THE UNIVERSITY OF BRITISH COLUMBIA

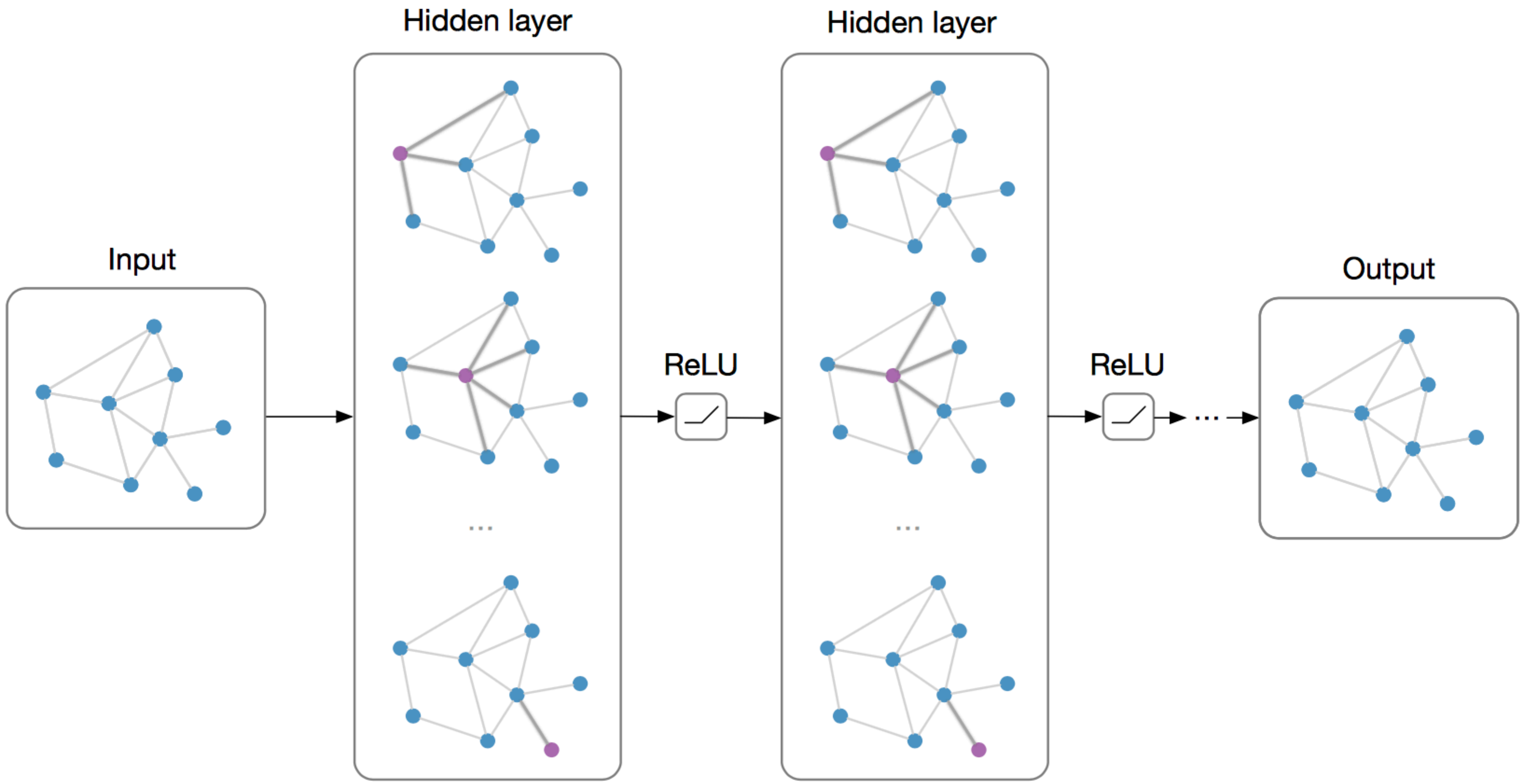
Topics in AI (CPSC 532S):
Multimodal Learning with Vision, Language and Sound

Lecture 20: Graph Neural Networks (cont)

Logistics

Relatively **short** lecture today … RL next class

Graph Neural Networks (GNNs)



Main Idea: Pass massages between pairs of nodes and agglomerate

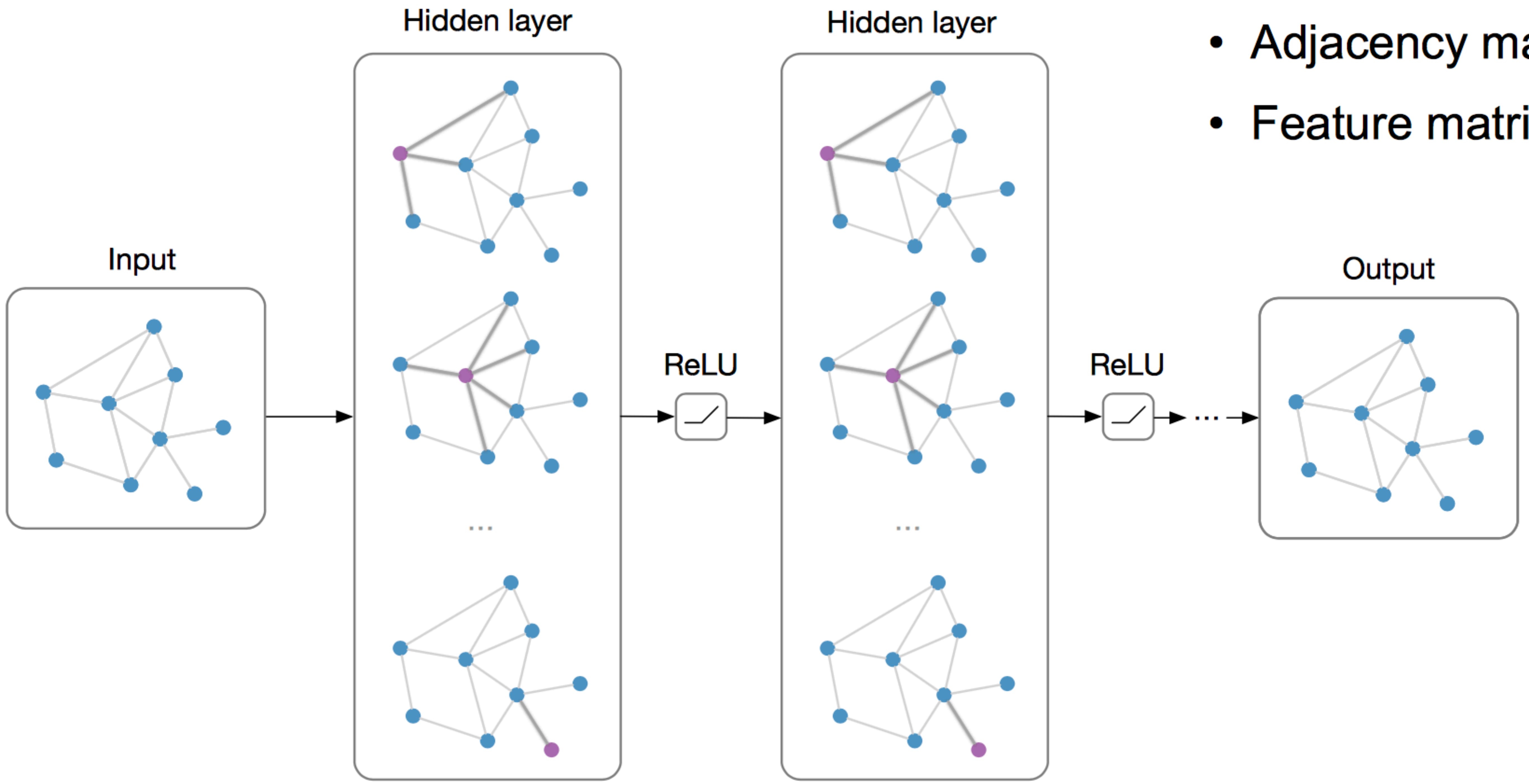
Alternative Interpretation: Pass massages between nodes to refine node (and possibly edge) representations

* slide from Thomas Kipf, **University of Amsterdam**

Graph Neural Networks (GNNs)

Notation: $\mathcal{G} = (\mathbf{A}, \mathbf{X})$

- Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
- Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$



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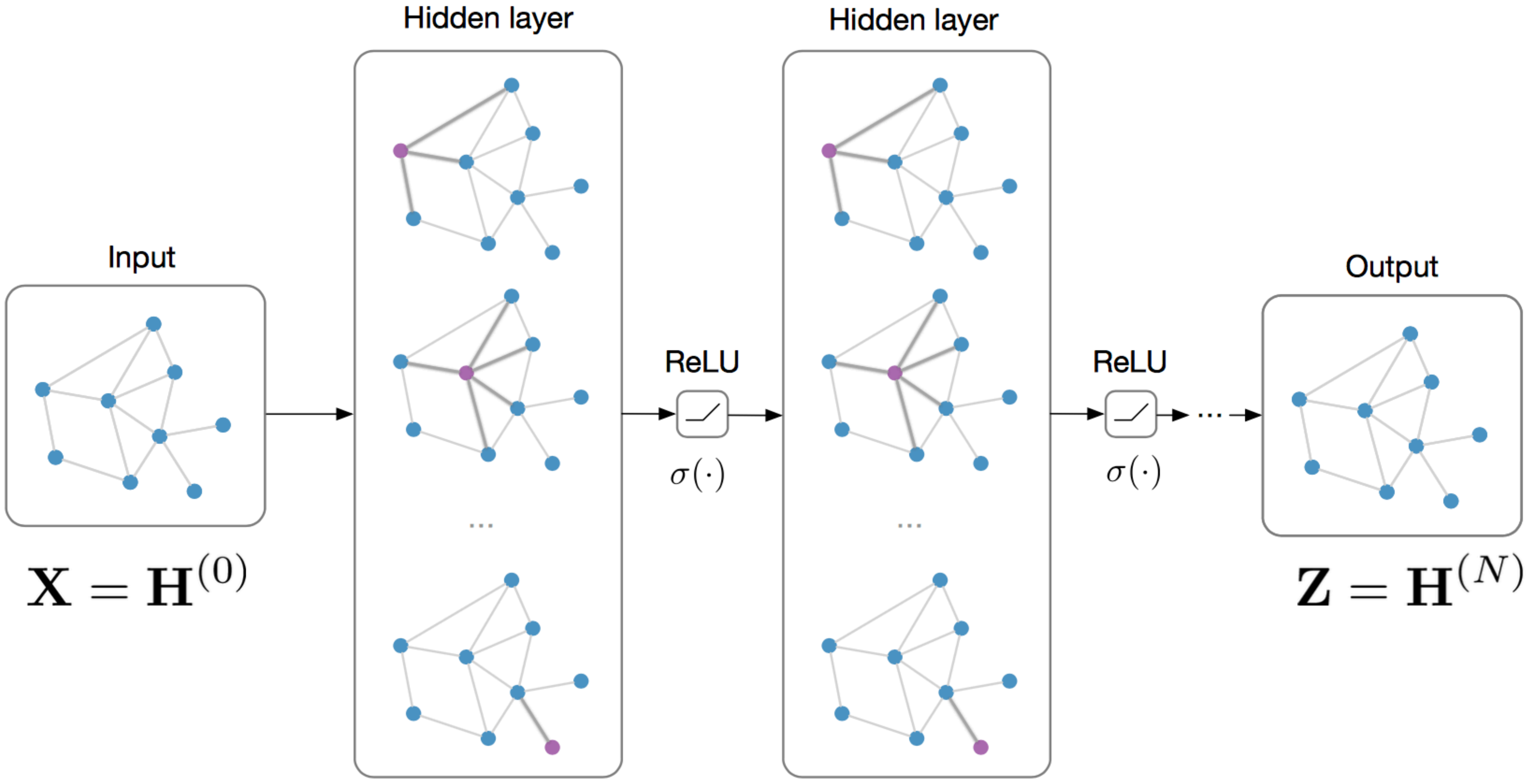
Classification and **Link Prediction** with GNNs / GCNs

Input: Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times E}$, preprocessed adjacency matrix $\hat{\mathbf{A}}$



$\mathbf{H}^{(l+1)} =$ Message Passing $(\mathbf{A}, \mathbf{H}^{(l)})$

* slide from Thomas Kipf, **University of Amsterdam**

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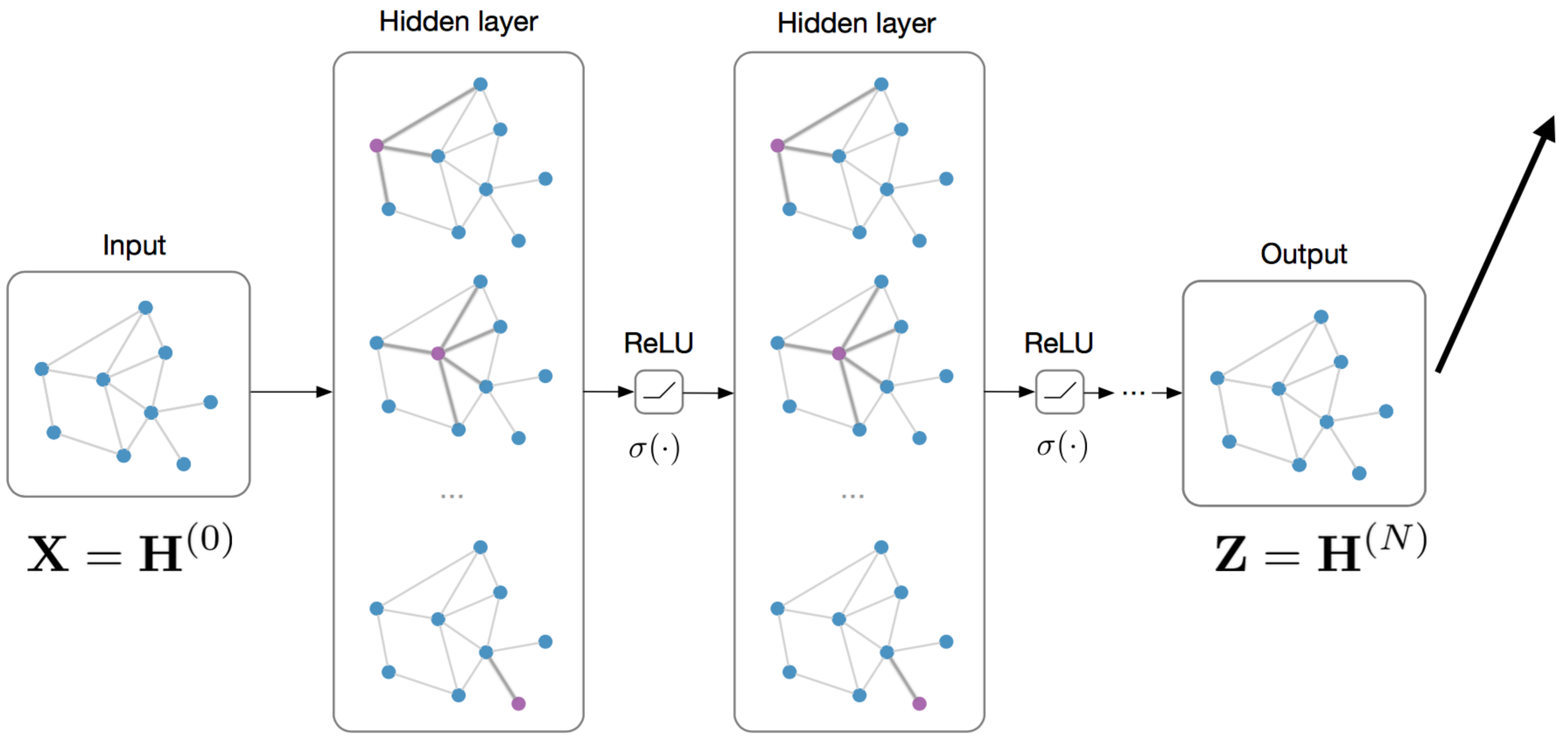

Node classification:

$\mathrm{softmax}(\mathbf{z_n})$

e.g. Kipf & Welling (ICLR 2017)

$$\mathbf{H}^{(l+1)} = \text{Message Passing}\left(\mathbf{A}, \mathbf{H}^{(l)}\right)$$

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Classification and **Link Prediction** with GNNs / GCNs

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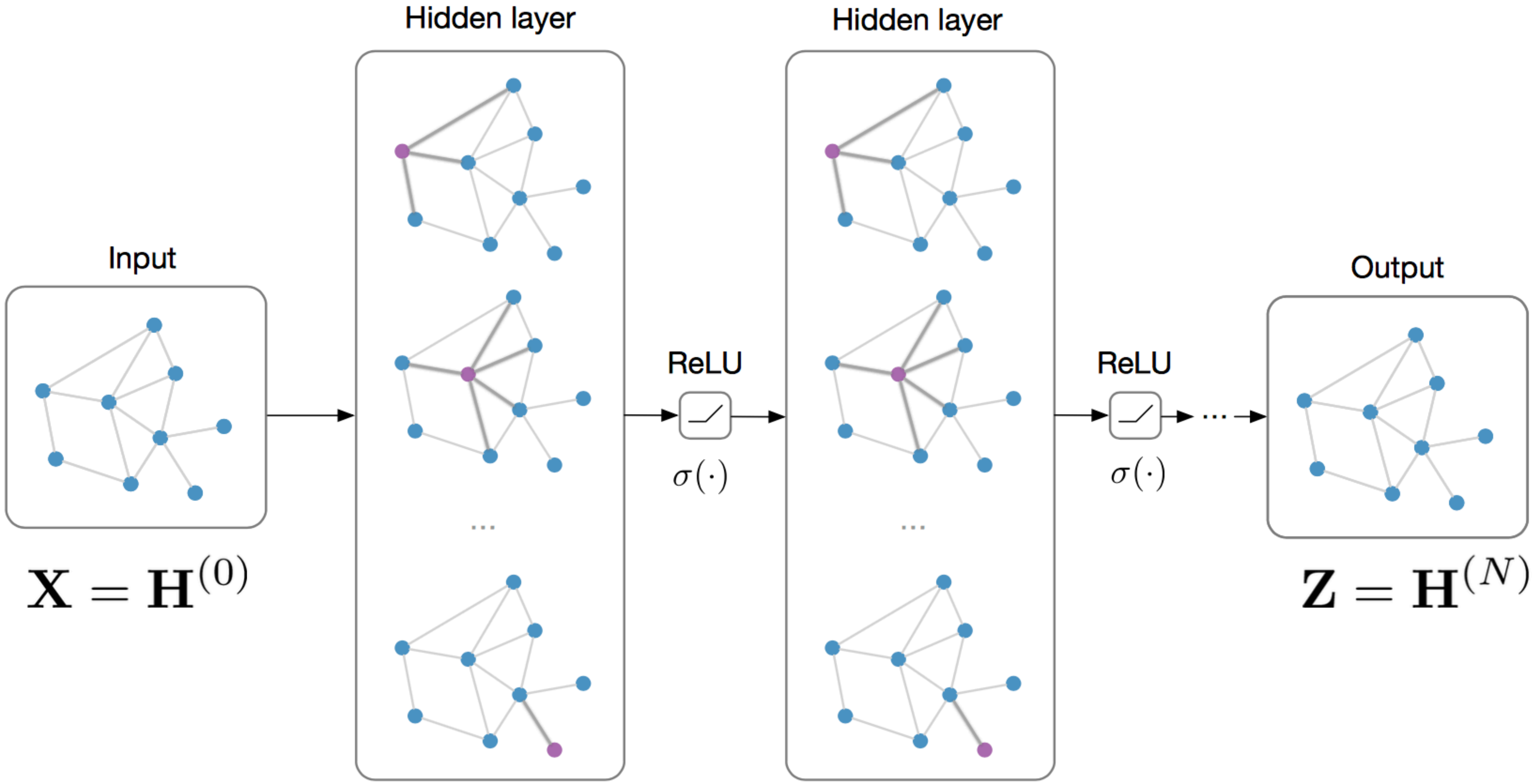

$\mathbf{X} = \mathbf{H}^{(0)}$

$\mathbf{Z} = \mathbf{H}^{(N)}$

Node classification:

$\mathrm{softmax}(\mathbf{z_n})$

e.g. Kipf & Welling (ICLR 2017)

Graph classification:

$\mathrm{softmax}(\sum_n \mathbf{z_n})$

e.g. Duvenaud et al. (NIPS 2015)

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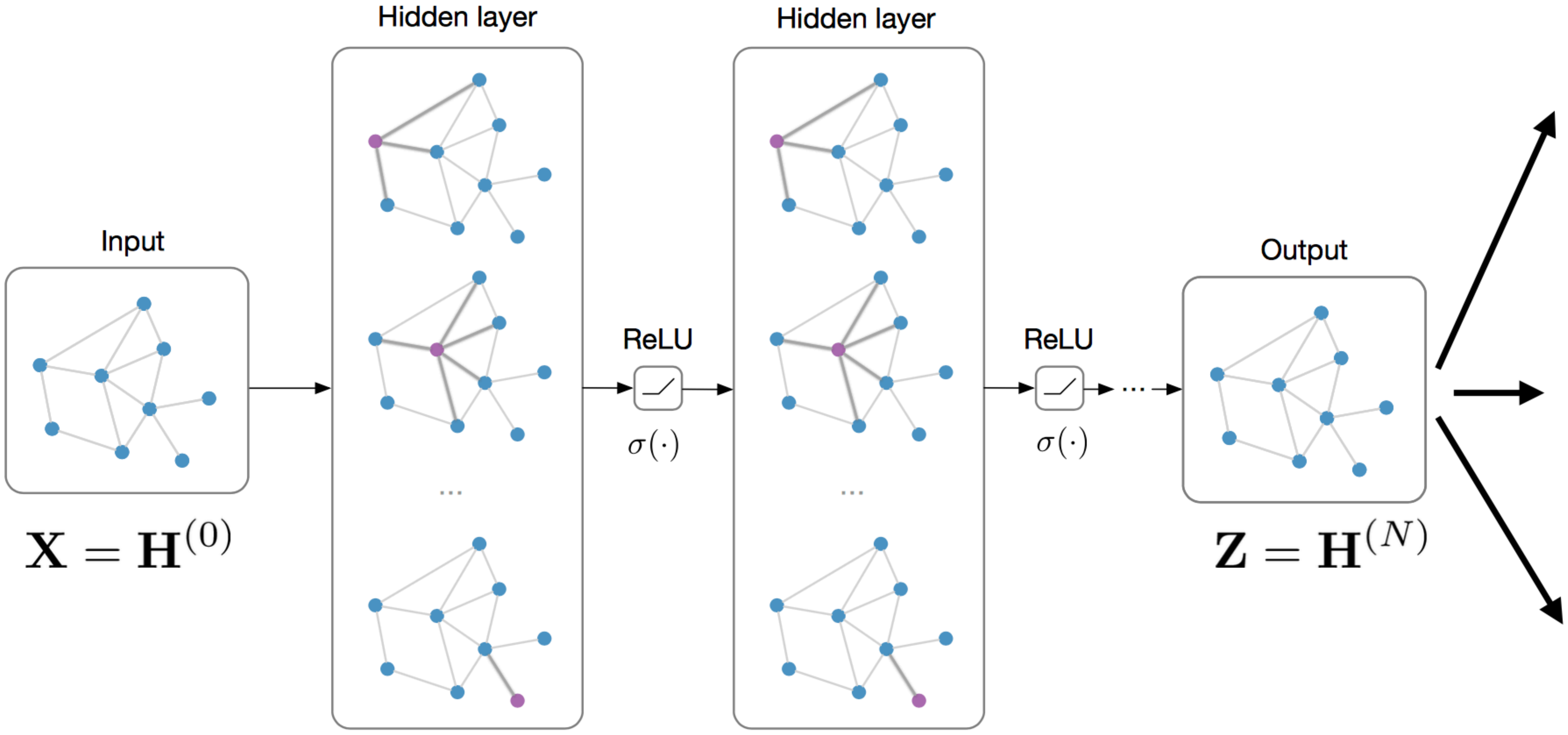

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e.g. Kipf & Welling (ICLR 2017)

Graph classification:

$\mathrm{softmax}(\sum_n \mathbf{z_n})$

e.g. Duvenaud et al. (NIPS 2015)

Link prediction:

$p(A_{ij}) = \sigma(\mathbf{z_i^T z_j})$

Kipf & Welling (NIPS BDL 2016)
"Graph Auto-Encoders"

* slide from Thomas Kipf, **University of Amsterdam**

Message Passing in GNNs

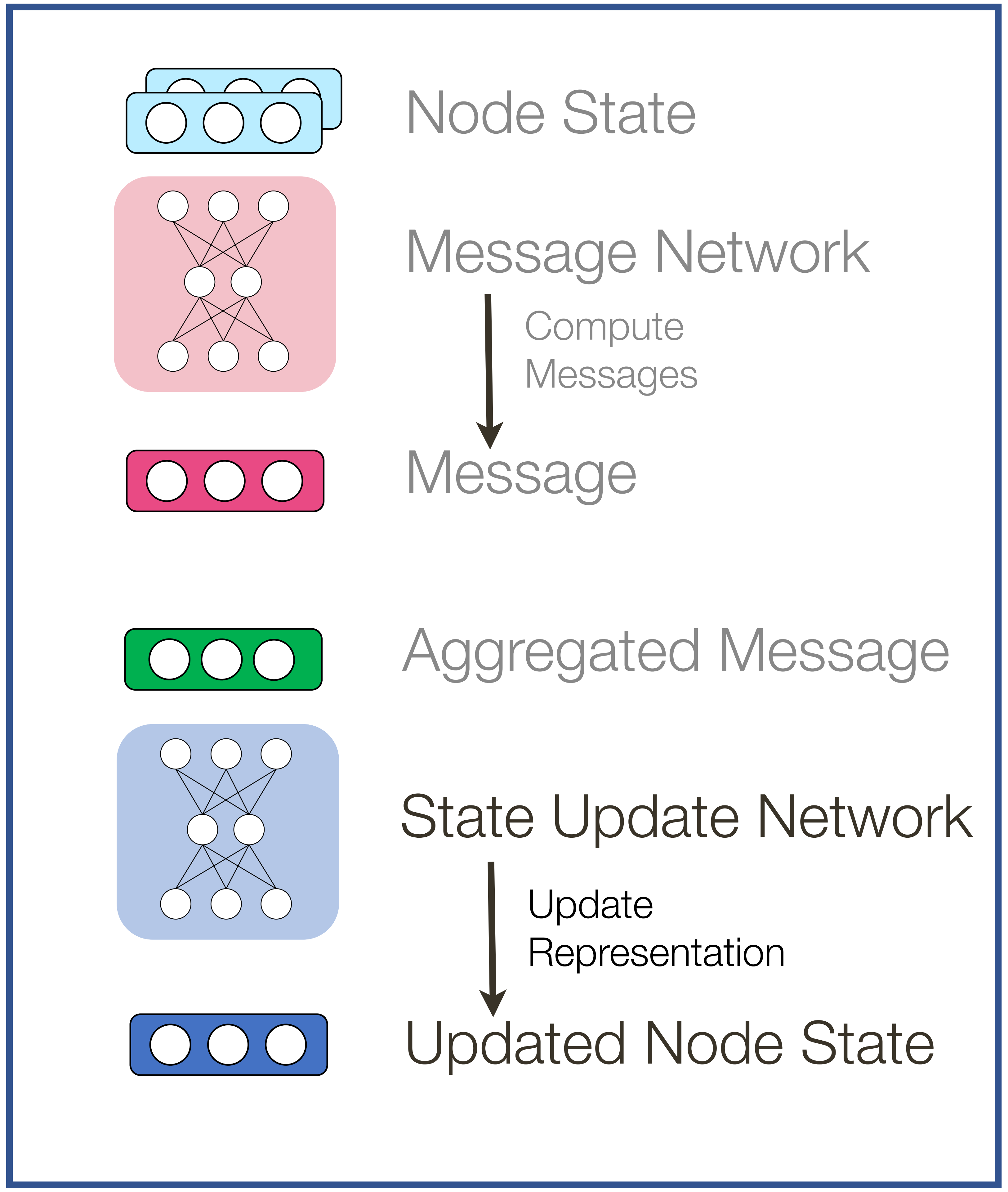
(t+1)-th message passing step/layer

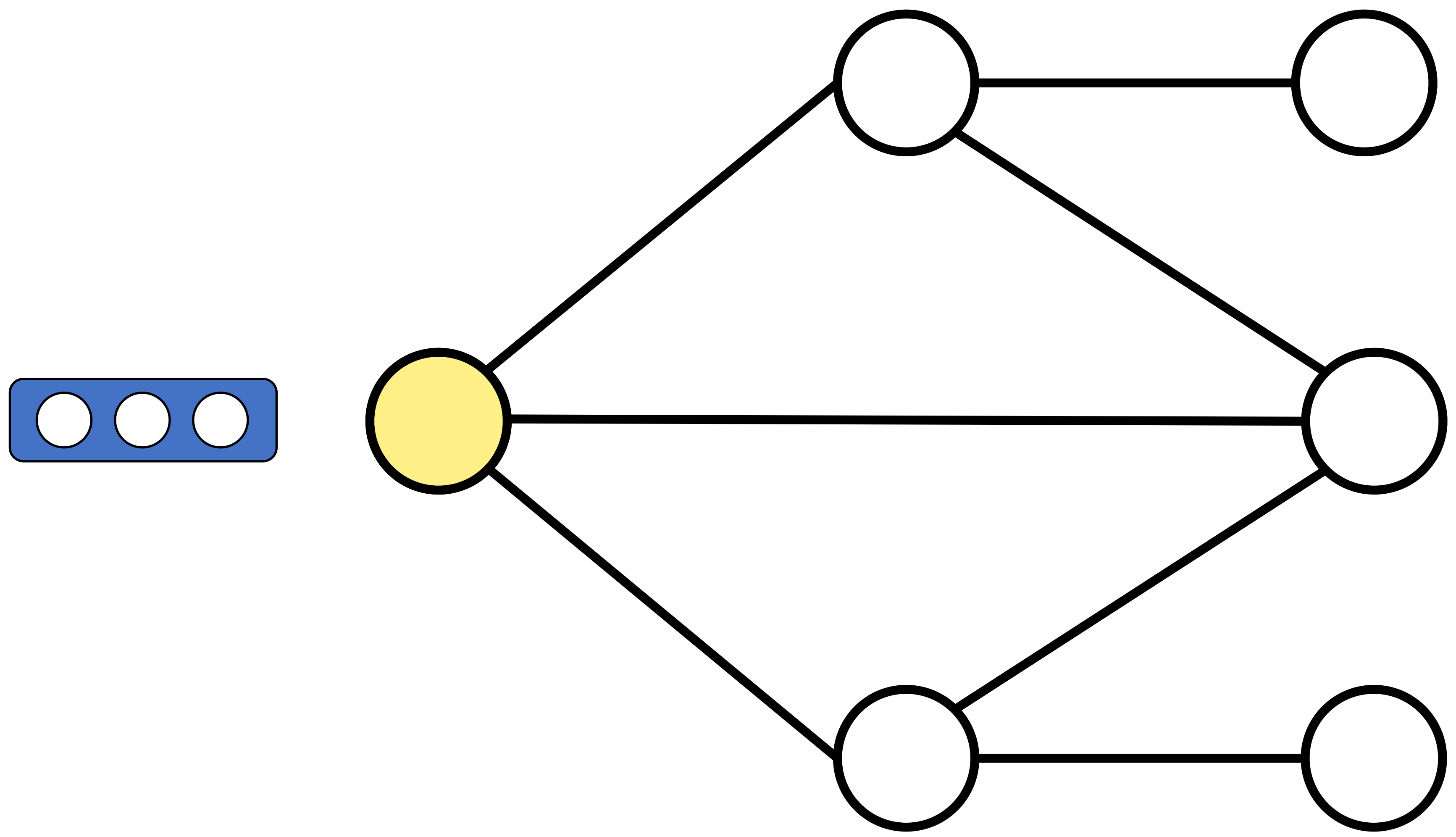
$\mathbf{h}_i^t \quad \mathbf{h}_j^t$

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

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

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





Note: We can do all updates in parallel! (but can also be serial)

Slide from Renjie Liao

GNN **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

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GNN **Instantiations**

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

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Edge Feature

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Edge Feature

$$f_{\text{agg}}\left(\{\mathbf{m}_{ji}^t | j \in \mathcal{N}_i\}\right) = \sum_{j \in \mathcal{N}_i} \mathbf{m}_{ji}^t \quad [4,5,7]$$

Slide from Renjie Liao

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Slide from Renjie Liao

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Slide from Renjie Liao

GNN **Readout**

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

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

Slide from Renjie Liao

GNN **Readout**

1. **Node Readout**

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

GNN **Readout**

1. Node Readout

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

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2. **Edge Readout**

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

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Edge Feature

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Edge Feature

3. **Graph Readout**

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

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

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

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

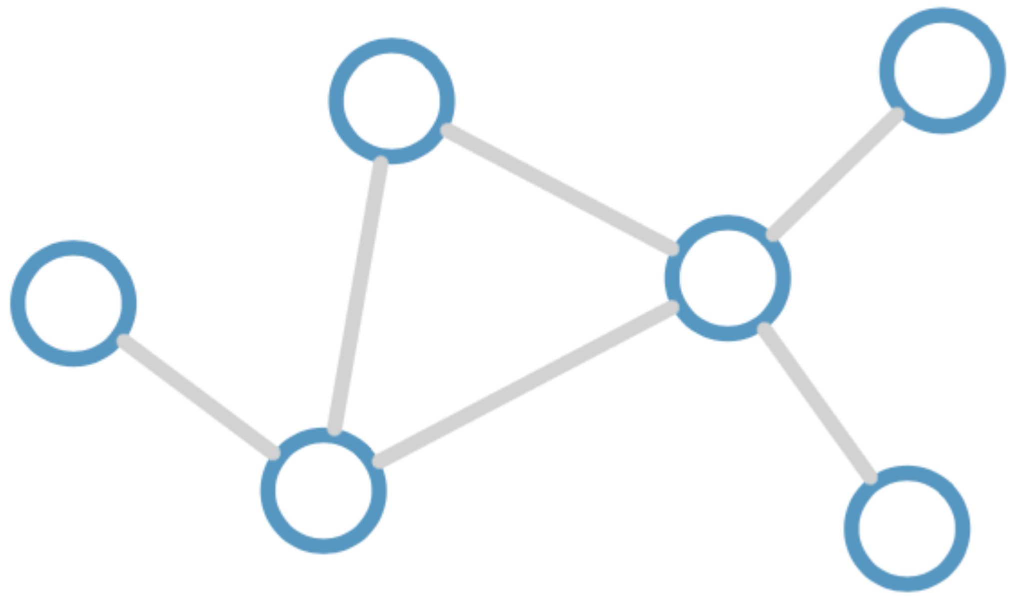
Graph Feature

Slide from Renjie Liao

Graph Convolutional Networks (GCNs)

Kipf & Welling (ICLR 2017), related previous works by Duvenaud et al. (NIPS 2015) and Li et al. (ICLR 2016)

Consider this undirected graph:



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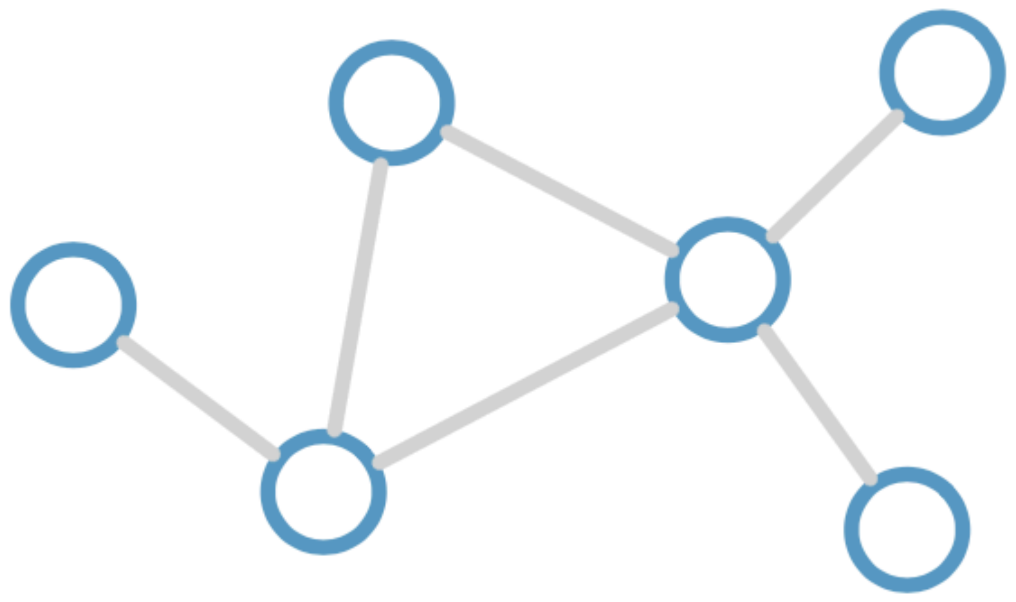
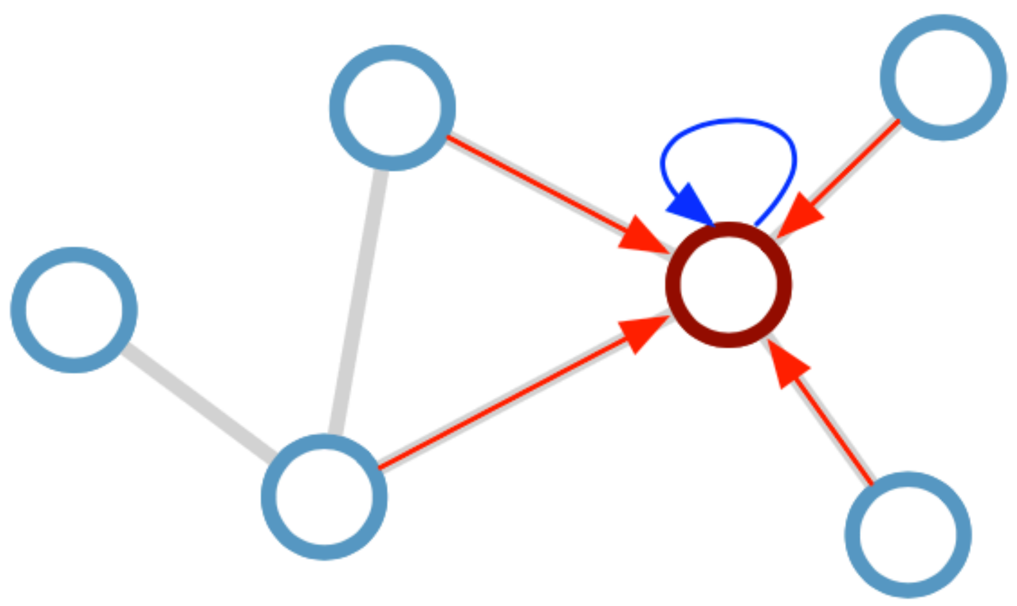


Calculate update for node in red:



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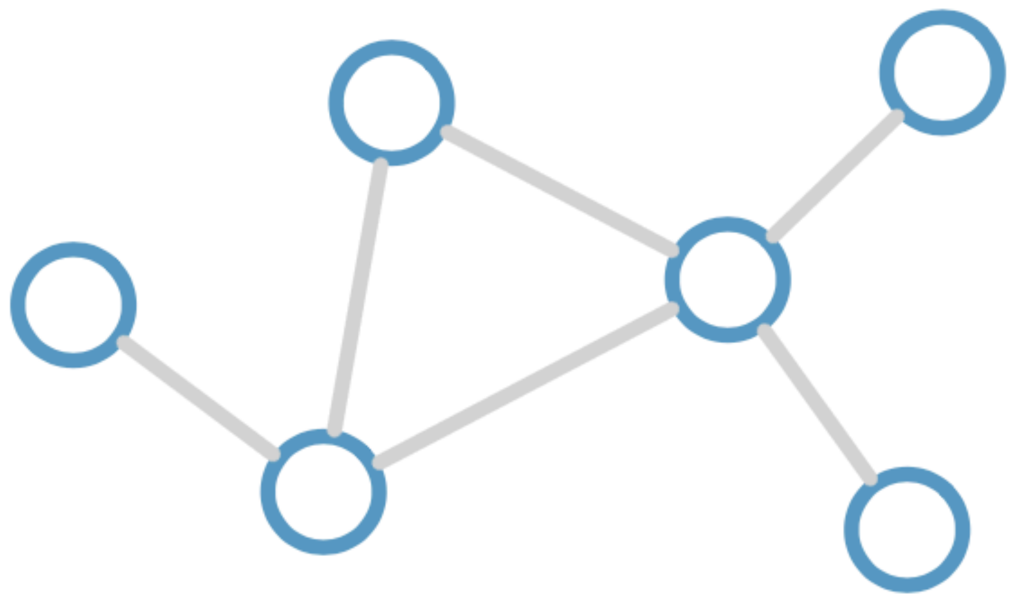

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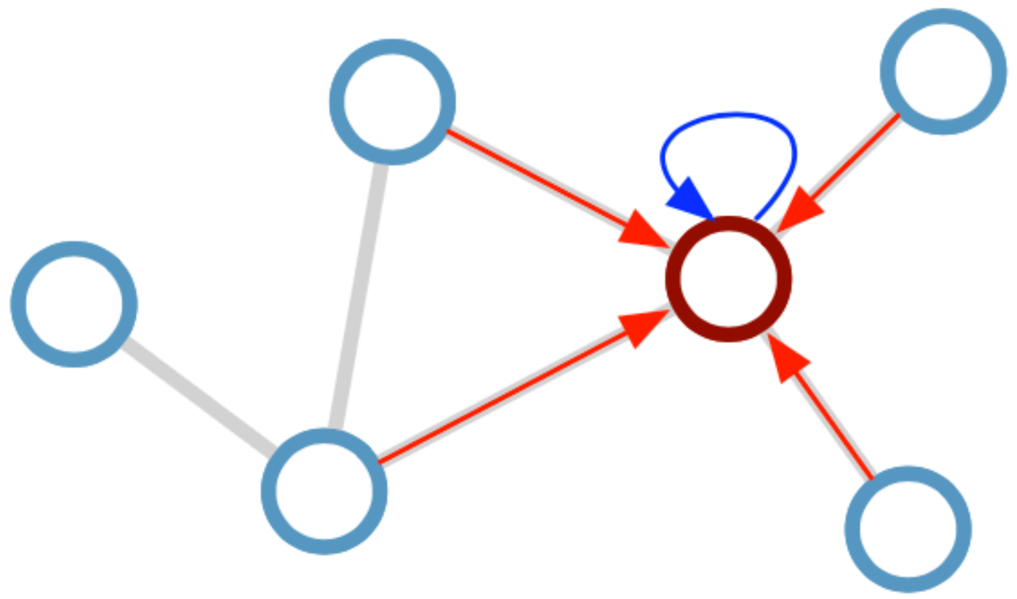


Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

$\mathcal{N}_i$: neighbor indices

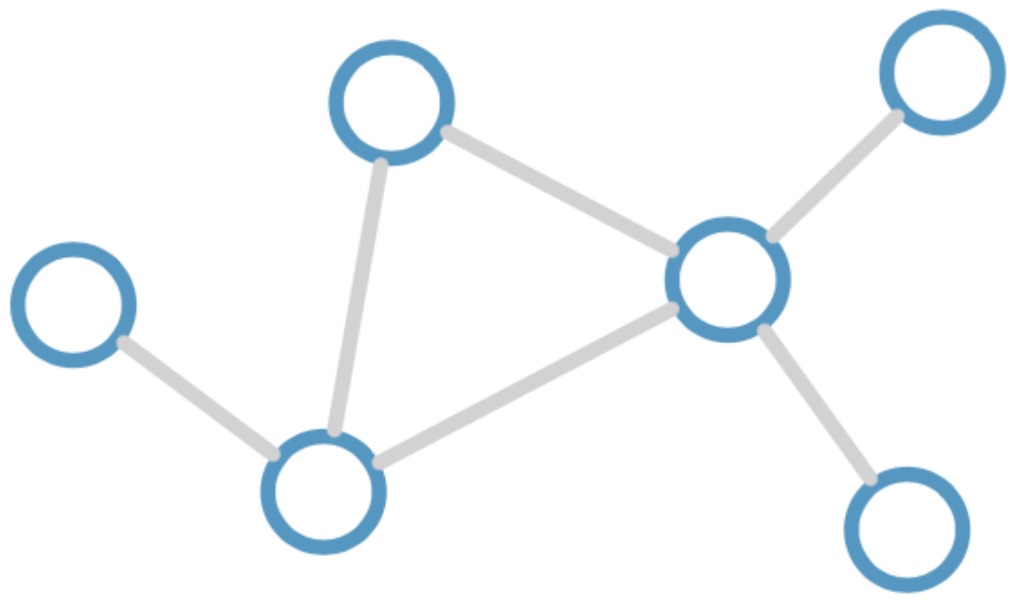
c_{ij} : norm. constant (fixed/trainable)

* slide from Thomas Kipf, **University of Amsterdam**

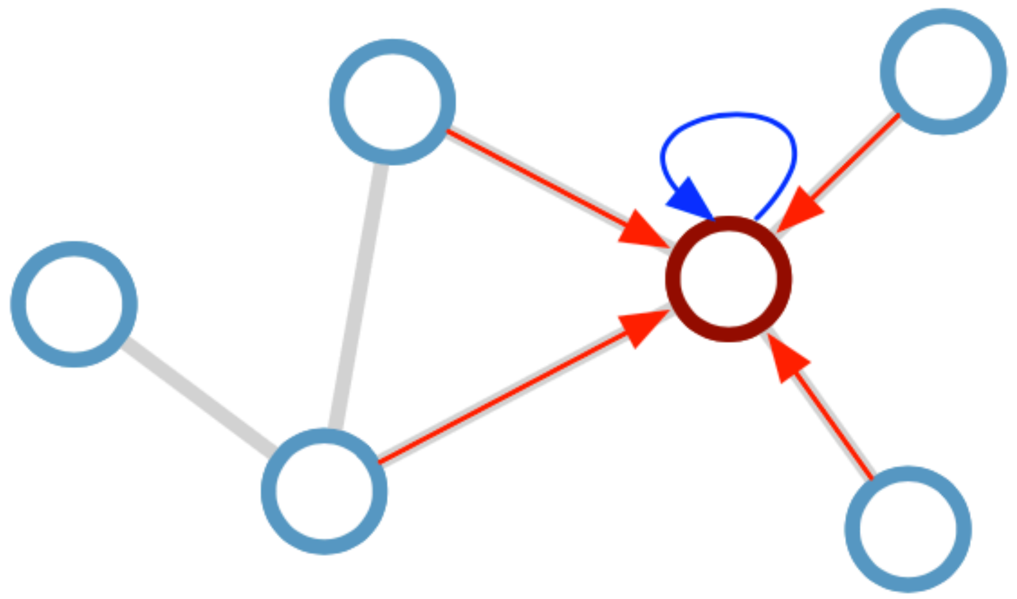
Graph Convolutional Networks (GCNs)

Kipf & Welling (ICLR 2017), related previous works by Duvenaud et al. (NIPS 2015) and Li et al. (ICLR 2016)

Consider this undirected graph:



Calculate update for node in red:



Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\underline{\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}}\right)$$

Compute Message

Aggregate Messages

Update Node Representation

$\mathcal{N}_i$: neighbor indices

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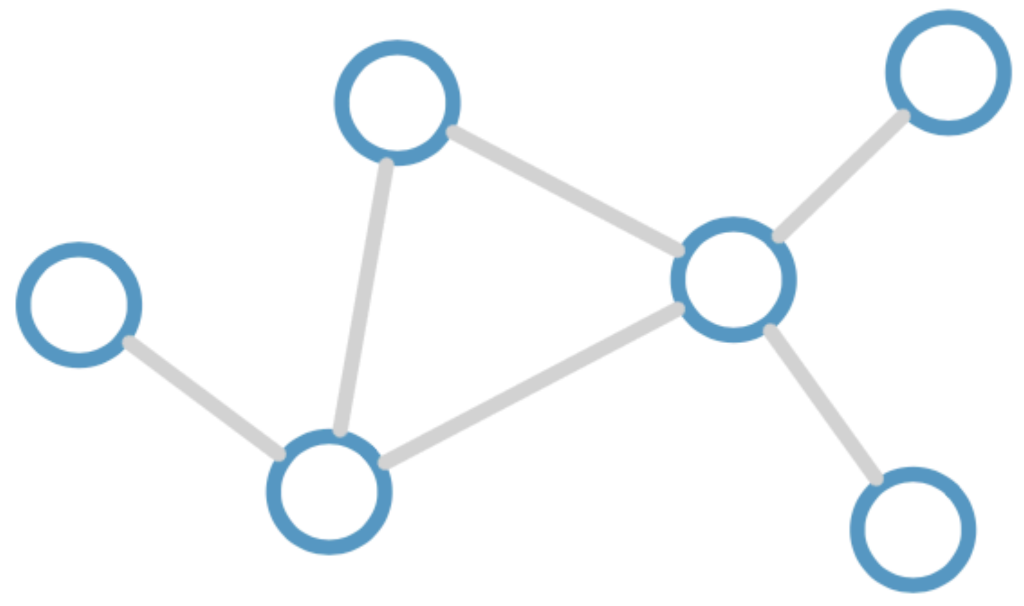

