EECE 571F: Advanced Topics in Deep Learning

Lecture 3: Graph Neural Networks I
Message Passing Models

Renjie Liao

University of British Columbia

Winter, Term 1, 2024

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

Outline

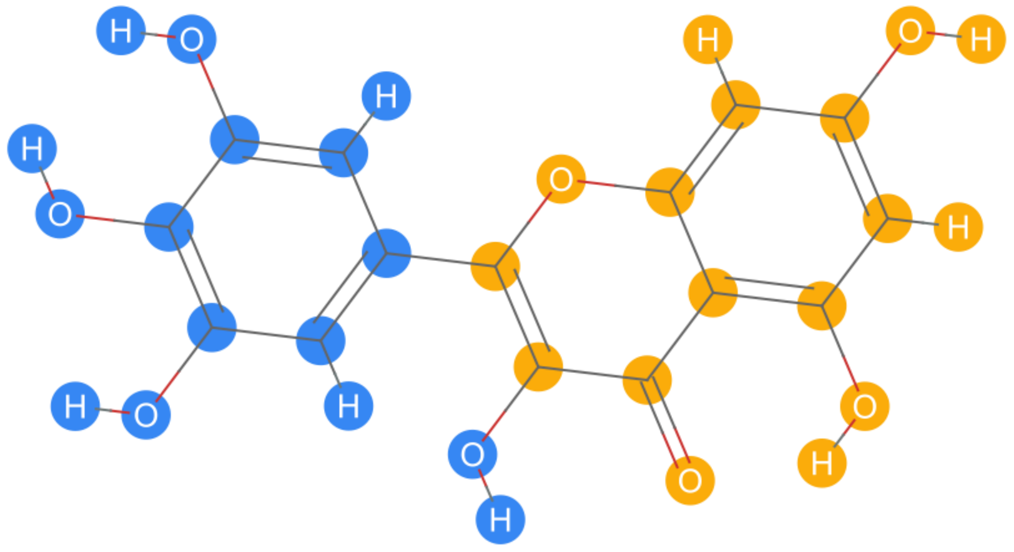
- **Motivating Applications**

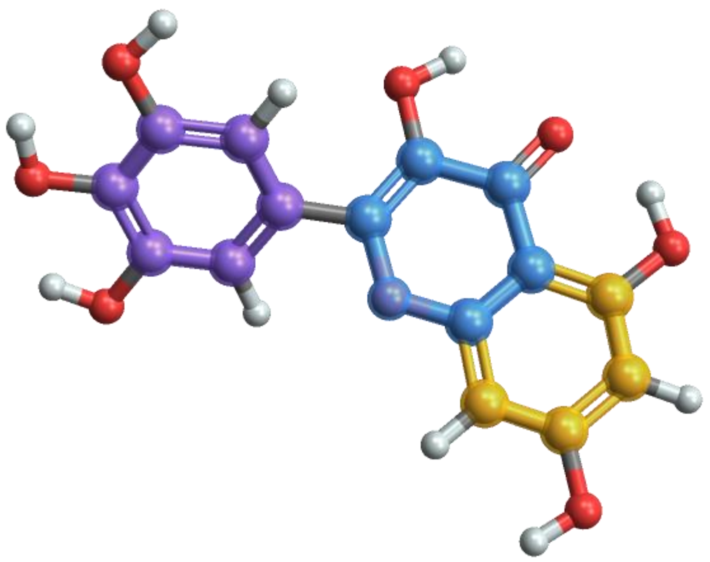
- Graph Neural Networks (GNNs)

    - 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

Motivating Applications of Graphs

- Molecules



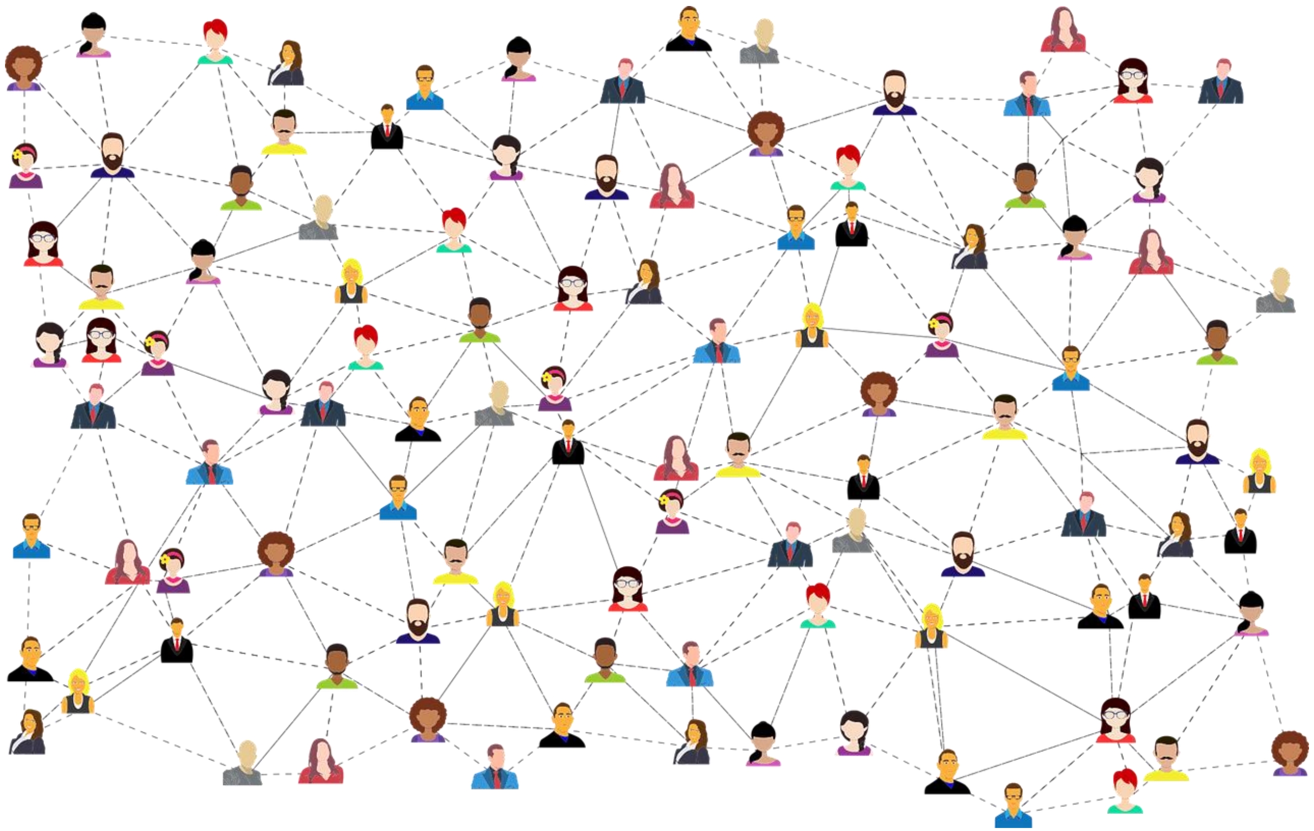


- Multi-edges exist
- Nodes have types
- Edges have types

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

Motivating Applications of Graphs

- Social Networks

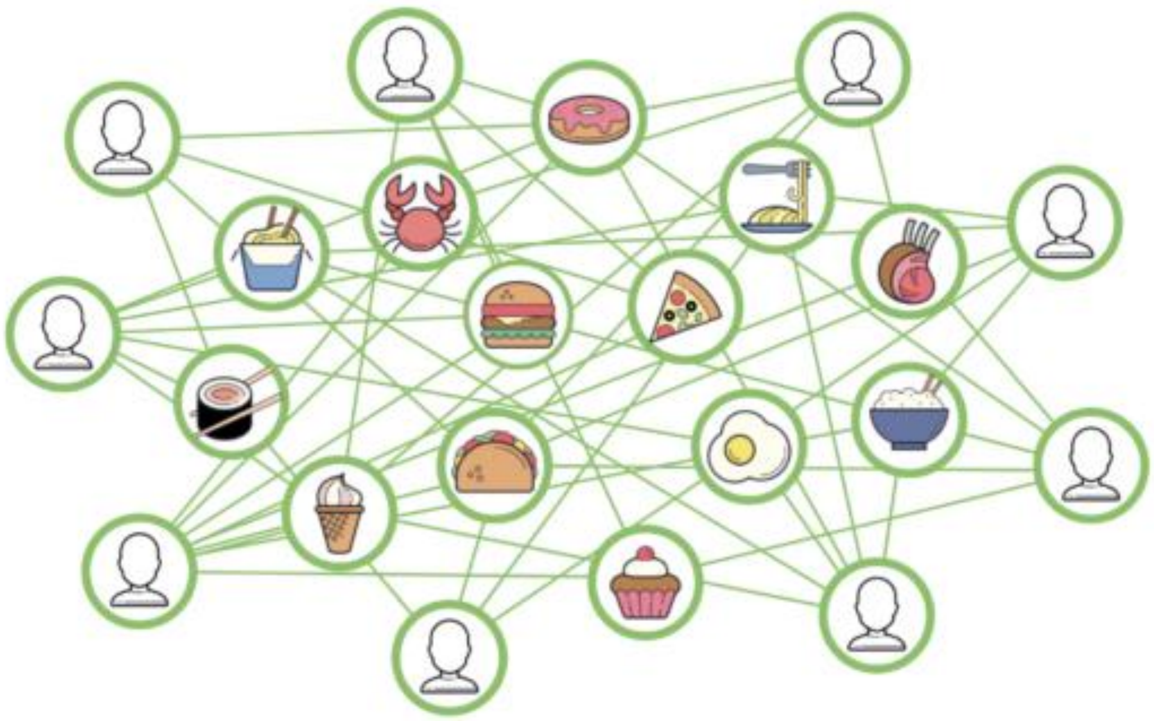


Link Prediction

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

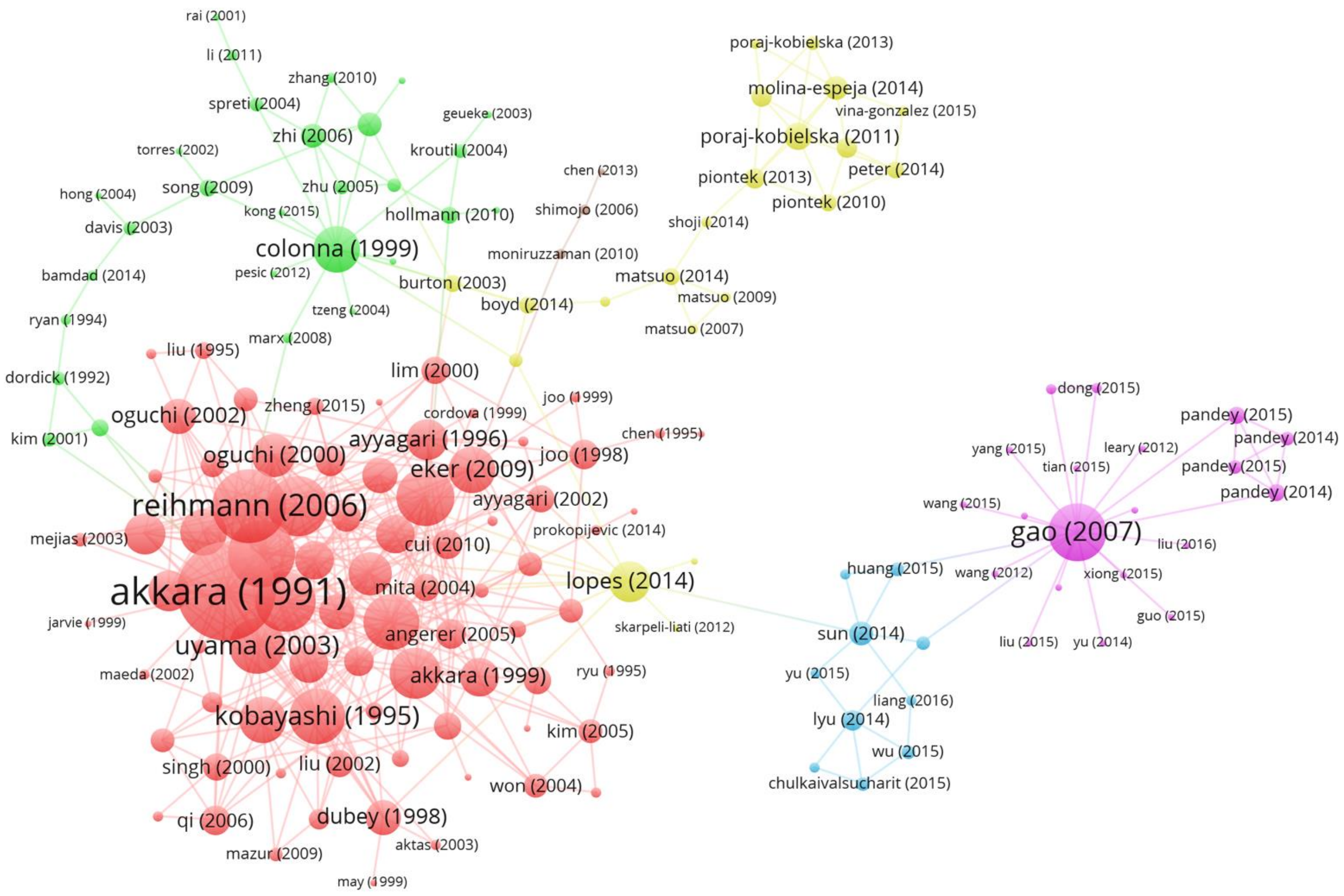
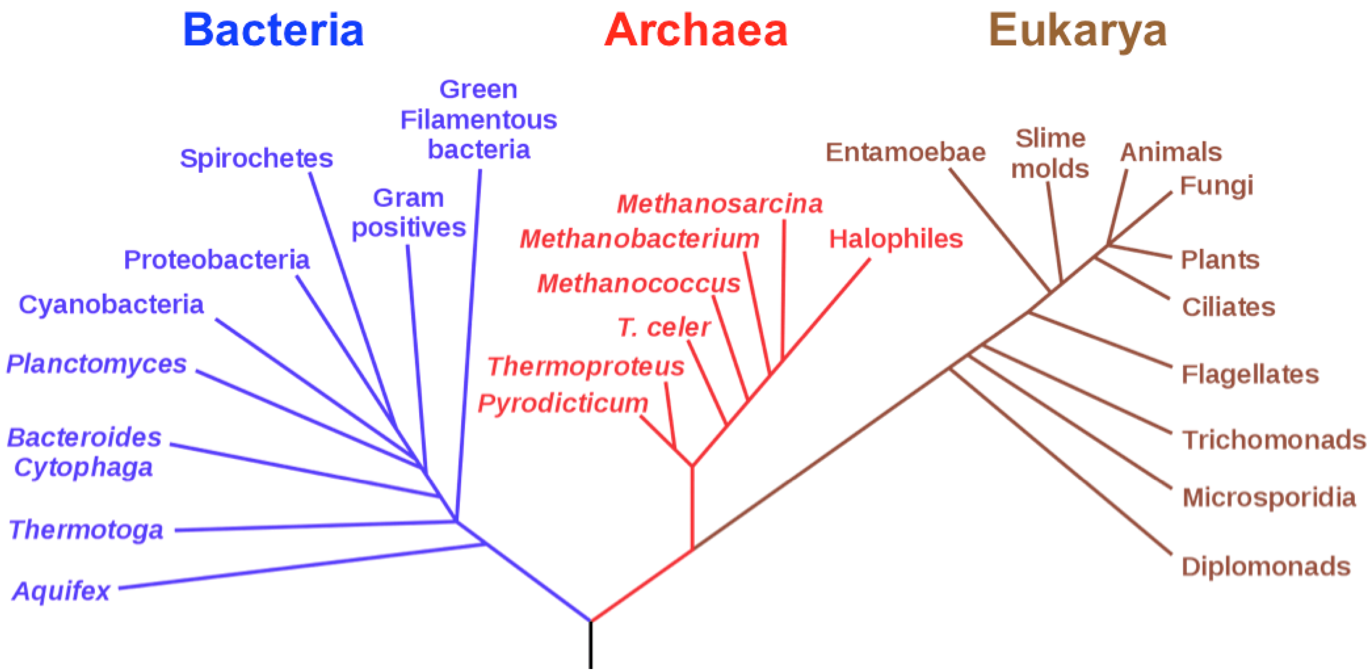


Image Credit: https://www.tudelft.nl/en/library/research-analytics/case-12-citation-networks-2

