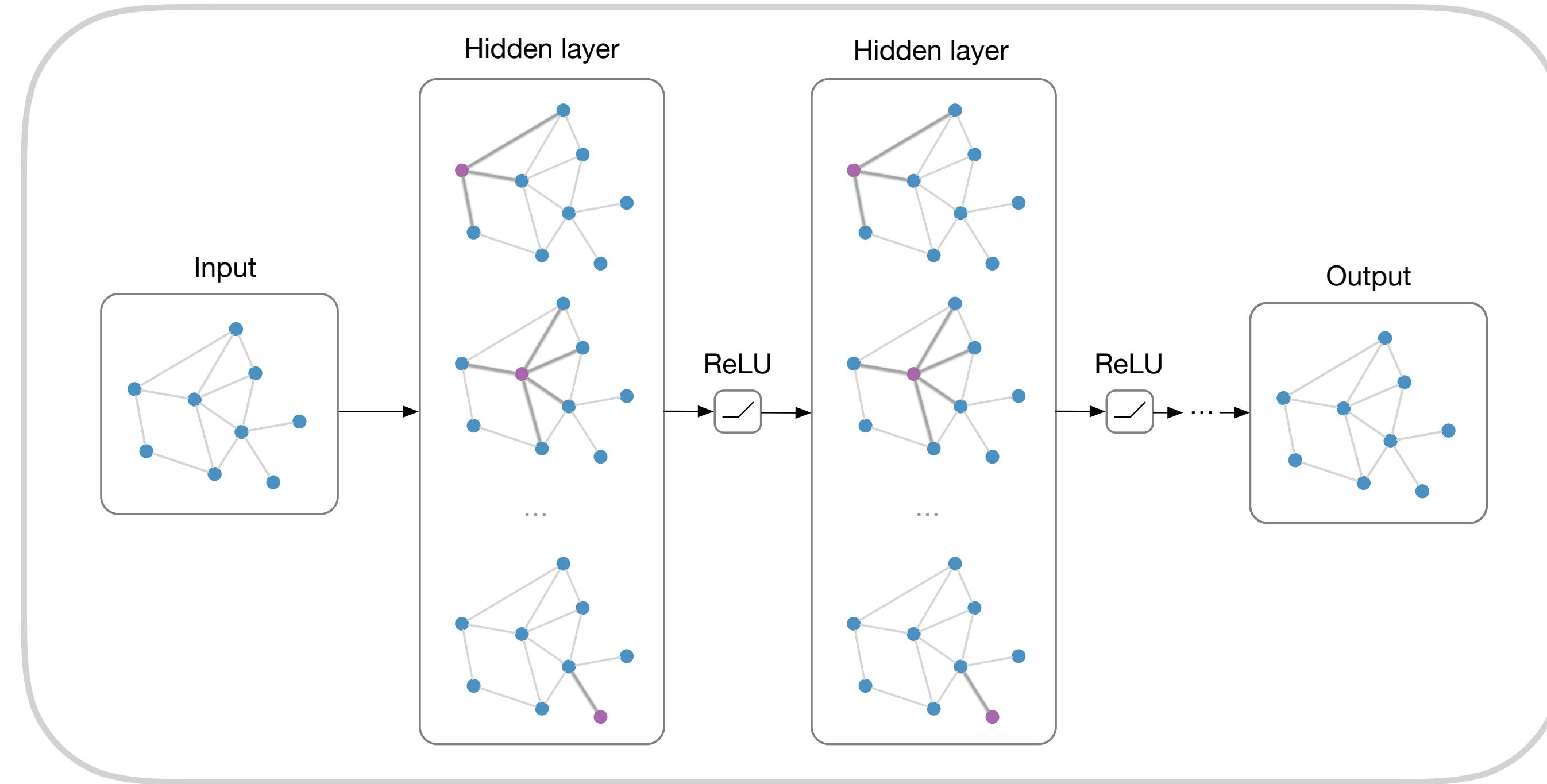


Structured deep models: Deep learning on graphs and beyond



Thomas Kipf, 25 May 2018

CompBio Seminar, University of Cambridge

The Deep Learning slide

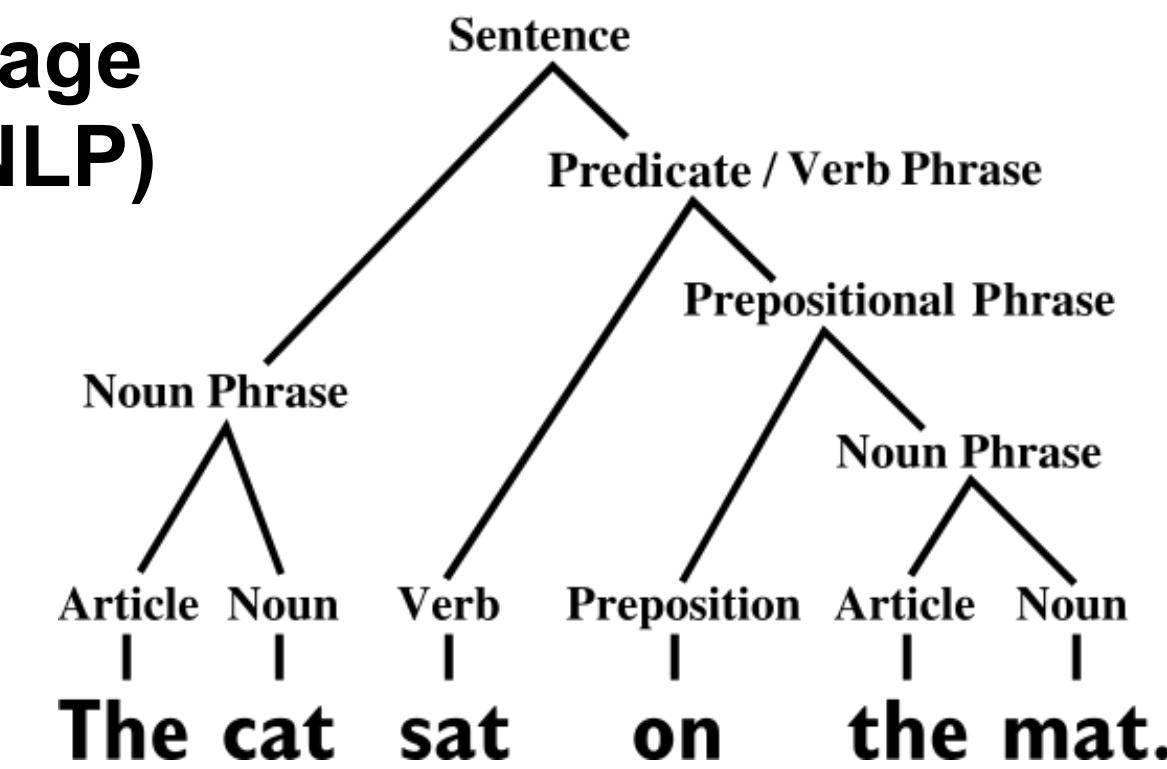


Speech data

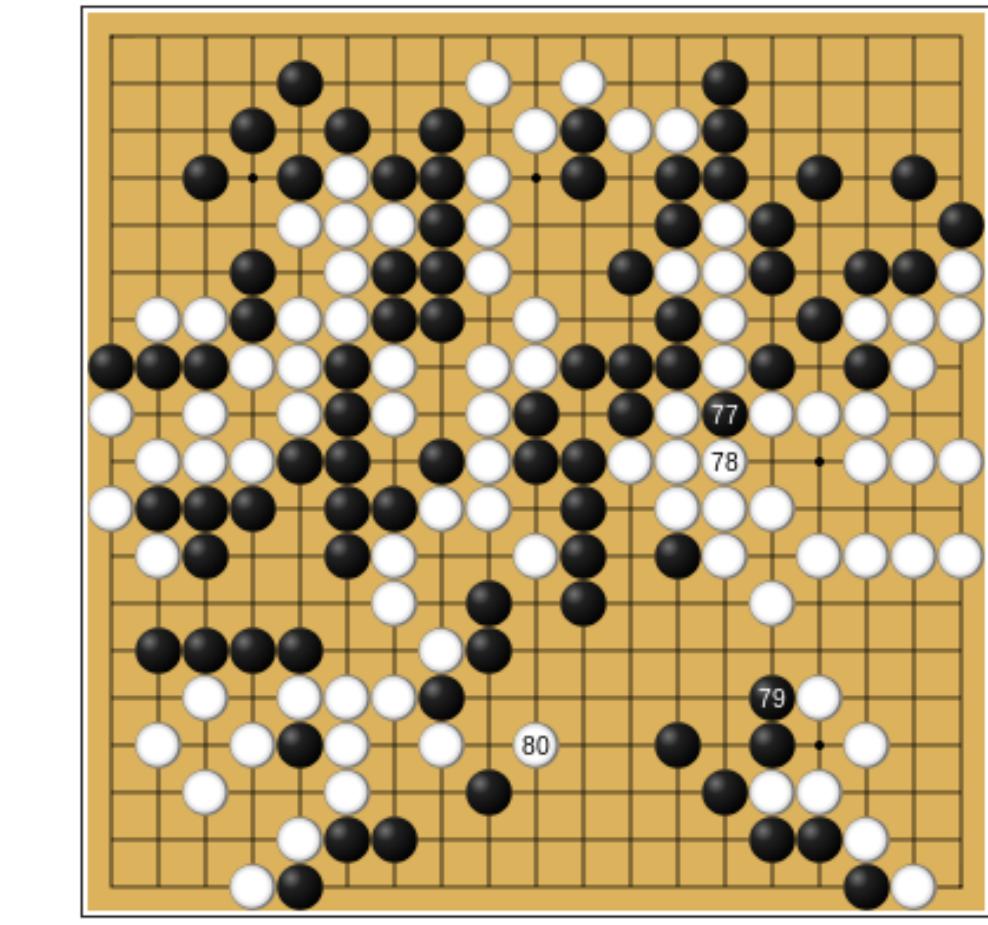


Natural language processing (NLP)

...



Grid games



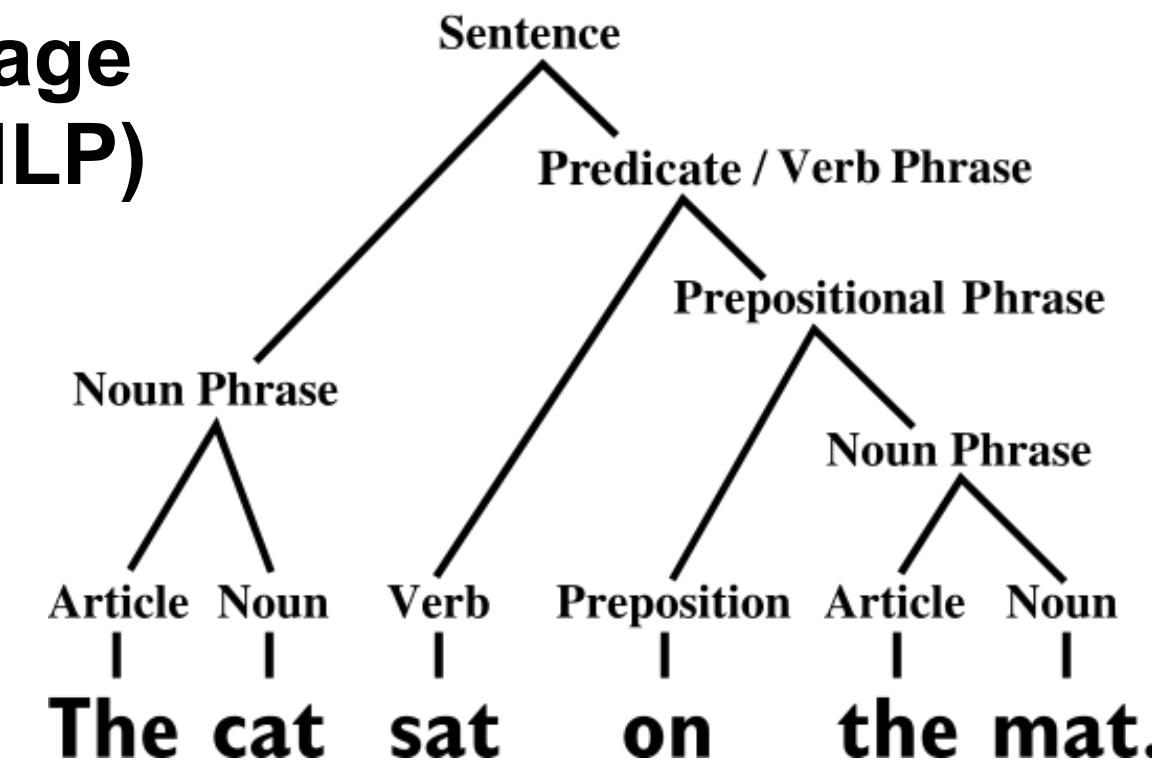
The Deep Learning slide



Speech data

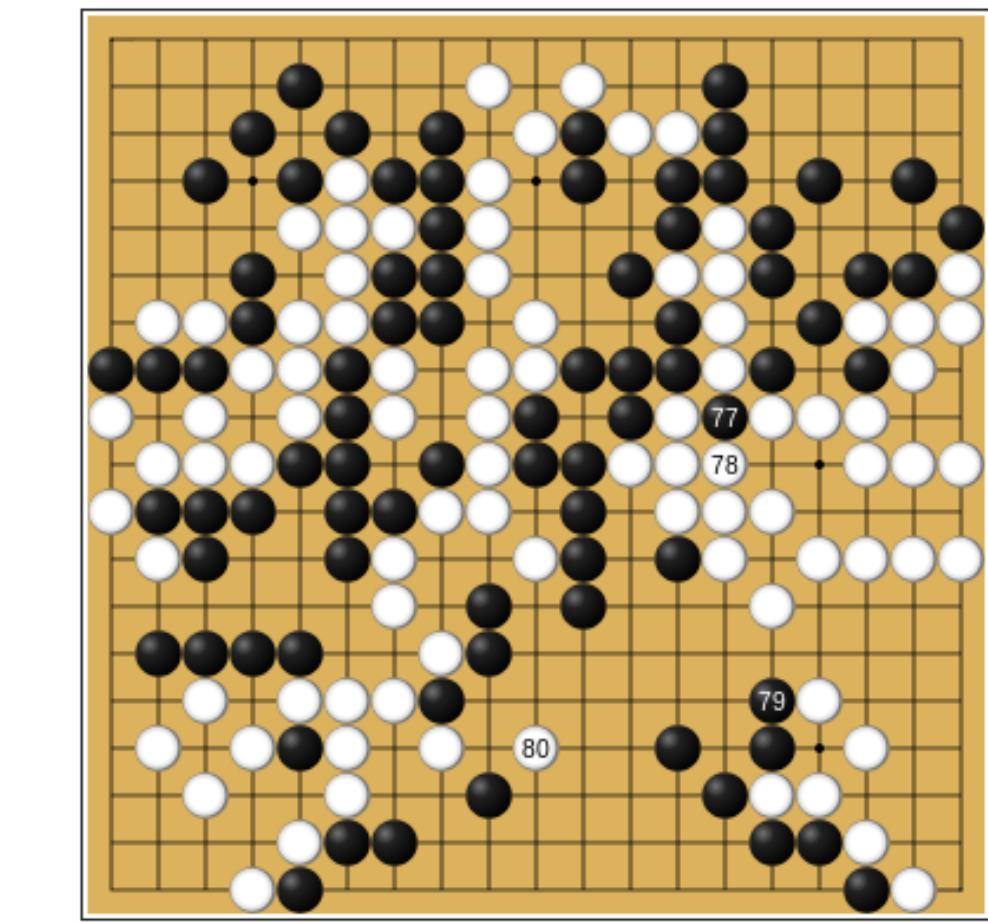


Natural language processing (NLP)



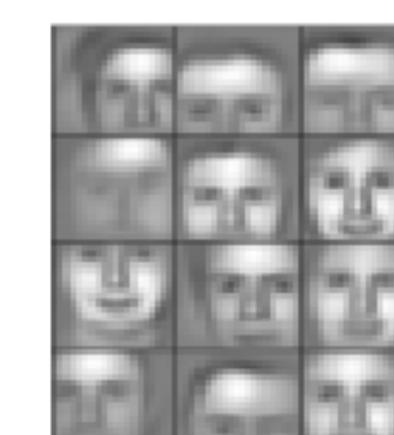
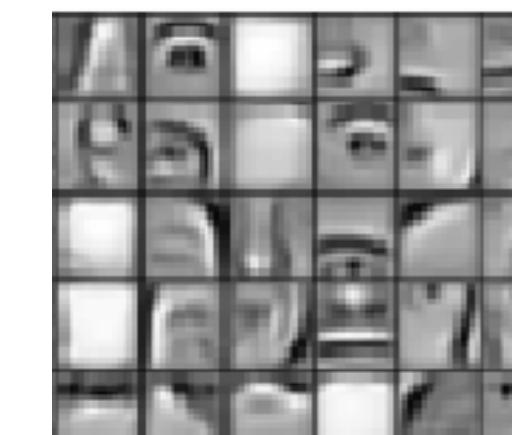
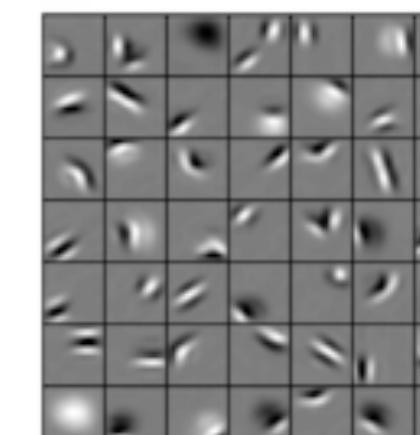
...

