Vaswani, A., Shazeer, N., Parmar, N., Uszkoreit, J., Jones, L., Gomez, A.N., Kaiser, Ł. and Polosukhin, I., 2017. Attention is all you need. In Advances in neural information processing systems (pp. 5998-6008).

[10] Veličković, P., Cucurull, G., Casanova, A., Romero, A., Lio, P. and Bengio, Y., 2017. Graph attention networks. arXiv preprint arXiv:1710.10903.

[11] Ying, C., Cai, T., Luo, S., Zheng, S., Ke, G., He, D., Shen, Y. and Liu, T.Y., 2021. Do Transformers Really Perform Bad for Graph Representation?. arXiv preprint arXiv:2106.05234.

Questions?