Motivating Applications of Graphs

- Phylogenetic Tree

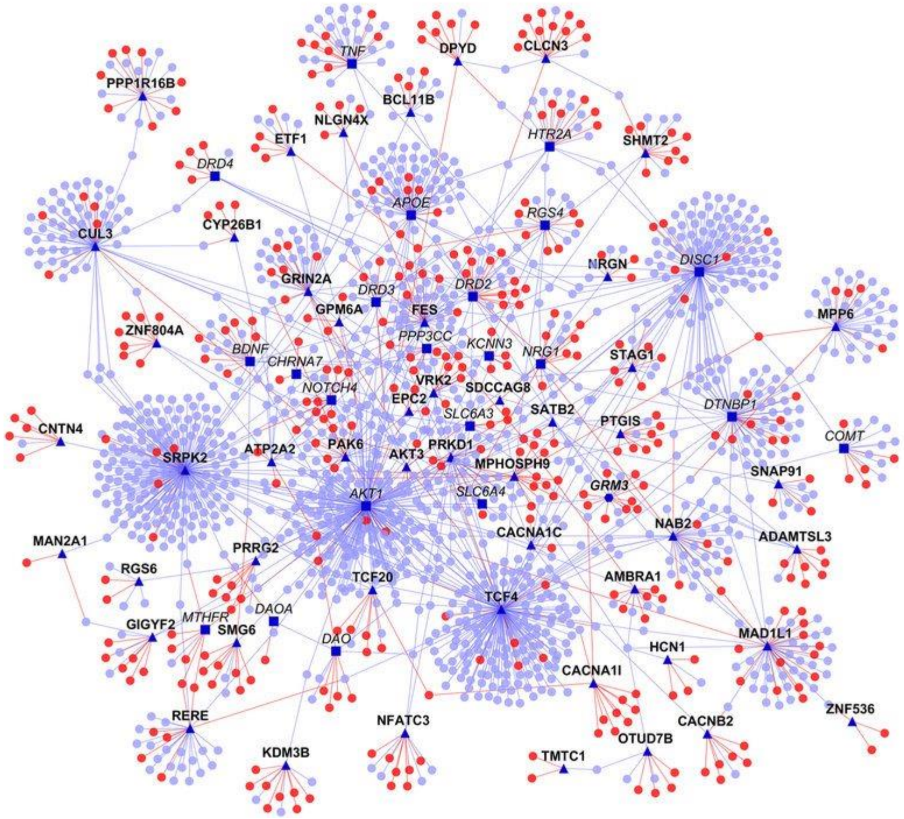


A phylogenetic tree based on rRNA genes showing the three life domains

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

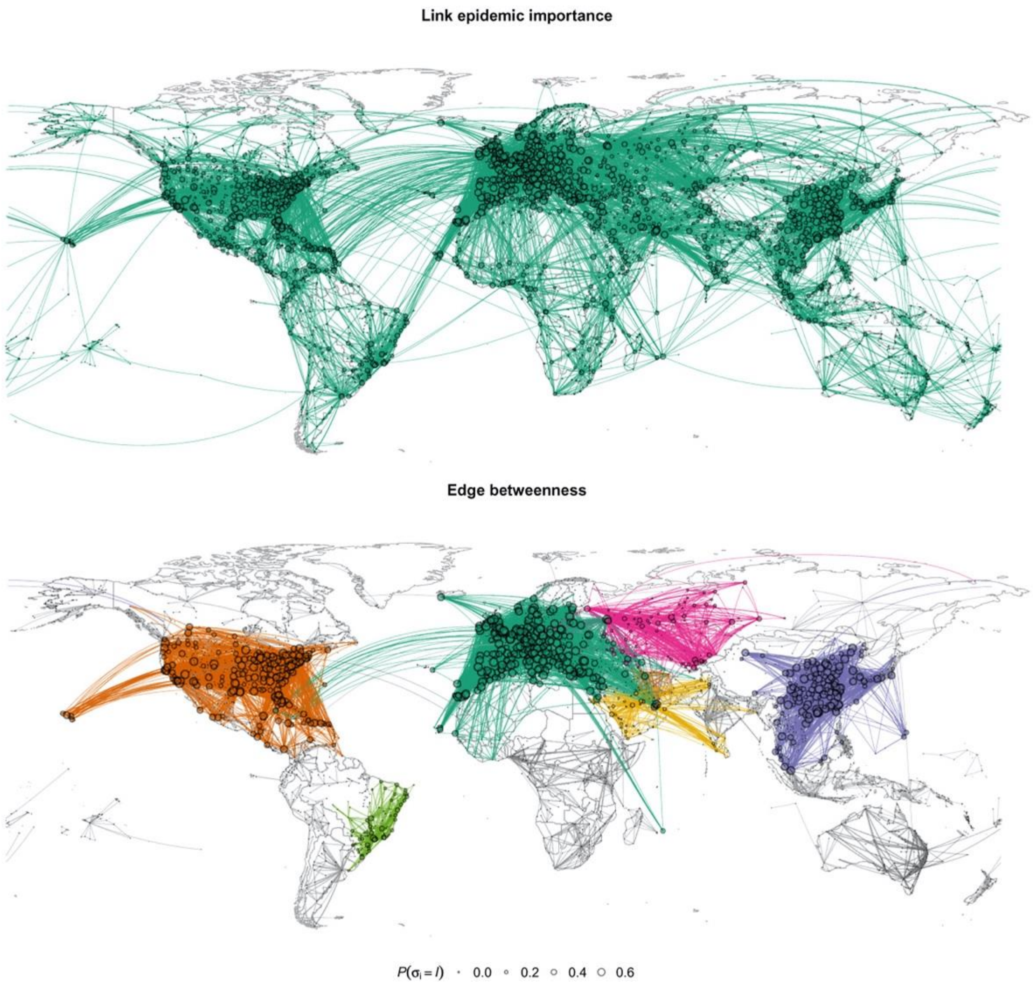


Image Credit: https://www.science.org/doi/10.1126/sciadv.aau4212

Outline

- Motivating Applications

- Graph Neural Networks (GNNs)

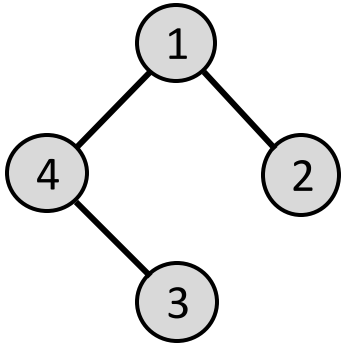
  - **Graph representations**
  - Graph isomorphism & automorphism
  - Challenges of graph data
  - Graph Neural Networks (GNNs): history & basics
  - Message passing framework of GNNs
  - Instantiation of message passing
  - Relationship with Transformers

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)}

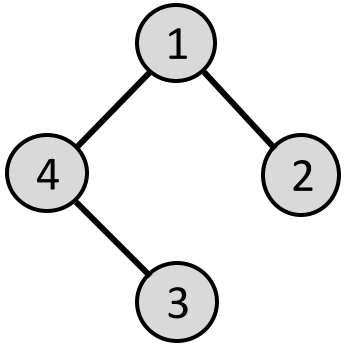
Deep Learning for Graphs

Graph Representations

- Connectivity

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

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



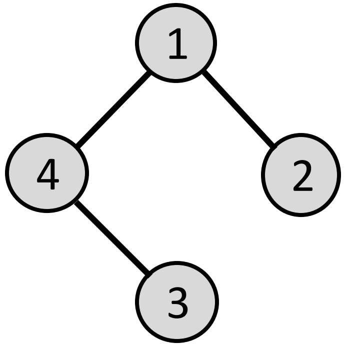
V = {1,2,3,4}, E = {(1,2), (1,4), (4,3)}

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

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



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

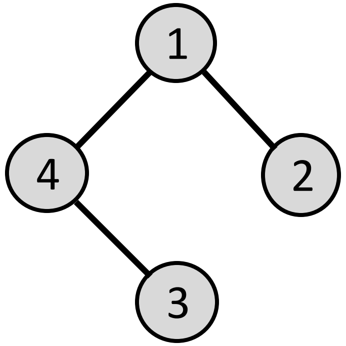
	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

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

Graph Data = (A, X)



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

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

Outline

- Motivating Applications

- Graph Neural Networks (GNNs)

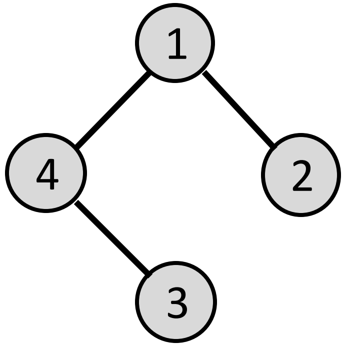
    - Graph representations
    - **Graph isomorphism & automorphism**
    - Challenges of graph data
    - Graph Neural Networks (GNNs): history & basics
    - Message passing framework of GNNs
    - Instantiation of message passing
    - Relationship with Transformers

Deep Learning for Graphs

Permutation

V = [1,2,3,4] => V’ = [2,1,3,4]

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



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

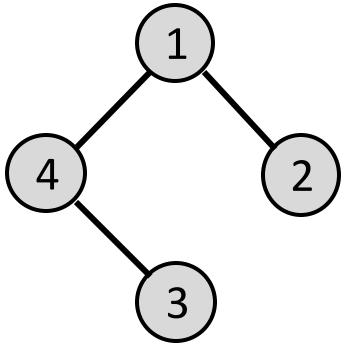
V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

Deep Learning for Graphs

Permutation

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

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



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

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

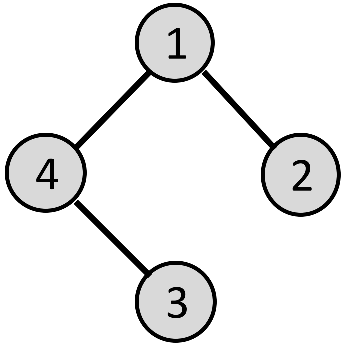
Original Adj Matrix

Deep Learning for Graphs

Permutation

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

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



	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 = [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
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

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

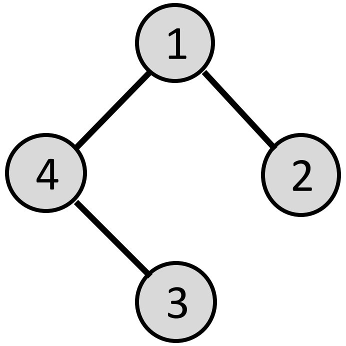
Transposed Permutation Matrix

Deep Learning for Graphs

Permutation

V = [1,2,3,4] => V’ = [2,1,3,4]

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



	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 = [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
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

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

=

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

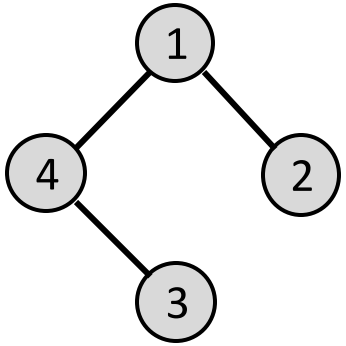
Permuted Adj Matrix

Deep Learning for Graphs

Permutation

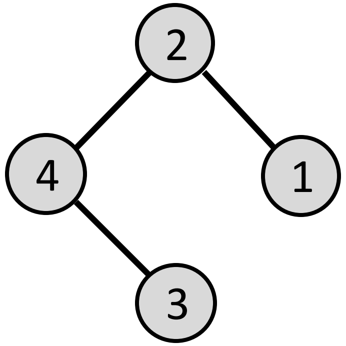
V = [1,2,3,4] => V’ = [2,1,3,4]

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



$$\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 0 & 1 \\ 2 & 1 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 1 & 0 & 1 & 0 \end{array}$$

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



$$\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 0 & 0 \\ 2 & 1 & 0 & 0 & 1 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 0 & 1 & 1 & 0 \end{array}$$

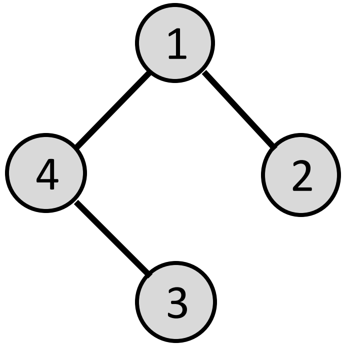
V’ = [2,1,3,4], E’ = [(2,1), (2,4), (4,3)]

Deep Learning for Graphs

Permutation

V = [1,2,3,4] => V’ = [2,1,3,4]

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



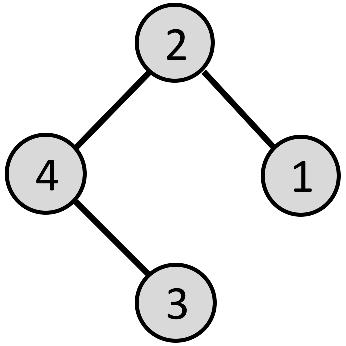
	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

V = [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.*

$$PA_1P^\top = A_2$$



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

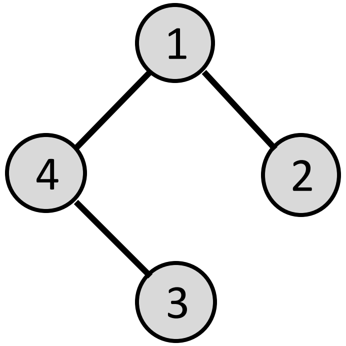
V’ = [2,1,3,4], E’ = [(2,1), (2,4), (4,3)]

Deep Learning for Graphs

Permutation

V = [1,2,3,4] => V’ = [4,3,2,1]

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



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

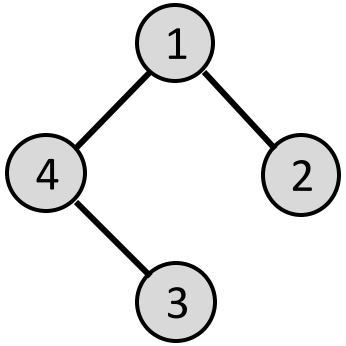
V = [1,2,3,4], E = [(1,2), (1,4), (4,3)]

Deep Learning for 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)]



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

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

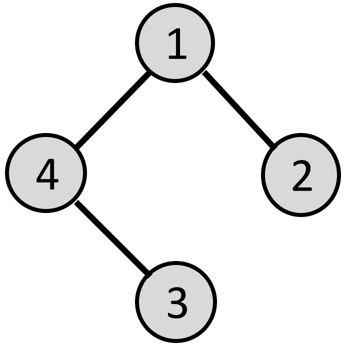
Original Adj Matrix

Deep Learning for 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)]



	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 = [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
4	1	0	1	0

Original Adj Matrix

Permute Columns

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

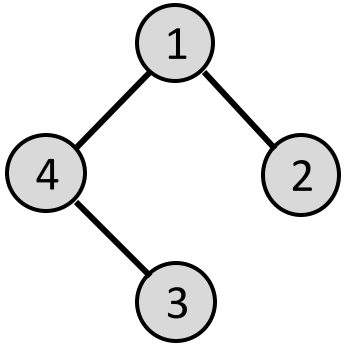
Transposed Permutation Matrix

Deep Learning for 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)]



$$\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 0 & 1 \\ 2 & 1 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 1 & 0 & 1 & 0 \end{array}$$

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

Permute Rows

Permute Columns

$$\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 0 & 0 & 1 \\ 2 & 0 & 0 & 1 & 0 \\ 3 & 0 & 1 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 \end{array} \quad \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 0 & 1 \\ 2 & 1 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 1 & 0 & 1 & 0 \end{array} \quad \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 0 & 0 & 1 \\ 2 & 0 & 0 & 1 & 0 \\ 3 & 0 & 1 & 0 & 0 \\ 4 & 1 & 0 & 0 & 0 \end{array} = \begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & 0 & 1 & 0 & 1 \\ 2 & 1 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 1 \\ 4 & 1 & 0 & 1 & 0 \end{array}$$

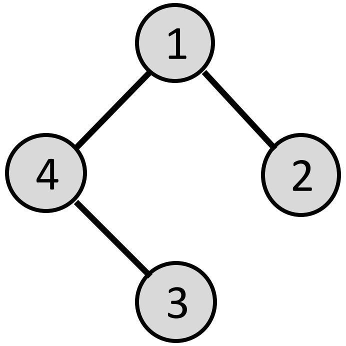
Permutation Matrix | Original Adj Matrix | Transposed Permutation Matrix | Permuted Adj Matrix

Deep Learning for Graphs

Permutation

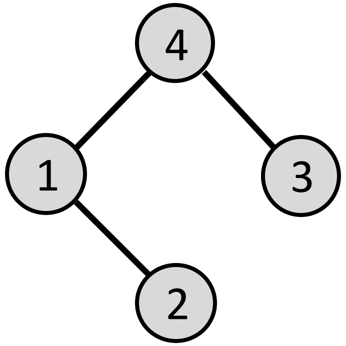
V = [1,2,3,4] => V’ = [4,3,2,1]

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



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



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

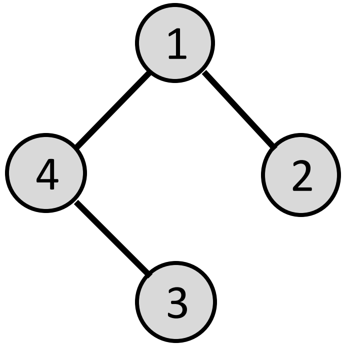
V’ = [4,3,2,1], E’ = [(4,3), (4,1), (1,2)]

Deep Learning for Graphs

Permutation

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

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



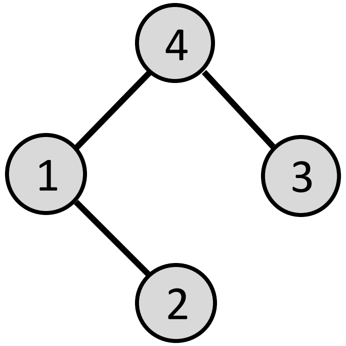
	1	2	3	4
1	0	1	0	1
2	1	0	0	0
3	0	0	0	1
4	1	0	1	0

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

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

Outline

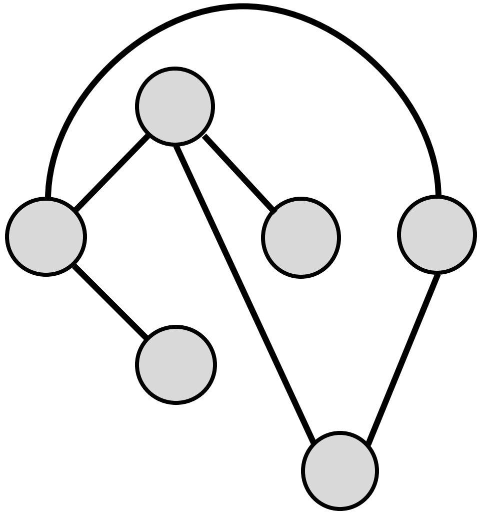
- Motivating Applications

- 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

Deep Learning for Graphs

Key Challenges:

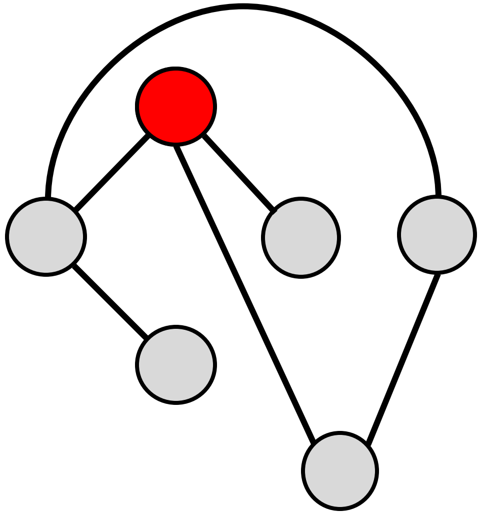
- **Unordered Neighbors**



Deep Learning for Graphs

Key Challenges:

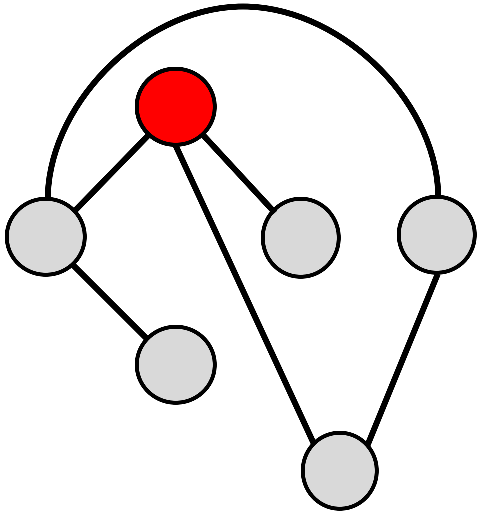
- **Unordered Neighbors**

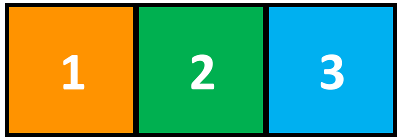


Deep Learning for Graphs

Key Challenges:

- **Unordered Neighbors**

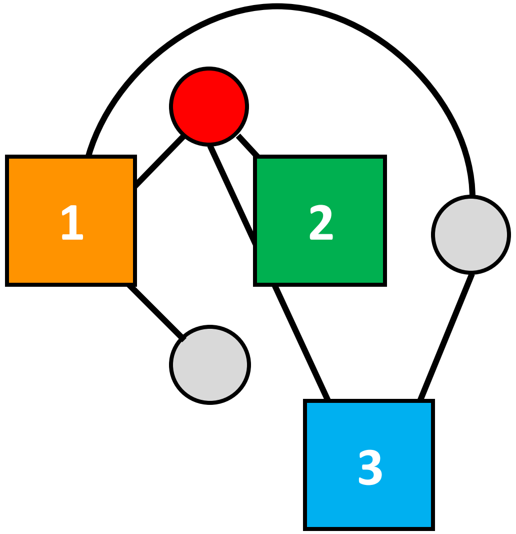




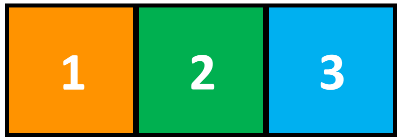
Deep Learning for Graphs

Key Challenges:

- **Unordered Neighbors**



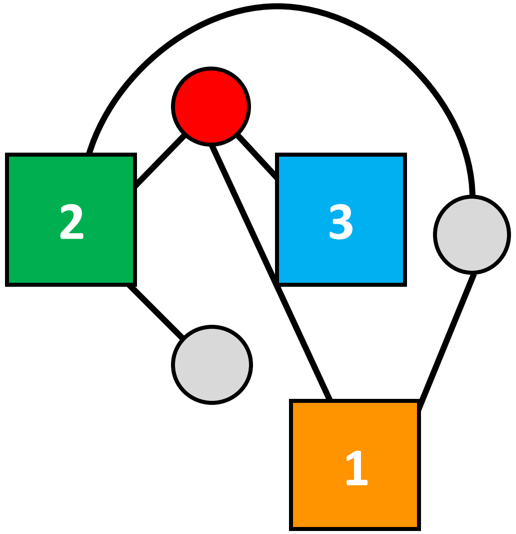
Option 1



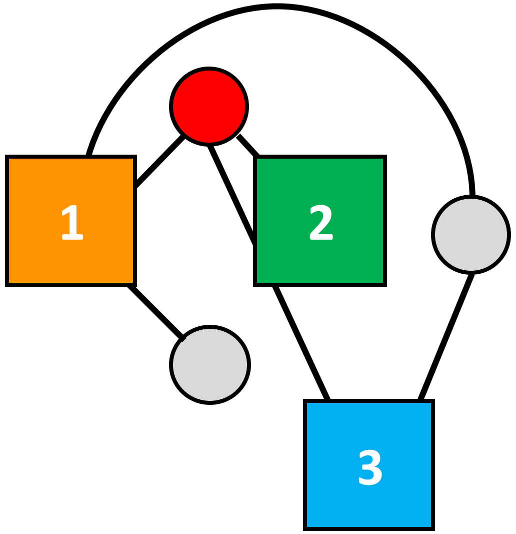
Deep Learning for Graphs

Key Challenges:

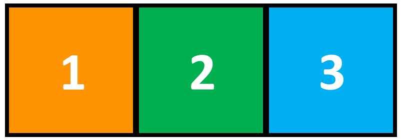
- **Unordered Neighbors**



Option 2



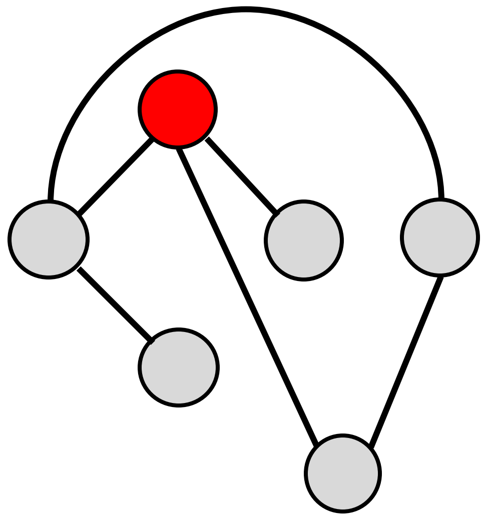
Option 1



Deep Learning for Graphs

Key Challenges:

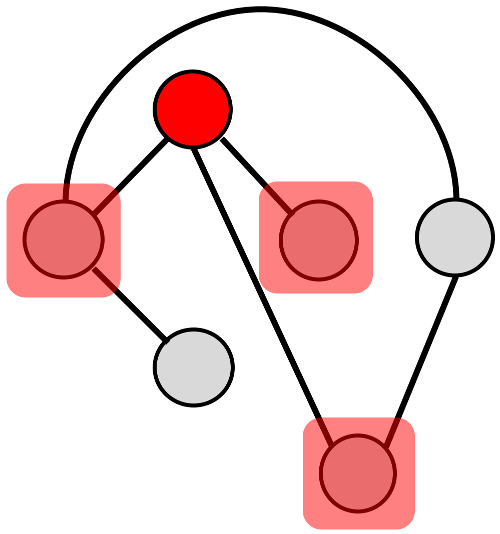
- Unordered Neighbors
- **Varying Neighborhood Sizes**



Deep Learning for Graphs

Key Challenges:

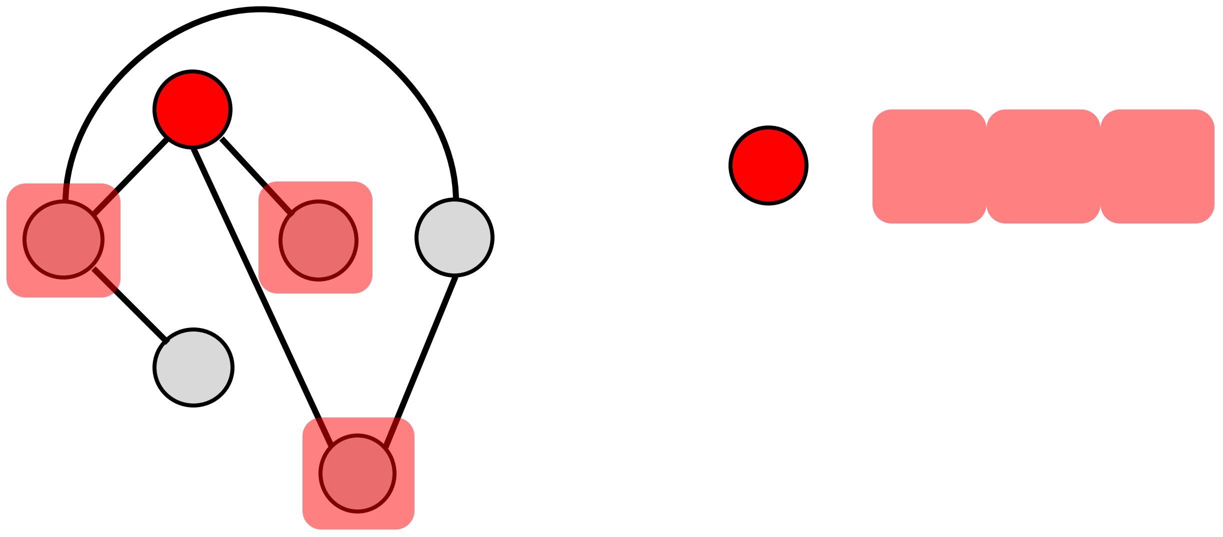
- Unordered Neighbors
- **Varying Neighborhood Sizes**



Deep Learning for Graphs

Key Challenges:

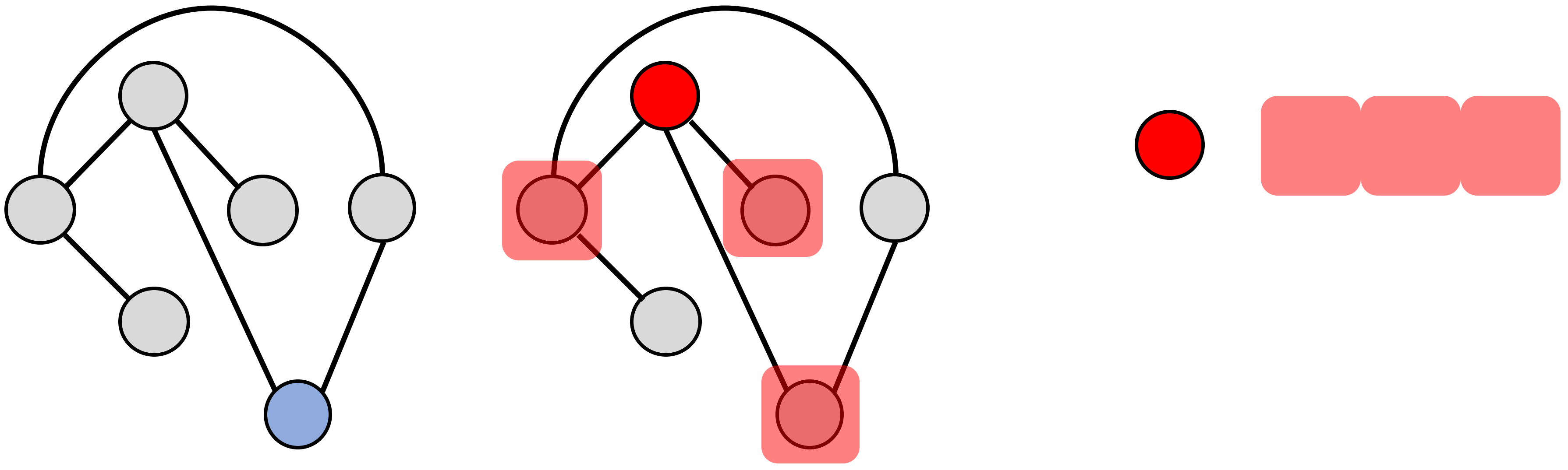
- Unordered Neighbors
- **Varying Neighborhood Sizes**



Deep Learning for Graphs

Key Challenges:

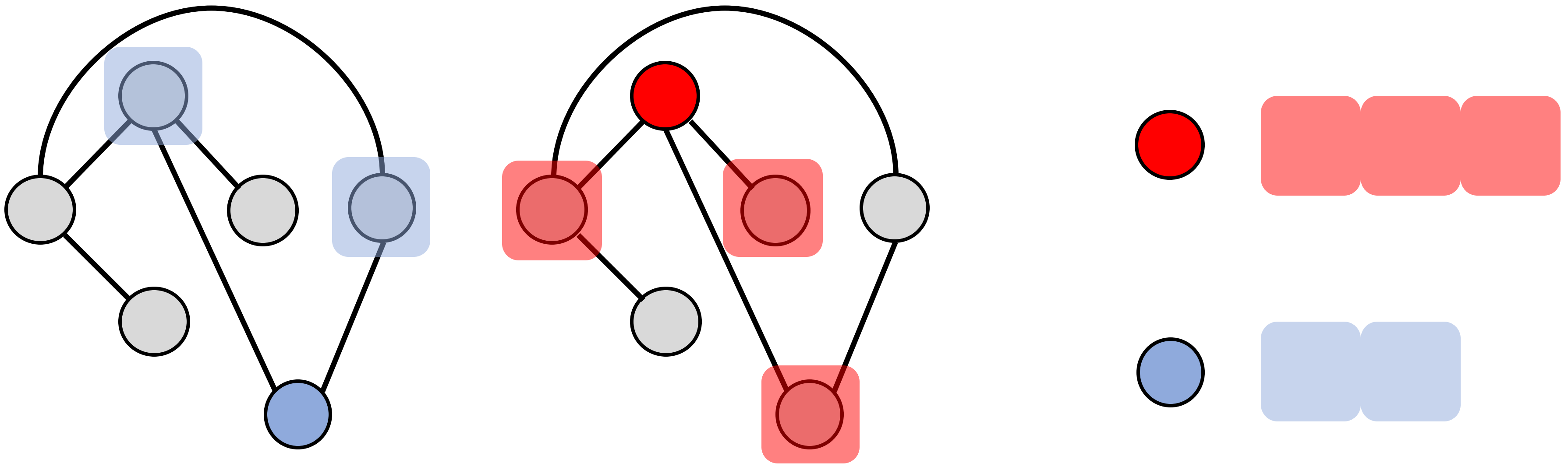
- Unordered Neighbors
- **Varying Neighborhood Sizes**



Deep Learning for Graphs

Key Challenges:

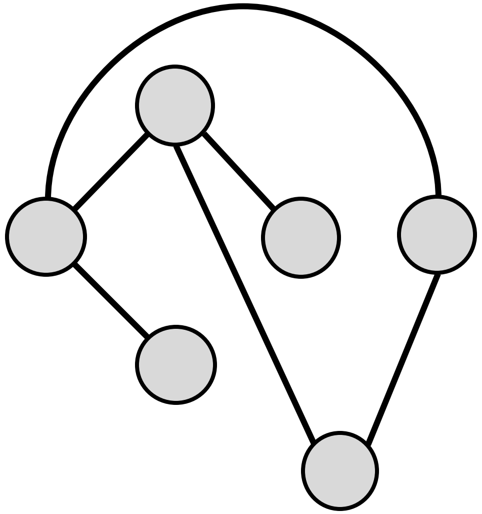
- Unordered Neighbors
- **Varying Neighborhood Sizes**



Deep Learning for Graphs

Key Challenges:

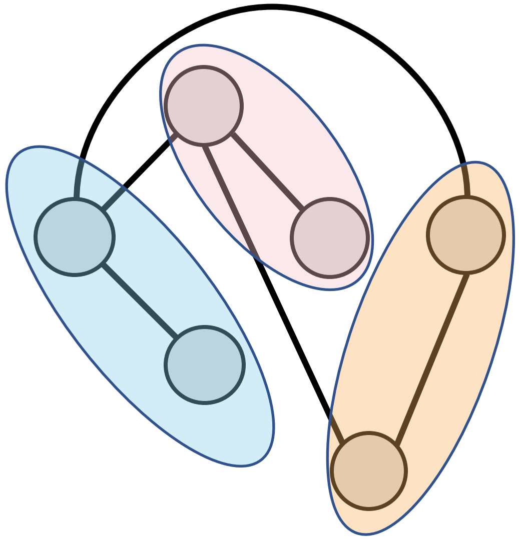
- Unordered Neighbors
- Varying Neighborhood Sizes
- **Varying Graph Partitions**



Deep Learning for Graphs

Key Challenges:

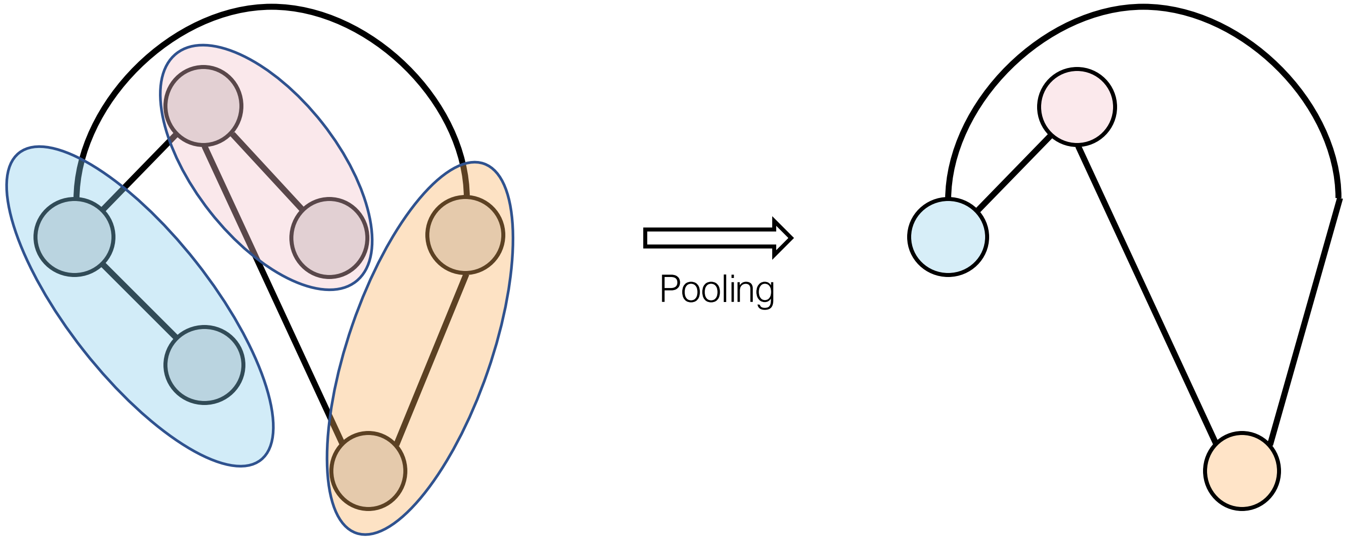
- Unordered Neighbors
- Varying Neighborhood Sizes
- **Varying Graph Partitions**