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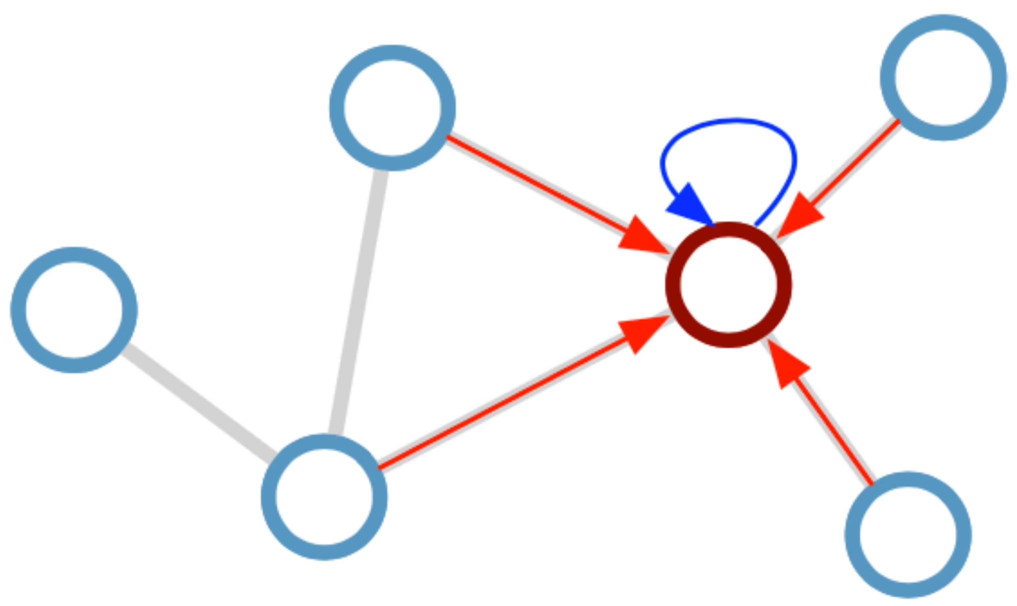

Compute Message

Aggregate Messages

Update Node Representation

Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \underbrace{\sum_{j\in\mathcal{N}_i}}_{} \frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

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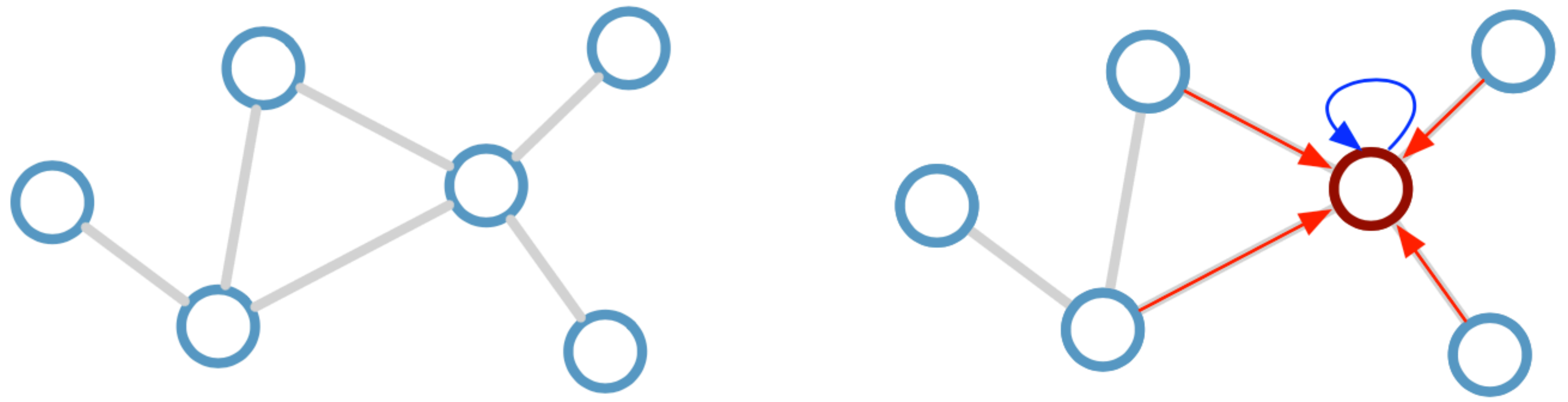

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Aggregate Messages

Update Node Representation

Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

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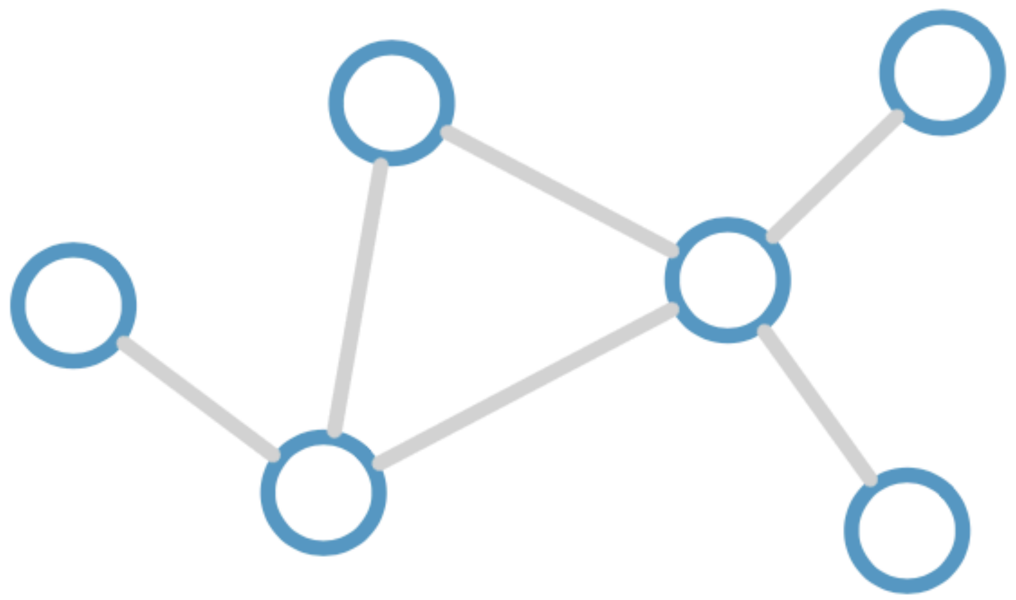

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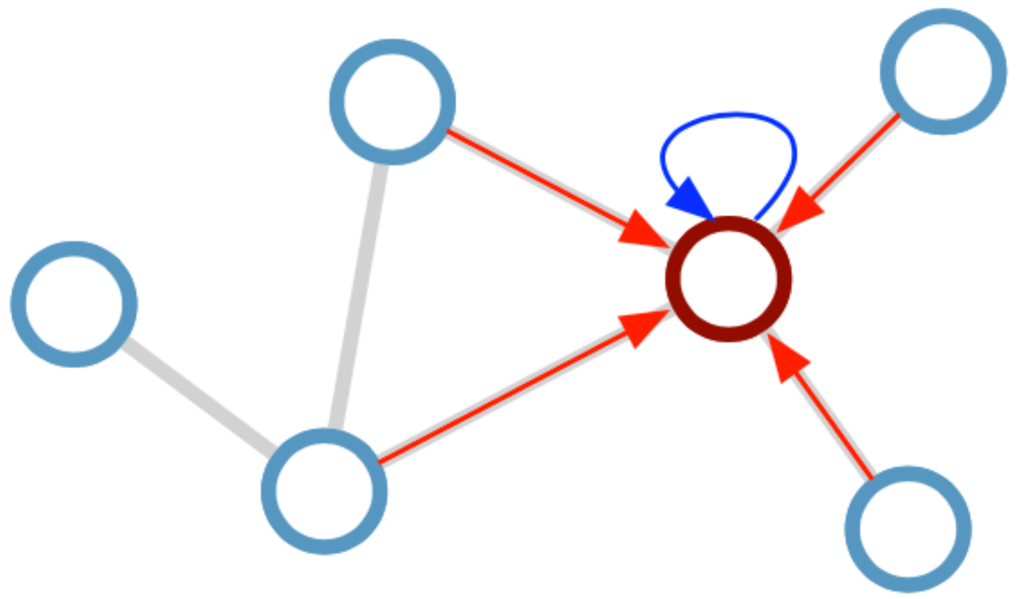

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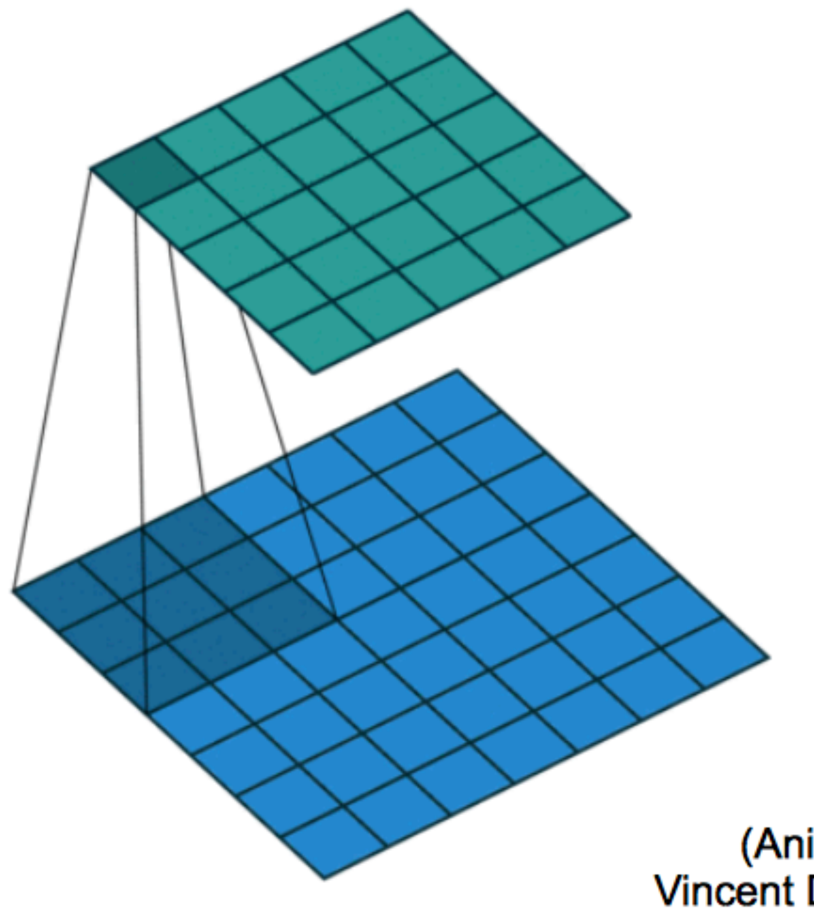
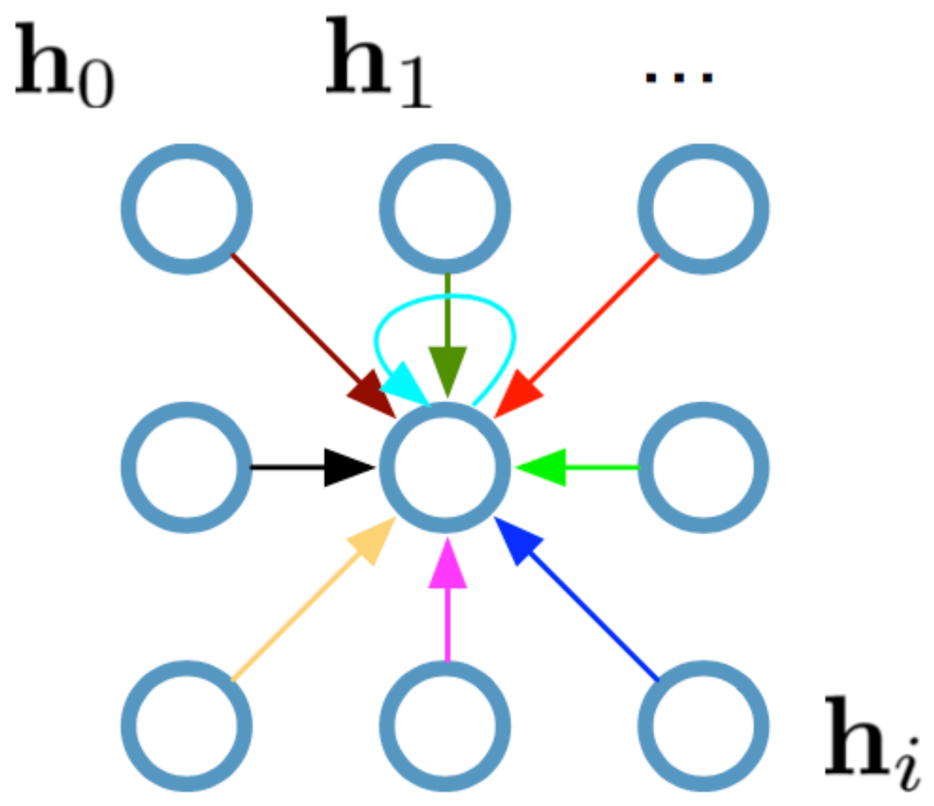
* slide from Thomas Kipf, **University of Amsterdam**

Recap: Convolutional Neural Networks (CNNs) on Grids

Single CNN layer with 3x3 filter:


(Animation by Vincent Dumoulin)



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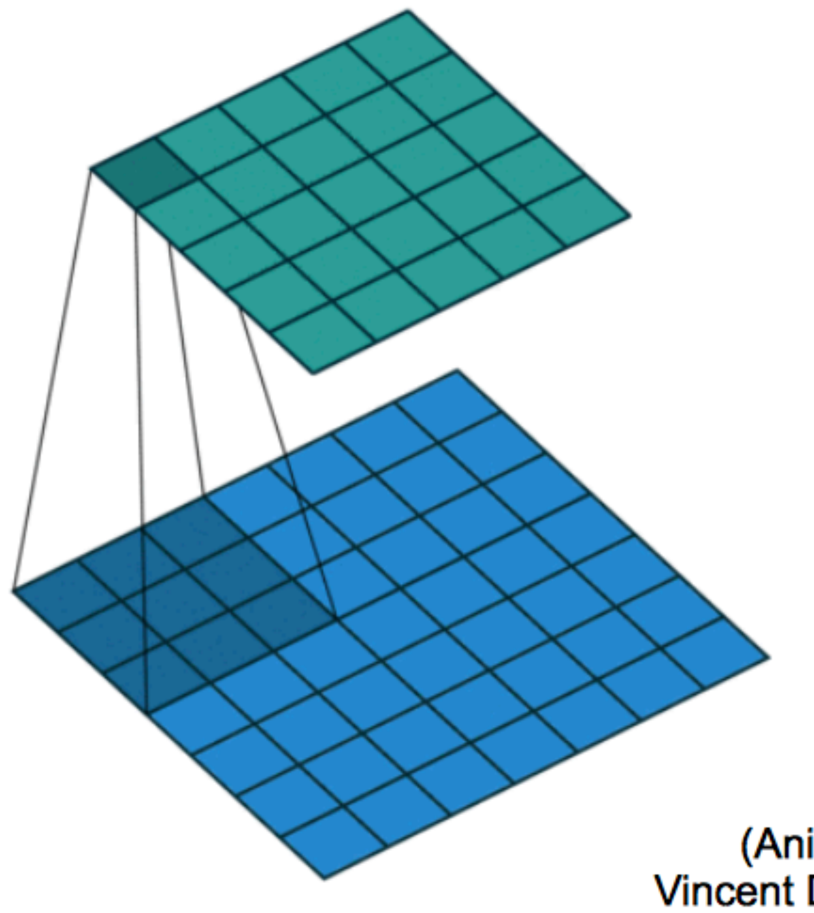

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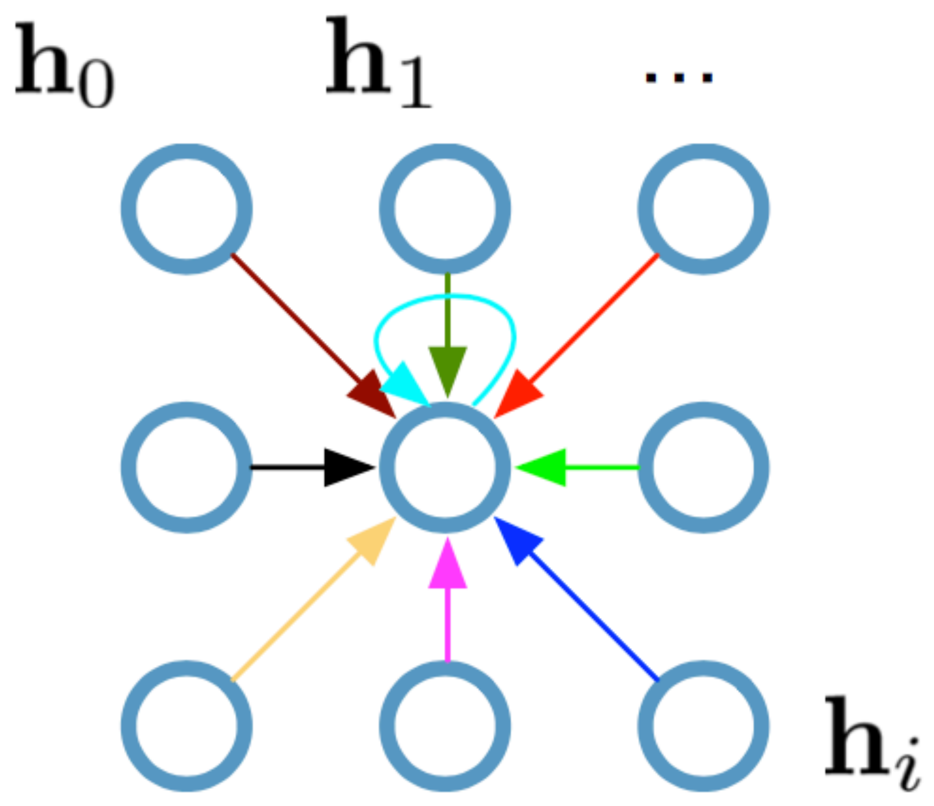

$\mathbf{h}_i \in \mathbb{R}^F$ are (hidden layer) activations of a pixel/node

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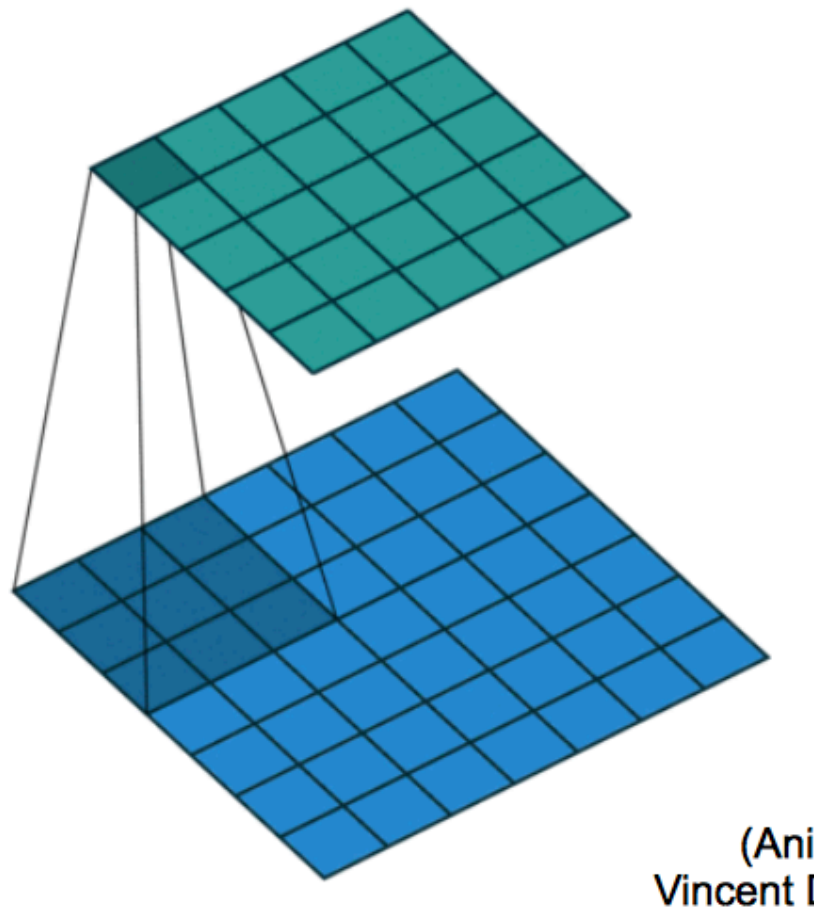

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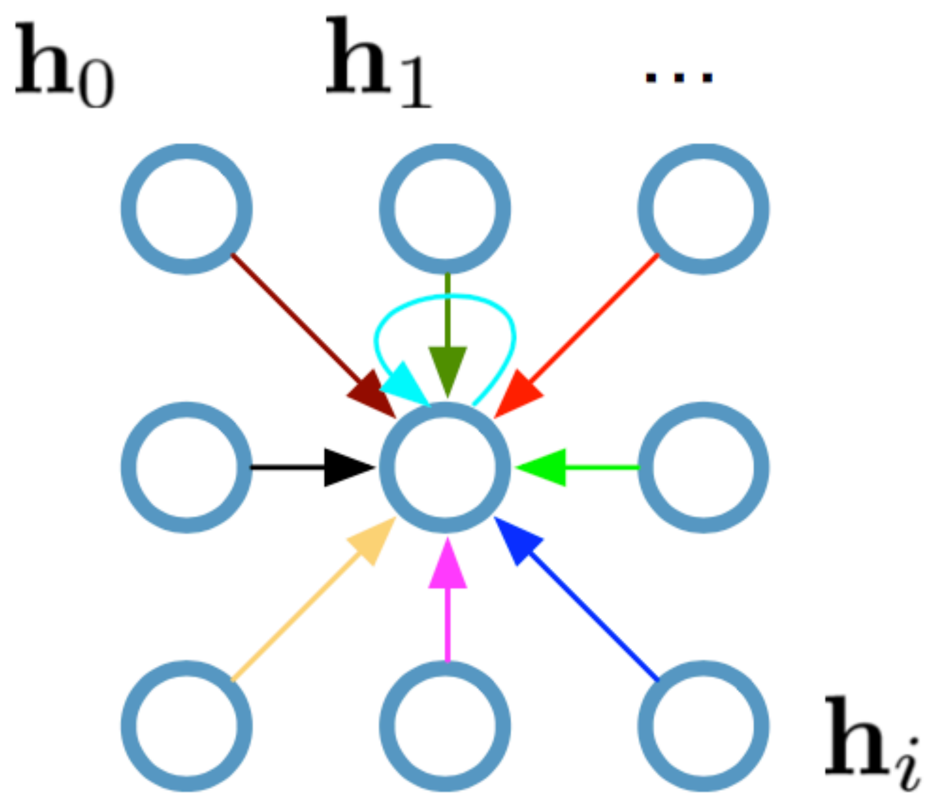

Update for a single pixel:

- Transform messages individually $\mathbf{W}_i \mathbf{h}_i$
- Add everything up $\sum_i \mathbf{W}_i \mathbf{h}_i$

$\mathbf{h}_i \in \mathbb{R}^F$ are (hidden layer) activations of a pixel/node

* slide from Thomas Kipf, **University of Amsterdam**

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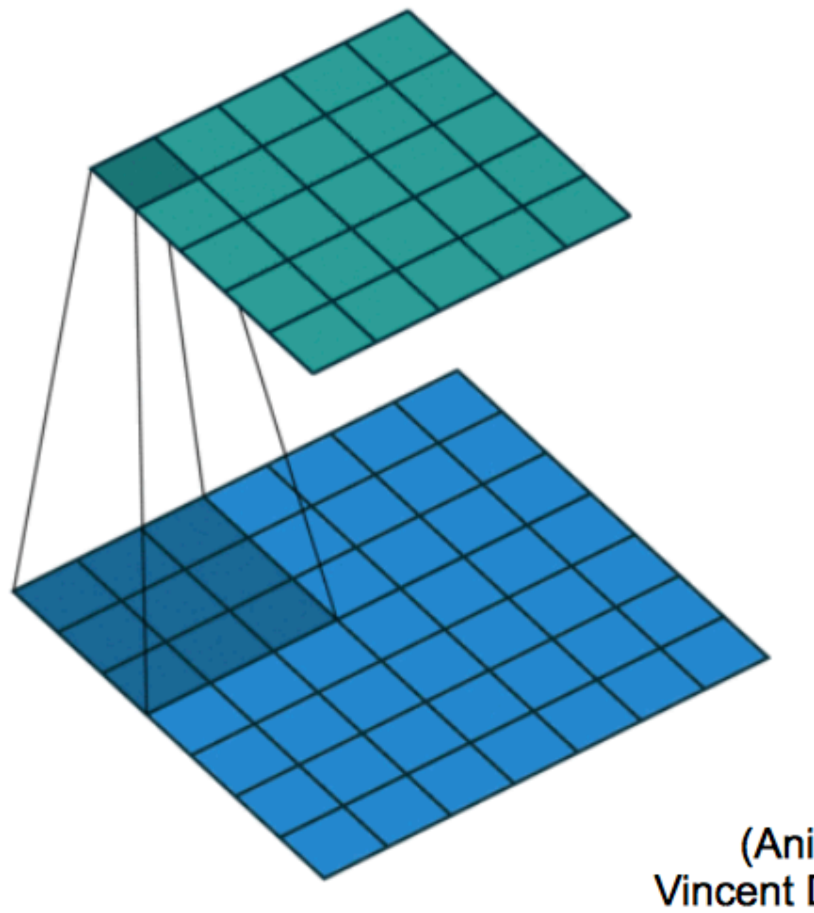

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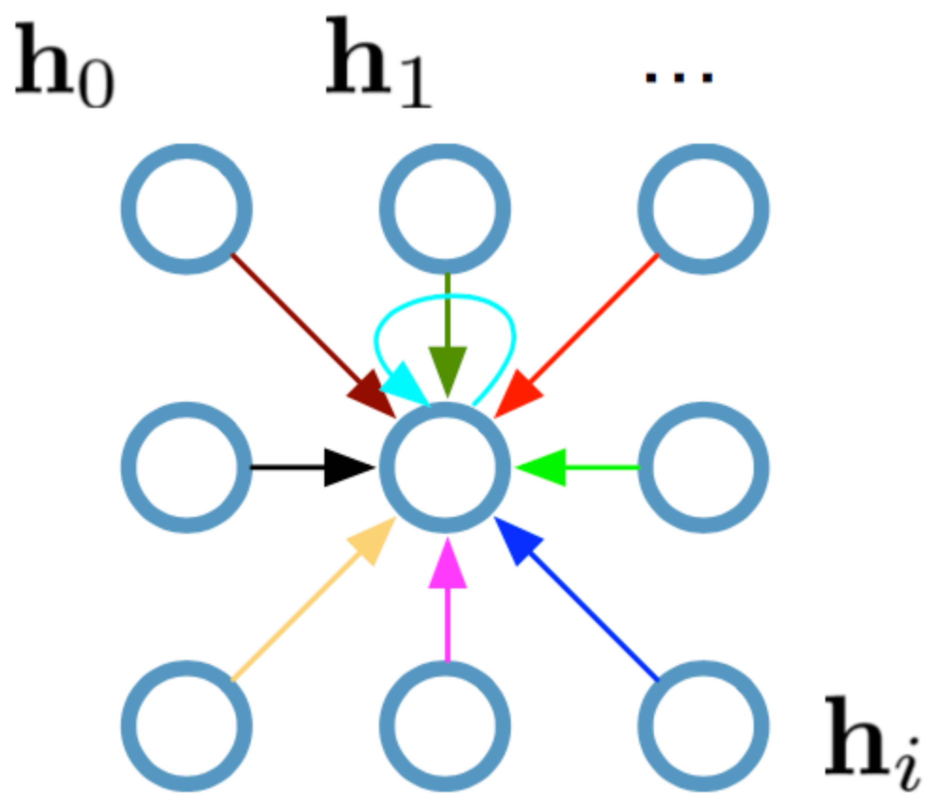

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$\mathbf{h}_i \in \mathbb{R}^F$ are (hidden layer) activations of a pixel/node

Full update:

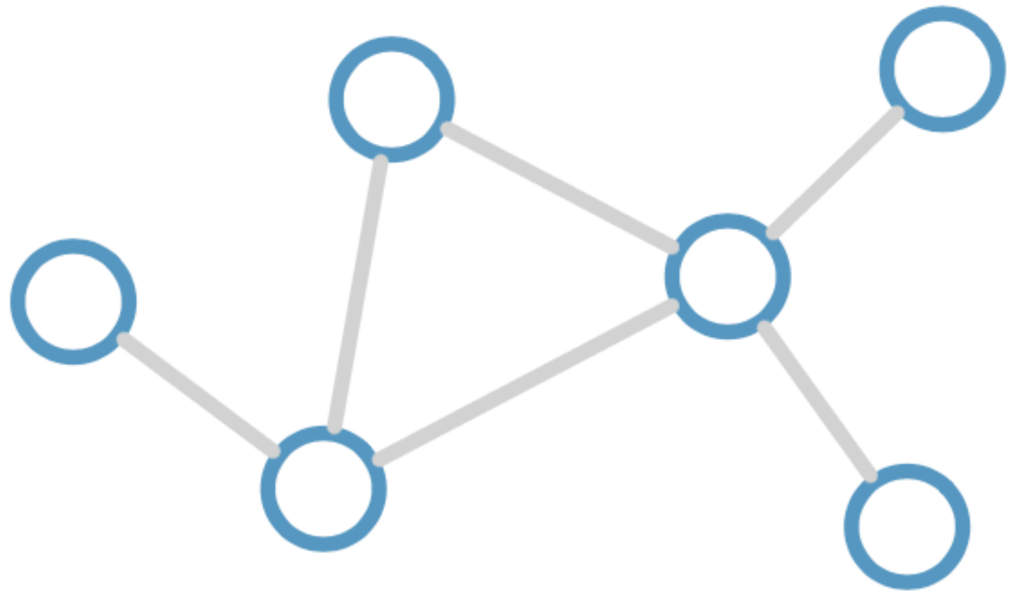
$$\mathbf{h}_4^{(l+1)} = \sigma\left(\mathbf{W}_0^{(l)}\mathbf{h}_0^{(l)} + \mathbf{W}_1^{(l)}\mathbf{h}_1^{(l)} + \cdots + \mathbf{W}_8^{(l)}\mathbf{h}_8^{(l)}\right)$$

* slide from Thomas Kipf, **University of Amsterdam**

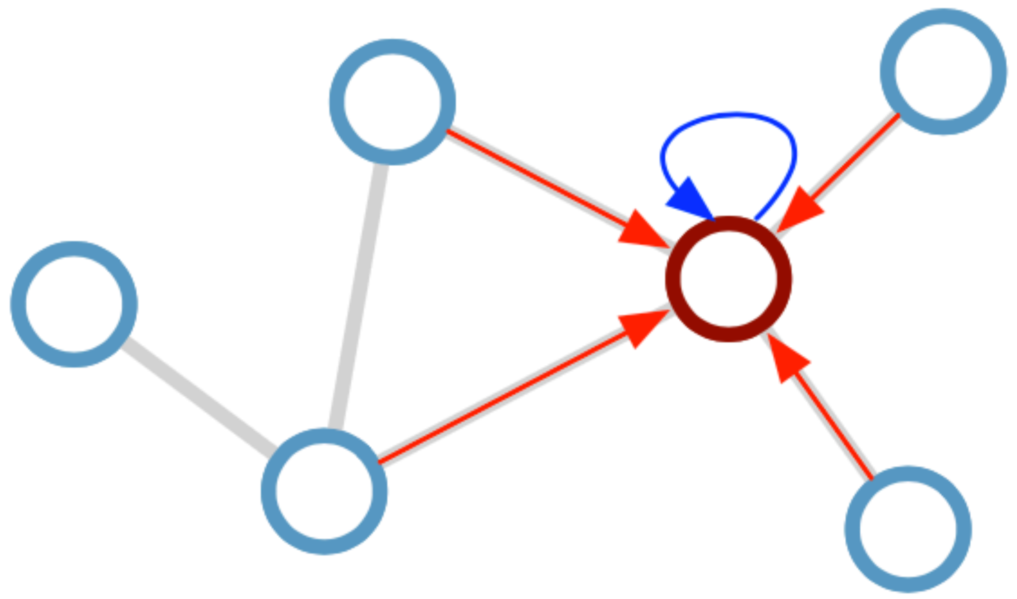
Graph Convolutional Networks (GCNs)

Kipf & Welling (ICLR 2017), related previous works by Duvenaud et al. (NIPS 2015) and Li et al. (ICLR 2016)

Consider this undirected graph:



Calculate update for node in red:



Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (fixed/trainable)

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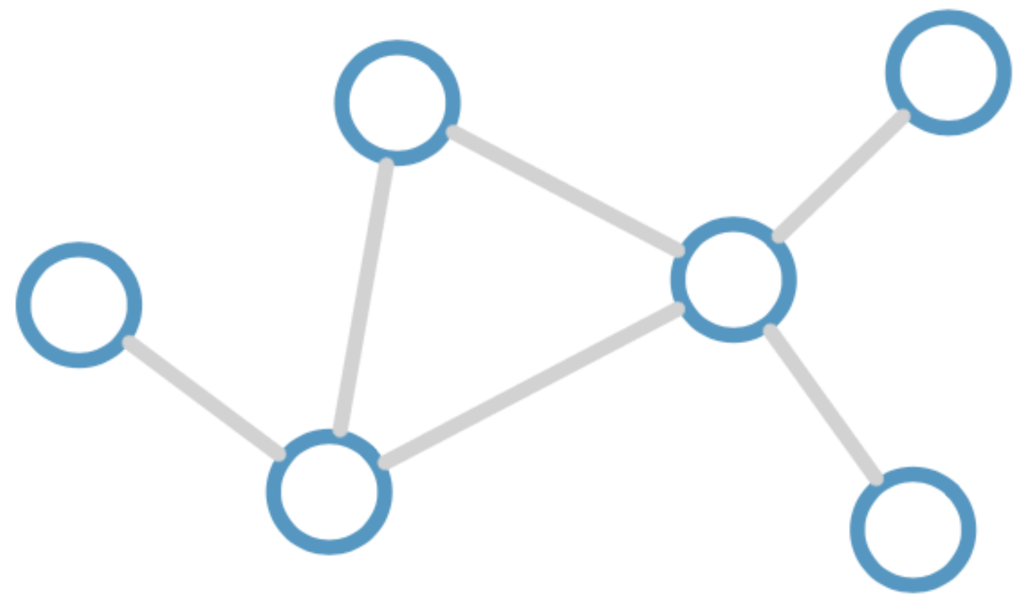

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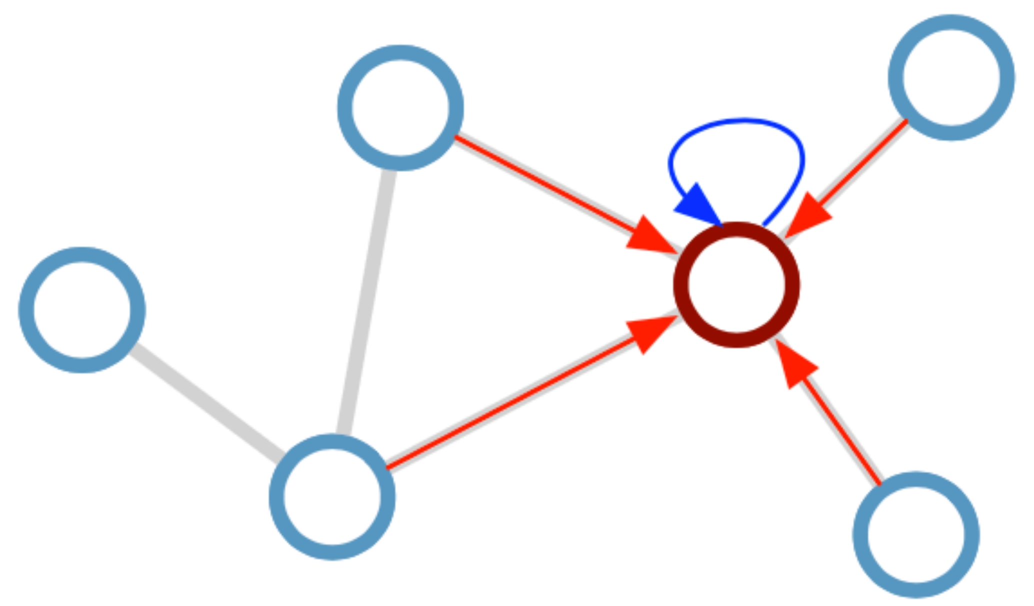

No self loops, or normalization:

$$\sigma(\mathbf{A}\mathbf{H}\mathbf{W}_1^{(l)})$$

Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

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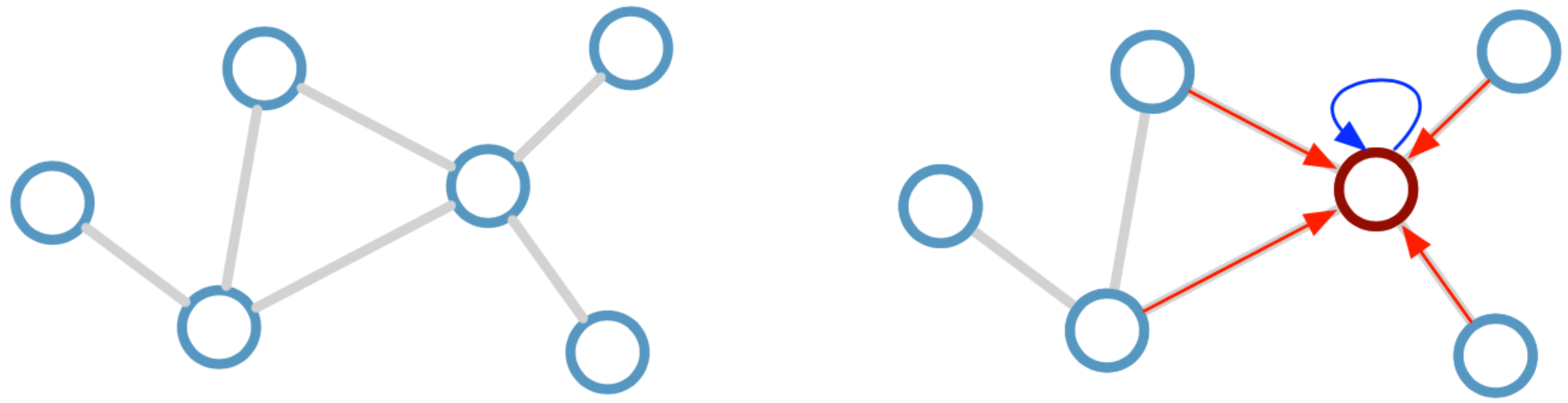

No self loops, or normalization:

$$\sigma(\mathbf{A}\mathbf{H}\mathbf{W}_1^{(l)})$$

Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\qquad \sum_{j \in \mathcal{N}_i} \mathbf{h}_j^{(l)} \mathbf{W}_1^{(l)} \right)$$

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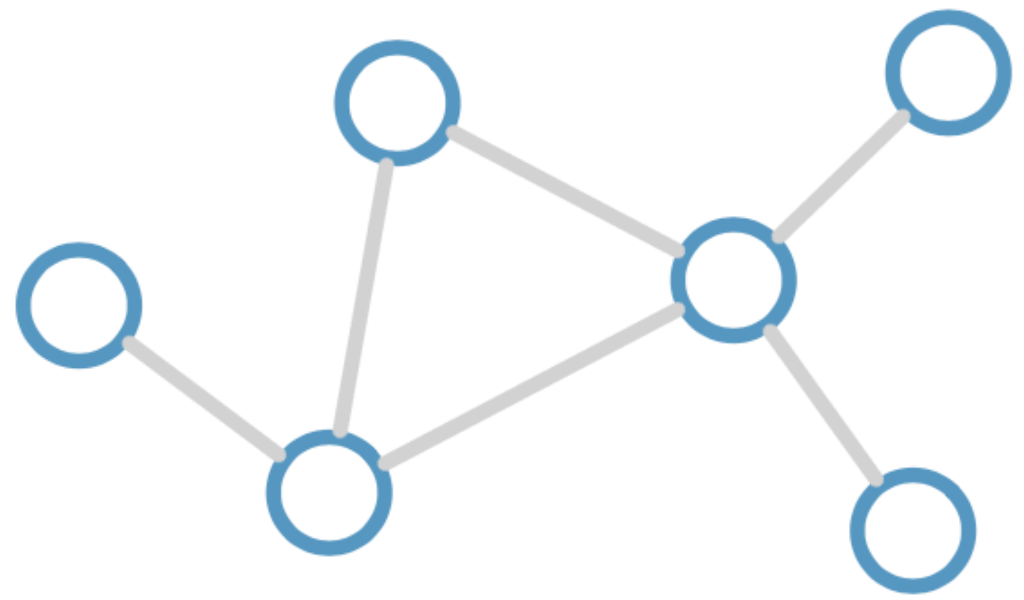

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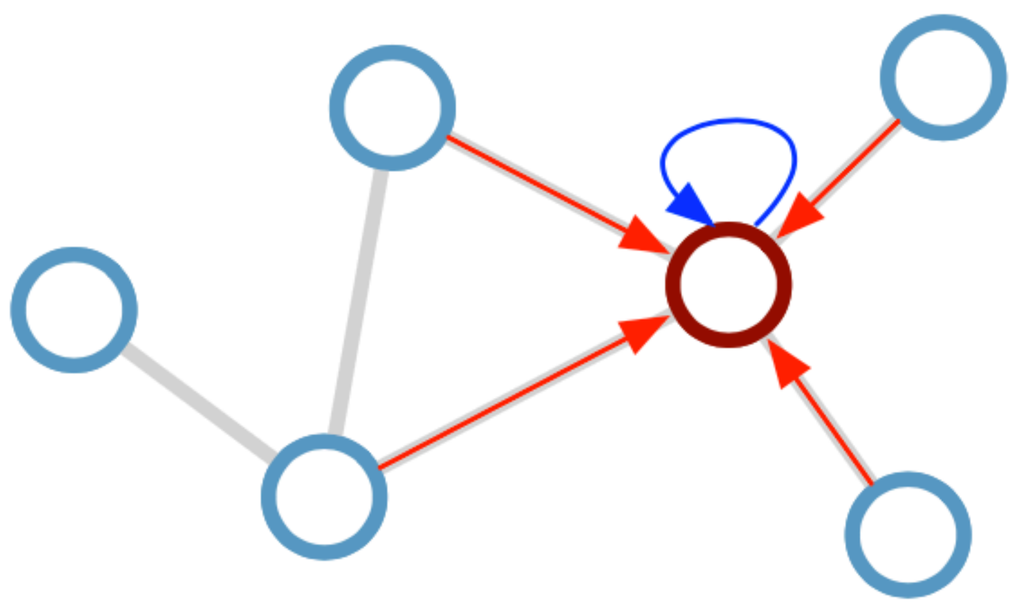

No self loops, or normalization:

$$\sigma(\mathbf{A}\mathbf{H}\mathbf{W}_1^{(l)})$$

+ self loops:

$$\sigma((\mathbf{A}+\mathbf{I})\mathbf{H}\mathbf{W}_1^{(l)})$$

Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i} \mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (fixed/trainable)

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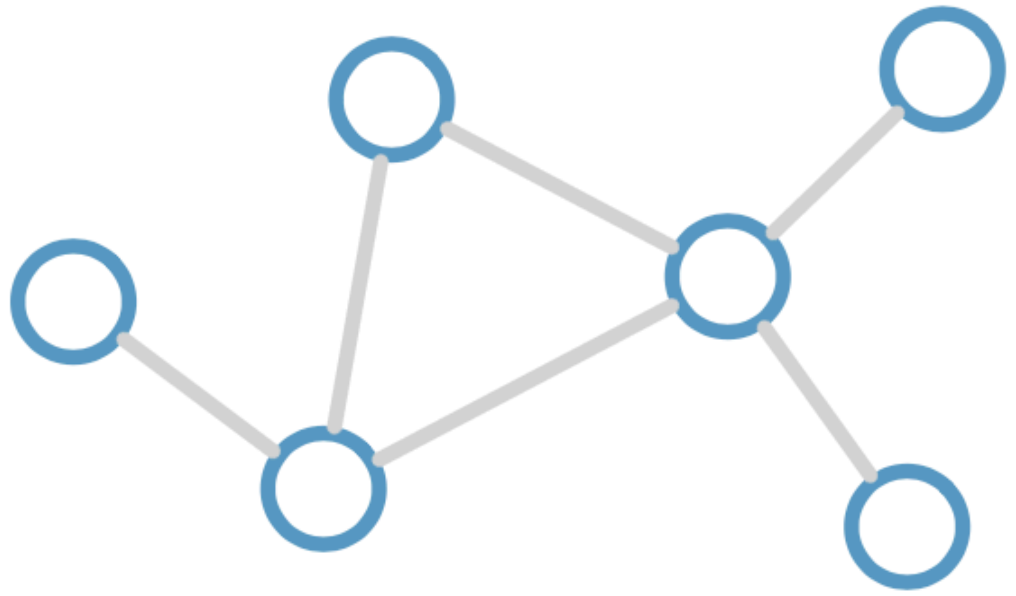

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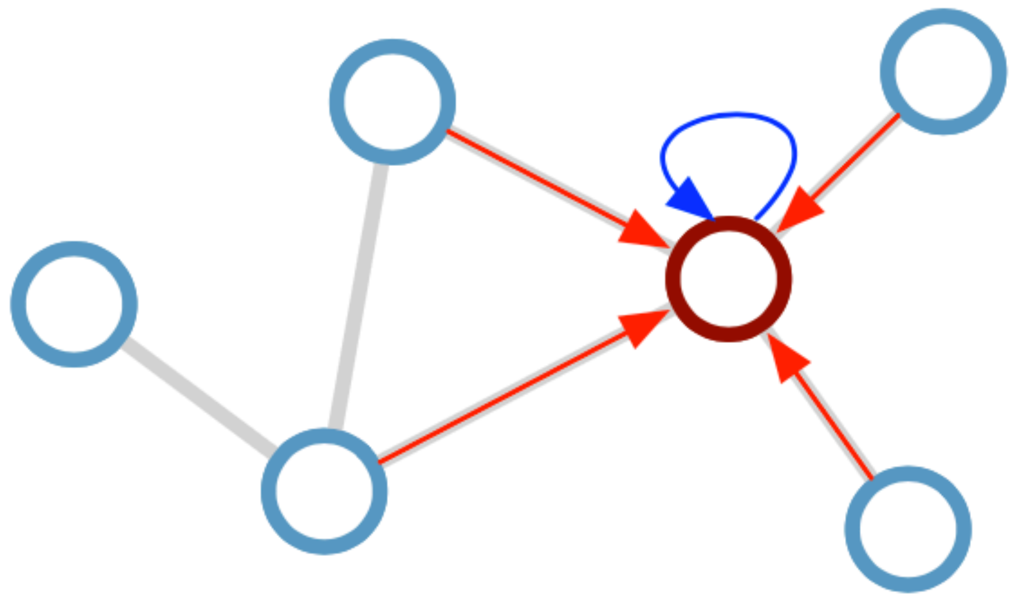


Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

No self loops, or normalization:

$$\sigma(\mathbf{A}\mathbf{H}\mathbf{W}_1^{(l)})$$

\+ self loops:

$$\sigma((\mathbf{A}+\mathbf{I})\mathbf{H}\mathbf{W}_1^{(l)})$$

\+ normalization:

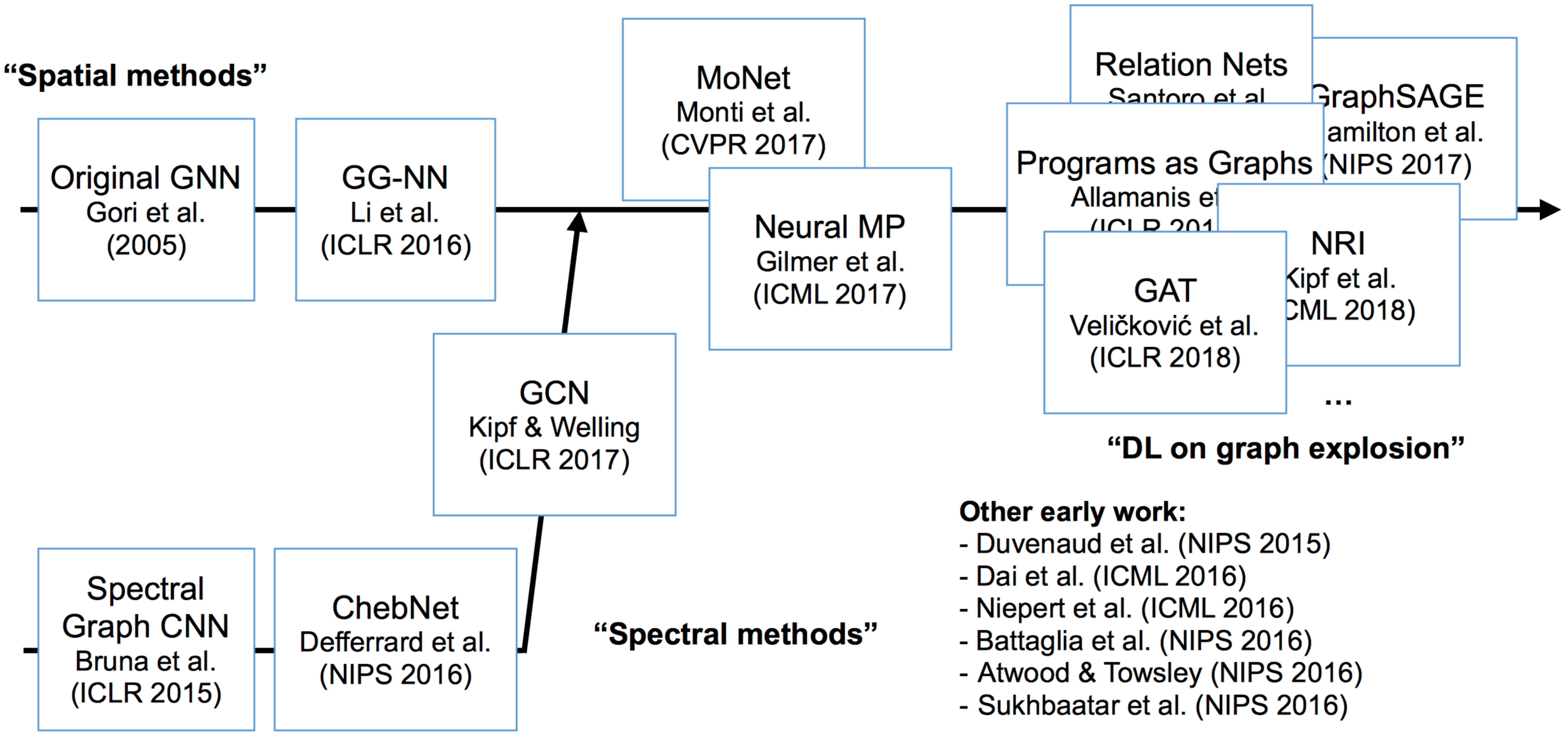
$$\sigma([\mathbf{D}^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}]\mathbf{H}\mathbf{W}_1^{(l)})$$

