THE UNIVERSITY OF BRITISH COLUMBIA

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

Lecture 18: Graph Neural Networks

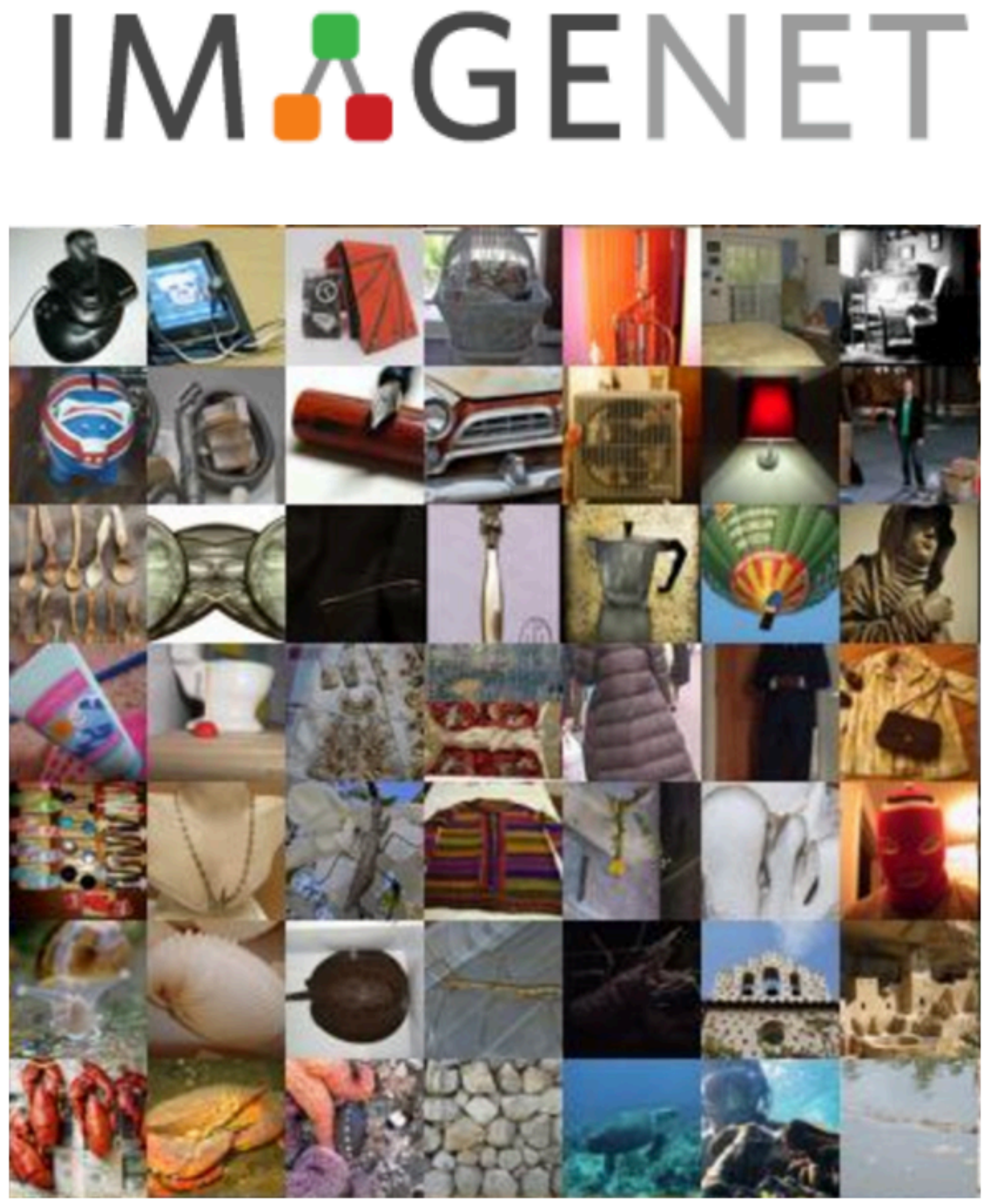
Logistics

— All **slides** will be up **today**!

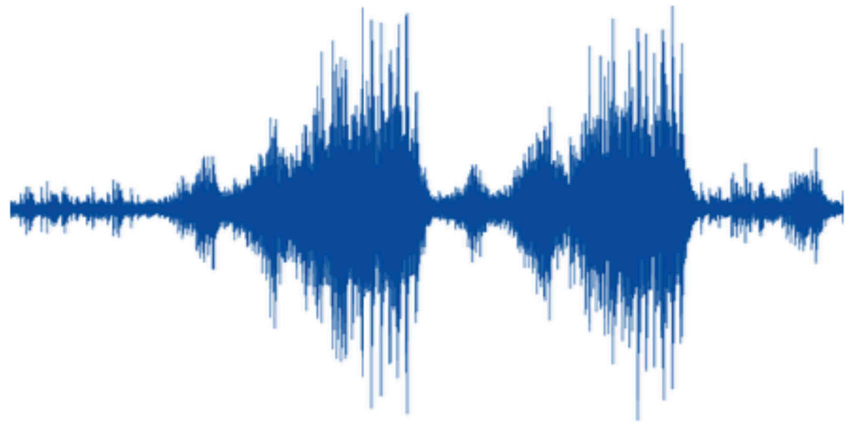
— Last **lecture** by me

— **Paper list** is up (volunteers)?

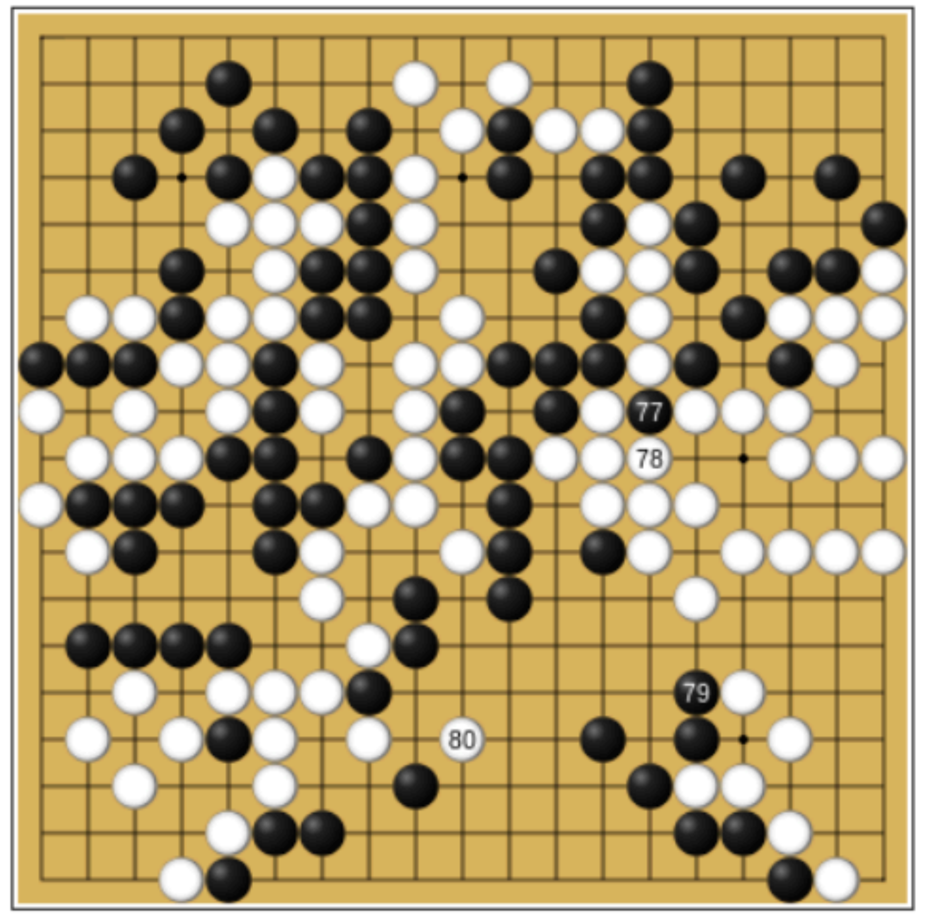
Traditional **Neural Networks**



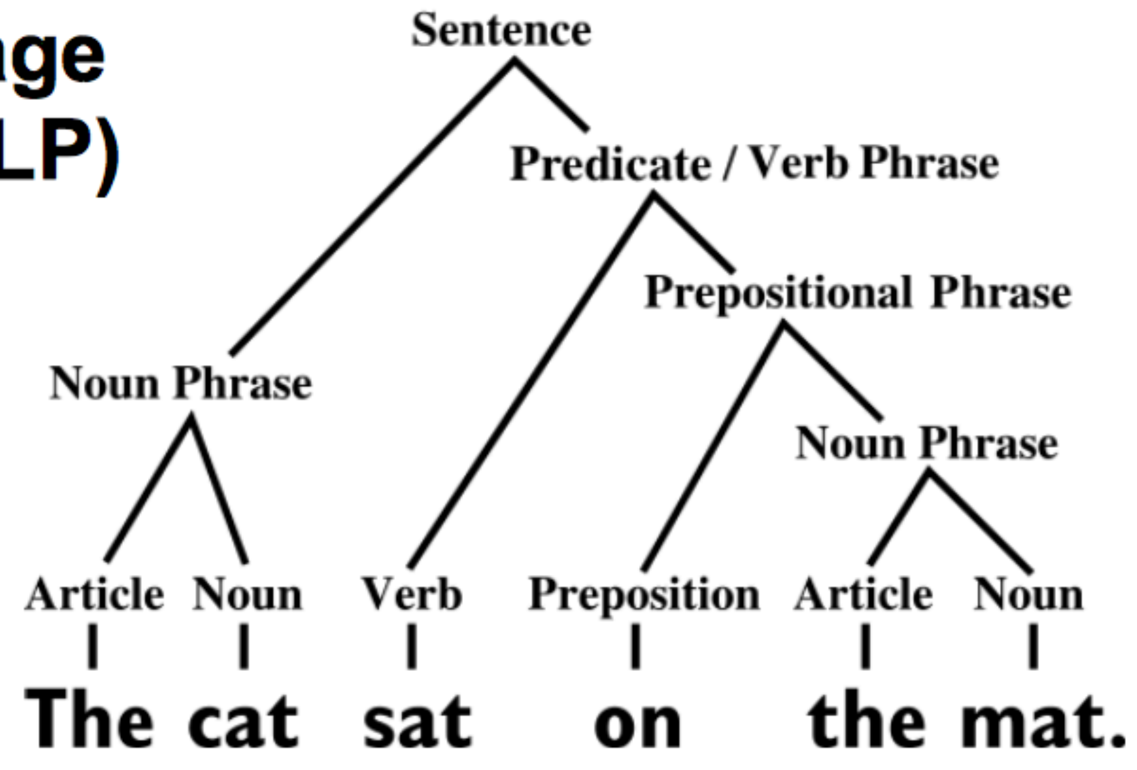
Speech data



Grid games



Natural language processing (NLP)



...

Deep neural nets that exploit:

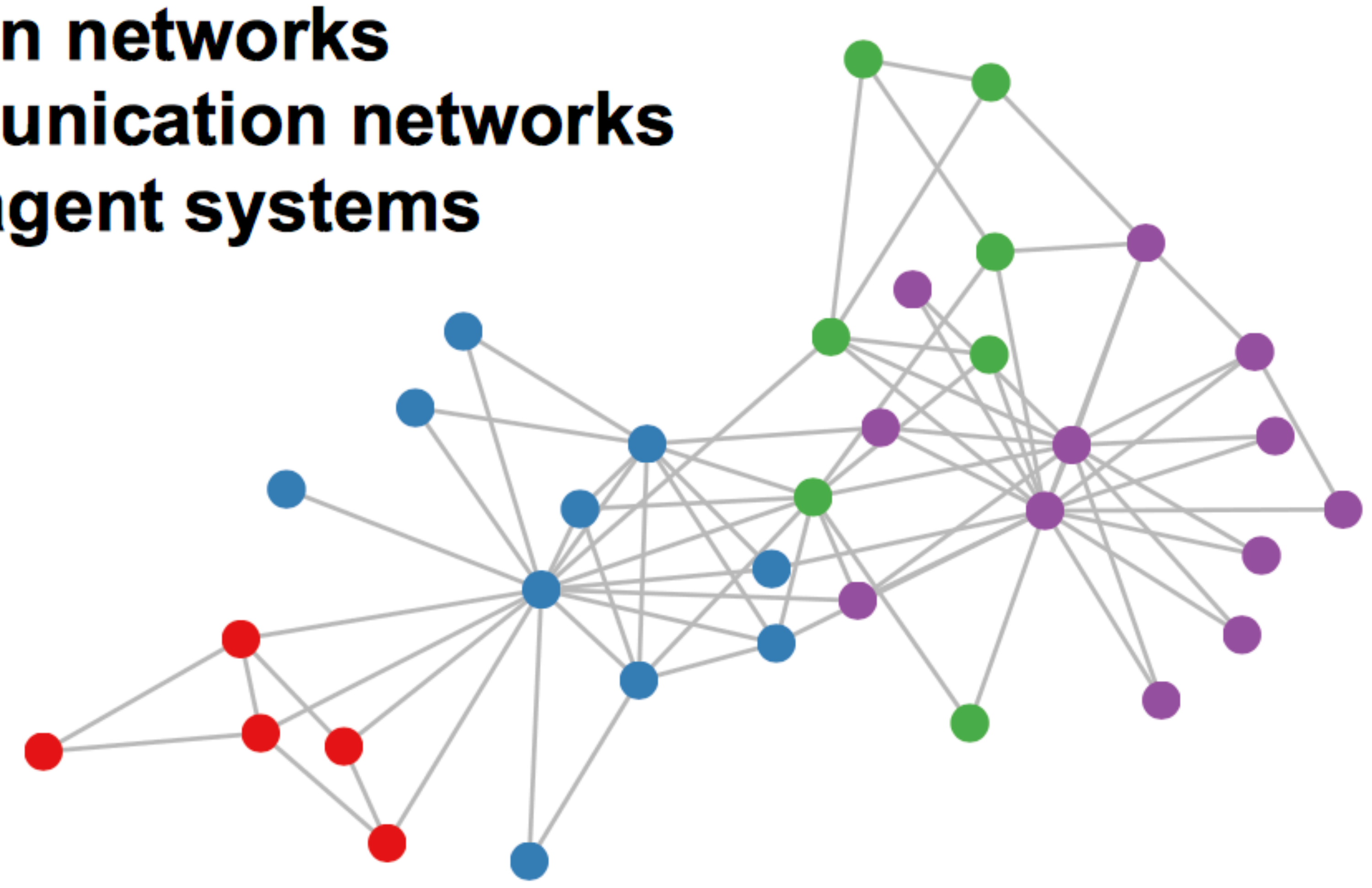
- translation equivariance (weight sharing)
- hierarchical compositionality

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

Graph-structured Data

A lot of real-world data does not “live” on grids

Social networks
Citation networks
Communication networks
Multi-agent systems



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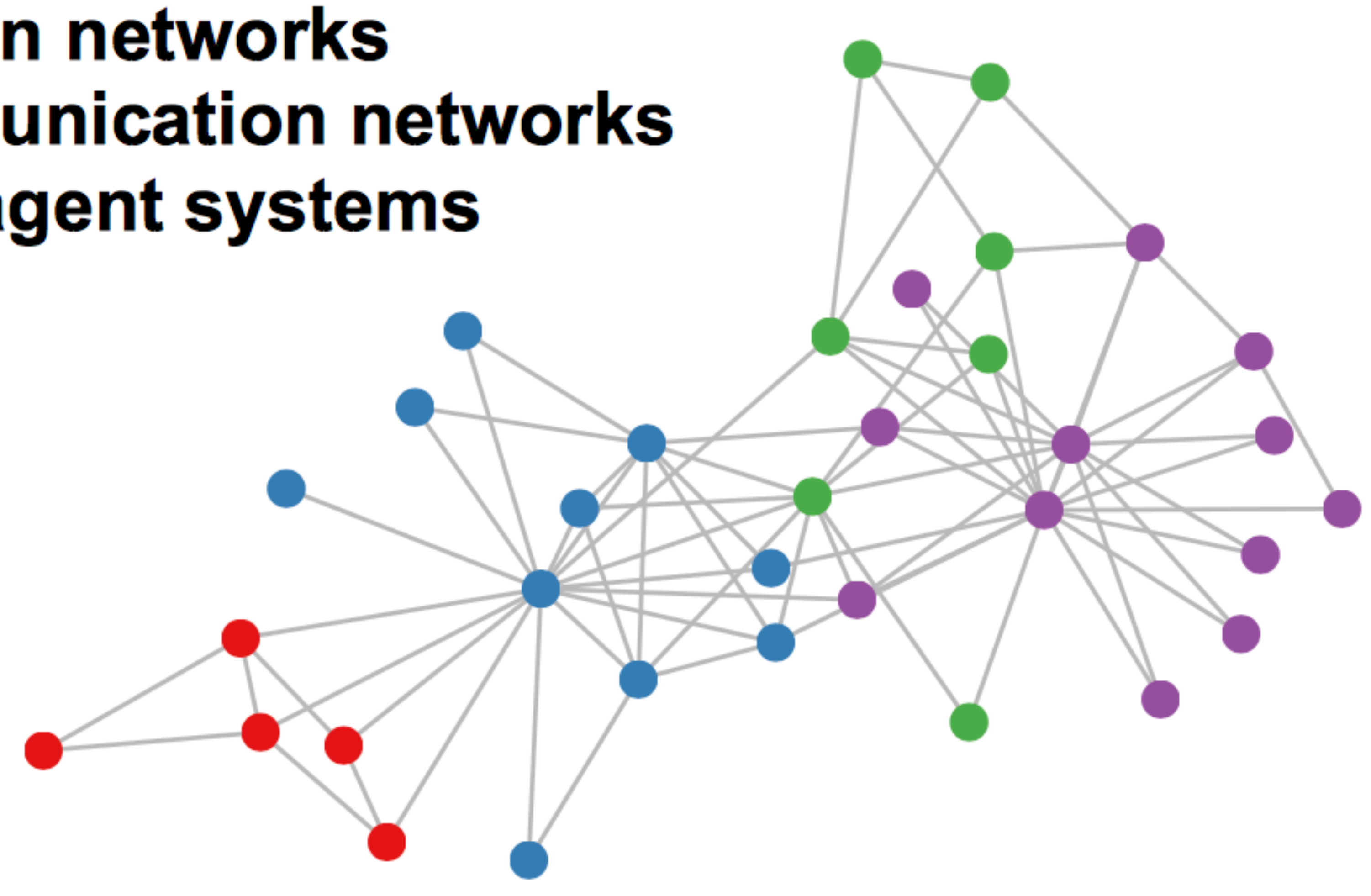