Deep Learning for Graphs

Key Challenges:

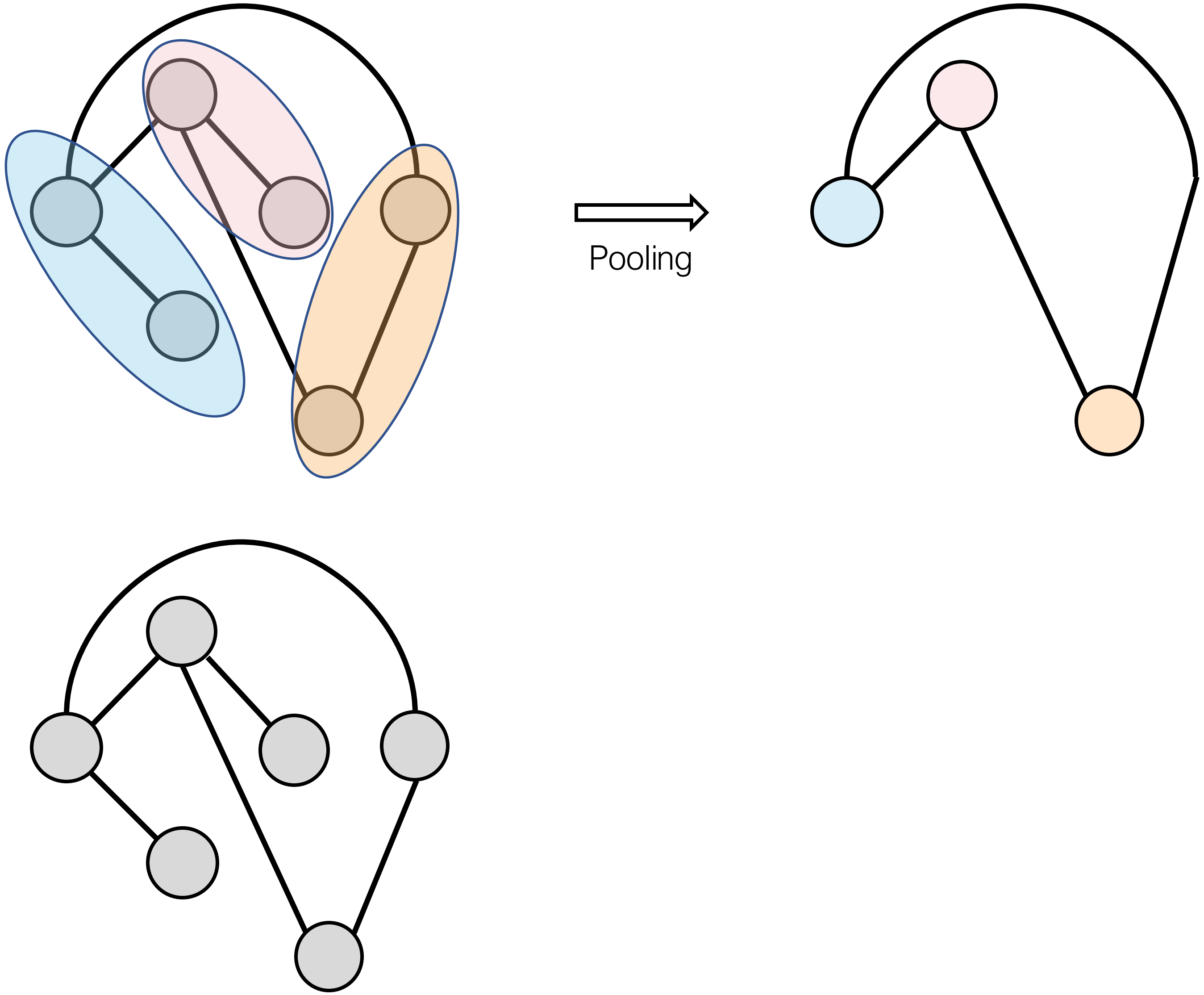
- Unordered Neighbors
- Varying Neighborhood Sizes
- **Varying Graph Partitions**



Deep Learning for Graphs

Key Challenges:

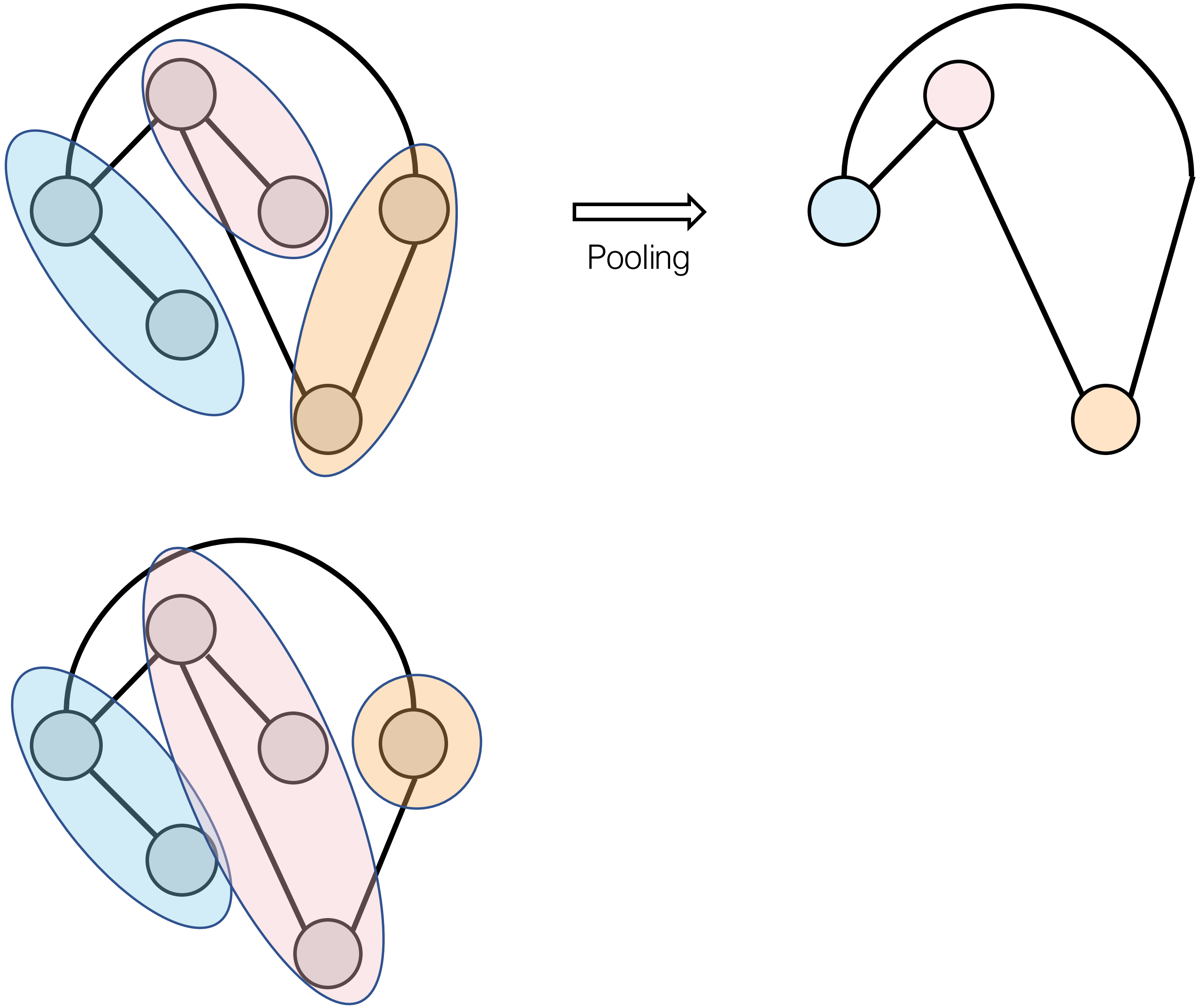
- Unordered Neighbors
- Varying Neighborhood Sizes
- **Varying Graph Partitions**



Deep Learning for Graphs

Key Challenges:

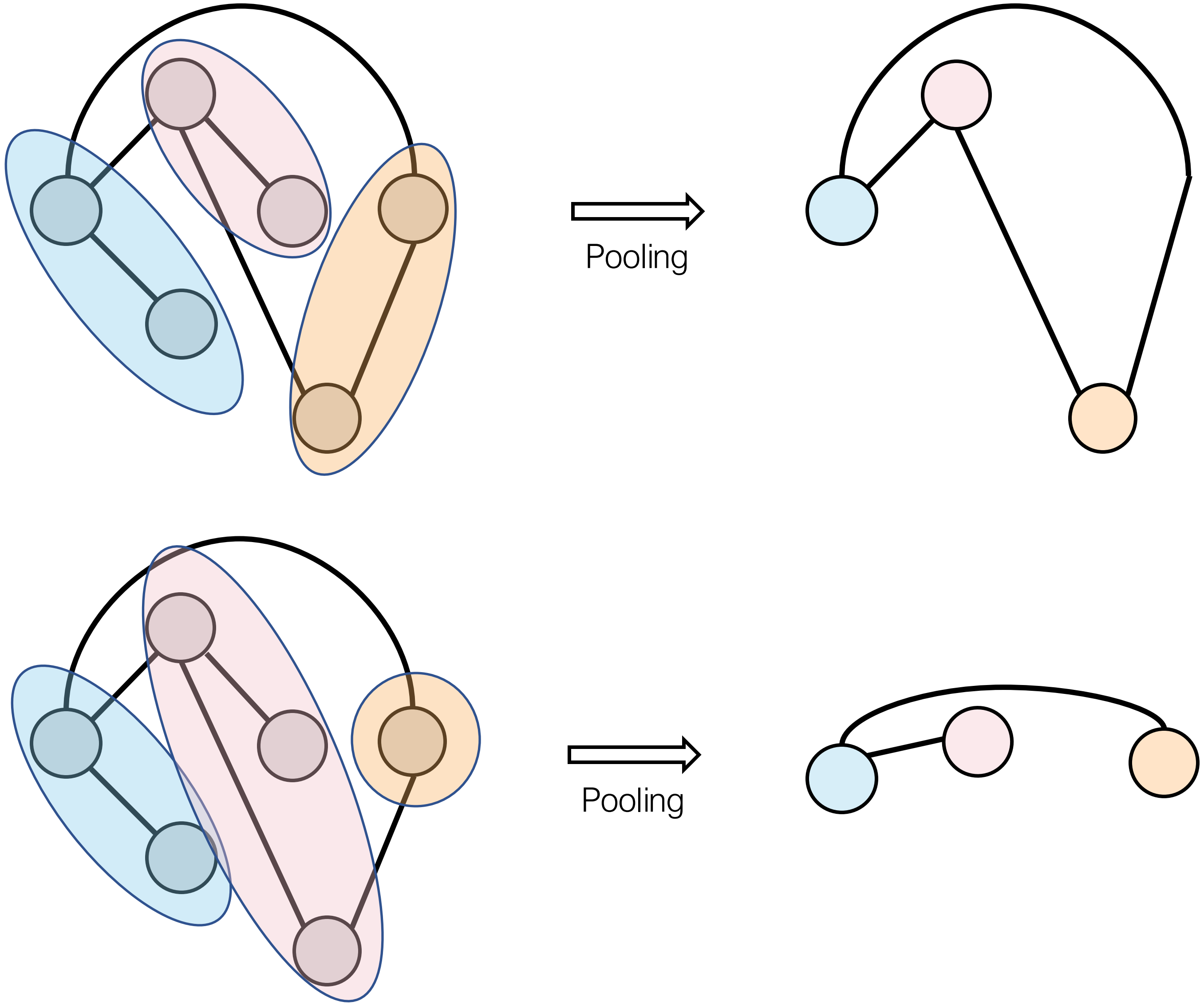
- Unordered Neighbors
- Varying Neighborhood Sizes
- **Varying Graph Partitions**



Deep Learning for Graphs

Key Challenges:

- Unordered Neighbors
- Varying Neighborhood Sizes
- **Varying Graph Partitions**



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

Deep Learning for Graphs

Graph Neural Networks (GNNs)

- Neural networks that can process general graph structured data

Deep Learning for Graphs

Graph Neural Networks (GNNs)

- Neural networks that can process general graph structured data
- First proposed in 2008 [1] and dates back to Recursive Neural Networks (mainly processing trees) in 90s [2]
- In fact, Boltzmann Machines [3] (fully connected graphs with binary units) in 80s can be viewed as GNNs

[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.

Deep Learning for Graphs

Graph Neural Networks (GNNs)

- Neural networks that can process general graph structured data
- First proposed in 2008 [1] and dates back to Recursive Neural Networks (mainly processing trees) in 90s [2]
- In fact, Boltzmann Machines [3] (fully connected graphs with binary units) in 80s can be viewed as GNNs
- Most of GNNs (if not all) can be incorporated by the **Message Passing** paradigm

[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.

Deep Learning for Graphs

Graph Neural Networks (GNNs)

- Neural networks that can process general graph structured data
- First proposed in 2008 [1] and dates back to Recursive Neural Networks (mainly processing trees) in 90s [2]
- In fact, Boltzmann Machines [3] (fully connected graphs with binary units) in 80s can be viewed as GNNs
- Most of GNNs (if not all) can be incorporated by the **Message Passing** paradigm
- GNNs have been independently studied in signal processing community under **Graph Signal Processing**

[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.

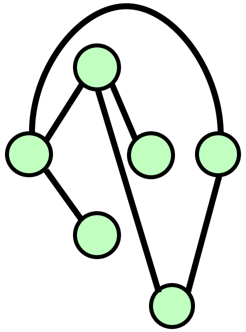
Deep Learning for Graphs

Graph Neural Networks (GNNs)

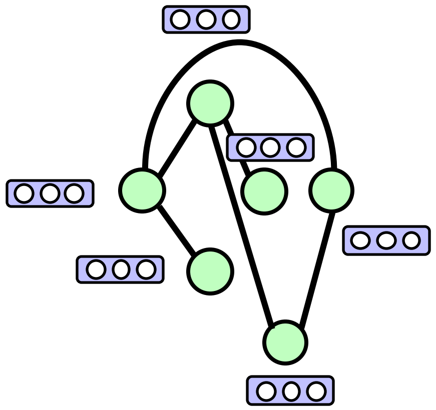
- Neural networks that can process general graph structured data
- First proposed in 2008 [1] and dates back to Recursive Neural Networks (mainly processing trees) in 90s [2]
- In fact, Boltzmann Machines [3] (fully connected graphs with binary units) in 80s can be viewed as GNNs
- Most of GNNs (if not all) can be incorporated by the **Message Passing** paradigm
- GNNs have been independently studied in signal processing community under **Graph Signal Processing**
- The study of GNNs for geometric processing are also called **Geometric Deep Learning**

[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.