$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (fixed/trainable)

* slide from Thomas Kipf, **University of Amsterdam**

A **Brief History** of Graph Neural Nets



Other early work:
- Duvenaud et al. (NIPS 2015)
- Dai et al. (ICML 2016)
- Niepert et al. (ICML 2016)
- Battaglia et al. (NIPS 2016)
- Atwood & Towsley (NIPS 2016)
- Sukhbaatar et al. (NIPS 2016)

(slide inspired by Alexander Gaunt's talk on GNNs)

Graph Convolutional Networks (GCNs)

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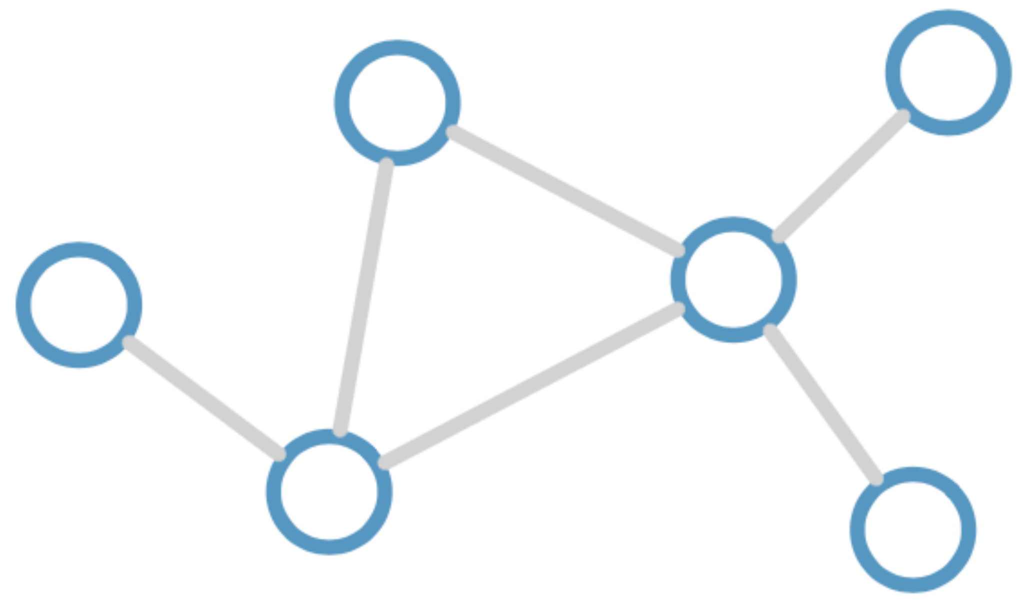
Consider this undirected graph:



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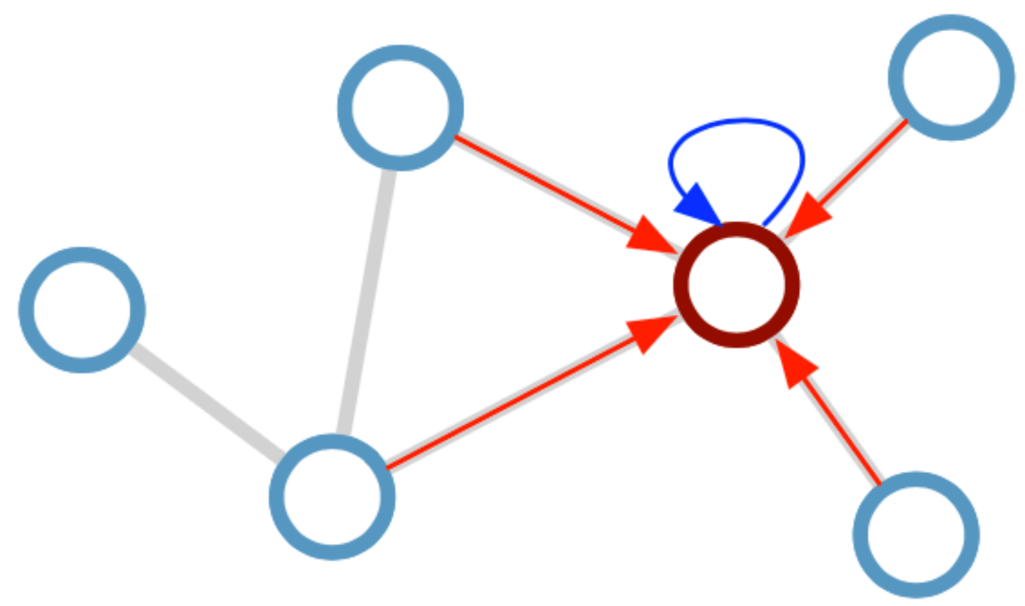


Update rule: $$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

No self loops, or normalization:

$$\sigma(\mathbf{AHW}_1^{(l)})$$

+ self loops:

$$\sigma((\mathbf{A}+\mathbf{I})\mathbf{HW}_1^{(l)})$$

+ normalization:

$$\sigma([\mathbf{D}^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}]\mathbf{HW}_1^{(l)})$$

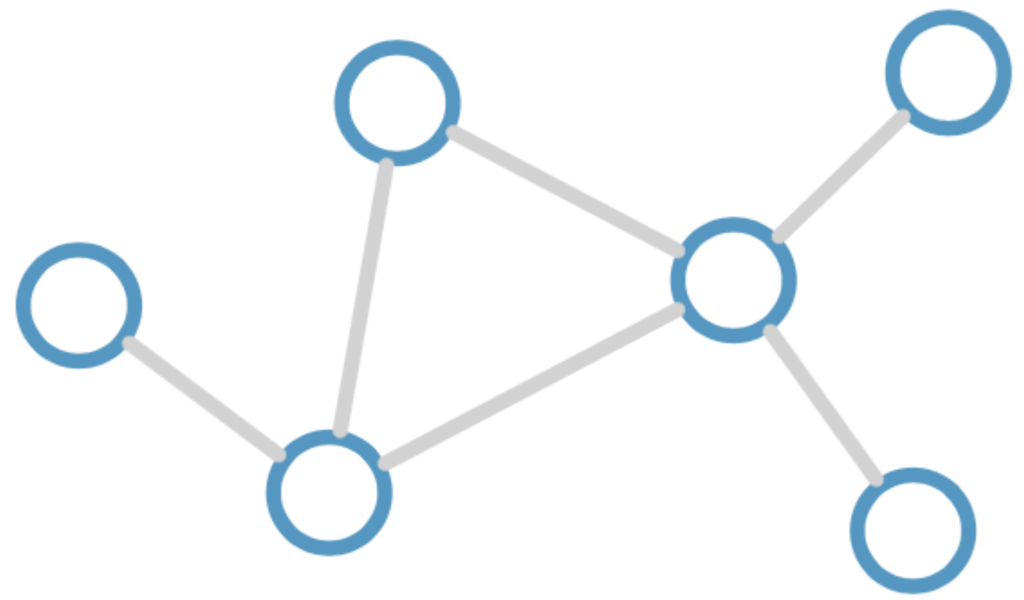
$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (fixed/trainable)

* slide from Thomas Kipf, **University of Amsterdam**

GCN with **different** node types and feature dimensions

Consider this undirected graph:



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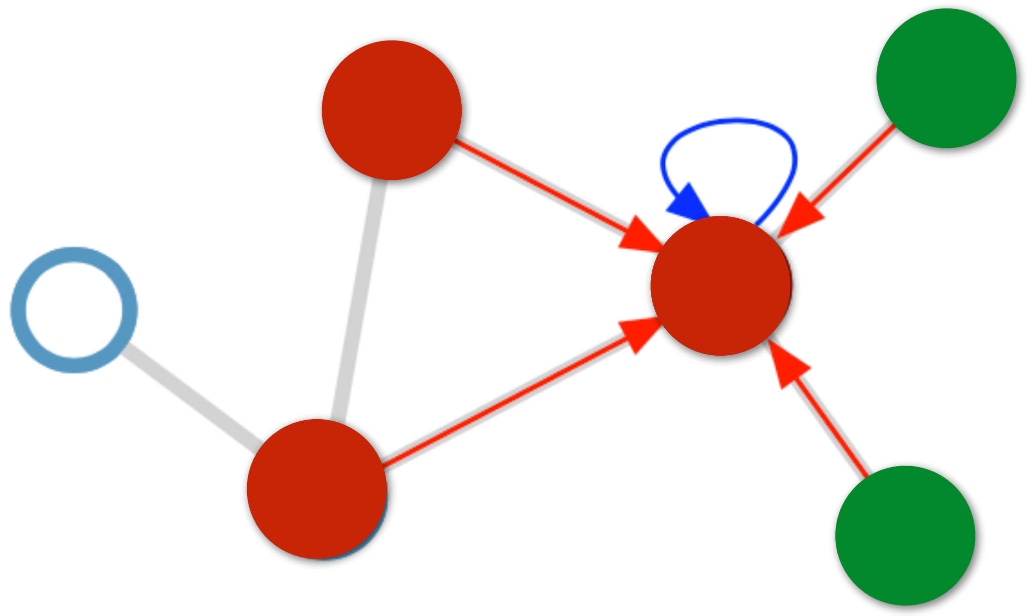


$$\mathbf{W}_0, \mathbf{W}_1 \in \mathbb{R}^{\mathbf{F}\times\mathbf{F}}$$

$$\mathbf{W}_2 \in \mathbb{R}^{\mathbf{F}\times\mathbf{F}'}$$

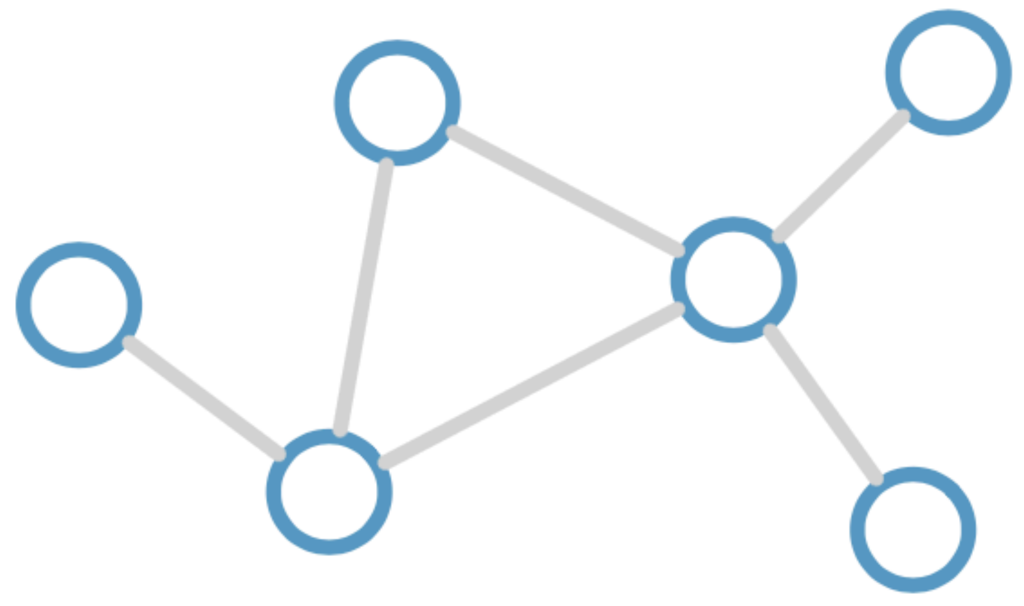
Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_2^{(l)}\right)$$

Graph Convolutional Networks (GCNs)

Kipf & Welling (ICLR 2017), related previous works by Duvenaud et al. (NIPS 2015) and Li et al. (ICLR 2016)

Consider this undirected graph:



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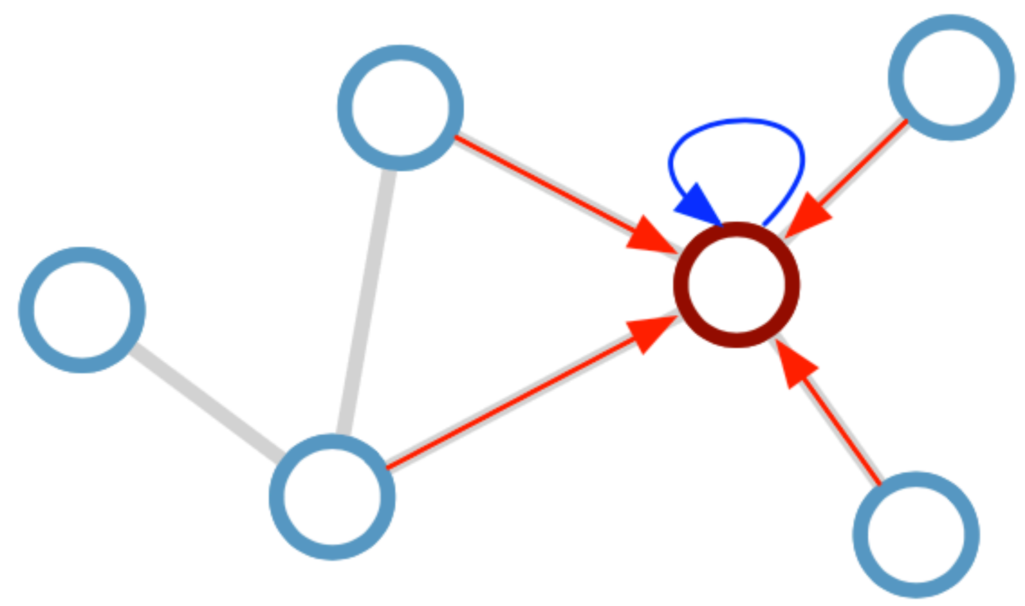


Update rule:

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

Desirable properties:

- Weight sharing over all locations
- Invariance to permutations
- Linear complexity O(E)
- Applicable both in transductive and inductive settings

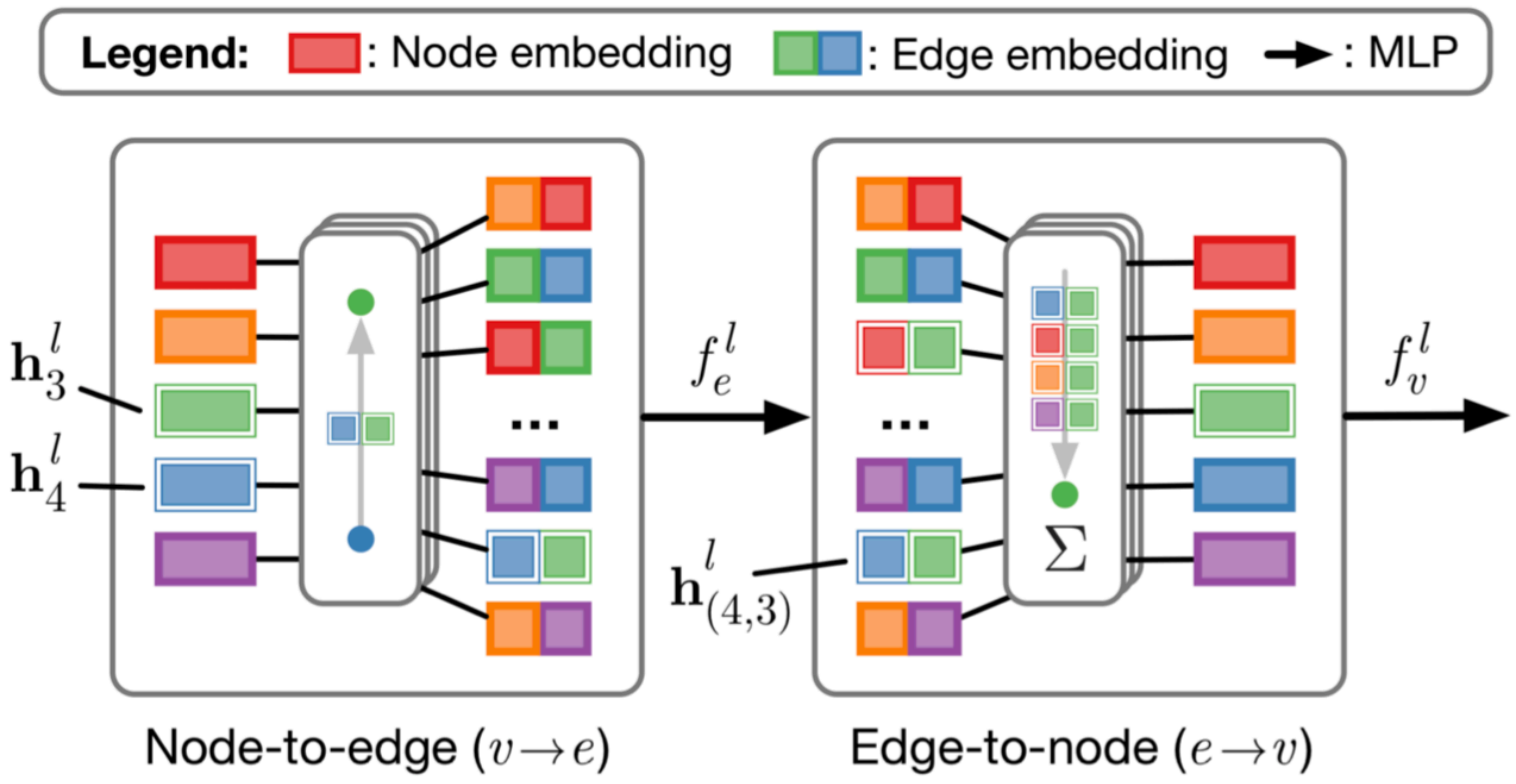
$\mathcal{N}_i$: neighbor indices

c_{ij} : norm. constant (fixed/trainable)

* slide from Thomas Kipf, **University of Amsterdam**

GNNs with **Edge** Embeddings

Battaglia et al. (NIPS 2016), Gilmer et al. (ICML 2017), Kipf et al. (ICML 2018)



Note: The nodes and edges need not to have same dimensional representations; (the FC layers) will take care of this

Formally:

$$v \to e: \quad \mathbf{h}_{(i,j)}^l = f_e^l([\mathbf{h}_i^l, \mathbf{h}_j^l, \mathbf{x}_{(i,j)}])$$

$$e \to v: \quad \mathbf{h}_j^{l+1} = f_v^l([\textstyle\sum_{i \in \mathcal{N}_j} \mathbf{h}_{(i,j)}^l, \mathbf{x}_j])$$

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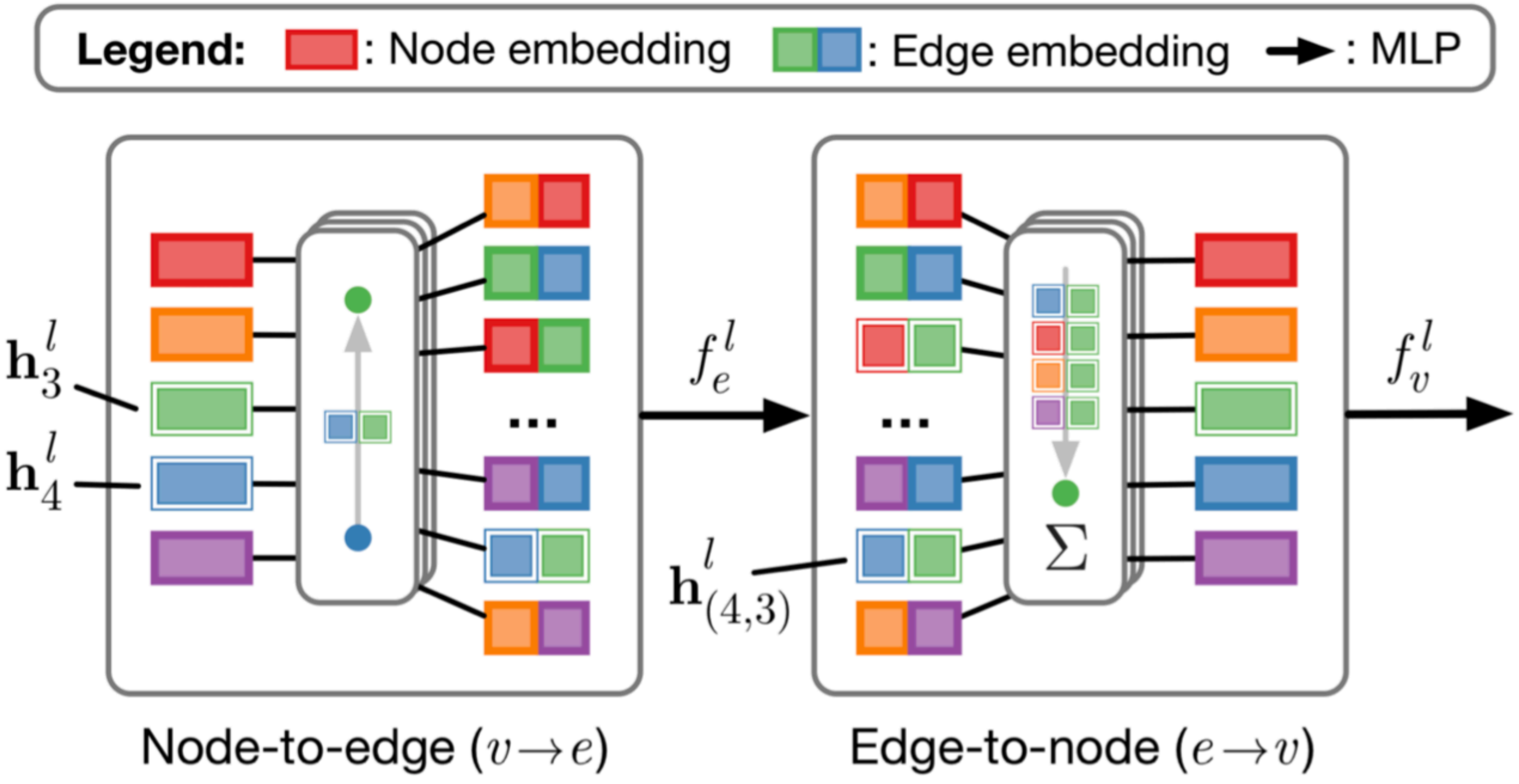

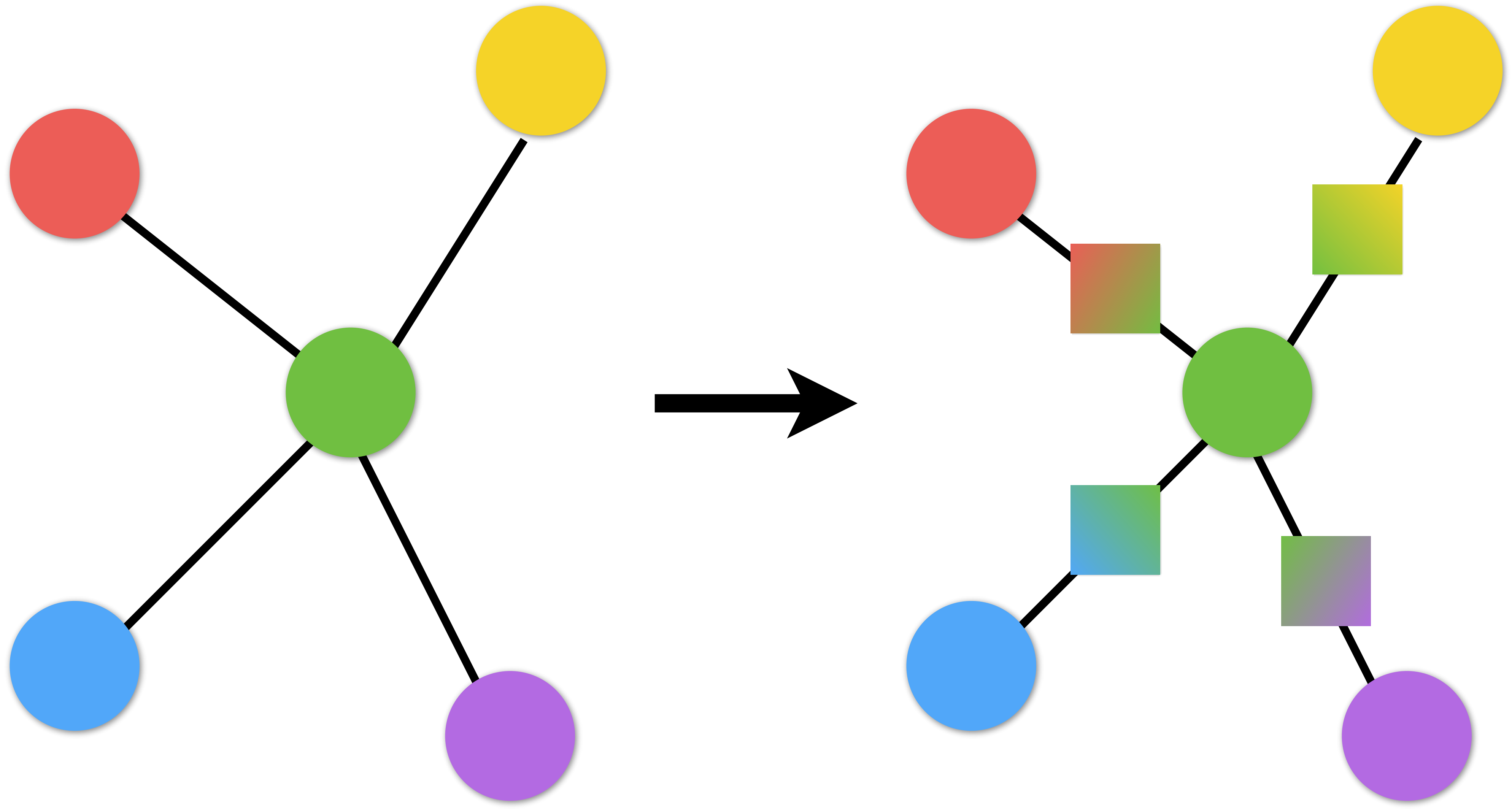

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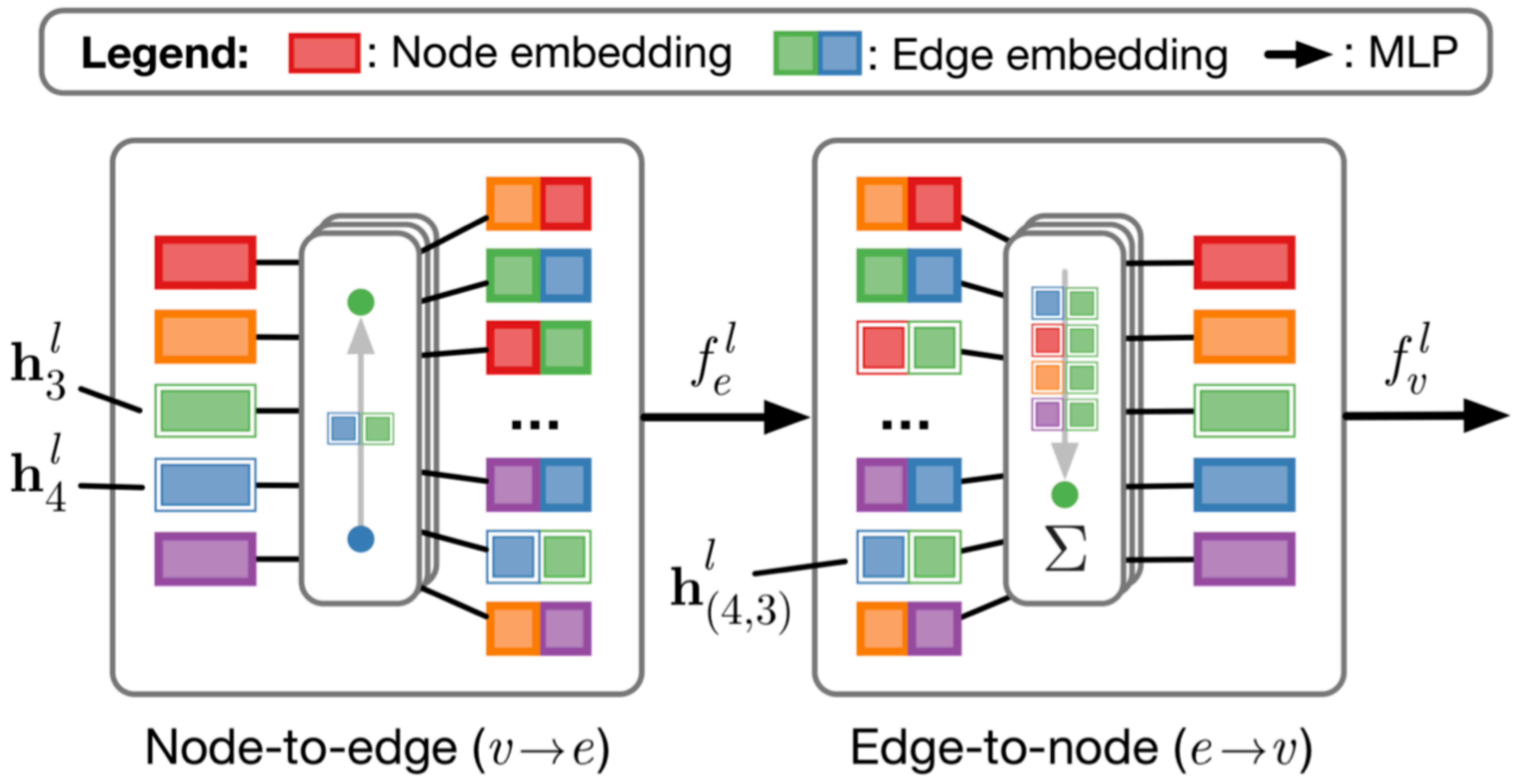

Pros:

- Supports edge features
- More expressive than GCN
- As general as it gets (?)
- Supports sparse matrix ops

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$$v \rightarrow e: \quad \mathbf{h}_{(i,j)}^l = f_e^l([\mathbf{h}_i^l, \mathbf{h}_j^l, \mathbf{x}_{(i,j)}])$$

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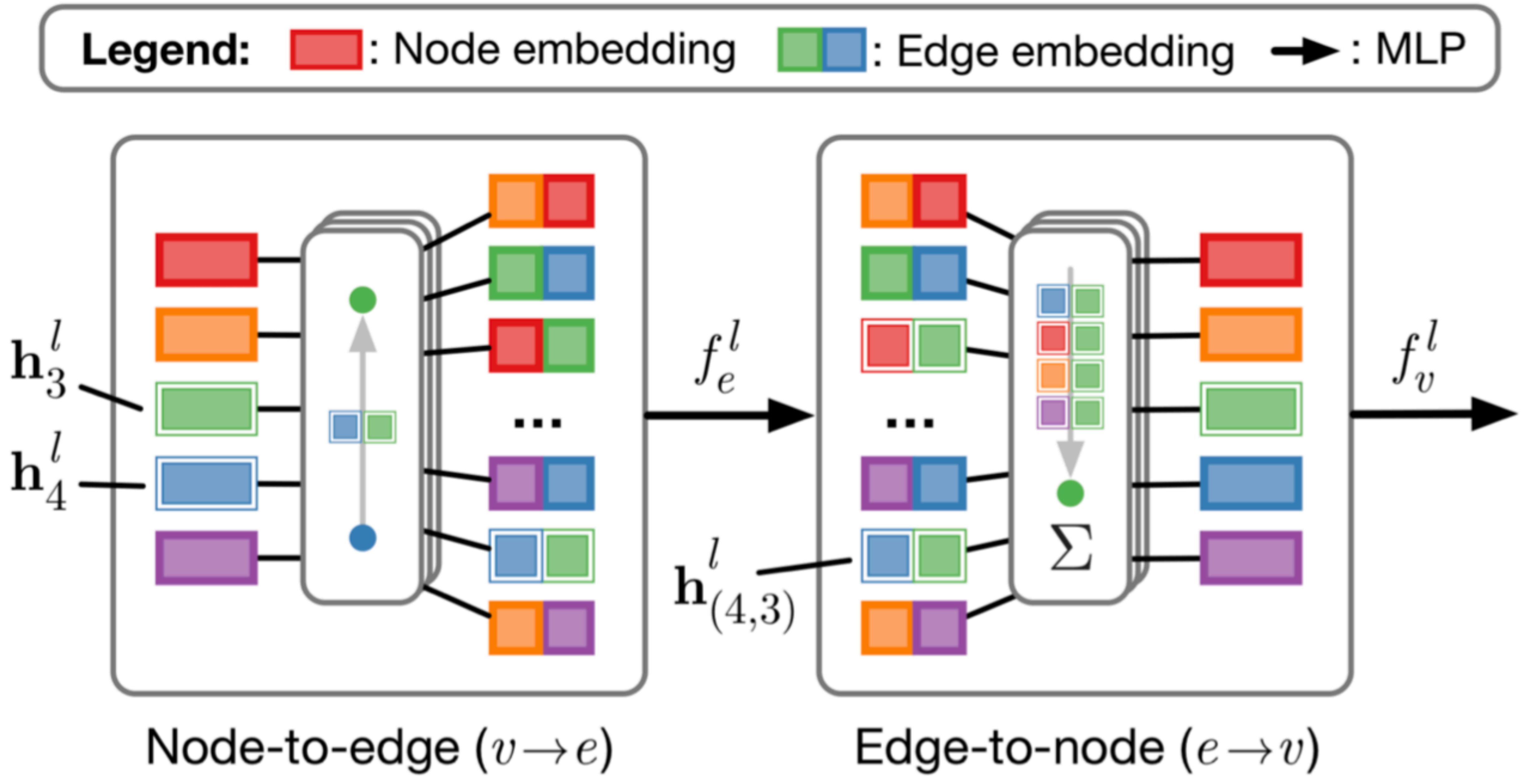

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$$e \to v: \quad \mathbf{h}_j^{l+1} = f_v^l([\textstyle\sum_{i \in \mathcal{N}_j} \mathbf{h}_{(i,j)}^l, \mathbf{x}_j])$$

Pros:

- Supports edge features
- More expressive than GCN
- As general as it gets (?)
- Supports sparse matrix ops

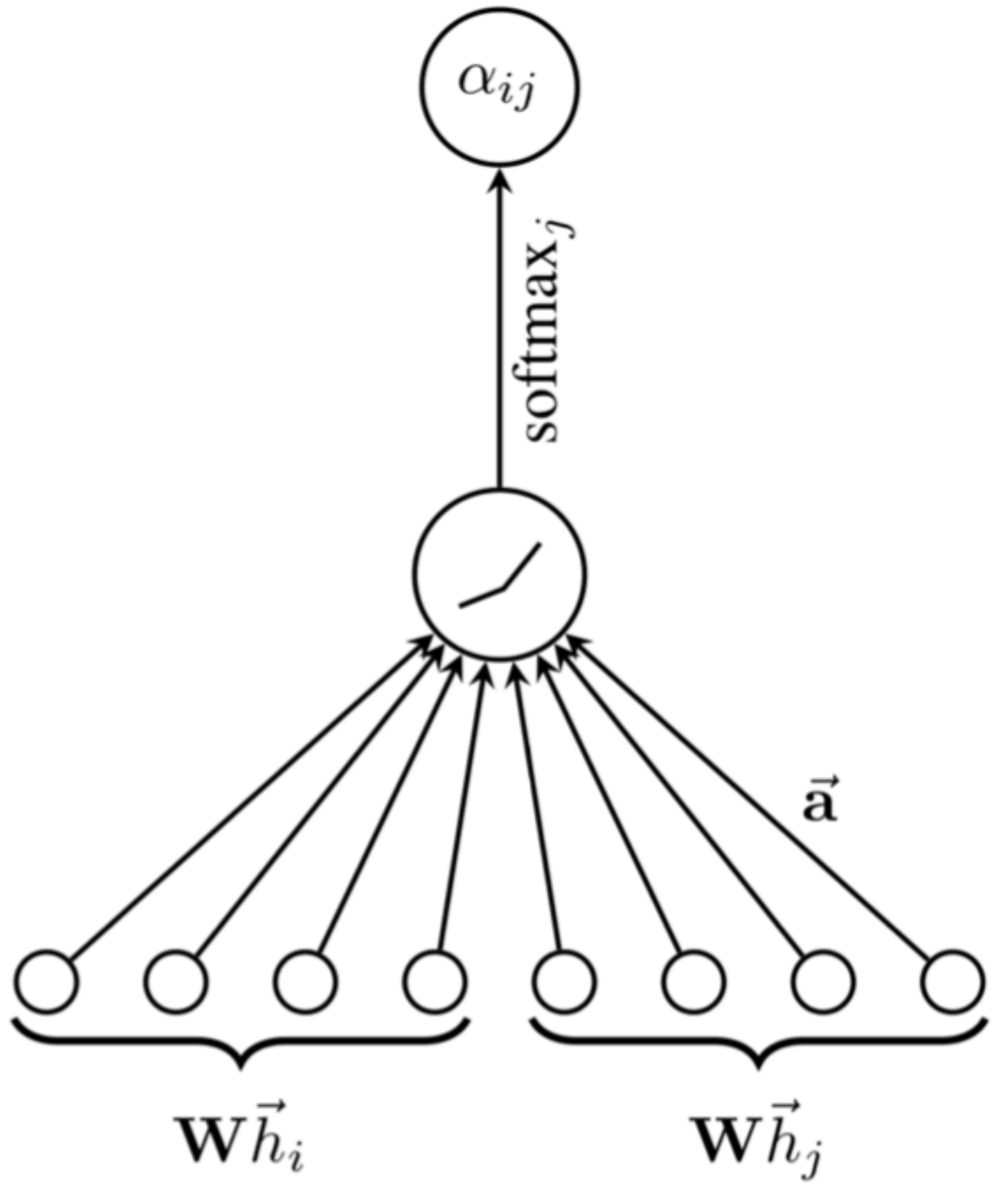
Cons:

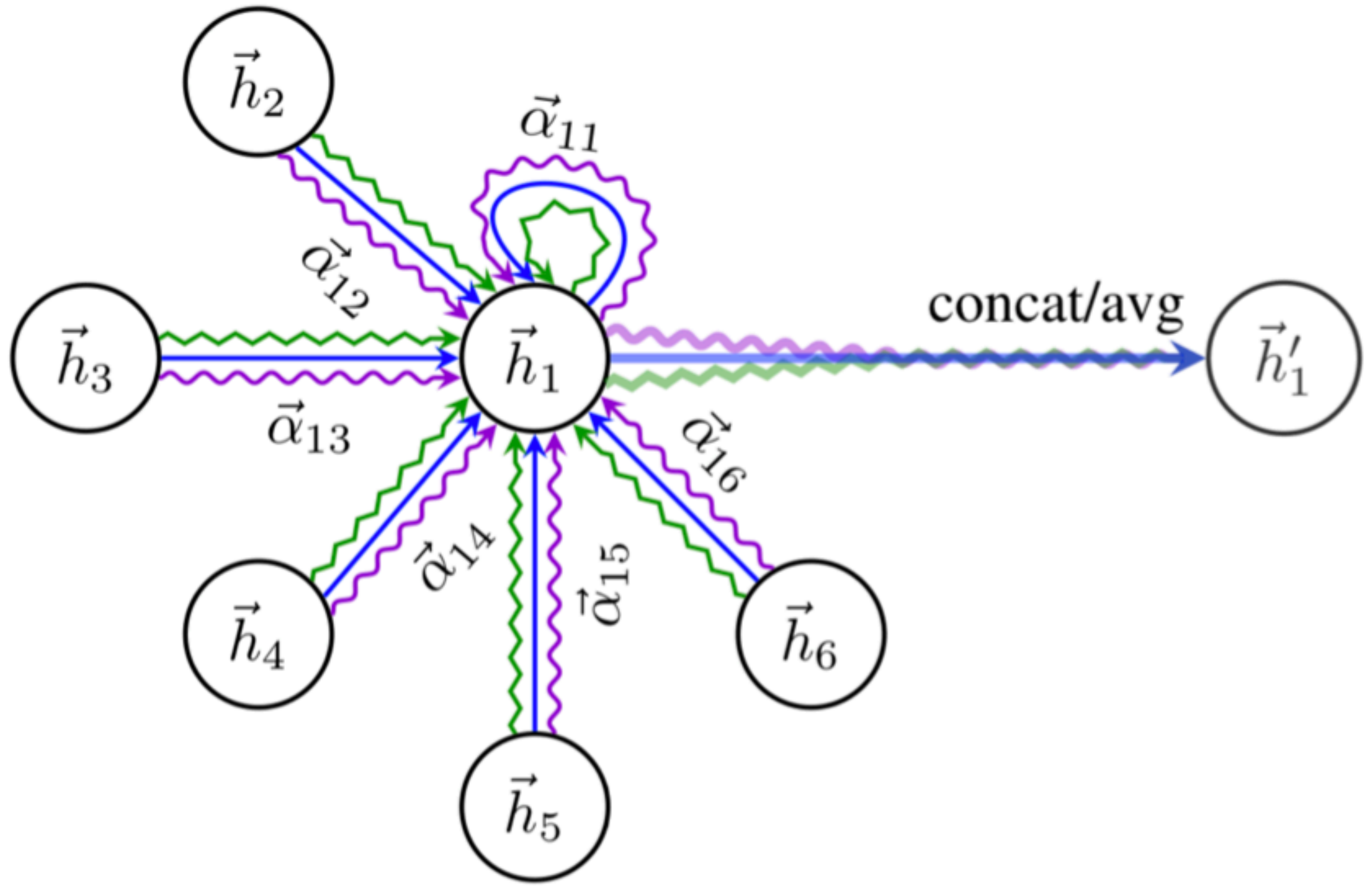
- Need to store intermediate edge-based activations
- Difficult to implement with subsampling

➡ In practice limited to small graphs

Graph Neural Networks (GNNs) with **Attention**

Monti et al. (CVPR 2017), Hoshen (NIPS 2017), Veličković et al. (ICLR 2018)





[Figure from Veličković et al. (ICLR 2018)]

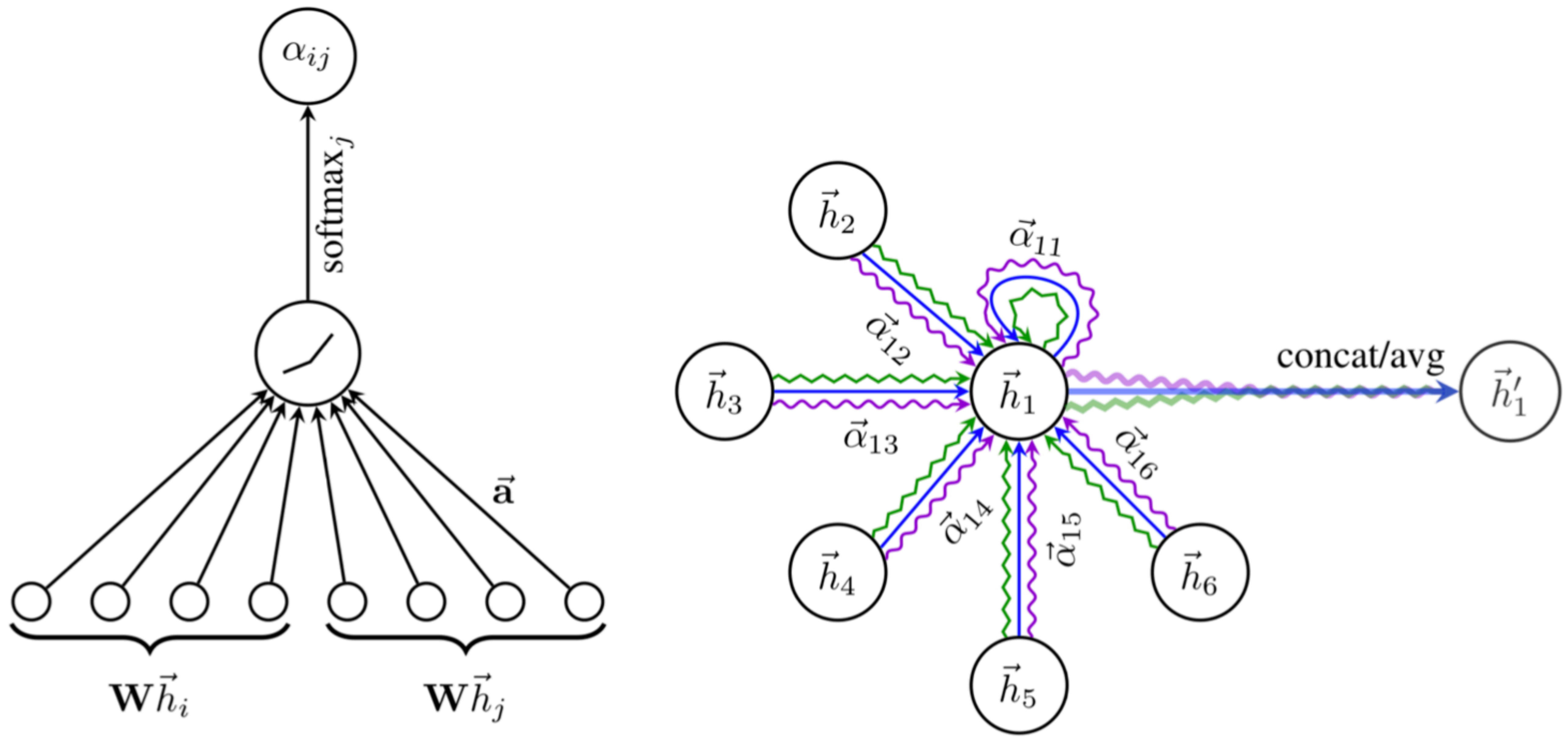
$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\alpha_{ij}^k \mathbf{W}^k \vec{h}_j\right)$$

Multi-graph (k-type edges), a.k.a., can think of it as K attention heads

* slide from Thomas Kipf, **University of Amsterdam**

Graph Neural Networks (GNNs) with **Attention**

Monti et al. (CVPR 2017), Hoshen (NIPS 2017), Veličković et al. (ICLR 2018)



[Figure from Veličković et al. (ICLR 2018)]

$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\alpha_{ij}^{k}\mathbf{W}^k\vec{h}_j\right) \qquad \alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_k]\right)\right)}$$

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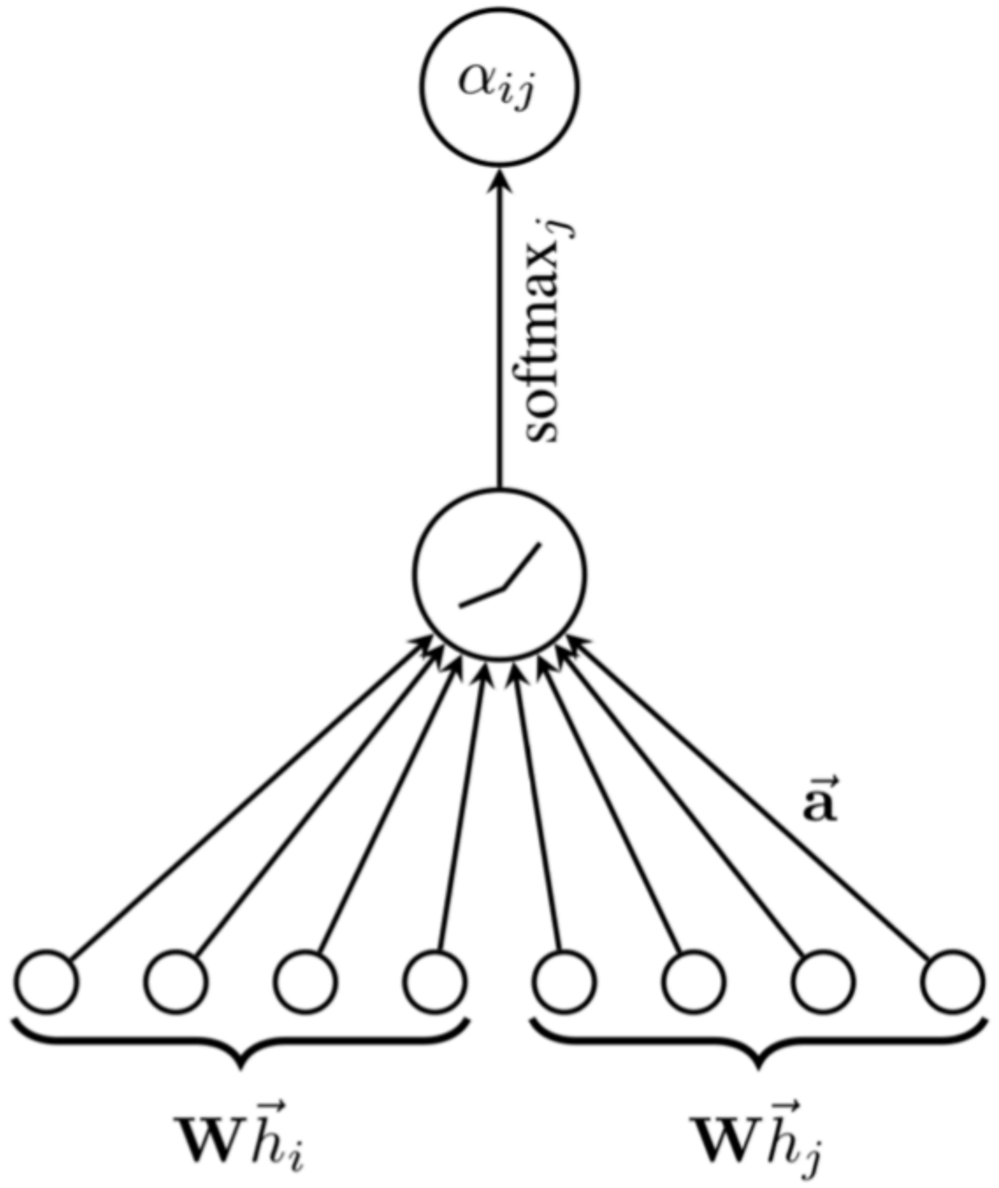