Grid games



Deep neural nets that exploit:

- translation equivariance (weight sharing)
- hierarchical compositionality



Graph-structured data

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

Graph-structured data

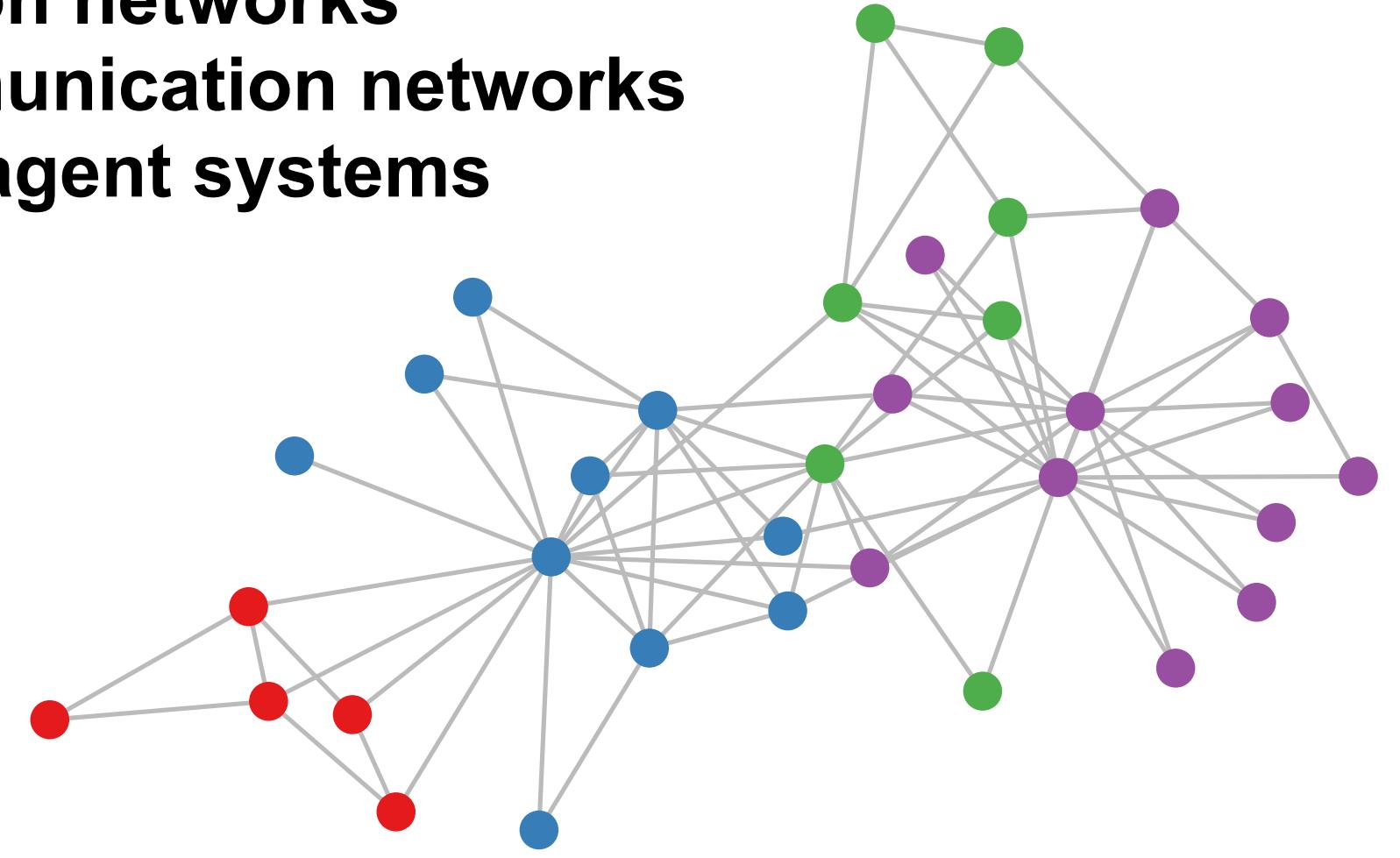
A lot of real-world data does not “live” on grids

Social networks

Citation networks

Communication networks

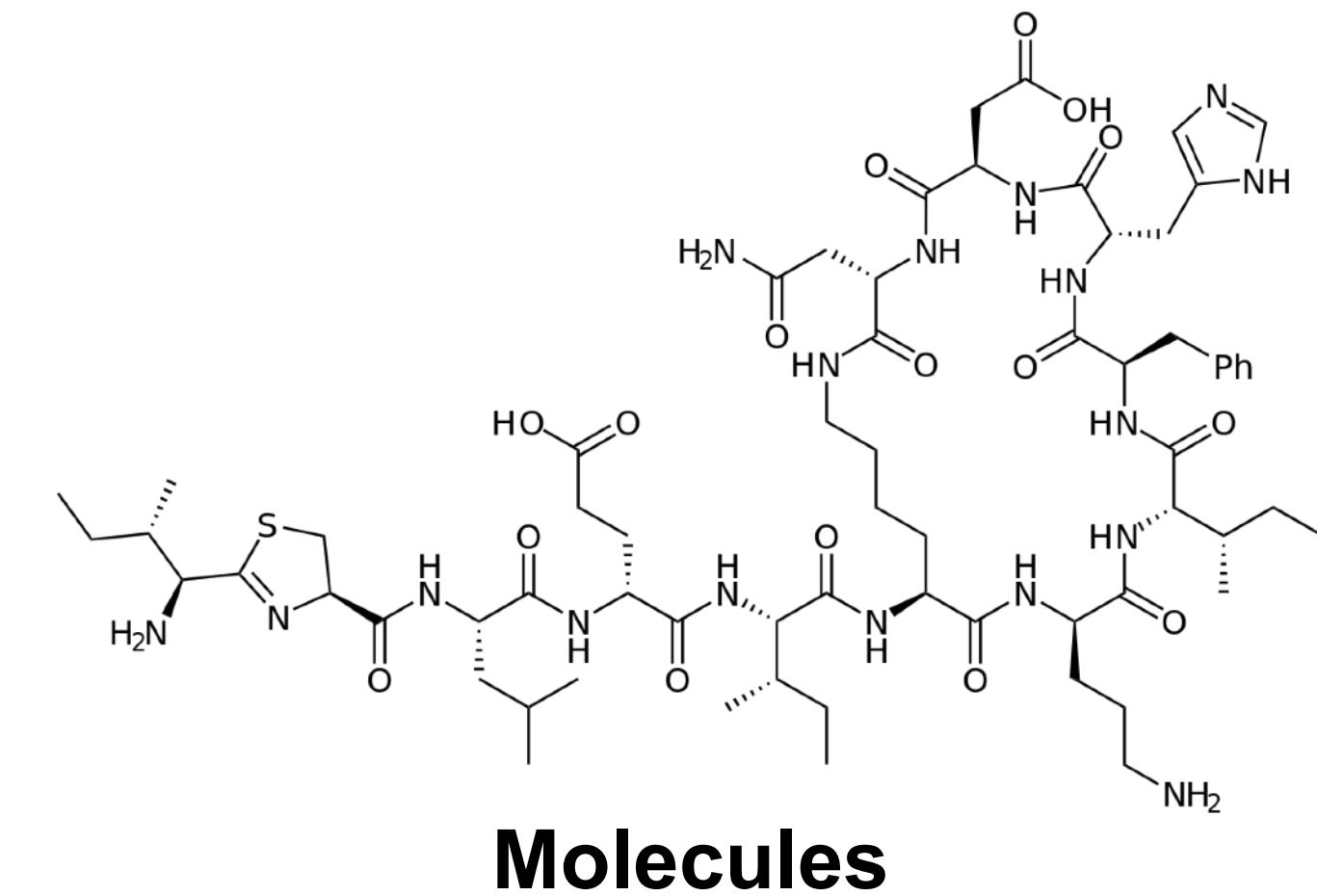
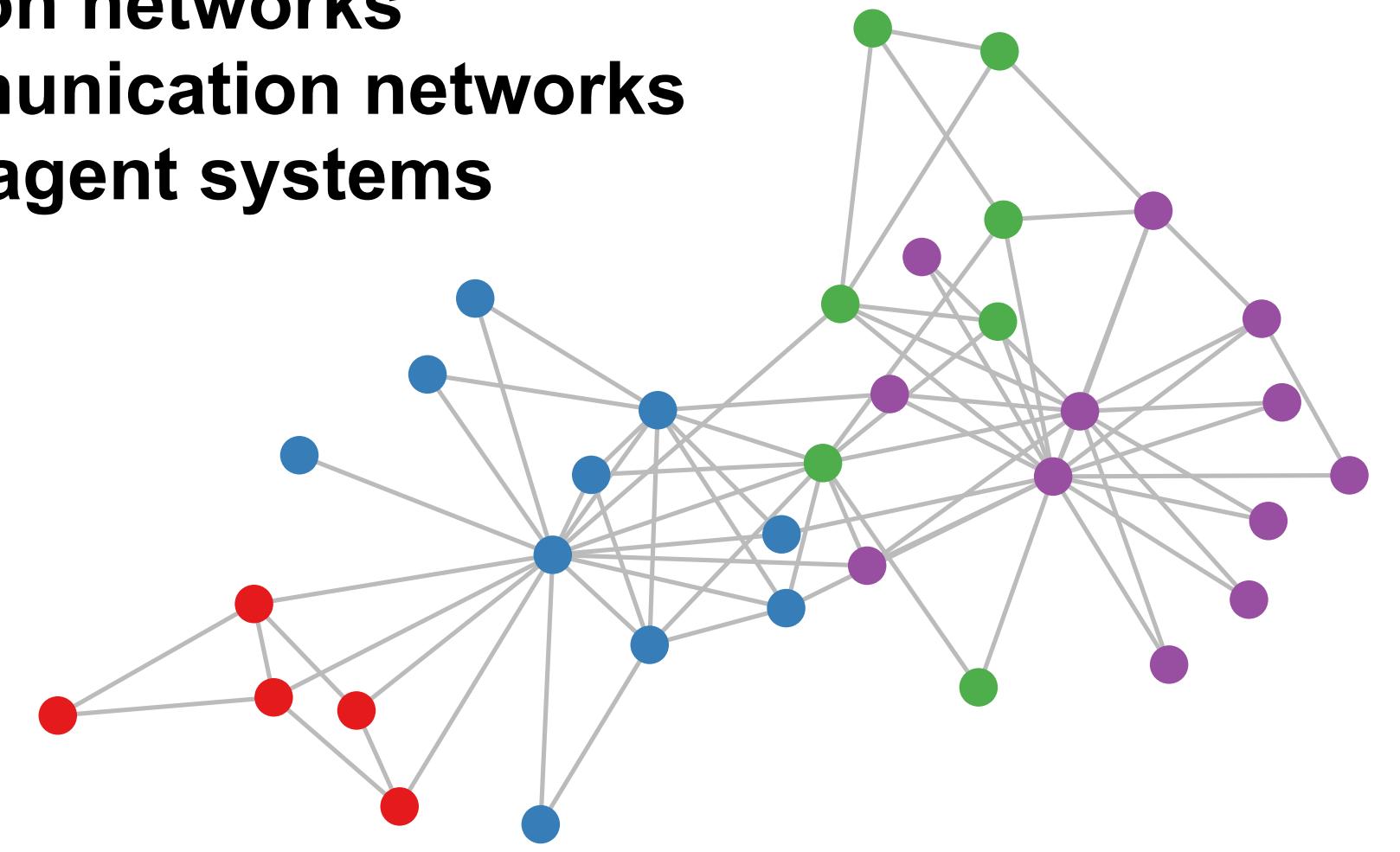
Multi-agent systems



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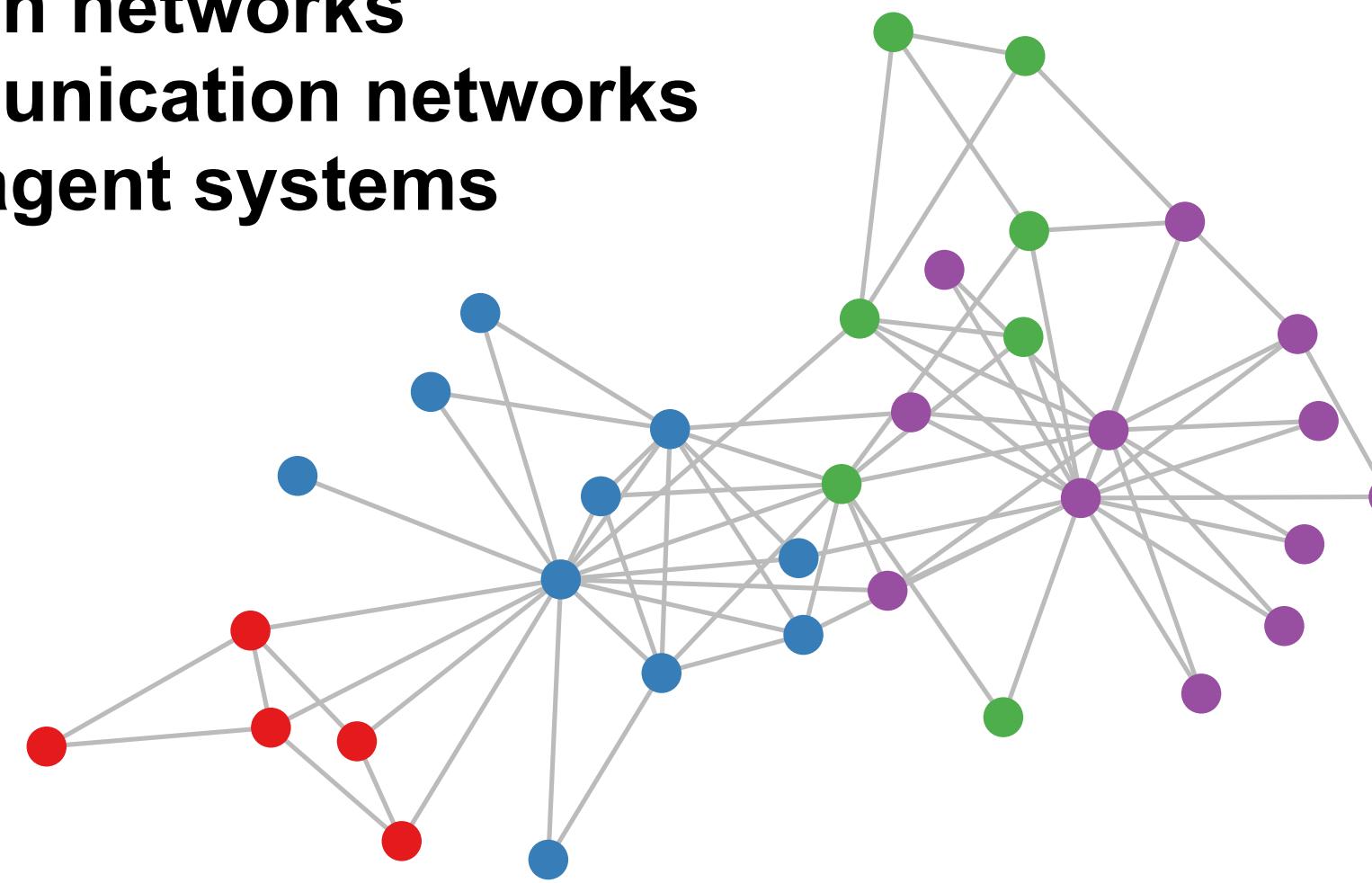
Social networks
Citation networks
Communication networks
Multi-agent systems



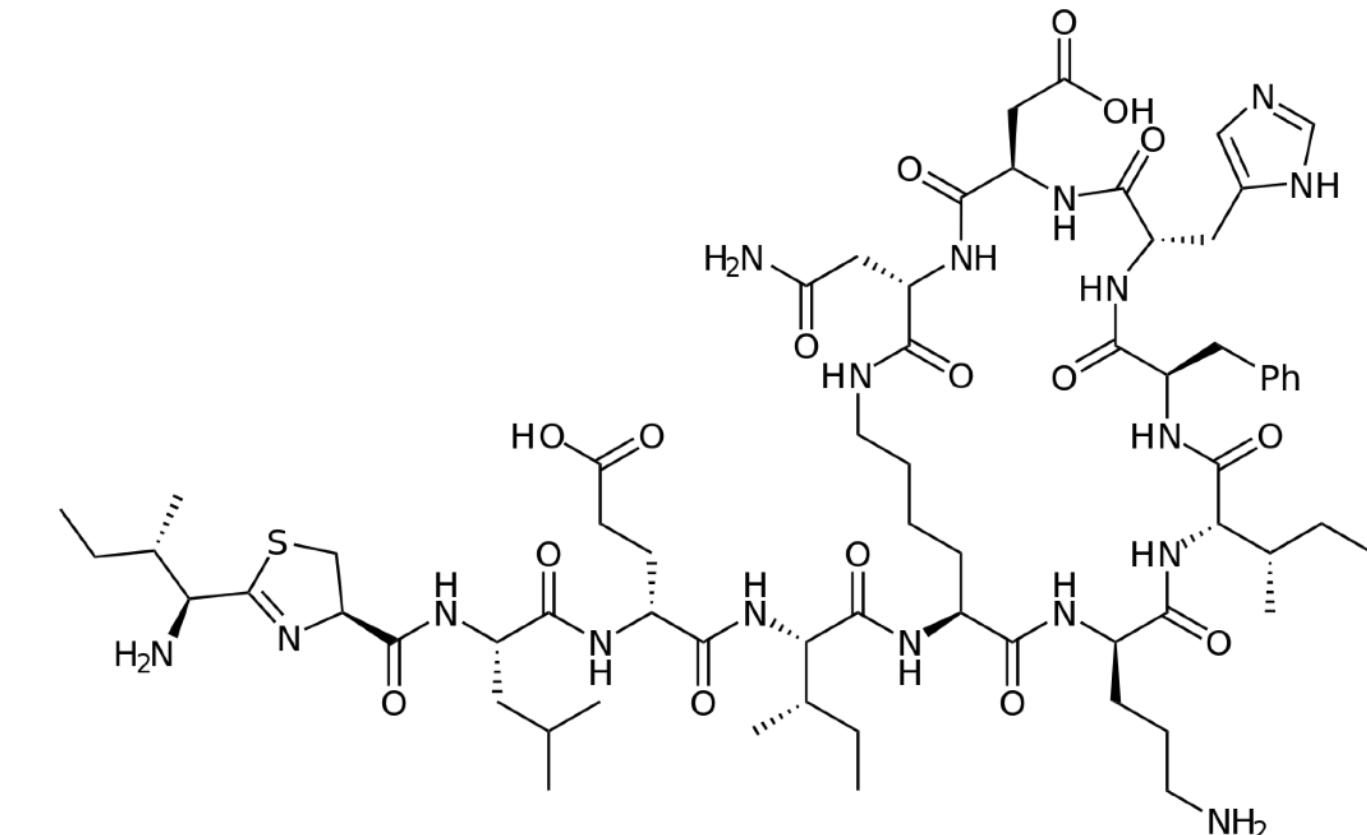
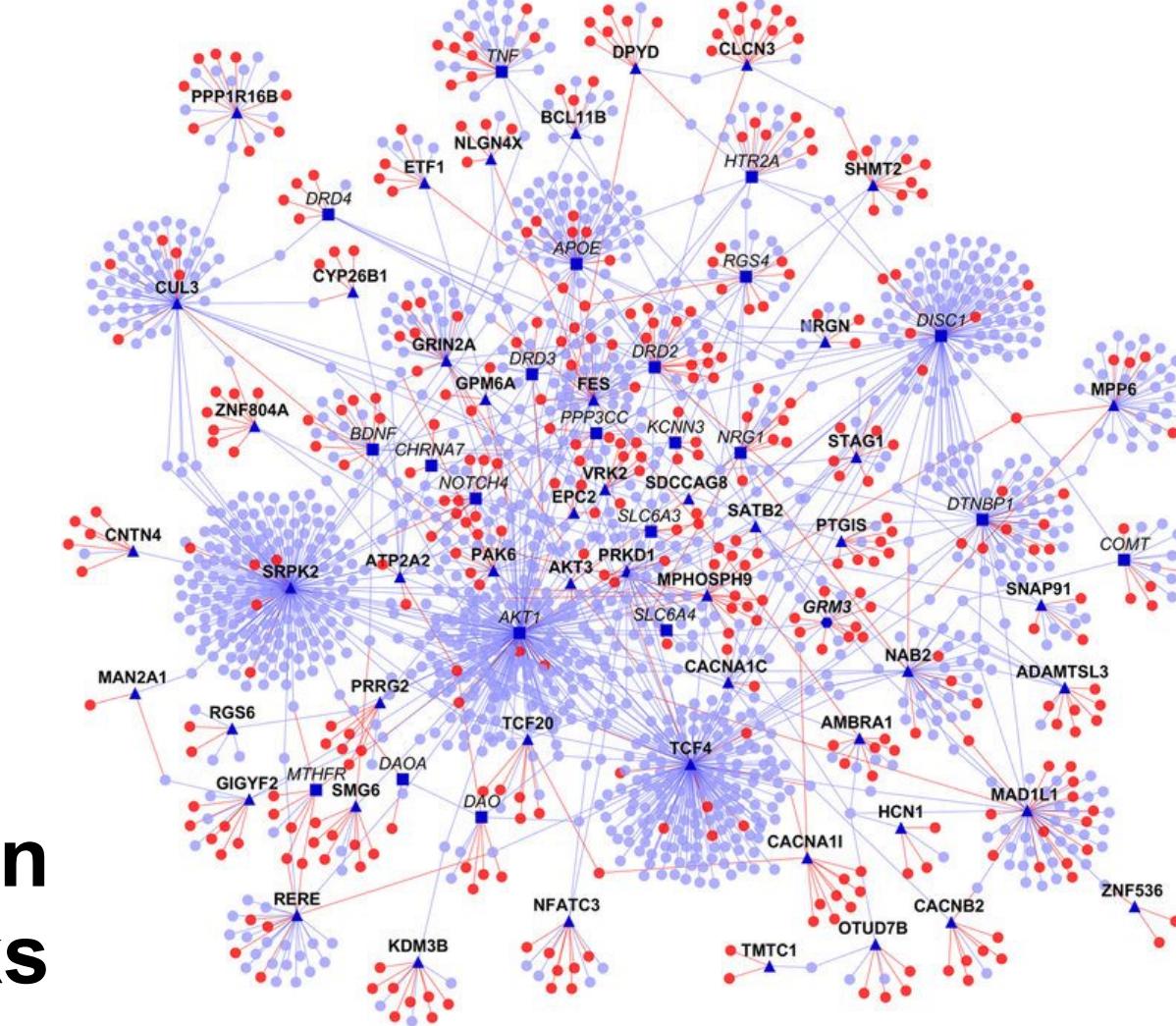
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A lot of real-world data does not “live” on grids