Graph Neural Networks (GNNs)

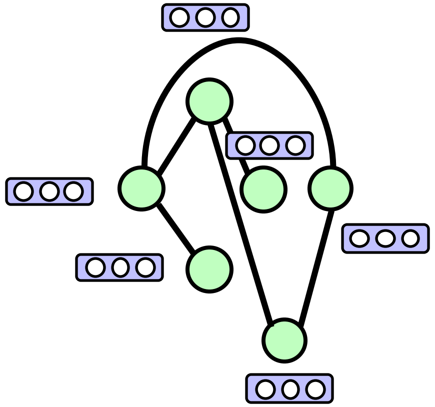


Graph Neural Networks (GNNs)



Input Encoding

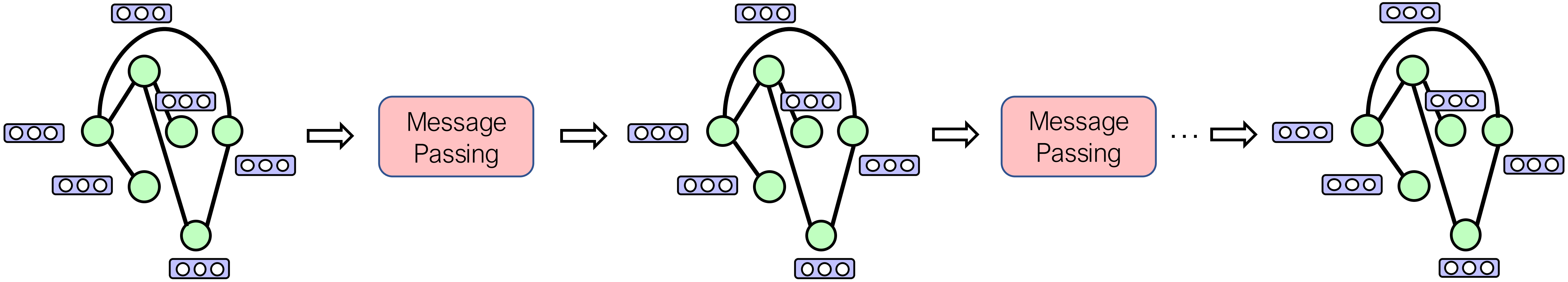
Graph Neural Networks (GNNs)



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*

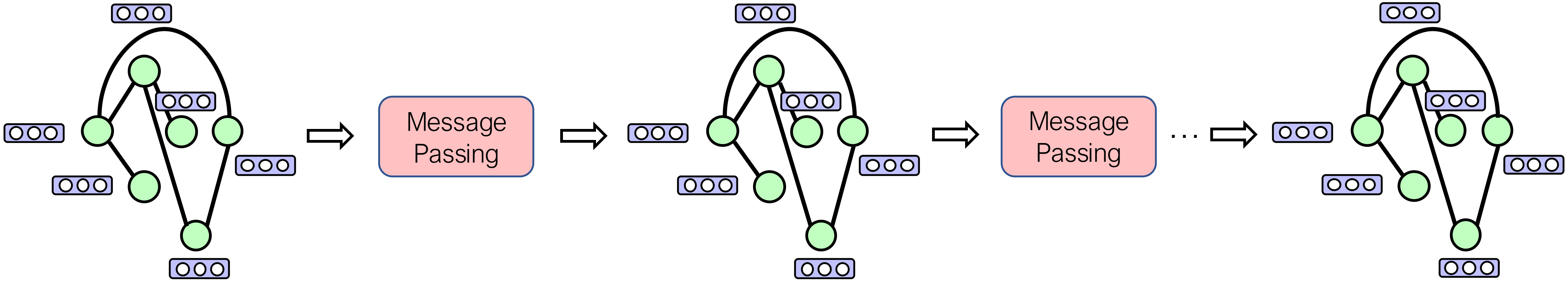
Graph Neural Networks (GNNs)



Input Encoding

Message Passing Layers/Steps

Graph Neural Networks (GNNs)

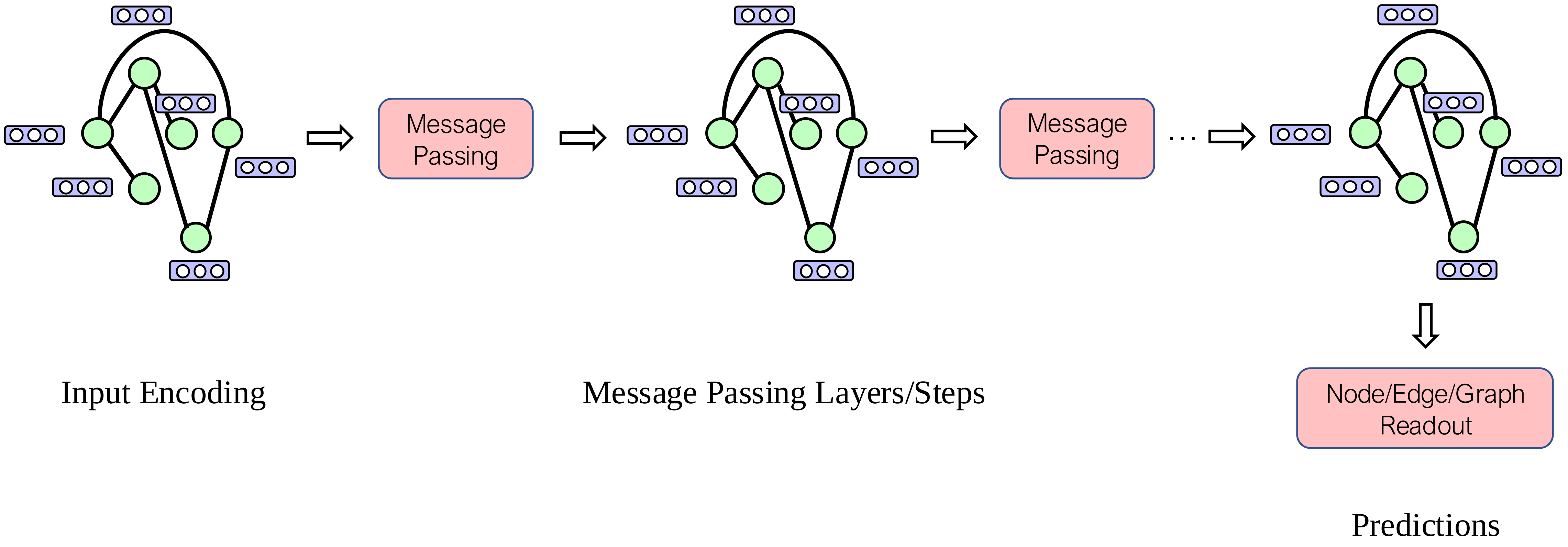


Input Encoding

Message Passing Layers/Steps

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

Graph Neural Networks (GNNs)



Outline

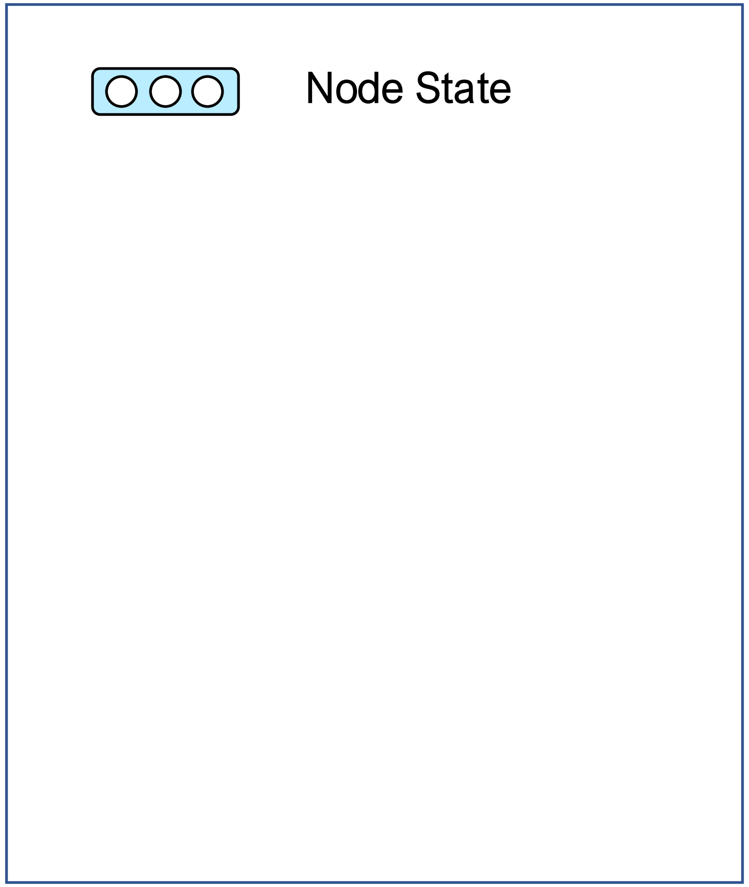
- Motivating Applications

- Graph Neural Networks (GNNs)

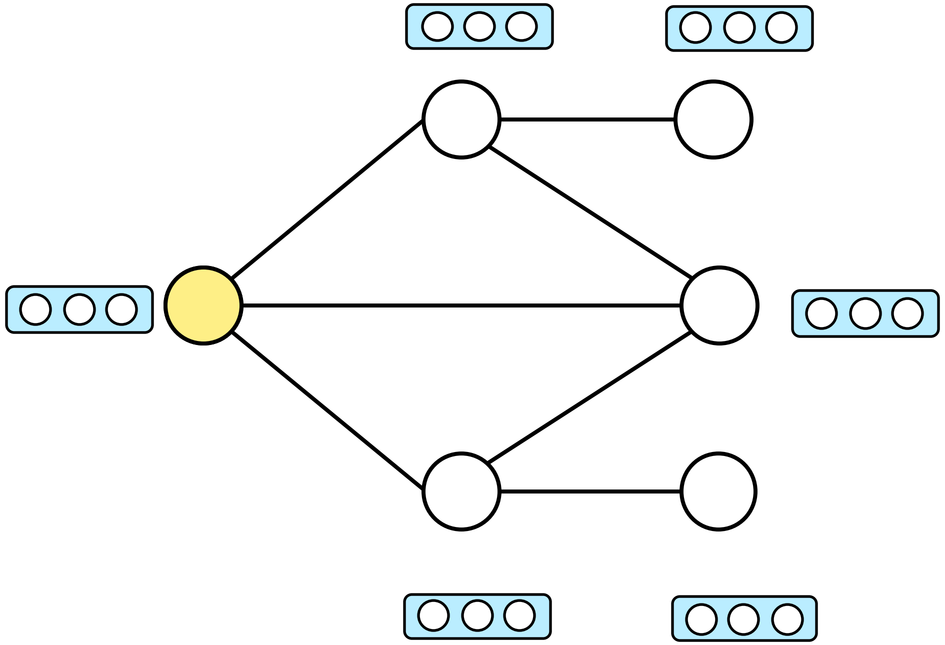
    - Graph representations
    - Graph isomorphism & automorphism
    - Challenges of graph data
    - Graph Neural Networks (GNNs): history & basics
    - **Message passing framework of GNNs**
    - Instantiation of message passing
    - Relationship with Transformers