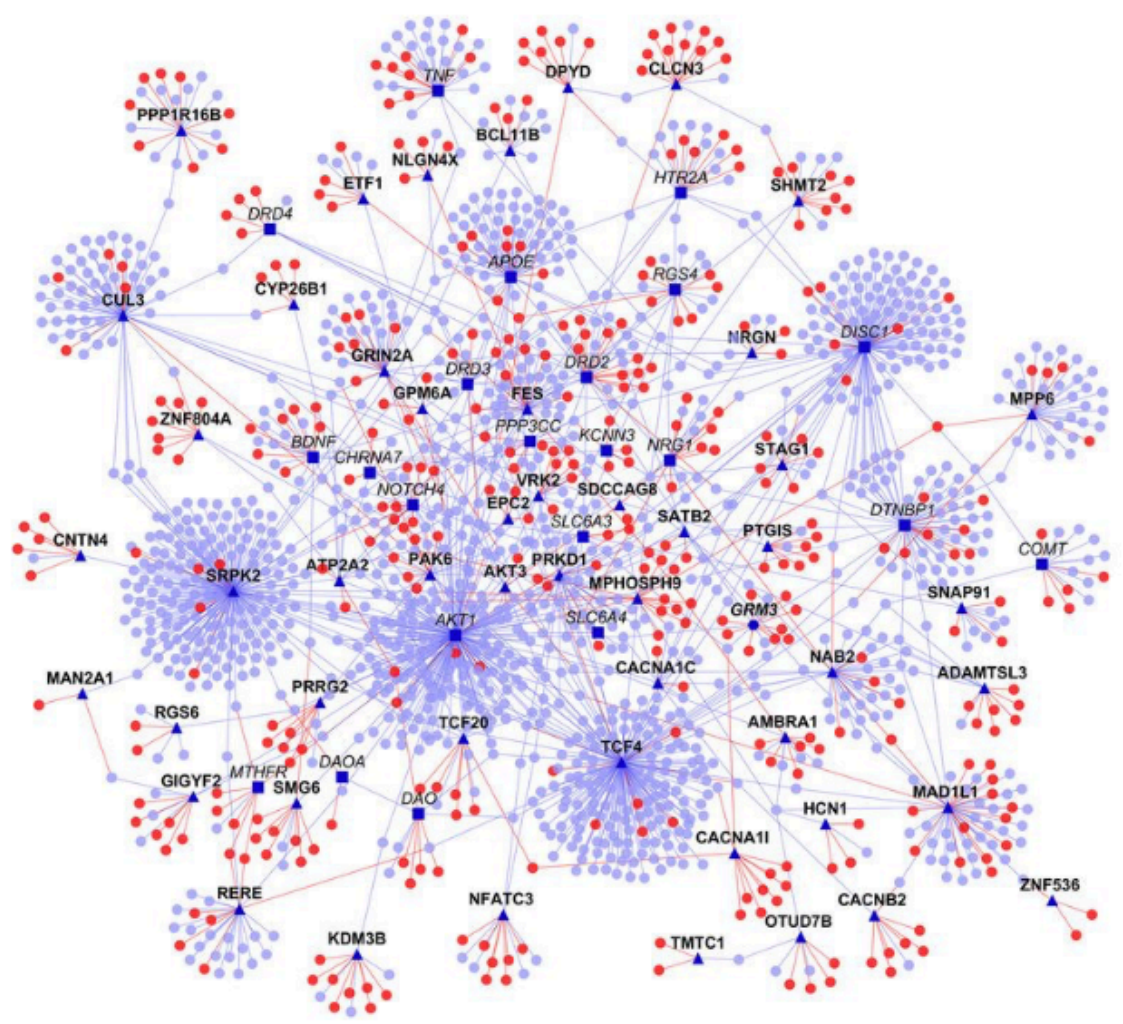

Protein interaction networks

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

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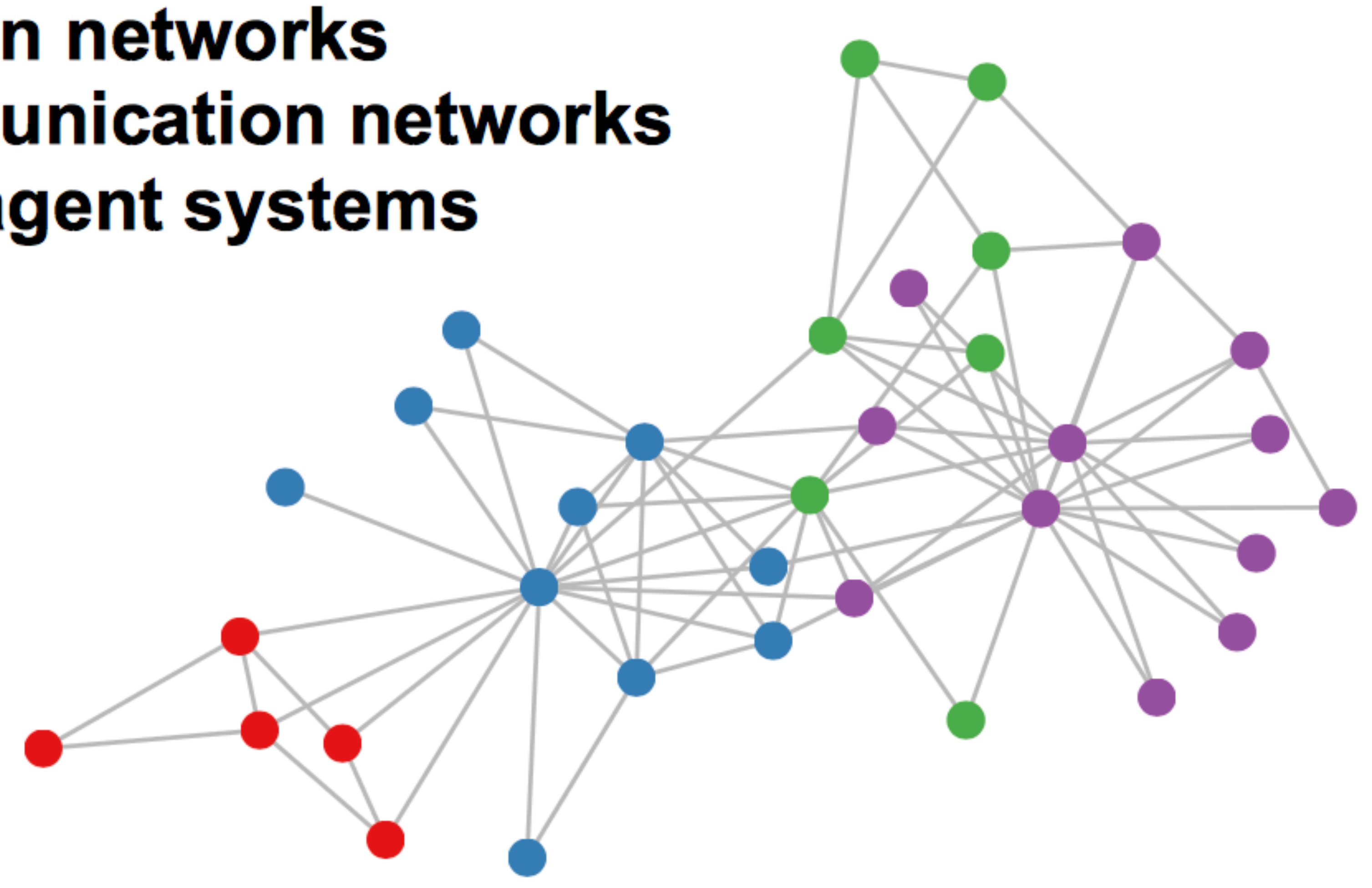
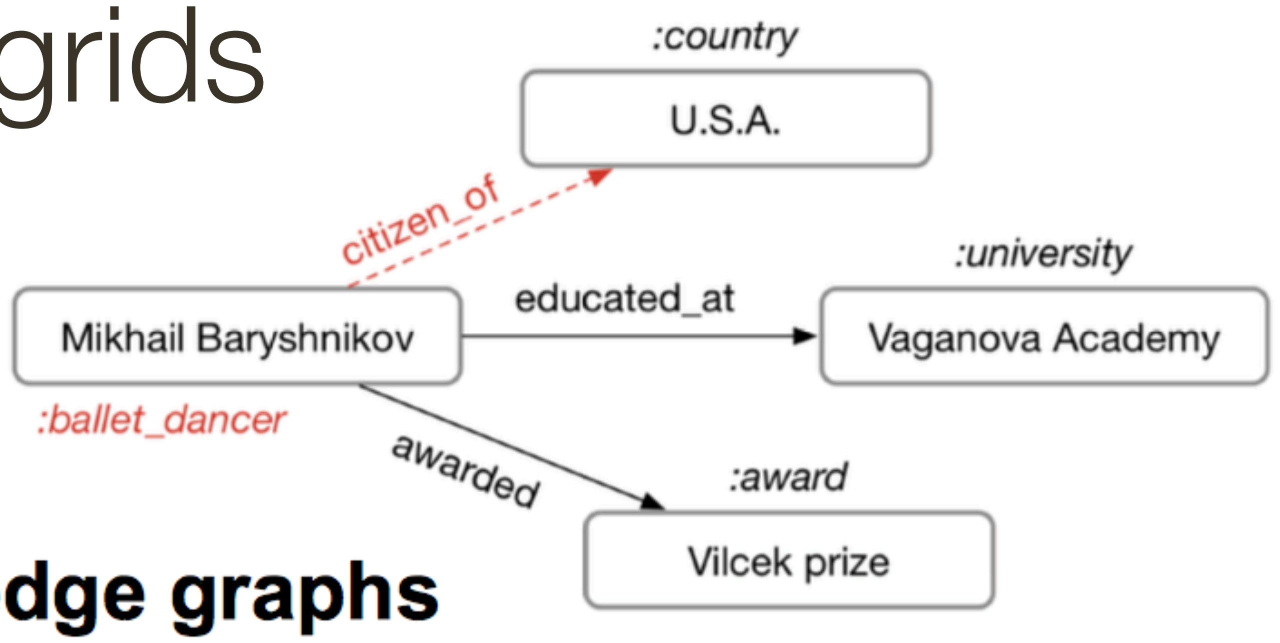


Knowledge graphs



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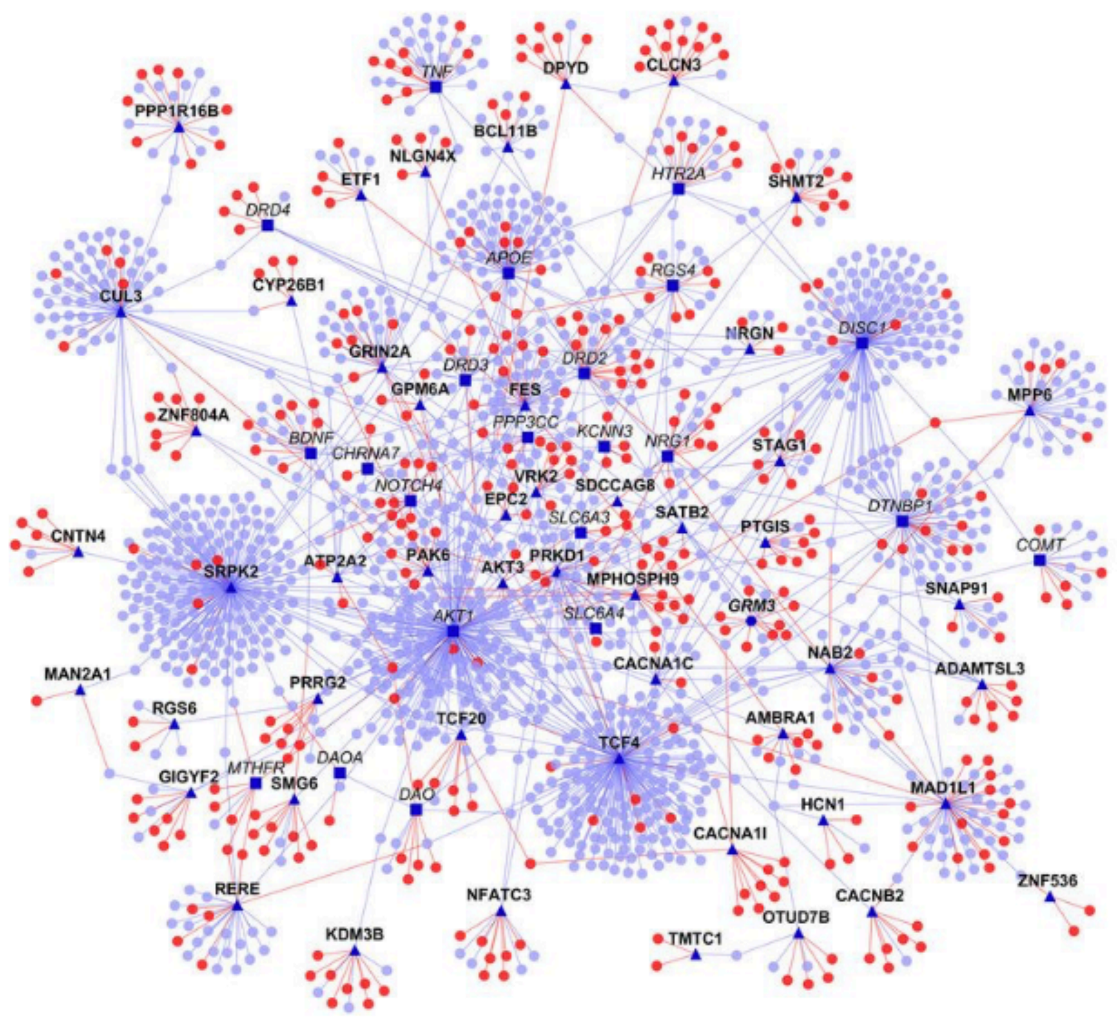

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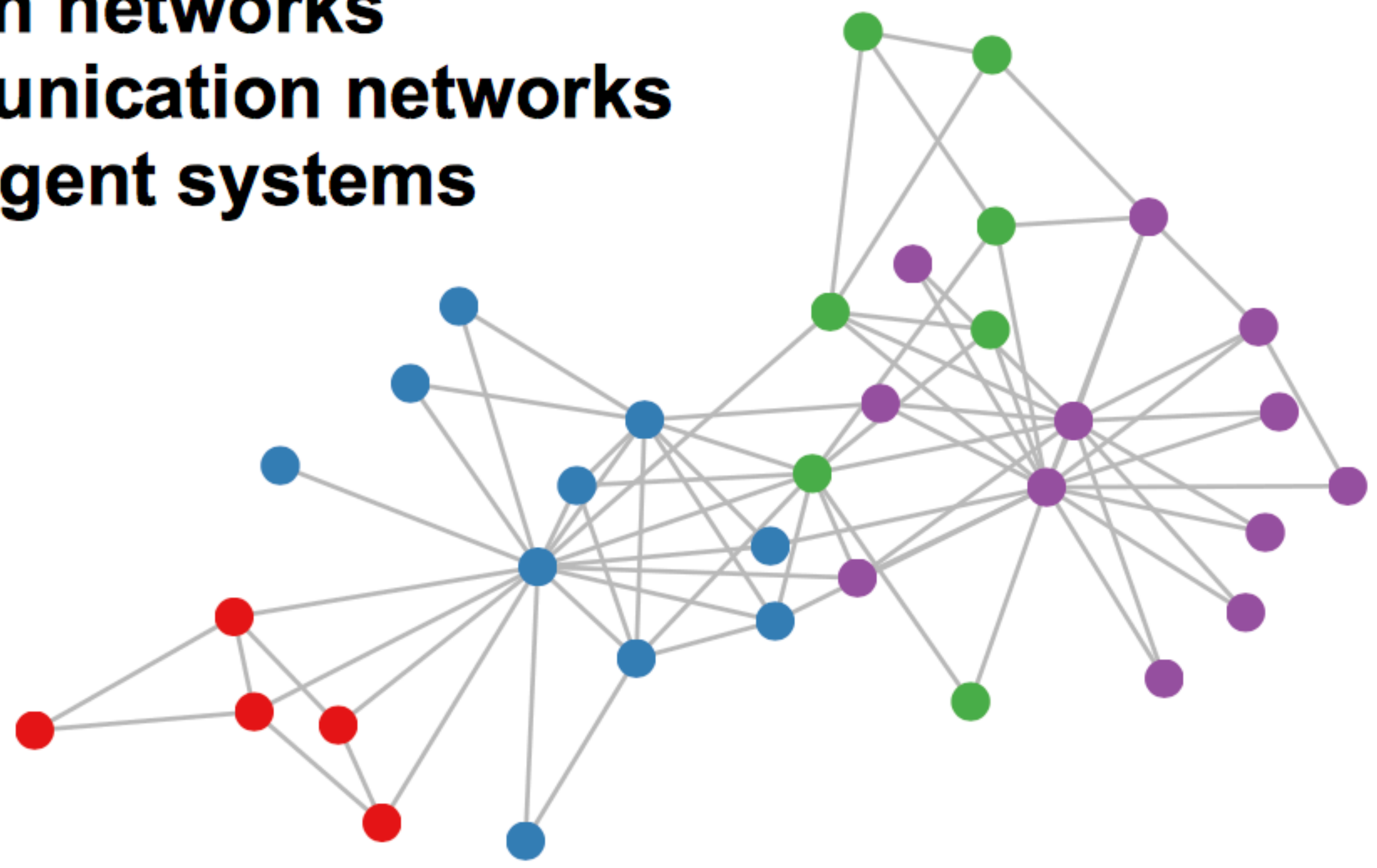