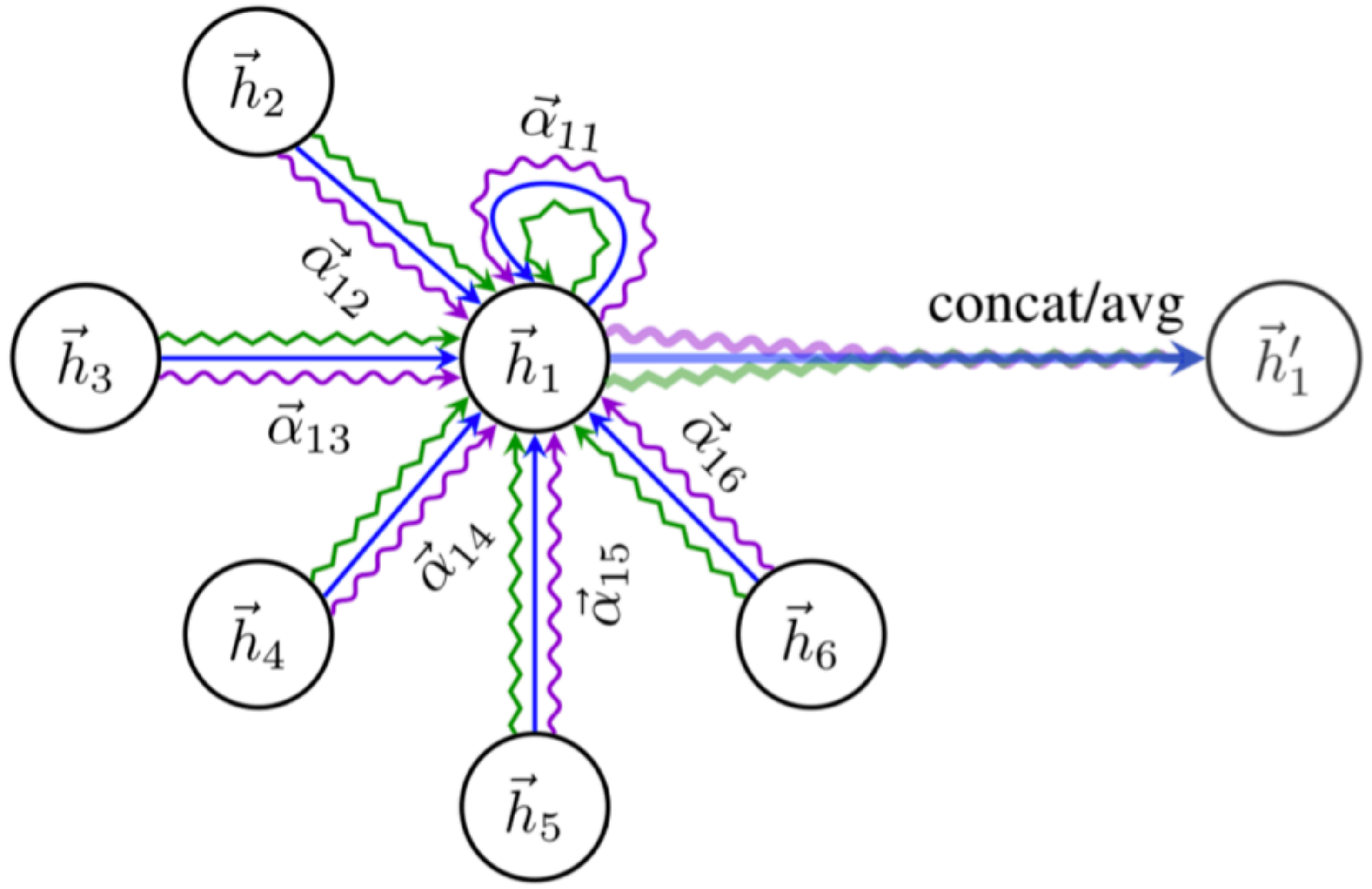

[Figure from Veličković et al. (ICLR 2018)]

Pros:

- No need to store intermediate edge-based activation vectors (when using dot-product attn.)
- Slower than GCNs but faster than GNNs with edge embeddings

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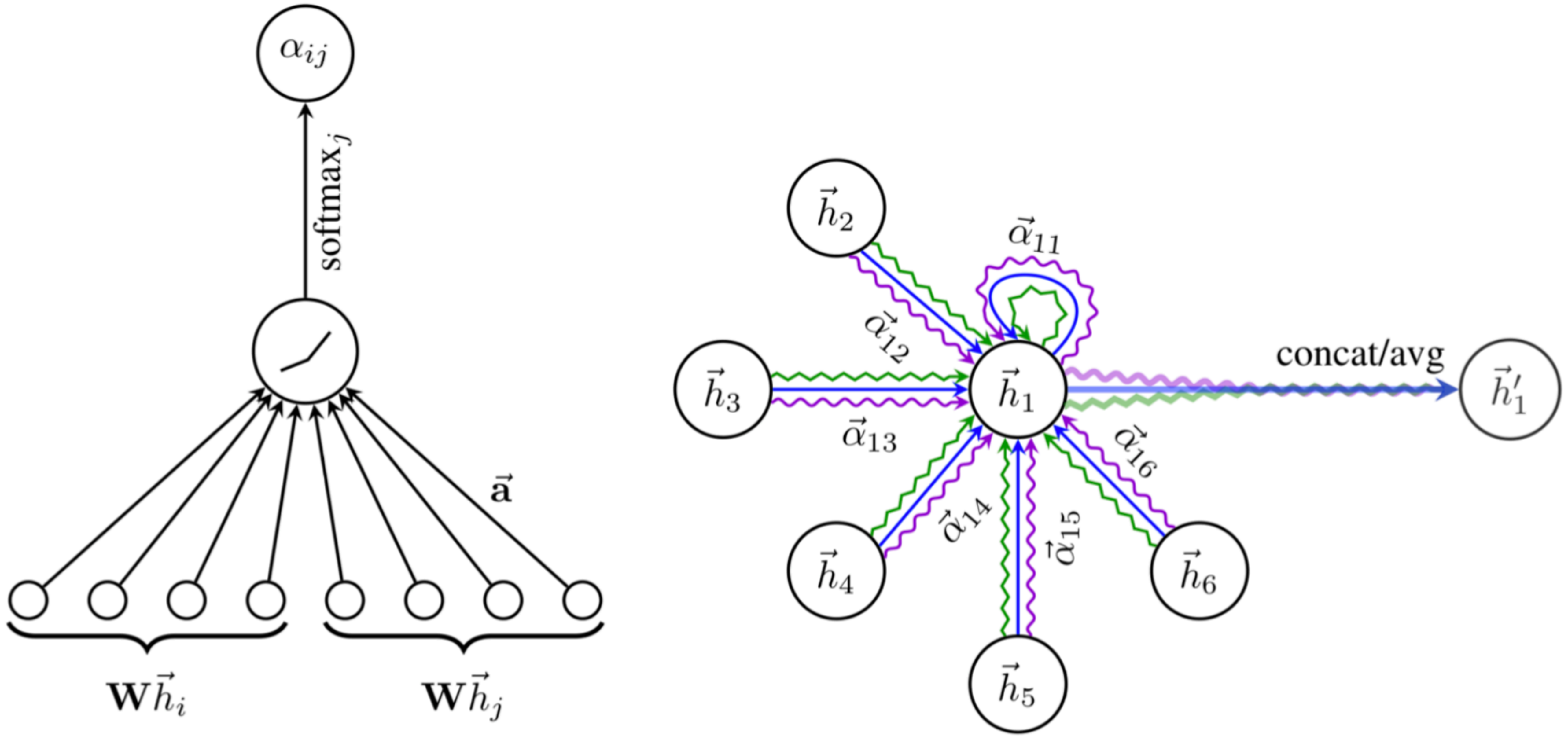


[Figure from Veličković et al. (ICLR 2018)]

Pros:

- No need to store intermediate edge-based activation vectors (when using dot-product attn.)
- Slower than GCNs but faster than GNNs with edge embeddings

Cons:

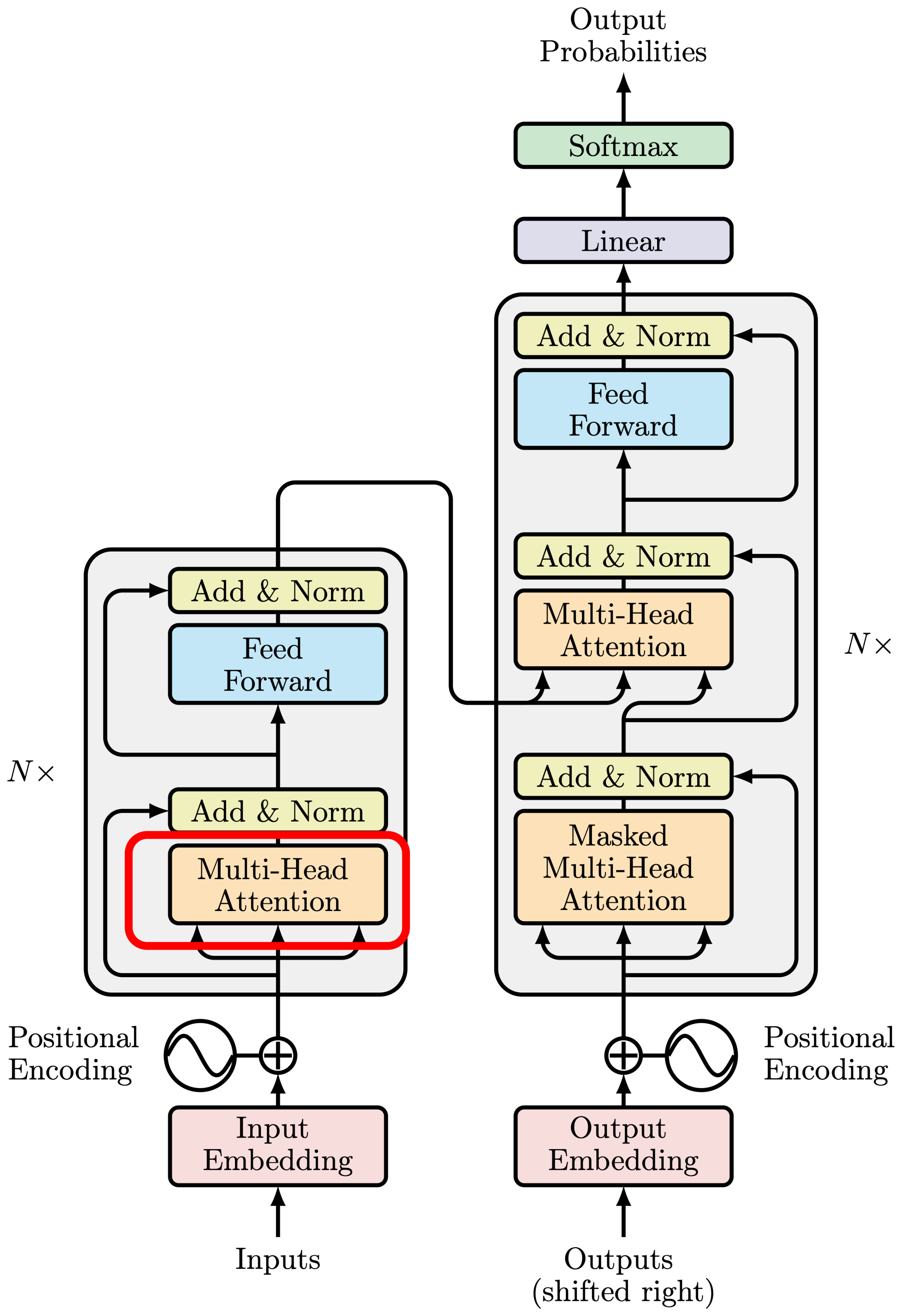
- (Most likely) less expressive than GNNs with edge embeddings
- Can be more difficult to optimize

$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\alpha_{ij}^k \mathbf{W}^k\vec{h}_j\right) \qquad \alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i\|\mathbf{W}\vec{h}_k]\right)\right)}$$

Multi-graph (k-type edges), a.k.a., can think of it as K attention heads

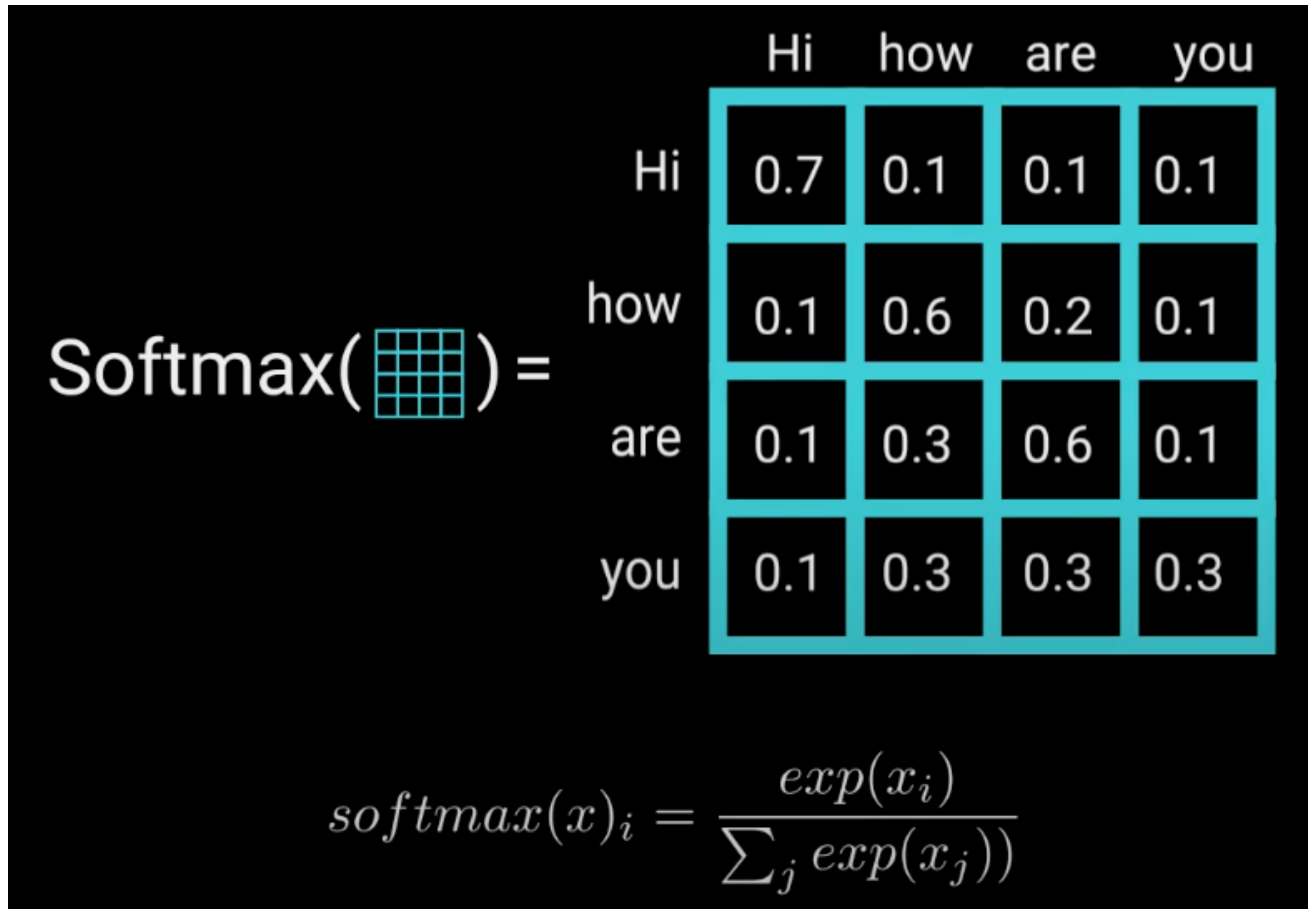
* slide from Thomas Kipf, **University of Amsterdam**

GNN **Relationship** to **Transformers**



— 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!



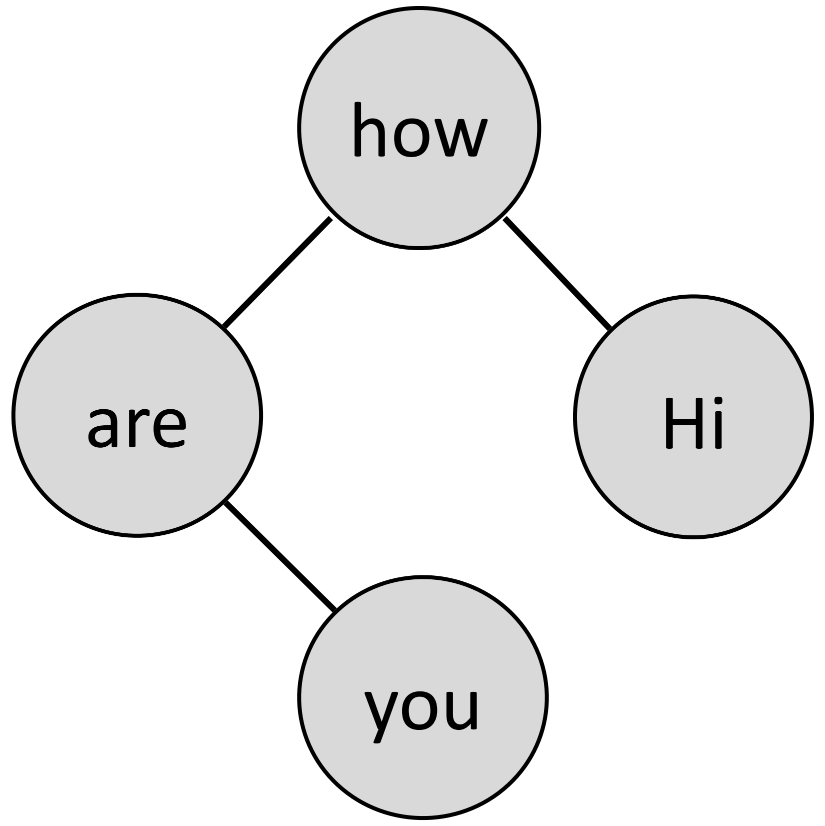
Slide from Renjie Liao

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

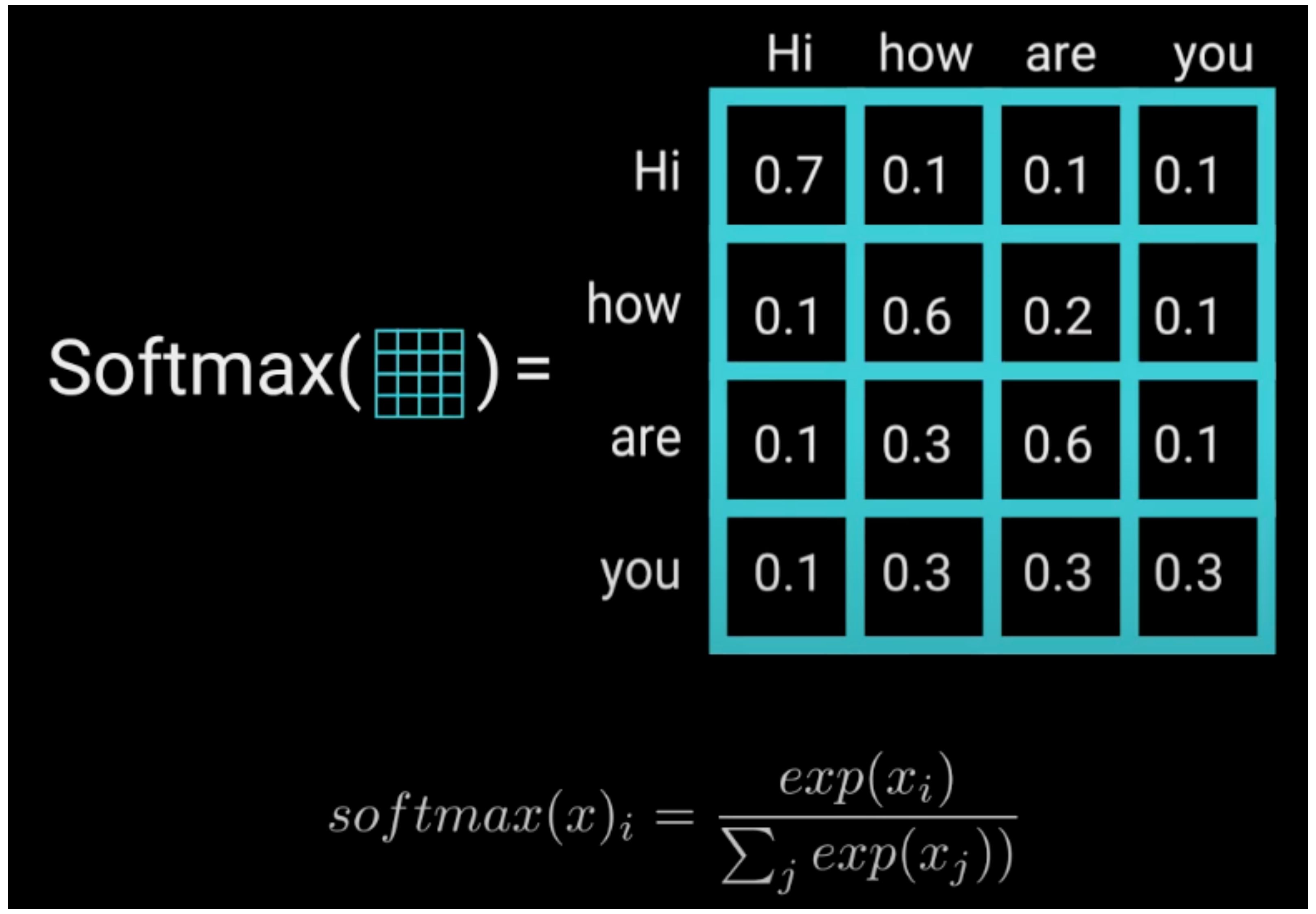
GNN **Relationship** to **Transformers**

— Apply the adjacency matrix as a mask to the attention and renormalize it, is like Graph Attention Networks (GAT) [10]

— Encoder 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

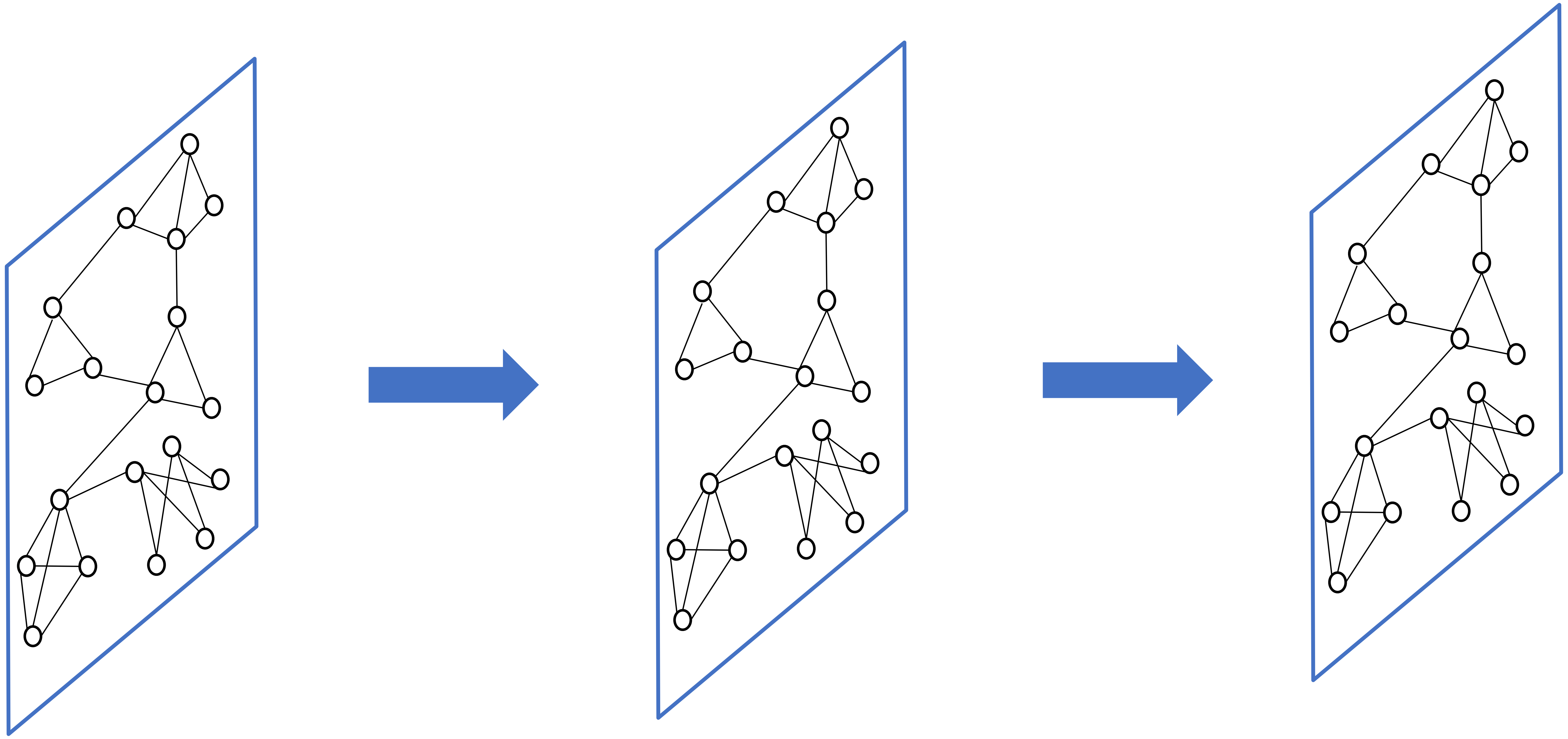


Slide from Renjie Liao

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

So far … we mainly focused on **graph filtering**

Goal: Refine node (or possibly) edge feature

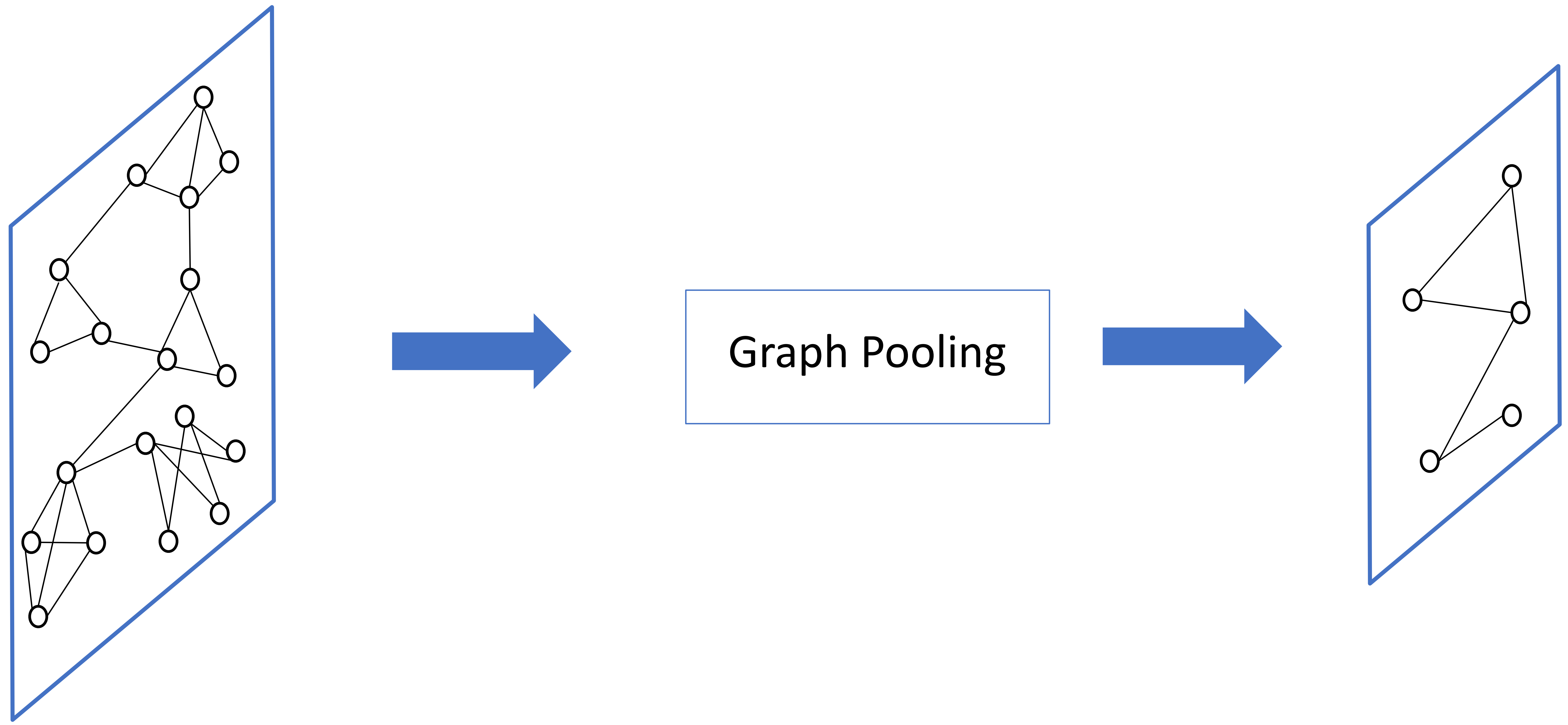


$\mathbf{A} \in \{0,1\}^{n\times n}, \mathbf{X} \in \mathbb{R}^{n\times d}$

$\mathbf{A} \in \{0,1\}^{n\times n}, \mathbf{X}_f \in \mathbb{R}^{n\times d}$

We can also do **graph pooling**

Goal: Generate a smaller graph that captures original graphs information



$\mathbf{A} \in \{0,1\}^{n \times n}, \mathbf{X} \in \mathbb{R}^{n \times d}$

$\mathbf{A}_p \in \{0,1\}^{n_p \times n_p}, \mathbf{X}_p \in \mathbb{R}^{n \times d}, n_p < n$

Global pooling vs. **Graph** Pooling

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

Global pooling vs. **Graph** Pooling

Issue: Global pooling over a (large) graph will lose information

Toy example: we use 1-dim node embeddings

Node embeddings for $G1 = \{-1, -2, 0, 1, 2\}$

Node embeddings for $G2 = \{-10, -20, 0, 10, 20\}$

Clearly $G1$ and $G2$ (have very different node embeddings)

Global pooling vs. **Graph** Pooling

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Node embeddings for $G1$ = {−1, −2, 0, 1, 2}

Node embeddings for $G2$ = {−10, −20, 0, 10, 20}

Clearly $G1$ and $G2$ (have very different node embeddings)

If we do global ReLU(Sum()) pooling:

Prediction for $G1$ = 0

Prediction for $G2$ = 0

We cannot differentiate $G1$ and $G2$

Global pooling vs. **Graph** Pooling

A solution: Let's aggregate all the node embeddings **hierarchically**

Toy example: We will aggregate via ReLU(Sum()). We first separately aggregate the first 2 nodes and last 3 nodes. Then we aggregate again to make the final prediction.

G1 node embeddings: {–1, –2, 0, 1, 2}

Round 1: ReLU(Sum({–1, –2})) = 0, ReLU(Sum({0,1,2})) = 3

Round 2: ReLU(Sum({0,3})) = **3**

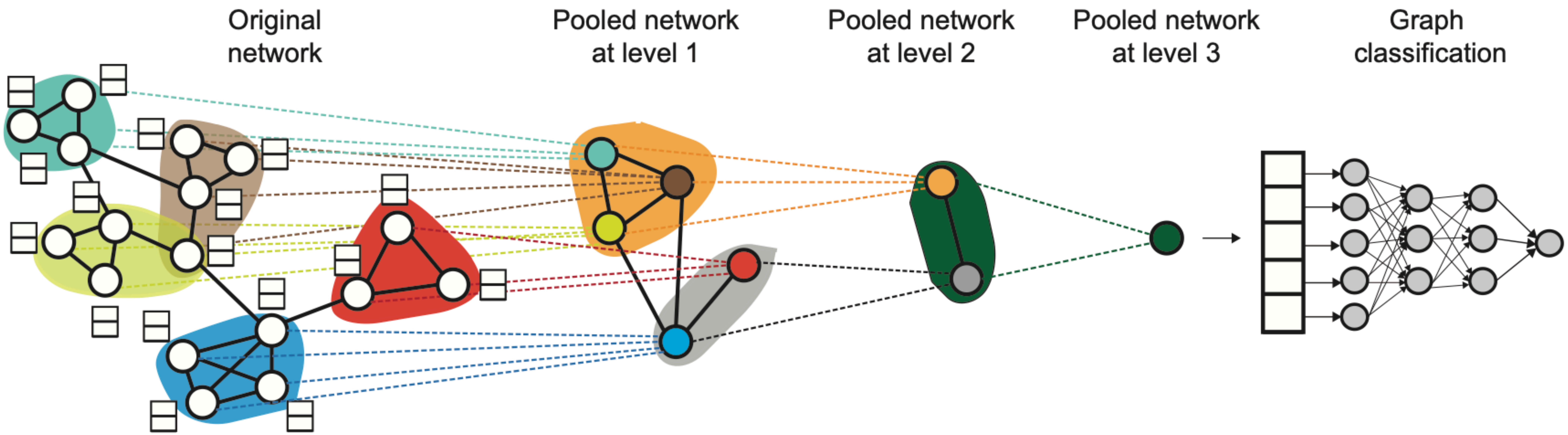
G2 node embeddings: {–10, –20, 0, 10, 20}

Round 1: ReLU(Sum({–10, –20})) = 0, ReLU(Sum({0,10, 20})) = 30

Round 2: ReLU(Sum({0, 30})) =**30**

Now we can tell the difference!

Diff**Pool** — Differentiable Graph Pooling

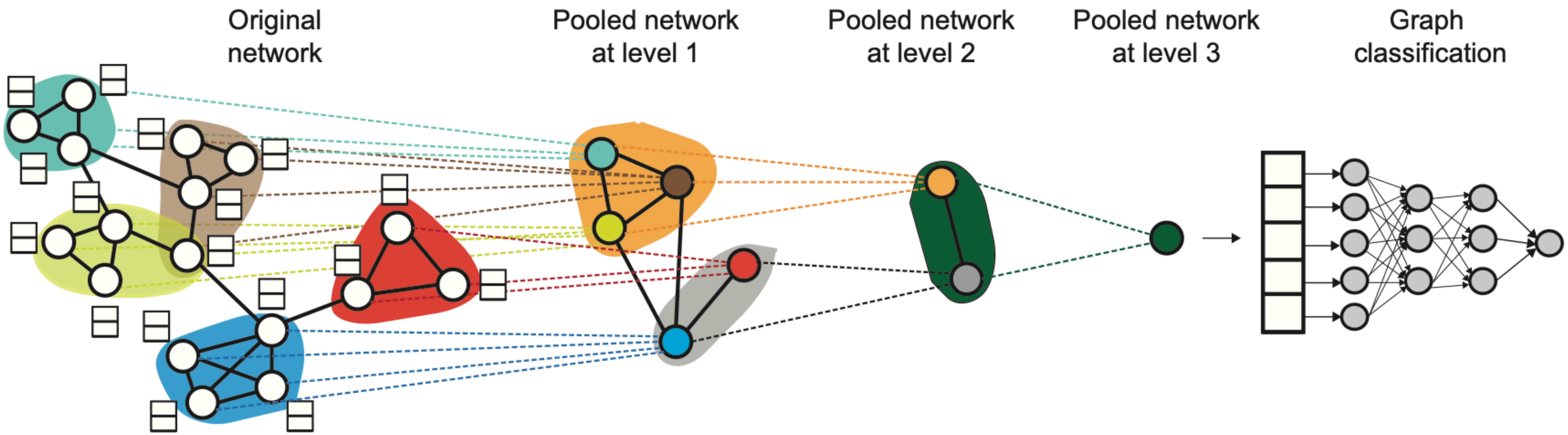


Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$

Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$

Diff**Pool** — Differentiable Graph Pooling

Assignment matrix $\mathbf{S} \in \mathbb{R}^{n \times N}$



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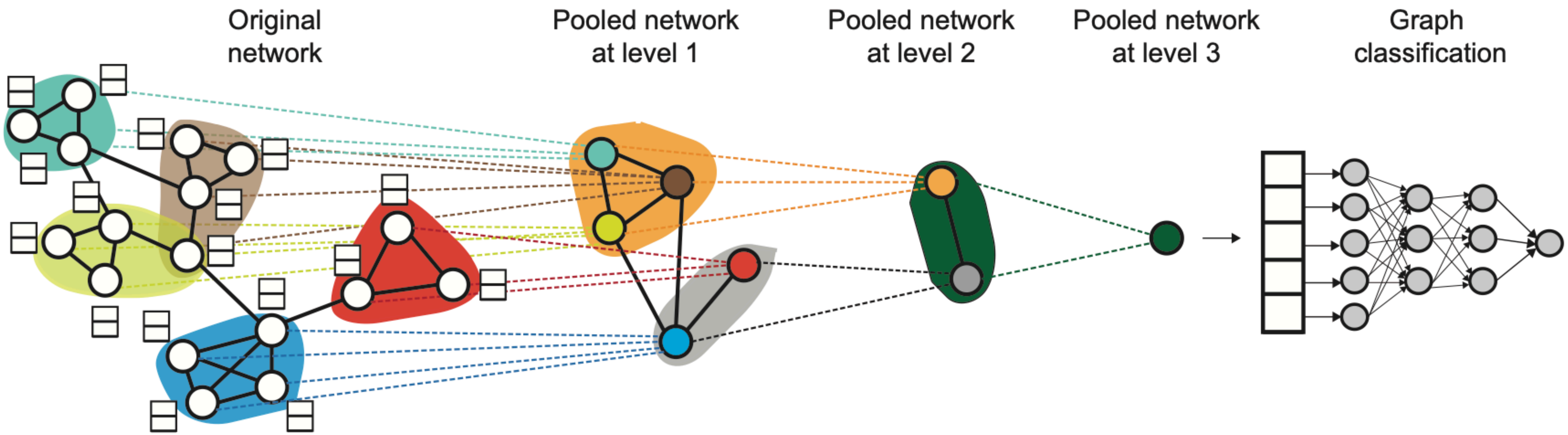


Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$

Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$

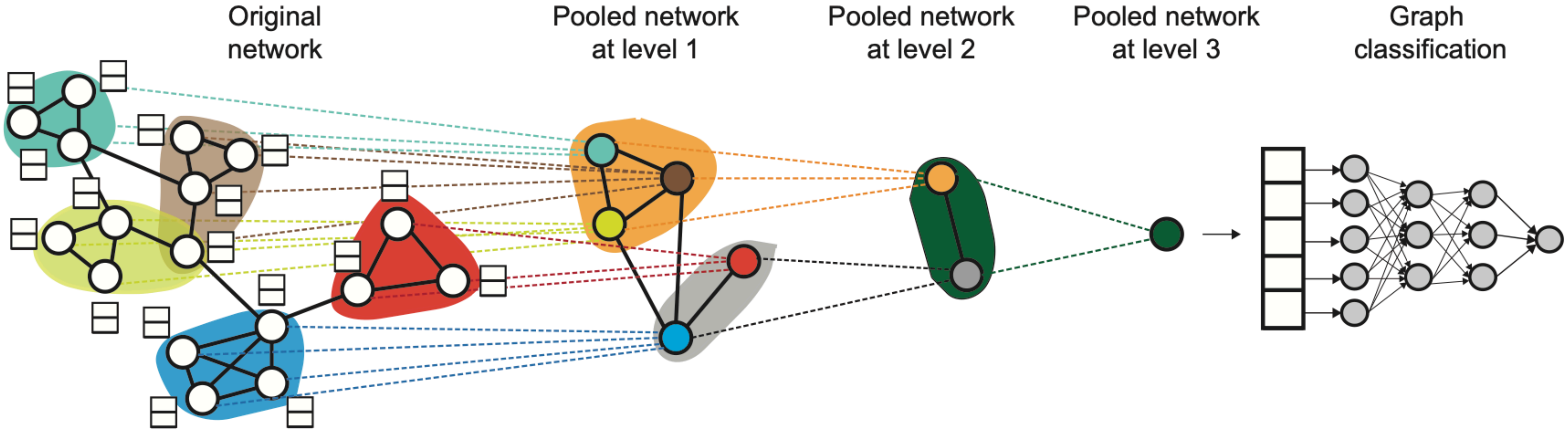
Coarsened adjacent matrix $\mathbf{A}' = \mathbf{SAS}^T \in \mathbb{R}^{n \times n}$

Coarsened feature matrix $\mathbf{X}' = \mathbf{SX} \in \mathbb{R}^{n \times F}$

Diff**Pool** — Differentiable Graph Pooling

Assignment matrix $\mathbf{S} \in \mathbb{R}^{n \times N}$

$$\mathbf{S} = Softmax(\mathbf{W} \cdot GNN_2(\mathbf{X}, \mathbf{A})); \mathbf{W} \in \mathbb{R}^{n \times N}$$



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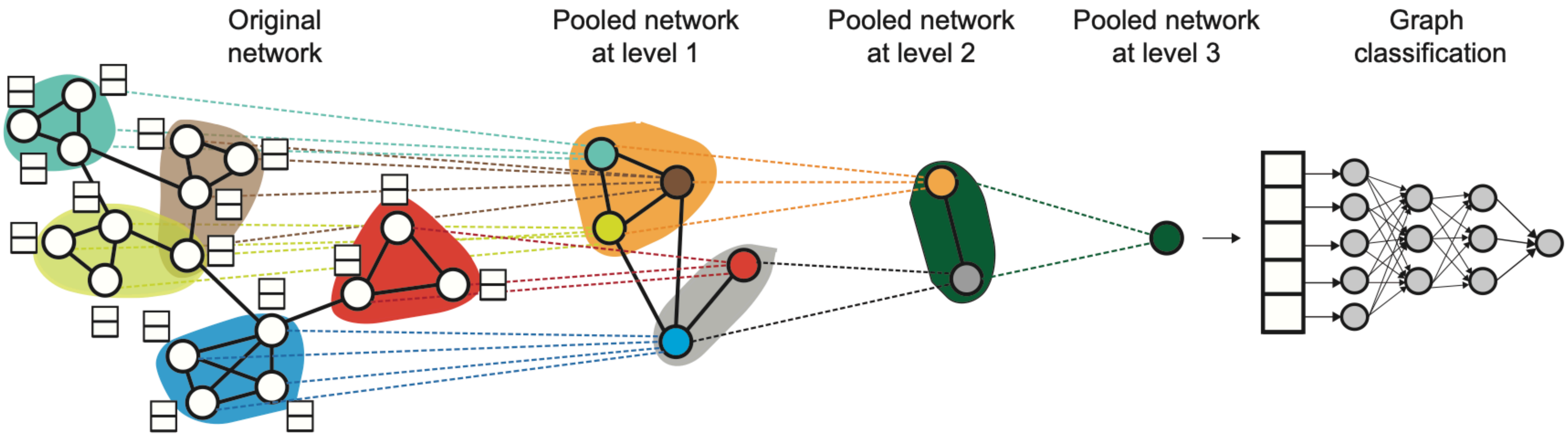


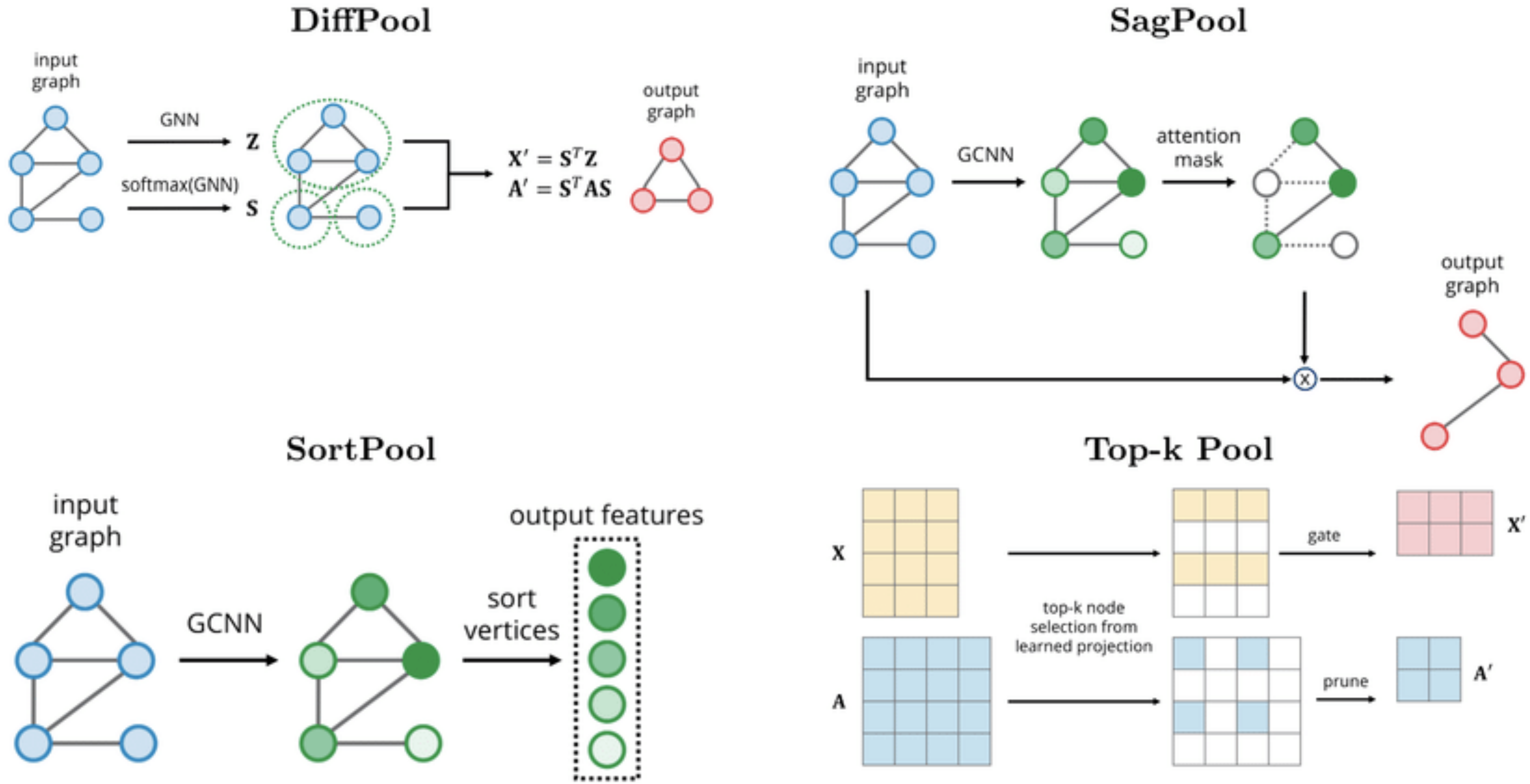
Adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$

Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times F}$

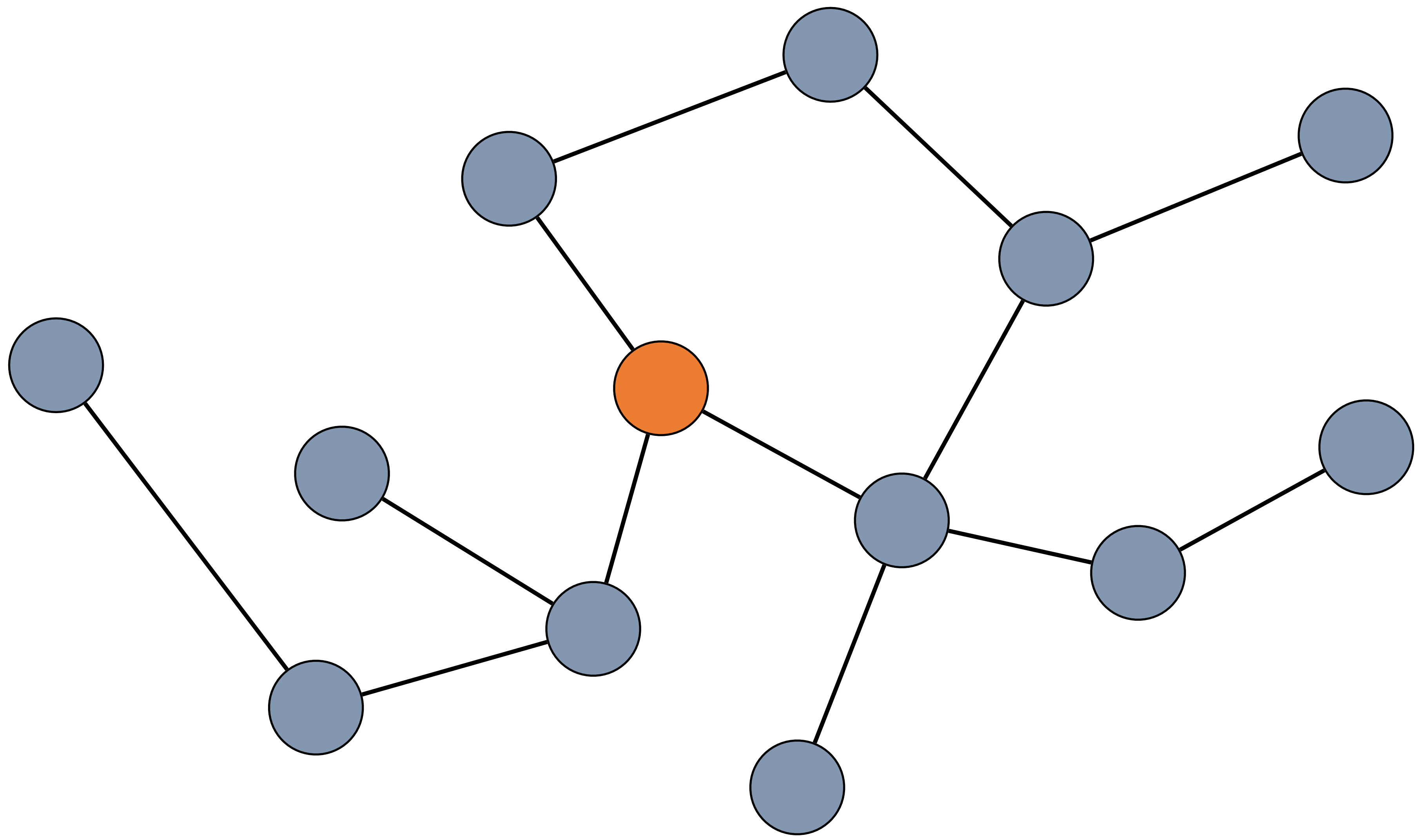
Coarsened adjacent matrix $\mathbf{A}' = \mathbf{S}\mathbf{A}\mathbf{S}^T \in \mathbb{R}^{n \times n}$

Coarsened feature matrix $\mathbf{X}' = \mathbf{S} \cdot GNN_1(\mathbf{X}, \mathbf{A})$

Graph Pooling

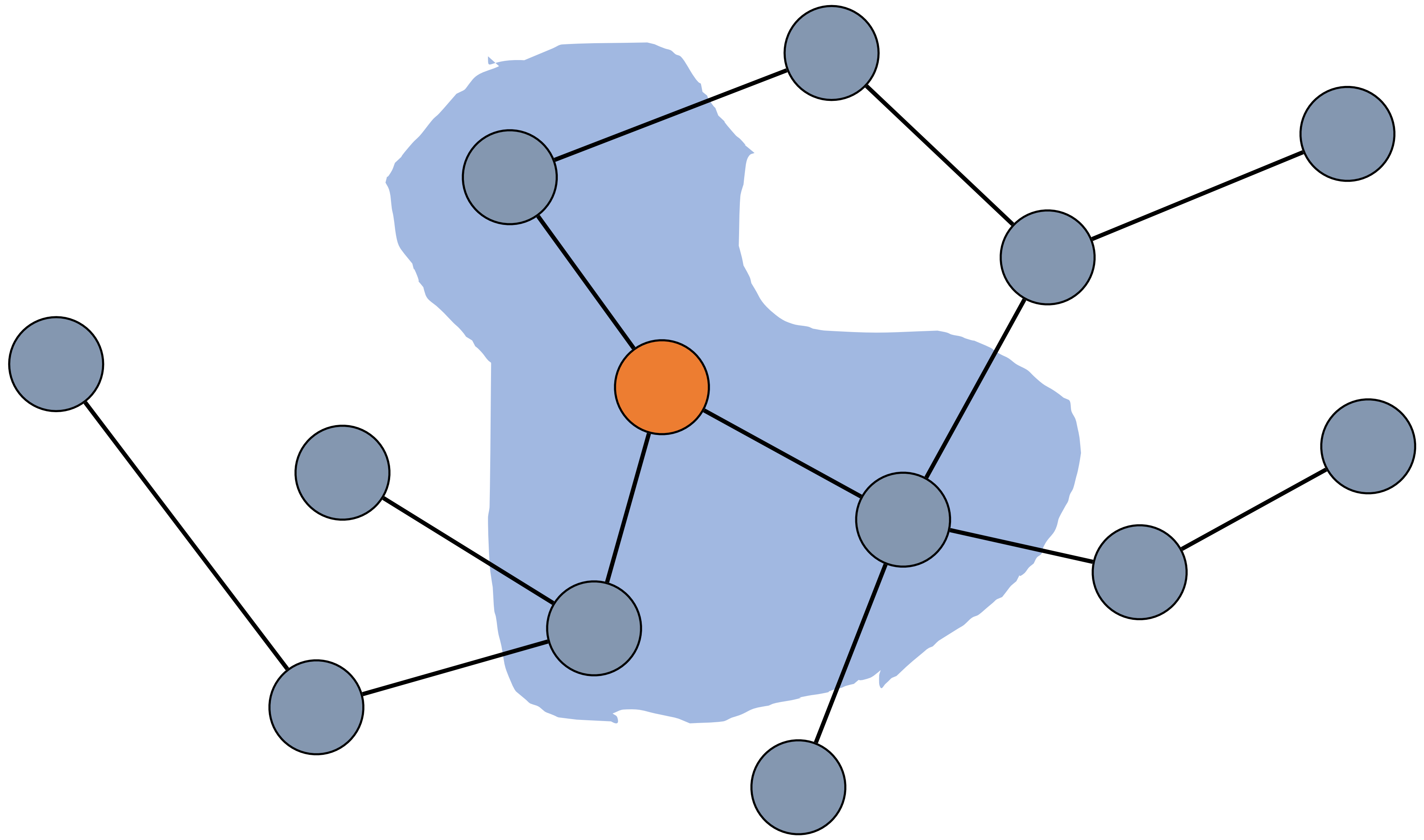


Deeper GNNs (more layers)



Depth in GNNs **increases receptive field** and **model capacity**

Deeper GNNs (more layers)



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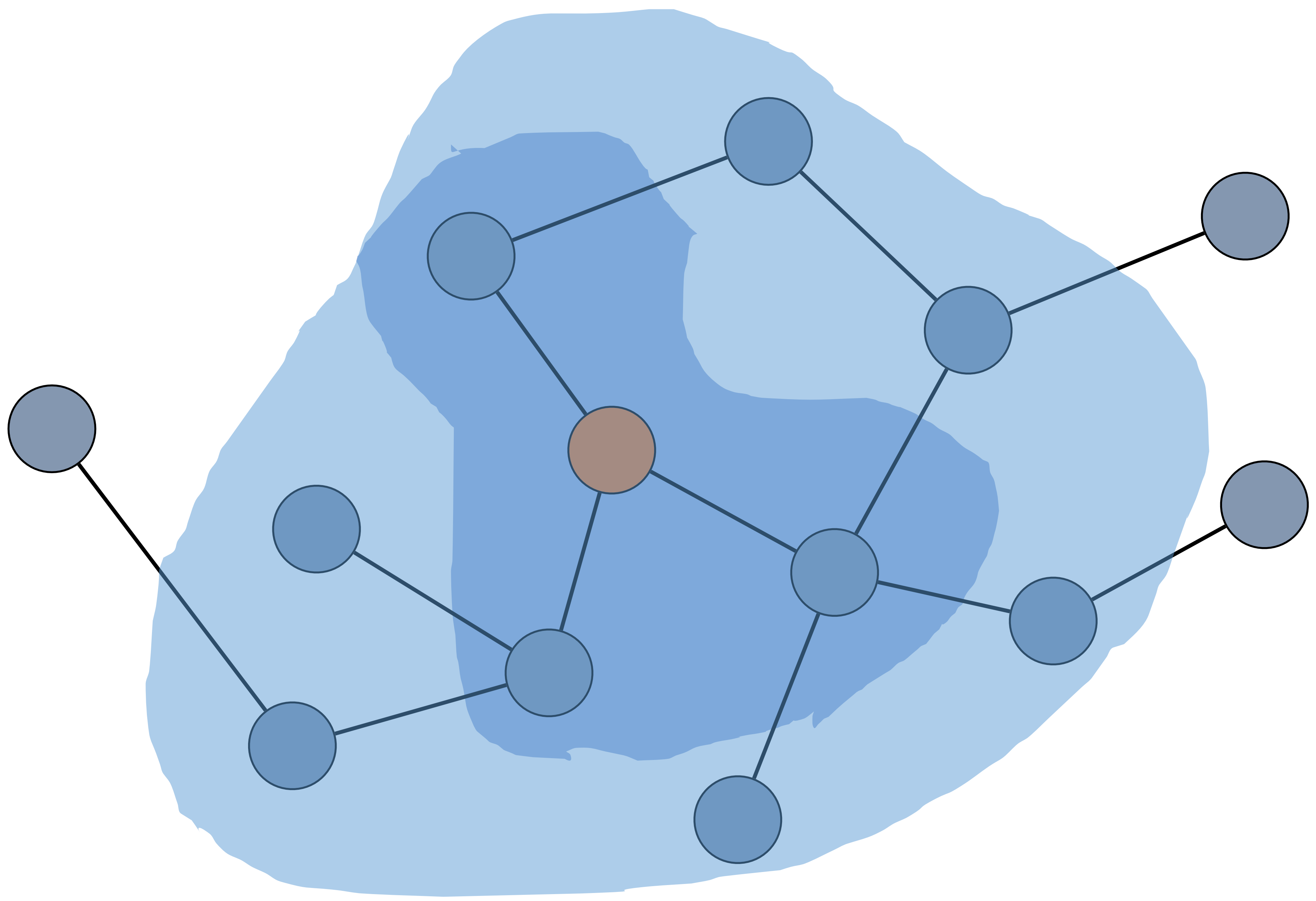

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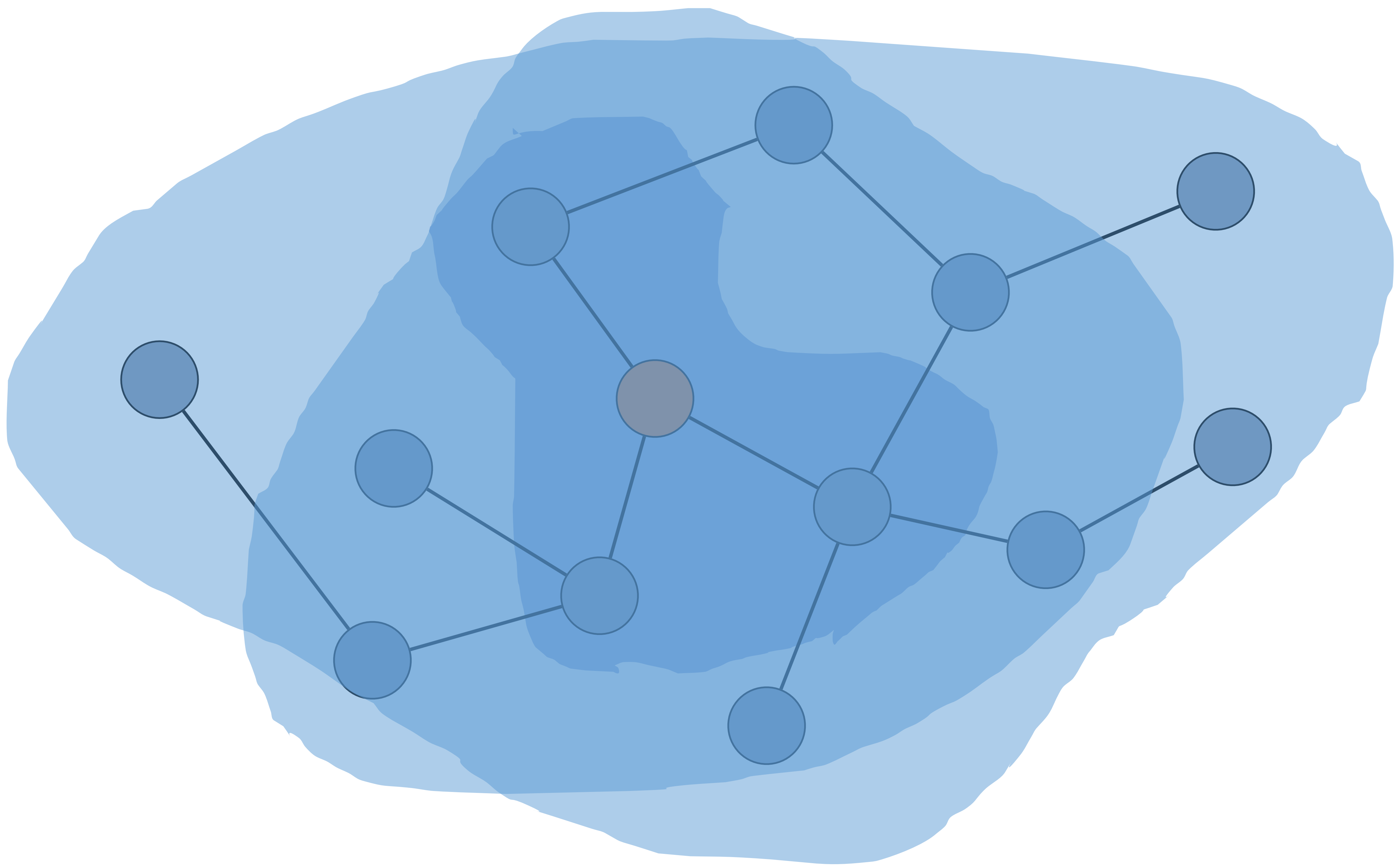
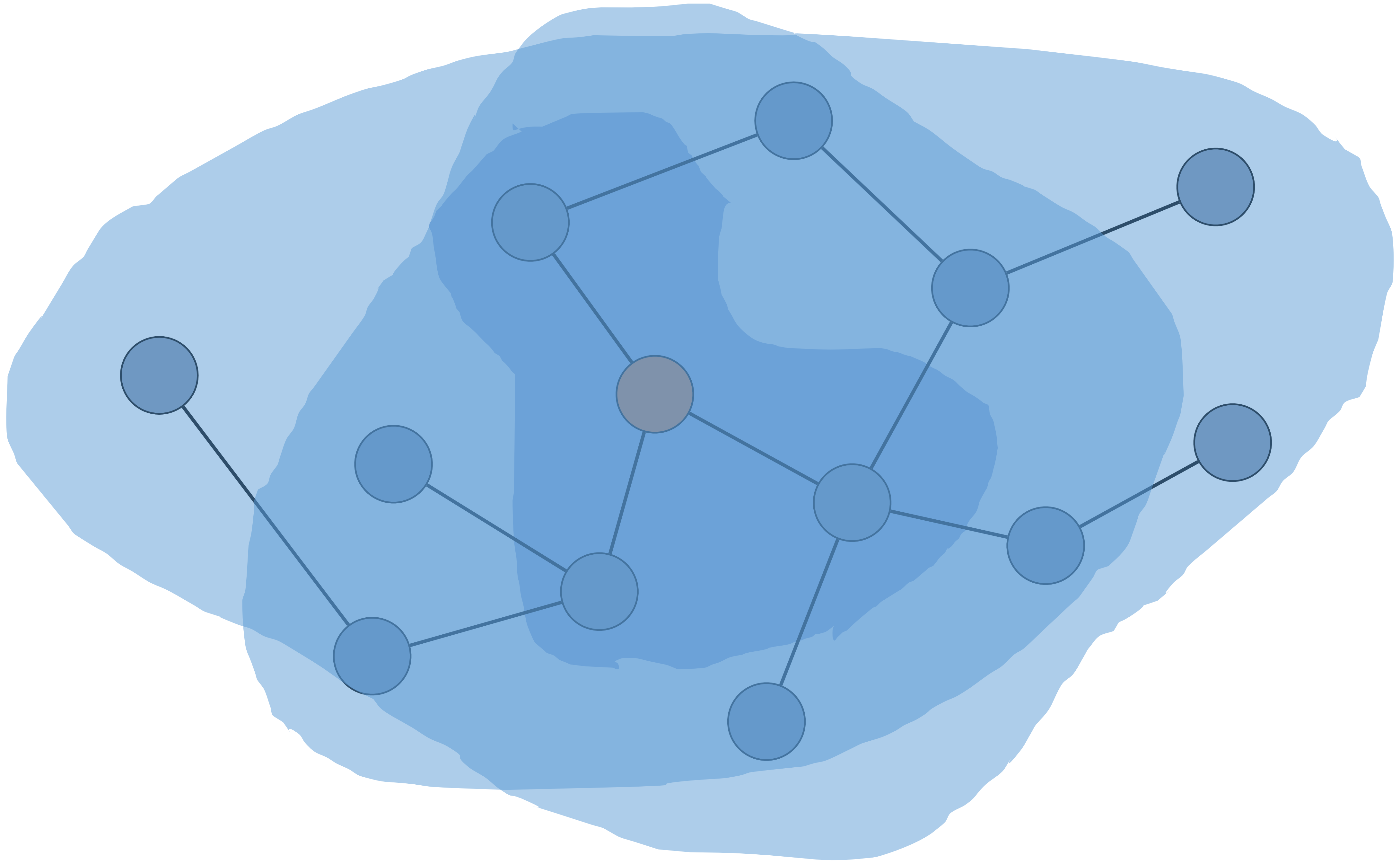


Depth in GNNs **increases receptive field** and **model capacity**

Deeper GNNs (more layers)

However, unlike in CNNs, deeper GNN models generally do not work well



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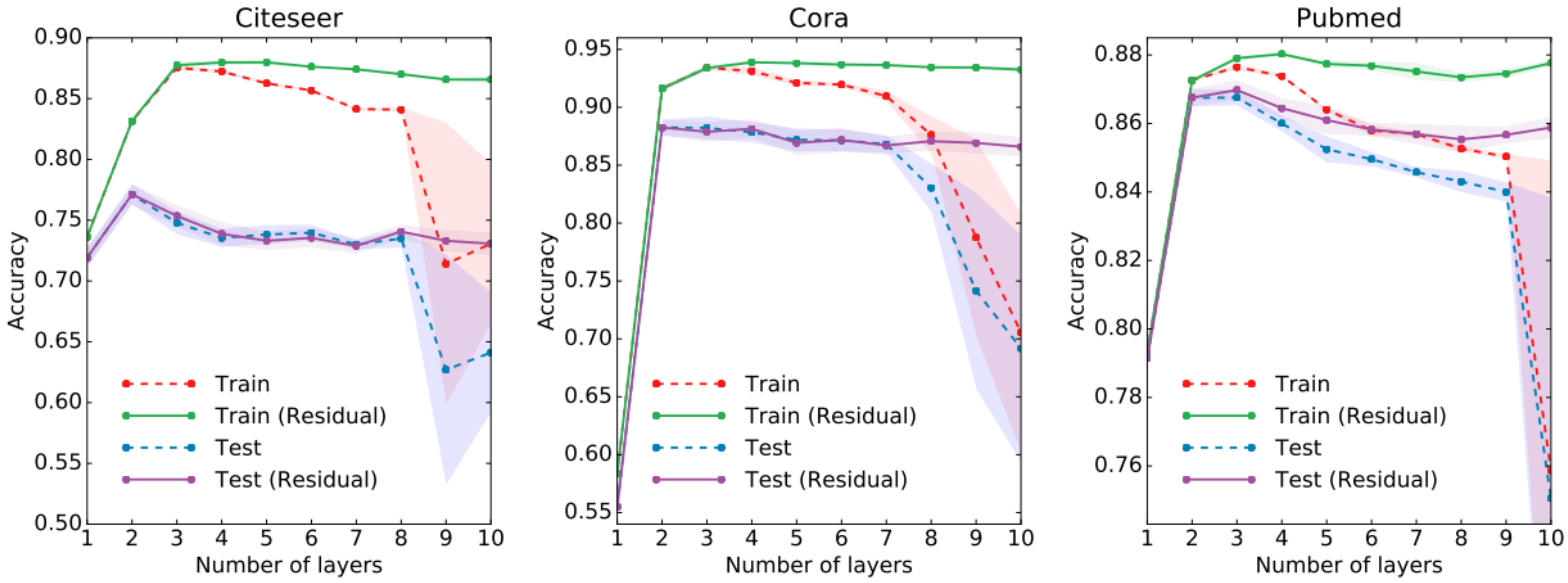
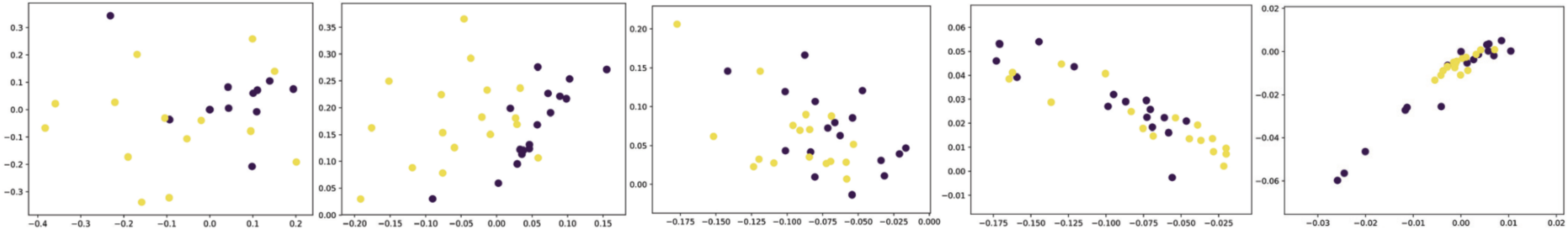
Deeper GNNs (more layers)



Deeper GNNs (more layers) — Oversmoothing

Latent node vectors get closer to each other as the number of GCN layers increases, this makes it difficult to distinguish nodes in deeper GCNs



(a) 1-layer (b) 2-layer (c) 3-layer (d) 4-layer (e) 5-layer

Figure 2: Vertex embeddings of Zachary's karate club network with GCNs with 1,2,3,4,5 layers.

Deeper Insights into Graph Convolutional Networks for Semi-Supervised Learning. AAAI 2018

Deeper GNNs (more layers) — Oversmoothing

Recall **GCN** propagation equation:

$$\sigma([\underline{\mathbf{D}^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}}]\underline{\mathbf{H}\mathbf{W}_1^{(l)}})$$

Lets assume we have no non-linearity

$$\lim_{k \to \inf} \mathbf{M}^k \mathbf{v} \propto \mathbf{u}_1$$

$$\underline{\mathbf{M} = \mathbf{D}^{-\frac{1}{2}}(\mathbf{A}+\mathbf{I})\mathbf{D}^{-\frac{1}{2}}} \qquad \underline{\mathbf{v} = \mathbf{h}_i \mathbf{W}_1^{(l)}}$$

where $\mathbf{u}_1$ is an **eigenvector** corresponding to largest **eigenvalue** of $\mathbf{M}$

GNN Oversmoothing

Oversmoothing is theoretically proven

— Deeper GCN converge to a solution where connected nodes will have similar latent vectors

— Such convergence in GCN happens very quickly (exponential to the depth), regardless of the initial node vectors

Similar results can be derived for other generic “vanilla” GNNs

GNN Oversmoothing

Combining a proper normalizer and a residual node update formulation addresses oversmoothing (in many cases)

— **Normalization** (PairNorm) **PairNorm: Tackling Oversmoothing in GNNs.** ICLR 2020

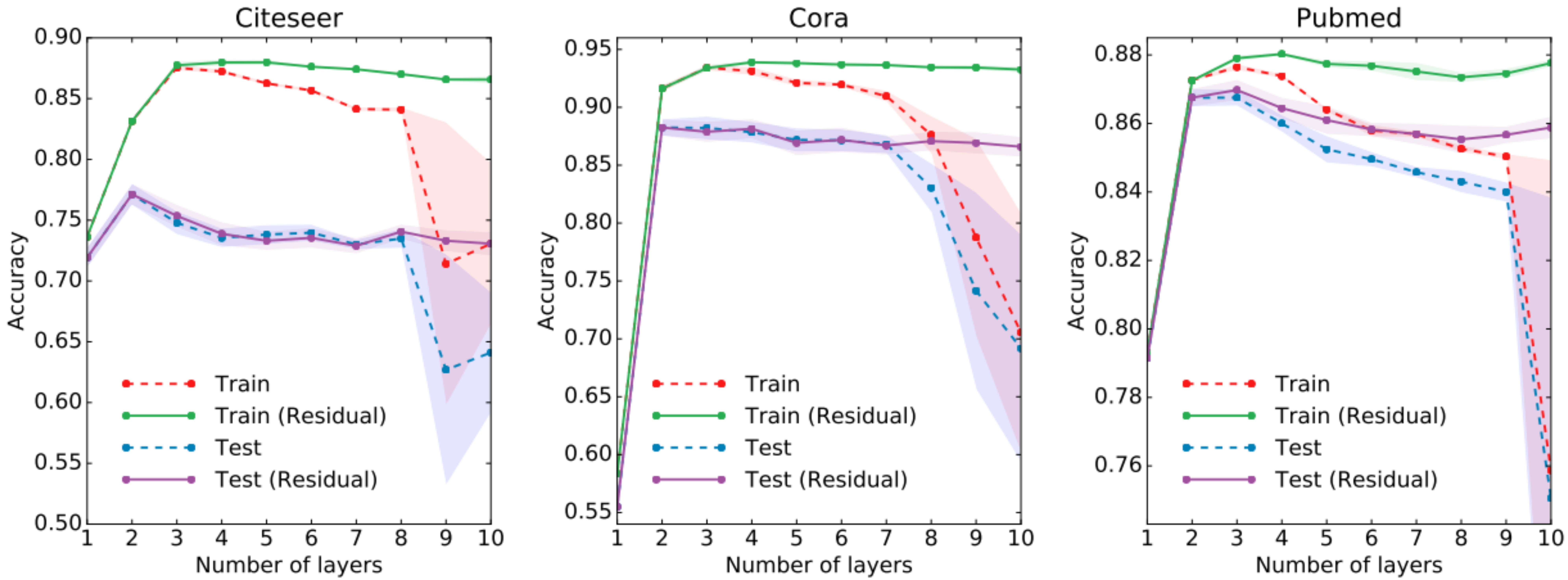
$$\tilde{\mathbf{x}}_i^c = \tilde{\mathbf{x}}_i - \frac{1}{n}\sum_{i=1}^{n}\tilde{\mathbf{x}}_i \qquad \text{(Center)}$$

$$\dot{\mathbf{x}}_i = s \cdot \frac{\tilde{\mathbf{x}}_i^c}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\|\tilde{\mathbf{x}}_i^c\|_2^2}} = s\sqrt{n} \cdot \frac{\tilde{\mathbf{x}}_i^c}{\sqrt{\|\tilde{\mathbf{X}}^c\|_F^2}} \qquad \text{(Scale)}$$

— **Residual** update

$$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right) \longrightarrow \mathbf{h}_i^{(l+1)} = \sigma\left(\sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right) + \mathbf{h}_i^{(l)}$$

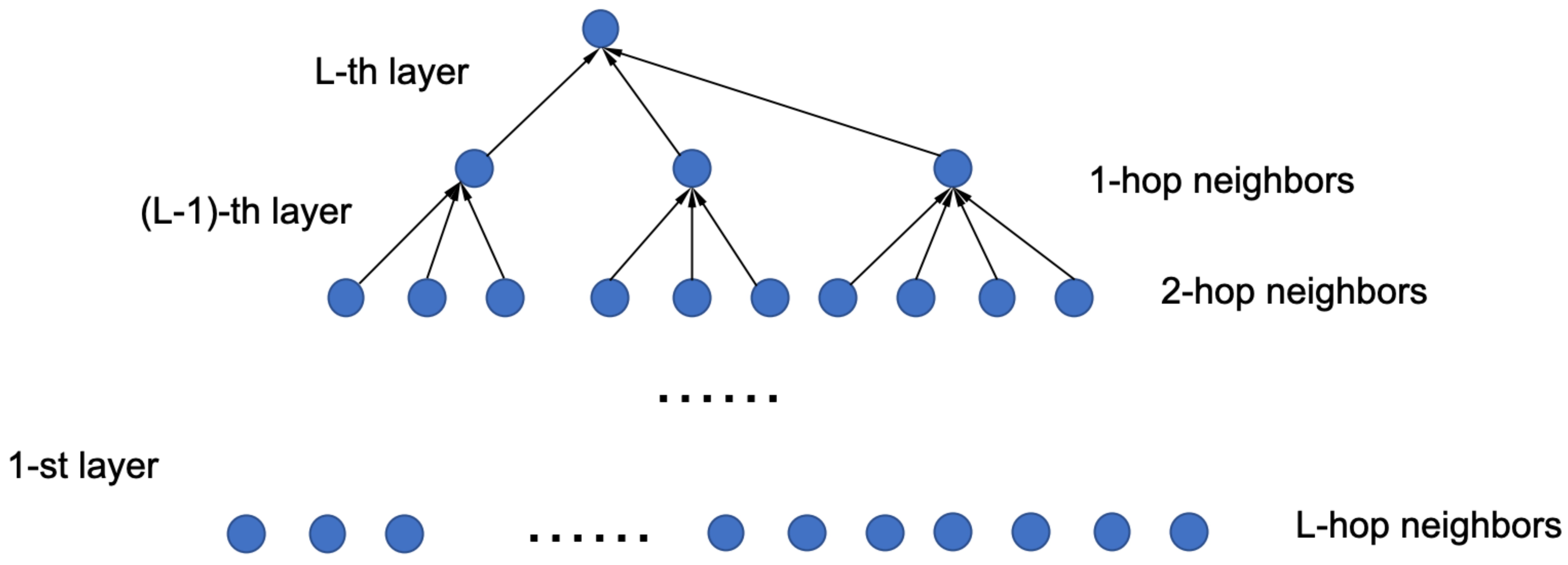
Deeper GNNs (more layers)



GNN **Scalability**

Node-wise **local neighborhood** sampling

— Sample a set of neighborhoods instead of using the entire local neighborhood



- Inductive Representation learning on Large Graphs (NIPS'17)

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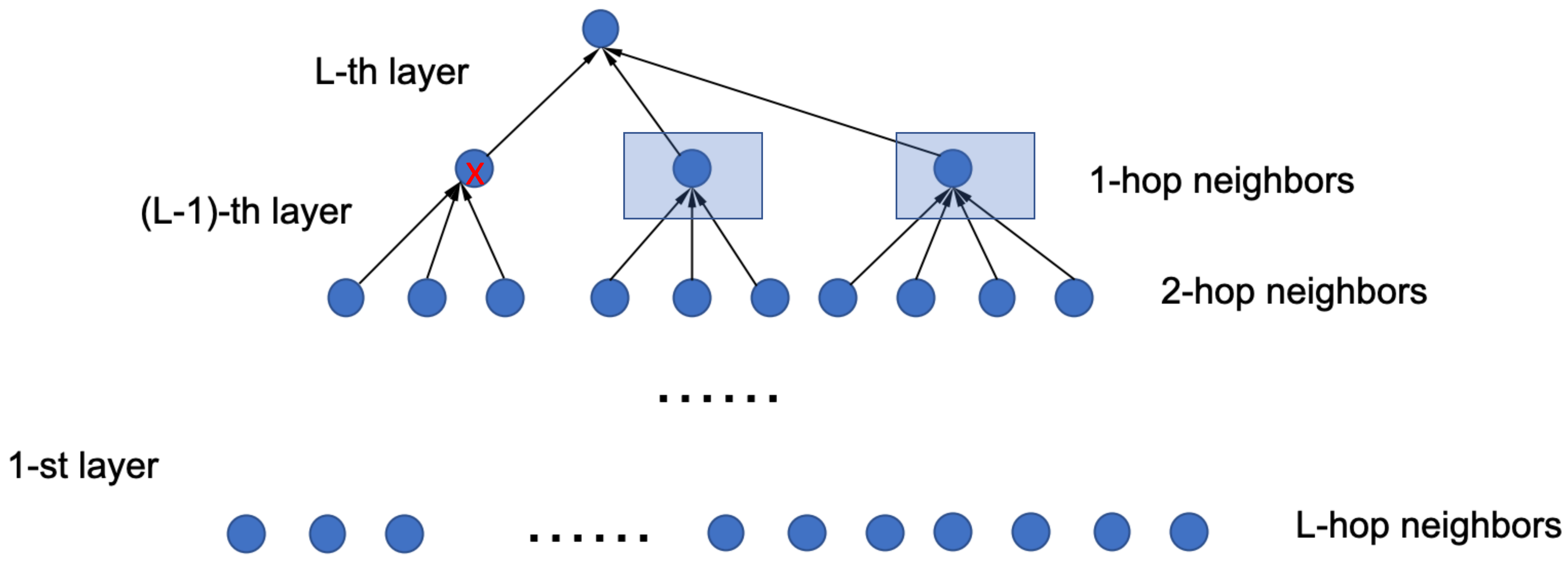

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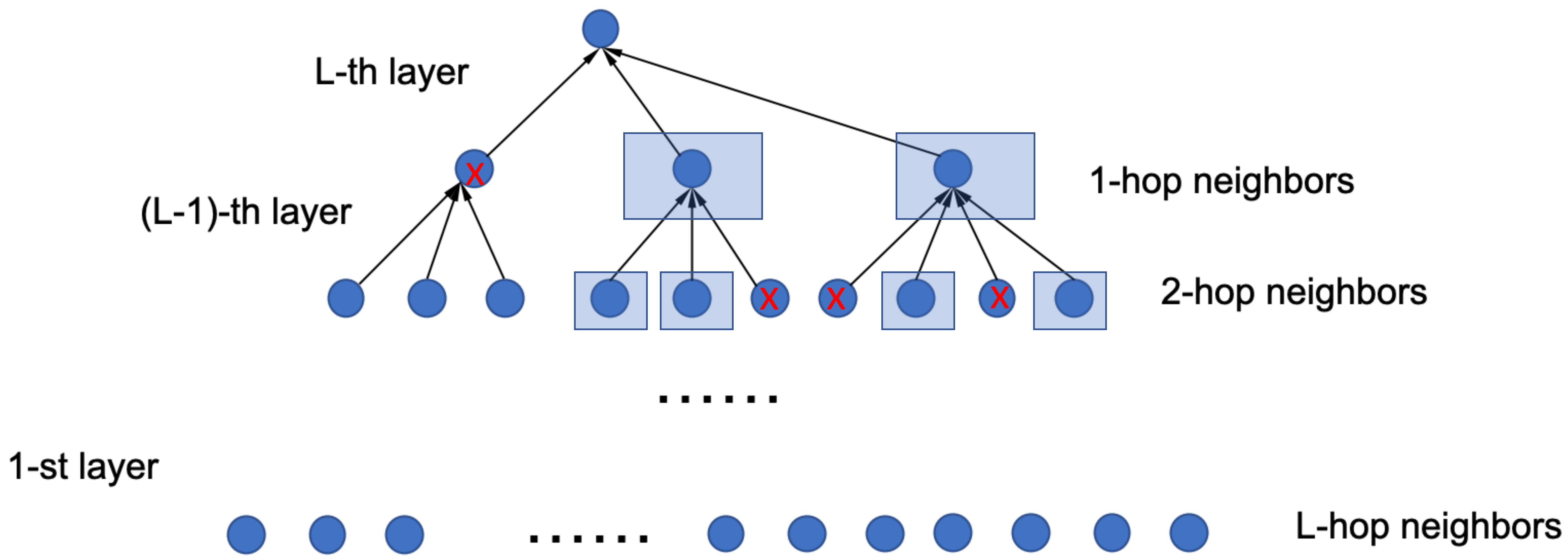

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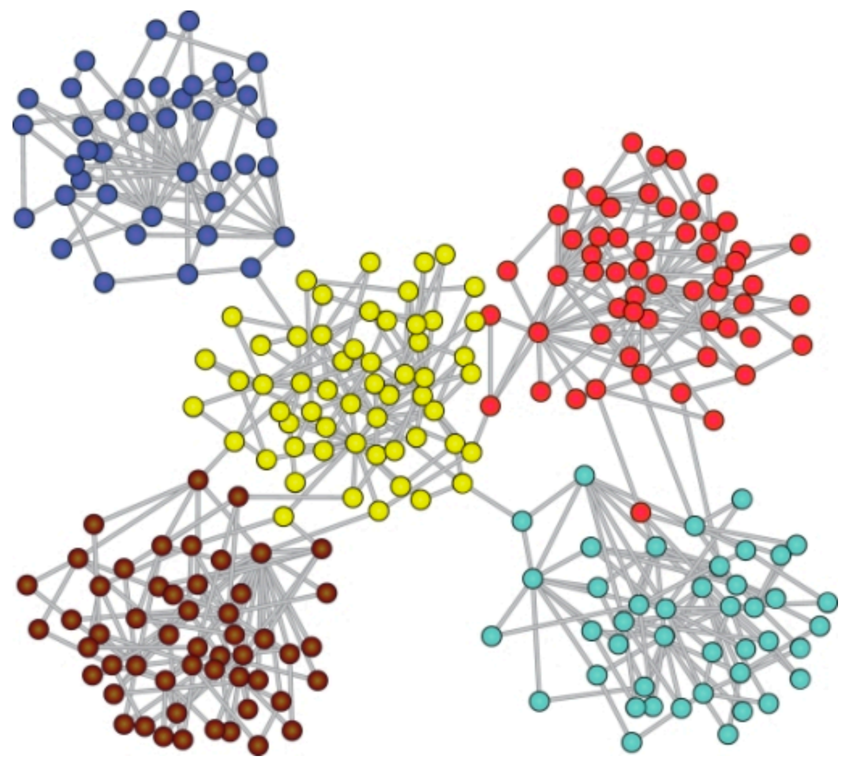
Subgraph-wise sampling



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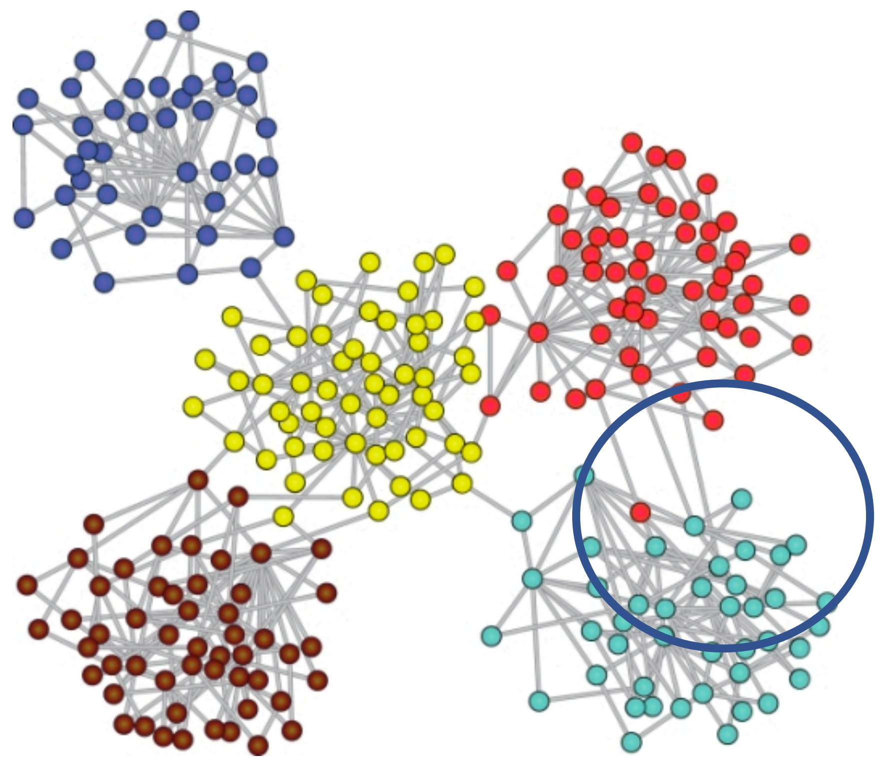
Subgraph-wise sampling

1. Select a subgraph



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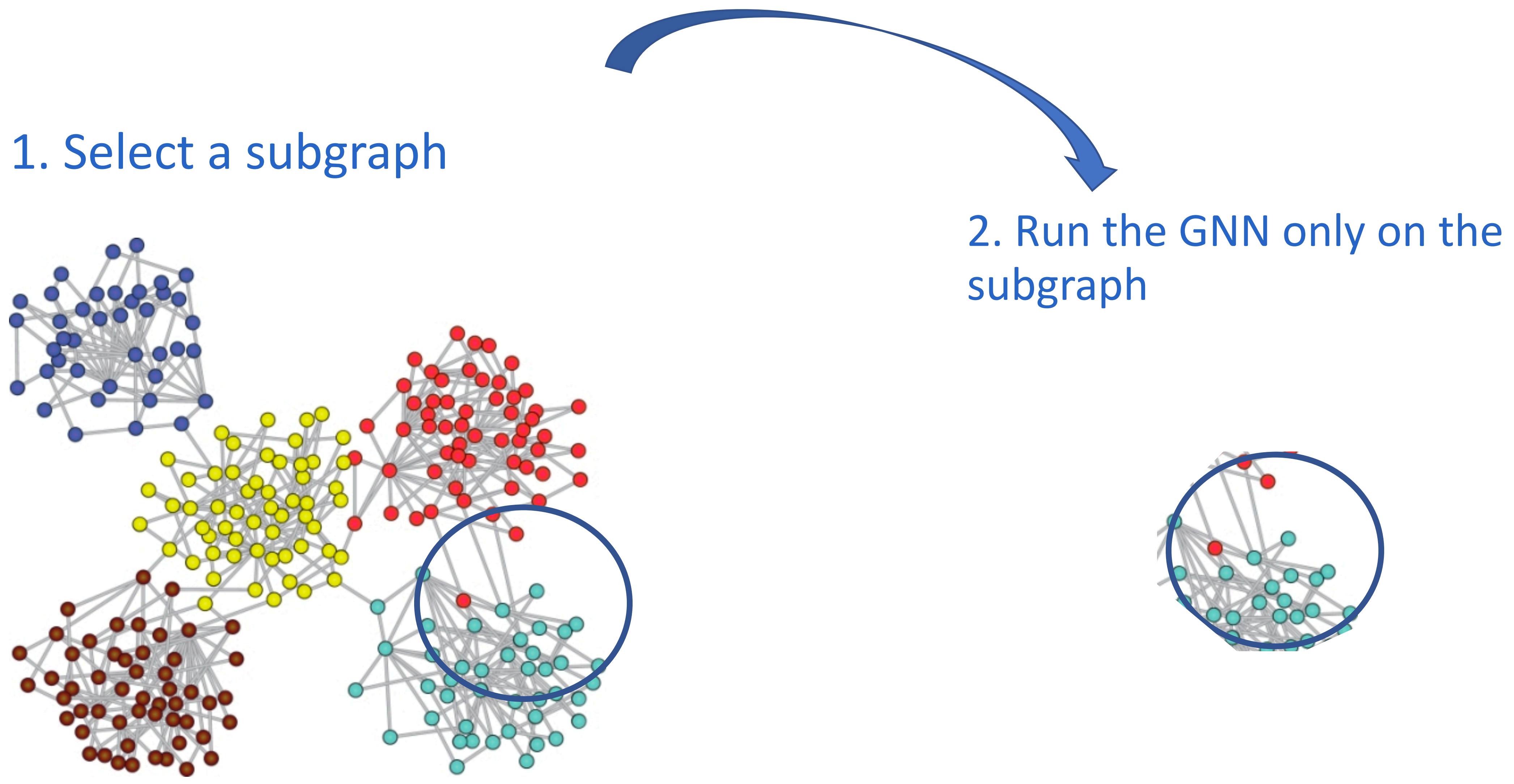
Subgraph-wise sampling



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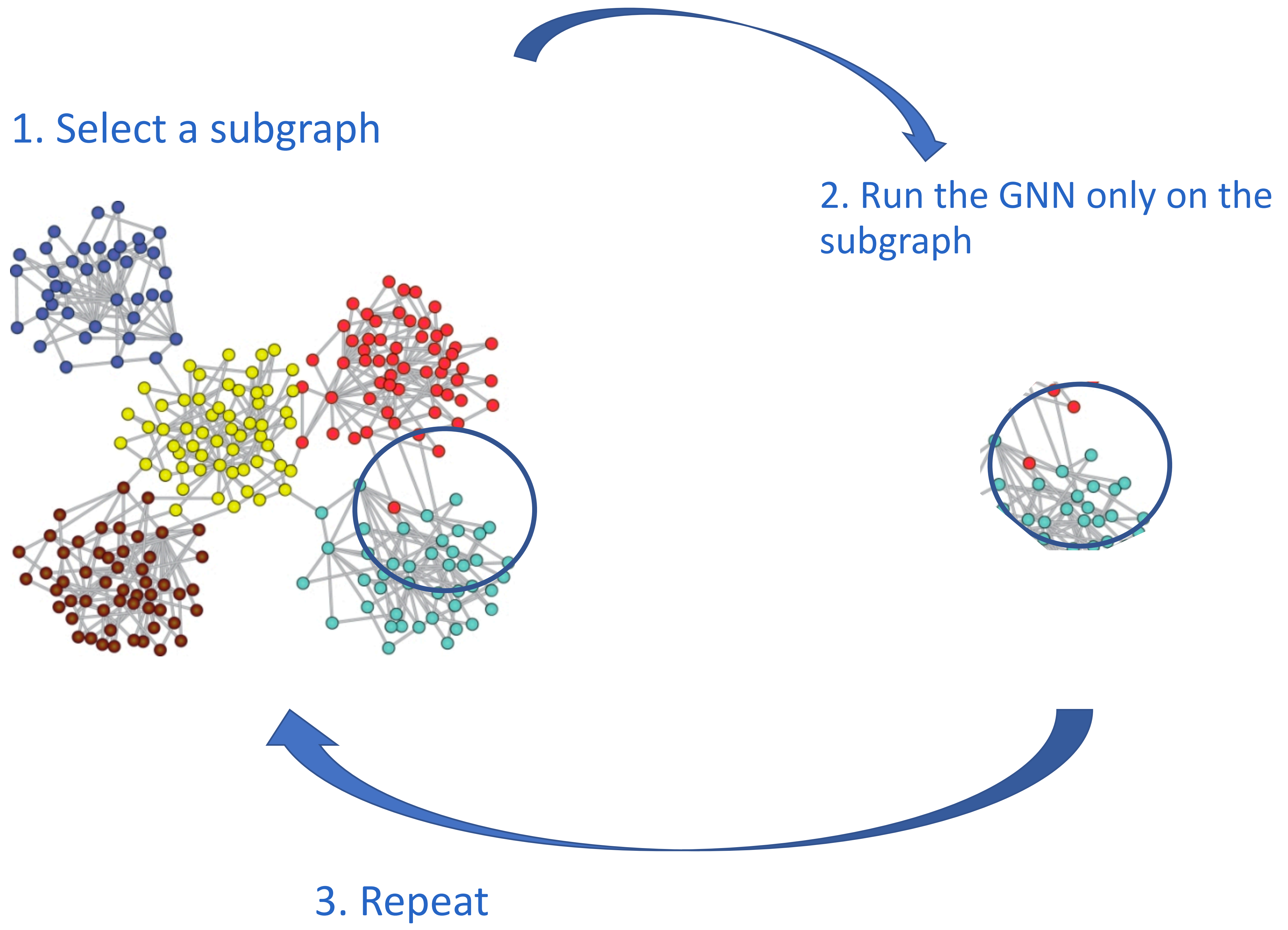
Subgraph-wise sampling



GNN **Scalability**

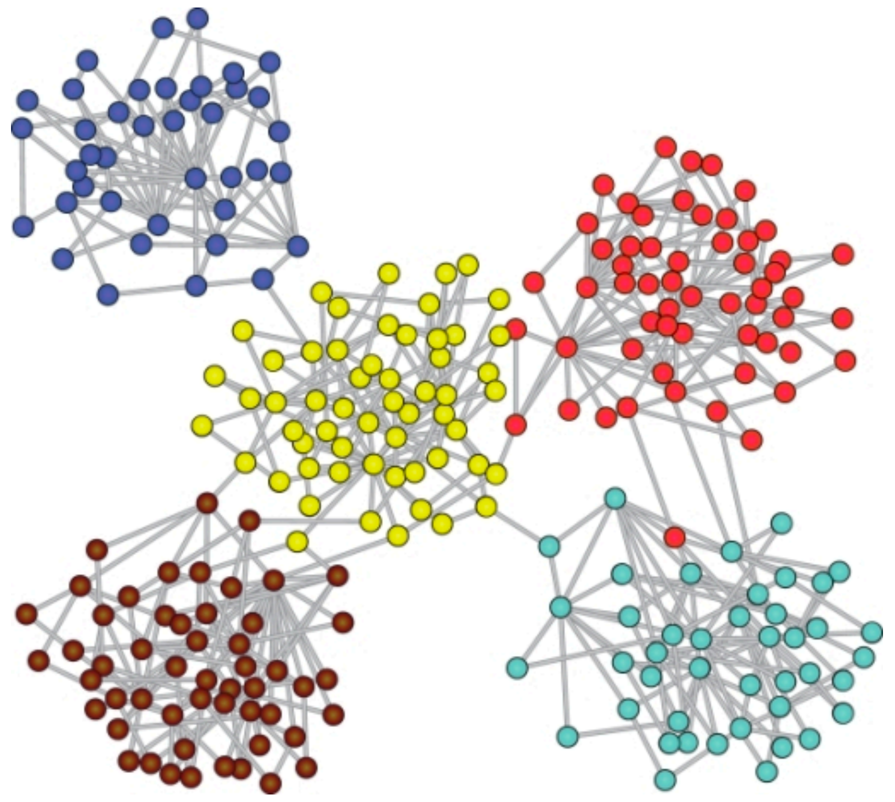
Node-wise **local neighborhood** sampling