Social networks
Citation networks
Communication networks
Multi-agent systems



Protein interaction networks

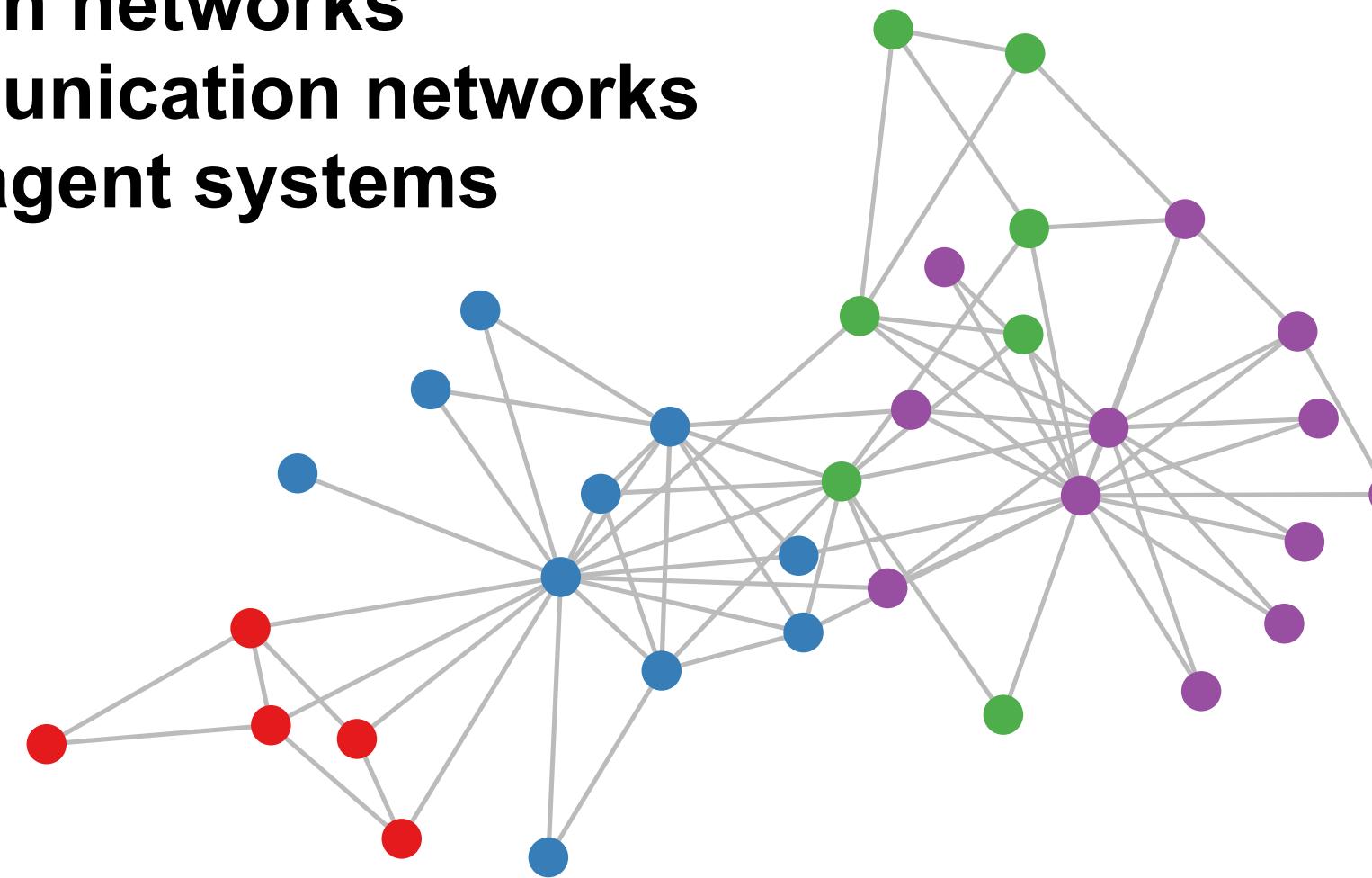


Molecules

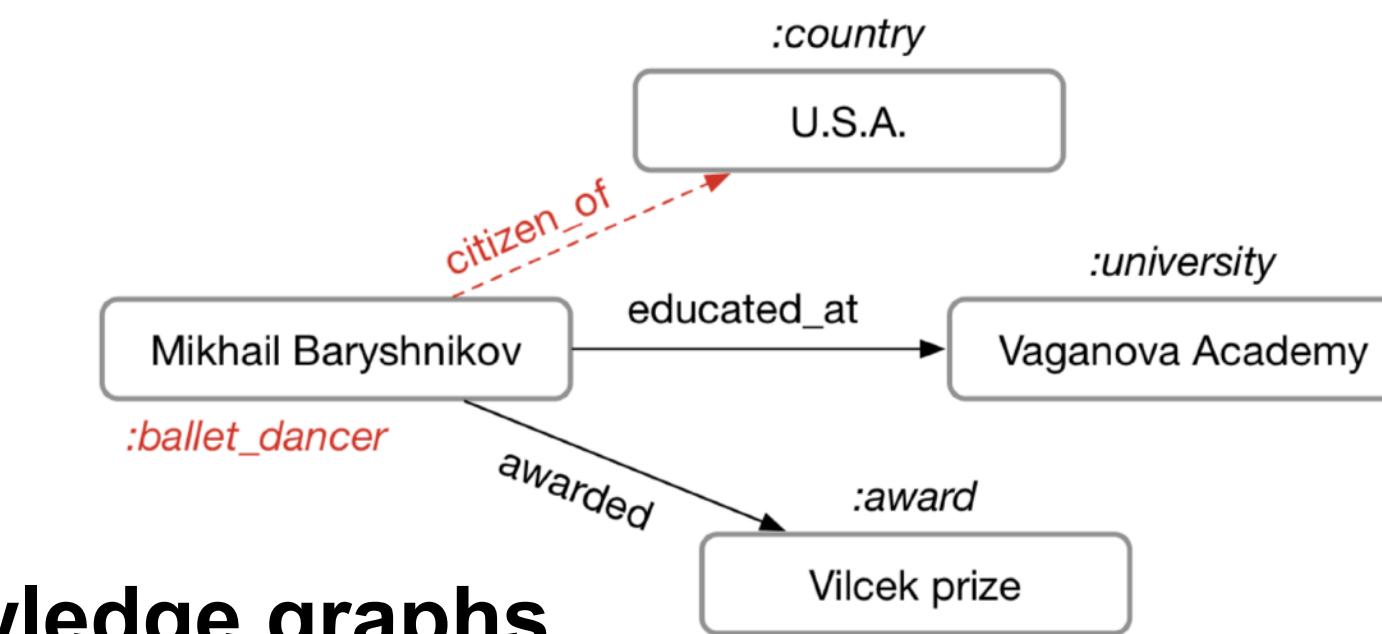
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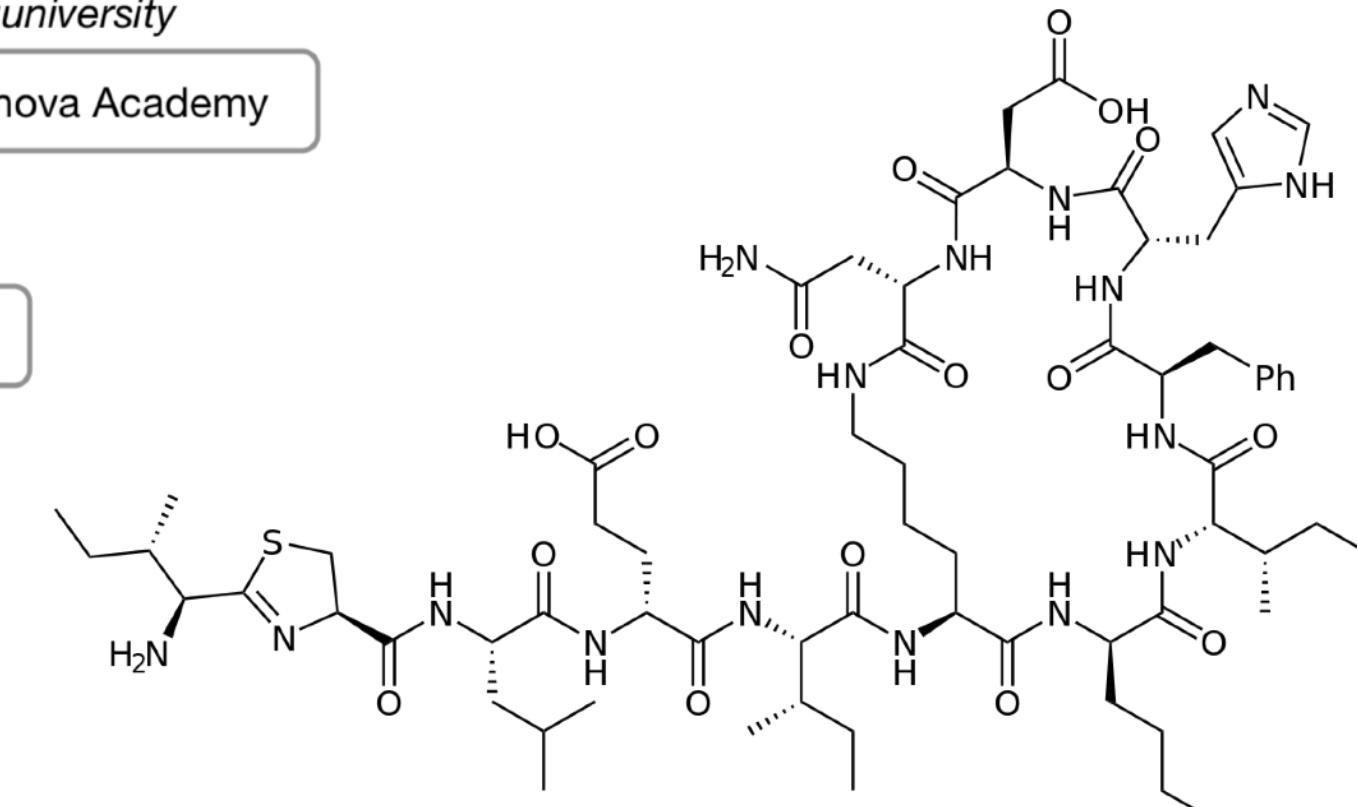
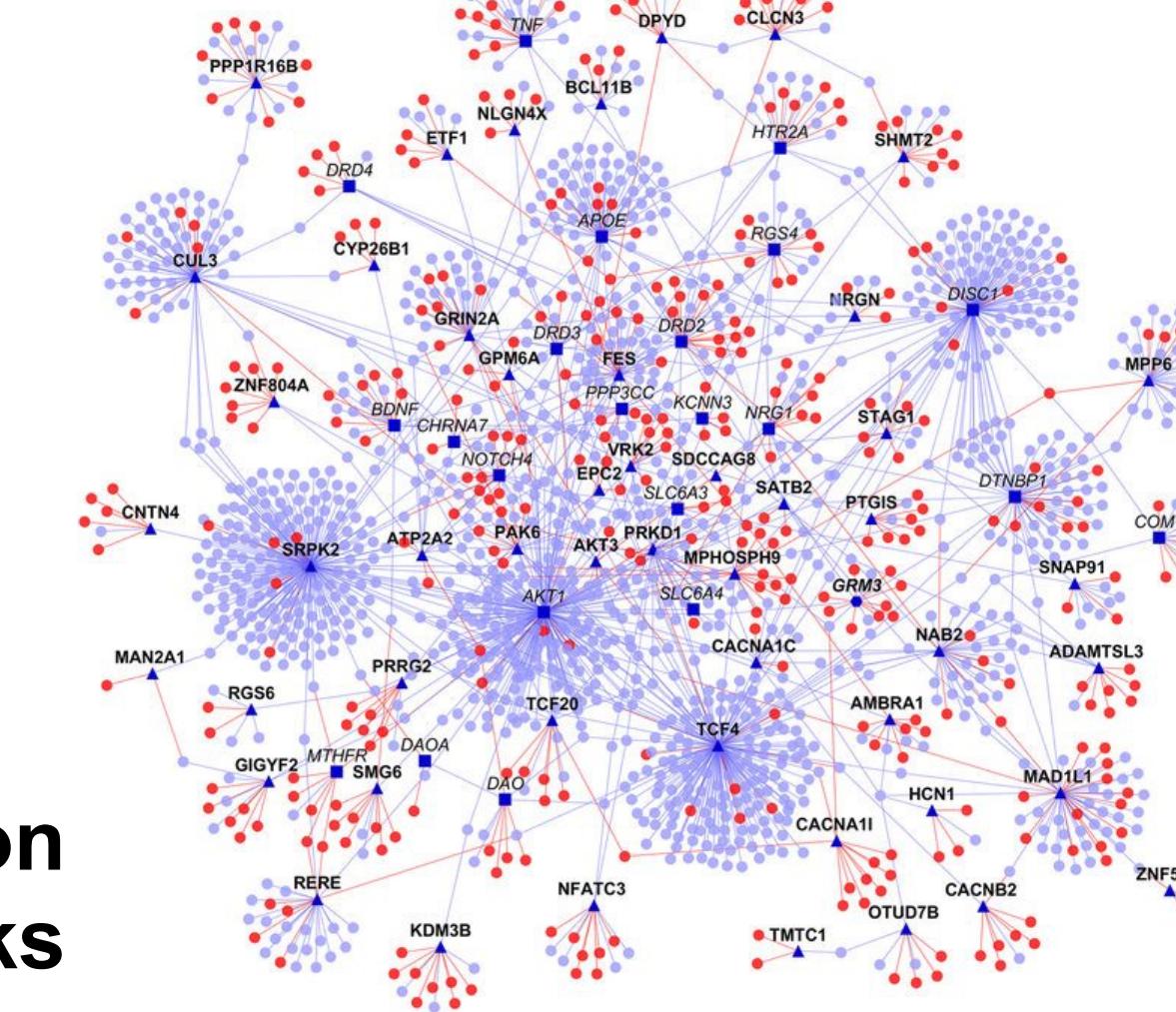
Social networks
Citation networks
Communication networks
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Protein interaction networks