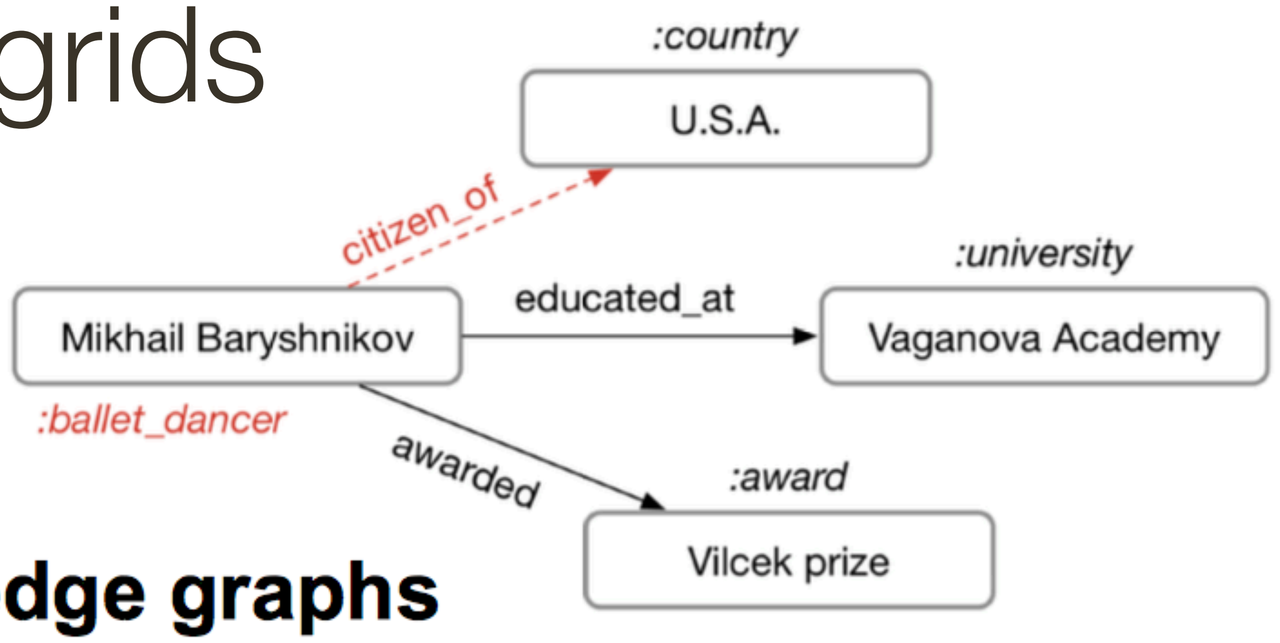

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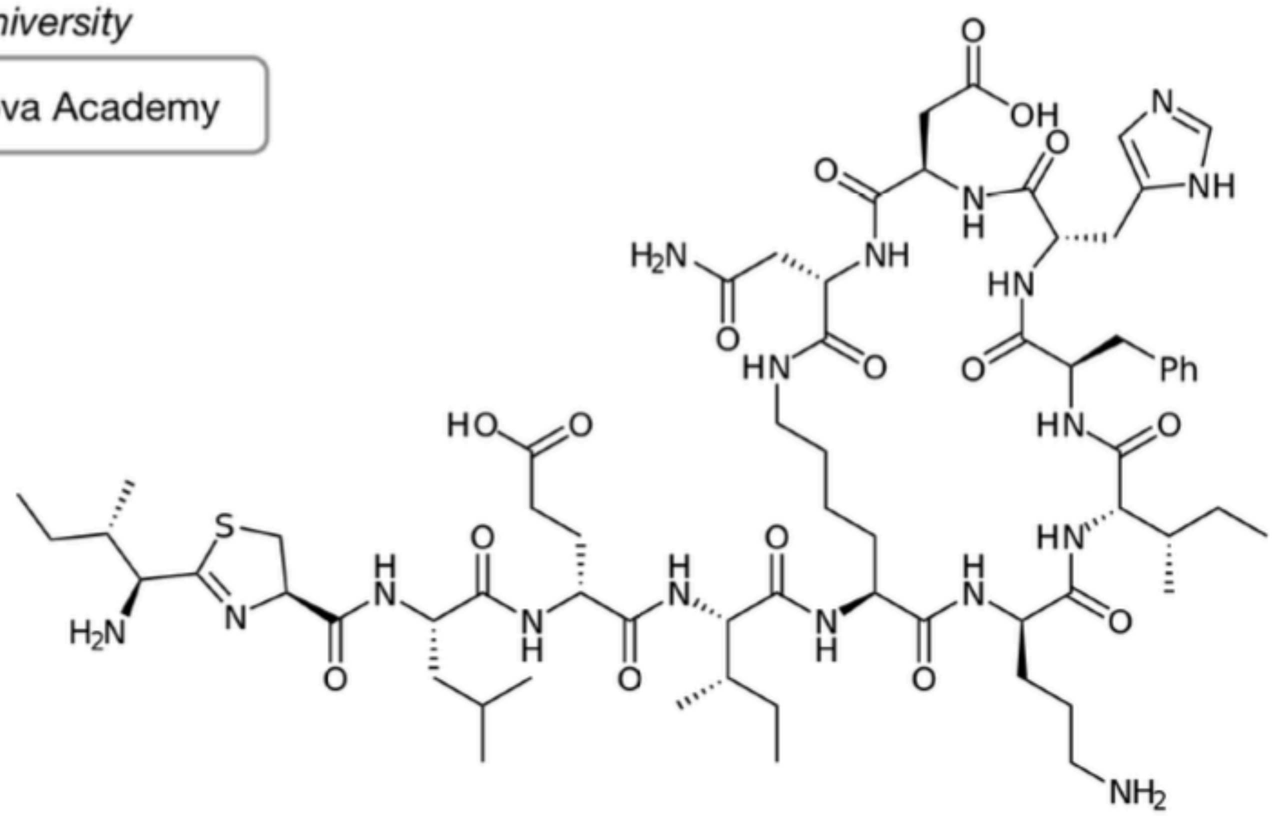
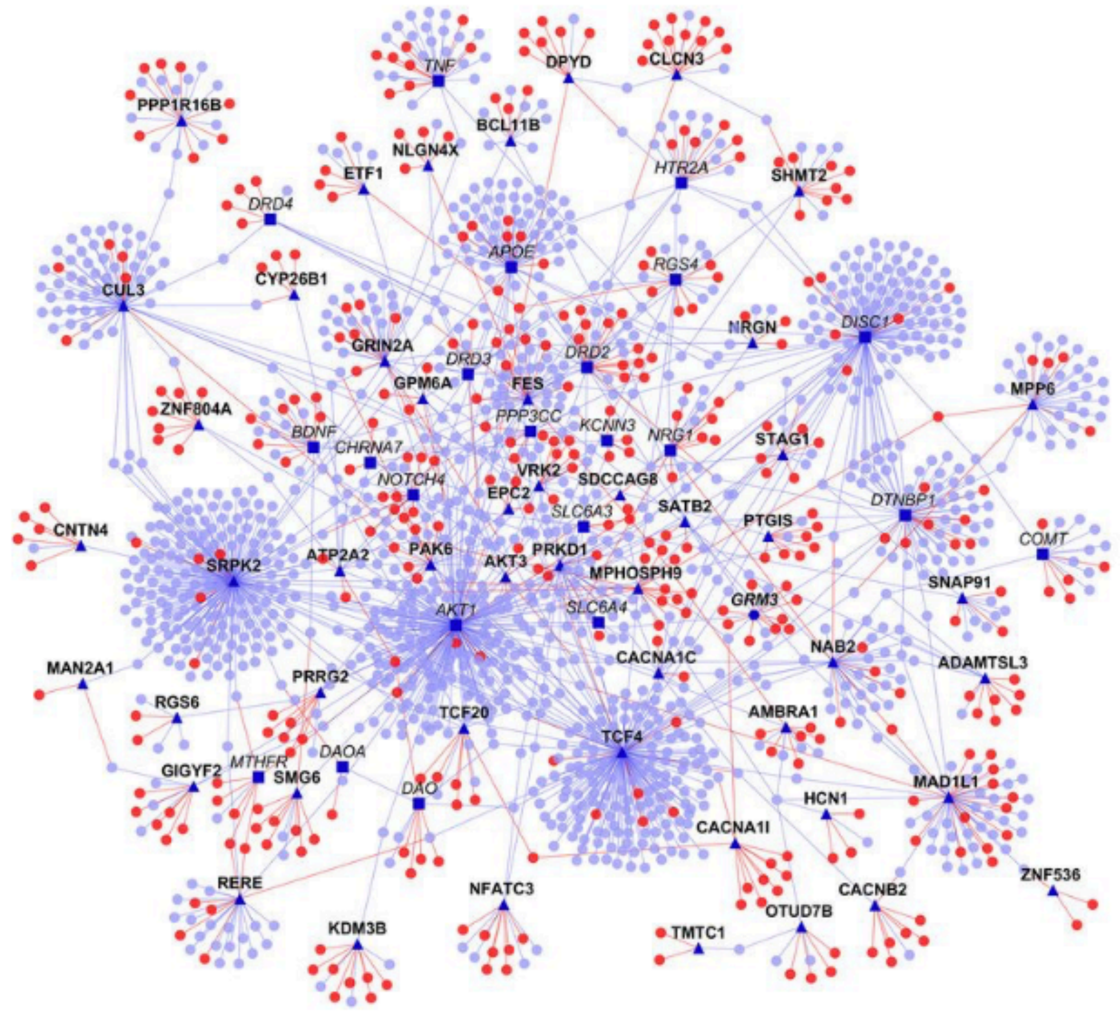
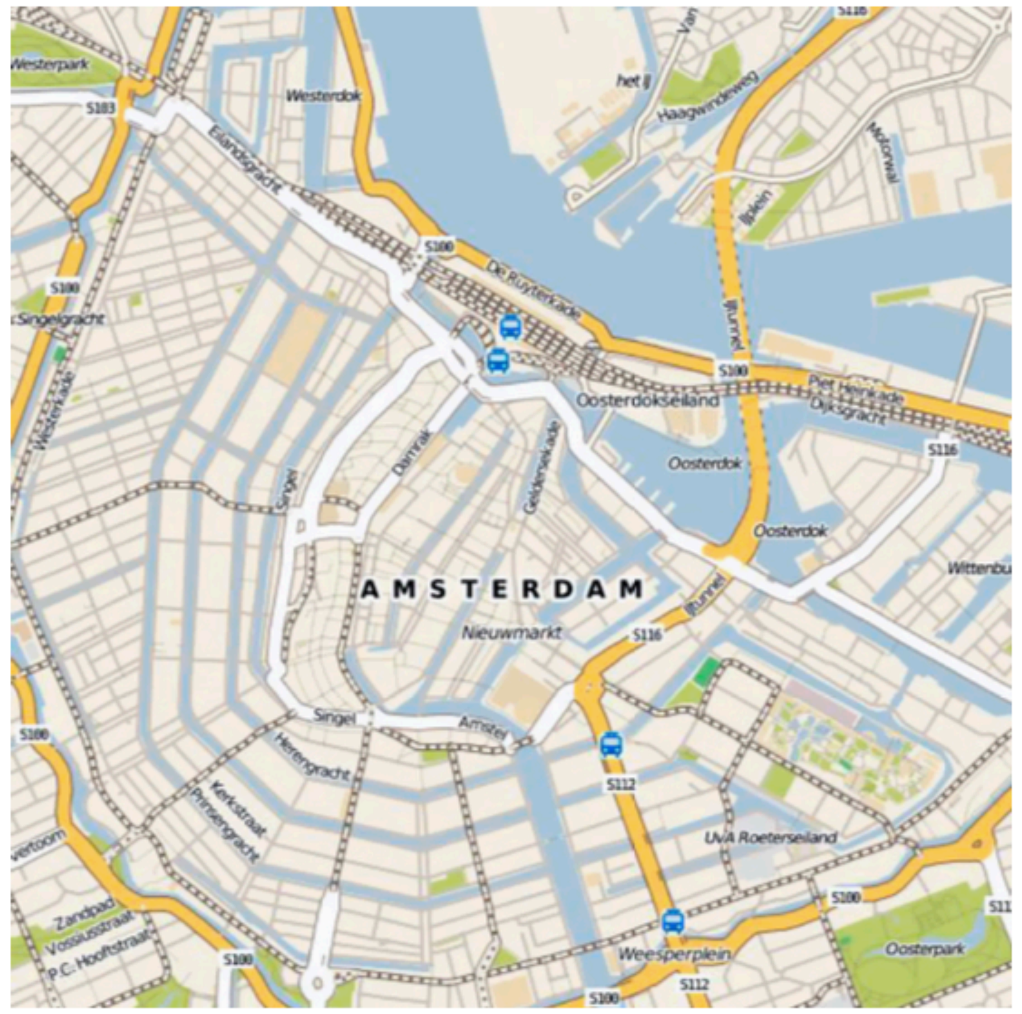


Molecules

Protein interaction networks



Road maps



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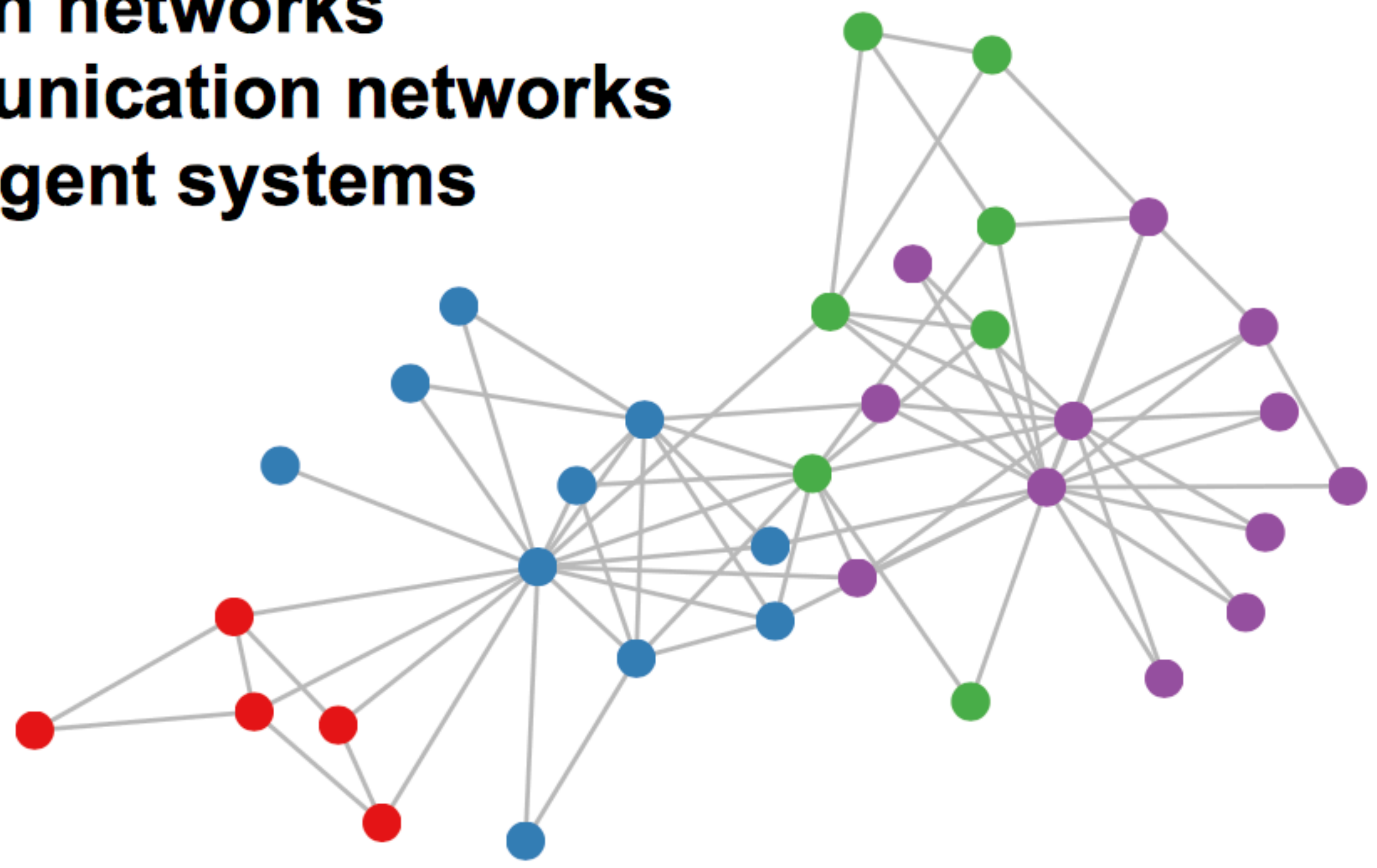

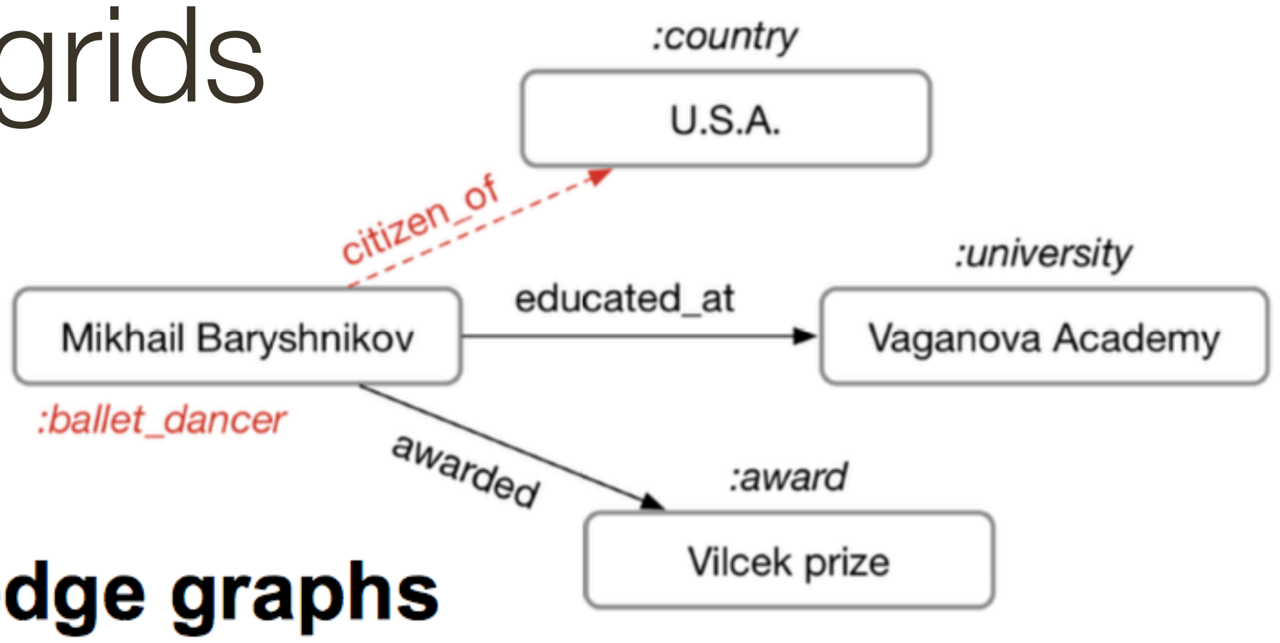

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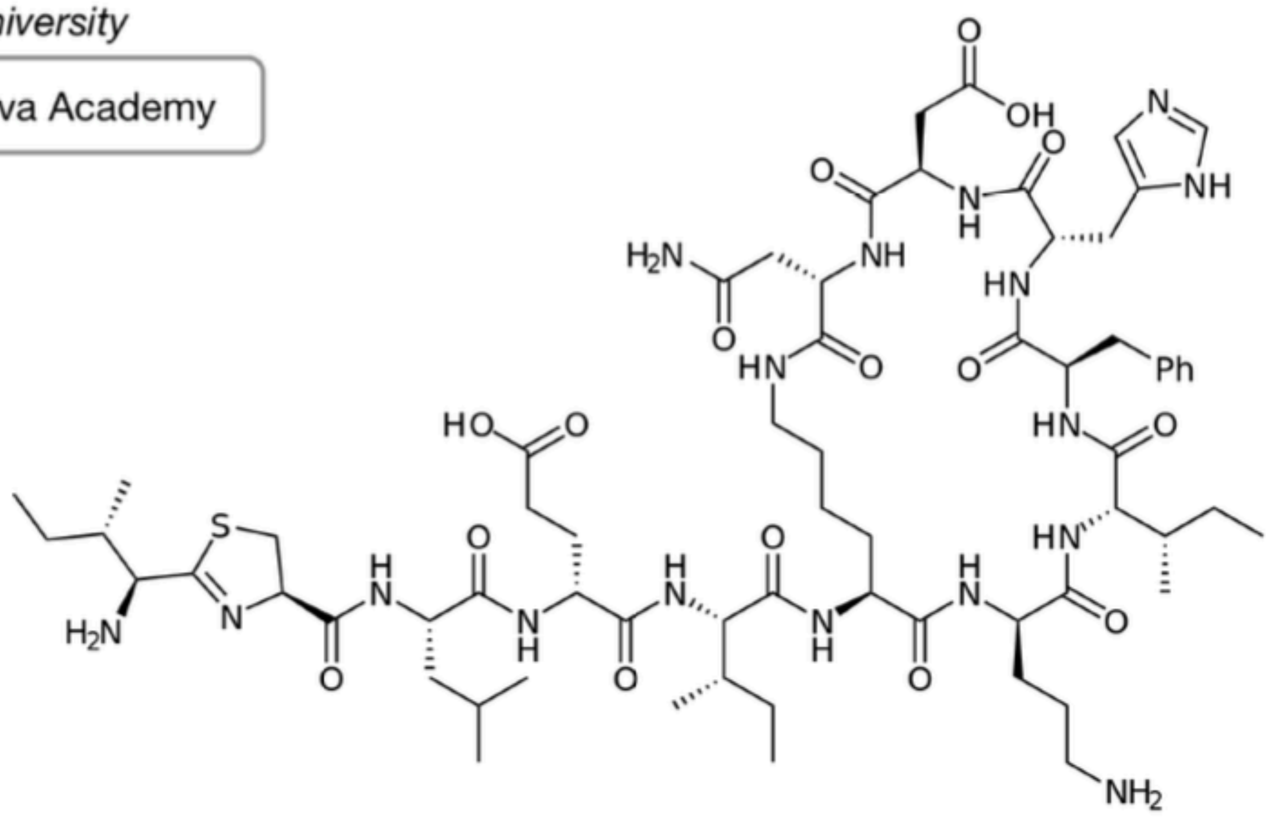

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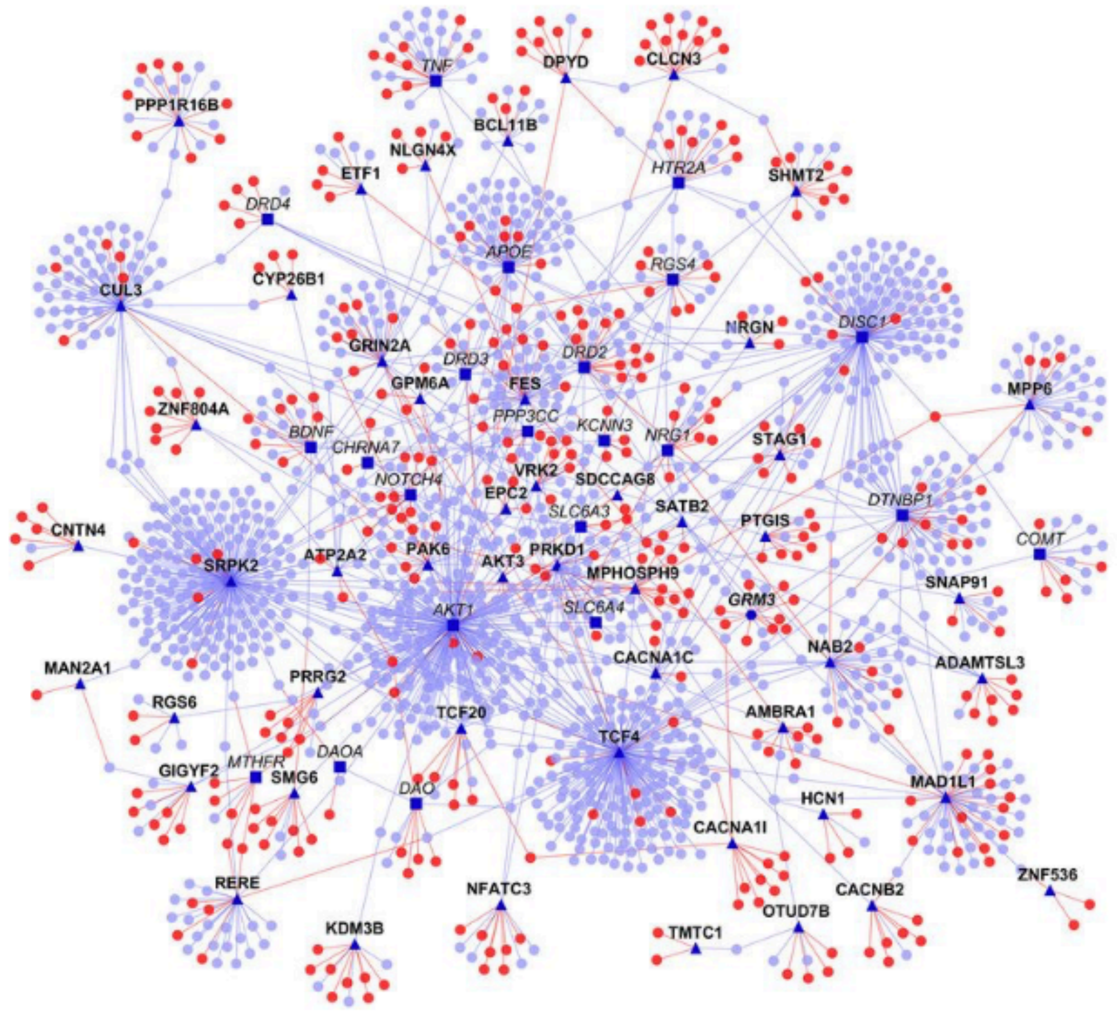
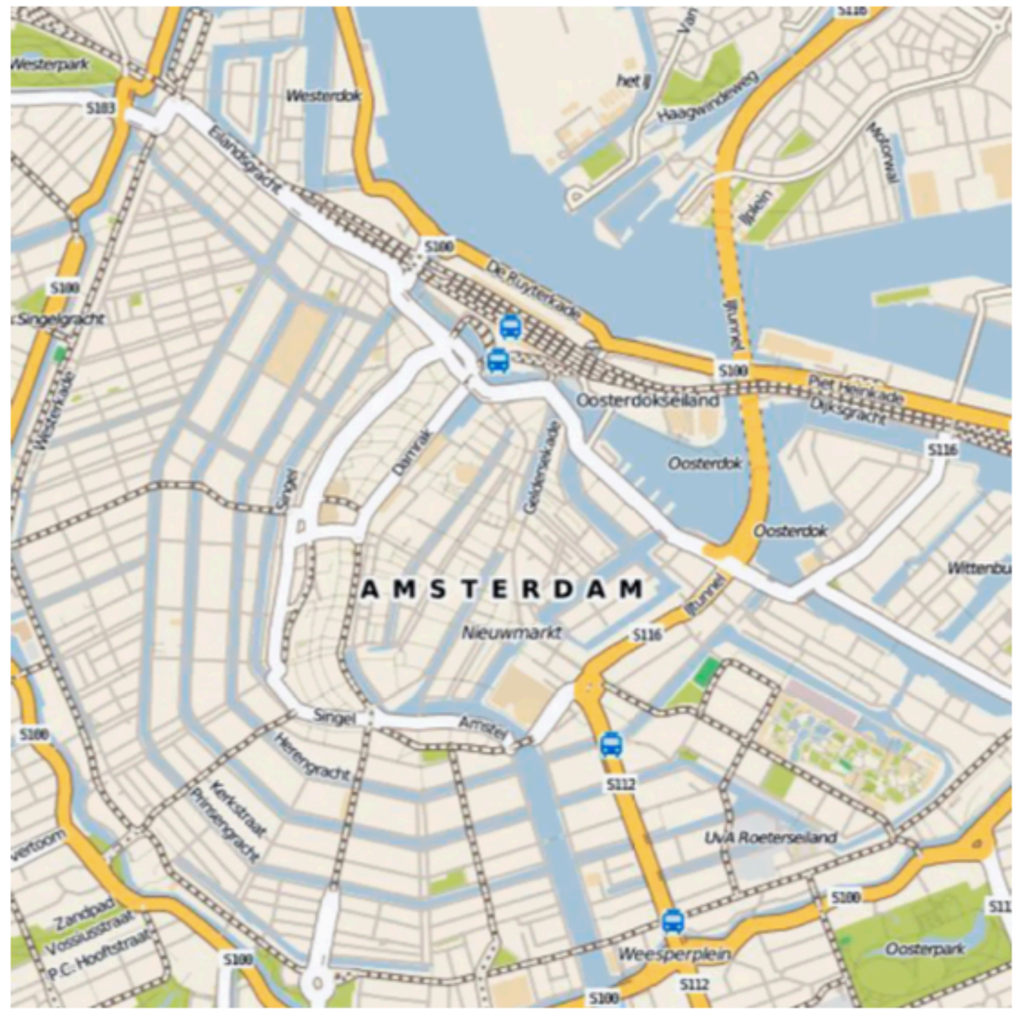