Message Passing in GNNs

$\mathbf{h}_i^t$

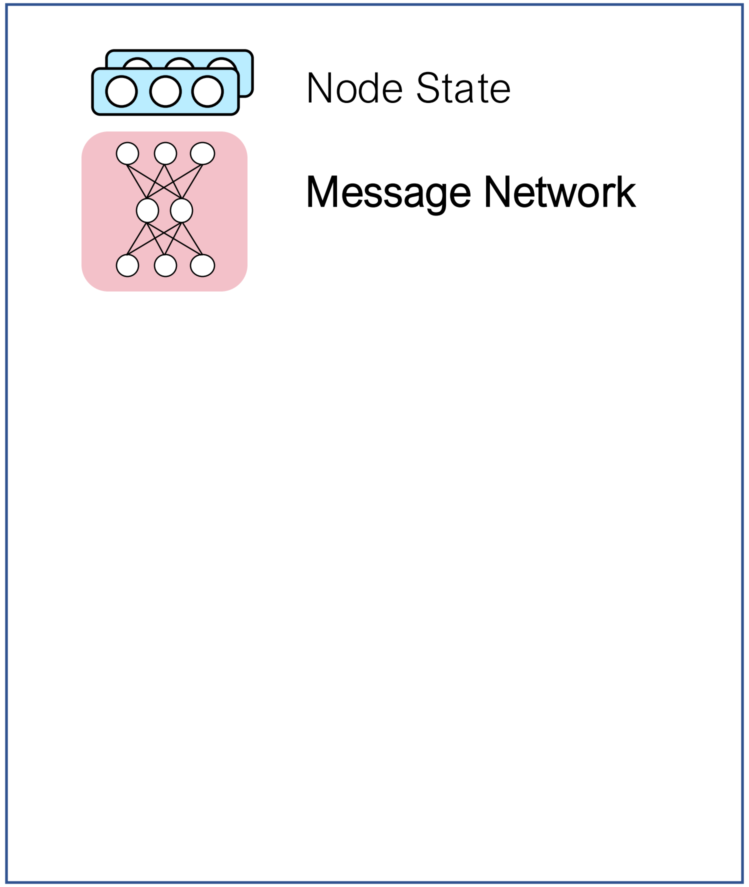


(t+1)-th message passing step/layer

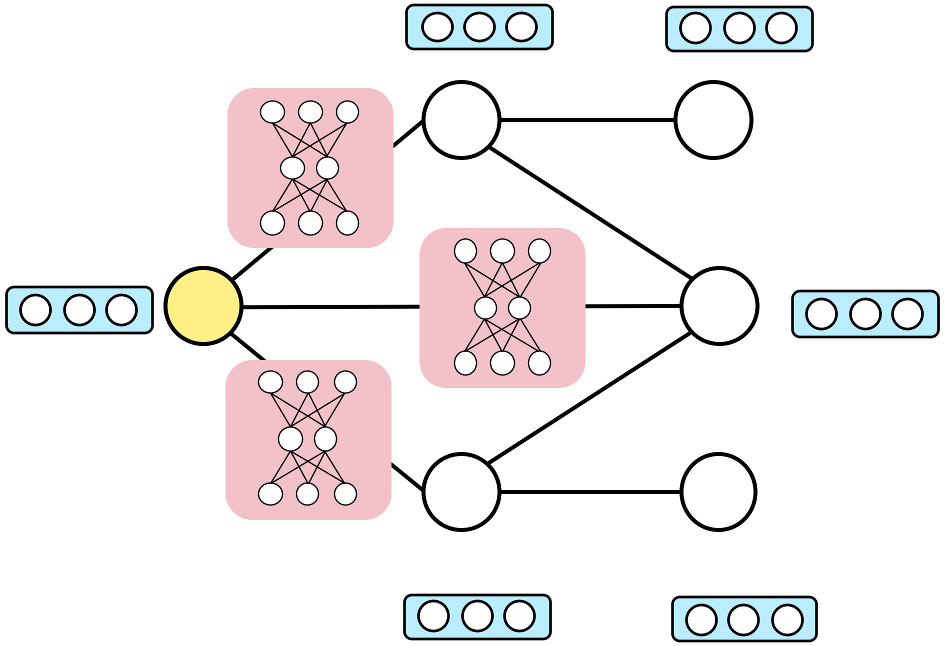


Message Passing in GNNs

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



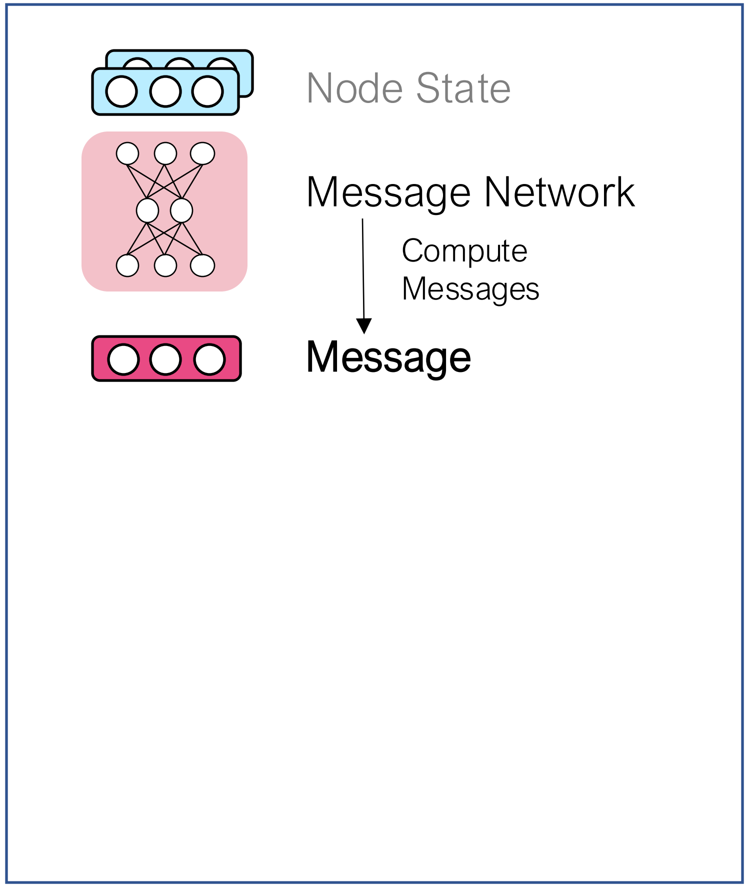
(t+1)-th message passing step/layer



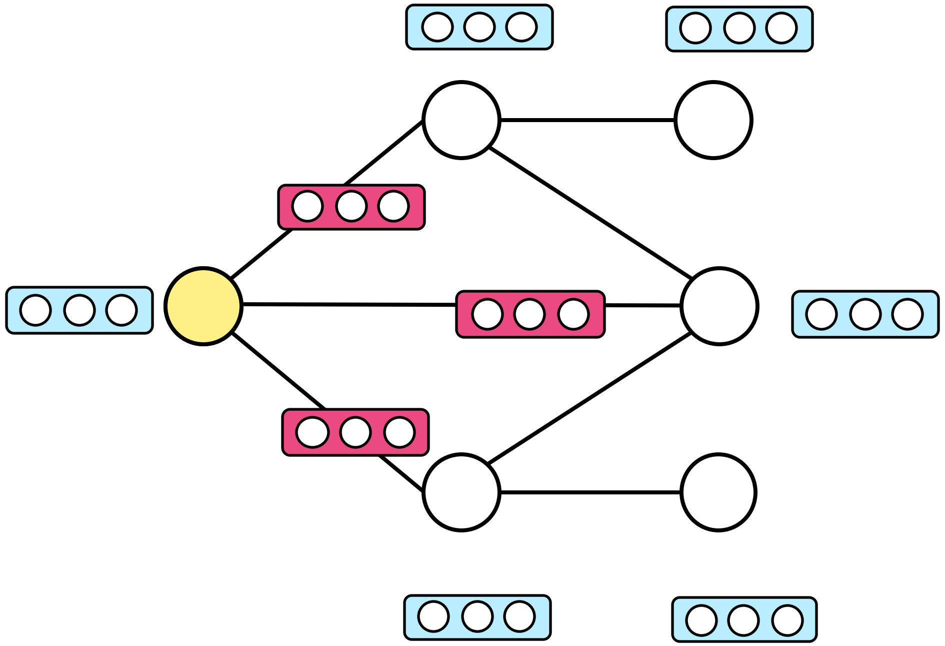
Message Passing in GNNs

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

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



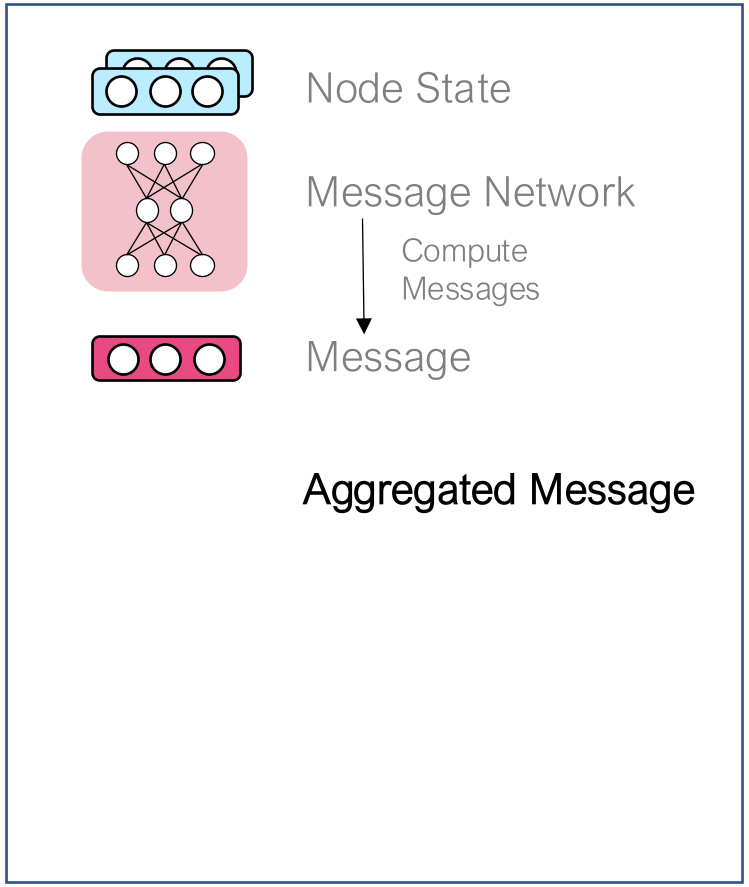
(t+1)-th message passing step/layer



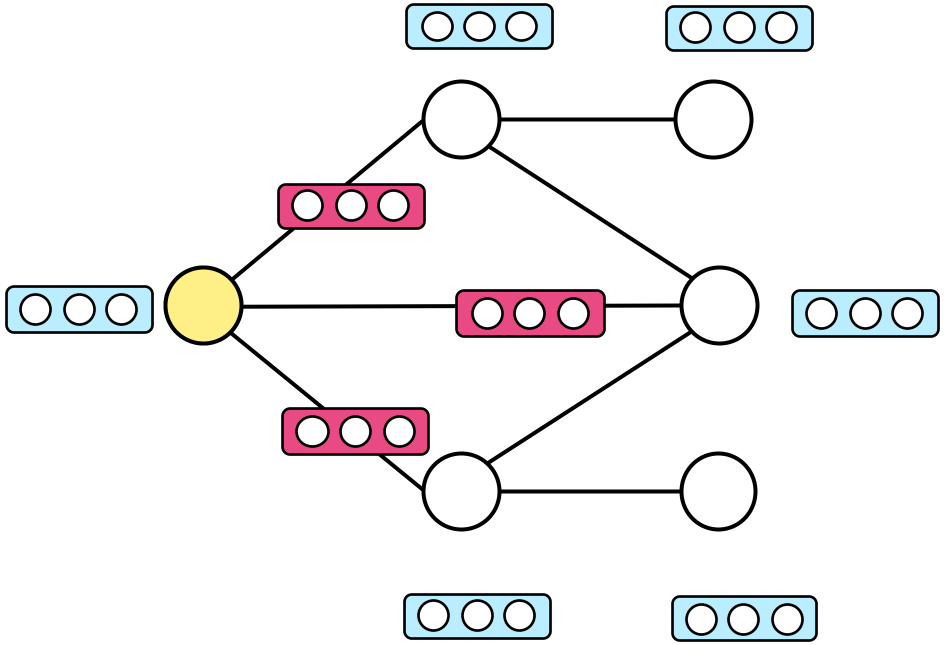
Message Passing in GNNs

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

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



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

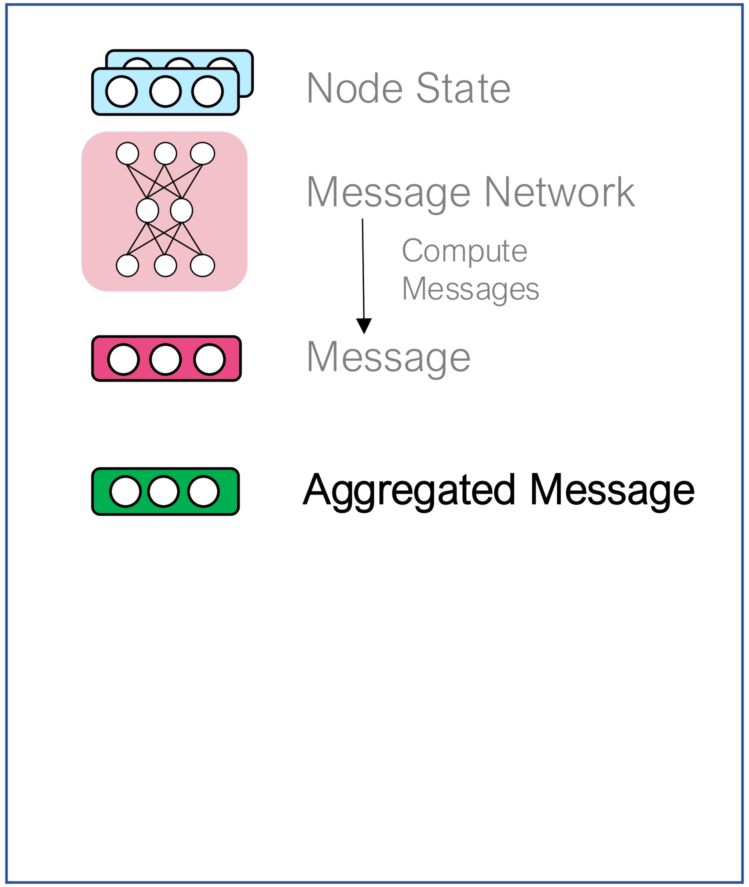


Message Passing in GNNs

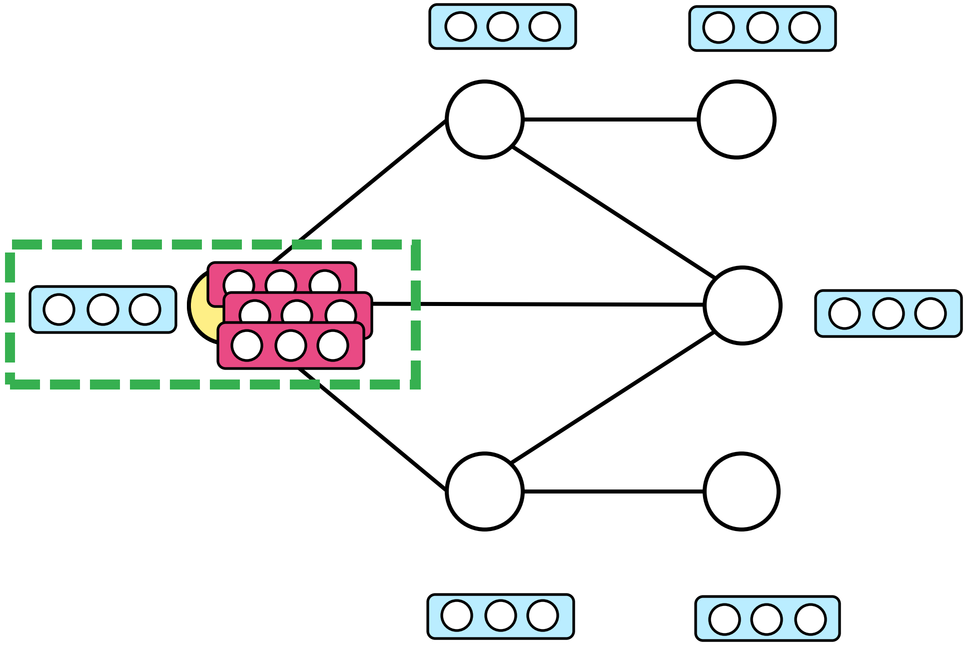
$\mathbf{h}_i^t \quad \mathbf{h}_j^t$

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

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



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

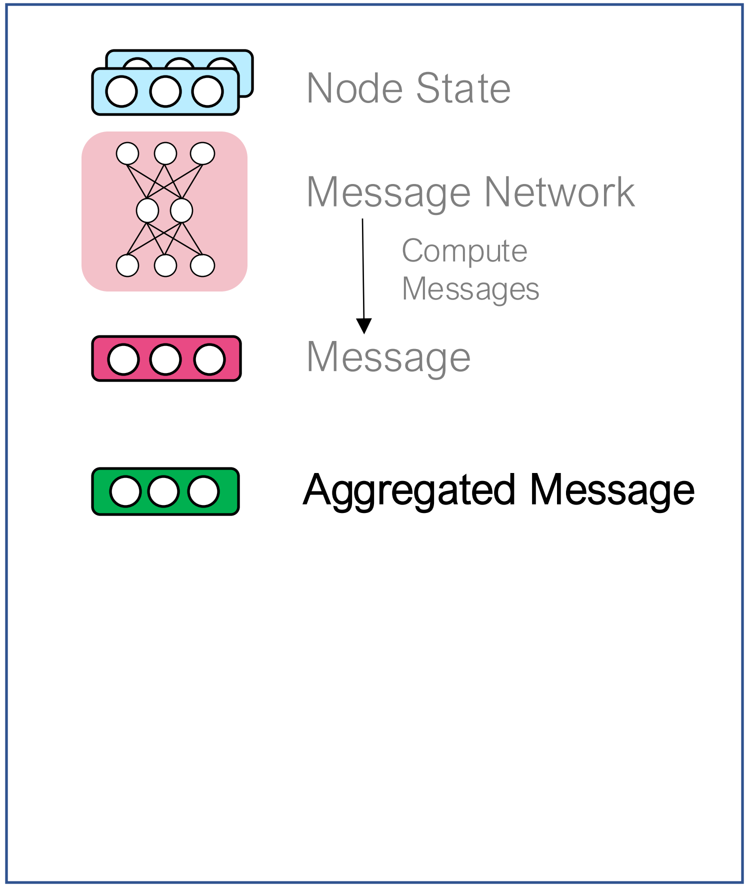


Message Passing in GNNs

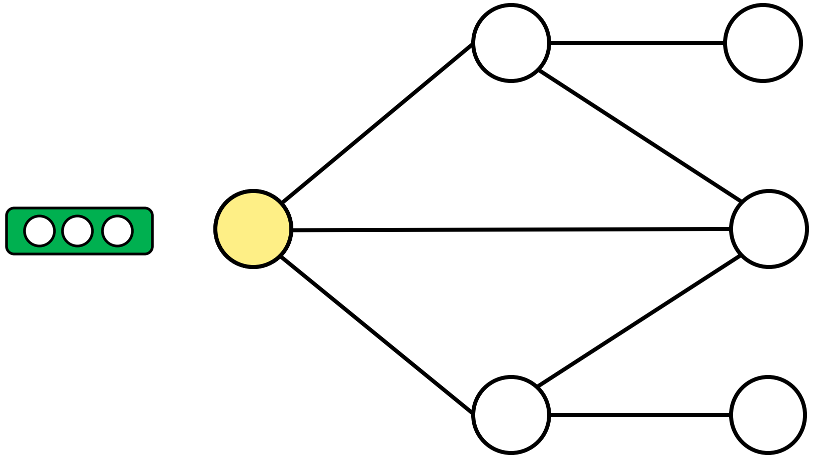
$\mathbf{h}_i^t \quad \mathbf{h}_j^t$

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

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



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

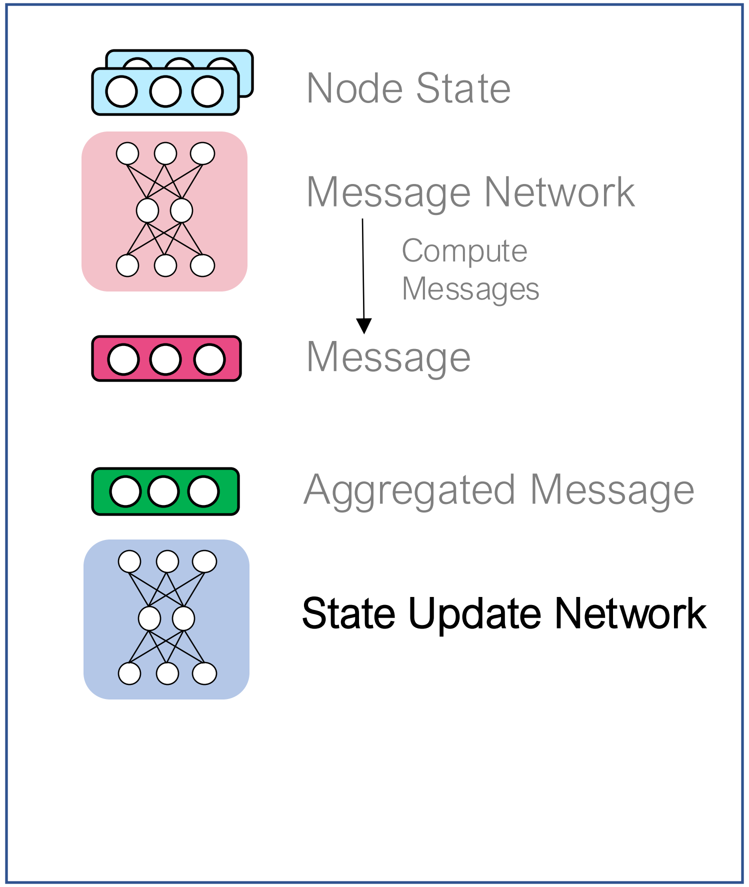


Message Passing in GNNs

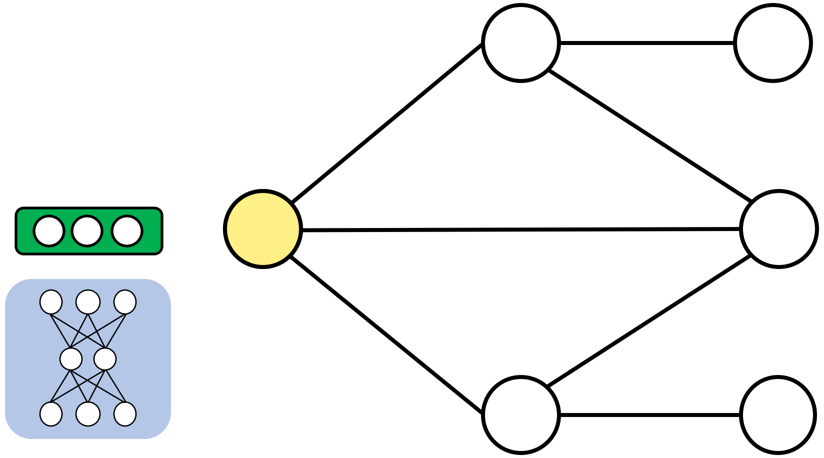
$\mathbf{h}_i^t \quad \mathbf{h}_j^t$

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

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



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



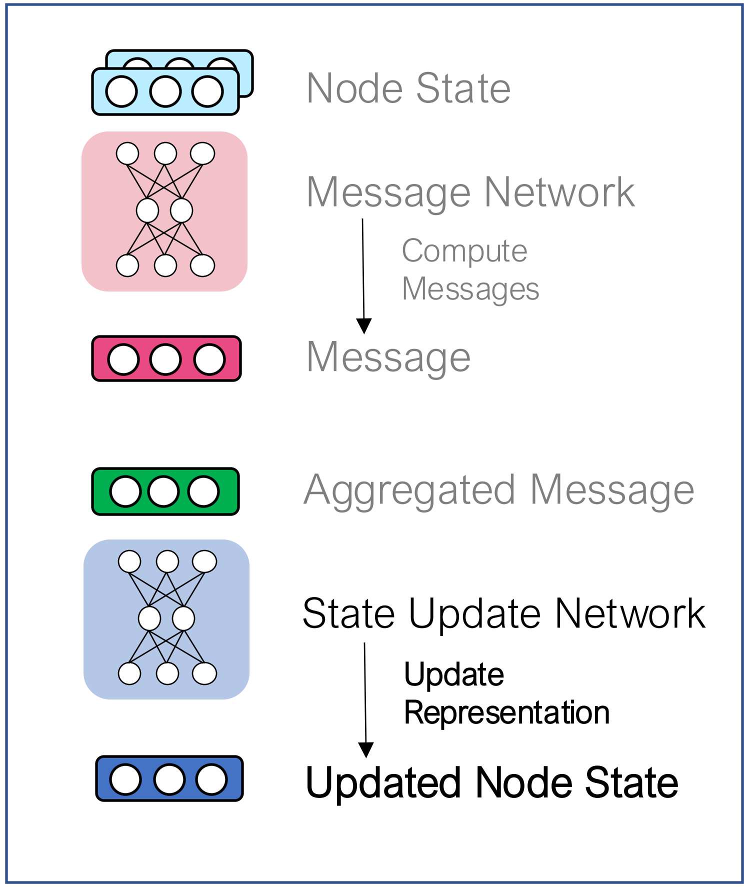
Message Passing in GNNs

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

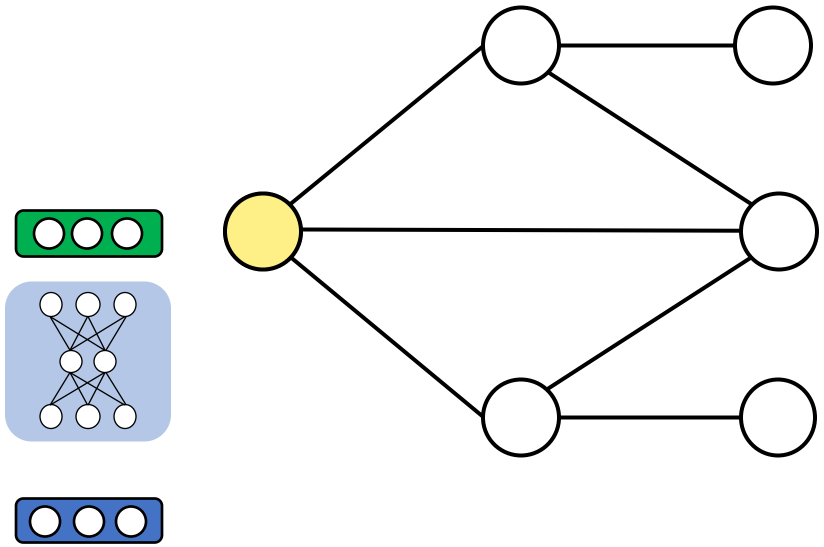
$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