— Sample a set of neighborhoods instead of using the entire local neighborhood

Subgraph-wise sampling

Clustering algorithms (**Cluster GCN**)

1. Run a clustering algorithm
2. Select subgraph/cluster
3. Run full-batch GNN on the small subgraph



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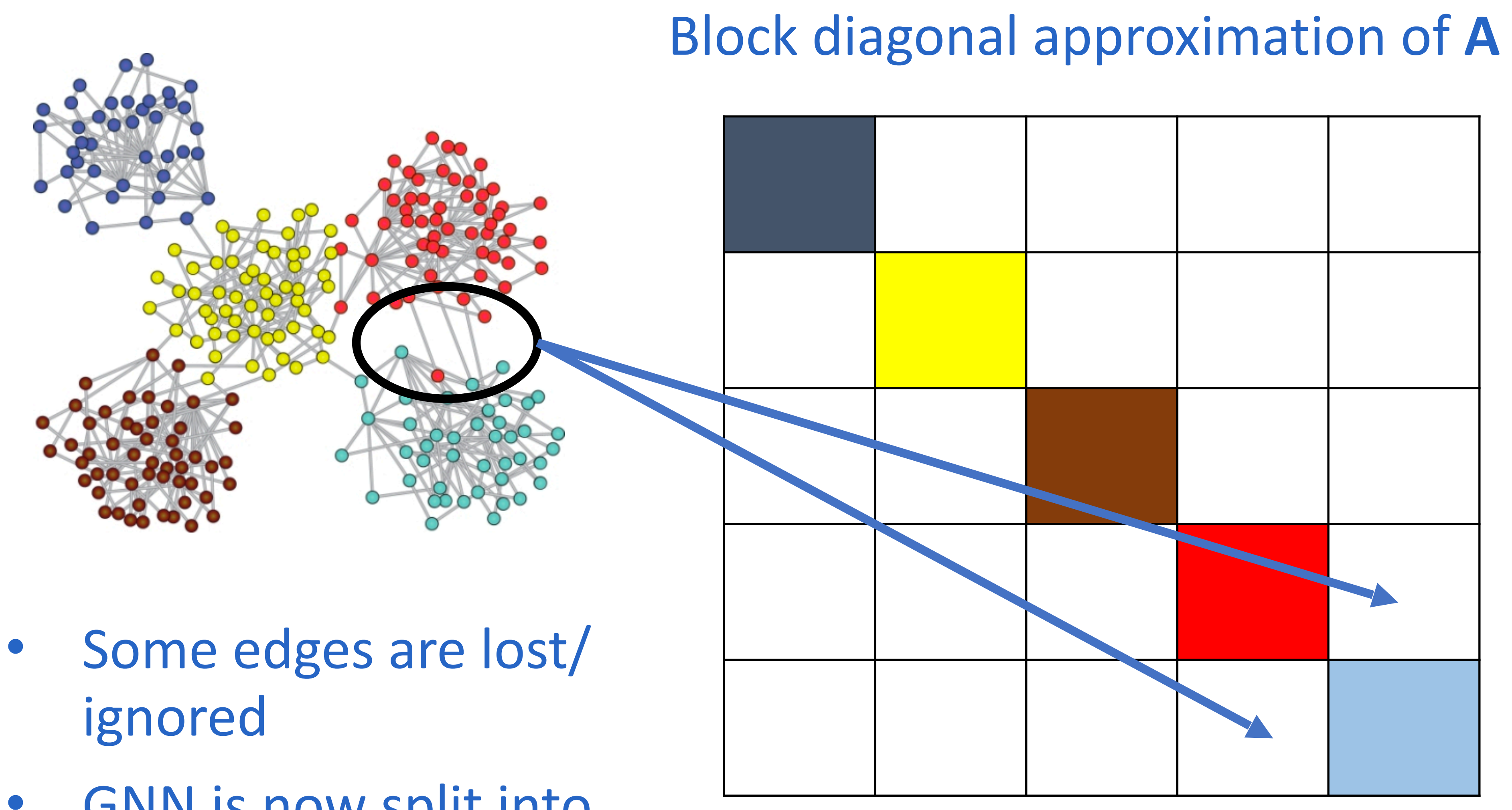
Subgraph-wise sampling

Clustering algorithms (**Cluster GCN**)



- Some edges are lost/ ignored
- GNN is now split into different batches/clusters

GNN **Scalability**

Node-wise **local neighborhood** sampling

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Subgraph-wise sampling

Clustering algorithms (**Cluster GCN**)

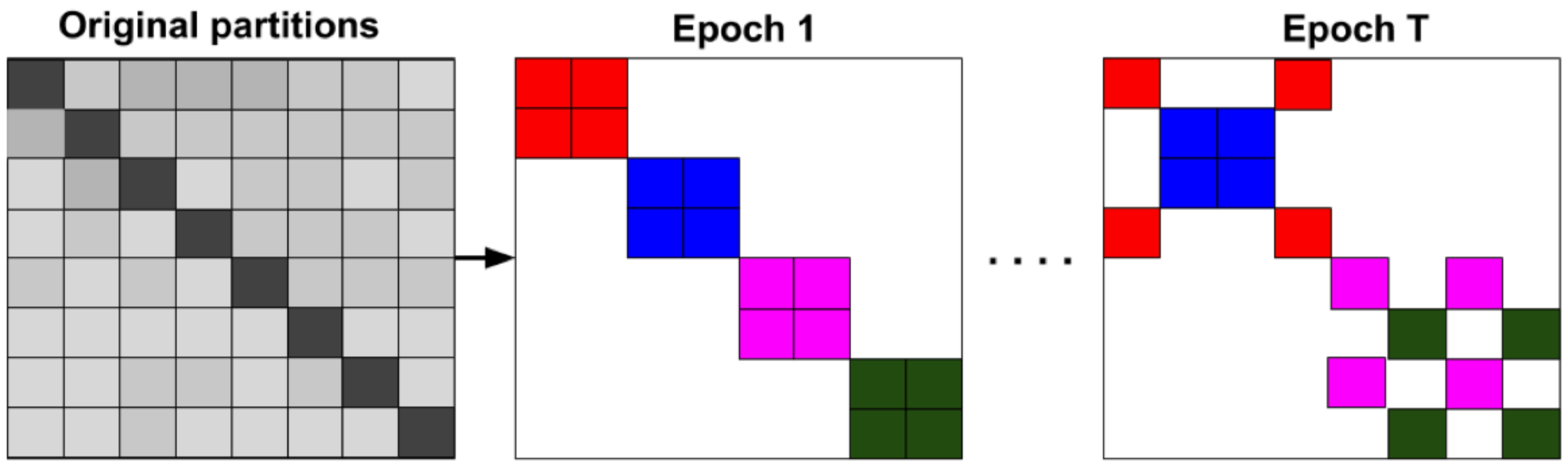
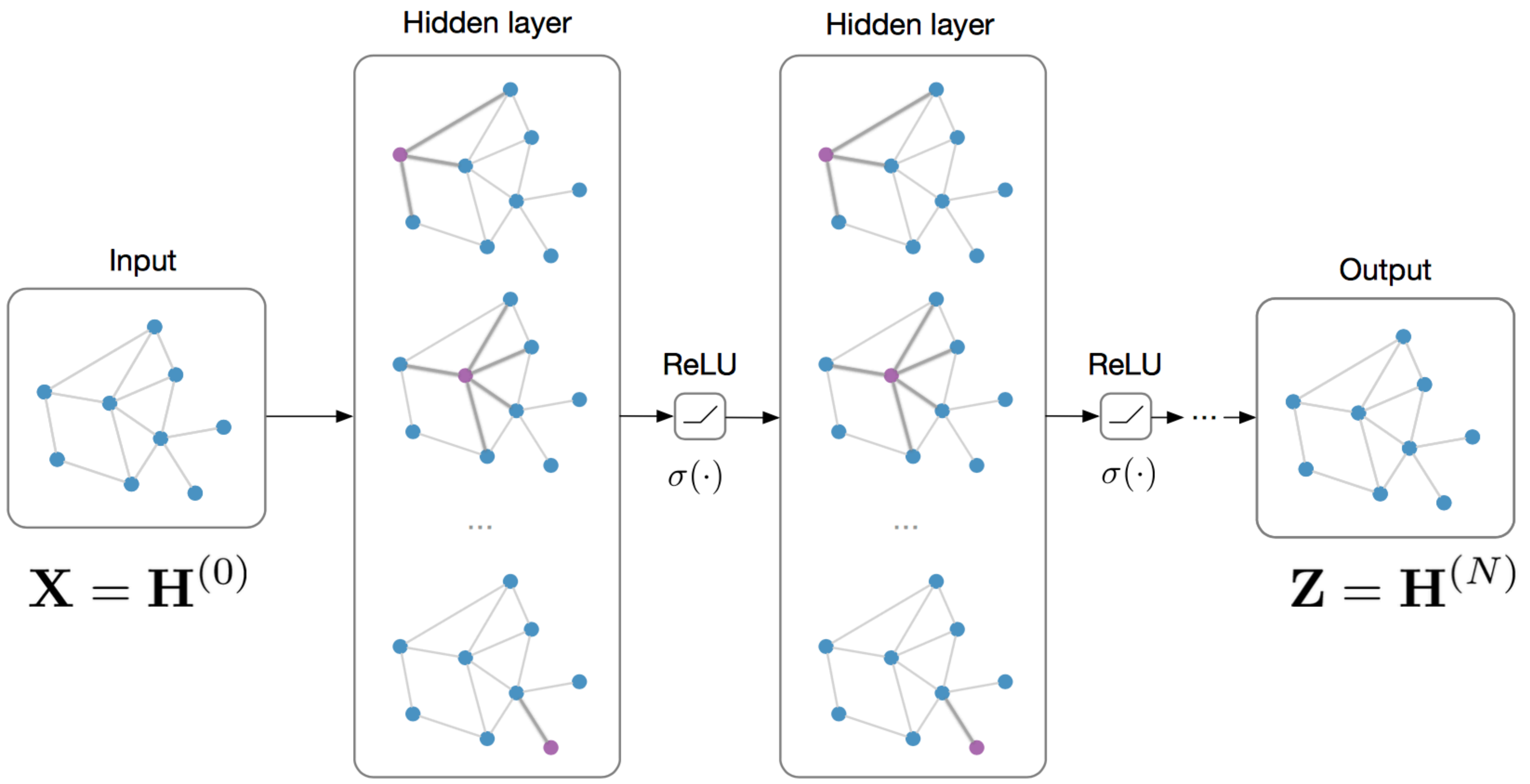


Figure 3: The proposed stochastic multiple partitions scheme. In each epoch, we randomly sample q clusters ($q = 2$ is used in this example) and their between-cluster links to form a new batch. Same color blocks are in the same batch.

How do we use GNN / GCN for real problems?

Classification and **Link Prediction** with GNNs / GCNs

Input: Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times E}$, preprocessed adjacency matrix $\hat{\mathbf{A}}$

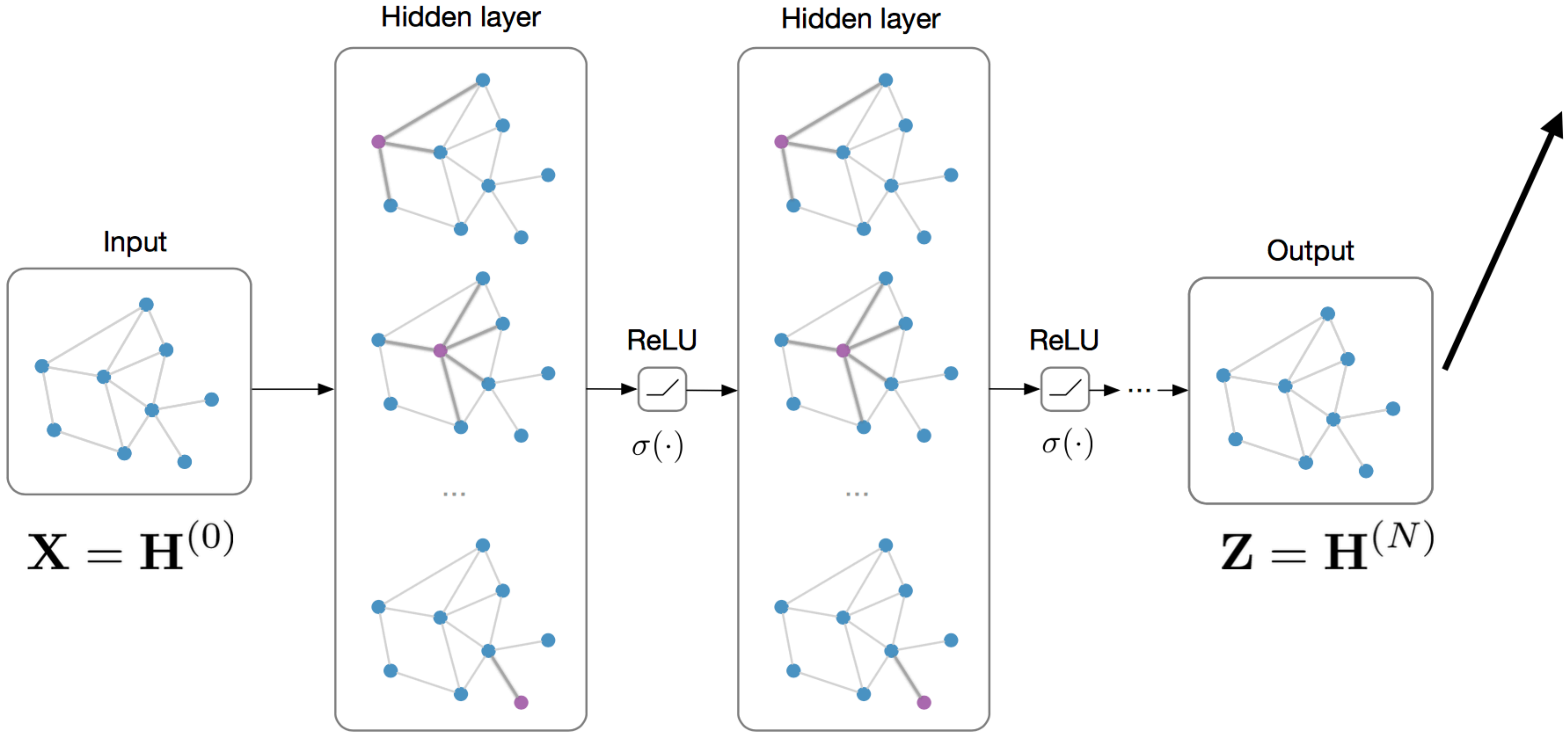


$$\mathbf{H}^{(l+1)} = \sigma\left(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)}\right)$$

* slide from Thomas Kipf, **University of Amsterdam**

Classification and **Link Prediction** with GNNs / GCNs

Input: Feature matrix $\mathbf{X} \in \mathbb{R}^{N \times E}$, preprocessed adjacency matrix $\hat{\mathbf{A}}$



$$\mathbf{H}^{(l+1)} = \sigma\left(\hat{\mathbf{A}}\mathbf{H}^{(l)}\mathbf{W}^{(l)}\right)$$

Node classification:

$$\mathrm{softmax}(\mathbf{z_n})$$

e.g. Kipf & Welling (ICLR 2017)

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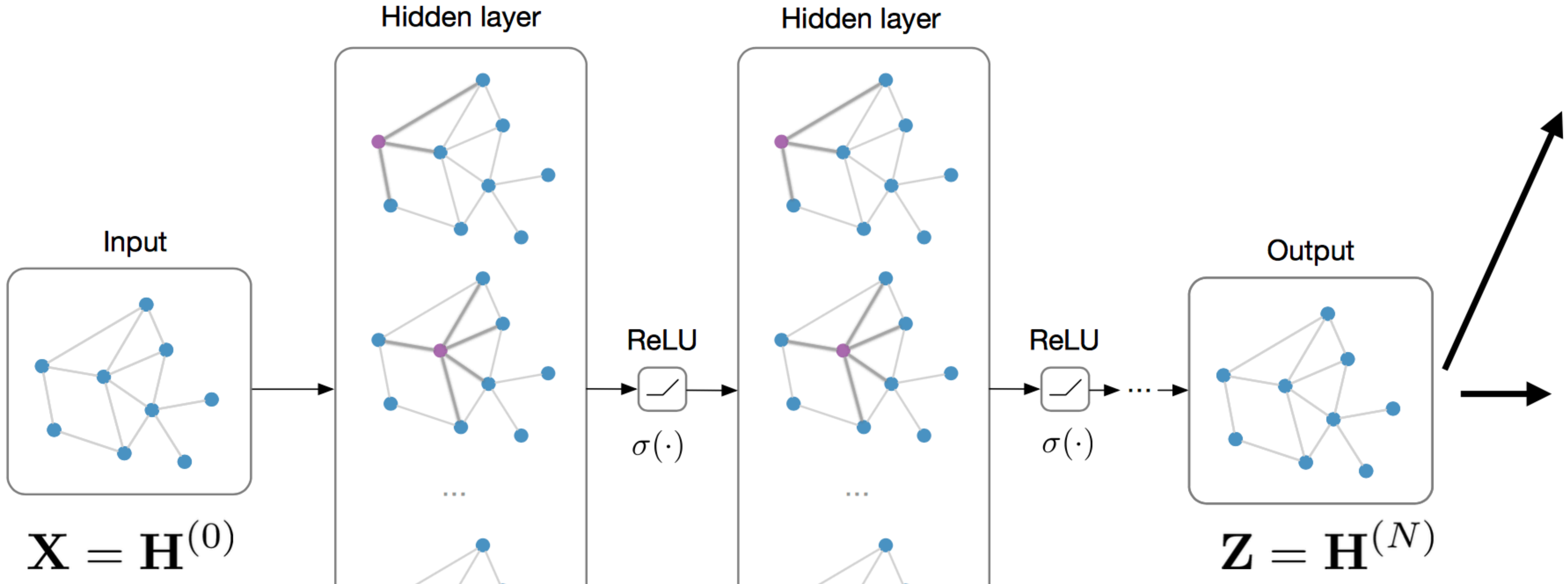

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Graph classification:

$$\mathrm{softmax}(\textstyle\sum_n \mathbf{z_n})$$

e.g. Duvenaud et al. (NIPS 2015)

* slide from Thomas Kipf, **University of Amsterdam**

Classification and **Link Prediction** with GNNs / GCNs

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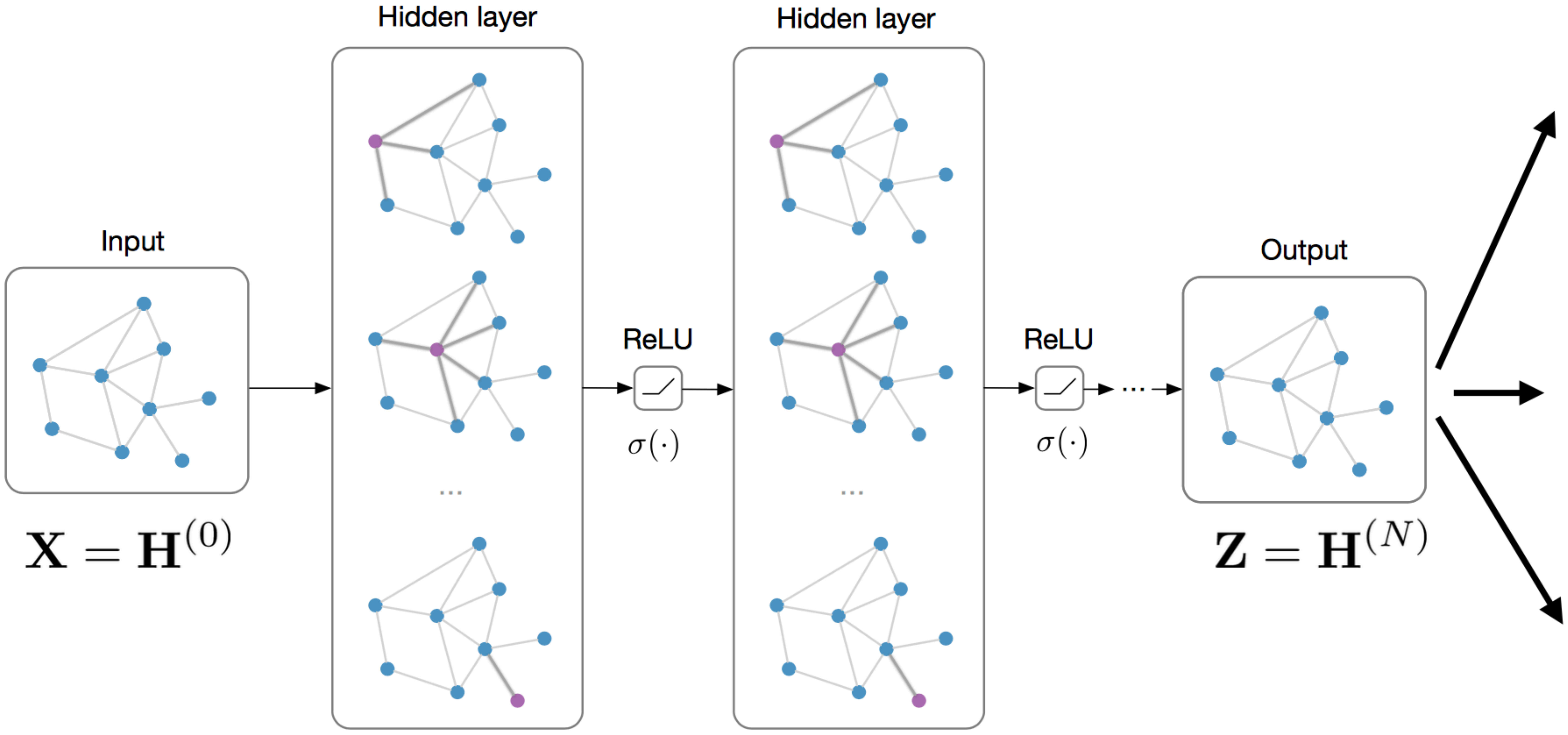

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Graph classification:

$$\mathrm{softmax}(\textstyle\sum_n \mathbf{z_n})$$

e.g. Duvenaud et al. (NIPS 2015)

Link prediction:

$$p(A_{ij}) = \sigma(\mathbf{z_i^T z_j})$$

Kipf & Welling (NIPS BDL 2016)
"Graph Auto-Encoders"

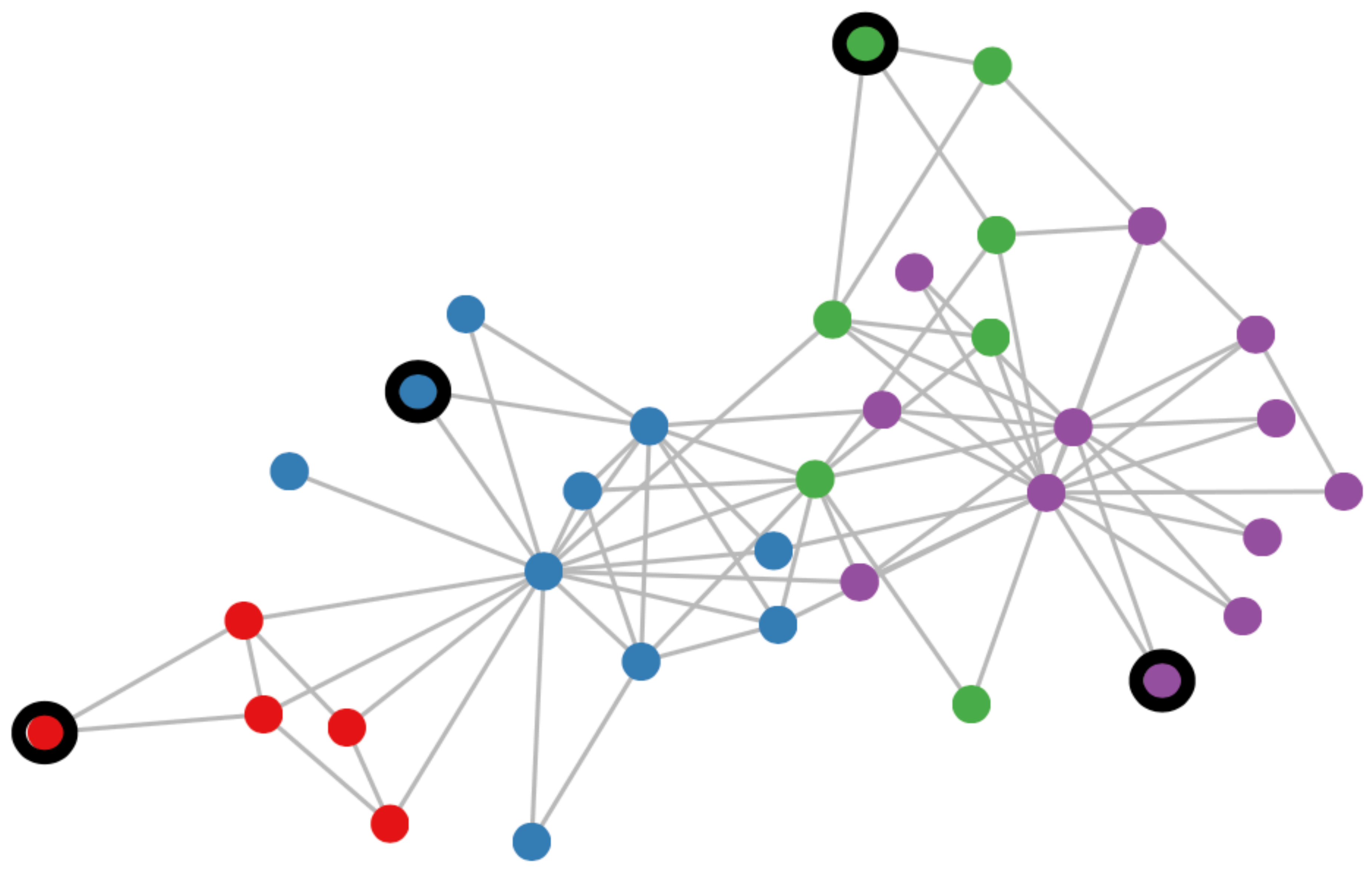
* slide from Thomas Kipf, **University of Amsterdam**

Semi-supervised Classification on Graphs

Setting:

Some nodes are labeled (black circle)
All other nodes are unlabeled

Task:
Predict node label of unlabeled nodes



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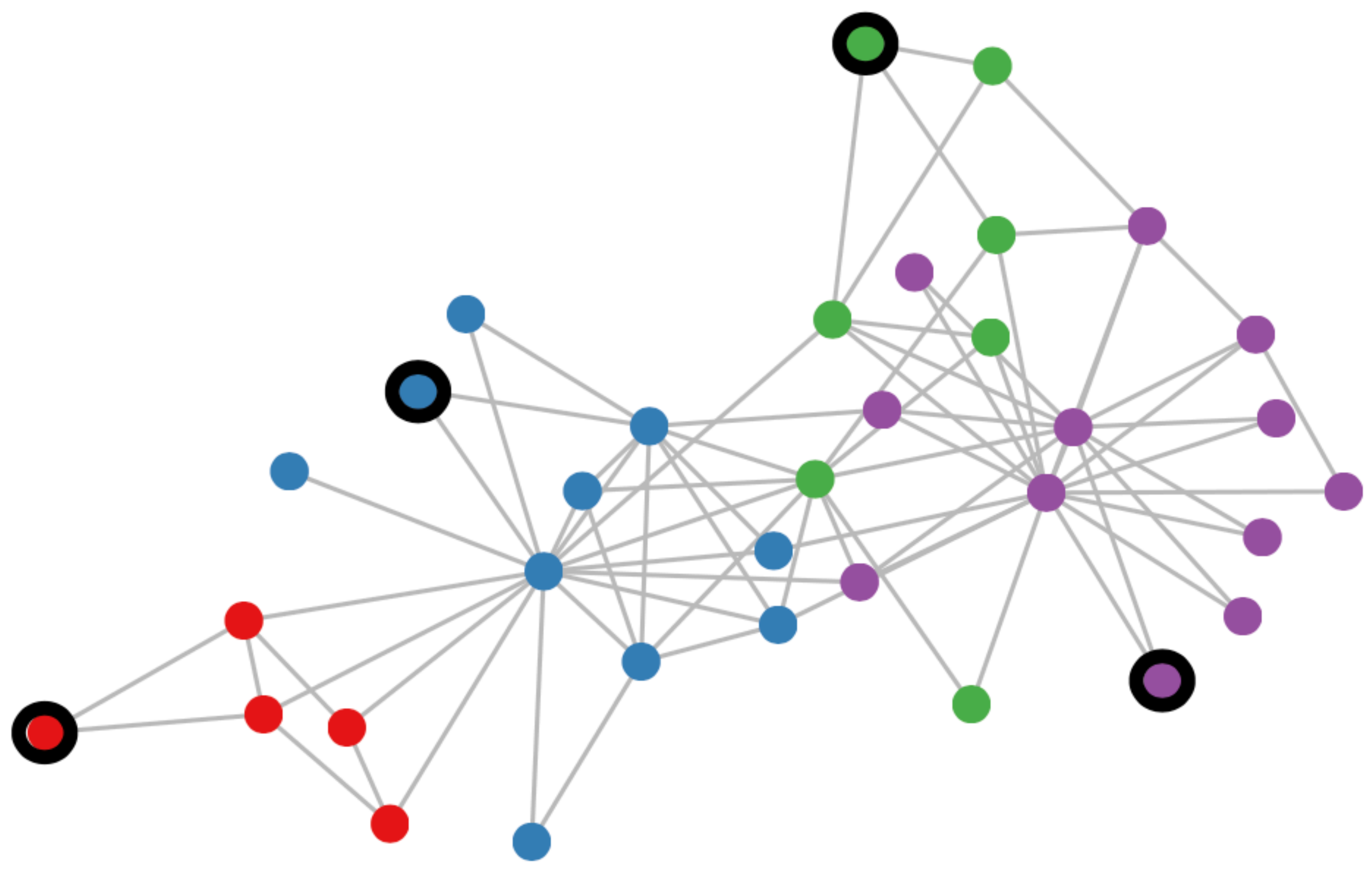


Evaluate loss on labeled nodes only:

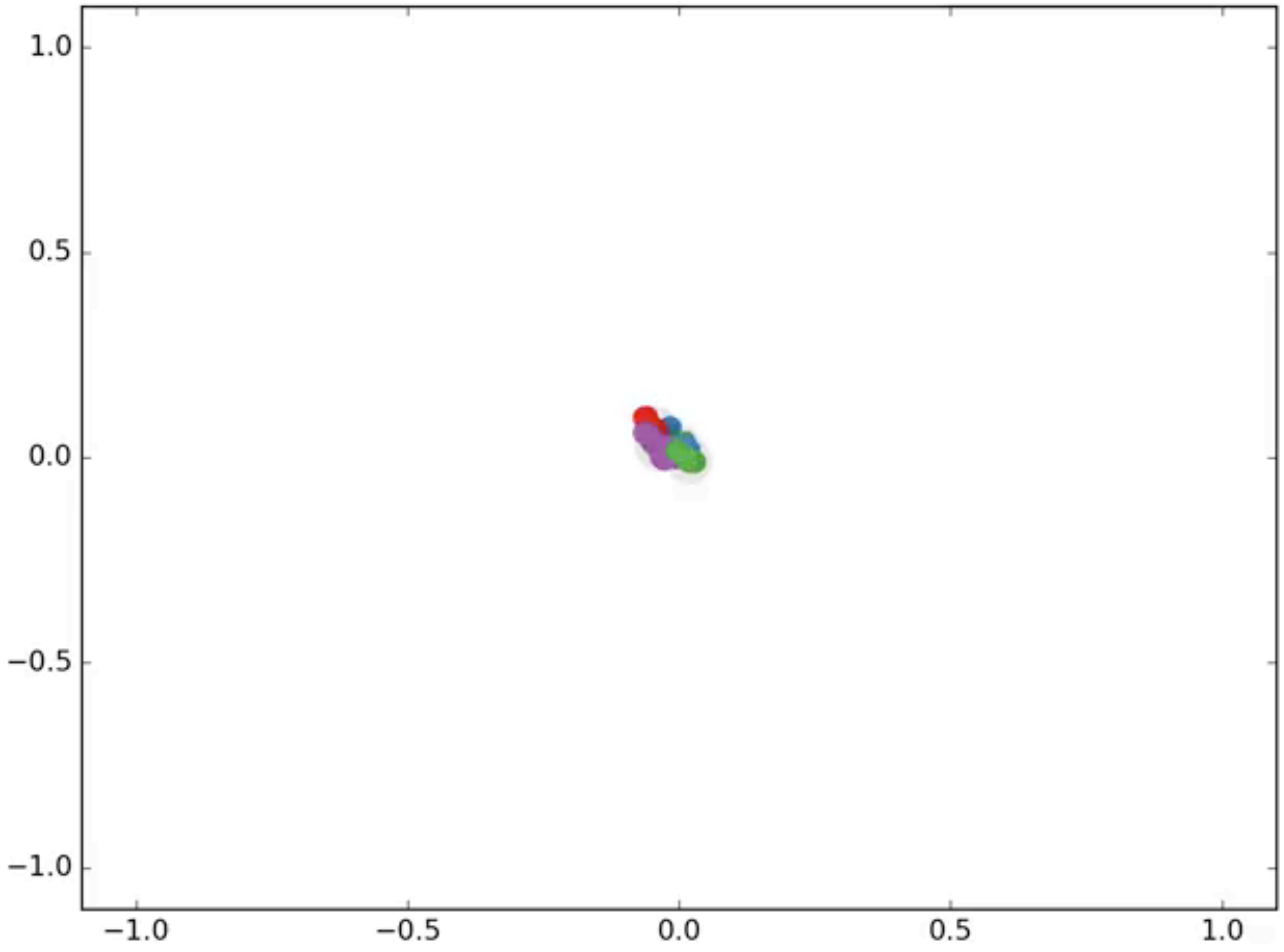
$$\mathcal{L} = -\sum_{l \in \mathcal{Y}_L} \sum_{f=1}^{F} Y_{lf} \ln Z_{lf}$$

$\mathcal{Y}_L$ set of labeled node indices

$\mathbf{Y}$ label matrix

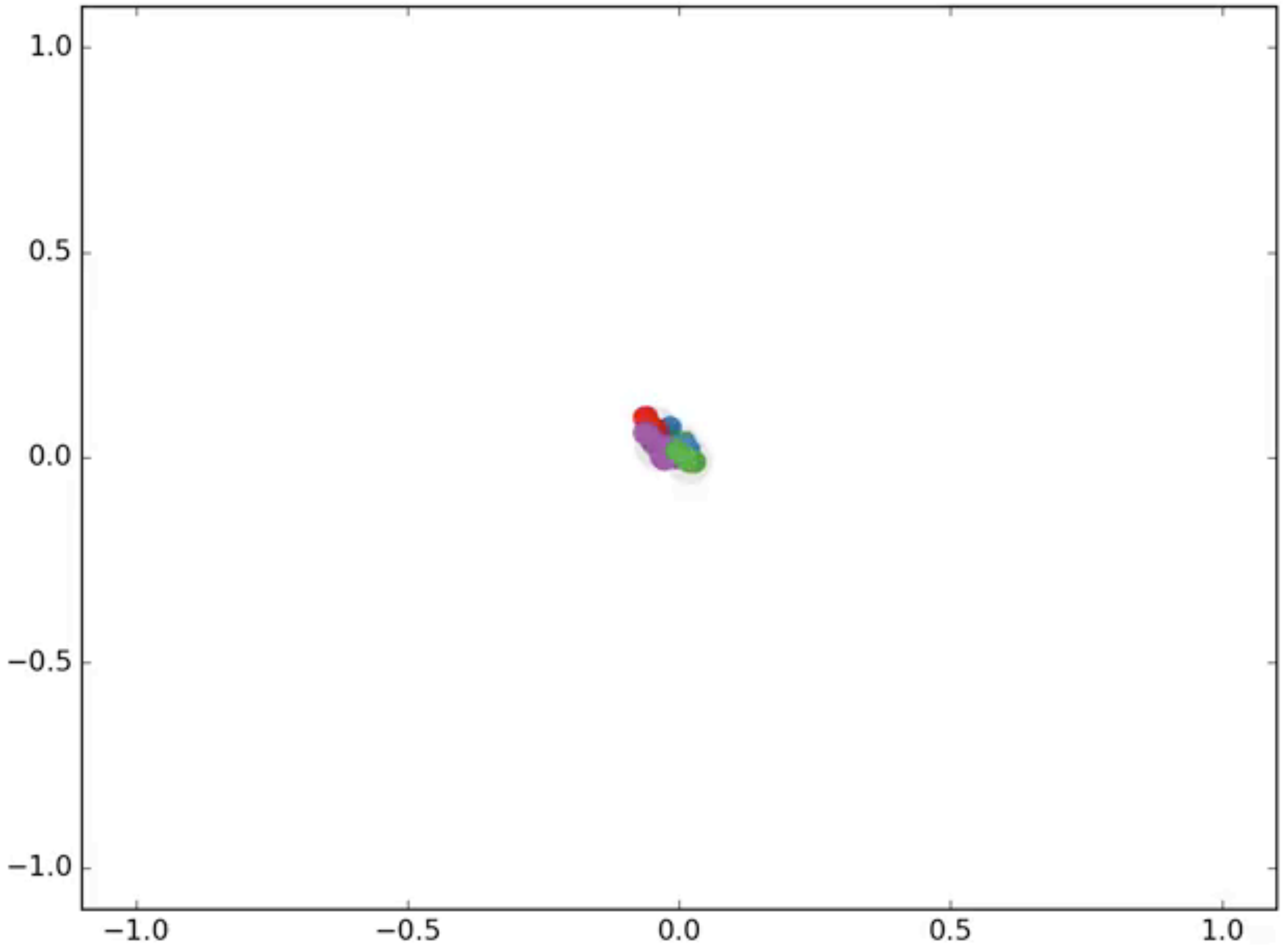
$\mathbf{Z}$ GCN output (after softmax)

Semi-supervised Classification on Graphs



* slide from Thomas Kipf, **University of Amsterdam**

Semi-supervised Classification on Graphs



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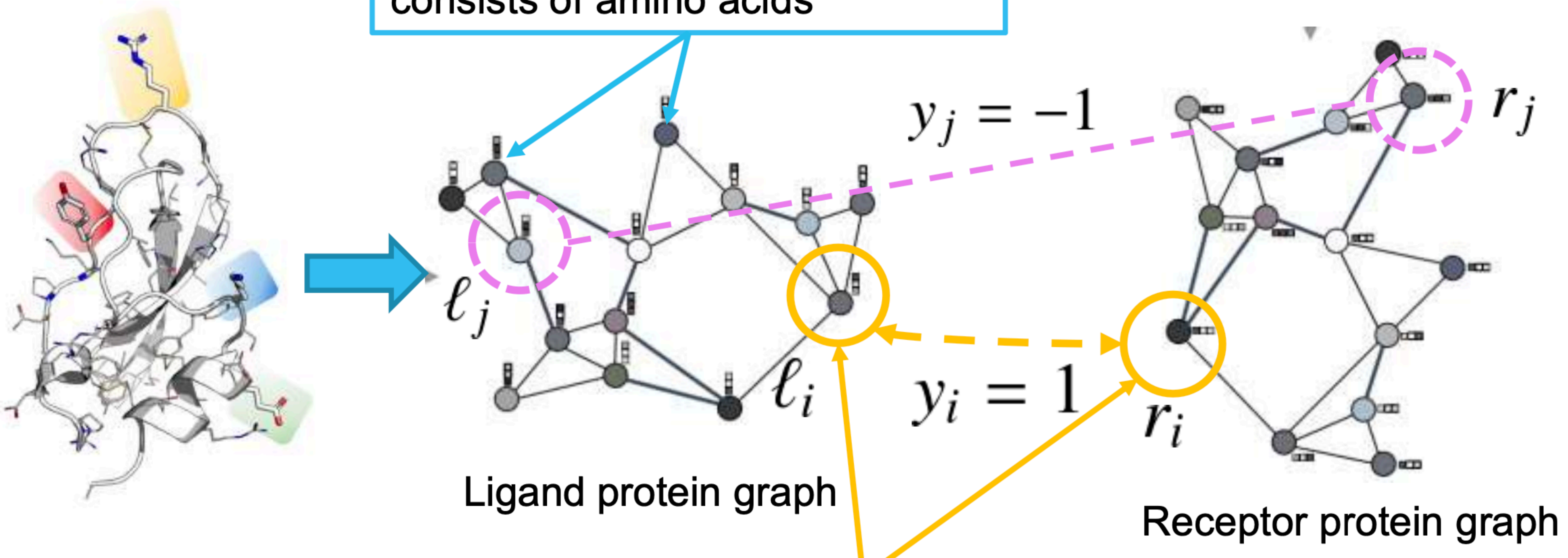
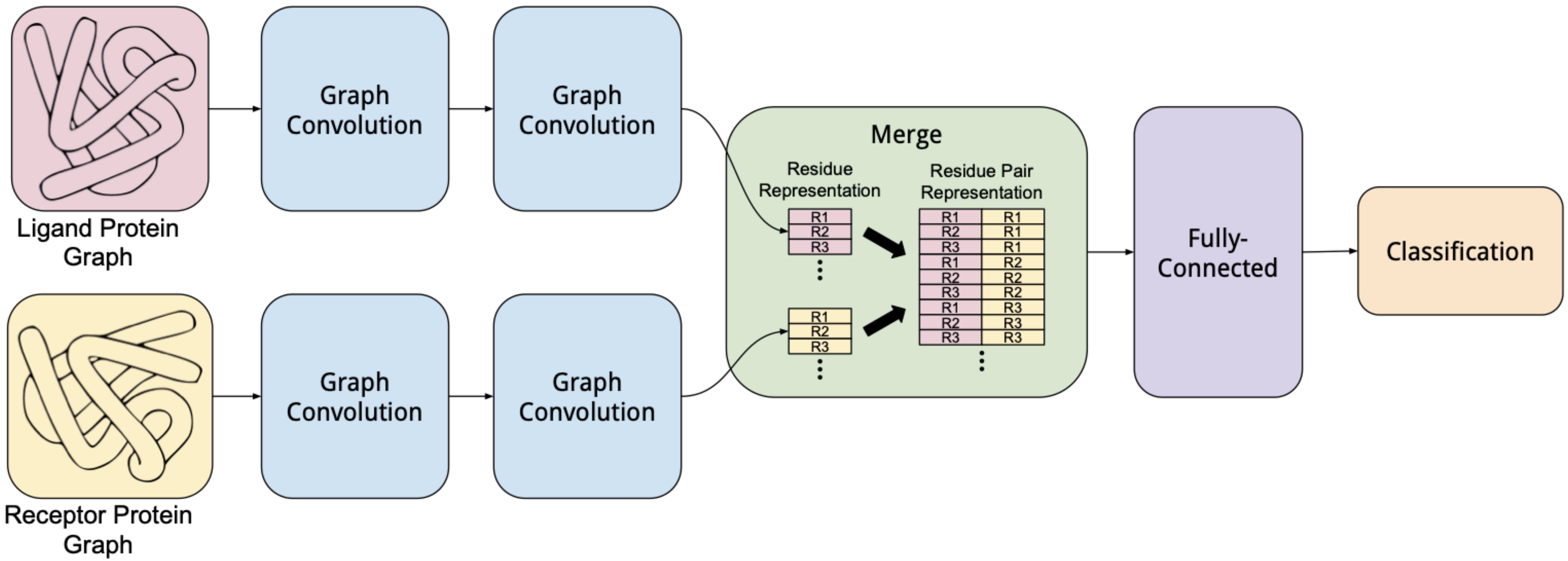
Protein Interface Prediction

Node **(residue)**: a sub-structure consists of amino acids



Binding sites: specific nodes **interact between ligand and receptor**

Protein Interface Prediction



Protein Interface Prediction

Node features only:

$$z_i = \sigma\left(W^{\mathrm{C}} x_i + \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} W^{\mathrm{N}} x_j + b\right)$$

Node features + **edge** features:

$$z_i = \sigma\left(W^{\mathrm{C}} x_i + \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} W^{\mathrm{N}} x_j + \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} W^{\mathrm{E}} A_{ij} + b\right)$$

Node features + **edge** features:

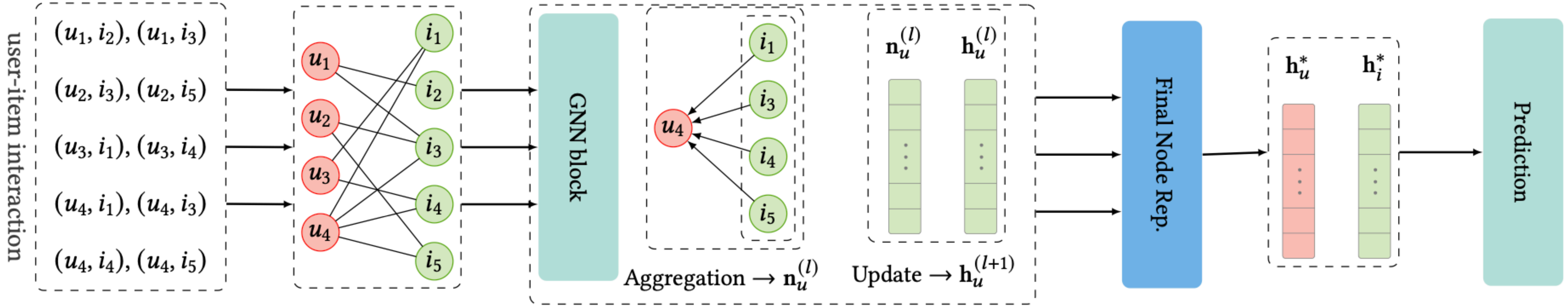
$$z_i = \sigma\left(W^{\mathrm{C}} x_i + \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} W_j^{\mathrm{N}} x_j + \frac{1}{|\mathcal{N}_i|} \sum_{j \in \mathcal{N}_i} W_j^{\mathrm{E}} A_{ij} + b\right)$$

Neighbor nodes j are ordered by distances from the node i

Protein Interface Prediction

Method	Convolutional Layers			
	1	2	3	4
No Convolution	**0.812 (0.007)**	0.810 (0.006)	0.808 (0.006)	0.796 (0.006)
Diffusion (DCNN) (2 hops) [5]	**0.790 (0.014)**	–	–	–
Diffusion (DCNN) (5 hops) [5])	**0.828 (0.018)**	–	–	–
Single Weight Matrix (MFN [9])	0.865 (0.007)	0.871 (0.013)	**0.873 (0.017)**	0.869 (0.017)
Node Average (Equation 1)	0.864 (0.007)	0.882 (0.007)	**0.891 (0.005)**	0.889 (0.005)
Node and Edge Average (Equation 2)	0.876 (0.005)	**0.898 (0.005)**	0.895 (0.006)	0.889 (0.007)
DTNN [21]	0.867 (0.007)	0.880 (0.007)	**0.882 (0.008)**	0.873 (0.012)
Order Dependent (Equation 3)	0.854 (0.004)	0.873 (0.005)	**0.891 (0.004)**	0.889 (0.008)

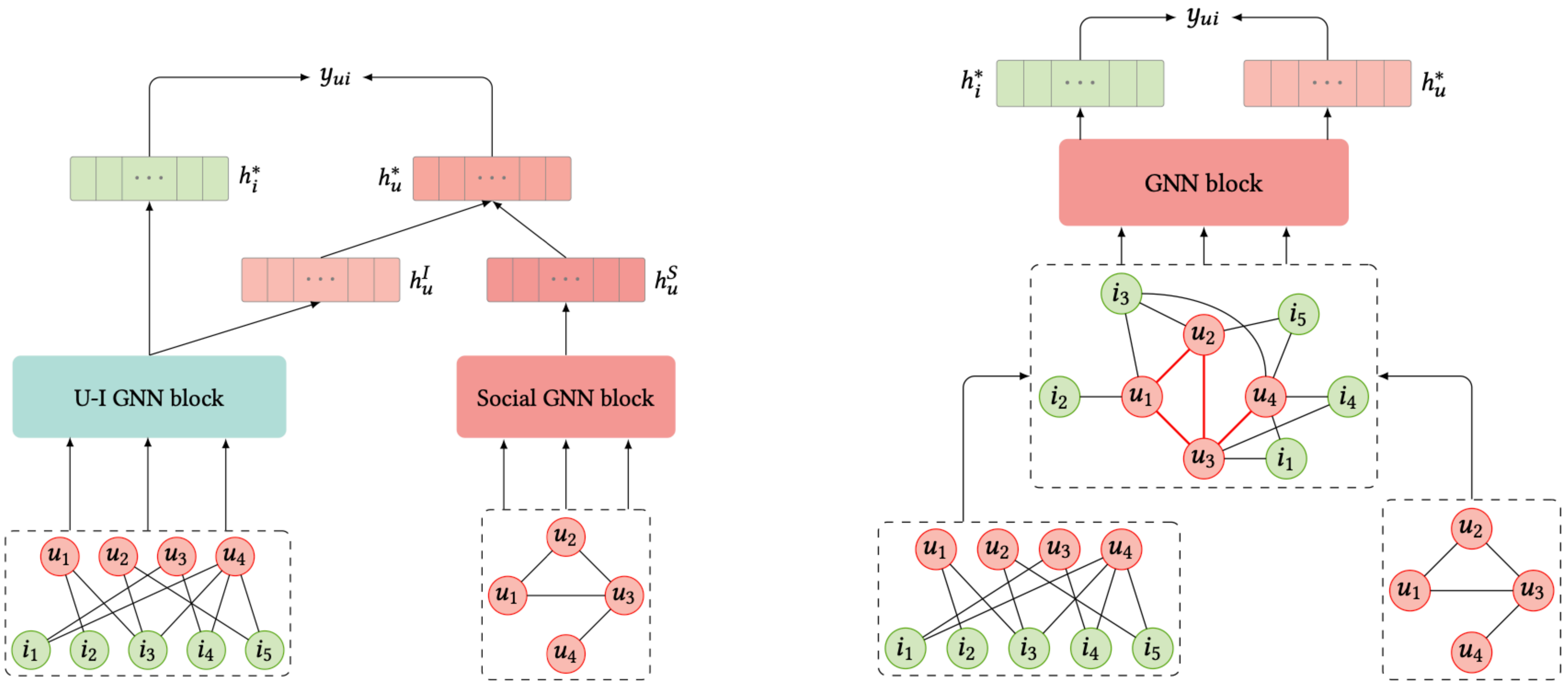
Recommender Systems



Typical framework of GNN in user-item collaborative filtering

Graph Neural Networks in Recommender Systems: A Survey, Wu et al

Recommender Systems



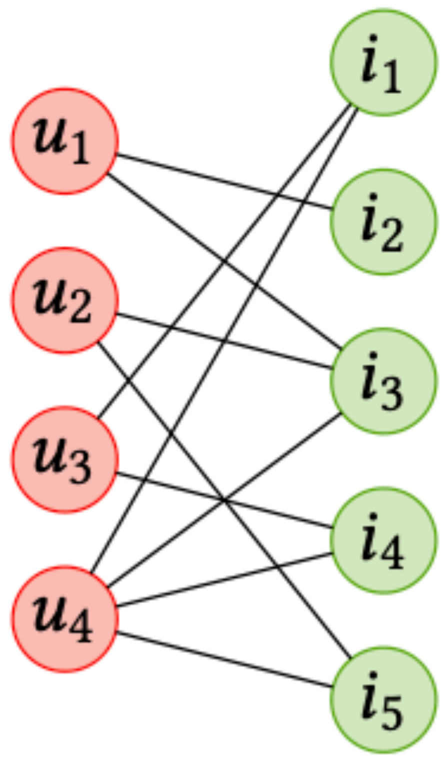
(a) The framework of GNN on the bipartite graph and social network graph separately.