Protein interaction networks

Standard **CNN** and **RNN** architectures don’t work on this data

Road maps



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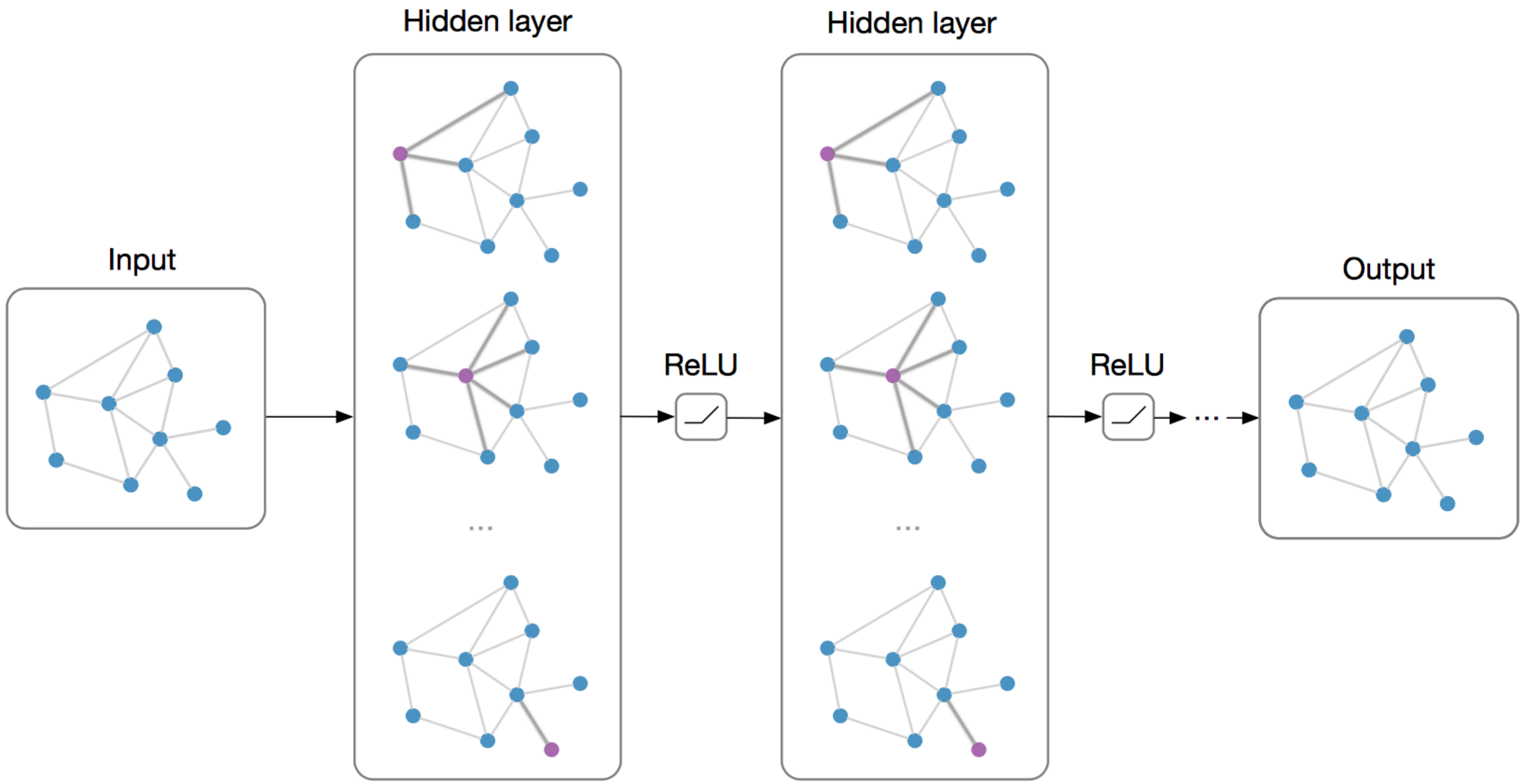
Graph Neural Networks (GNNs)



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**

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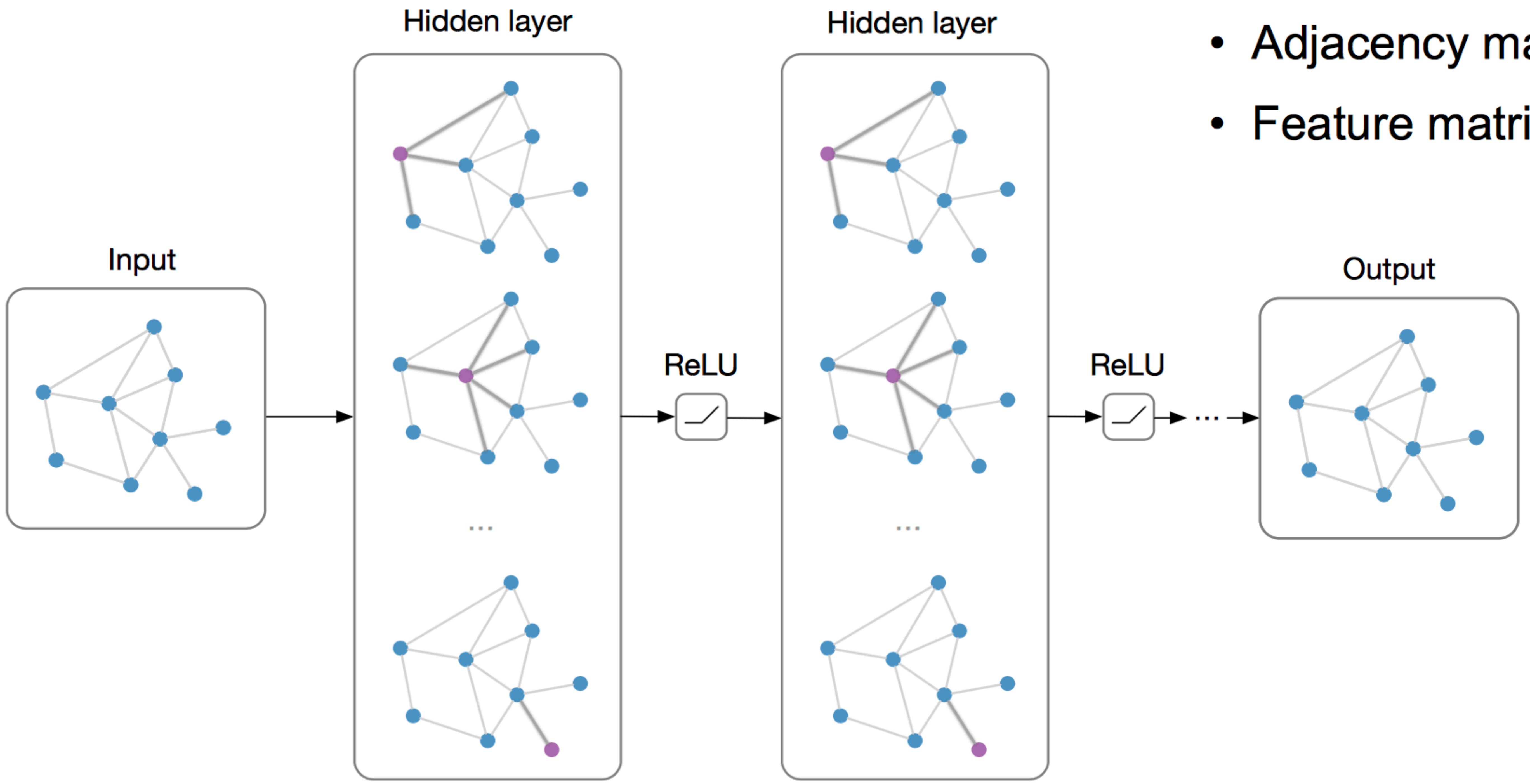

Notation: $\mathcal{G} = (\mathbf{A}, \mathbf{X})$

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

Main Idea: Pass massages between pairs of nodes and agglomerate

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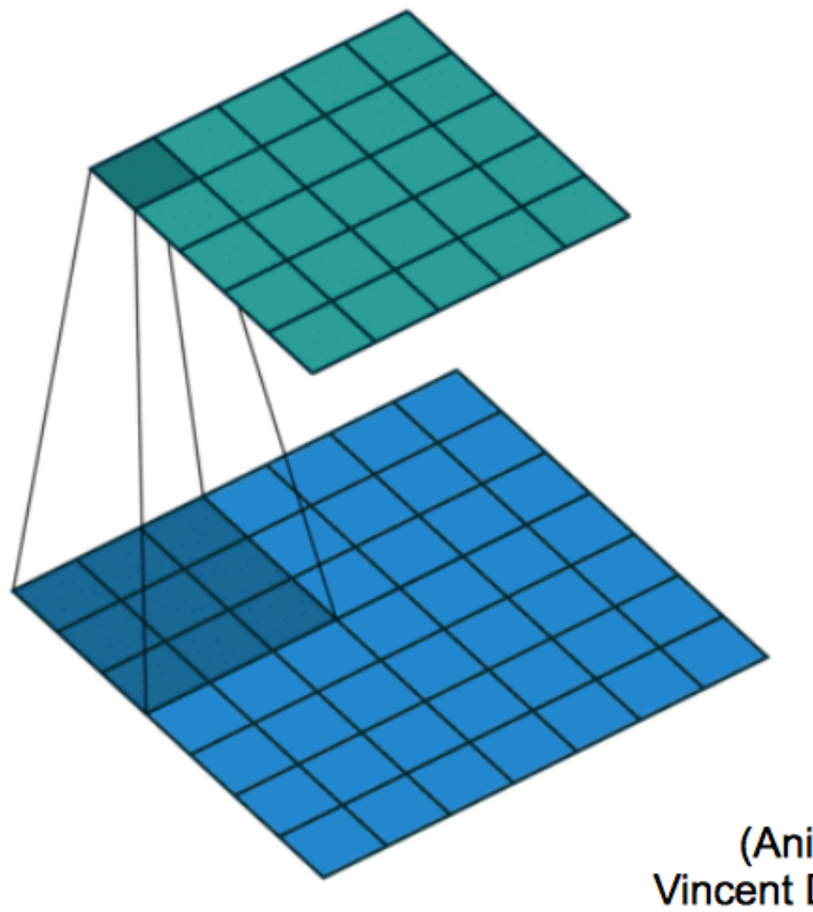
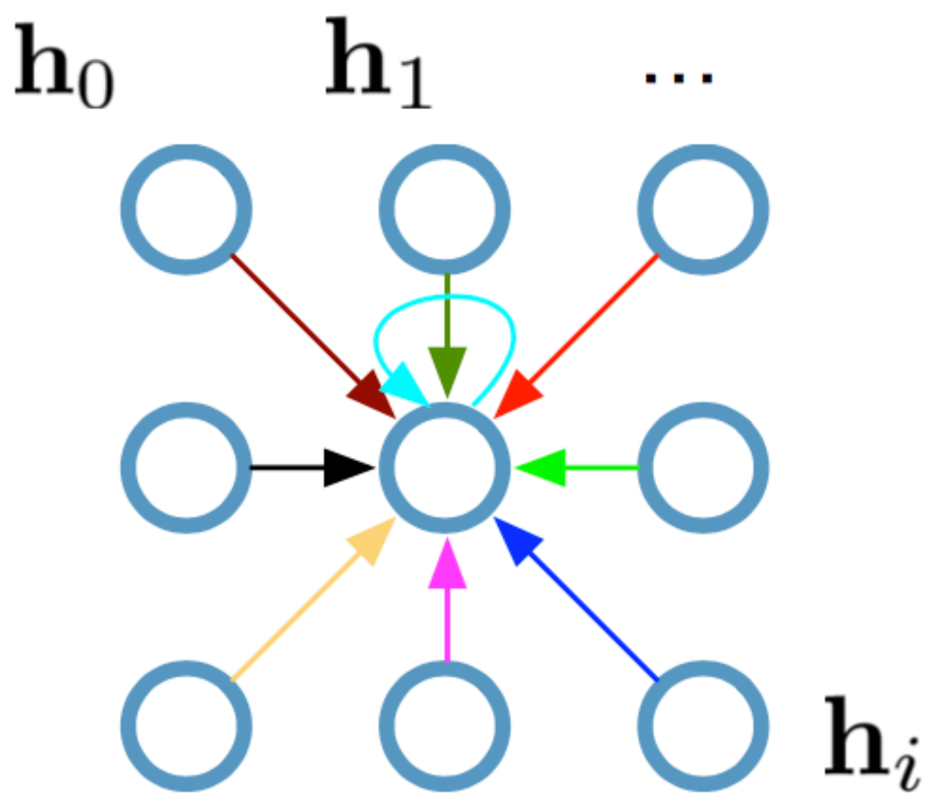
Recap: Convolutional Neural Networks (CNNs) on Grids

Single CNN layer with 3x3 filter:



(Animation by Vincent Dumoulin)



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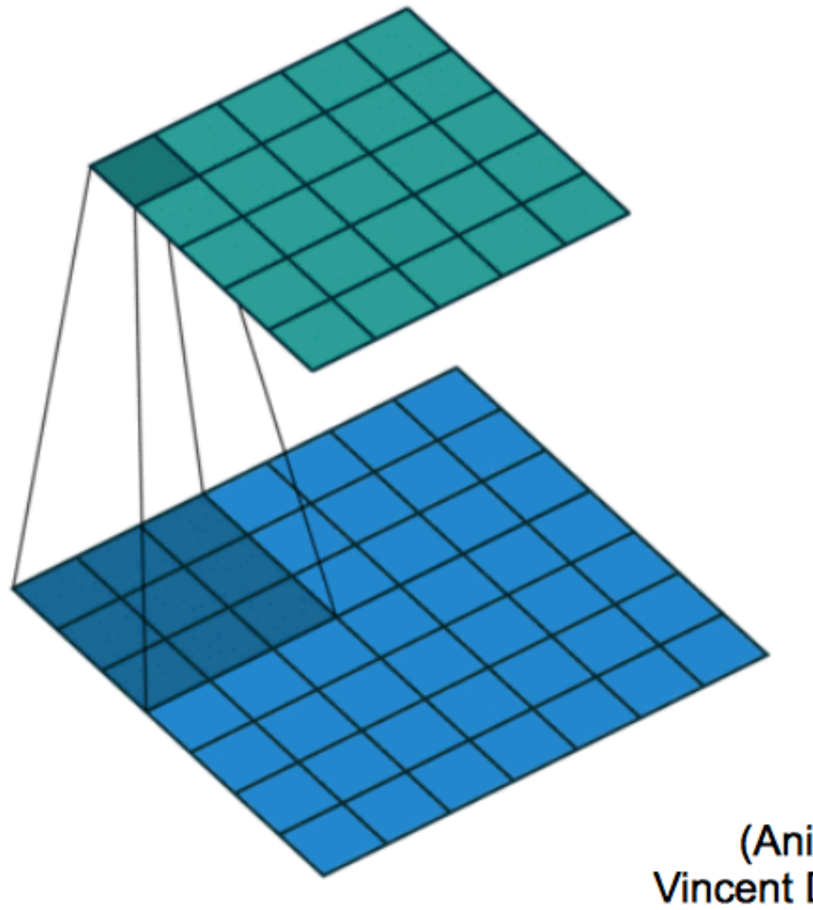

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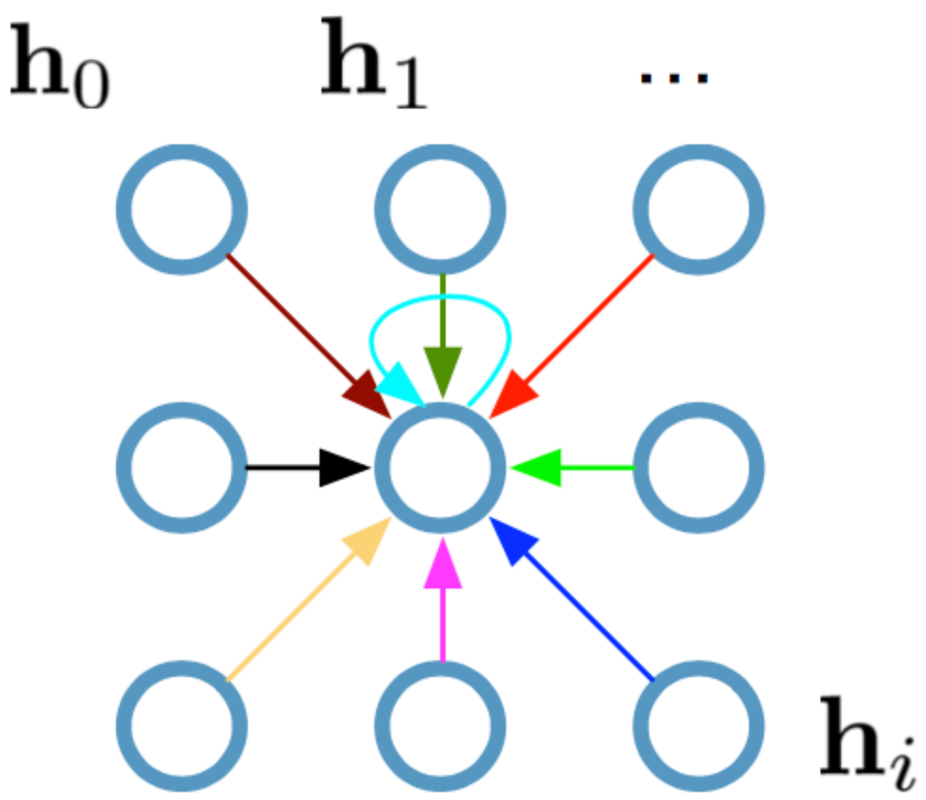