Knowledge graph

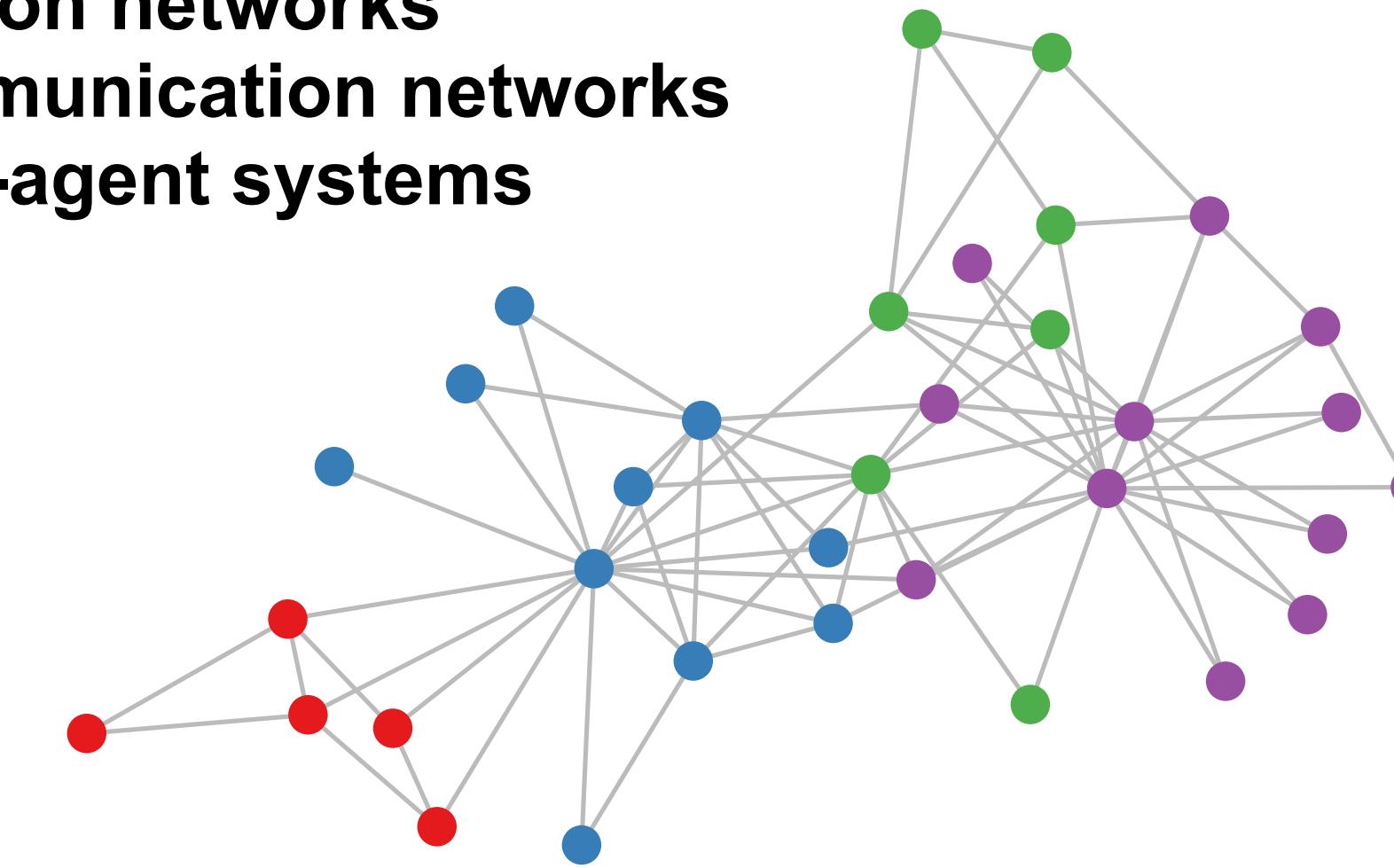


Molecules

Graph-structured data

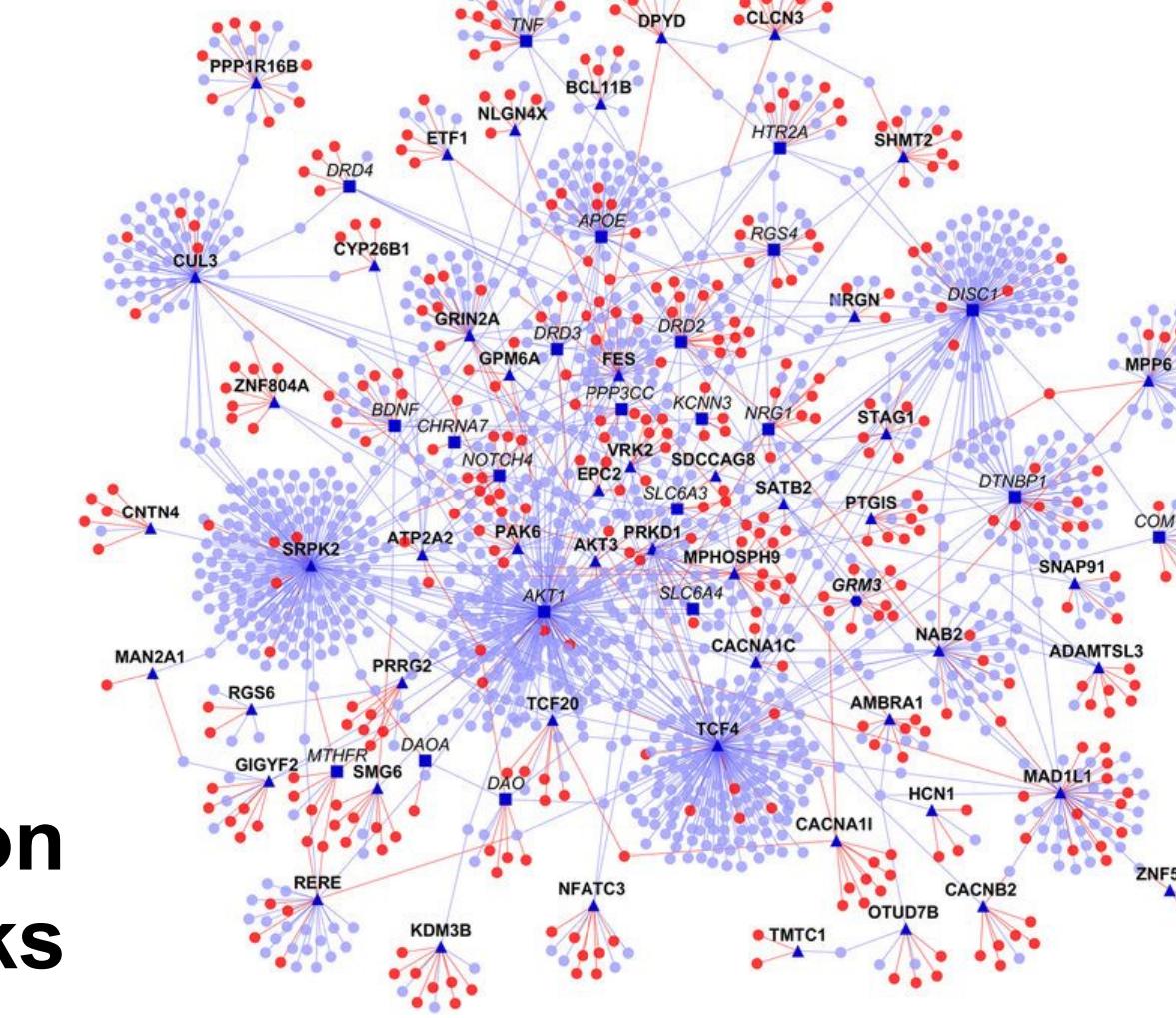
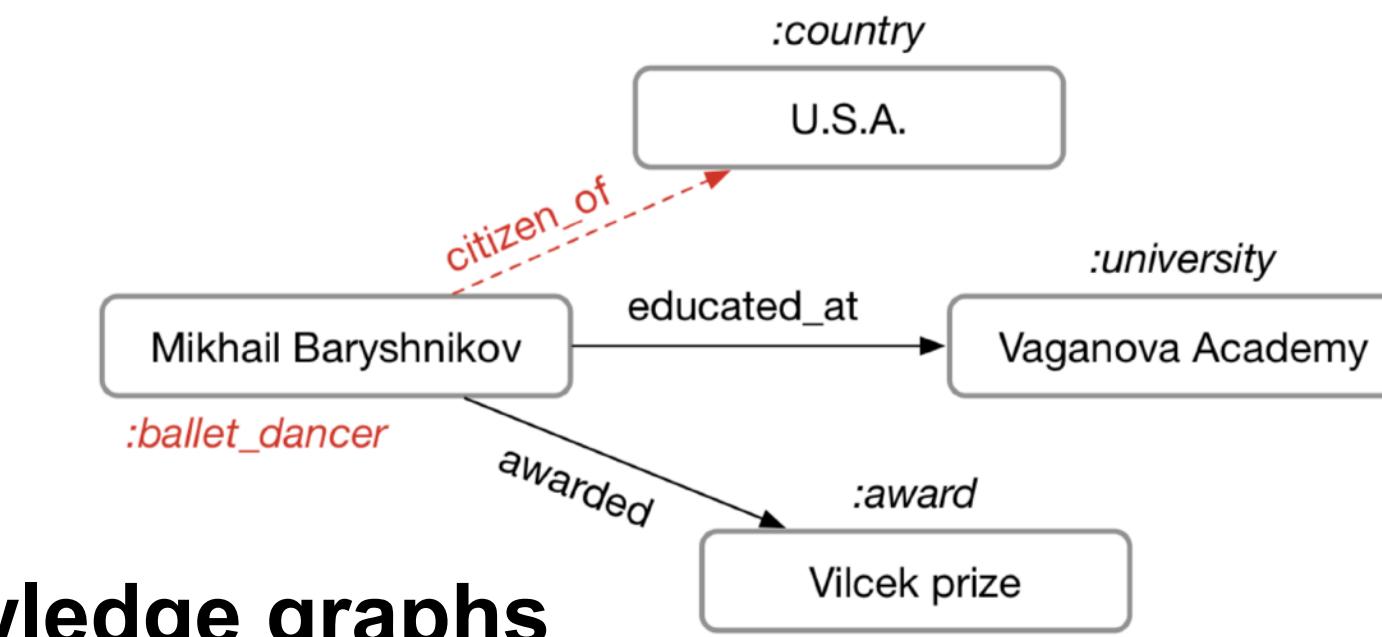
A lot of real-world data does not “live” on grids

Social networks
Citation networks
Communication networks
Multi-agent systems

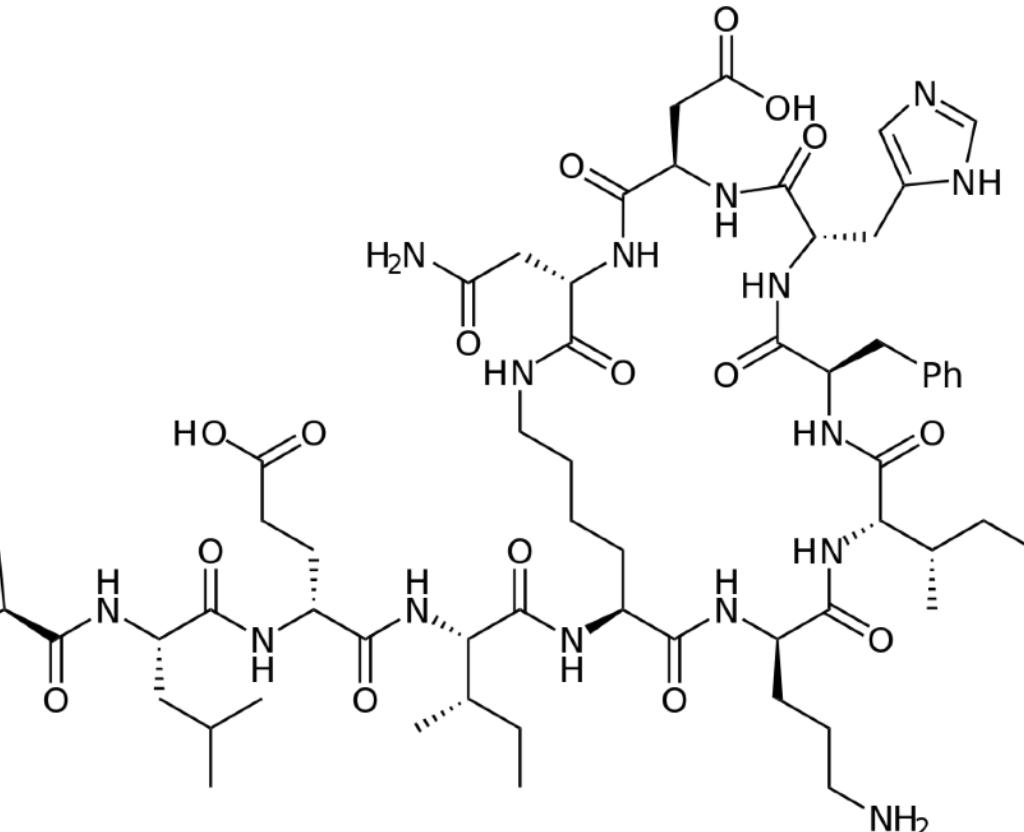
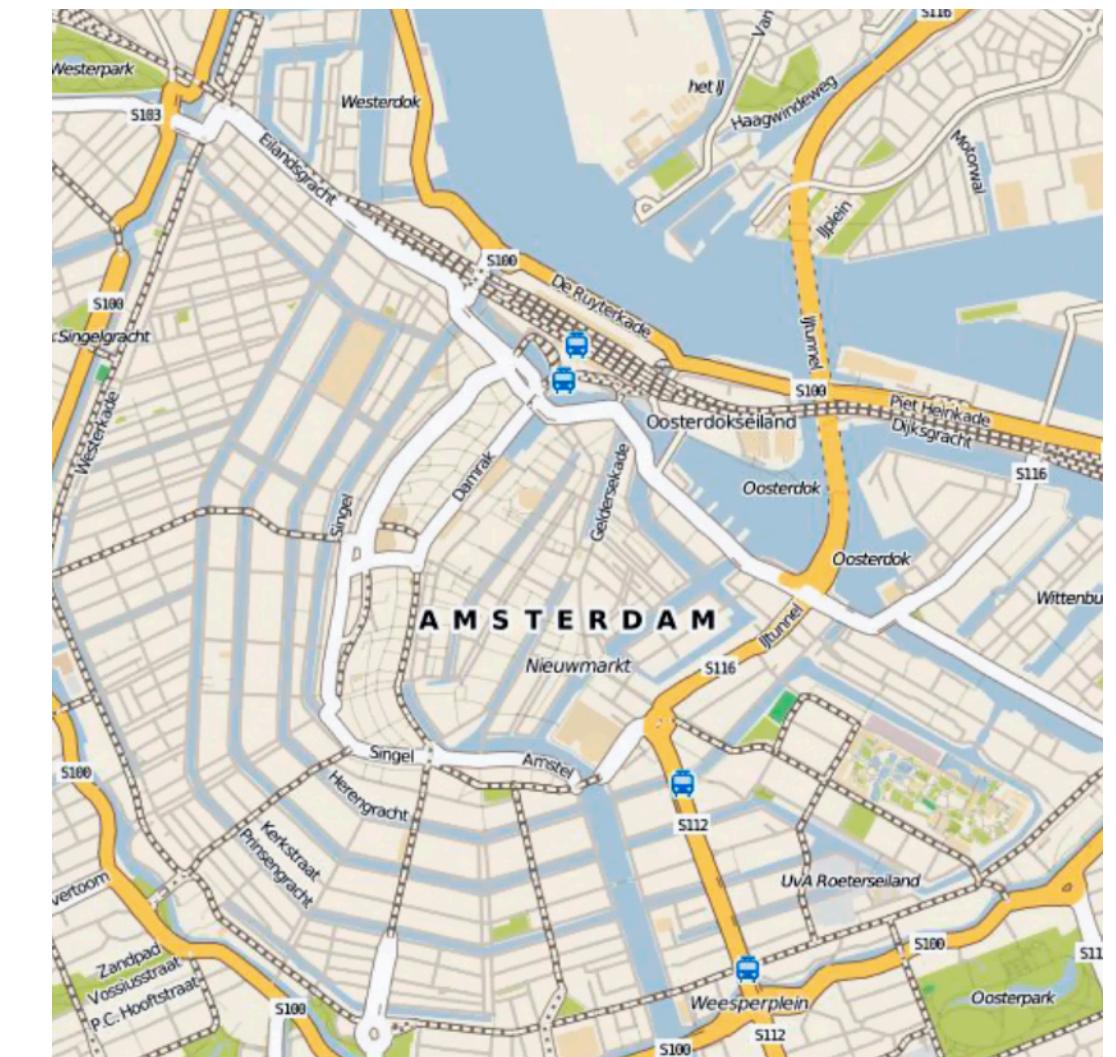


Protein interaction networks

Knowledge graphs



Road maps

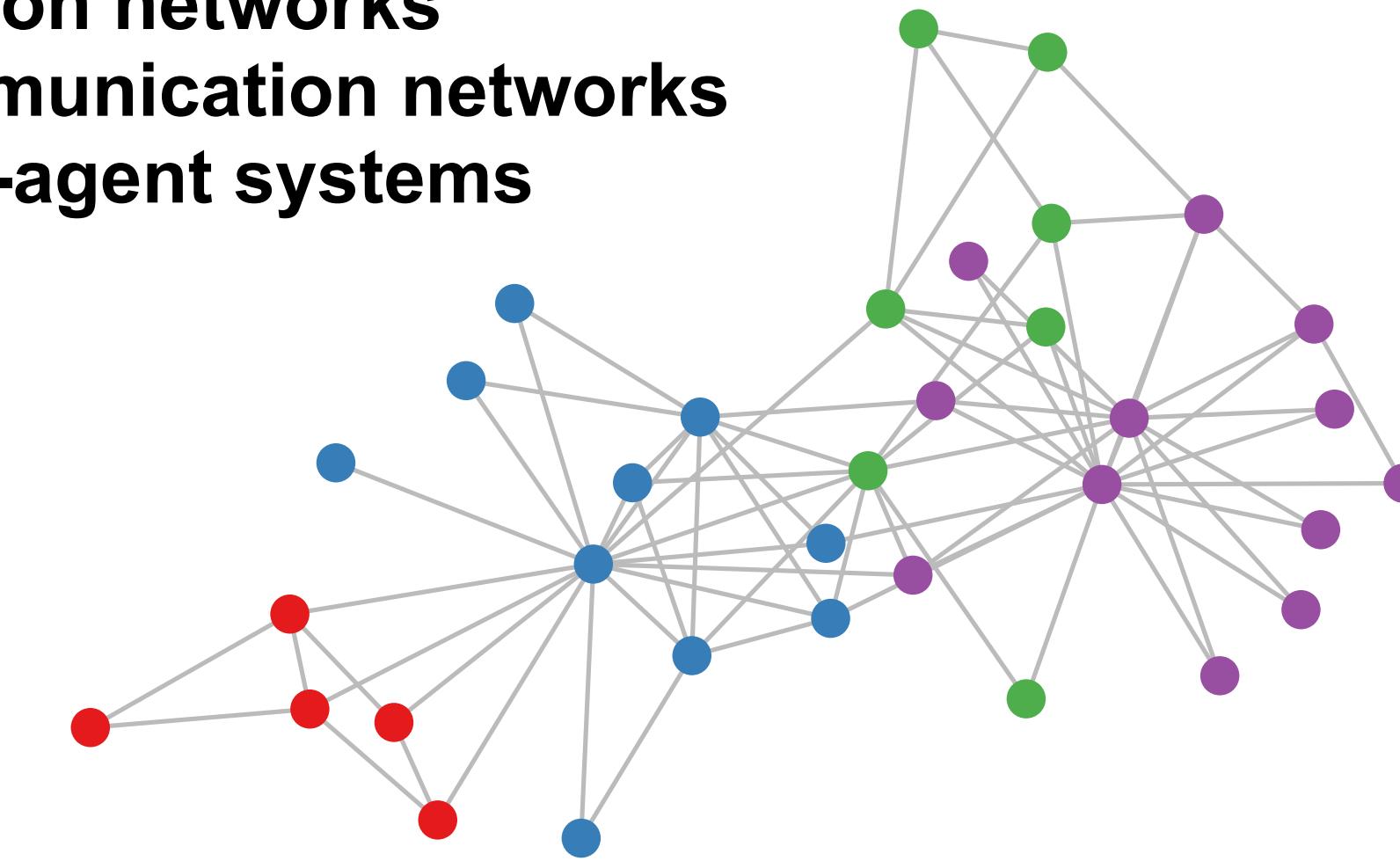


Molecules

Graph-structured data

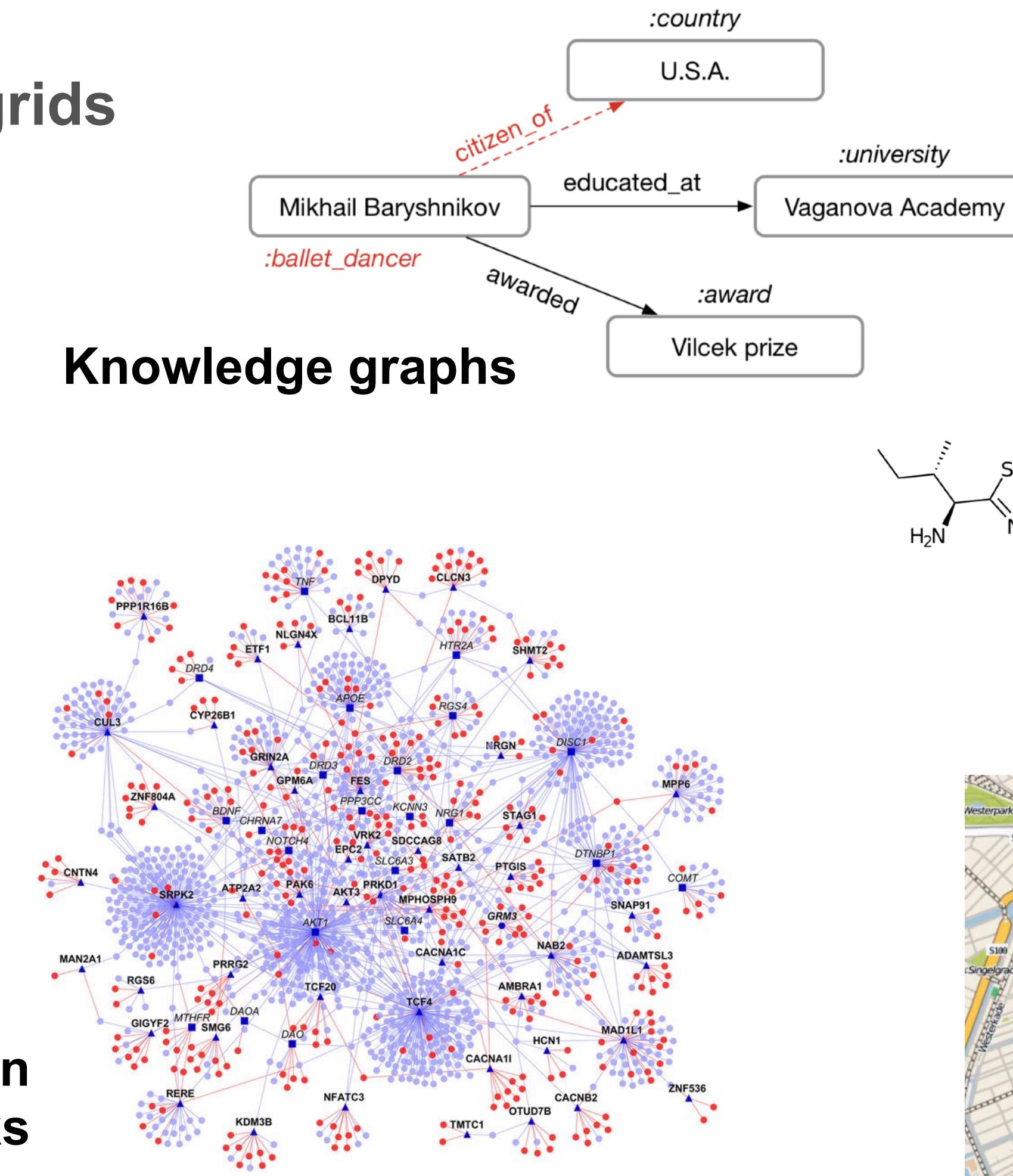
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Social networks
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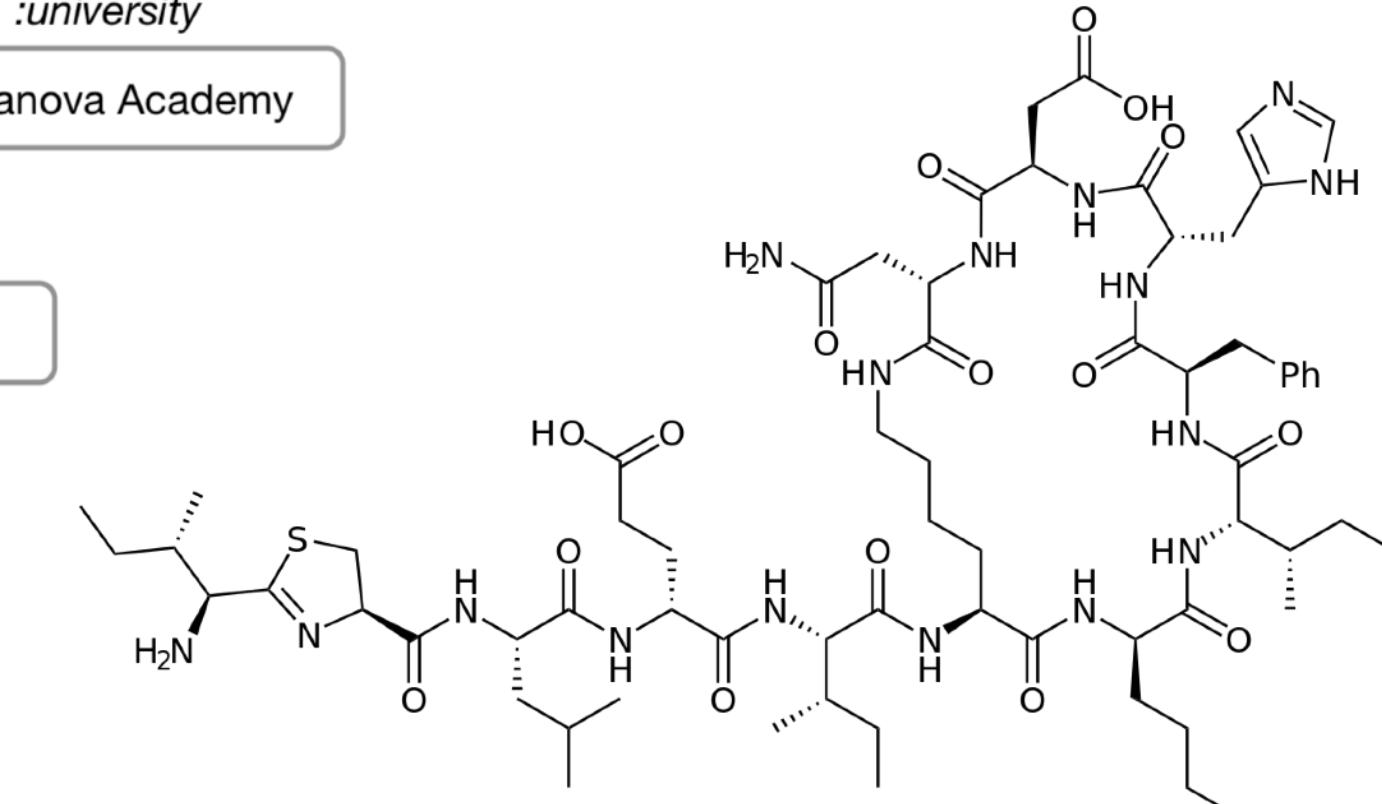