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

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



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



Message Passing in GNNs

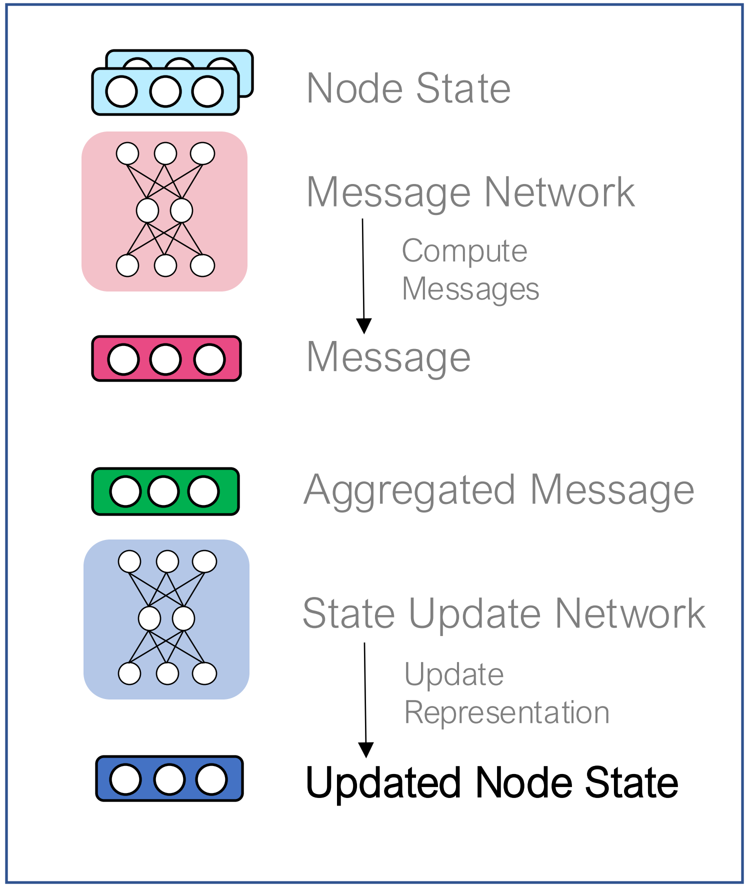
(t+1)-th message passing step/layer

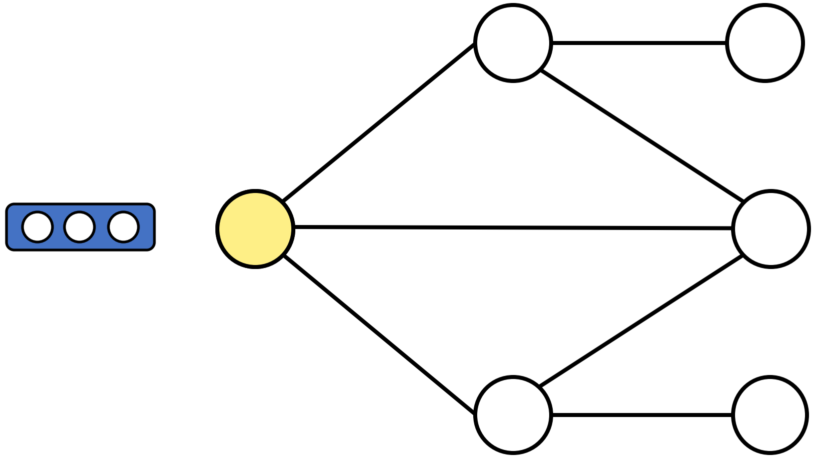
$$\mathbf{h}_i^t \quad \mathbf{h}_j^t$$

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

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

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





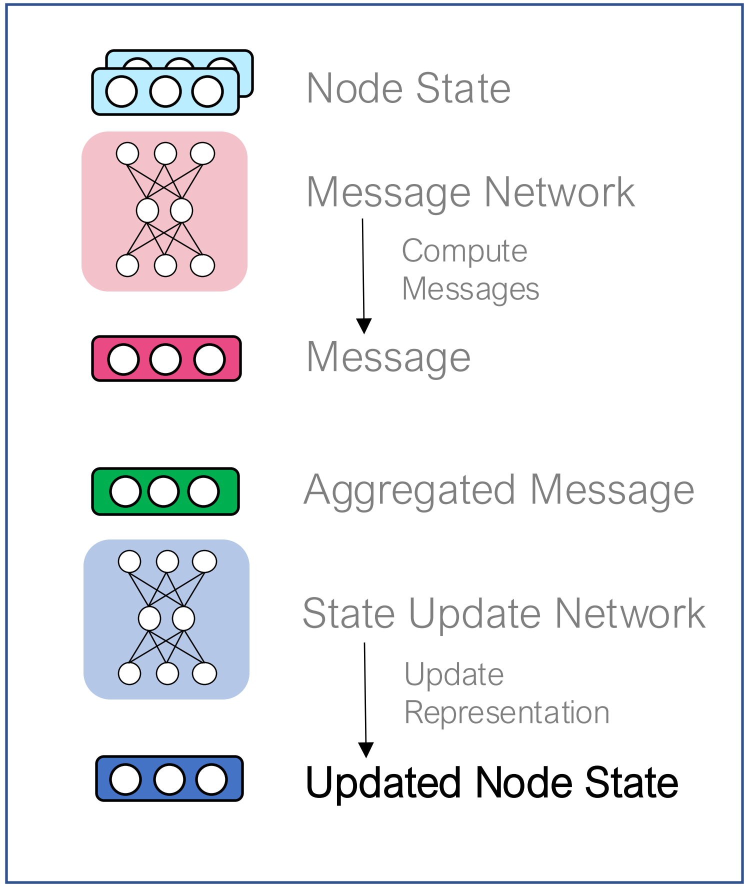
Message Passing in GNNs

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

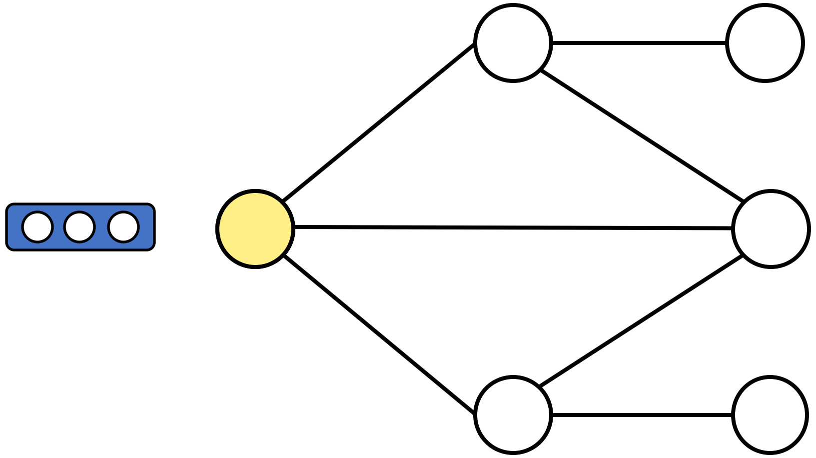
$$\mathbf{m}_{ji}^t = f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

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

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



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



- Parallel Schedule!

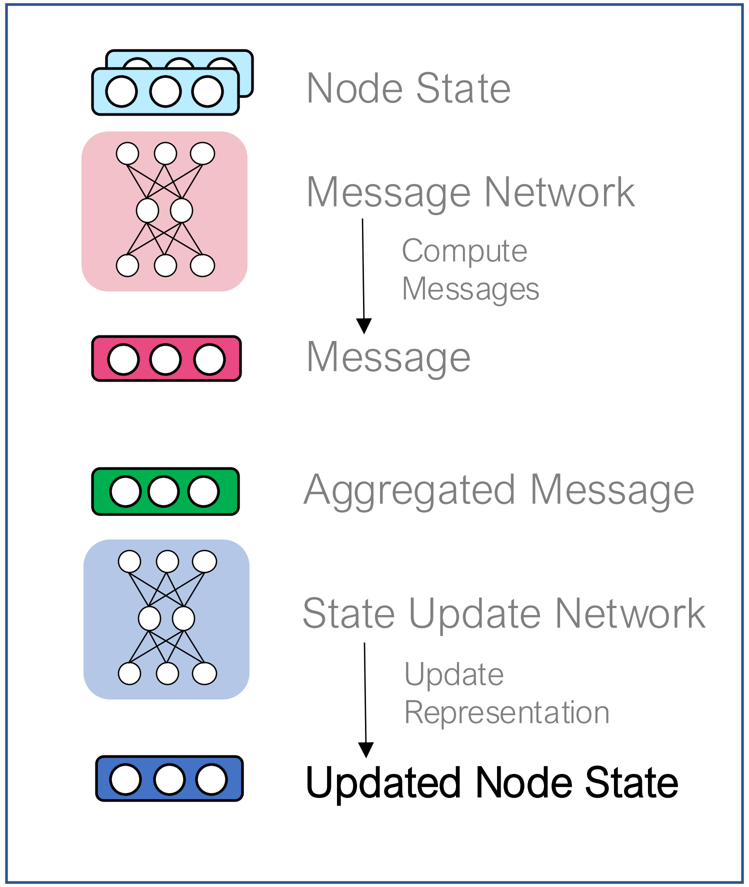
Message Passing in GNNs

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

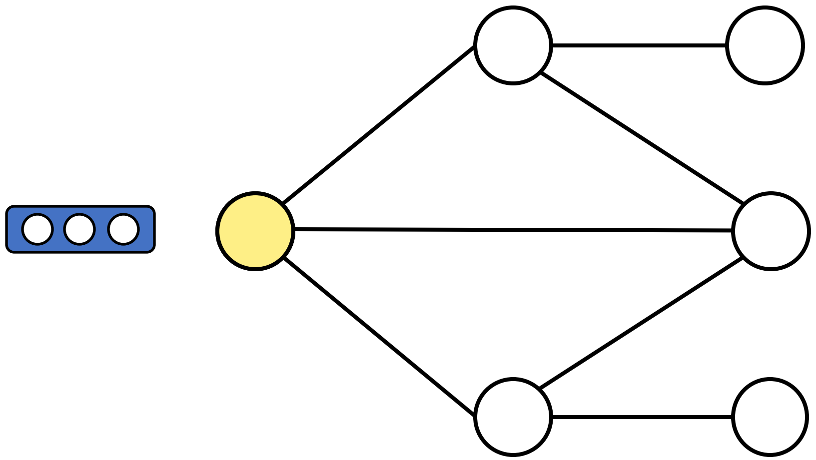
$$\mathbf{m}_{ji}^t = f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t)$$

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

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



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



- 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

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

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

Instantiations:

1. **Compute Messages**

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017.

Message Passing in GNNs

Instantiations:

1. **Compute Messages**

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

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019.

Message Passing in GNNs

Instantiations:

1. **Compute Messages**

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

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019.

Message Passing in GNNs

Instantiations:

1. **Compute Messages**

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\mathrm{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \mathrm{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. **Aggregate Messages**

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

$$f_{\mathrm{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. **Aggregate Messages**

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

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j\in\mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j\in\mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. **Aggregate Messages**

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

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. **Aggregate Messages**

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

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \text{LSTM}\left([\mathbf{m}_{ji}^t | j \in \mathcal{N}_i]\right)$$ [3]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. Aggregate Messages

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

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \textstyle\sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \textstyle\sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \text{LSTM}\left([\mathbf{m}_{ji}^t | j \in \mathcal{N}_i]\right)$$ [3]

3. **Update Node Representations**

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

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{GRU}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$ [1,4]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. Aggregate Messages

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

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \text{LSTM}\left([\mathbf{m}_{ji}^t | j \in \mathcal{N}_i]\right)$$ [3]

3. **Update Node Representations**

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

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{GRU}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$ [1,4]

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{MLP}_1(\mathbf{h}_i^t) + \text{MLP}_2(\bar{\mathbf{m}}_i^t)$$ [2]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

Message Passing in GNNs

Instantiations:

1. Compute Messages

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

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t])$$ [1]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t) = \mathbf{h}_j^t$$ [2]

$$f_{\text{msg}}(\mathbf{h}_j^t, \mathbf{h}_i^t, \boxed{\mathbf{e}_{ji}}) = \text{MLP}([\mathbf{h}_j^t, \mathbf{h}_i^t, \mathbf{e}_{ji}])$$ [1]

Edge Feature

2. Aggregate Messages

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

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [1,2,4]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \max_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t$$ [3]

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \text{LSTM}\left([\mathbf{m}_{ji}^t | j \in \mathcal{N}_i]\right)$$ [3]

3. **Update Node Representations**

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

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{GRU}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t)$$ [1,4]

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{MLP}_1(\mathbf{h}_i^t) + \text{MLP}_2(\bar{\mathbf{m}}_i^t)$$ [2]

$$f_{\text{update}}(\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t) = \text{MLP}([\mathbf{h}_i^t, \bar{\mathbf{m}}_i^t])$$ [3]

[1] Gilmer, Justin, et al. "Neural message passing for quantum chemistry." ICML. 2017. [2] Morris, Christopher, et al. "Weisfeiler and leman go neural: Higher-order graph neural networks." AAAI. 2019. [3] Hamilton, Will, et al. "Inductive representation learning on large graphs." NeurIPS. 2017. [4] Li, Yujia, et al. "Gated graph sequence neural networks." ICLR. 2016.

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**

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

Readout in GNNs

Instantiations:

1. Node Readout

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

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

2. **Edge Readout**

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

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

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

Edge Feature

Readout in GNNs

Instantiations:

1. Node Readout

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

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

2. Edge Readout

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

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

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

Edge Feature

3. Graph Readout

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

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

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

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!*

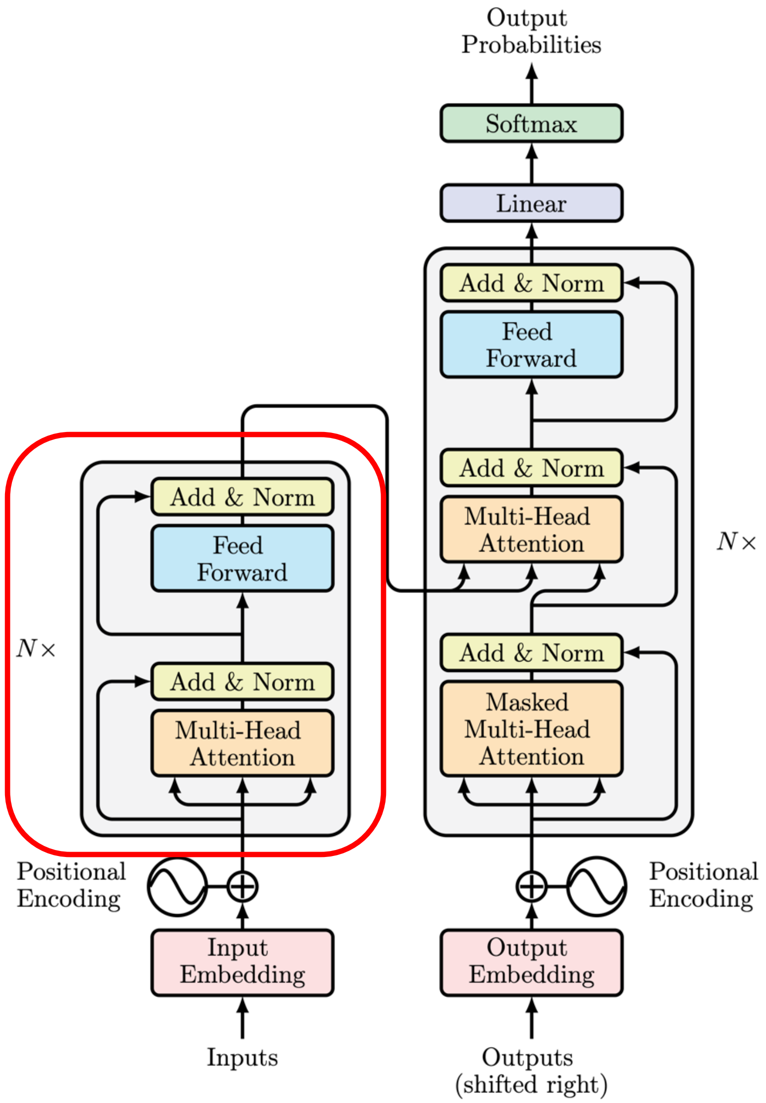
Tips:

- 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



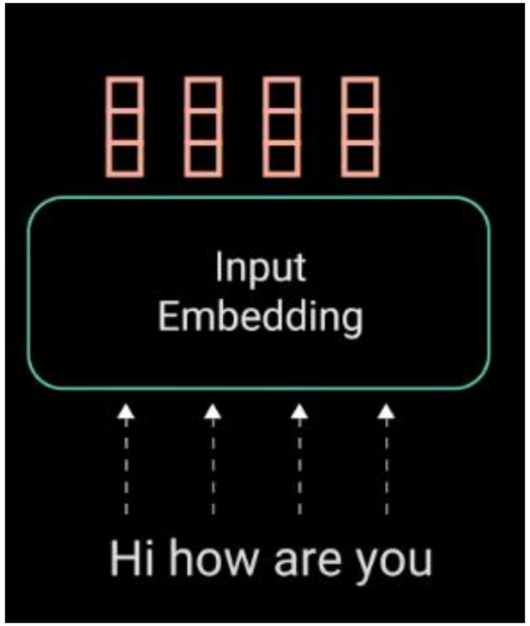
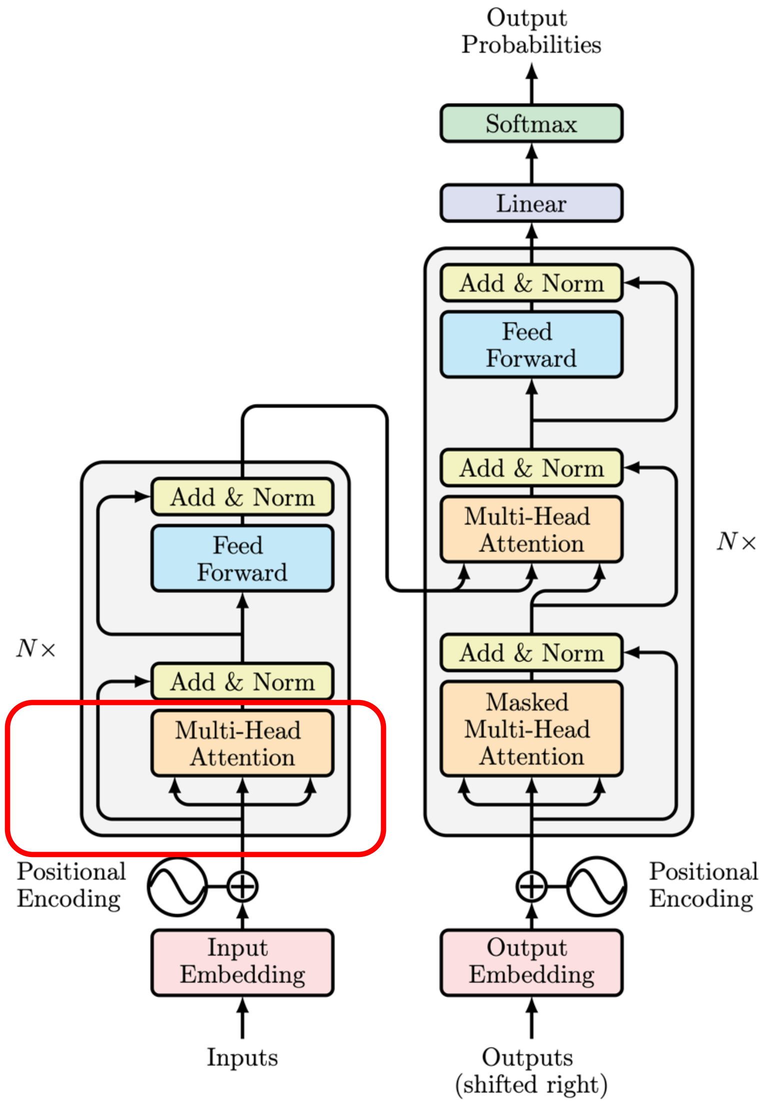
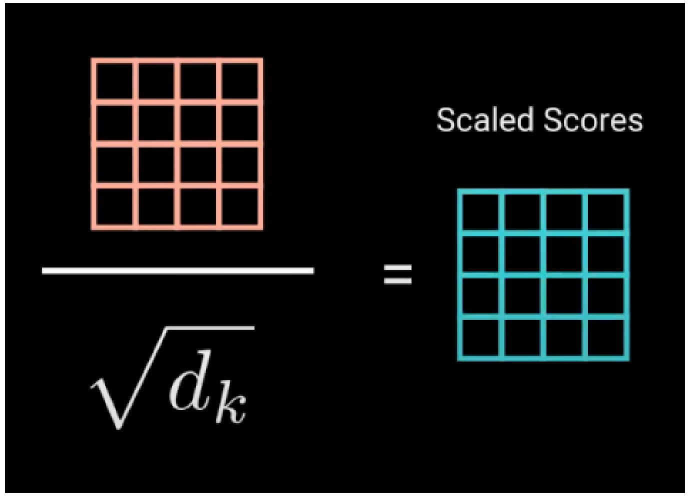


Image Credit: Vaswani, A., et al. Attention is all you need. NeurIPS 2017. https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Relationships with Transformer





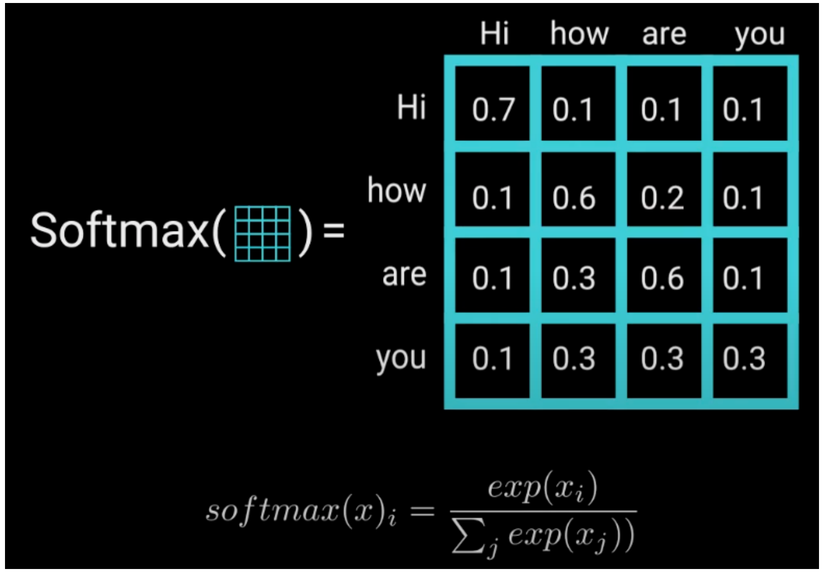
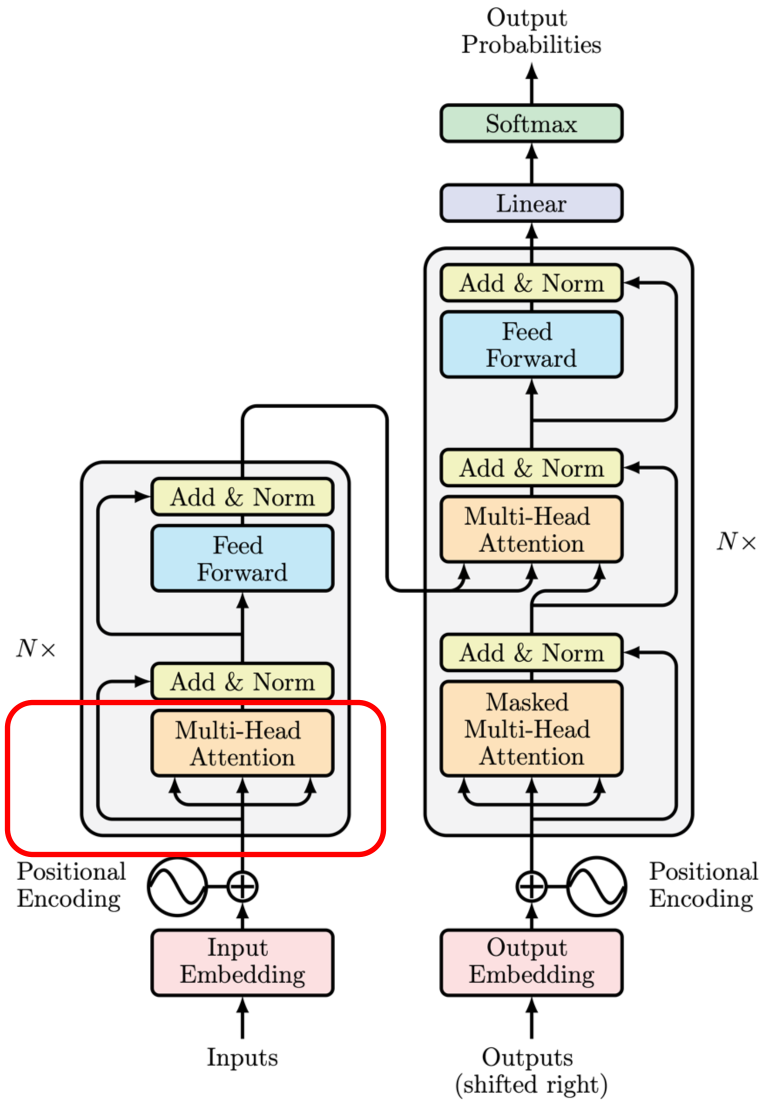


Image Credit: Vaswani, A., et al. Attention is all you need. NeurIPS 2017. https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Relationships with Transformer



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

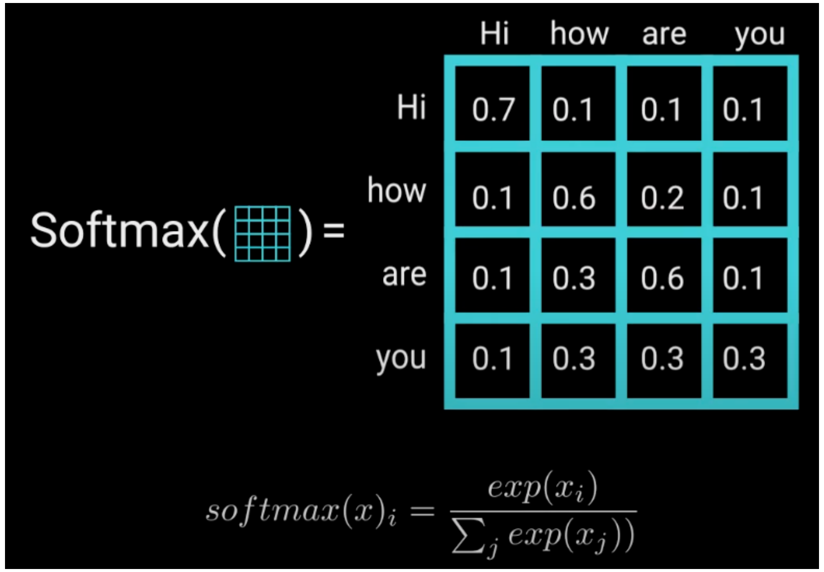
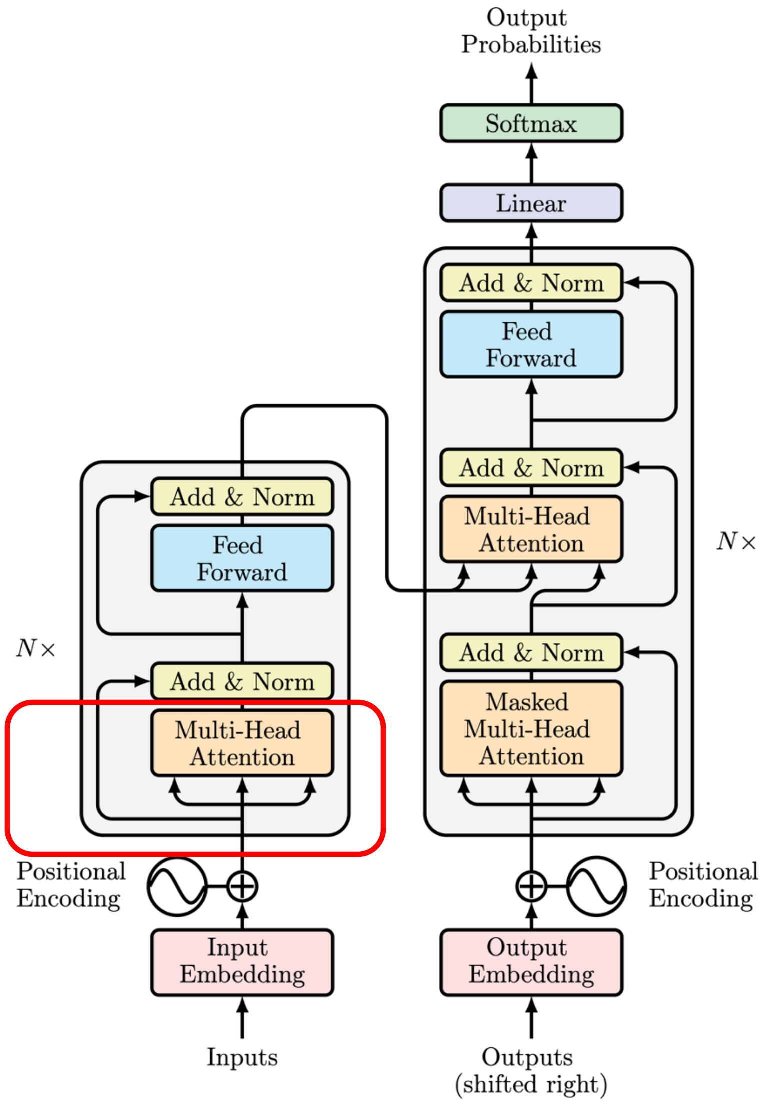


Image Credit: Vaswani, A., et al. Attention is all you need. NeurIPS 2017. https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Relationships with Transformer



- 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!

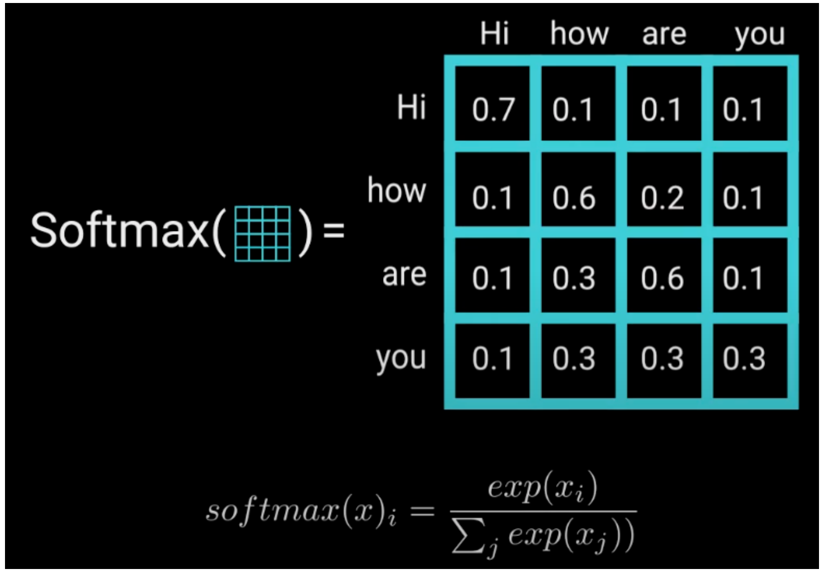


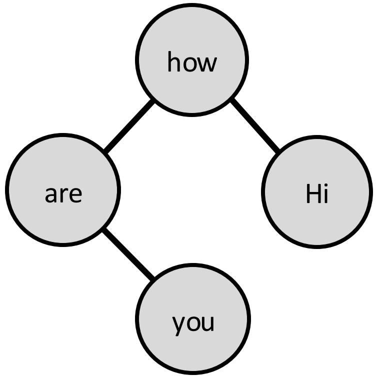
Image Credit: Vaswani, A., et al. Attention is all you need. NeurIPS 2017. https://towardsdatascience.com/illustrated-guide-to-transformers-step-by-step-explanation-f74876522bc0

Encode Graph Structures in Transformers

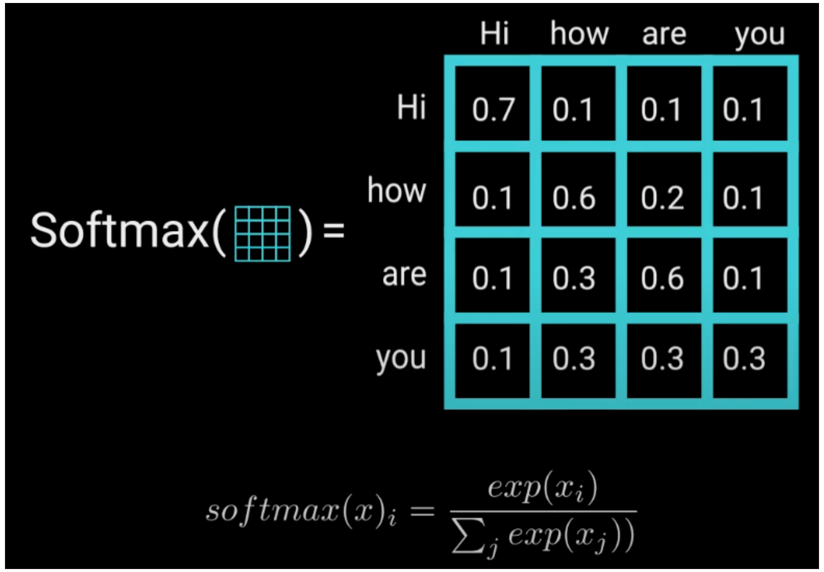
- Apply the adjacency matrix as a mask to the attention and renormalize it, like Graph Attention Networks (GAT) [1]

- 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?