$\mathbf{h}_i \in \mathbb{R}^F$ are (hidden layer) activations of a pixel/node

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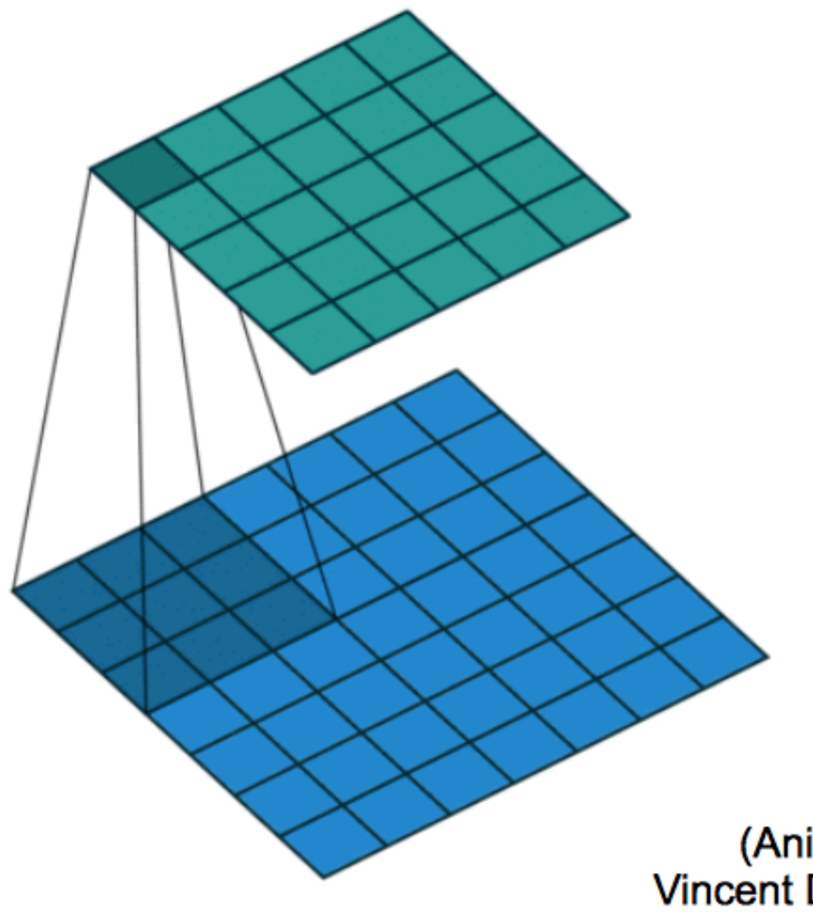

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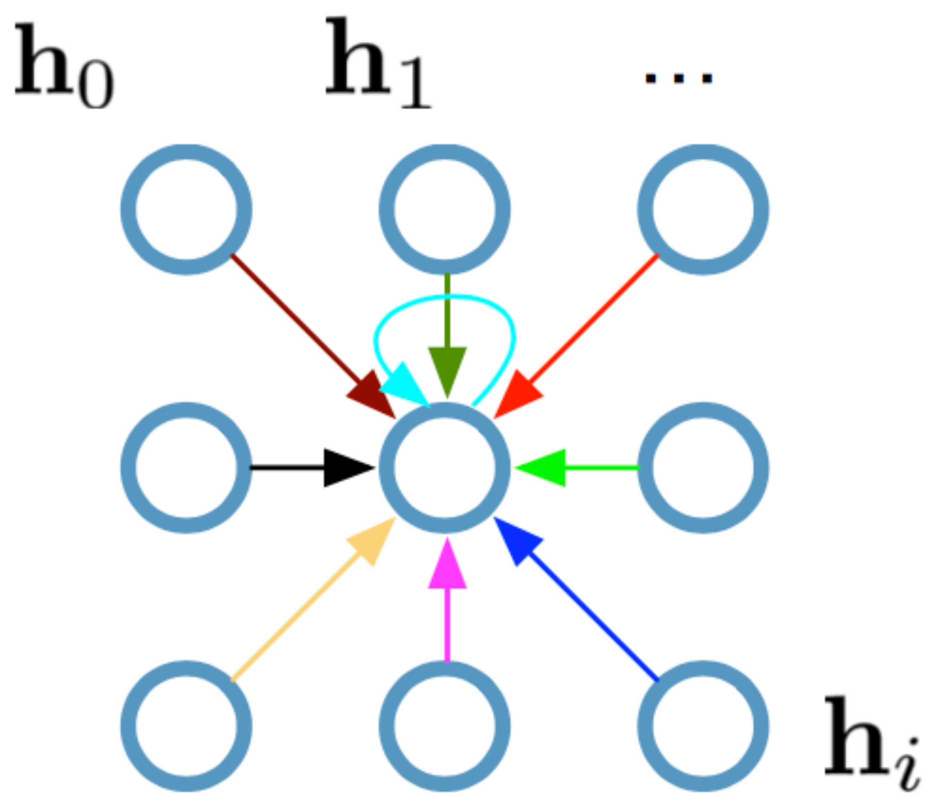

Update for a single pixel:

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

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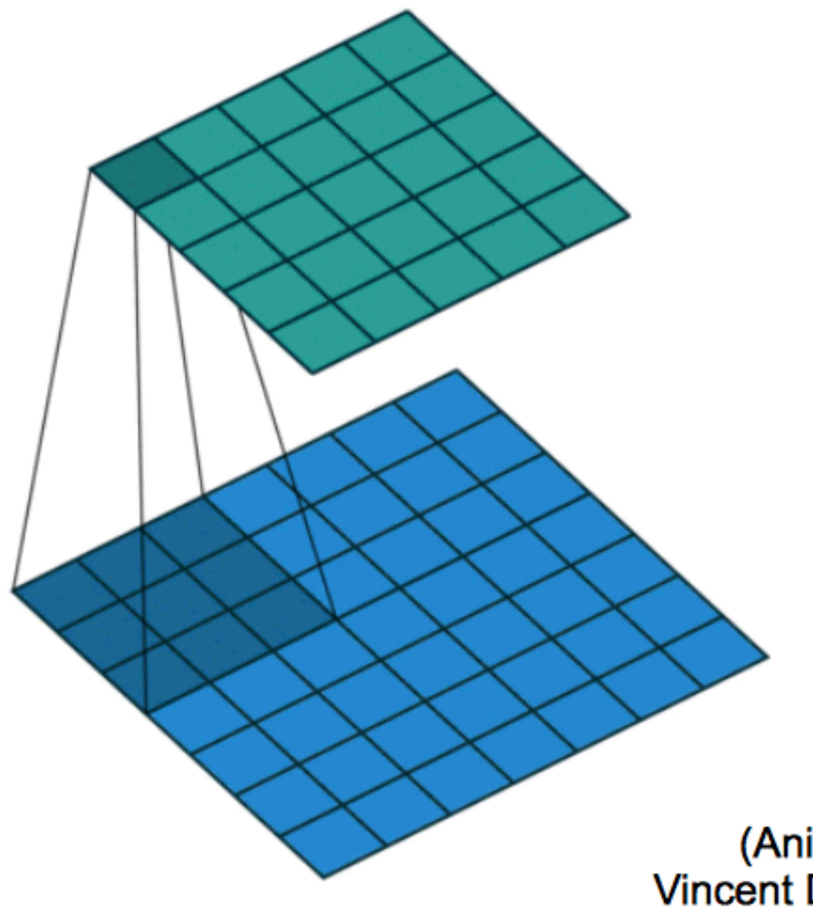

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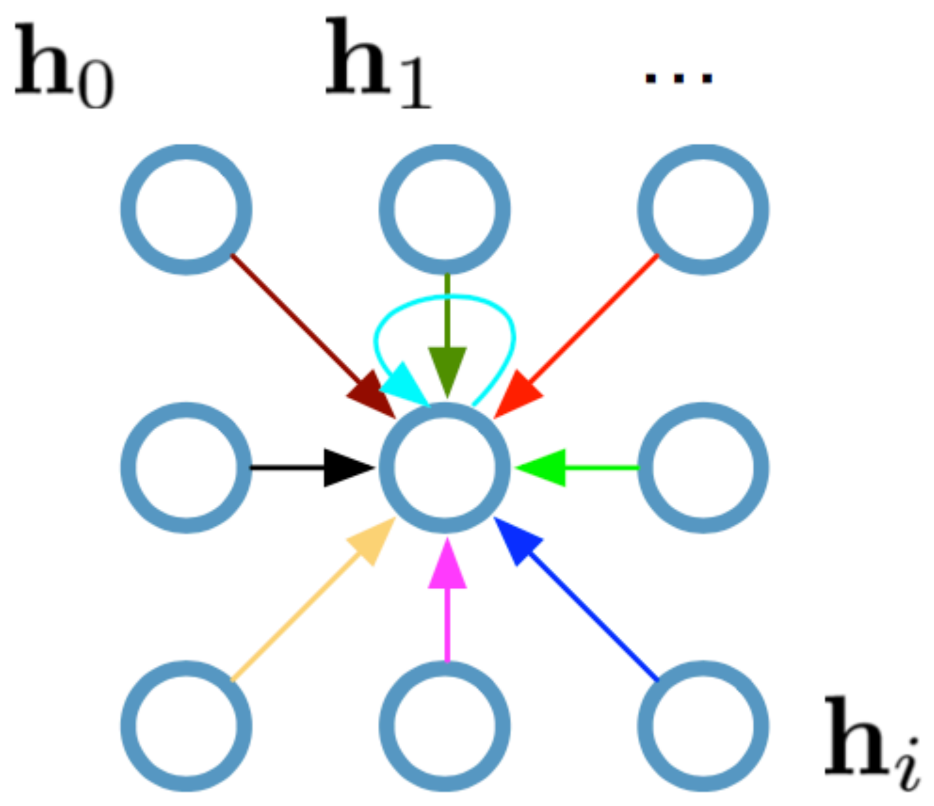

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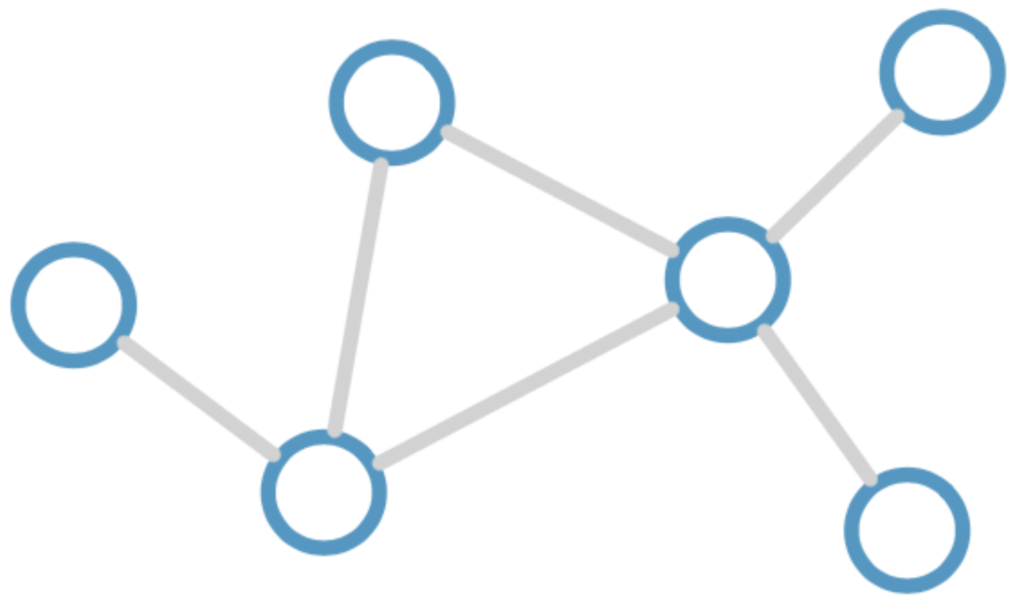
Full update:

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

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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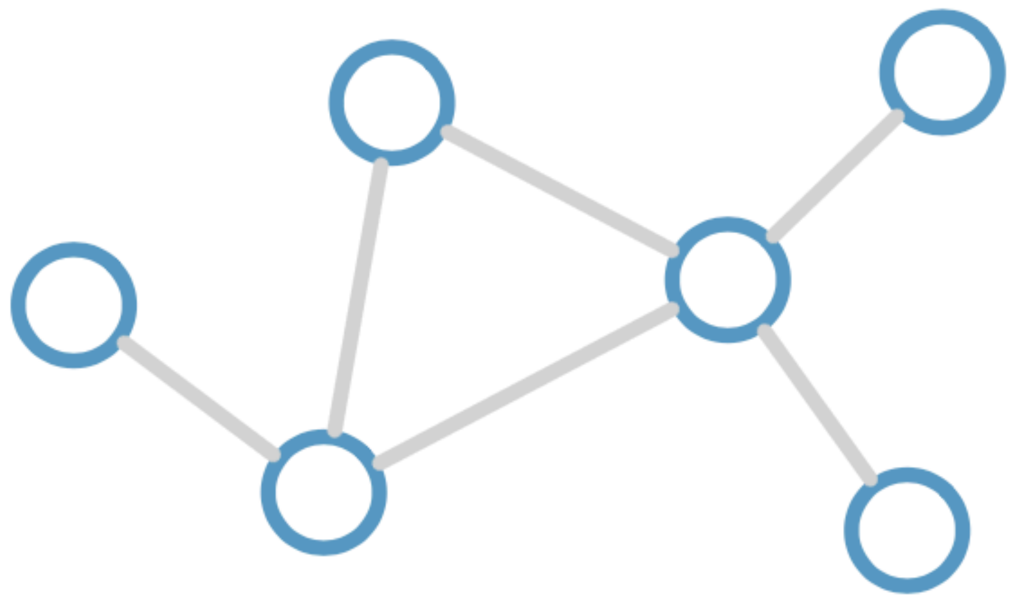
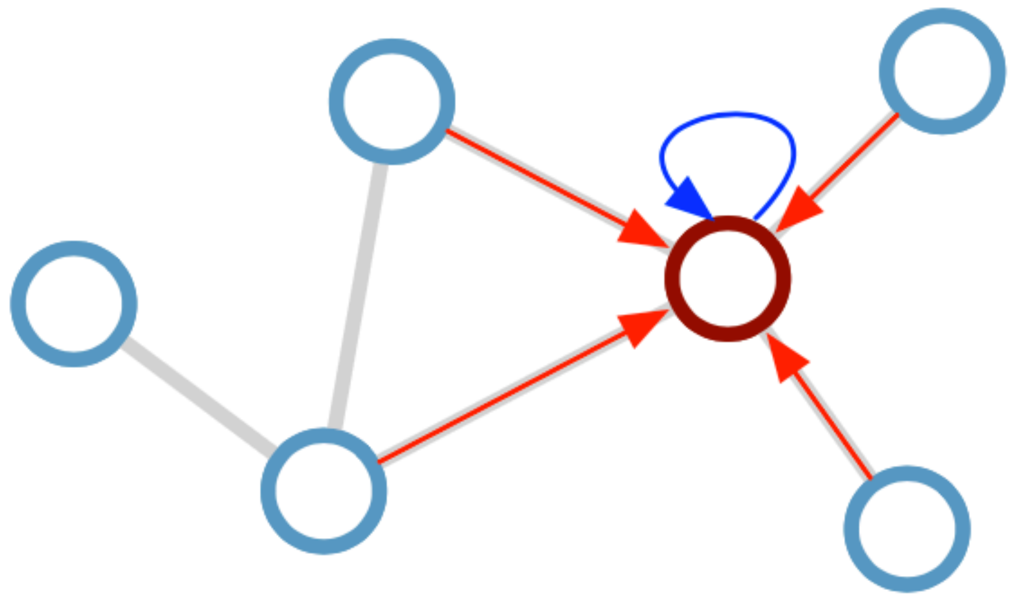


Calculate update for node in red:



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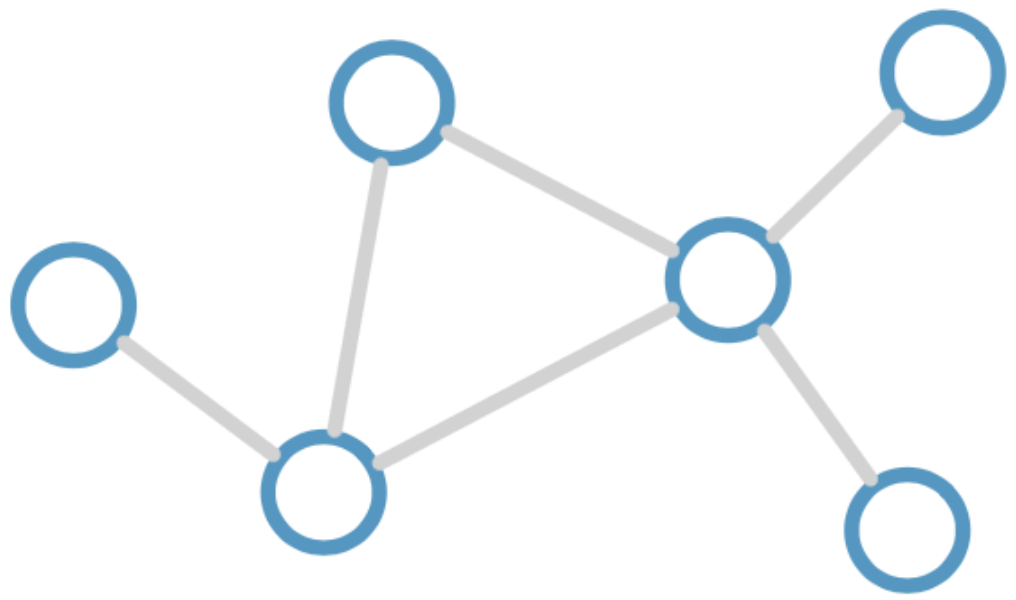

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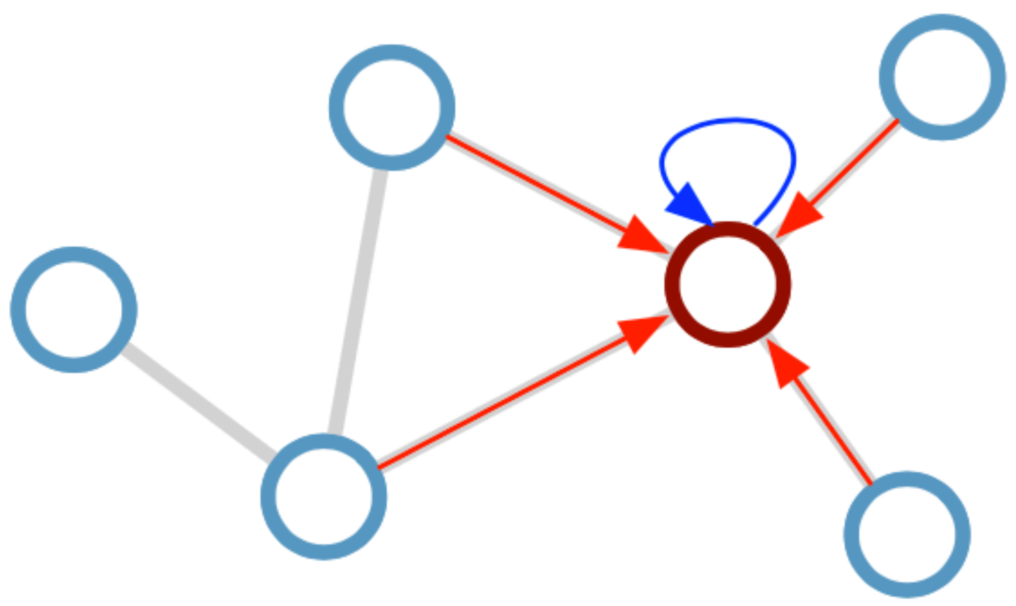

Update rule: $$\mathbf{h}_i^{(l+1)} = \sigma\left(\mathbf{h}_i^{(l)}\mathbf{W}_0^{(l)} + \sum_{j\in\mathcal{N}_i}\frac{1}{c_{ij}}\mathbf{h}_j^{(l)}\mathbf{W}_1^{(l)}\right)$$

Scalability: subsample messages [Hamilton et al., NIPS 2017]

$\mathcal{N}_i$: neighbor indices

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

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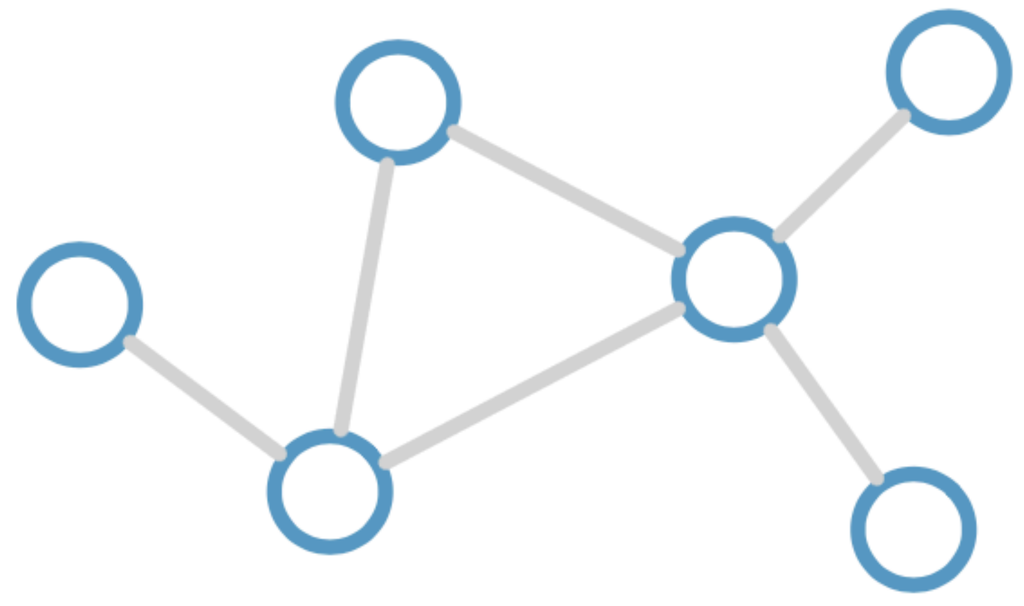