Protein interaction networks

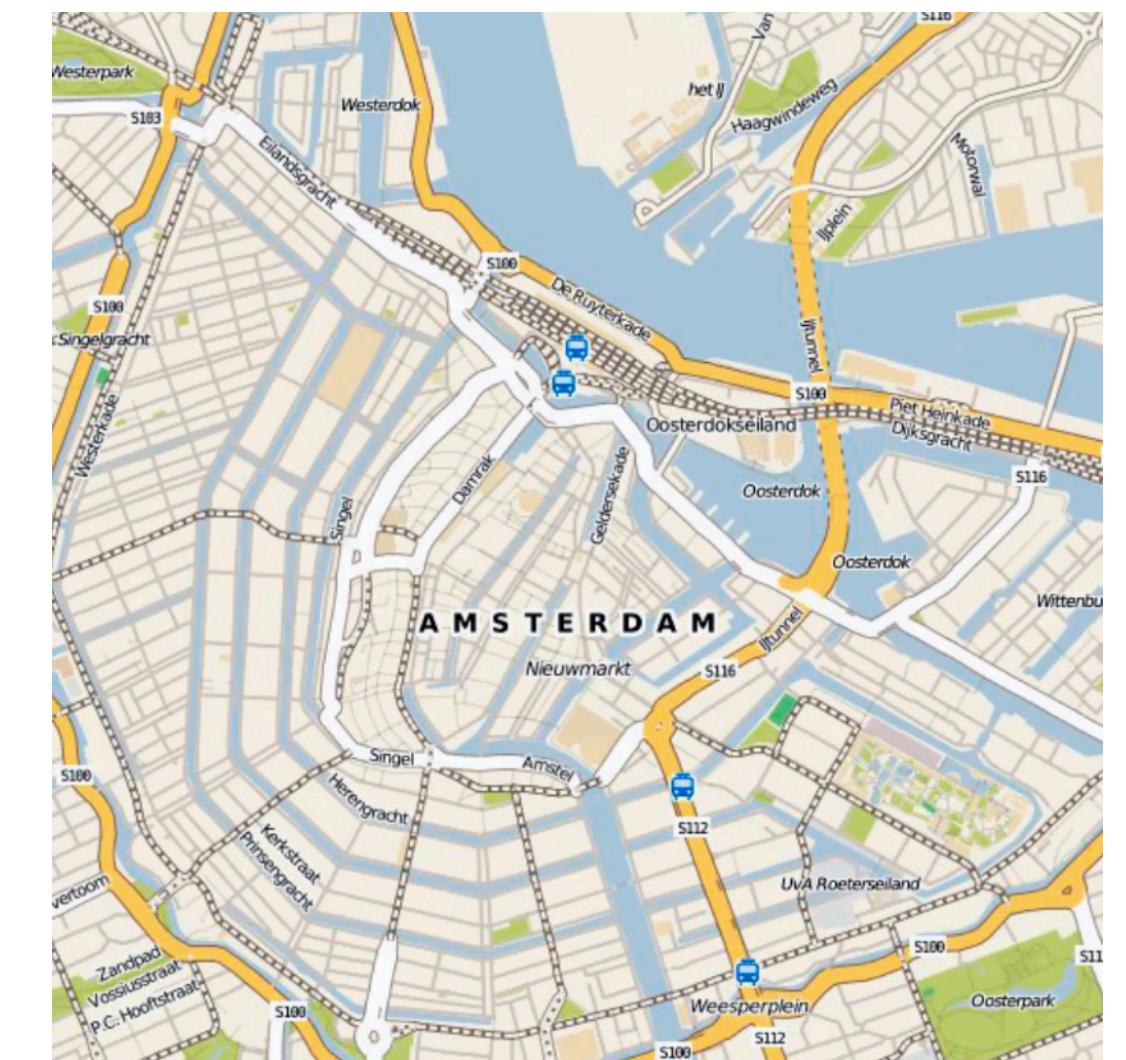
Standard deep learning architectures like CNNs and RNNs don't work here!



Knowledge graph



Molecules



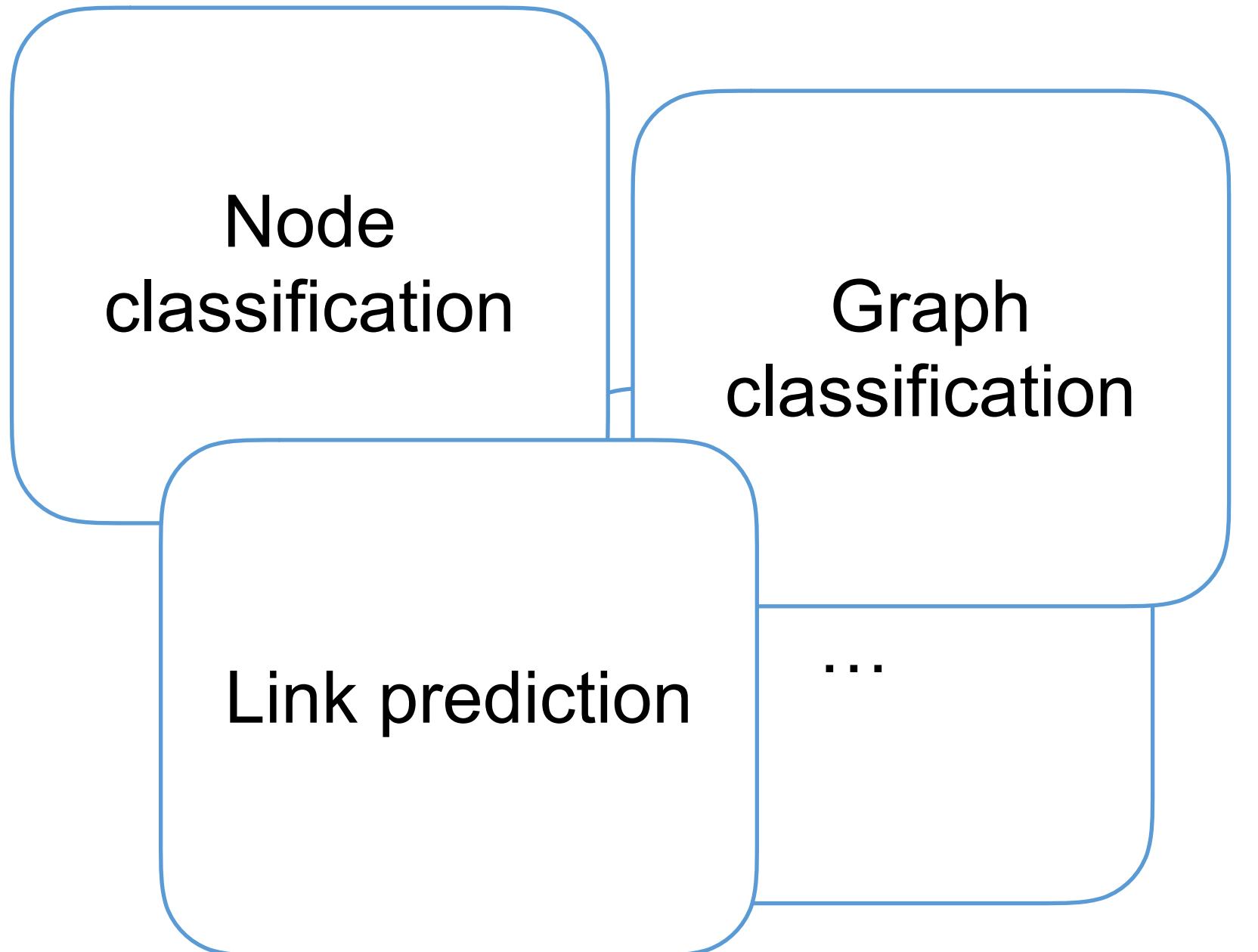
Road maps

Talk overview

1) Graph neural nets (GNNs):

Introduction & some history

2) GNNs for “classical” network problems

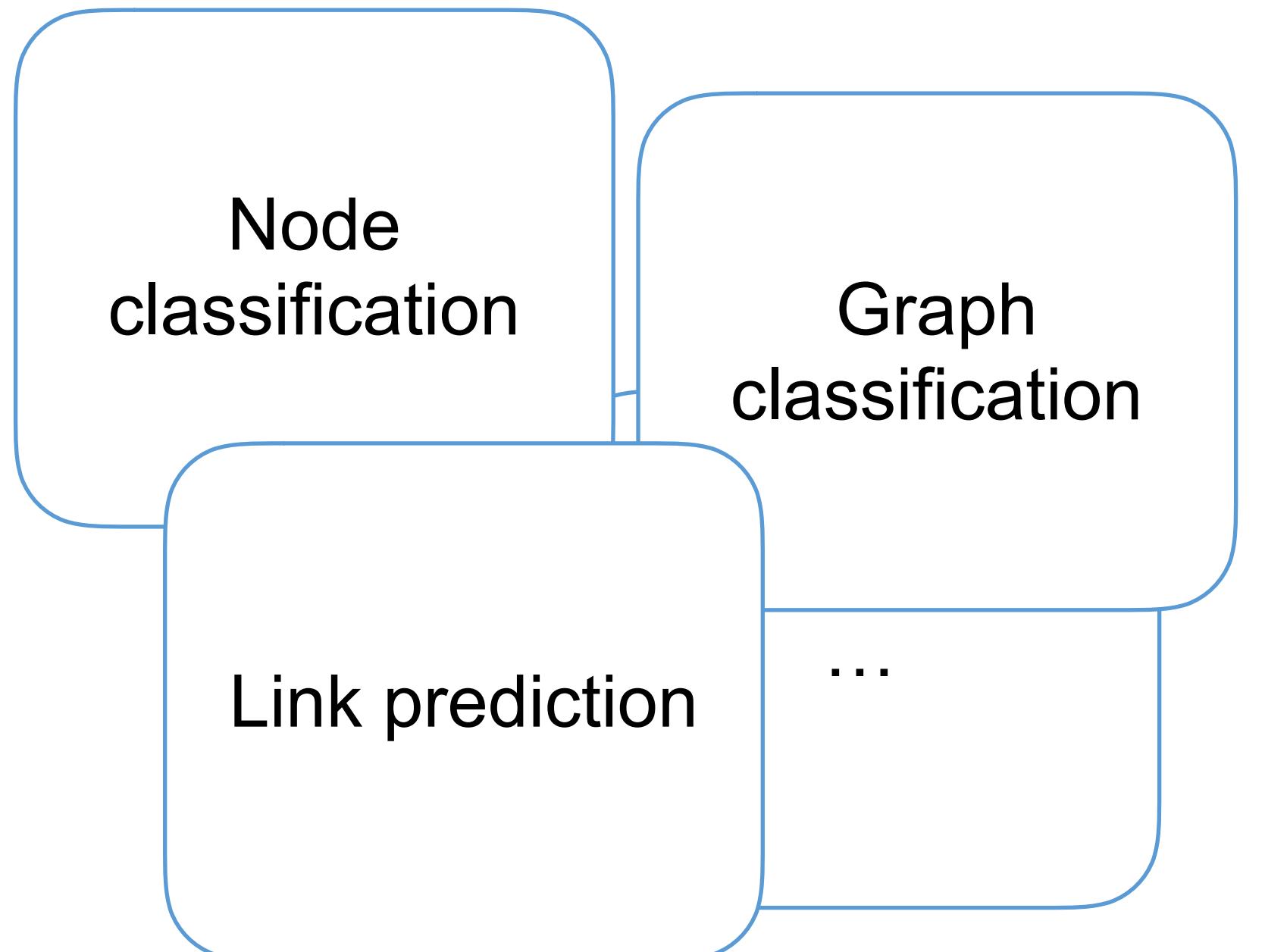


Talk overview

1) Graph neural nets (GNNs):

Introduction & some history

2) GNNs for “classical” network problems



3) Emerging research directions

Latent graph
inference

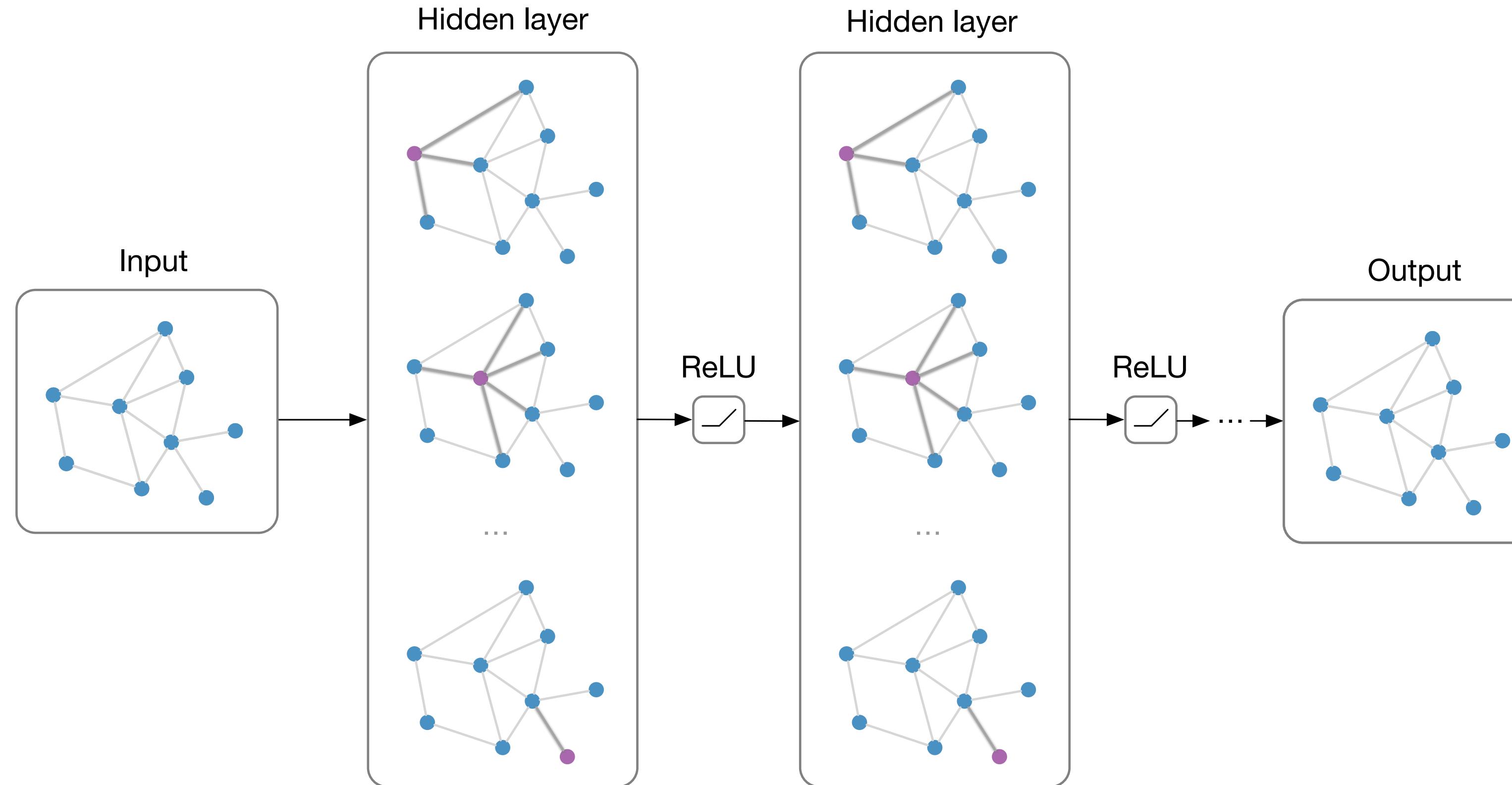
Generative models
of graphs

(Potential) applications:

- Interacting systems
(physics/multi-agent),
- Causal inference
- Program induction,
- Chemical synthesis,

Graph Neural Networks (GNNs)

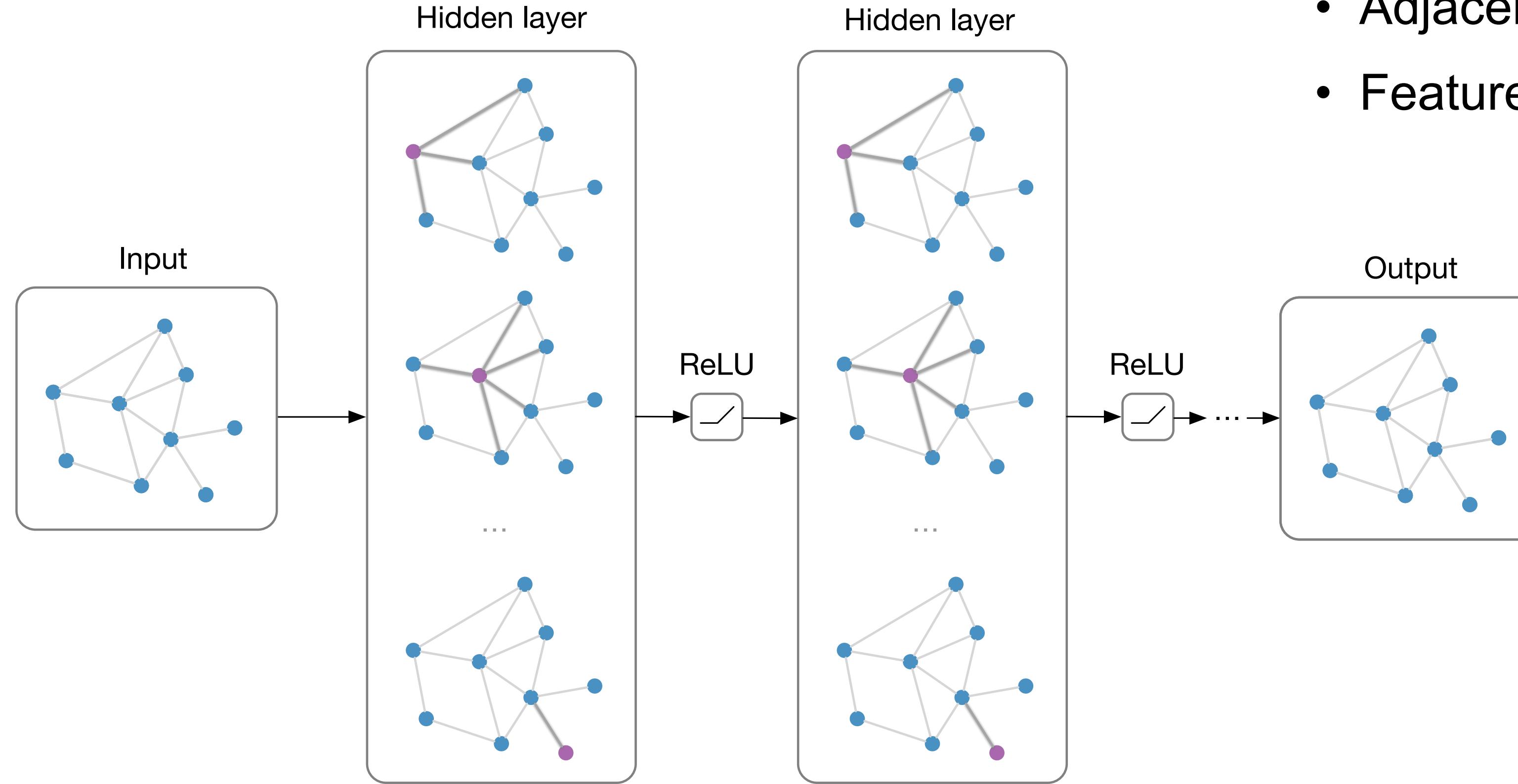
The bigger picture:



Main idea: Pass messages between pairs of nodes & agglomerate

Graph Neural Networks (GNNs)

The bigger picture:



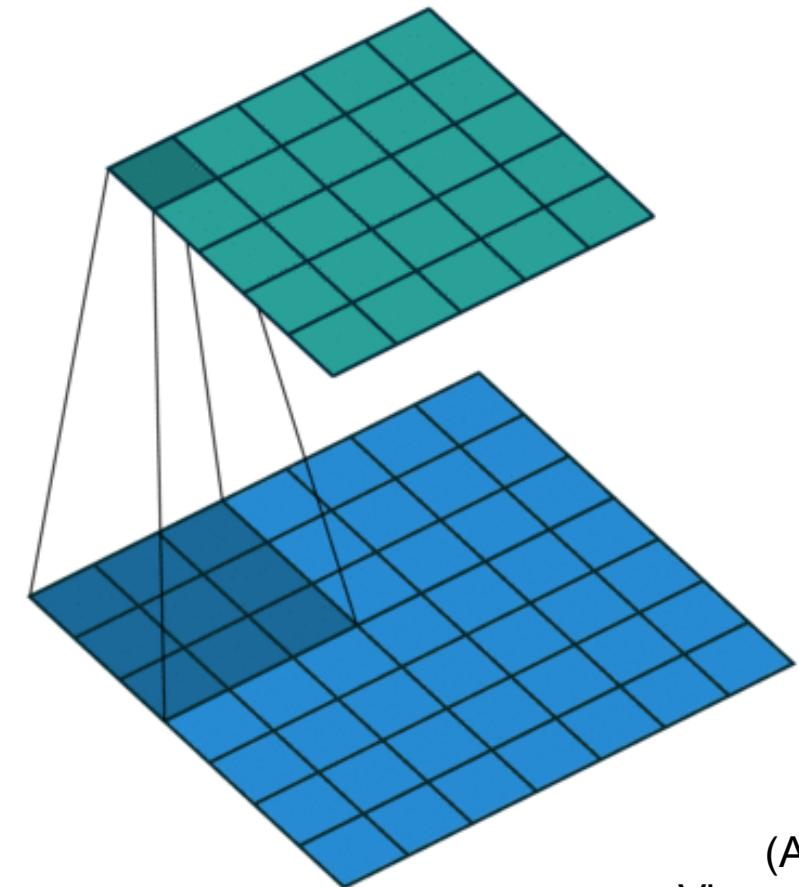
Notation: $\mathcal{G} = (\mathbf{A}, \mathbf{X})$

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

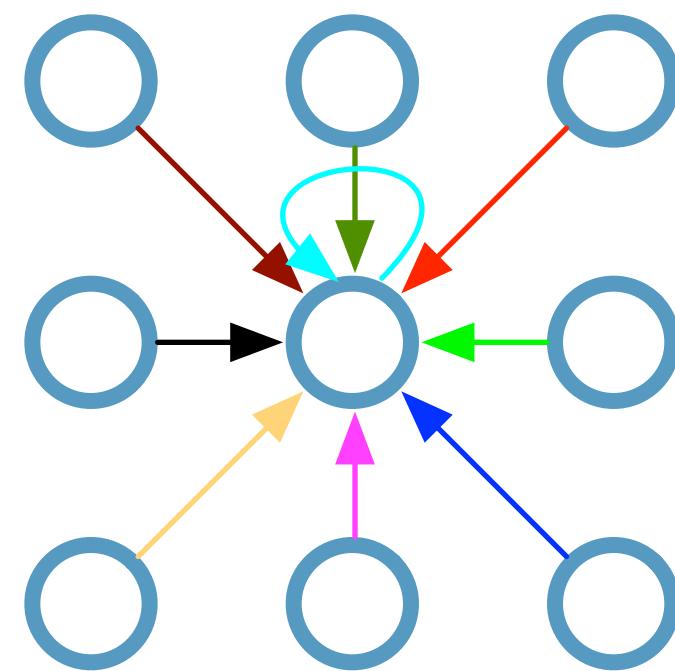
Main idea: Pass messages between pairs of nodes & agglomerate

Recap: Convolutional neural networks (on grids)

**Single CNN layer
with 3x3 filter:**

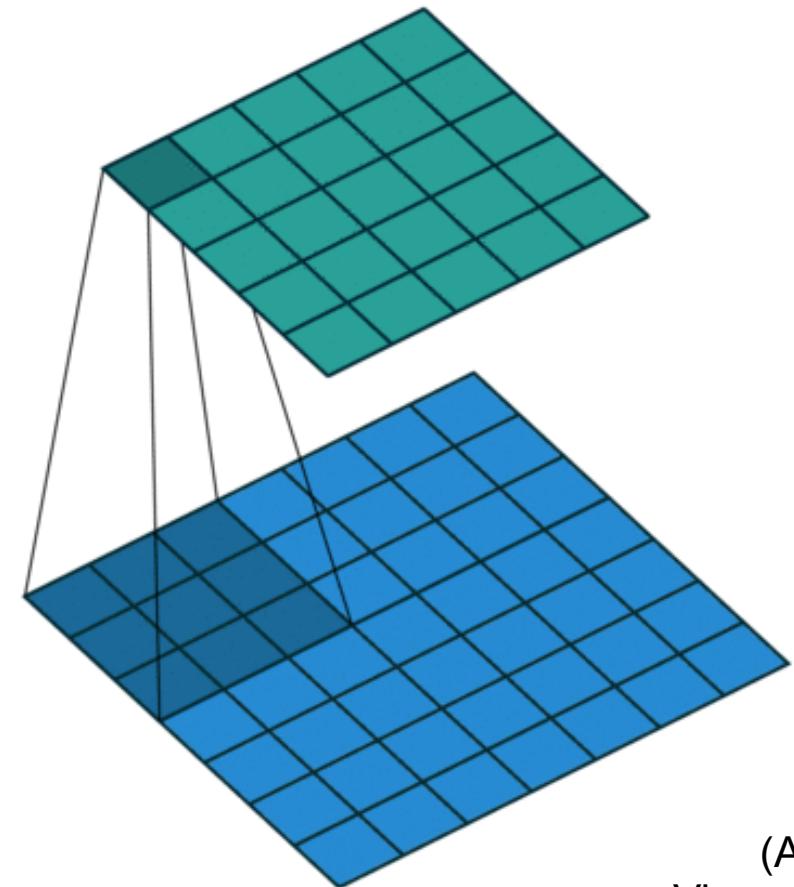


(Animation by
Vincent Dumoulin)

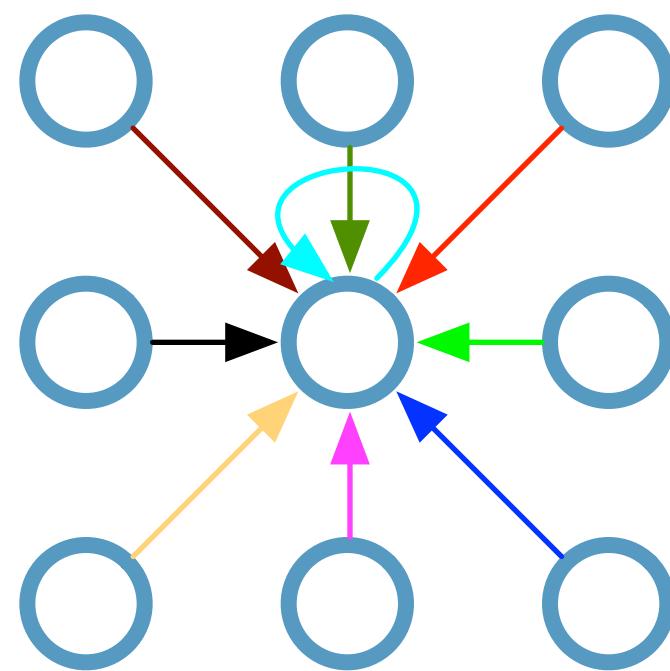


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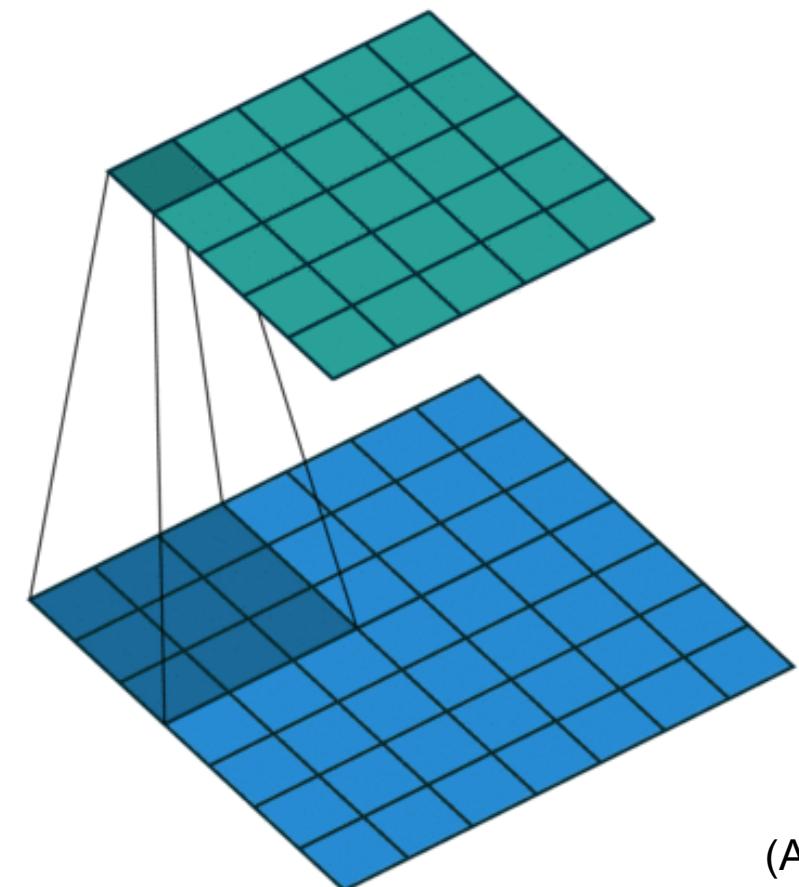


(Animation by
Vincent Dumoulin)

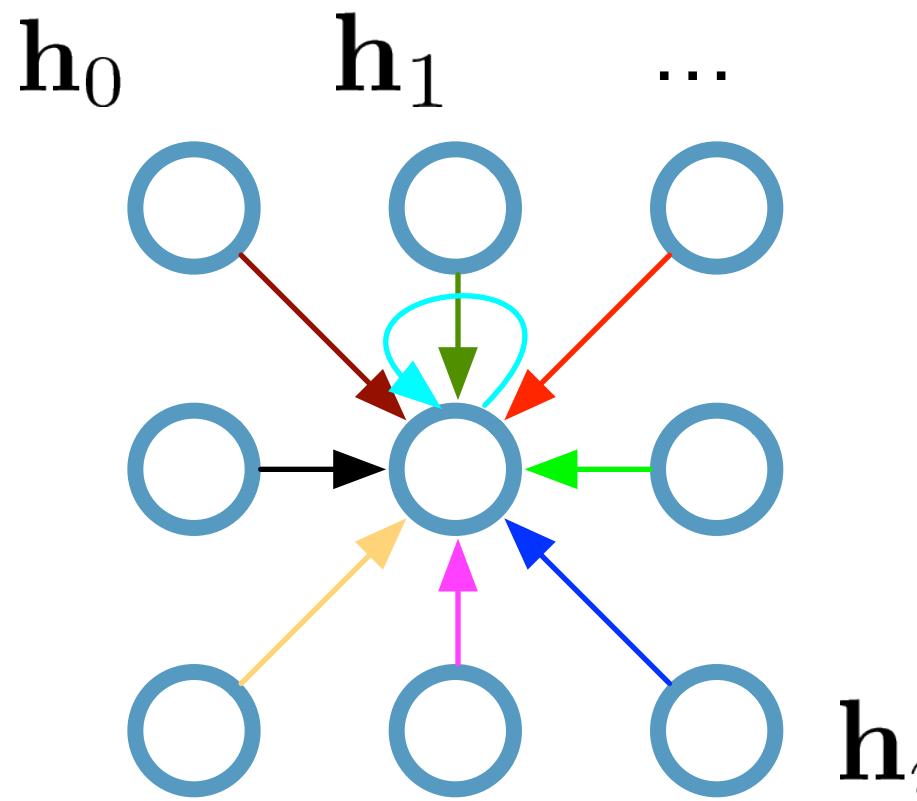


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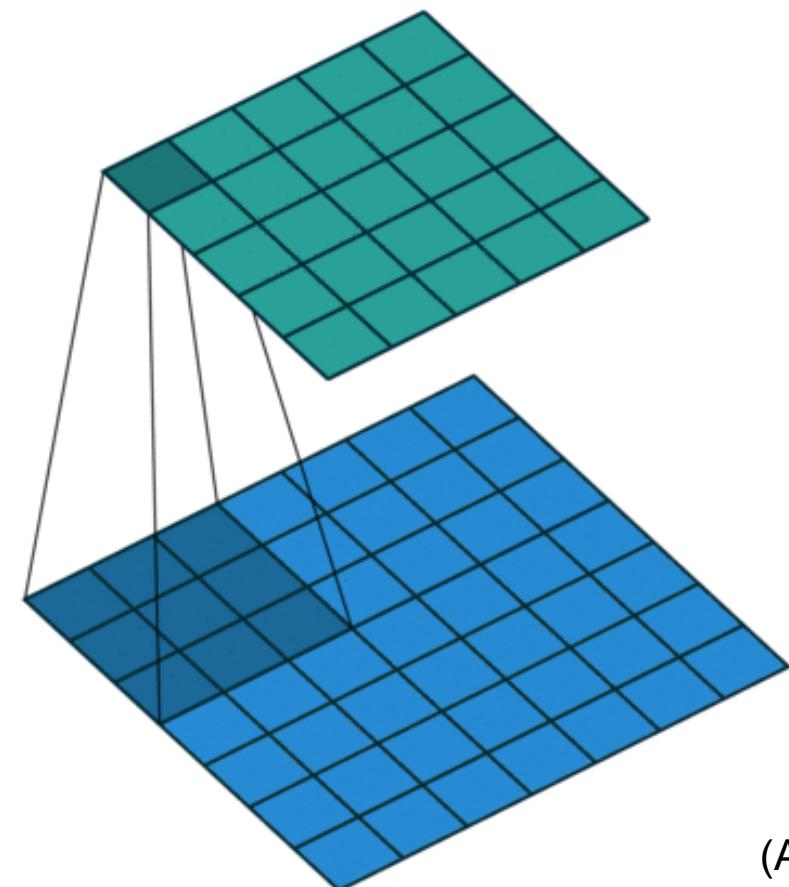


(Animation by
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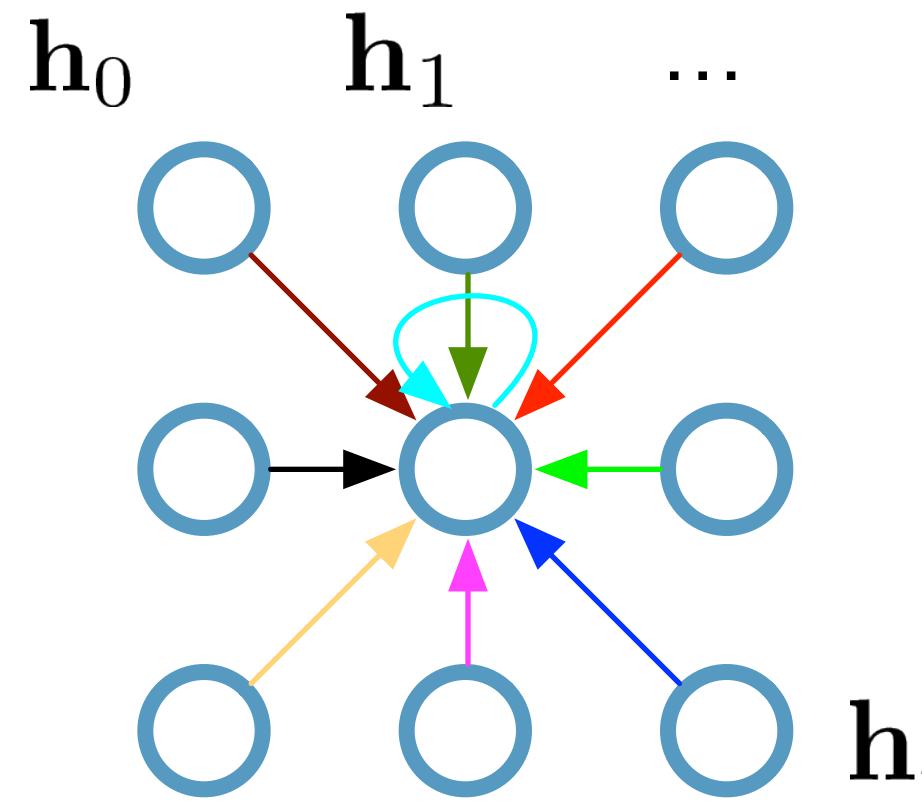


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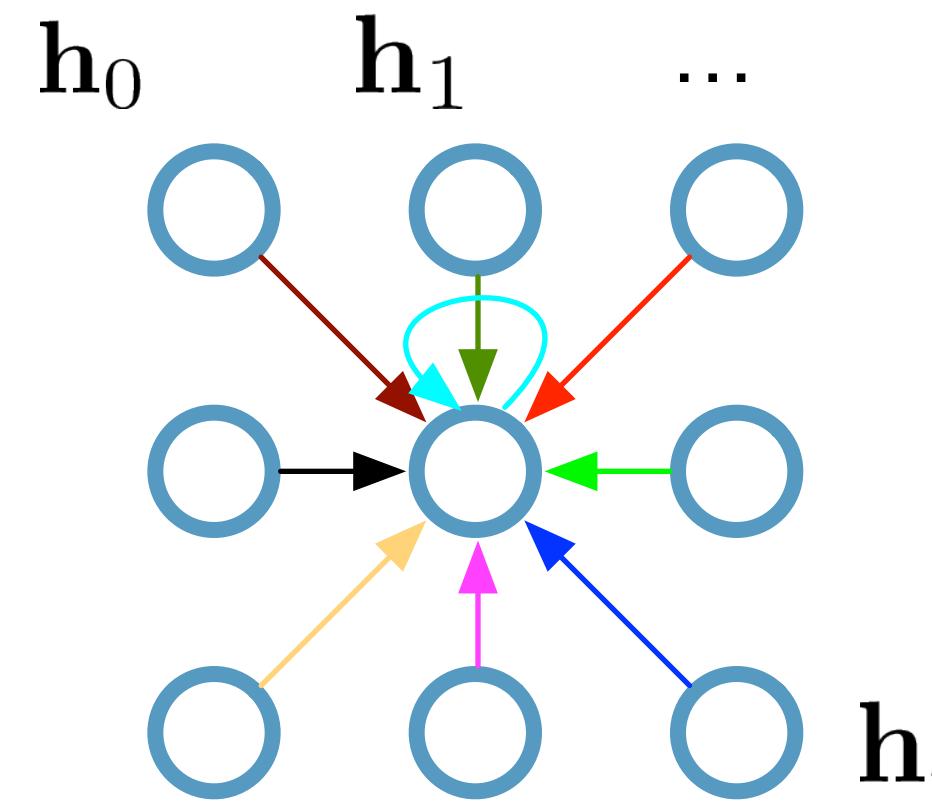
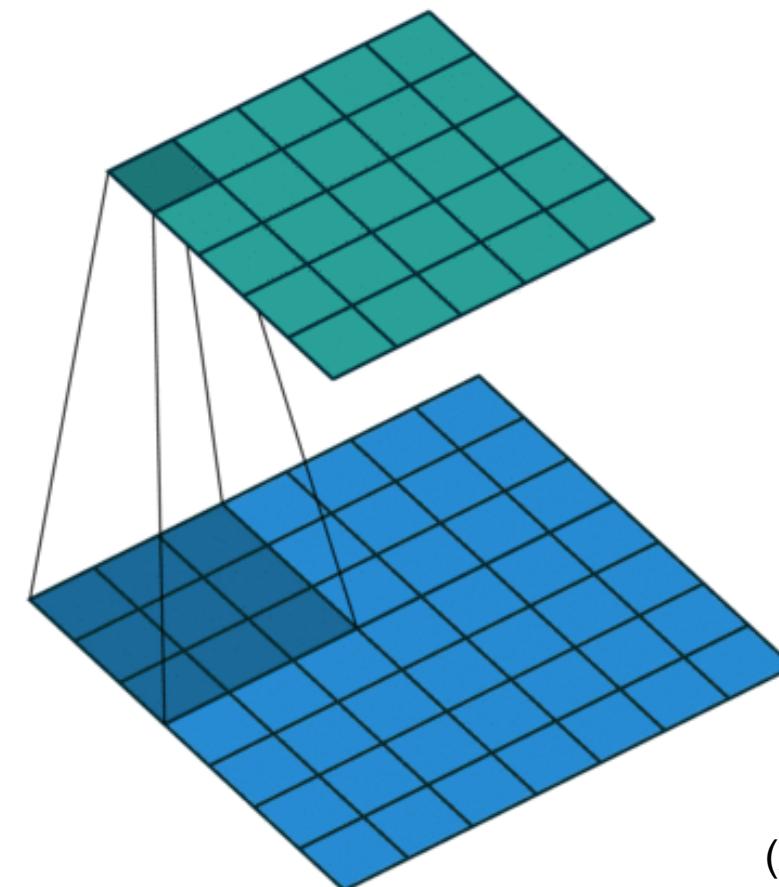
(Animation by
Vincent Dumoulin)