(b) The framework of GNN on the unified graph of user-item interactions and social network.

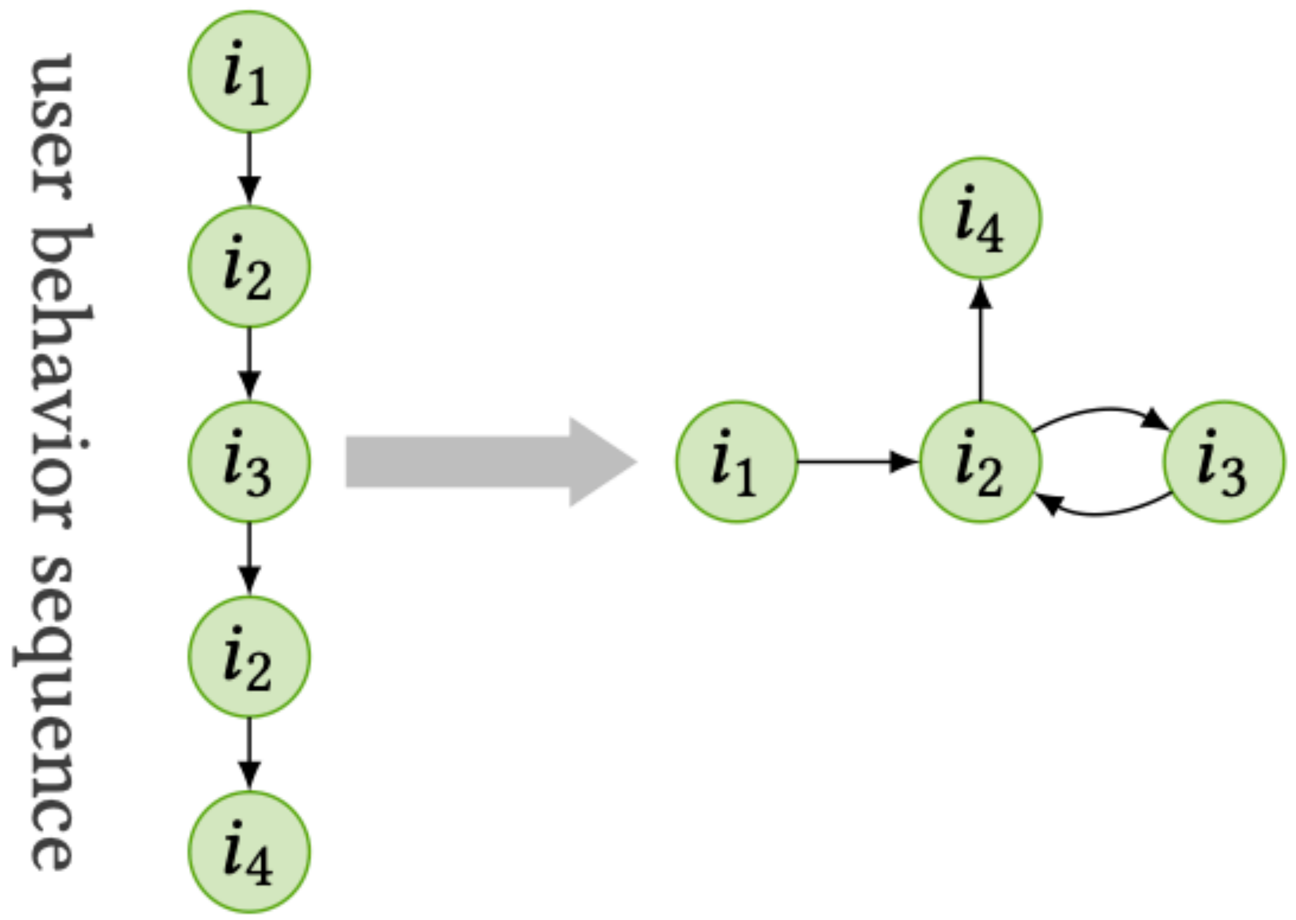
Graph Neural Networks in Recommender Systems: A Survey, Wu et al

Recommender Systems

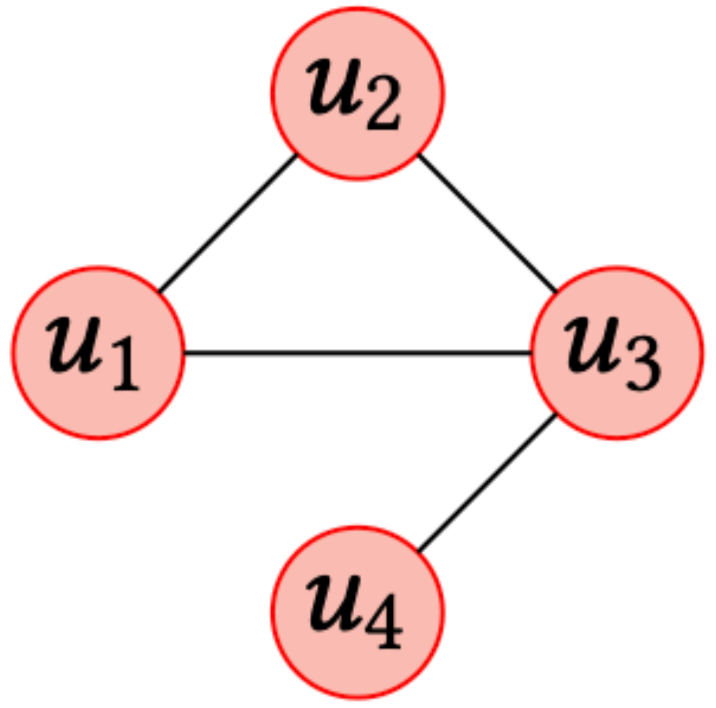
	i_1	i_2	i_3	i_4	i_5
u_1	0	1	1	0	0
u_2	0	0	1	0	1
u_3	1	0	0	1	0
u_4	1	0	1	1	1



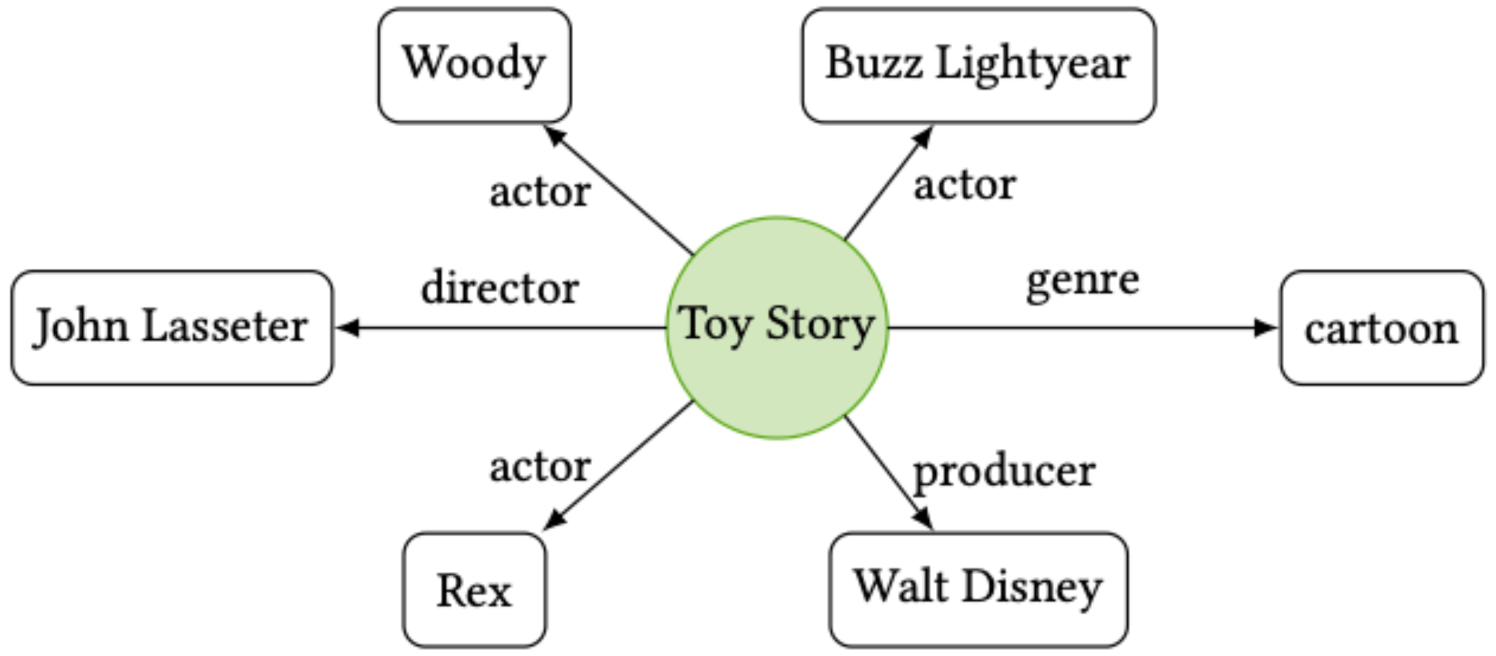
(a) User-item bipartite graph.



(b) Sequence graph.



(c) Social relationship between users.

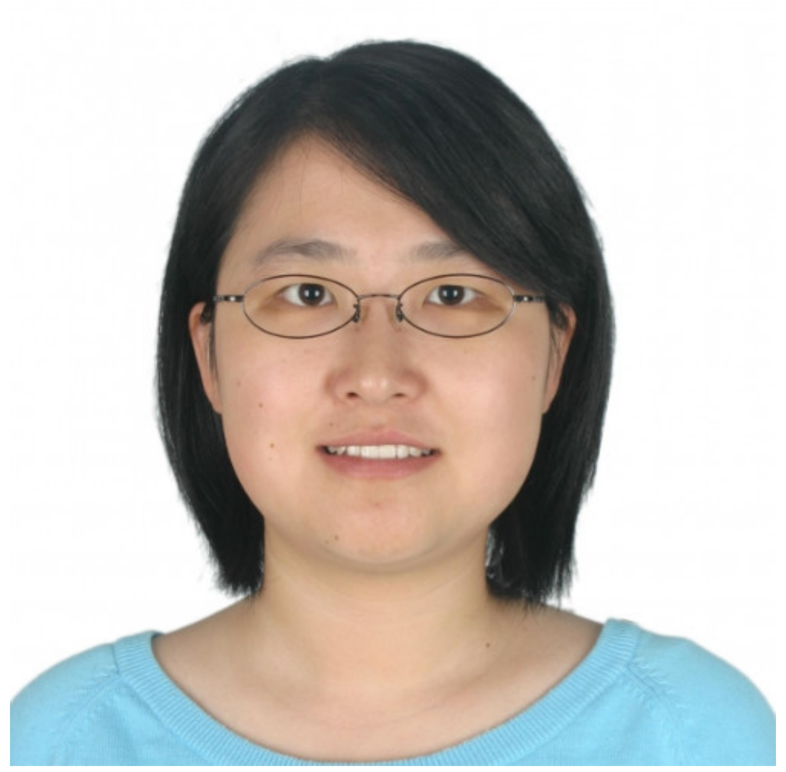


(d) Knowledge graph

Graph Neural Networks in Recommender Systems: A Survey, Wu et al

G³raphGround: Graph-based Language Grounding

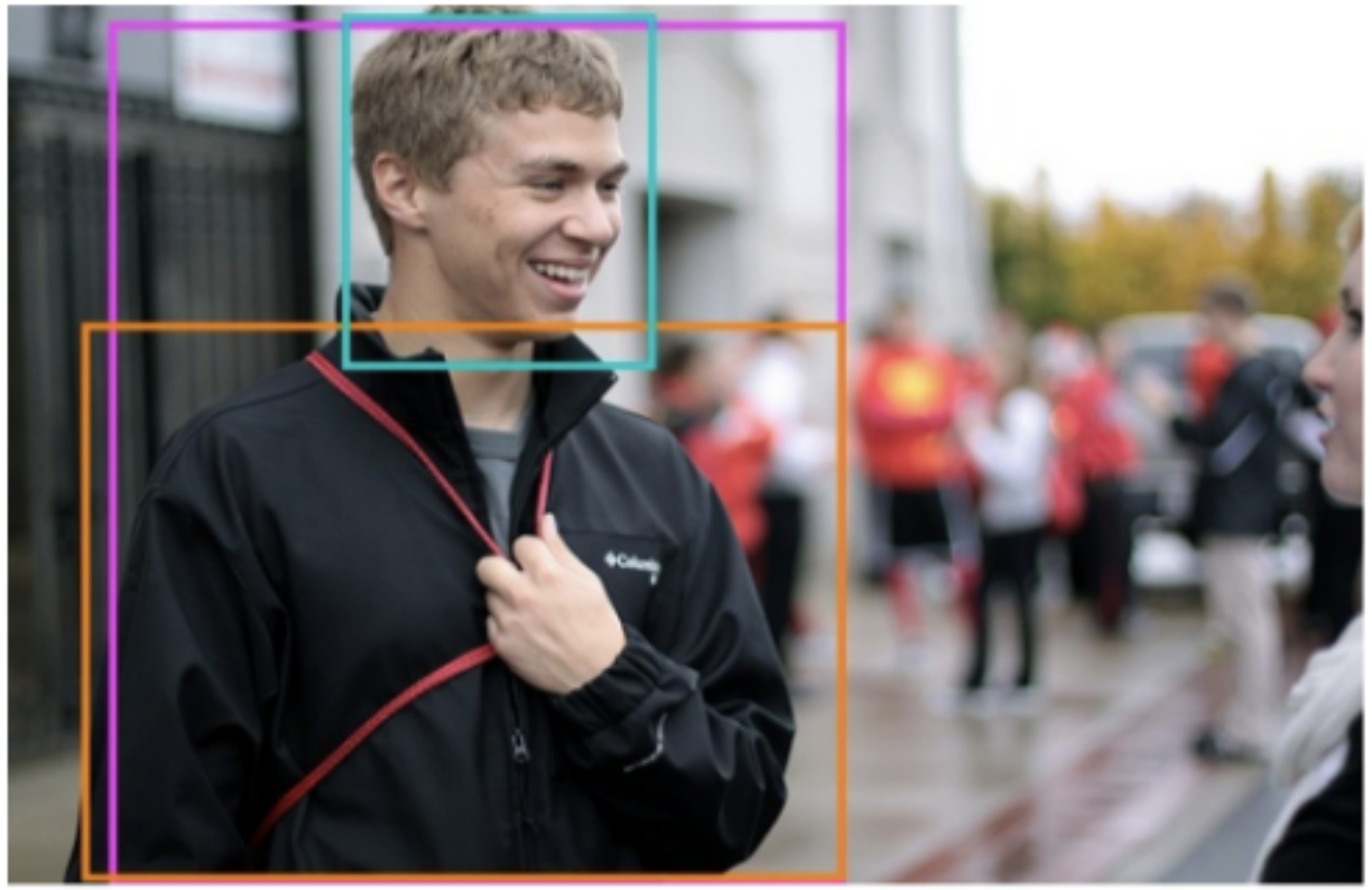
1



Mohit Bajaj Lanjun Wang Leonid Sigal

Image Grounding: Beyond Object Detection

Given the **image** and one or more **natural language phrases**, locate regions that correspond to those phrases.



A man wearing a black-jacket has a smile on his face.

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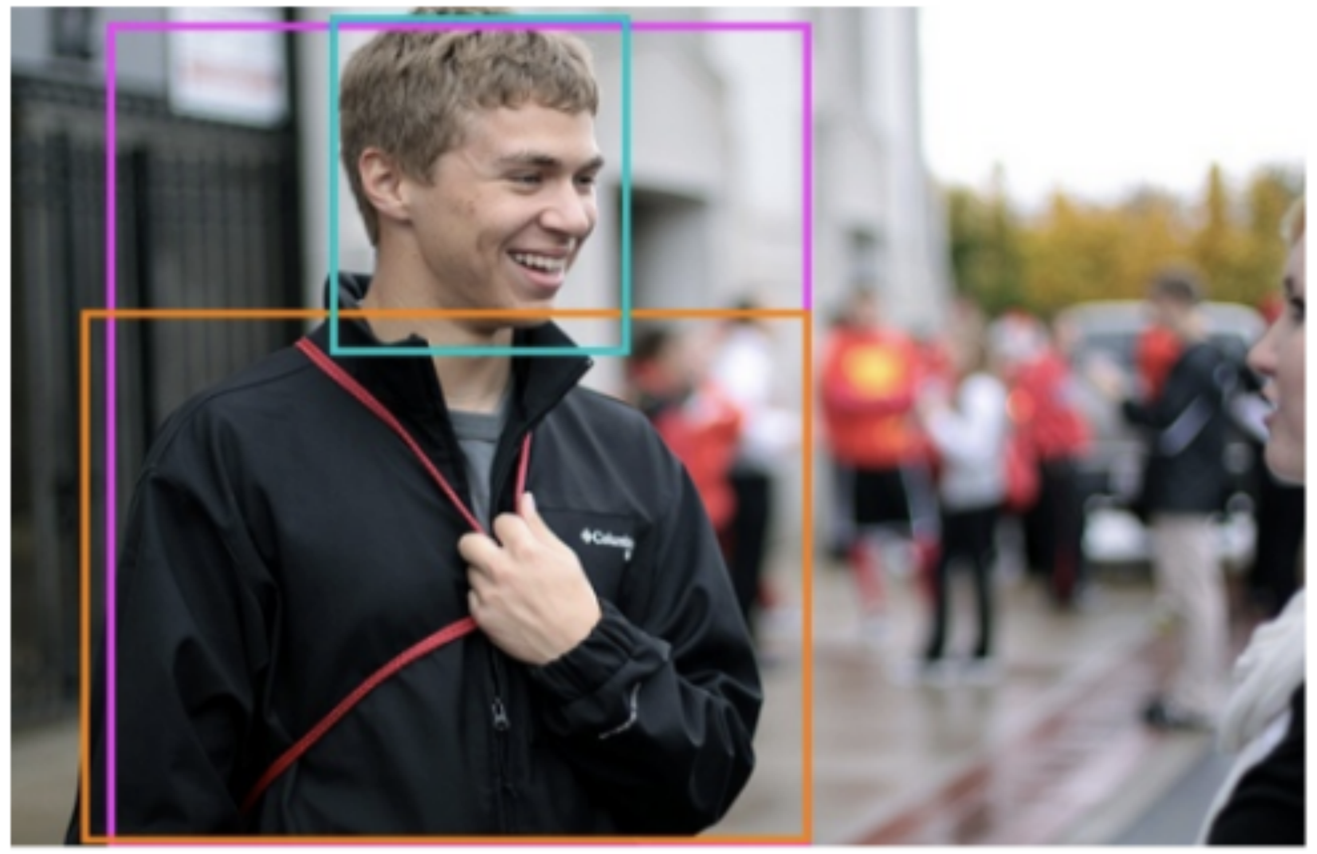

A man wearing a black-jacket has a smile on his face.

Fundamental task for **image / video understanding**

— Helps improve performance on other tasks (e.g., image captioning, VQA)

Proposed **Architecture**

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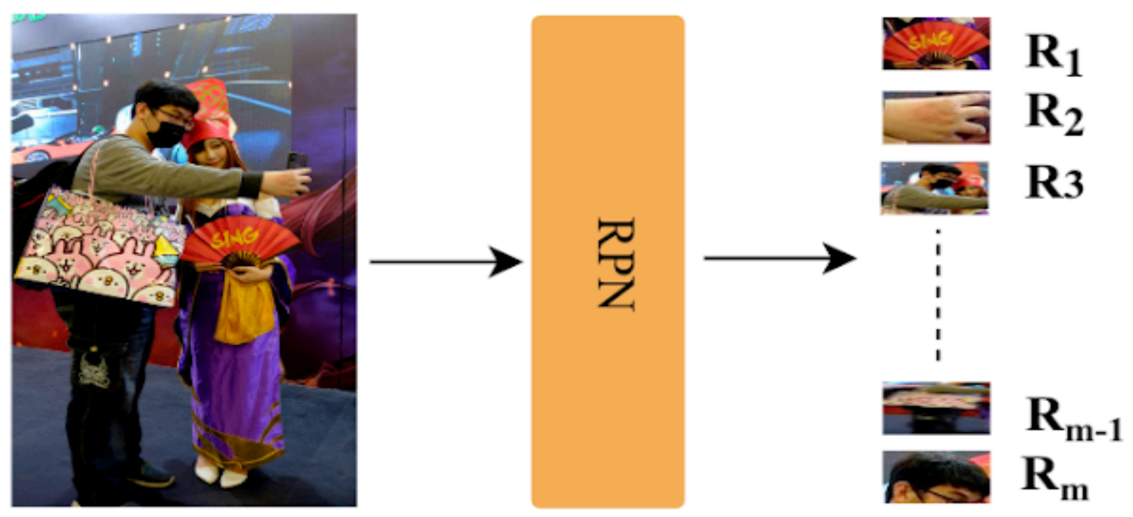

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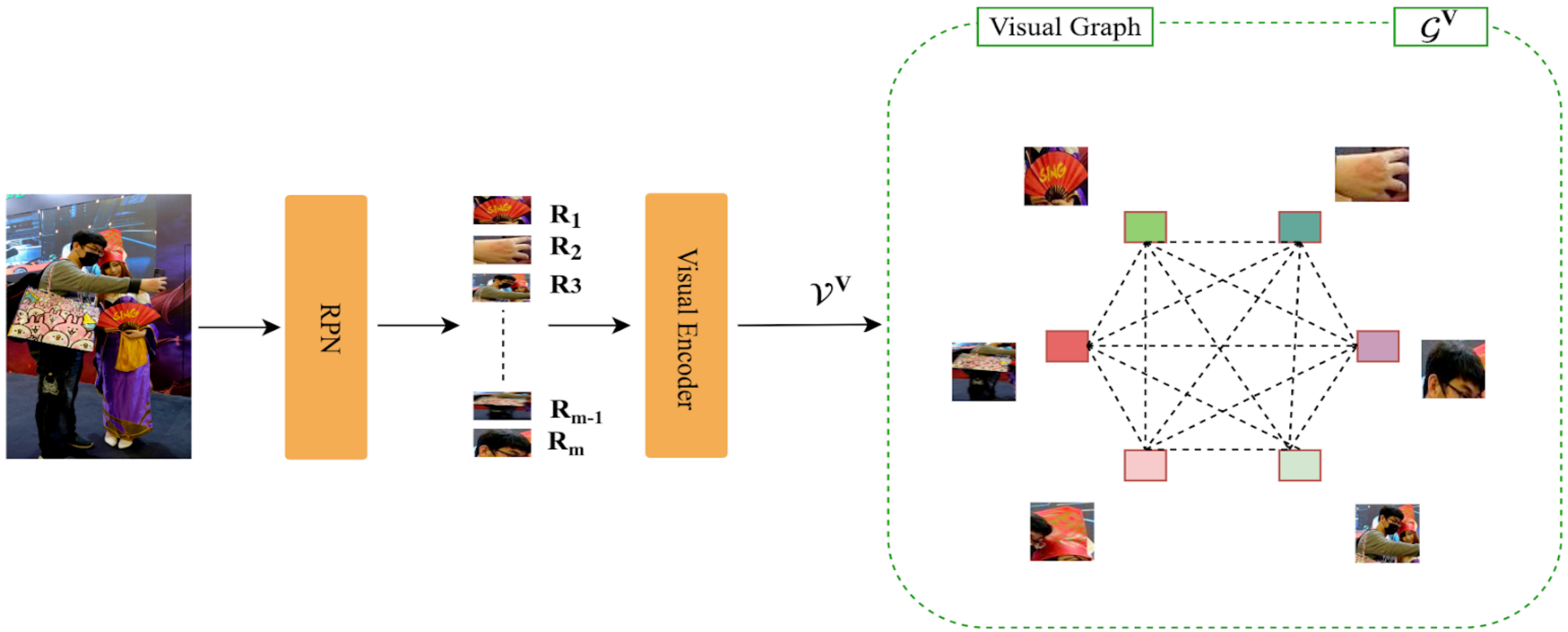

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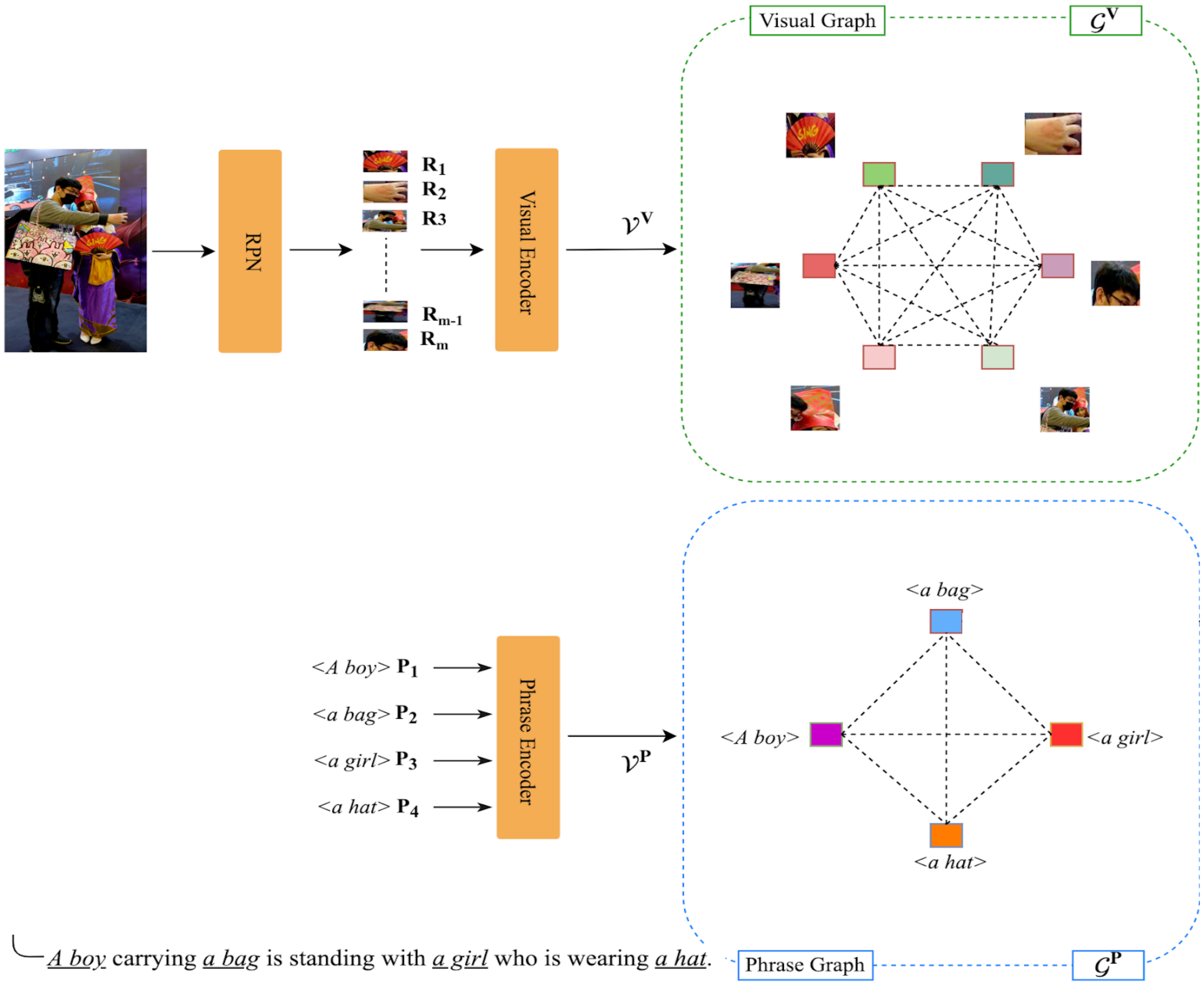

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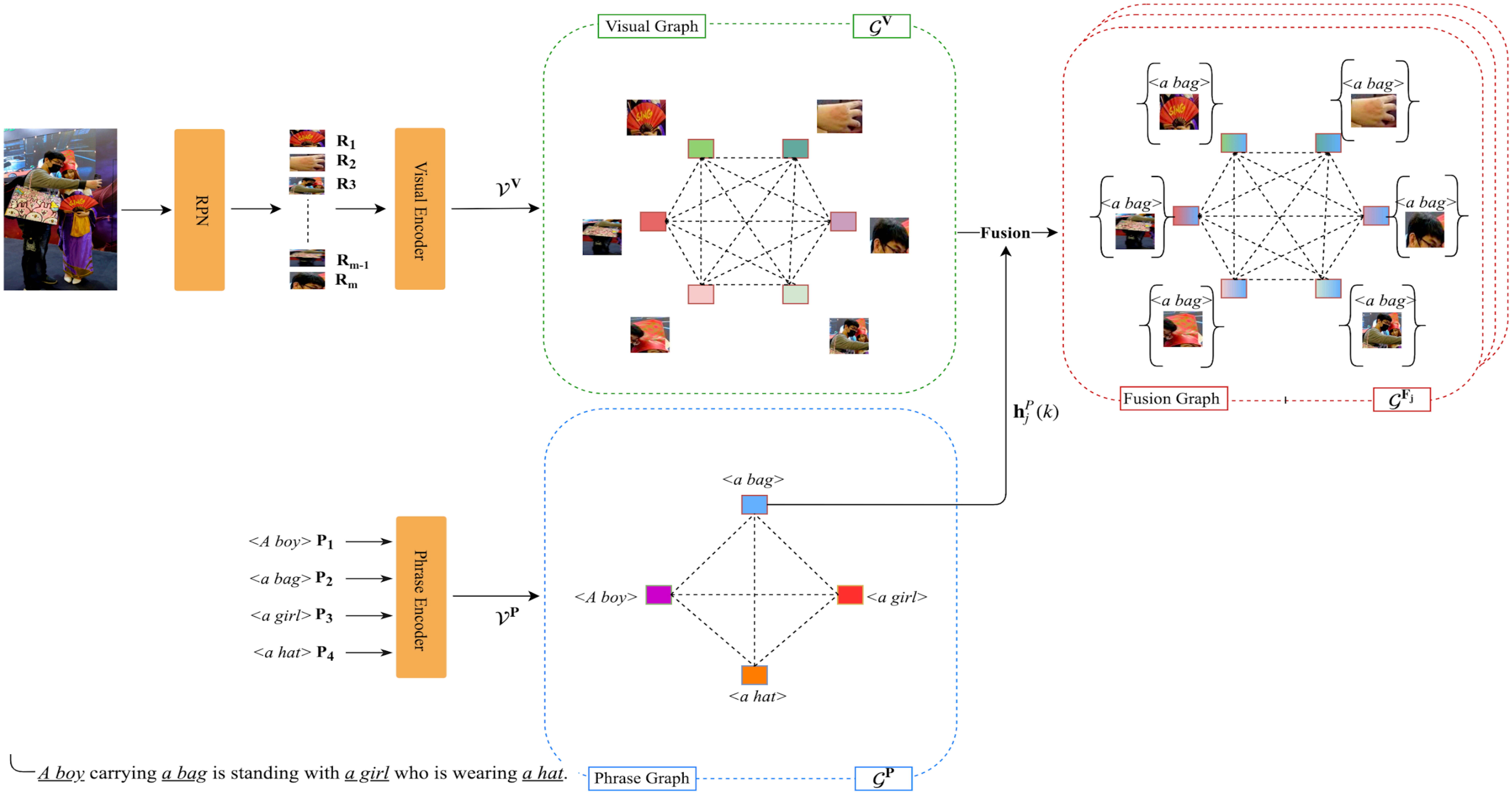

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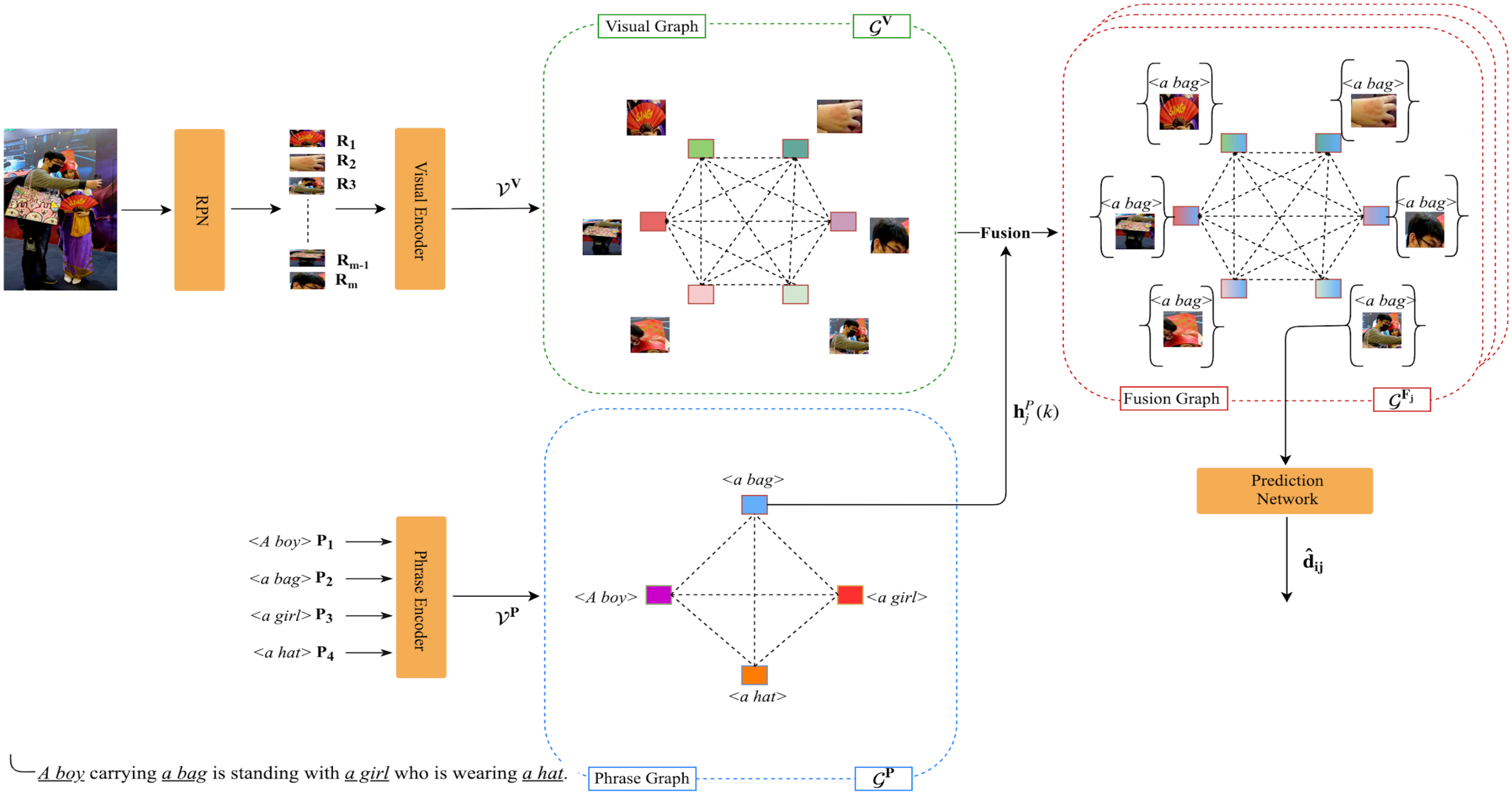

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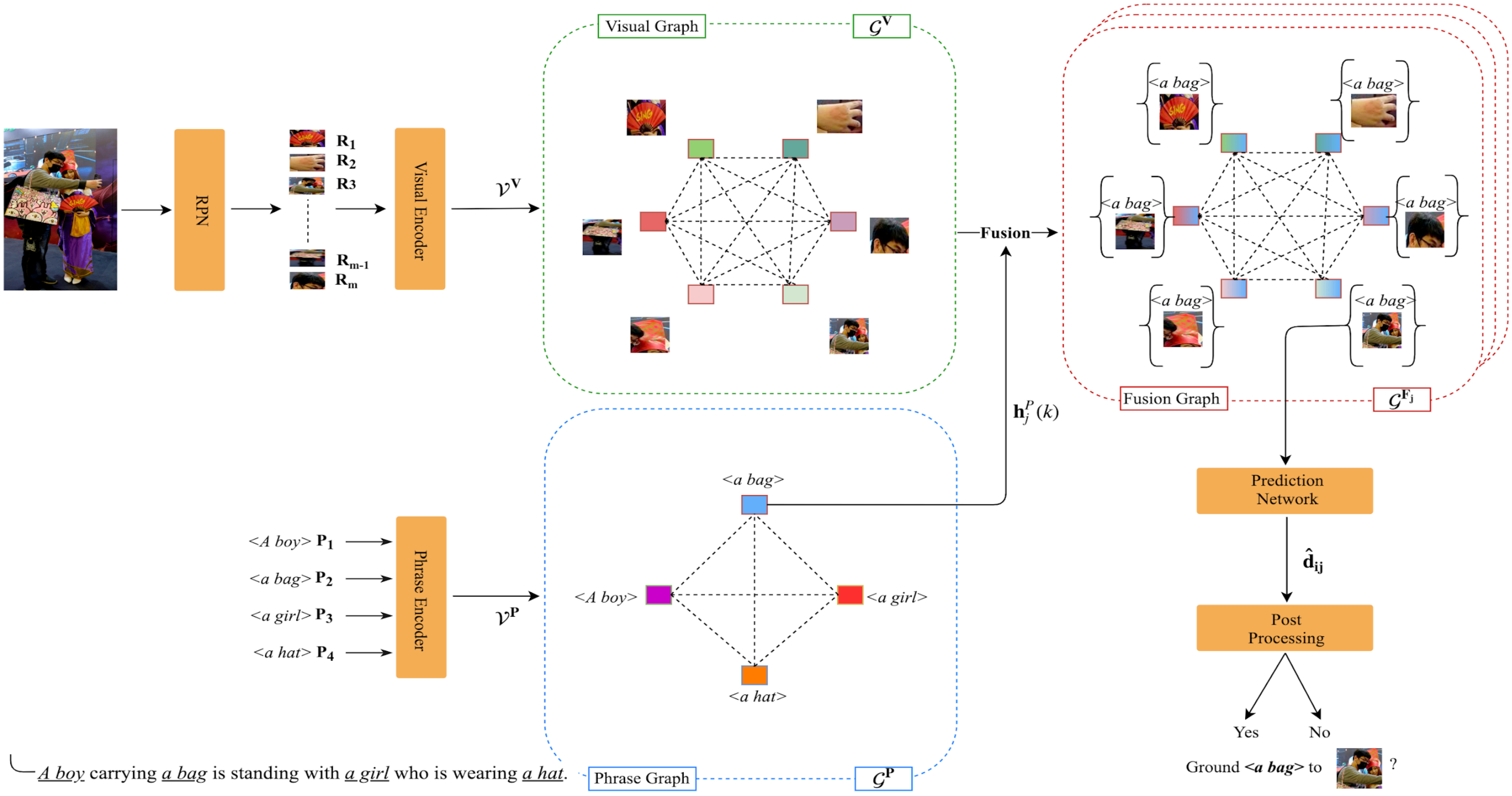

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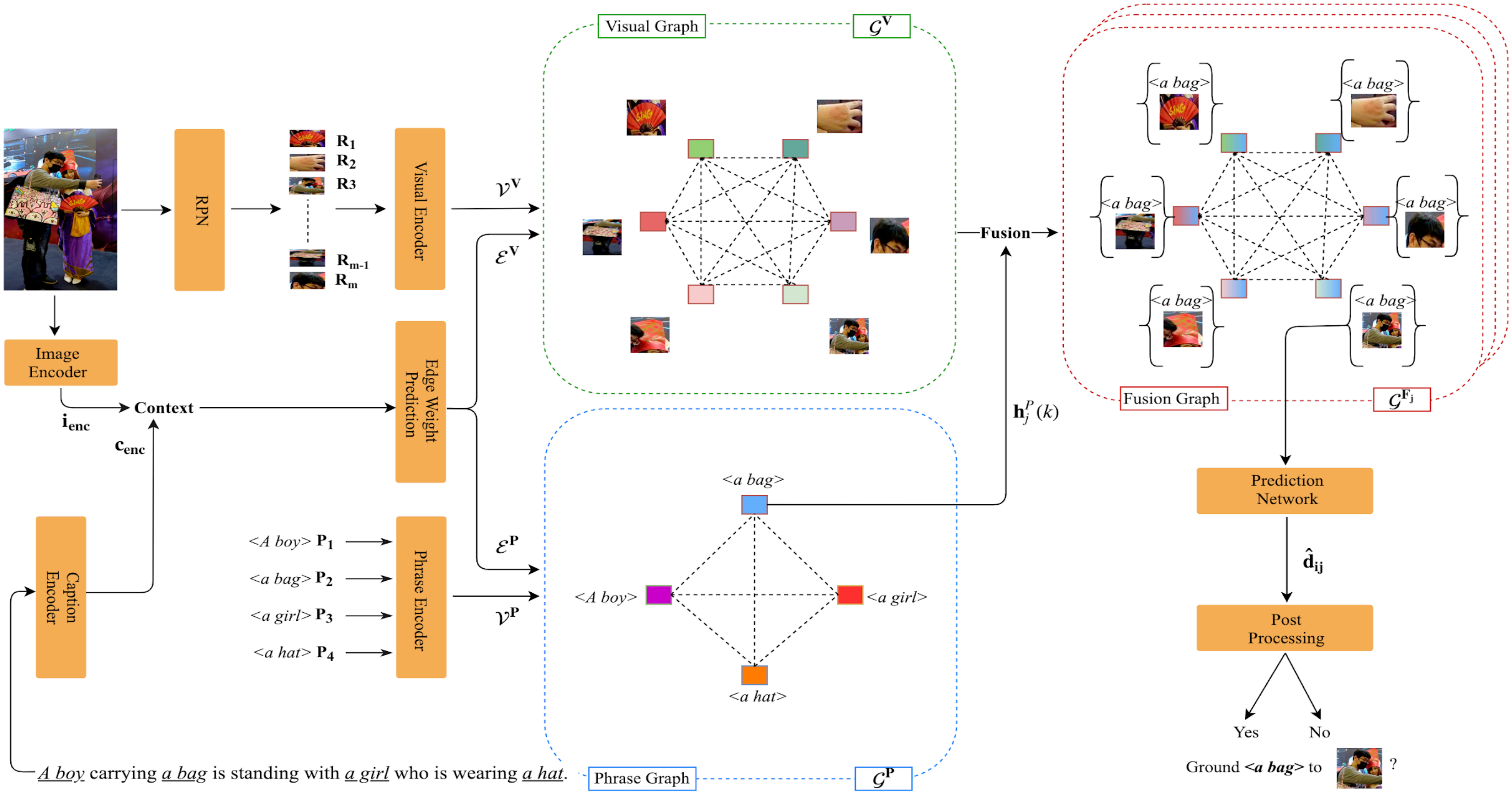


Experiments

Datasets

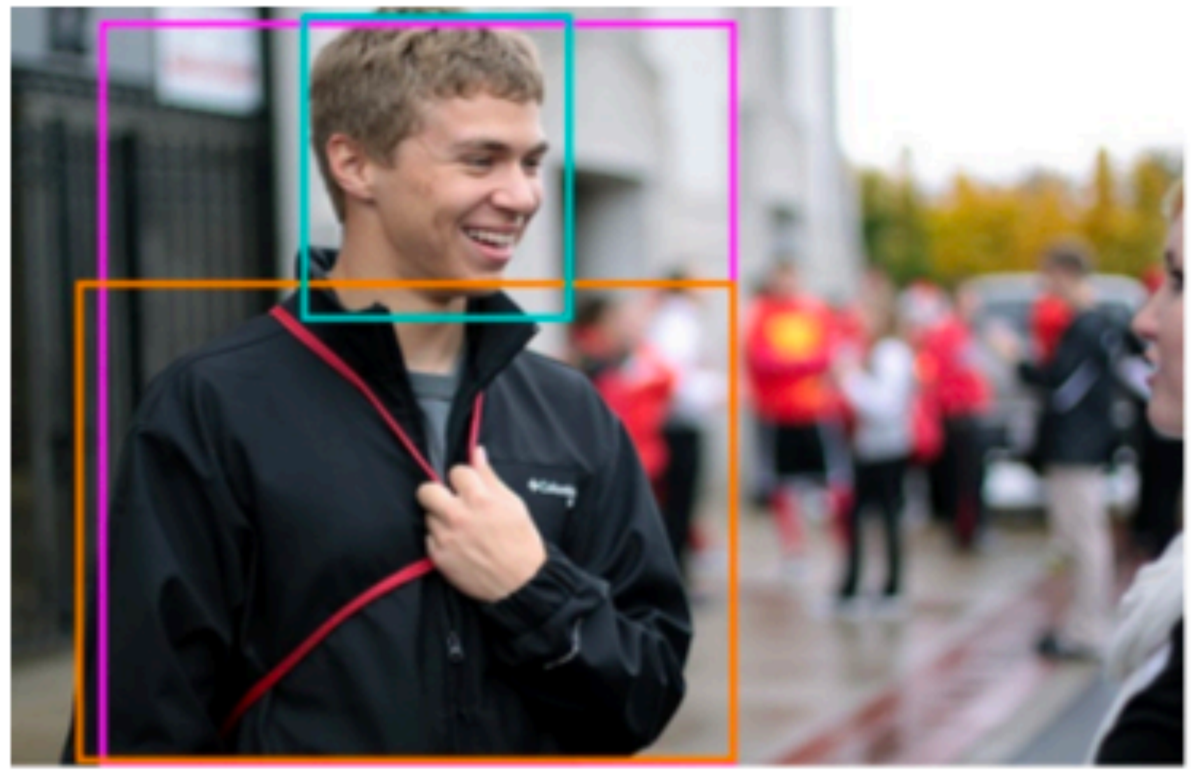
— **Flickr30K Entities**: (mostly noun) Phrases parsed from image captions

— **ReferIt Game**: Unambiguous single phrases

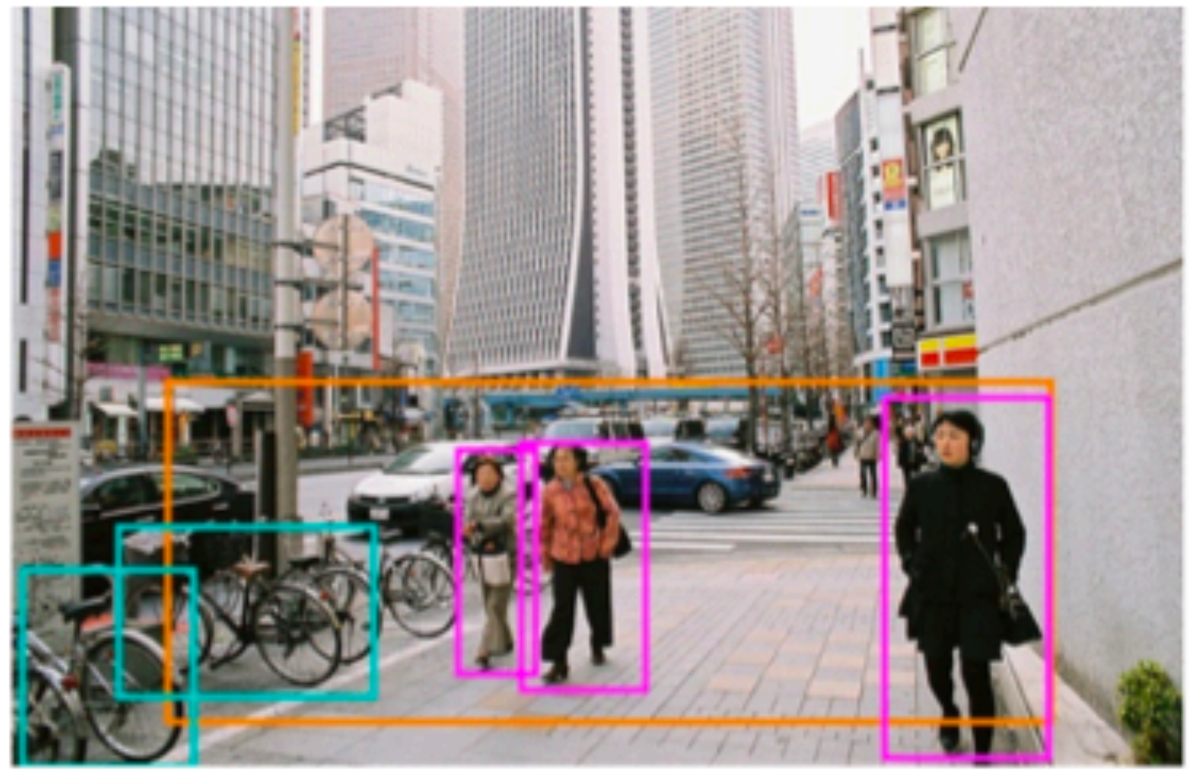
Evaluation

— Ratio of correctly grounded phrases to the total phrases

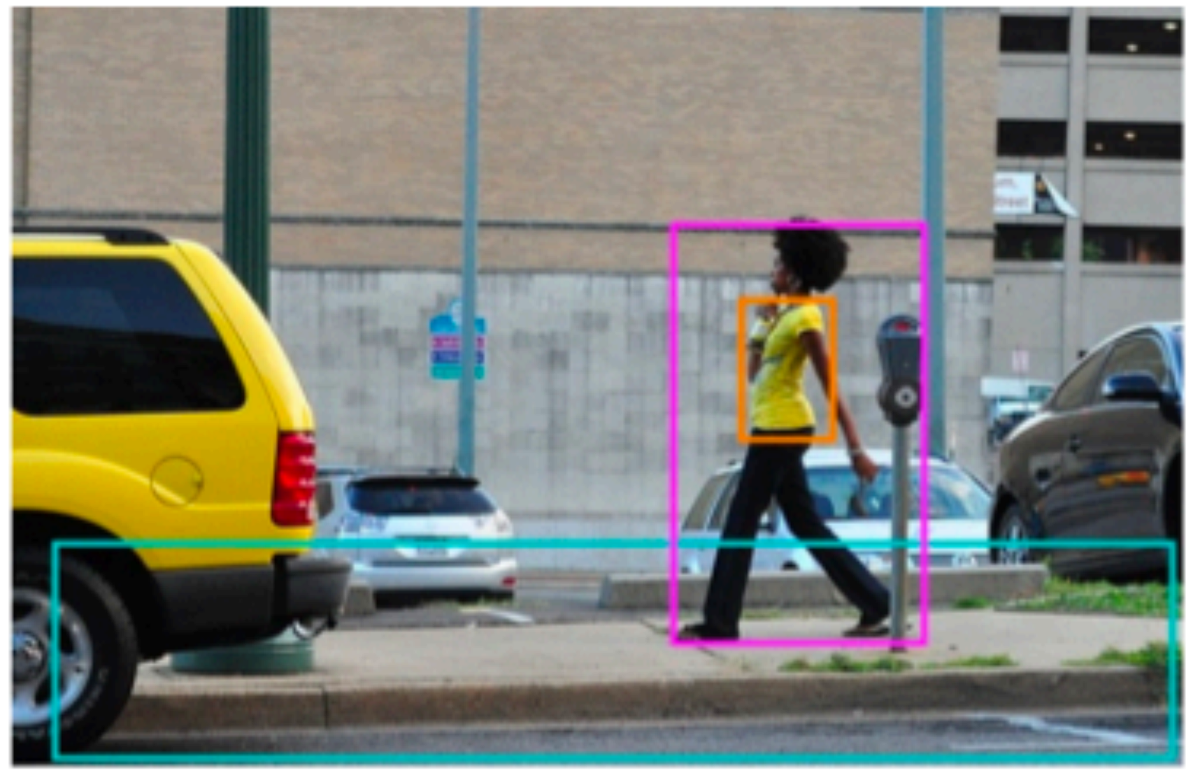
Qualitative Results: Flickr30K



(a) A man wearing a black-jacket has a smile on his face.