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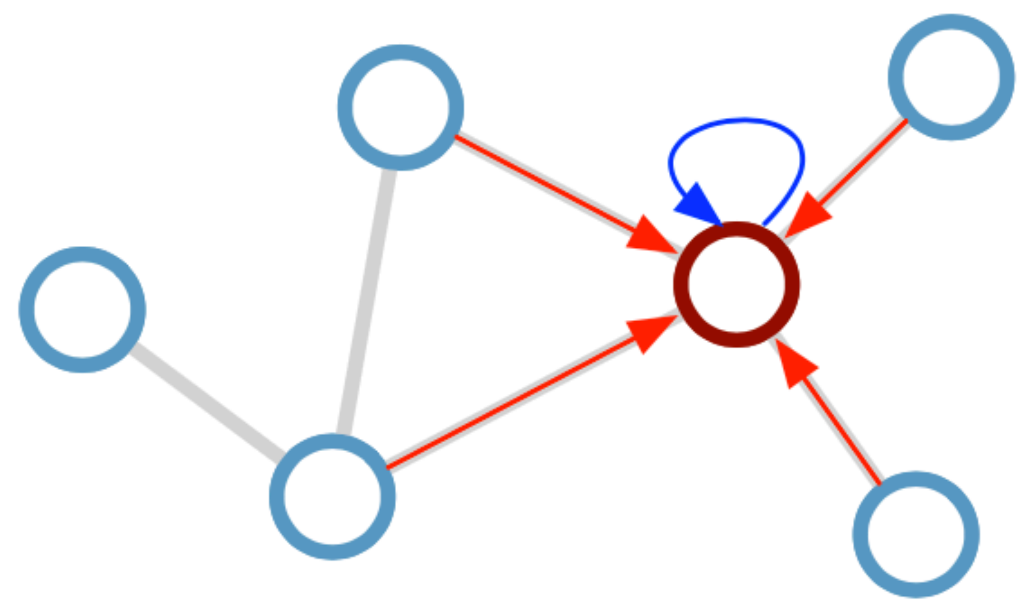

Desirable properties:

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

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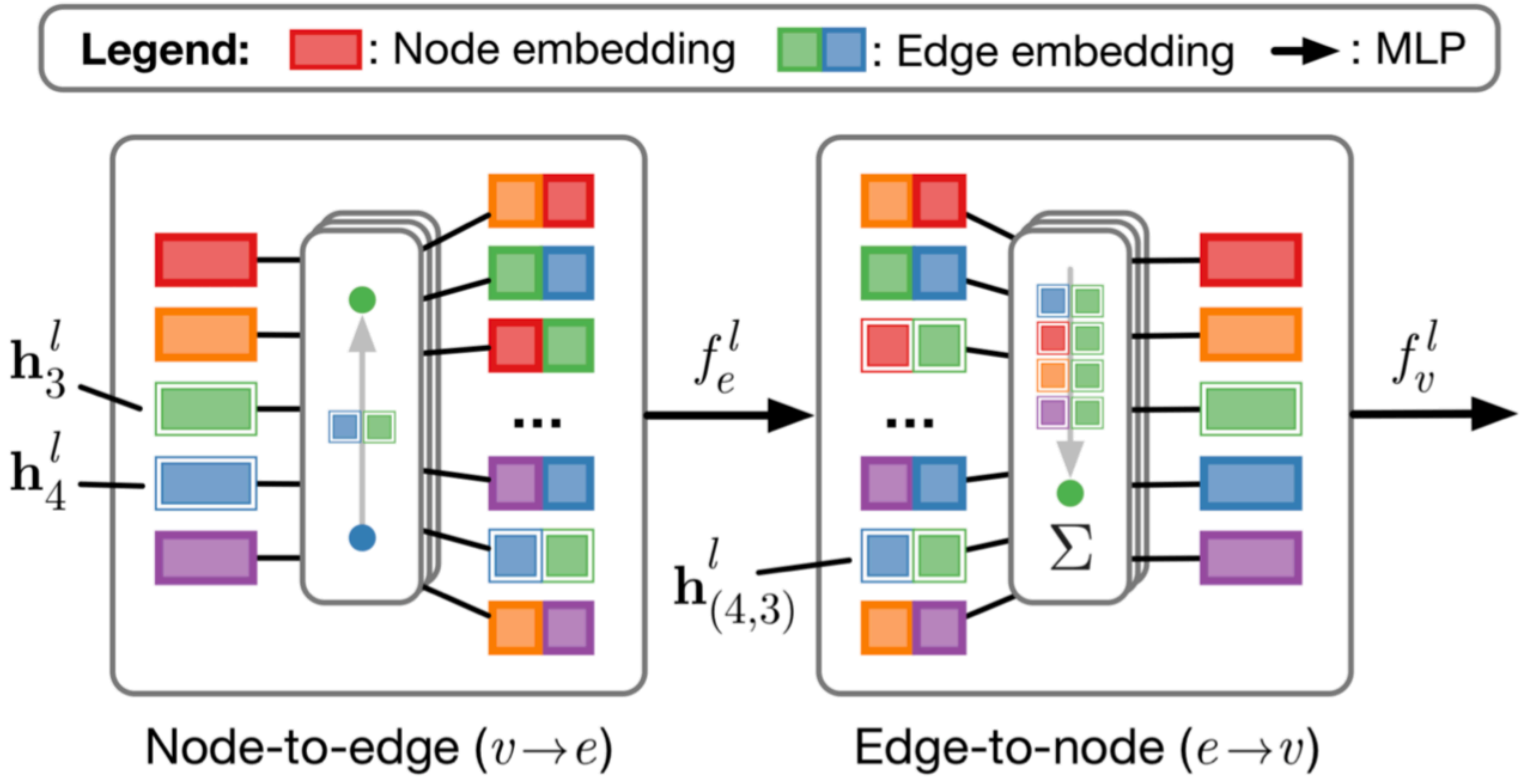
GNNs with **Edge** Embeddings

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



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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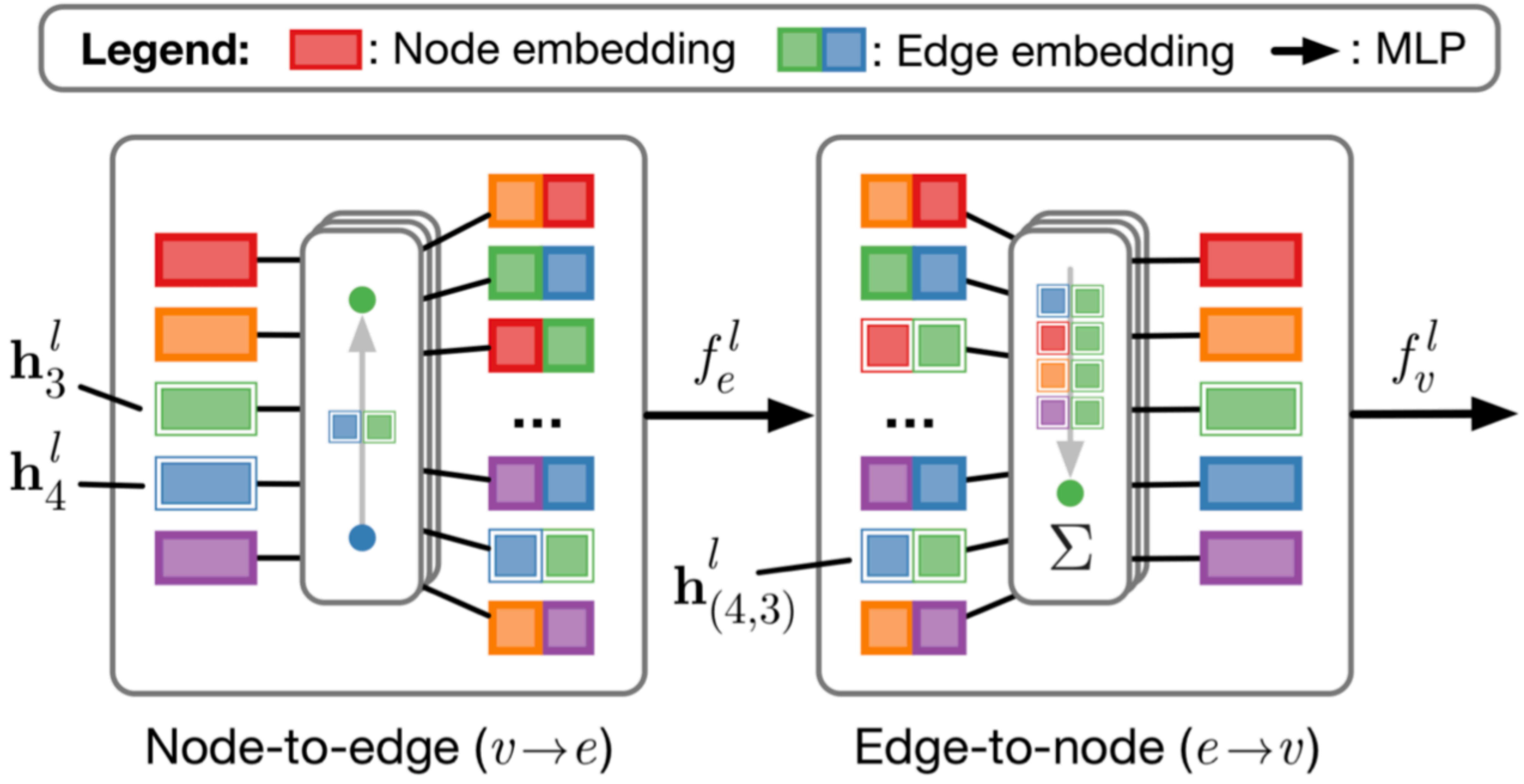

Pros:

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

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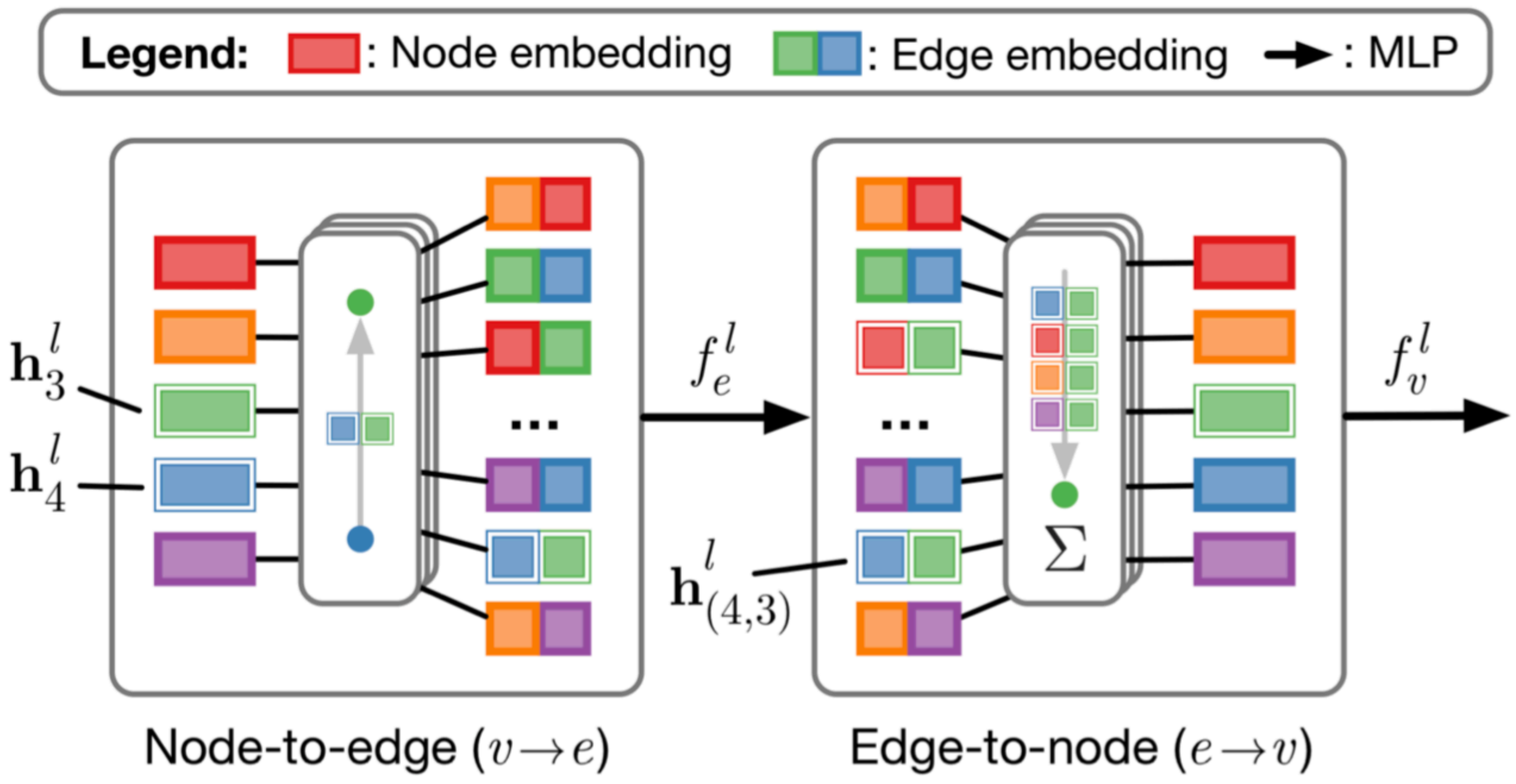

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Pros:

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

Cons:

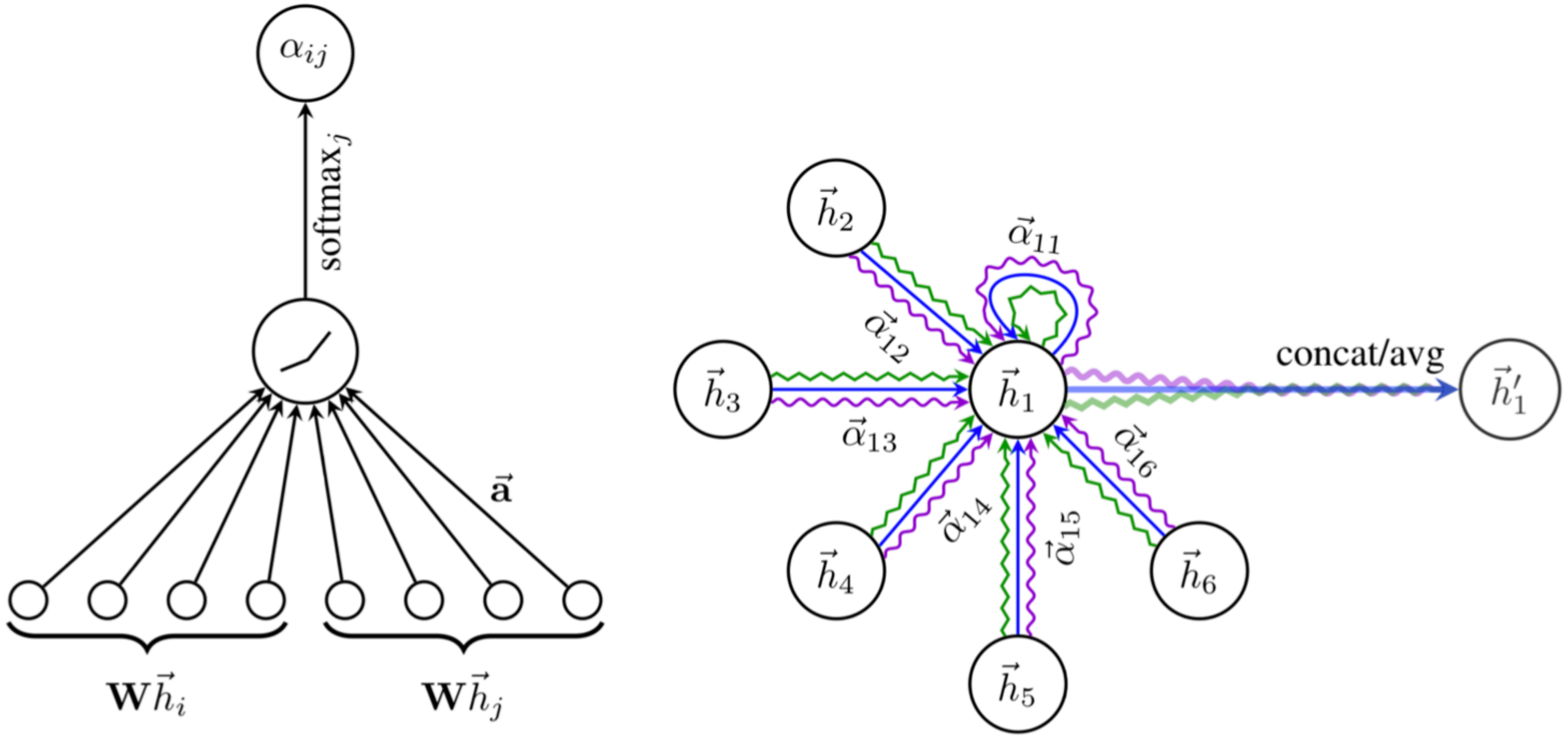
- Need to store intermediate edge-based activations
- Difficult to implement with subsampling

➡ In practice limited to small graphs

* 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)]

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

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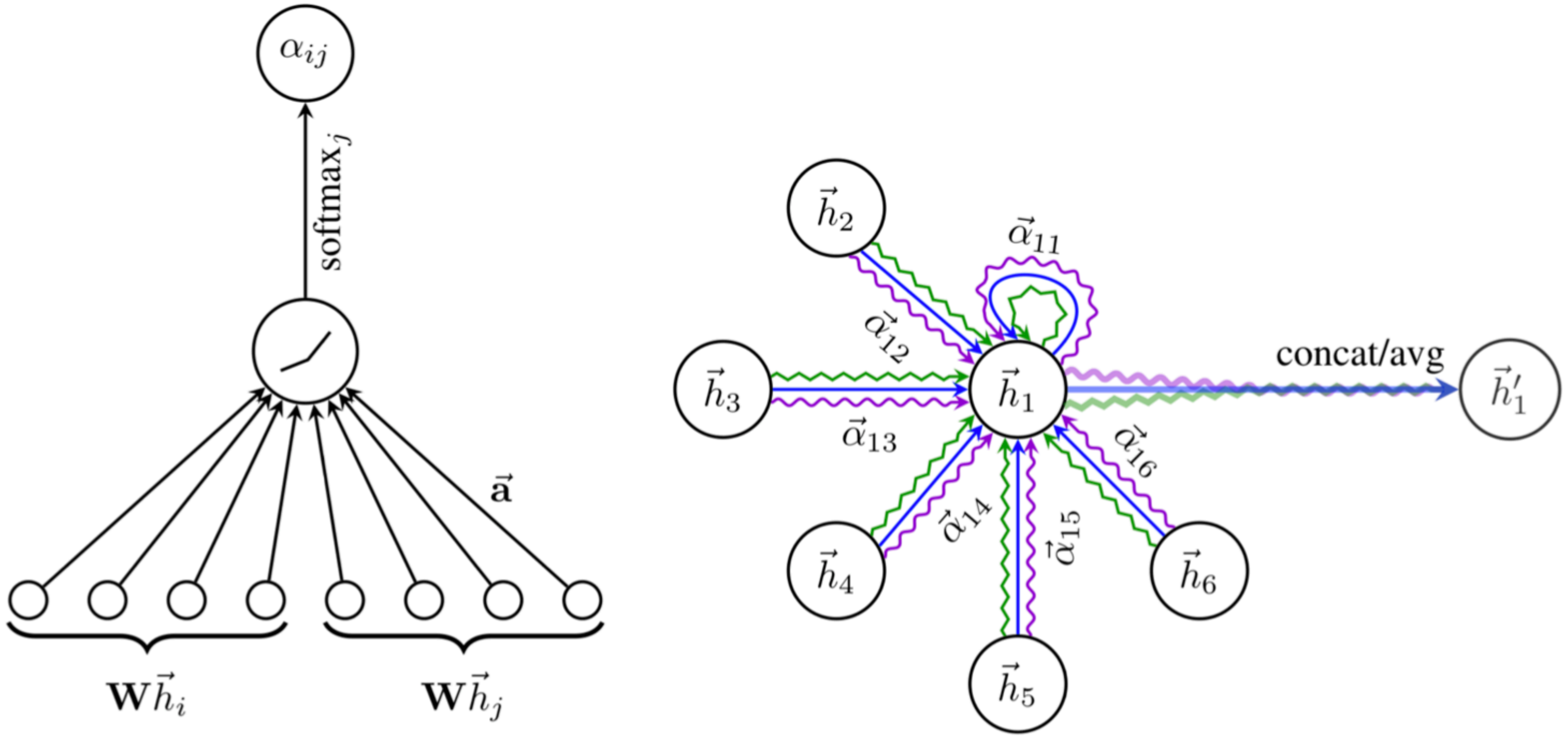