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

Recap: Convolutional neural networks (on grids)

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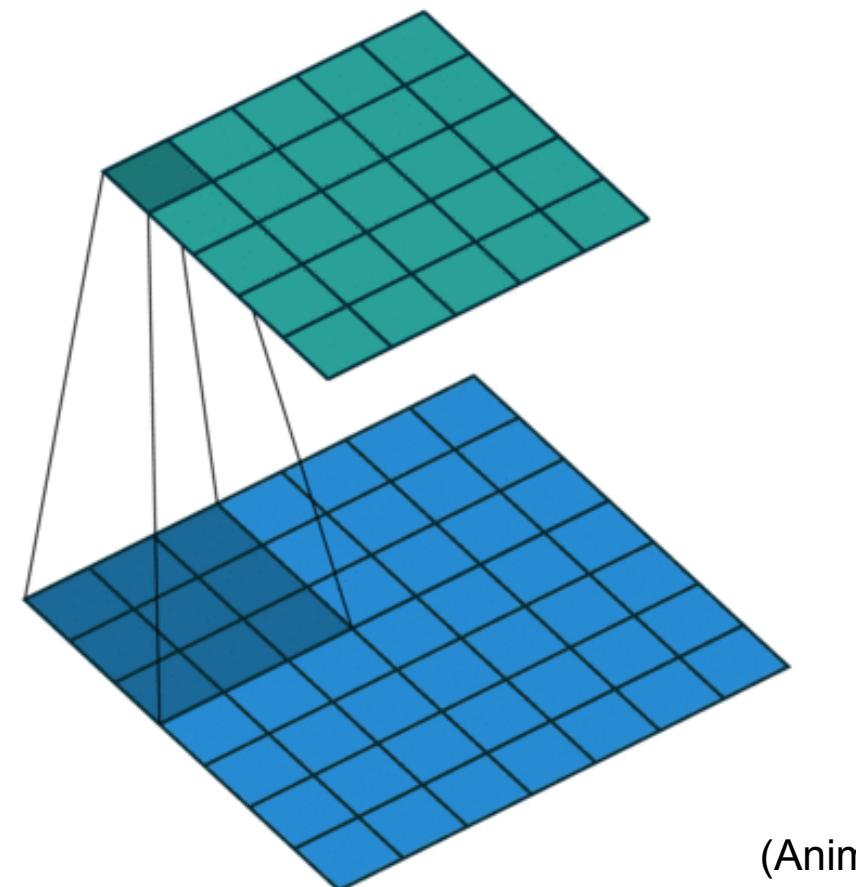
$\mathbf{h}_i \in \mathbb{R}^F$ are (hidden layer) activations of a pixel/node

Update for a single pixel:

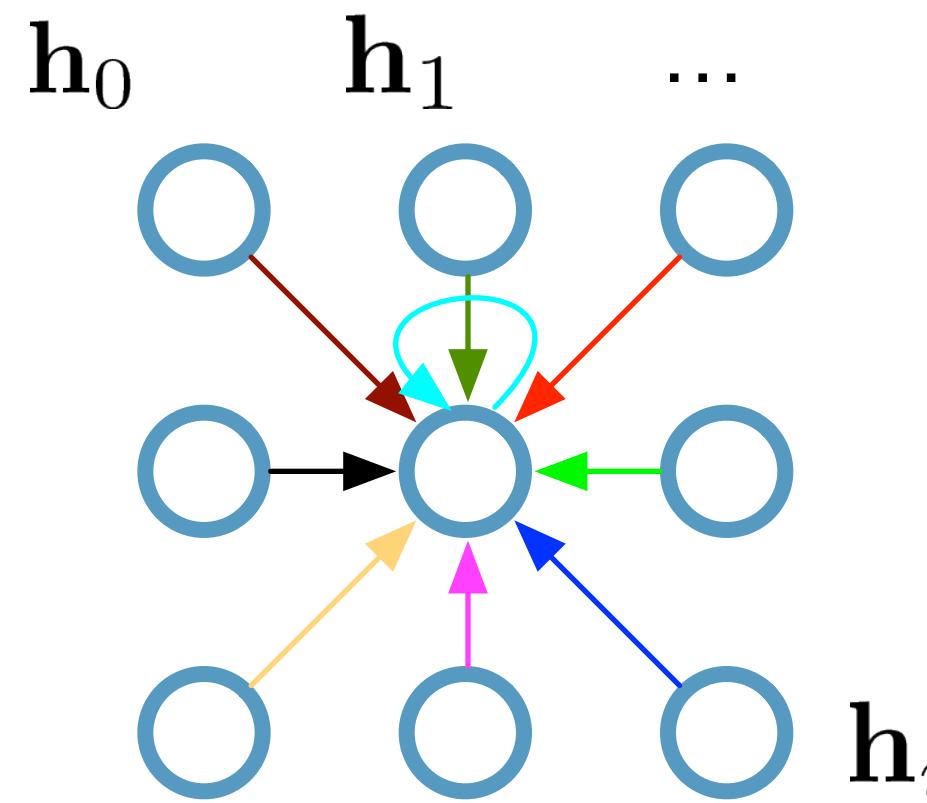
- Transform messages individually $\mathbf{W}_i \mathbf{h}_i$
- Add everything up $\sum_i \mathbf{W}_i \mathbf{h}_i$

Recap: Convolutional neural networks (on grids)

**Single CNN layer
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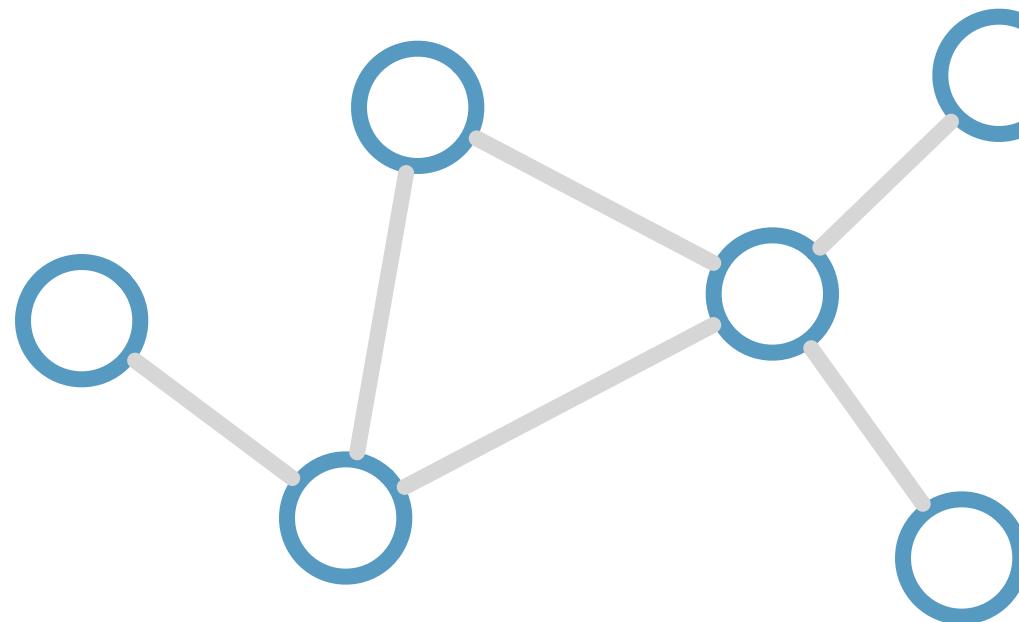
Full update:

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

Graph convolutional networks (GCNs)

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

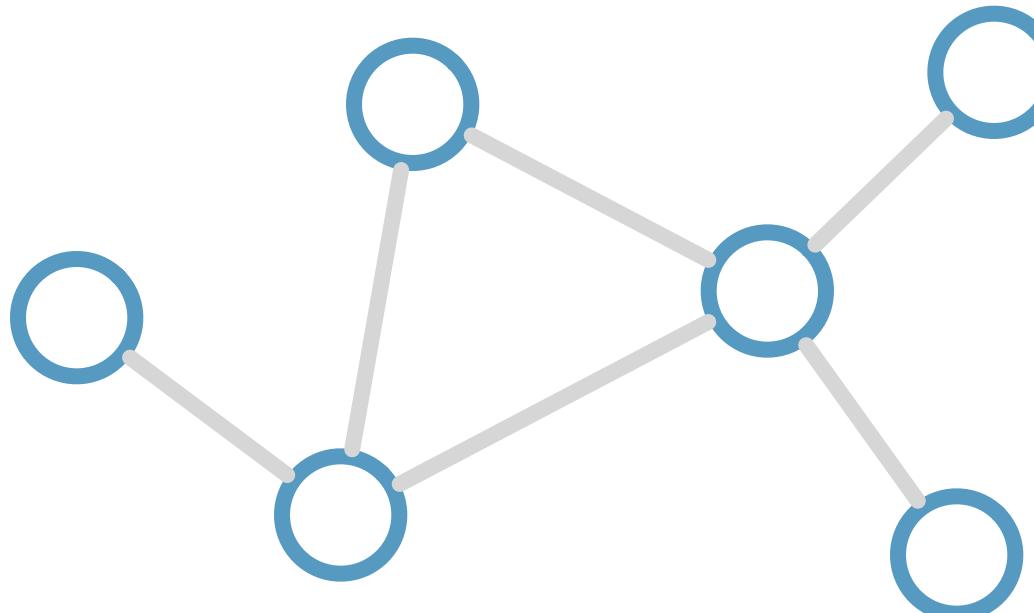
Consider this
undirected graph:



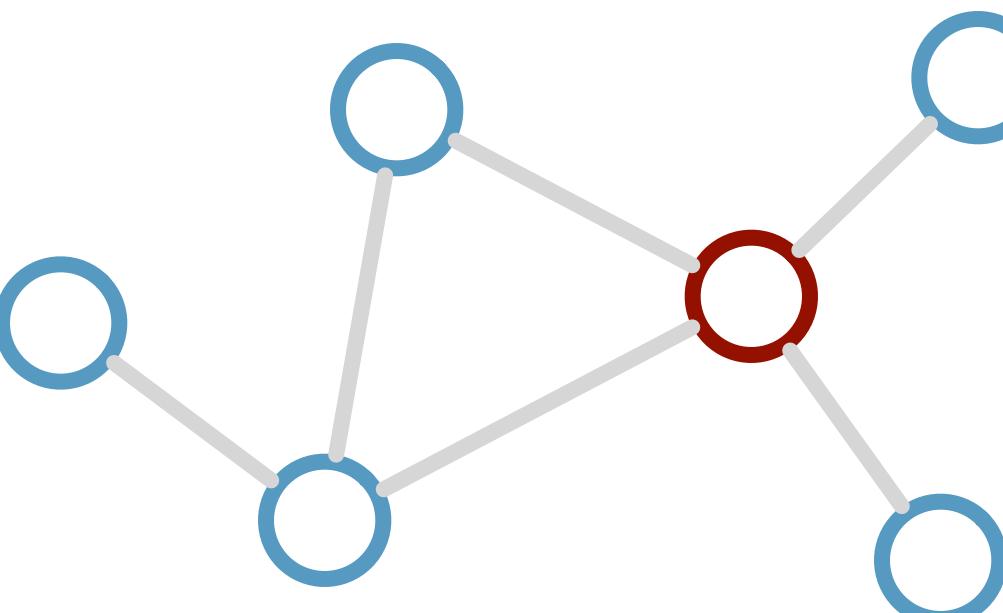
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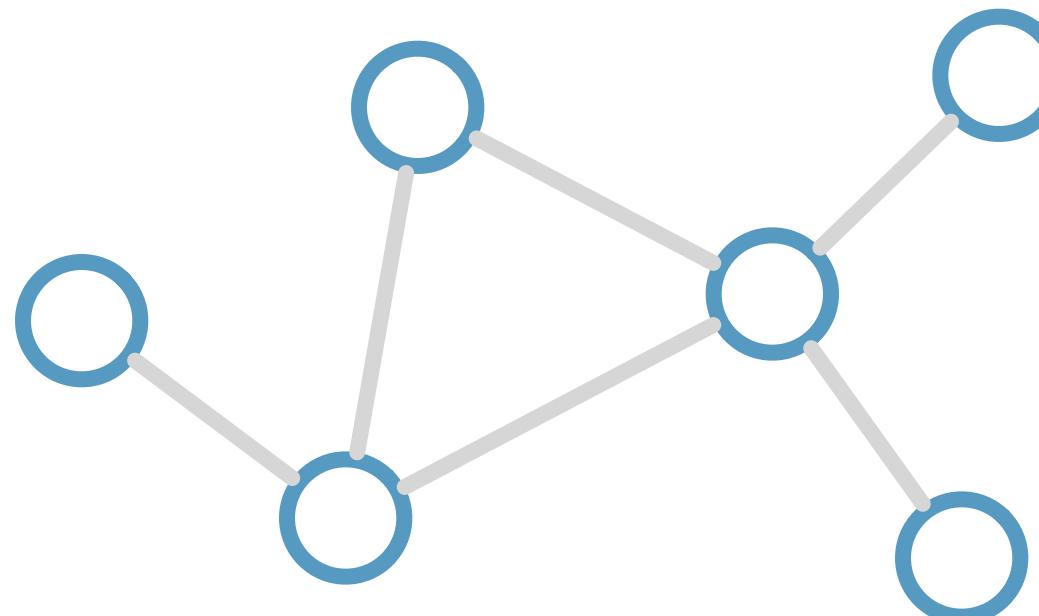
Calculate update
for node in red:



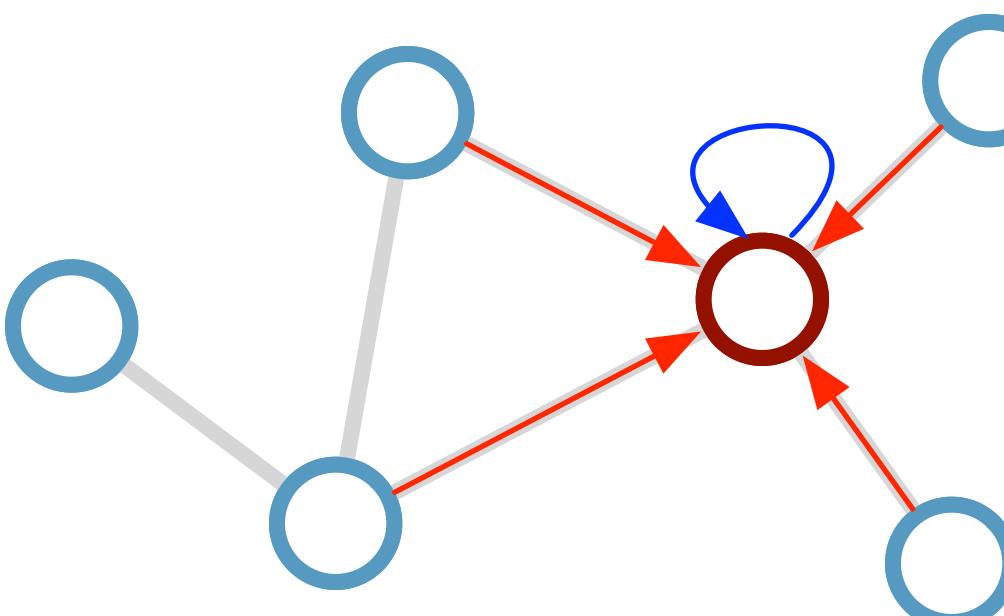
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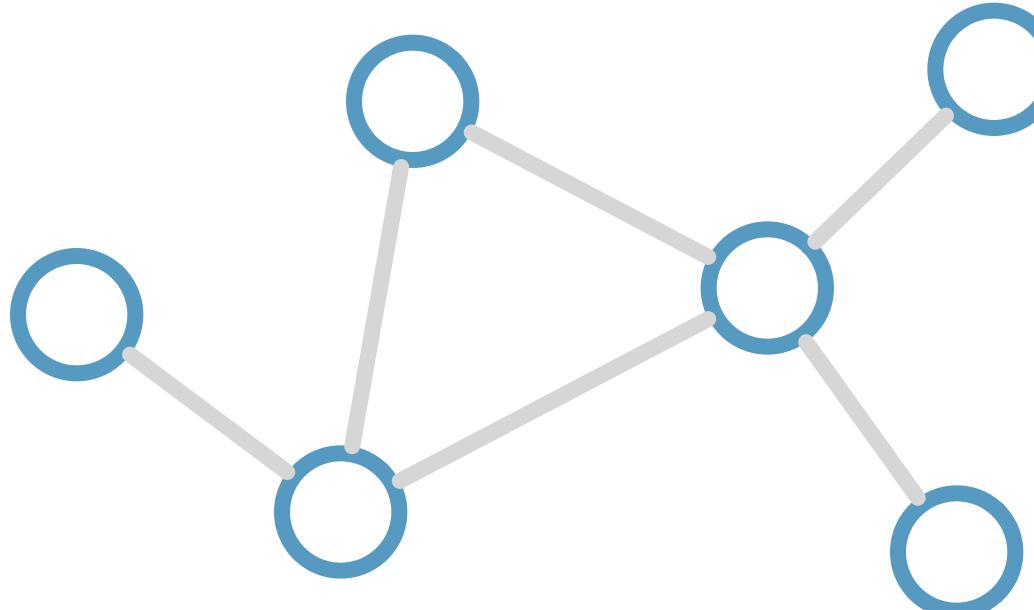
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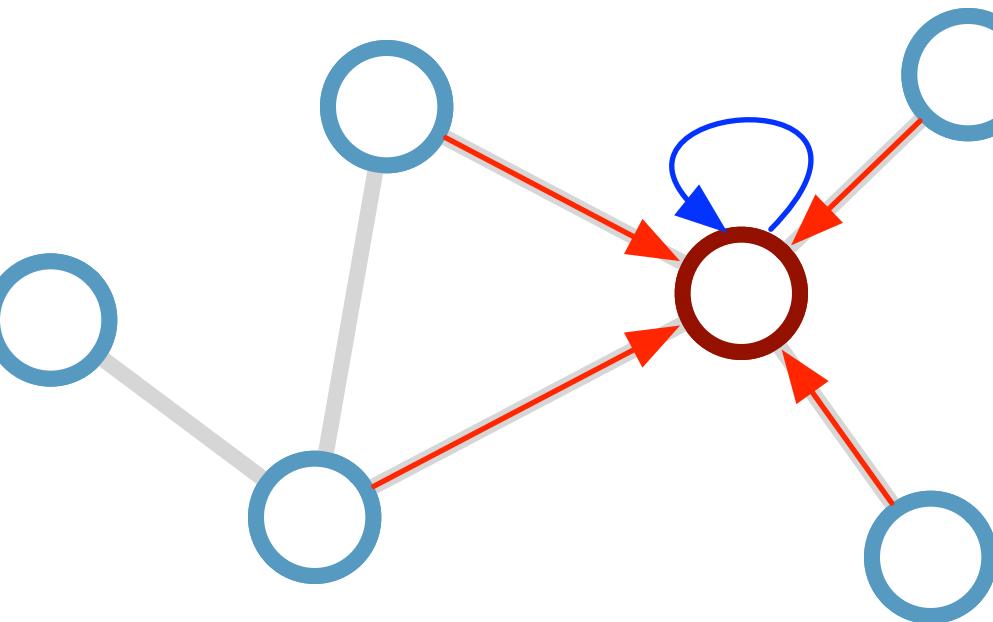
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**Update
rule:**