(b) People are walking on the street , with bikes parked up to the left of the picture.

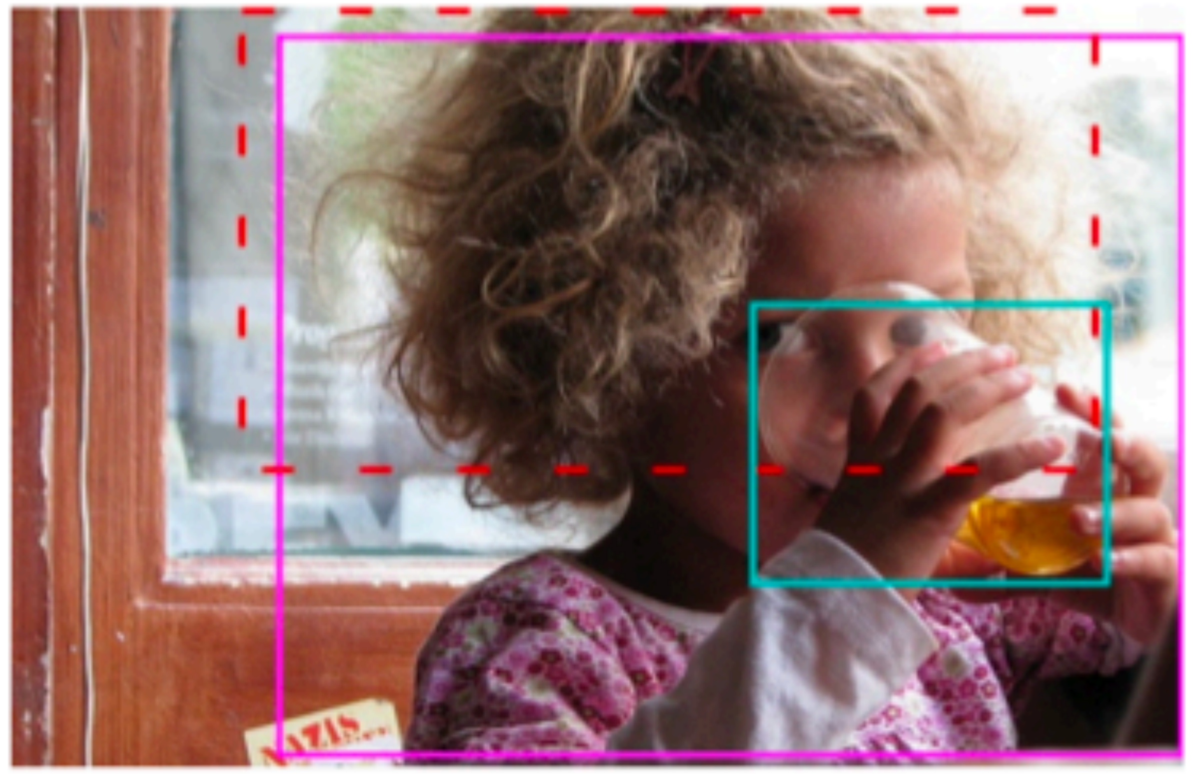


(c) A woman in a yellow shirt is walking down the sidewalk.

(d) A young boy is walking on wooden path in the middle of trees.

(e) Two women in colorful clothing are dancing inside a circle of other women.

(f) Lady wearing white shirt with blue umbrella in the rain.



(g) Young girl with curly hair is drinking out of a plastic cup.

(h) The bearded man keeps his blue Bic pen in hand while he plays the guitar.

Quantitative Results

Flickr30k Entities:

Method	Accuracy
SMPL [27]	42.08
NonlinearSP [26]	43.89
GroundeR [23]	47.81
MCB [7]	48.69
RtP [21]	50.89
Similarity Network [25]	51.05
IGOP [34]	53.97
SPC+PPC [20]	55.49
SS+QRN (VGGdet) [4]	55.99
CITE [19]	59.27
SeqGROUND	61.60
CITE [19] (finetuned)	61.89
QRC Net [4] (finetuned)	65.14
G^{3}RAPHGROUND++	**66.67**

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G^{3}RAPHGROUND++	**66.67**

ReferIt Game:

Method	Accuracy
SCRC [9]	17.93
MCB + Reg + Spatial [3]	26.54
GroundeR + Spatial [23]	26.93
Similarity Network + Spatial [25]	31.26
CGRE [17]	31.85
MNN + Reg + Spatial [3]	32.21
EB+QRN (VGGcls-SPAT) [4]	32.21
CITE [19]	34.13
IGOP [34]	34.70
QRC Net [4] (finetuned)	44.07
G^{3}RAPHGROUND++	**44.91**

Ablation

Method	Flickr30k	ReferIt
GG - VisualG - FusionG	56.32	32.89
GG - VisualG	62.23	38.82
GG - FusionG	59.13	36.54
GG - PhraseG	60.82	38.12
GGFusionBase	60.41	38.65
GG - ImageContext	62.32	40.92
GG - PhraseContext	62.73	*n.a.*
G^{3}RAPHGROUND (GG)	63.65	41.79
G^{3}RAPHGROUND++	**66.67**	**44.91**

Ablation

Method	Flickr30k	ReferIt
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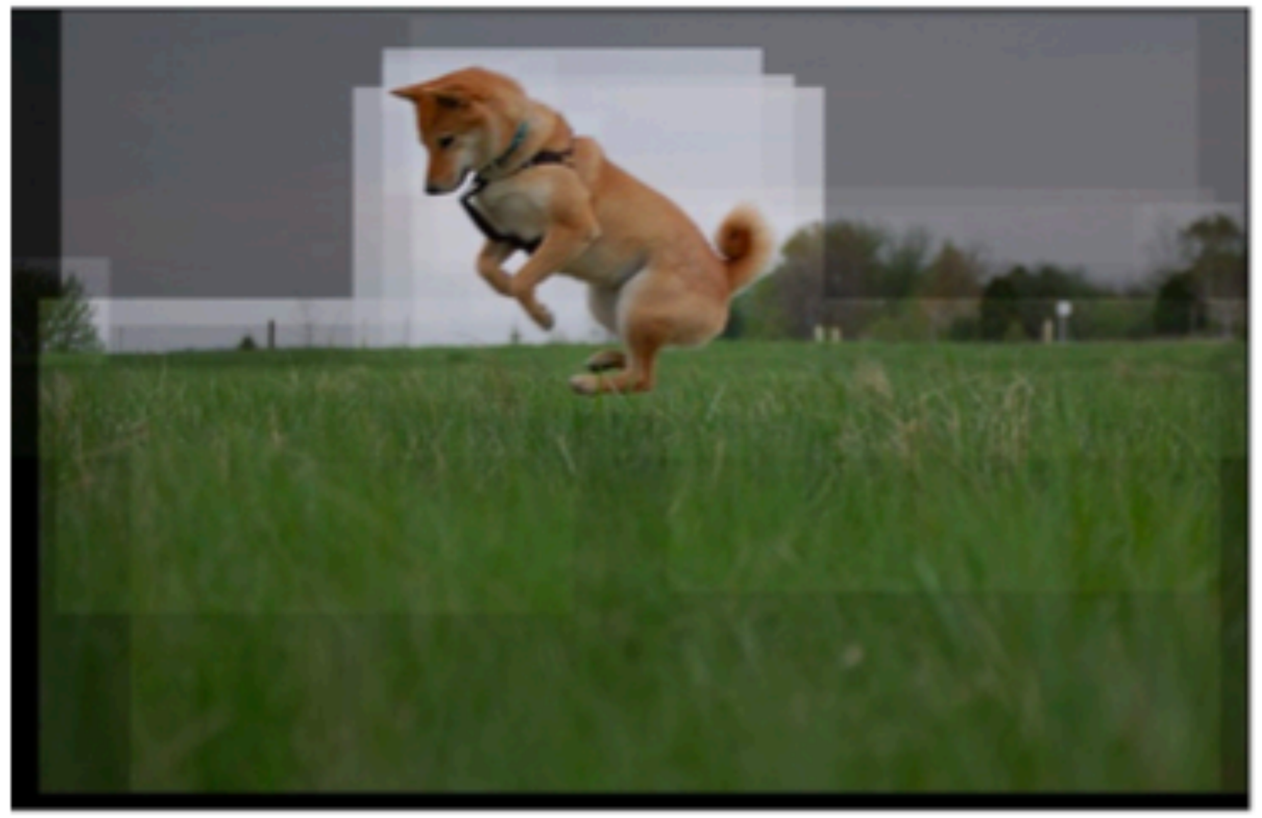
GG - PhraseContext	62.73	*n.a.*
G^{3}RAPHGROUND (GG)	63.65	41.79
G^{3}RAPHGROUND++	**66.67**	**44.91**

Visualizing Graph Attention

(a) A young boy is looking at a man painted in all gold.

(b) A man is checking his blue sneakers next to two men having a conversation.



(c) A brown dog jumps high on a field of grass.

(d) A woman stands in a field near a car and looks through binoculars.

THE UNIVERSITY OF BRITISH COLUMBIA

Energy-Based Learning for Scene Graph Generation

Mohammed Suhail

+ + +

Scene Graphs:

A **graph** based data structure for semantically representing image content

Scene Graphs

Scene Graphs

Scene Graphs

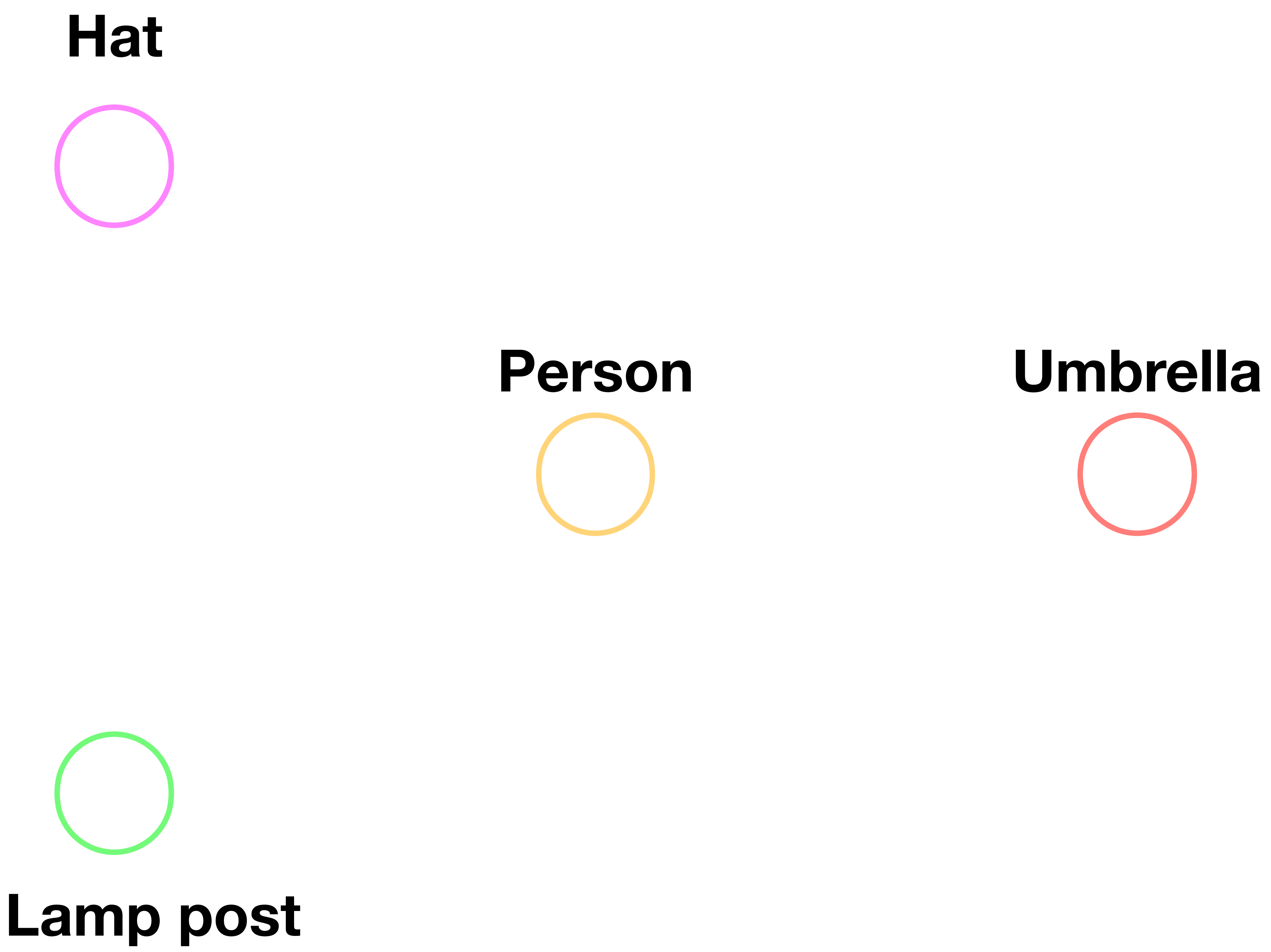
Hat

Umbrella

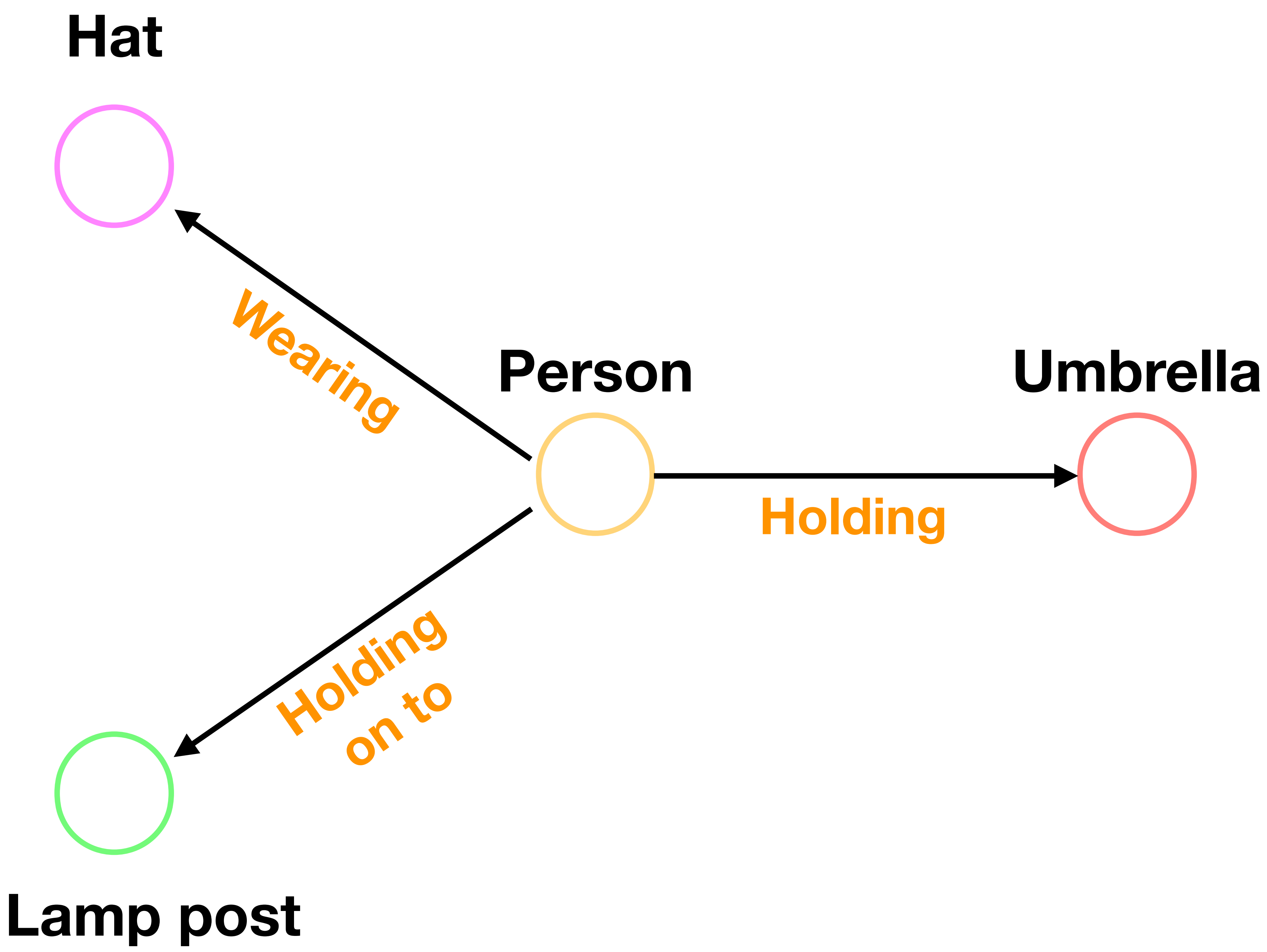
Lamp post

Person

Scene Graphs



Scene Graphs

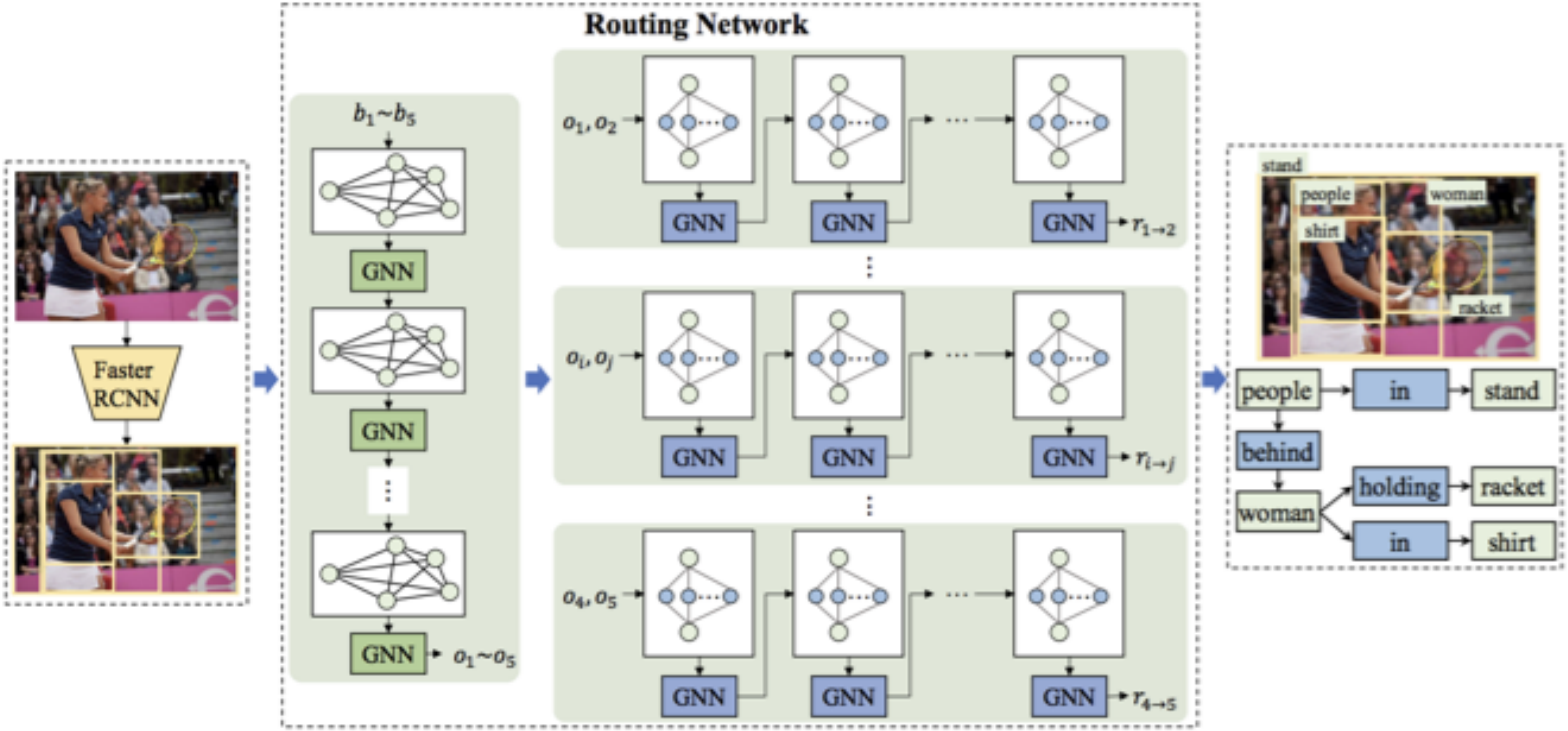


Scene Graph Generation Pipeline

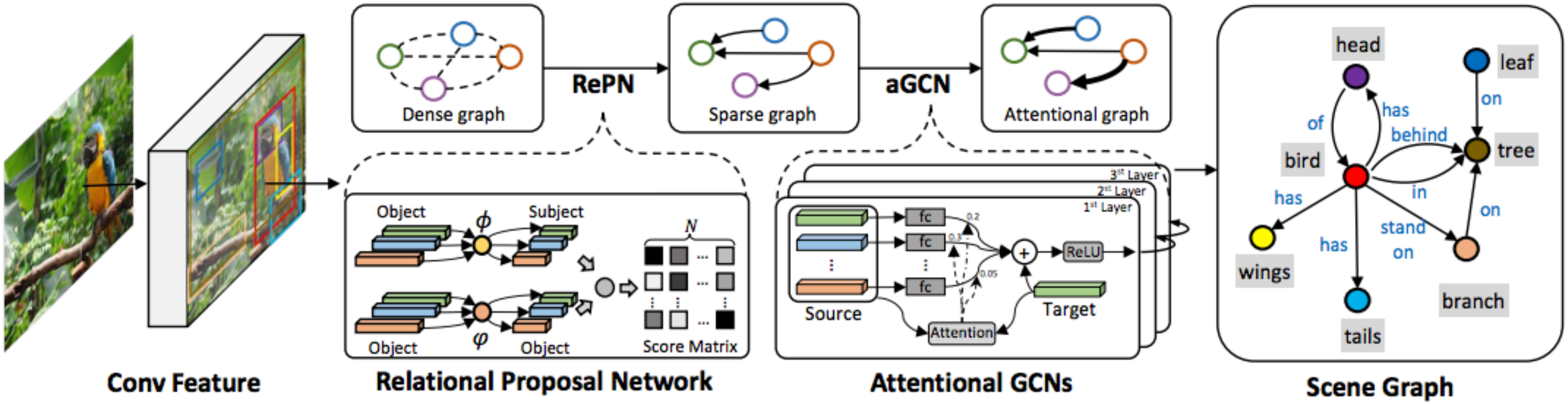
OBJECT DETECTOR
FEATURE EXTRACTION
STATE INITIALIZATION
CONTEXT
ENCODING
SCENE GRAPH
person
standing on
holding
beach
surfboard
FEATURE EMBEDDING
LABEL EMBEDDING
LABEL
PREDICTION
person
beach
surfboard
LOSS COMPUTATION
person
standing on
holding
beach
surfboard


OBJECT DETECTOR
FEATURE
EXTRACTION
STATE INITIALIZATION
CONTEXT
ENCODING
SCENE GRAPH
person
standing
on
holding
beach
surfboard
FEATURE
EMBEDDING
LABEL
EMBEDDING
LABEL
PREDICTION
person
beach
surfboard
LOSS
COMPUTATION
person
beach
surfboard
standing
on
holding
Cross
Entropy
Loss

KERN Architecture

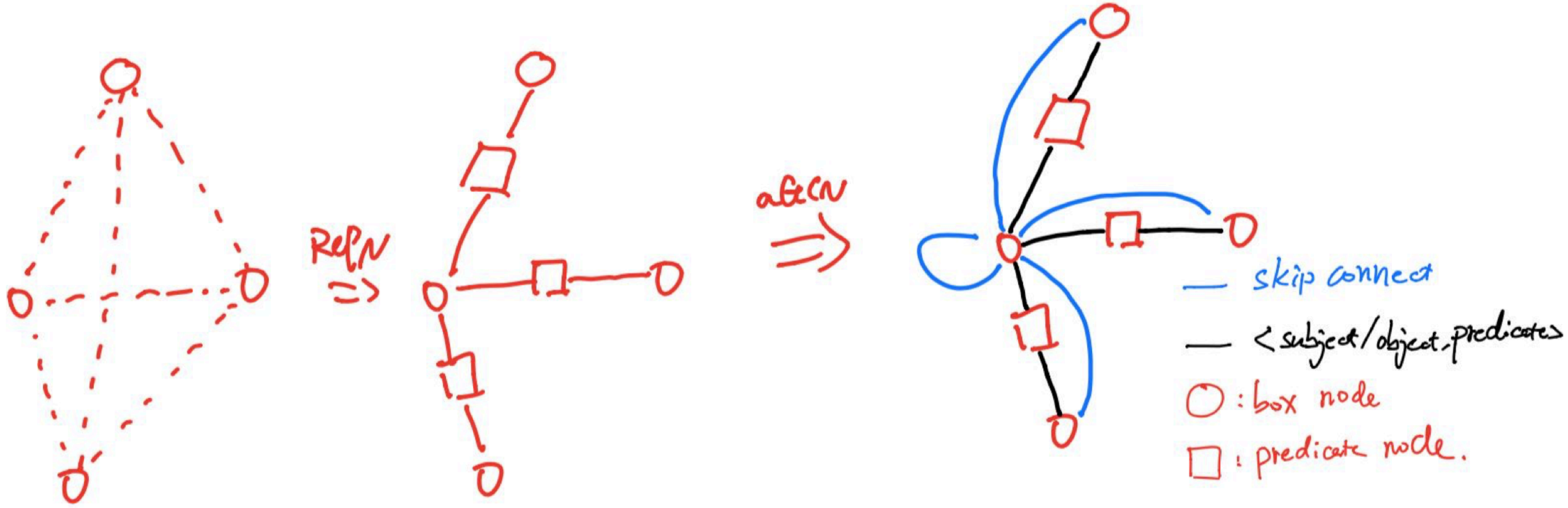


Graph RCNN



Dense graph
RePN
Sparse graph
aGCN
Attentional graph
Object
Subject
Object
Object
Score Matrix
N
Source
Target
fc
ReLU
Attention
1st Layer
2nd Layer
3rd Layer
head
leaf
of
has
behind
on
bird
tree
has
in
on
stand
on
has
wings
branch
tails
Conv Feature
Relational Proposal Network
Attentional GCNs
Scene Graph

Graph RCNN



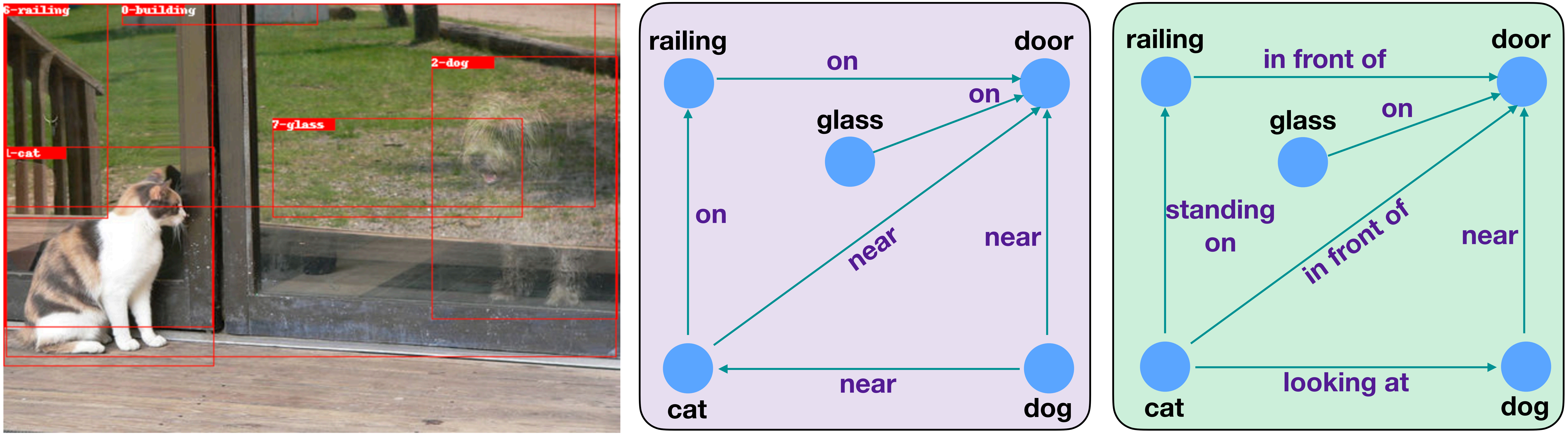
$$z_i^o = \sigma\Big(\overbrace{W^{\texttt{skip}} Z^o \boldsymbol{\alpha}^{\texttt{skip}}}^{\text{Message from Other Objects}} + \overbrace{W^{sr} Z^r \boldsymbol{\alpha}^{sr} + W^{or} Z^r \boldsymbol{\alpha}^{or}}^{\text{Messages from Neighboring Relationships}}\Big)$$

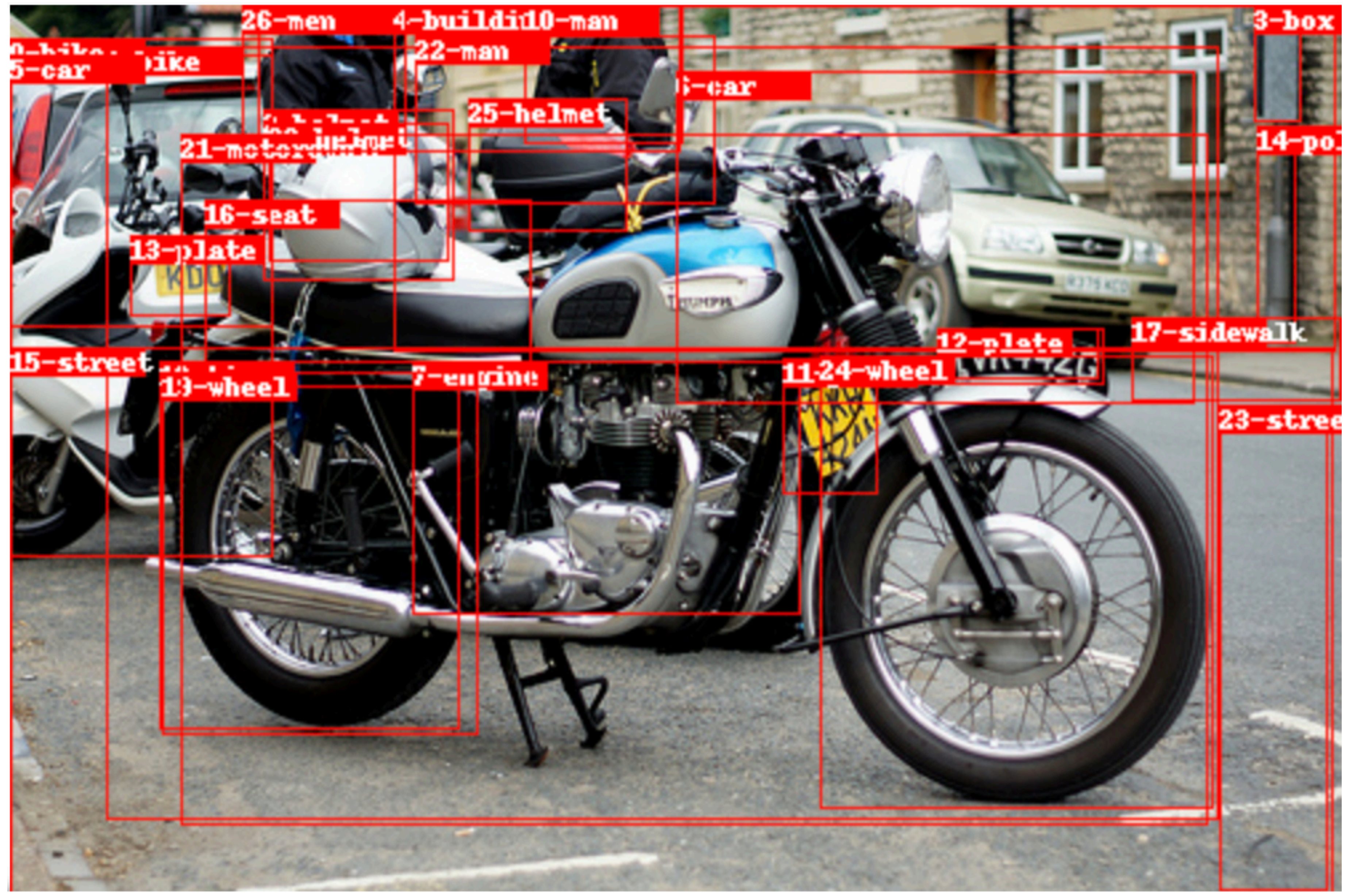
$$z_i^r = \sigma\Big(z_i^r + \underbrace{W^{rs} Z^o \boldsymbol{\alpha}^{rs} + W^{ro} Z^o \boldsymbol{\alpha}^{ro}}_{\text{Messages from Neighboring Objects}}\Big).$$

Structure information
is lost

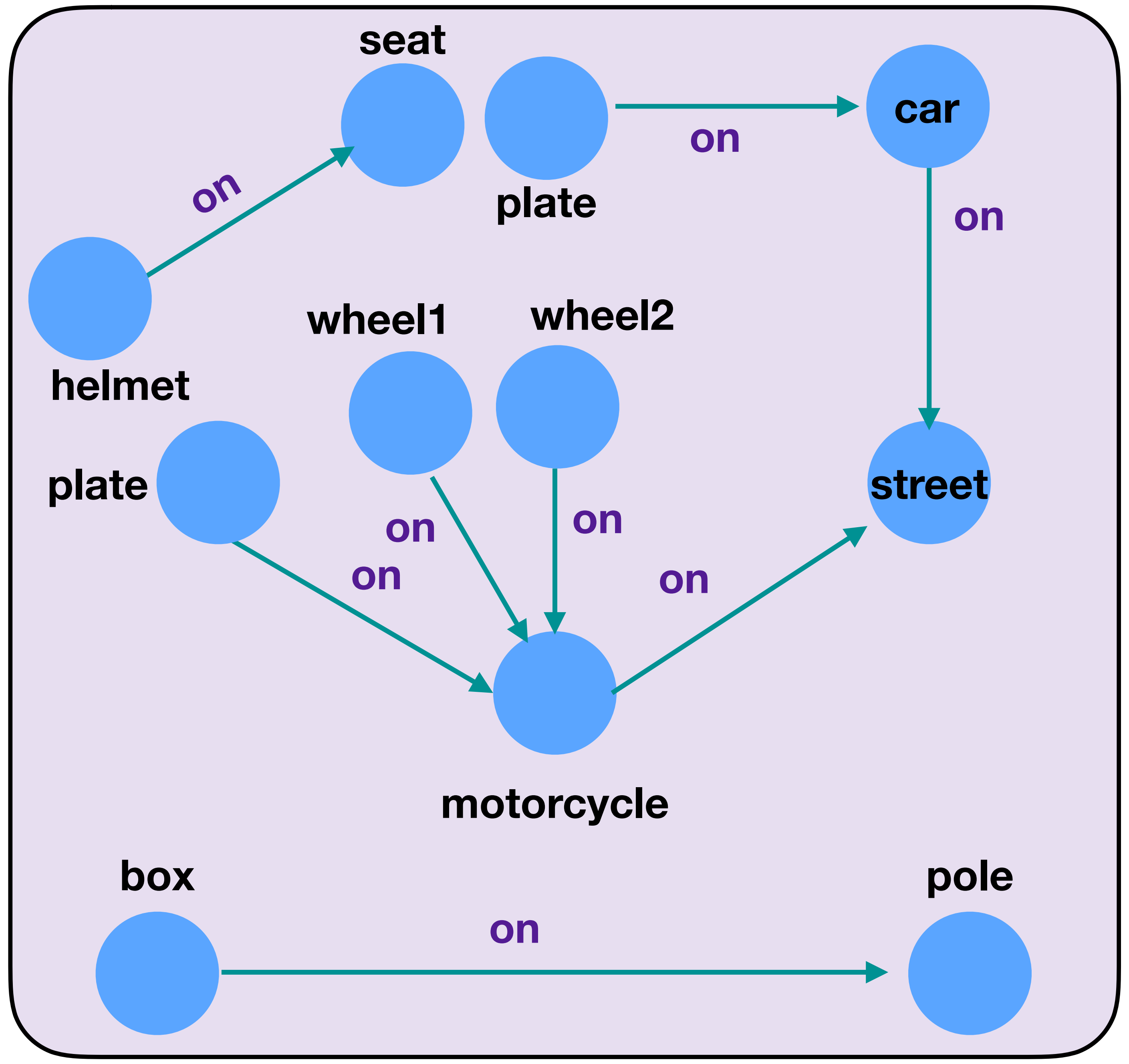

OBJECT DETECTOR
FEATURE
EXTRACTION
STATE INITIALIZATION
SCENE GRAPH
CONTEXT
ENCODING
person
standing
on
holding
beach
surfboard
FEATURE
EMBEDDING
LABEL
EMBEDDING
LABEL
PREDICTION
person
beach
surfboard
FEATURE
EMBEDDING
IMAGE GRAPH
person
standing
on
holding
beach
surfboard
EGNN
GNN
EDGED GATED
POOLING
GATED POOLING
MLP
ENERGY VALUE

Visualizations

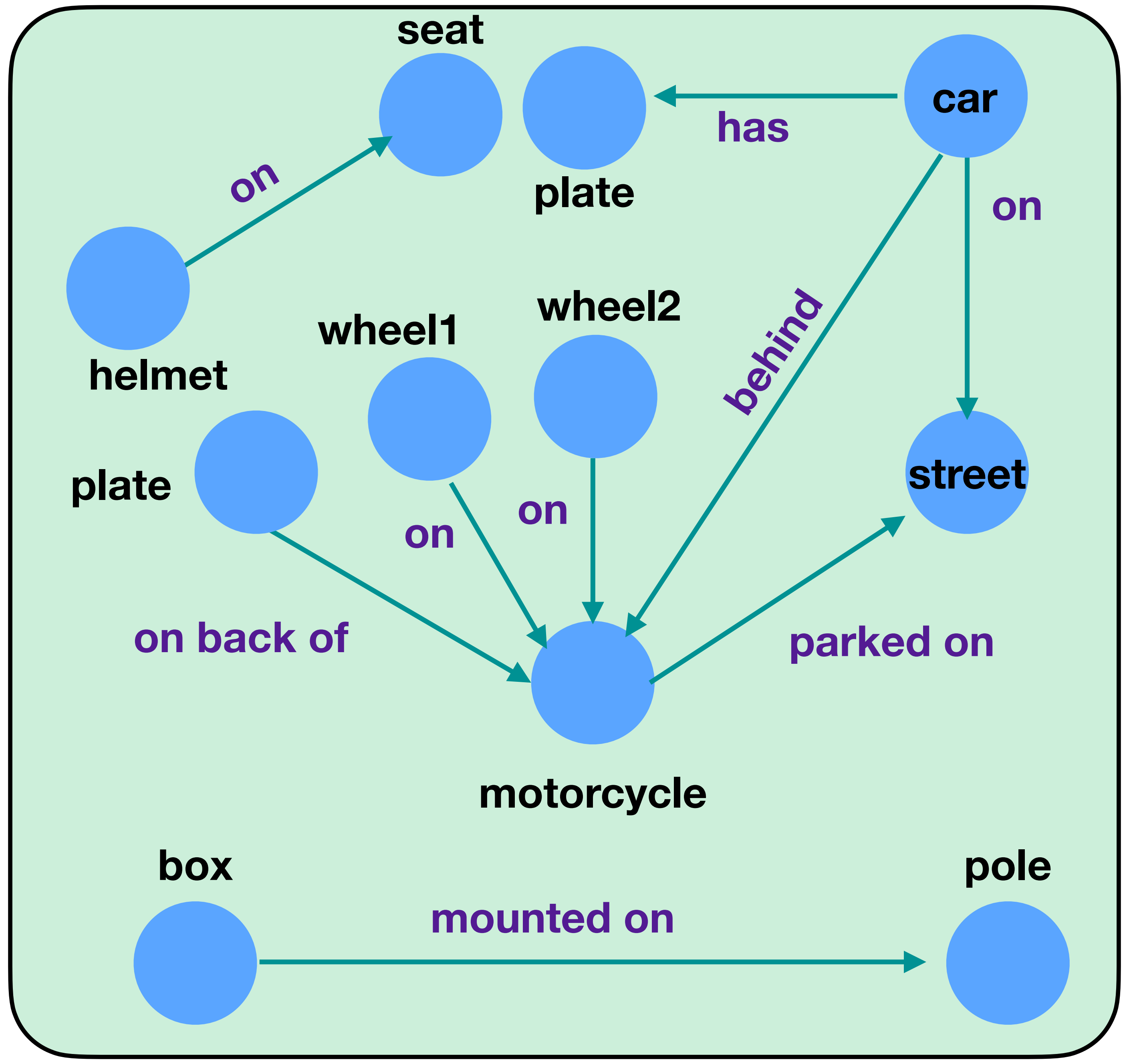

6-railing
0-building
2-dog
7-glass
1-cat
railing
door
on
glass
on
on
near
near
cat
near
dog
railing
in front of
door
glass
on
standing
on
in front of
near
cat
looking at
dog



26-men
22-man
25-helmet
16-seat
13-plate
5-car
7-engine
12-plate
17-sidewalk
3-box



seat
plate
car
helmet
wheel1
wheel2
plate
street
motorcycle
box
pole
on
on
on
on
on
on
on
on



seat
plate
car
has
on
on
helmet
wheel1
wheel2
behind
plate
street
on
on
on back of
parked on
motorcycle
box
pole
mounted on


railing
on
door
on
glass
on
near
near
cat
near
dog
railing
in front of
door
glass
on
standing on
in front of
near
cat
looking at
dog
seat
plate
on
car
on
helmet
wheel1 wheel2
plate
street
on
on
on
on
motorcycle
box
on
pole
seat
plate
has
car
on
on
helmet
wheel1
wheel2
behind
plate
street
on
on
on back of
parked on
motorcycle
box
mounted on
pole
person1
behind
person4
on
near
on
person0
on
street
person1
behind
person4
walking on
walking on
with
person0
walking on
street
girl
wearing
shirt
on
person1
street
on
wheel
behind
has
person2
on
horse
girl
wearing
shirt
standing on
person1
street
on
wheel
behind
has
person2
riding
horse
elephant
has
trunk
glasses
on
wearing
wearing
pant
woman
wearing
shirt
elephant
has
trunk
has
glasses
behind
pant
wearing
woman
wearing
shirt
Zero Shot
elephant
has
glasses
stand
near
door
coat
above
near
on
cabinet
near
table
stand
near
door
coat
on
near
over
over
on
cabinet
near
table
Zero Shot
coat
on
door

Conclusions

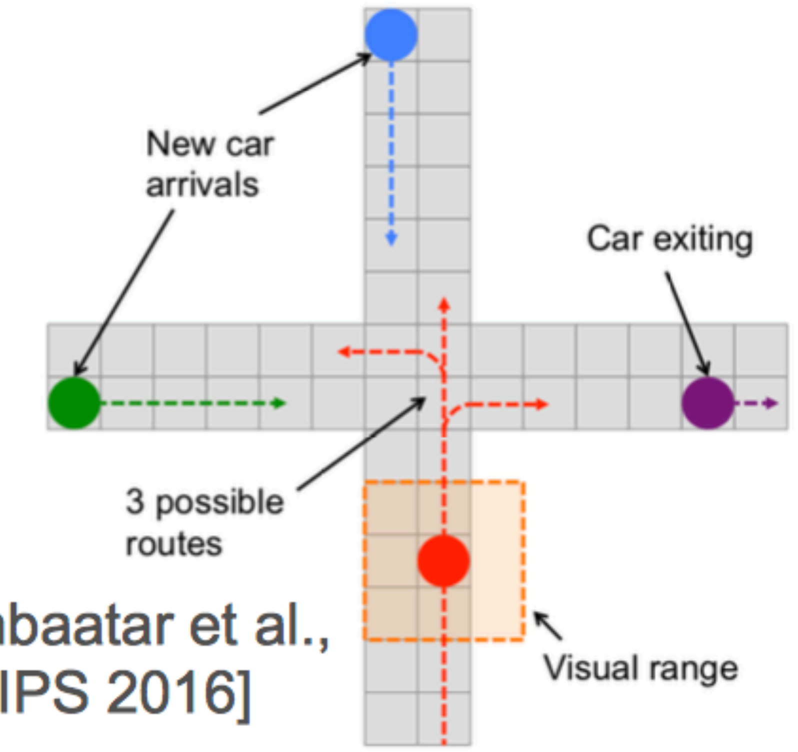
— **Deep learning on graphs works and is very effective!**

— Exciting area: lots of new applications and extensions (hard to keep up)

Relational reasoning

[Santoro et al., NIPS 2017]

Multi-Agent RL



[Sukhbaatar et al., NIPS 2016]

GCN for recommendation on 16 billion edge graph!

[Leskovec lab, Stanford]

Open problems:

— Theory

— Scalable, stable generative models

— Learning on large, evolving data

— Multi-modal and cross-model learning (e.g., sequence2graph)

* slide from Thomas Kipf, **University of Amsterdam**

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