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$$\vec{h}'_i = \sigma\left(\frac{1}{K}\sum_{k=1}^{K}\sum_{j\in\mathcal{N}_i}\alpha_{ij}^k \mathbf{W}^k \vec{h}_j\right) \qquad \alpha_{ij} = \frac{\exp\left(\mathrm{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\mathrm{LeakyReLU}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

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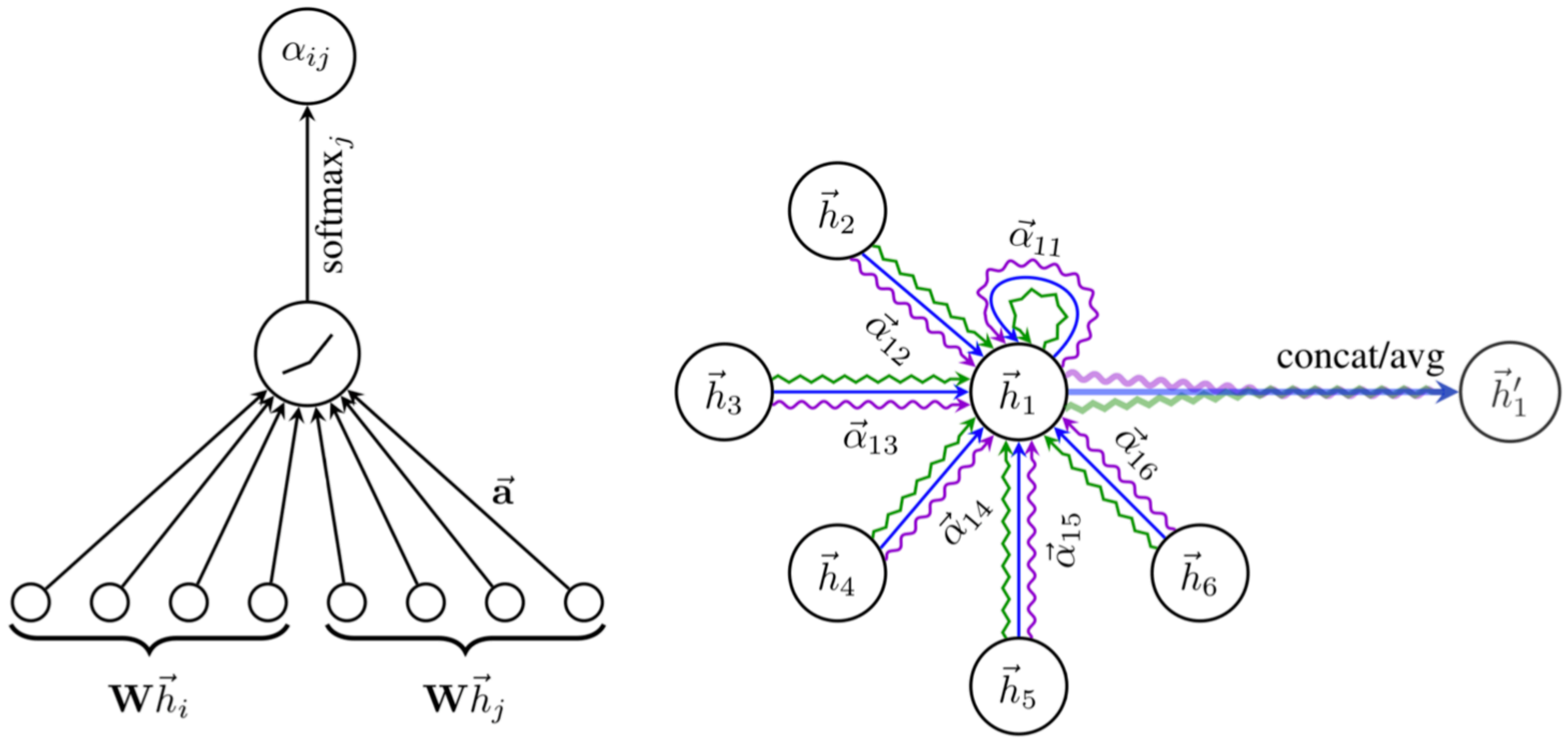

[Figure from Veličković et al. (ICLR 2018)]

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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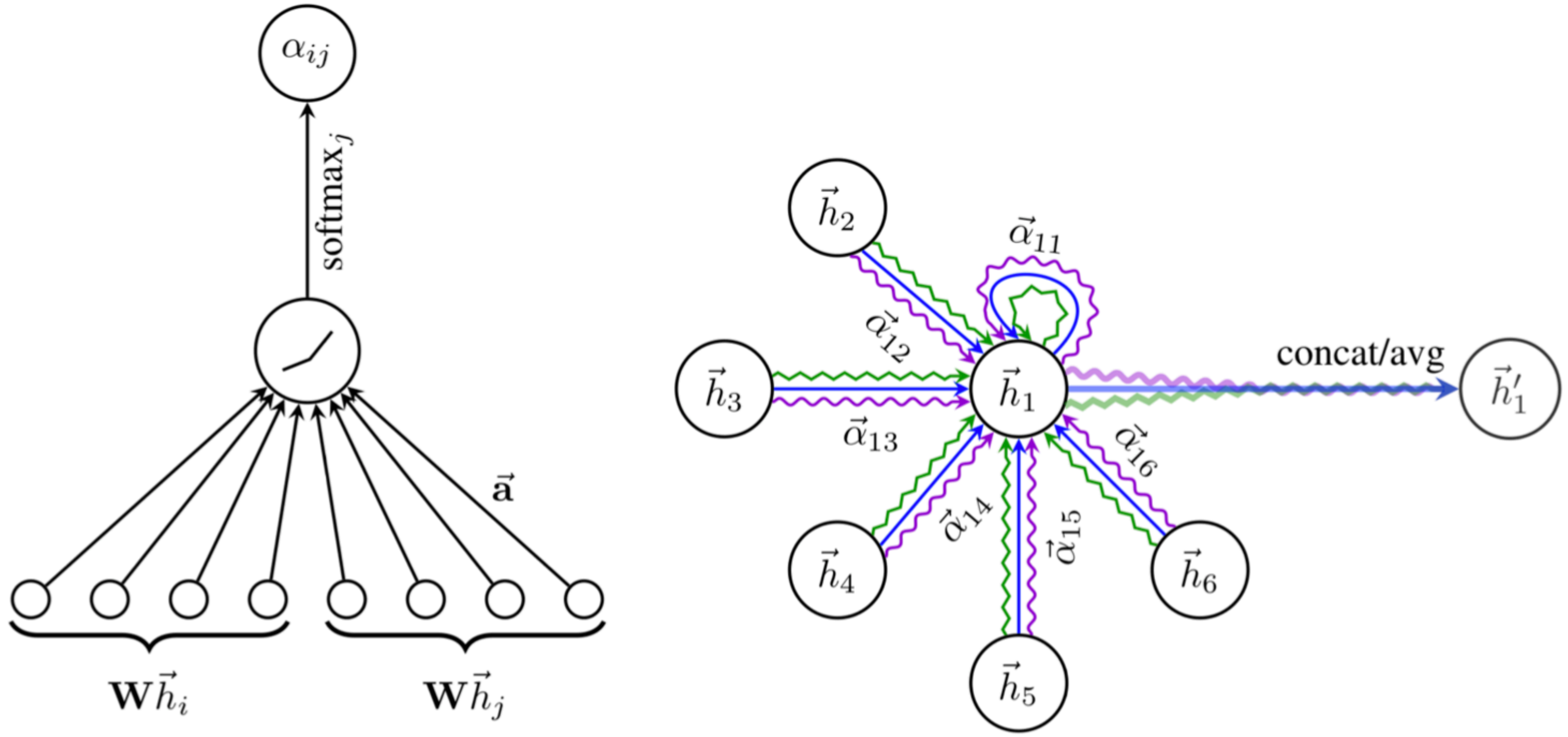

[Figure from Veličković et al. (ICLR 2018)]

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

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

$$\alpha_{ij} = \frac{\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_j]\right)\right)}{\sum_{k\in\mathcal{N}_i}\exp\left(\text{LeakyReLU}\left(\vec{\mathbf{a}}^T[\mathbf{W}\vec{h}_i \| \mathbf{W}\vec{h}_k]\right)\right)}$$

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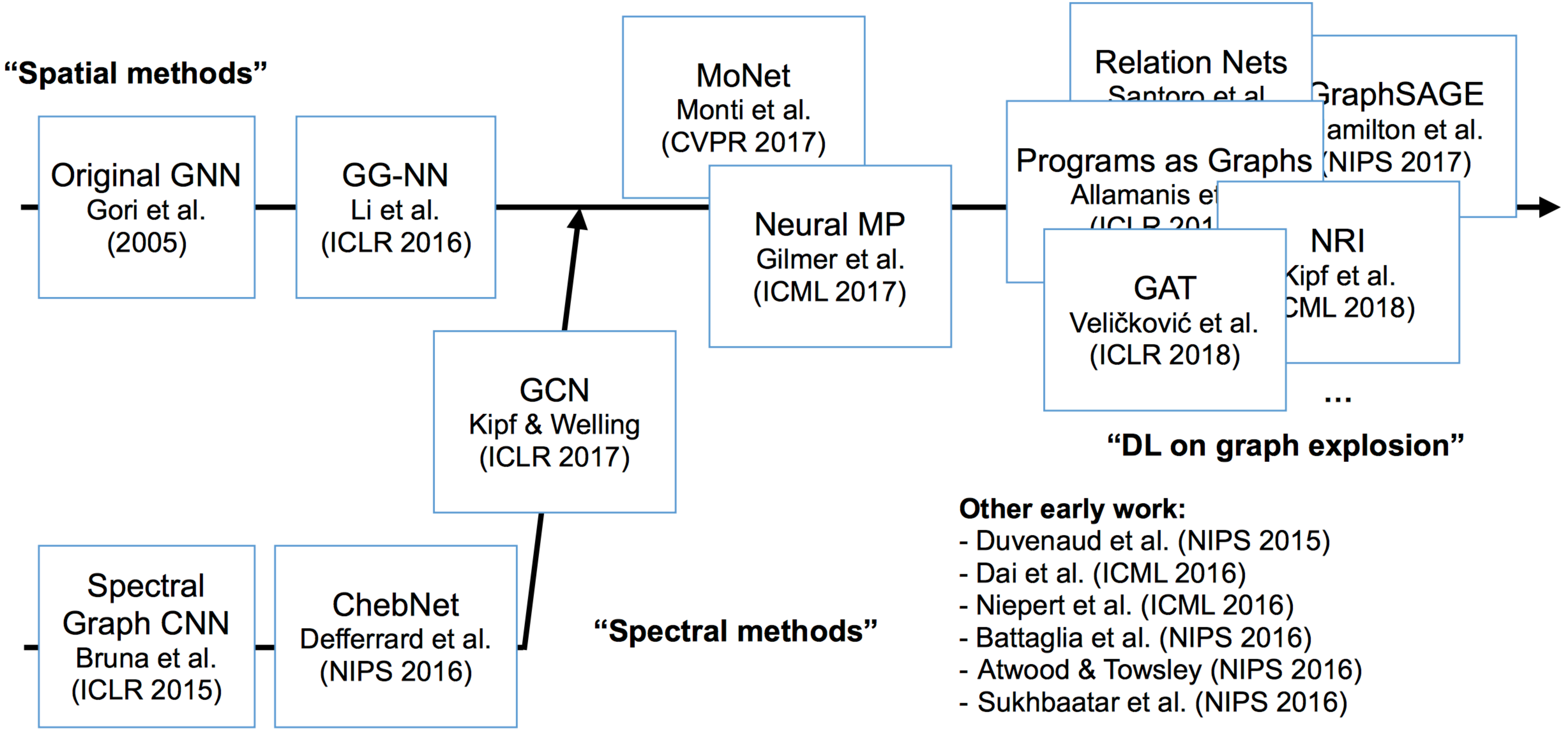
A **Brief History** of Graph Neural Nets



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)

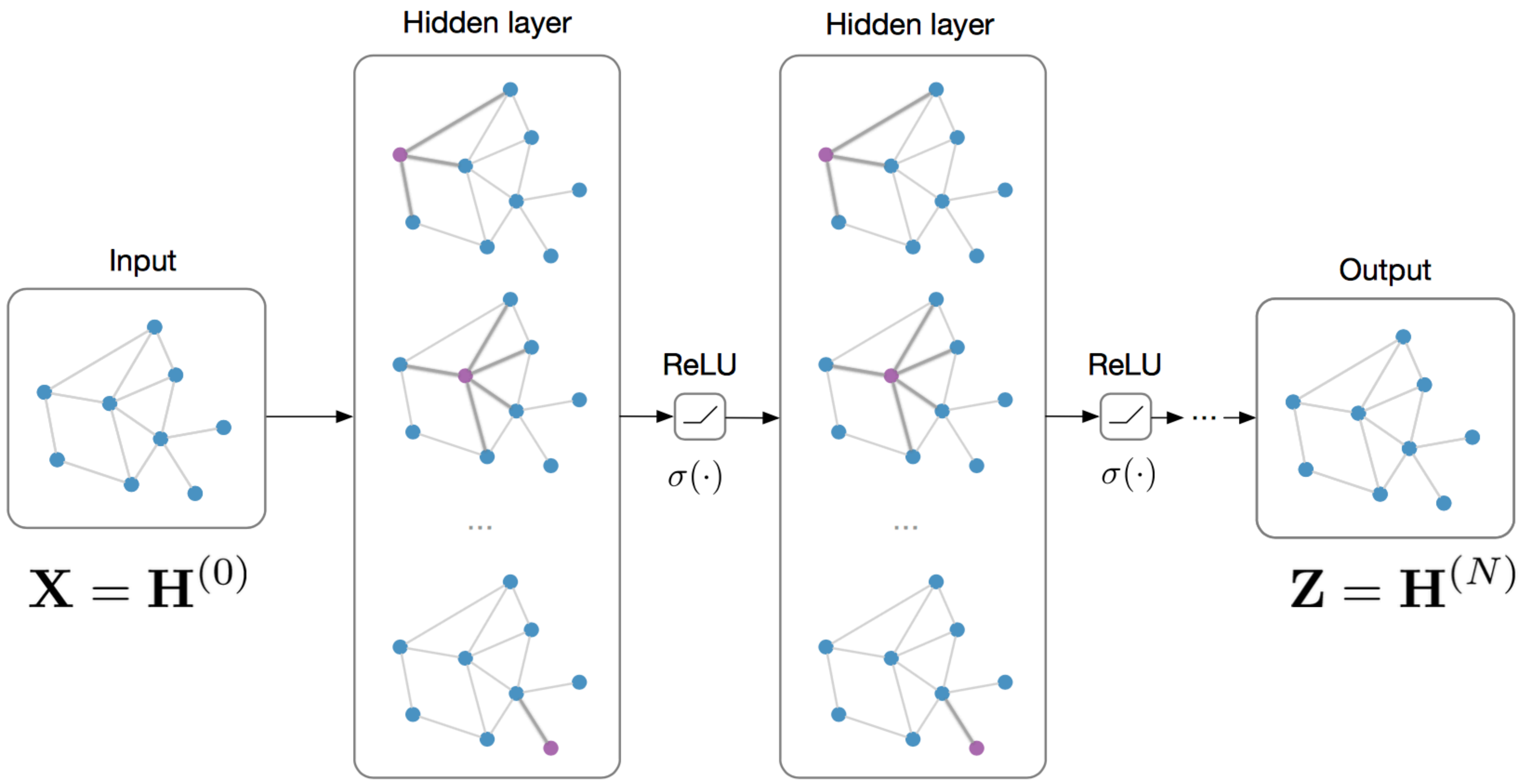
(slide inspired by Alexander Gaunt's talk on GNNs)

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

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 $\hat{\mathbf{A}}$



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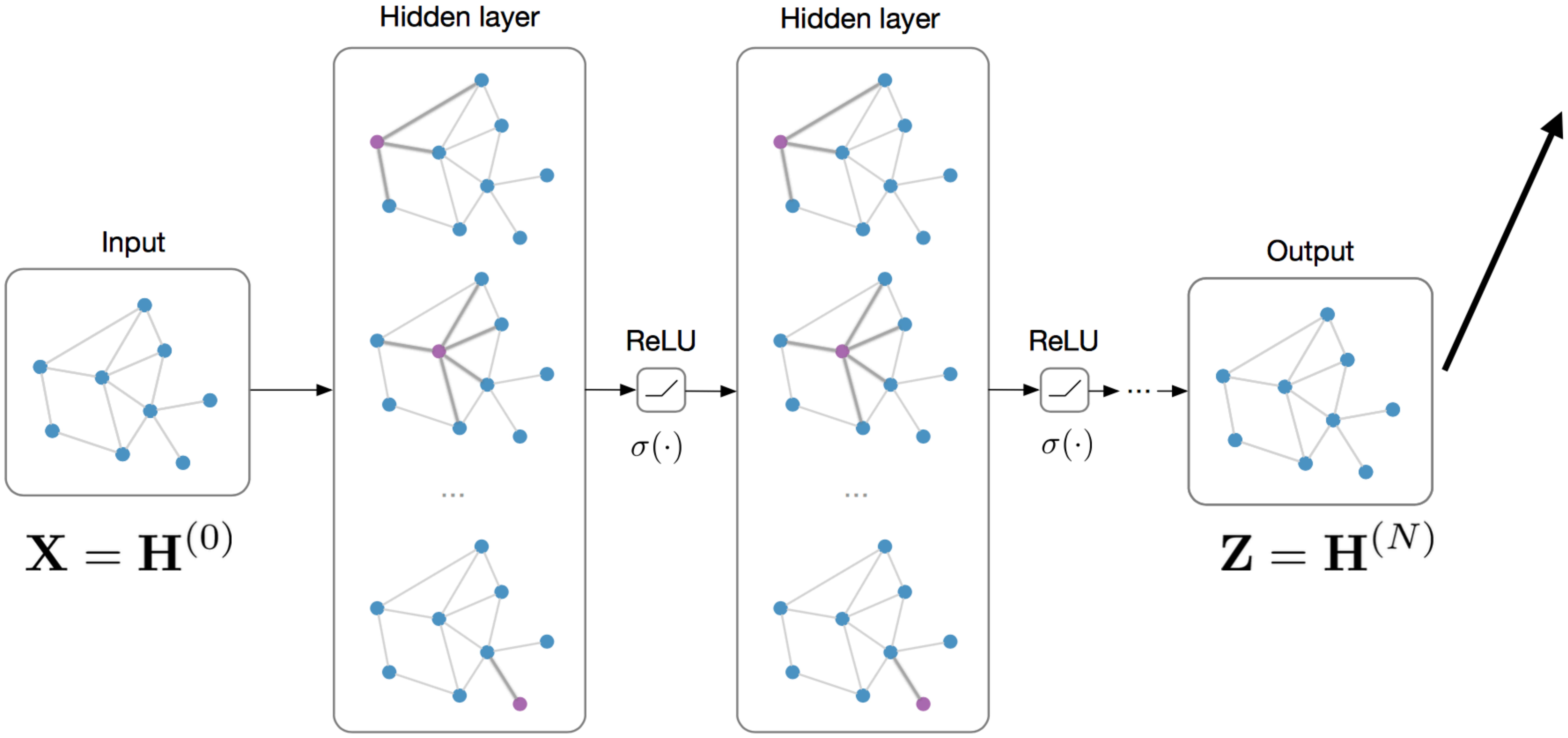

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Node classification:

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

e.g. Kipf & Welling (ICLR 2017)

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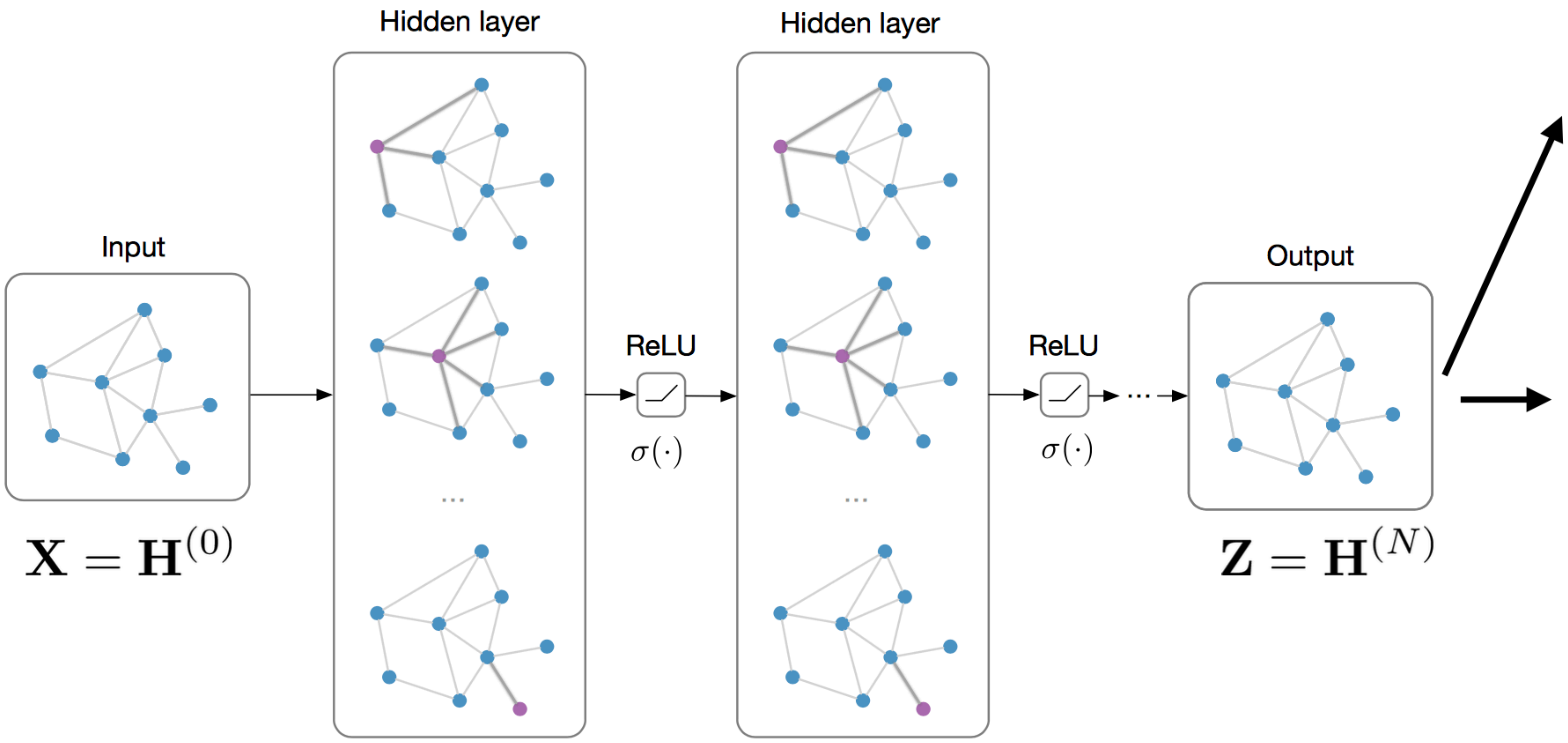

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e.g. Duvenaud et al. (NIPS 2015)

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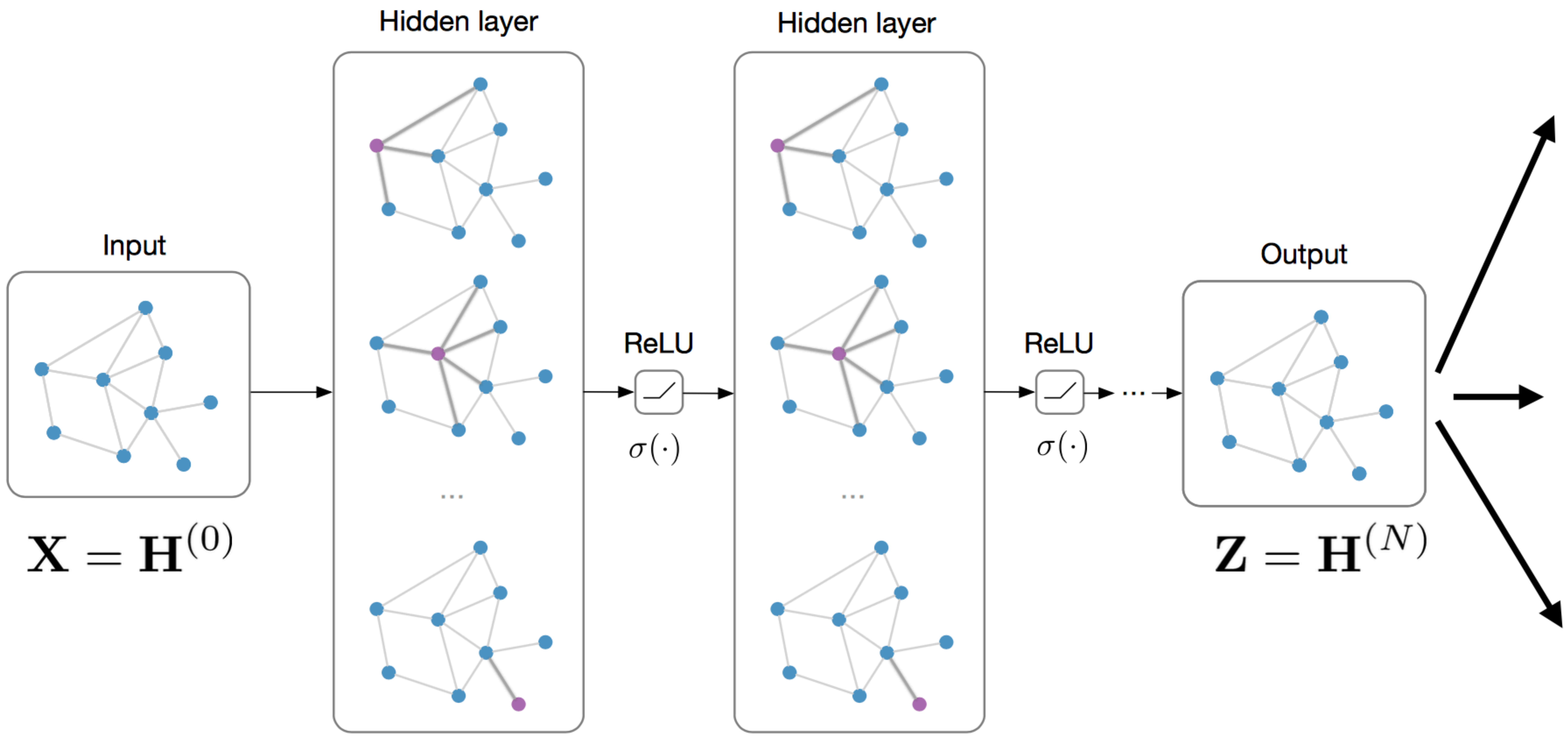

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Link prediction:

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

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

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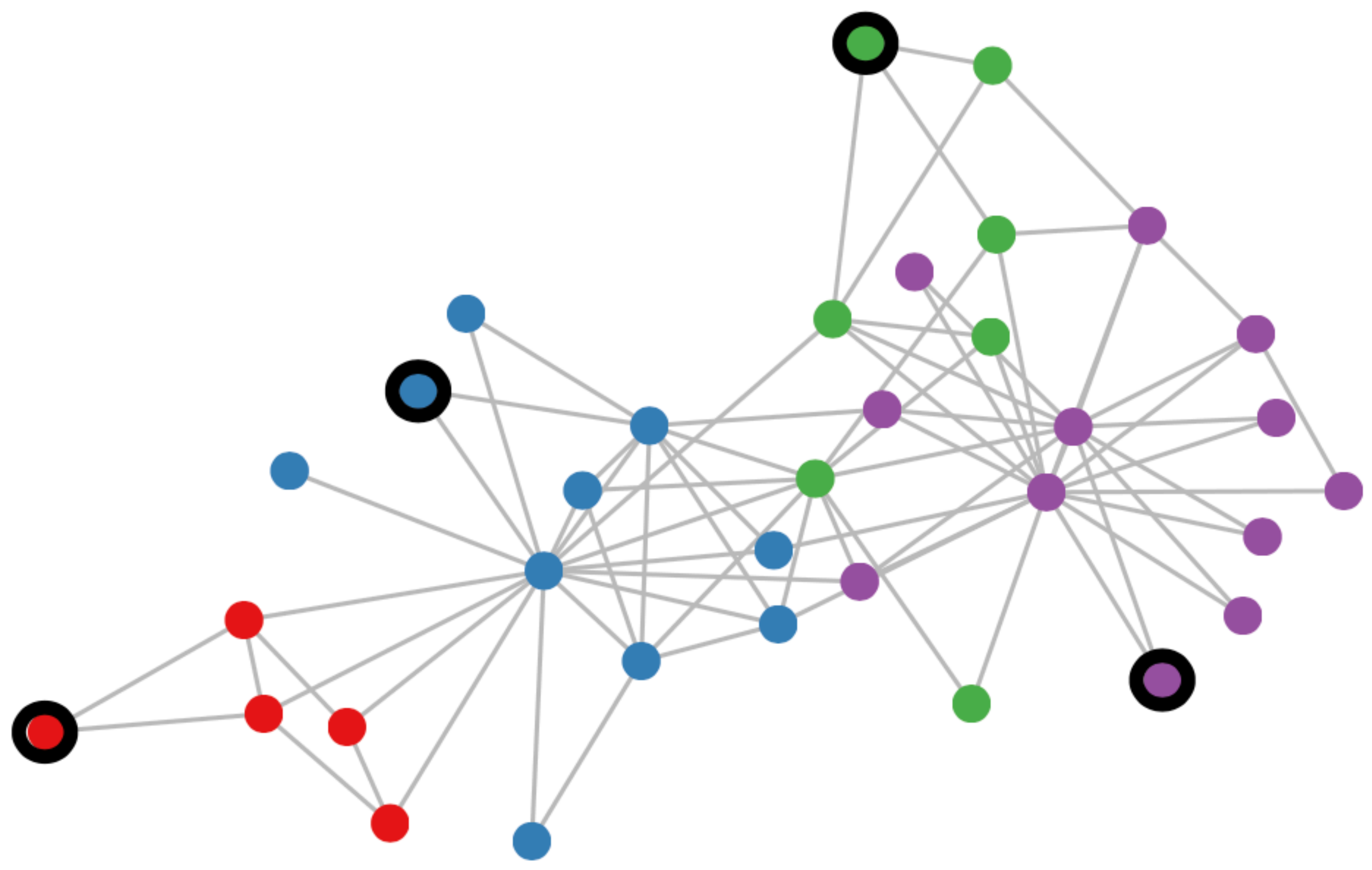
Semi-supervised Classification on Graphs

Setting:

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

Task:
Predict node label of unlabeled nodes



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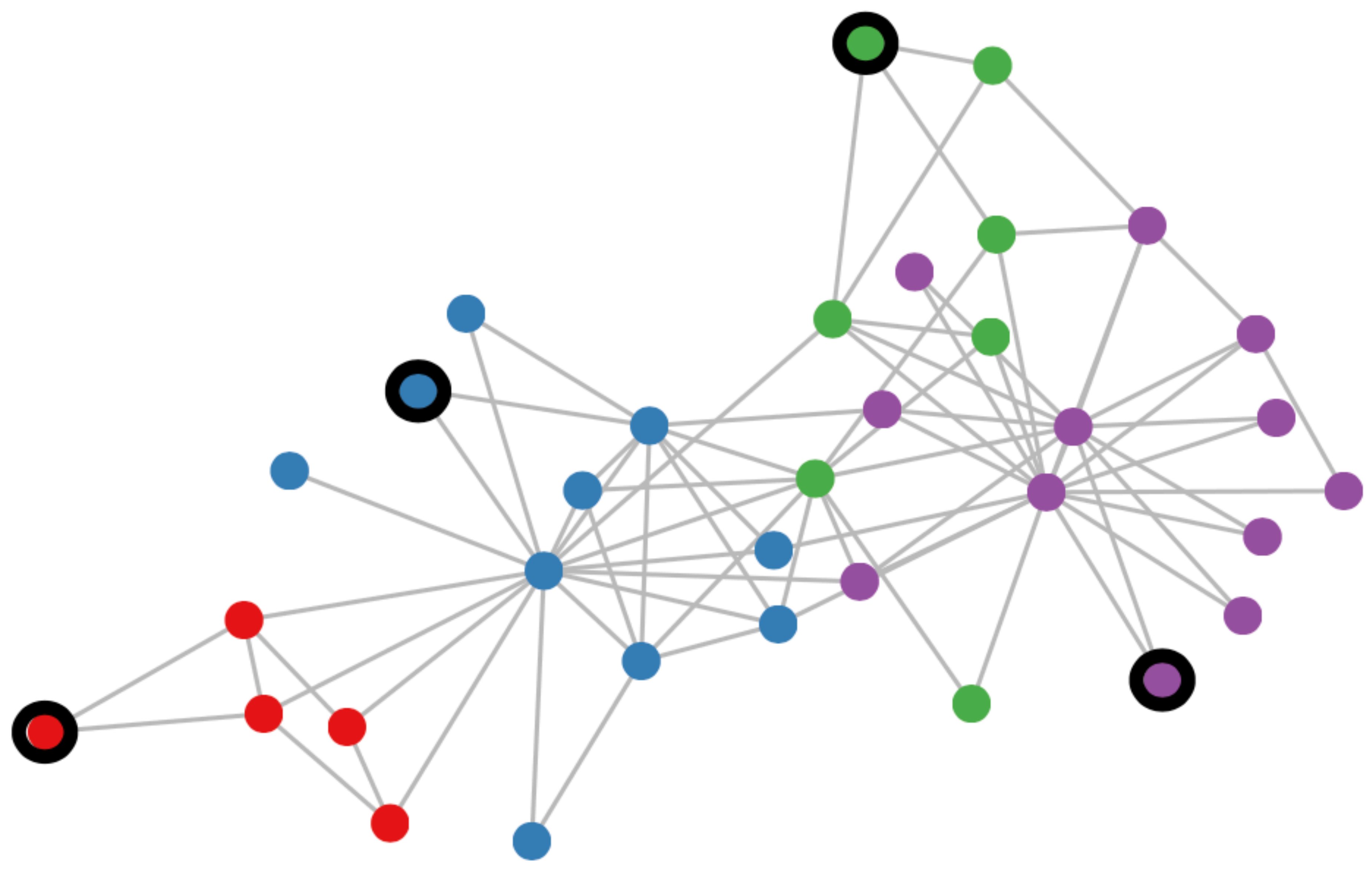


Evaluate loss on labeled nodes only:

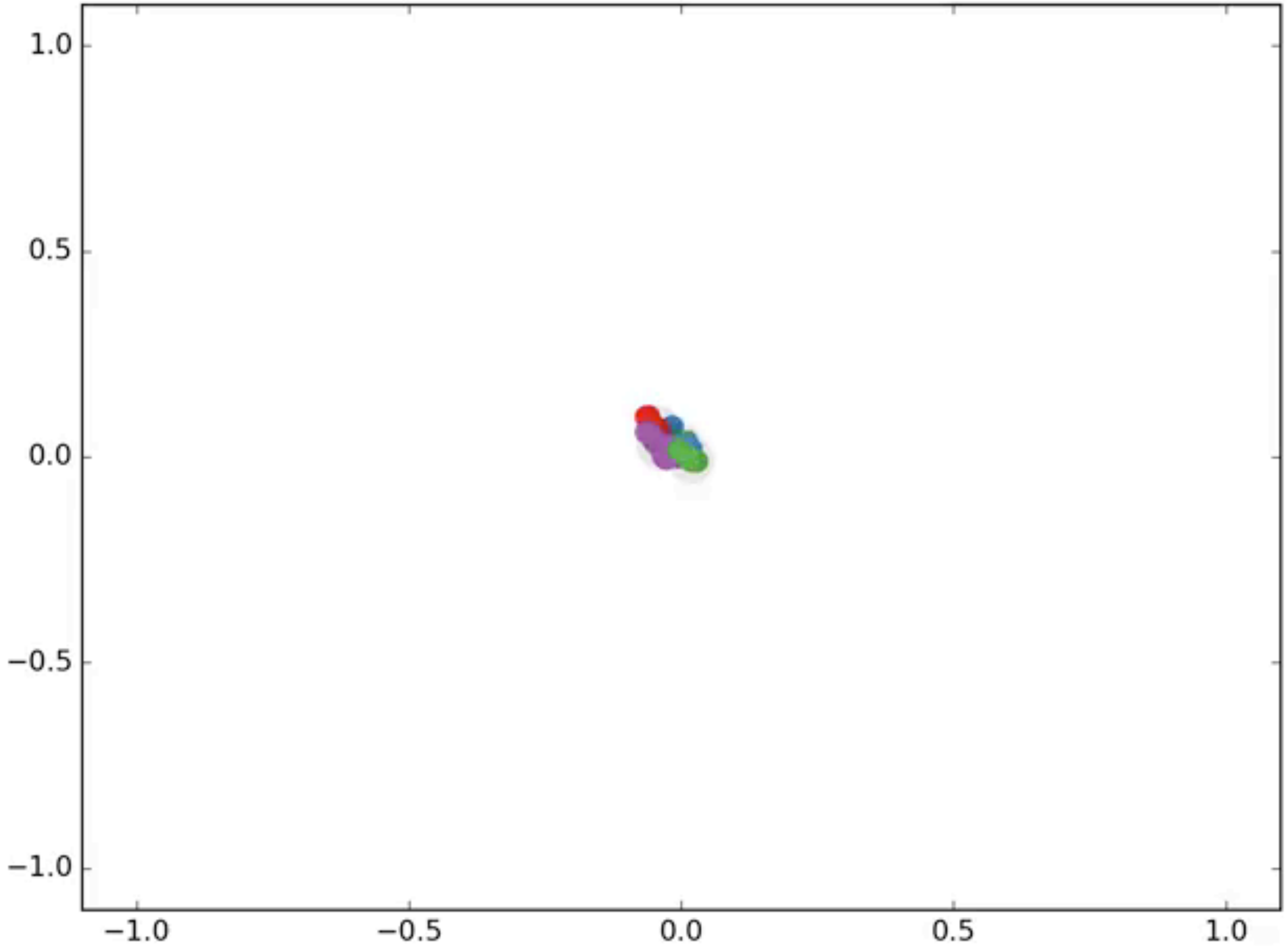
$$\mathcal{L} = -\sum_{l \in \mathcal{Y}_L} \sum_{f=1}^{F} Y_{lf} \ln Z_{lf}$$

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

$\mathbf{Y}$ label matrix

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

Semi-supervised Classification on Graphs



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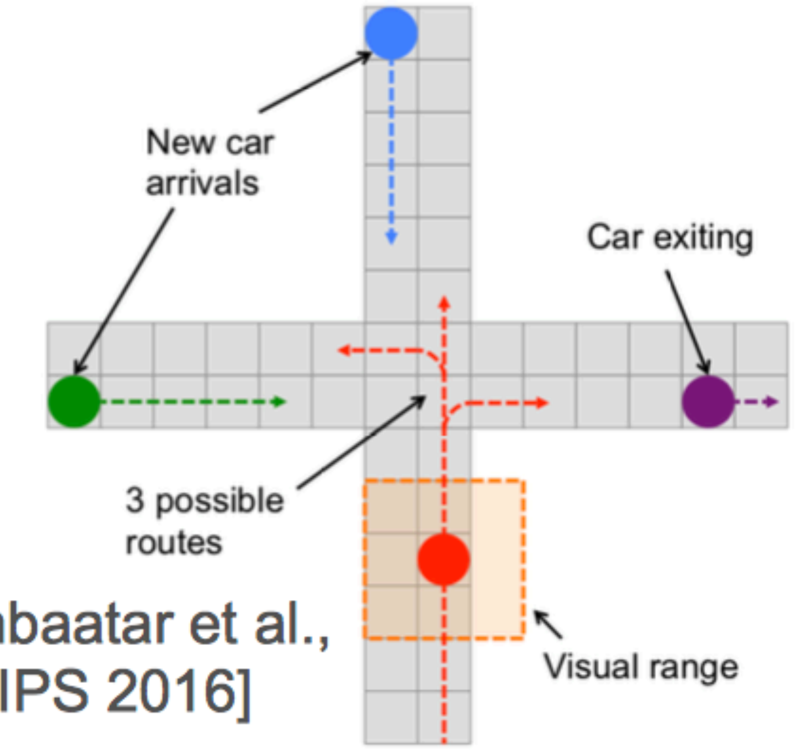
Conclusions

- **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 <u>billion</u> 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)

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Graph Neural Nets (GNNs) are strict Generalizations of Traditional Neural Nets

(CNNs / RNNs can be implemented using GNNs / GCNs, but this is inefficient)