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

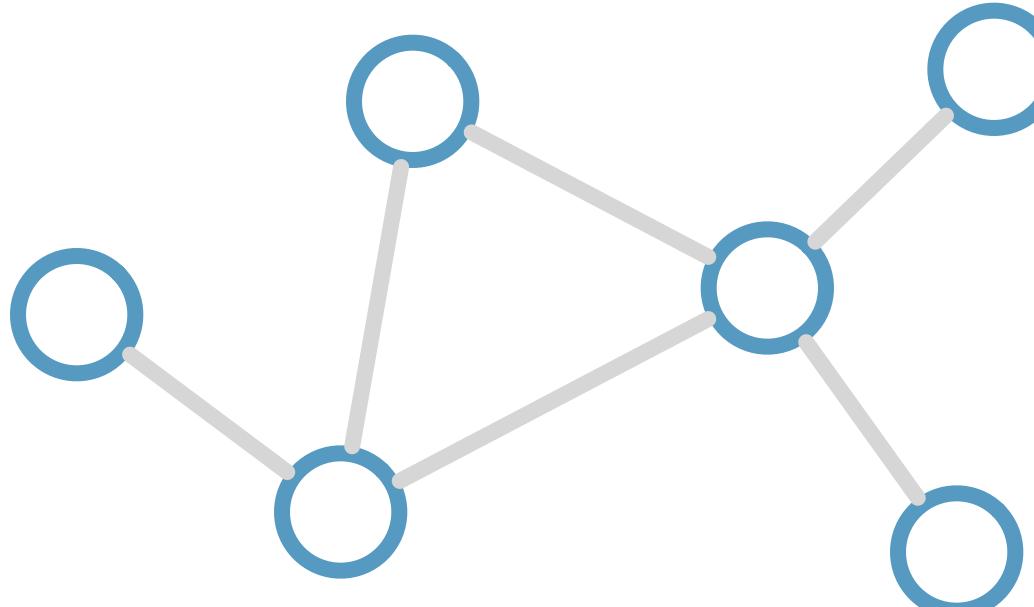
\mathcal{N}_i : neighbor indices

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

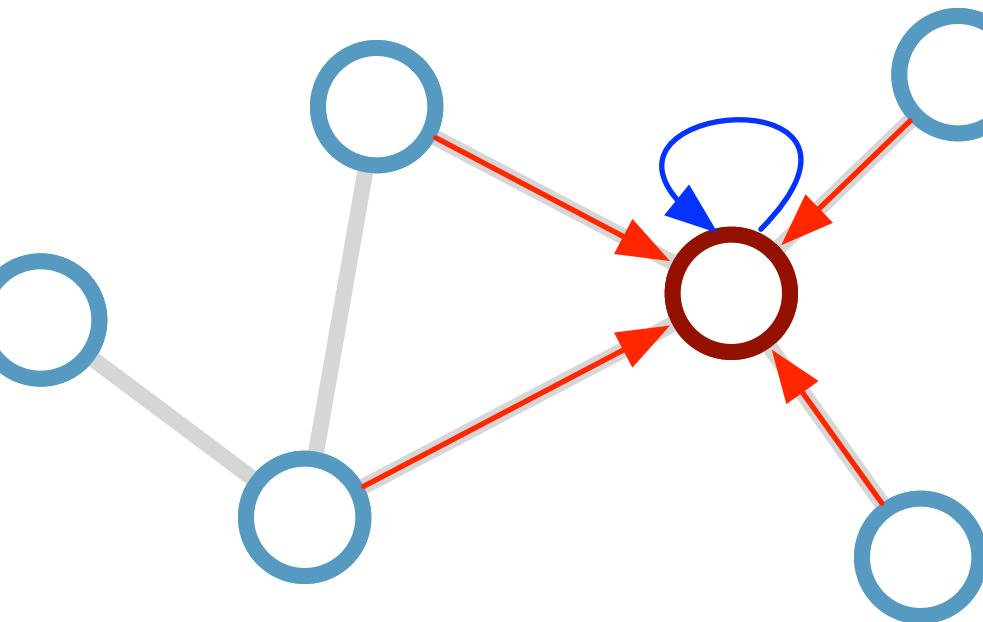
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Scalability: subsample messages [Hamilton et al., NIPS 2017]

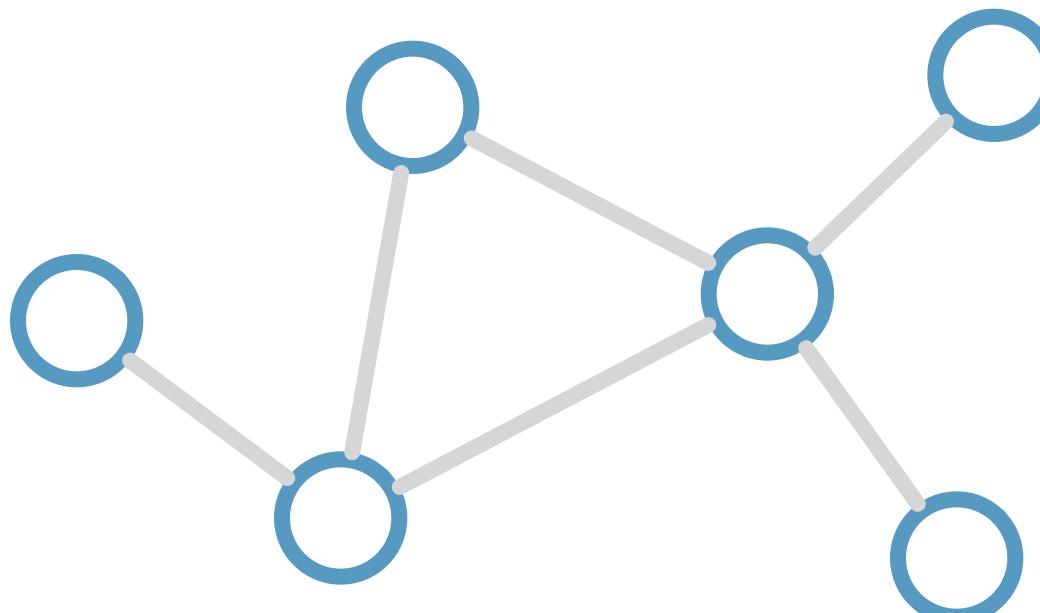
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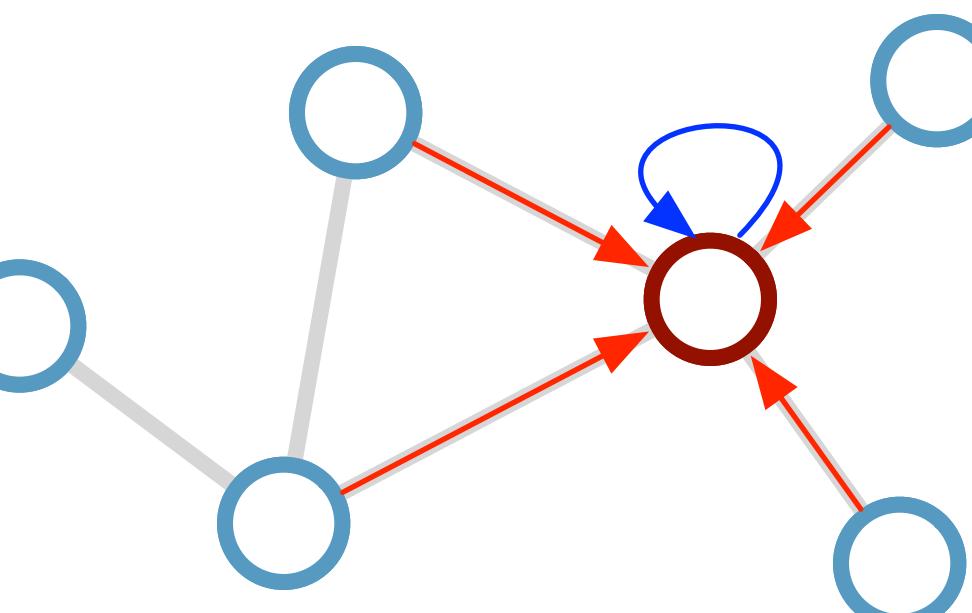
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Consider this
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Calculate update
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Desirable properties:

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

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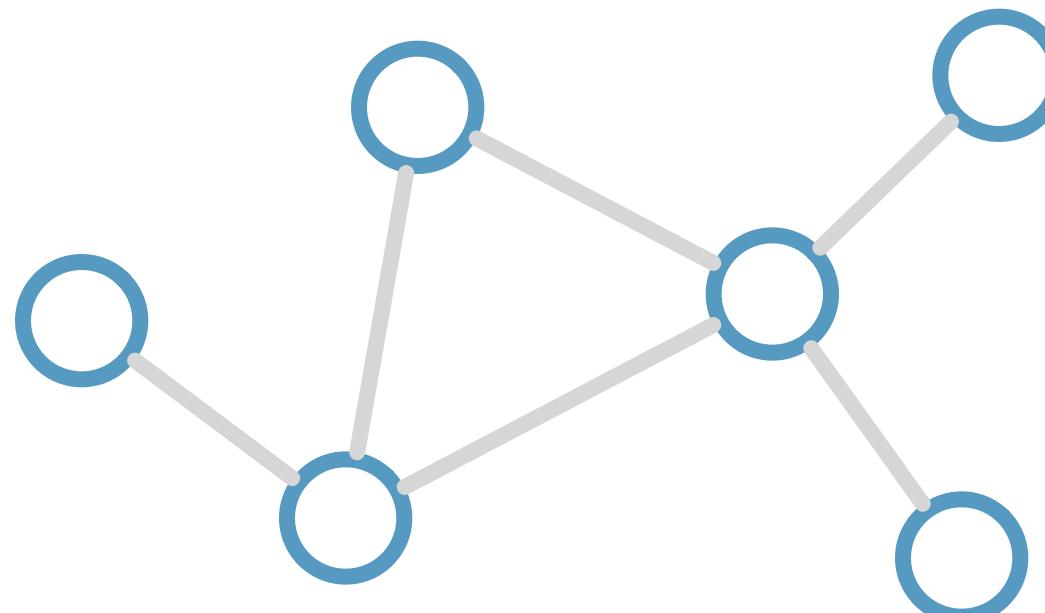
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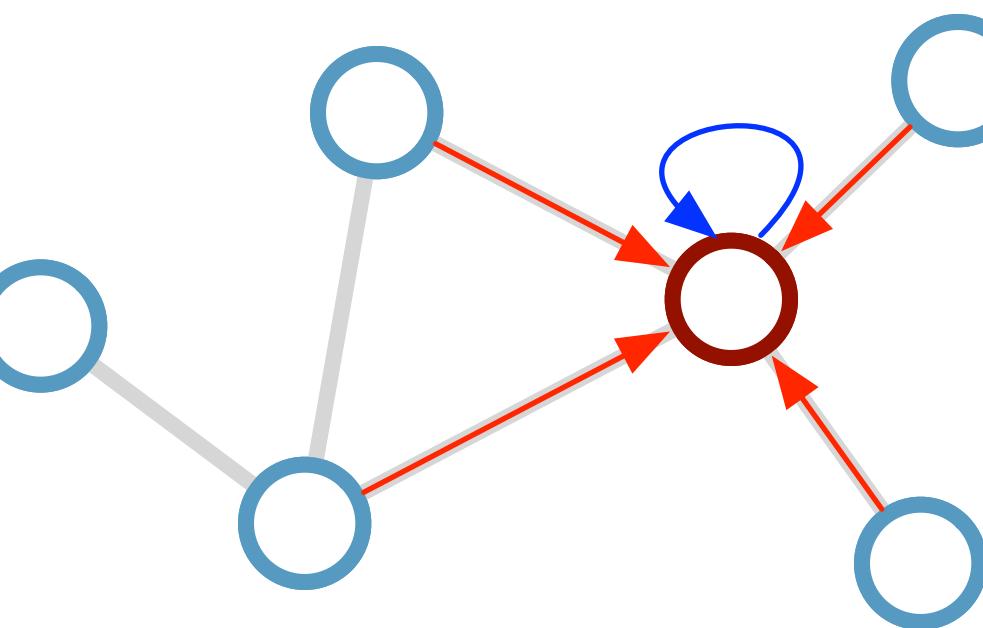
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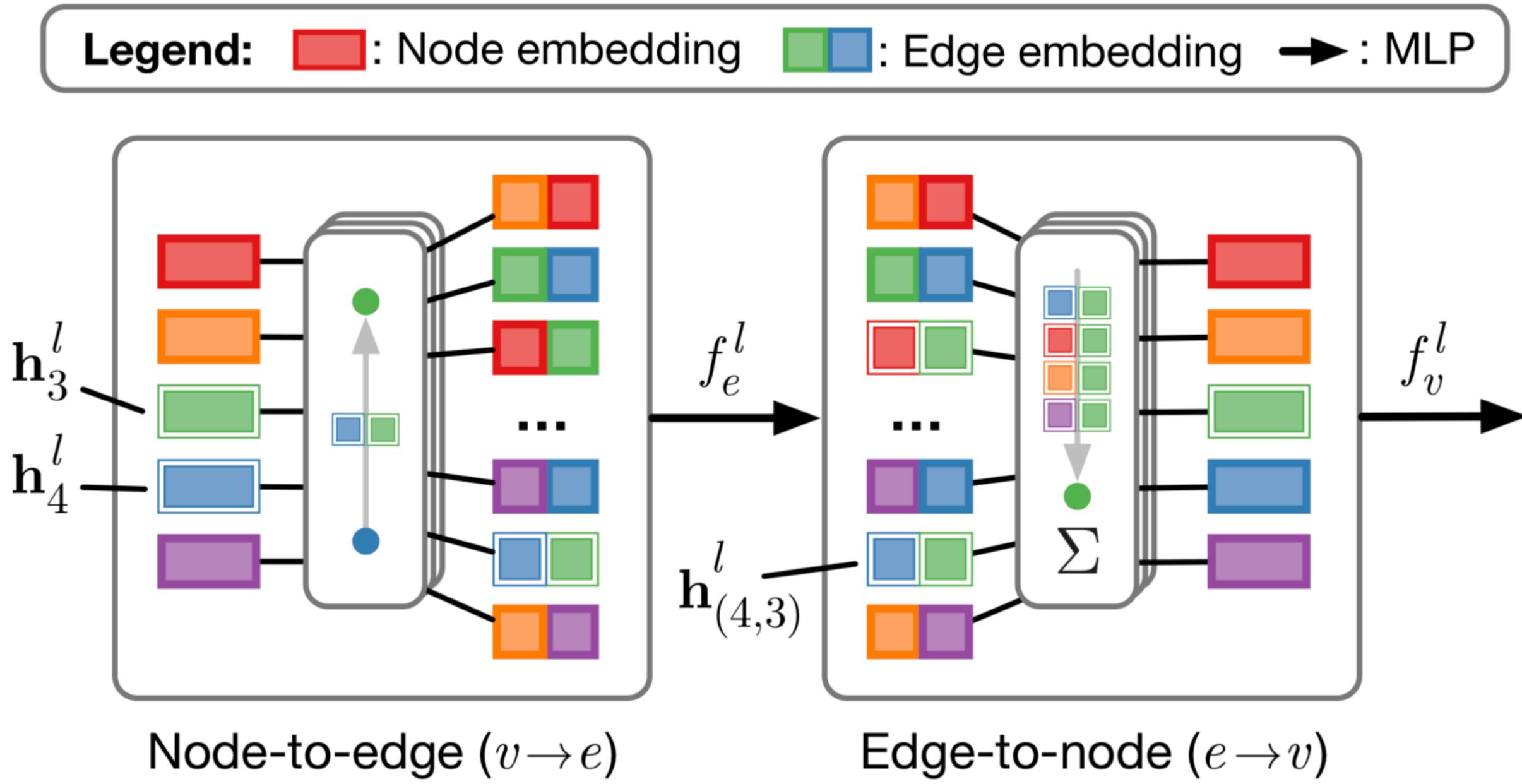
Limitations:

- Requires gating mechanism / residual connections for depth
- Only indirect support for edge features

\mathcal{N}_i : neighbor indices c_{ij} : norm. constant
(fixed/trainable)

GNNs with edge embeddings

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

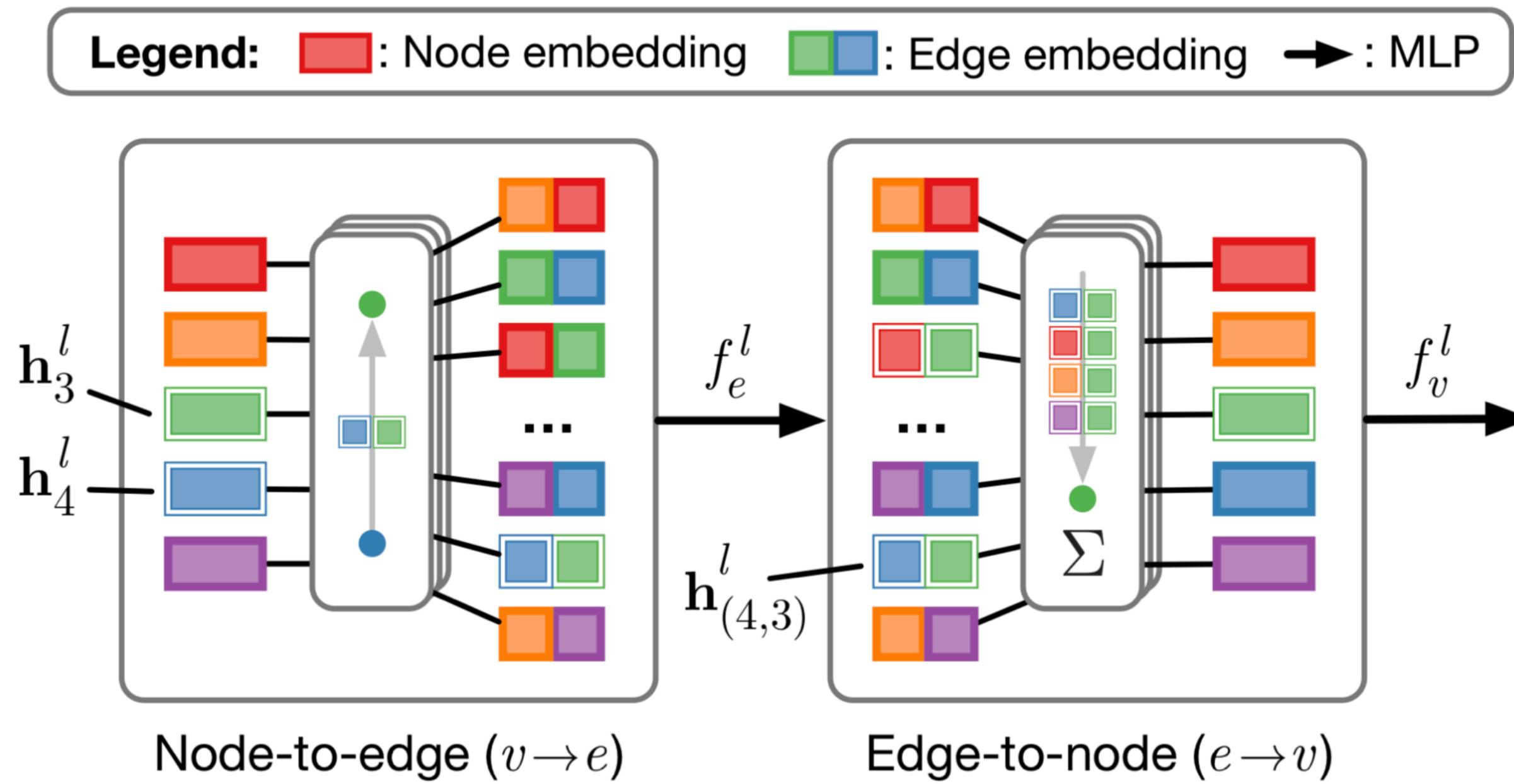


Formally:

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

GNNs with edge embeddings

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



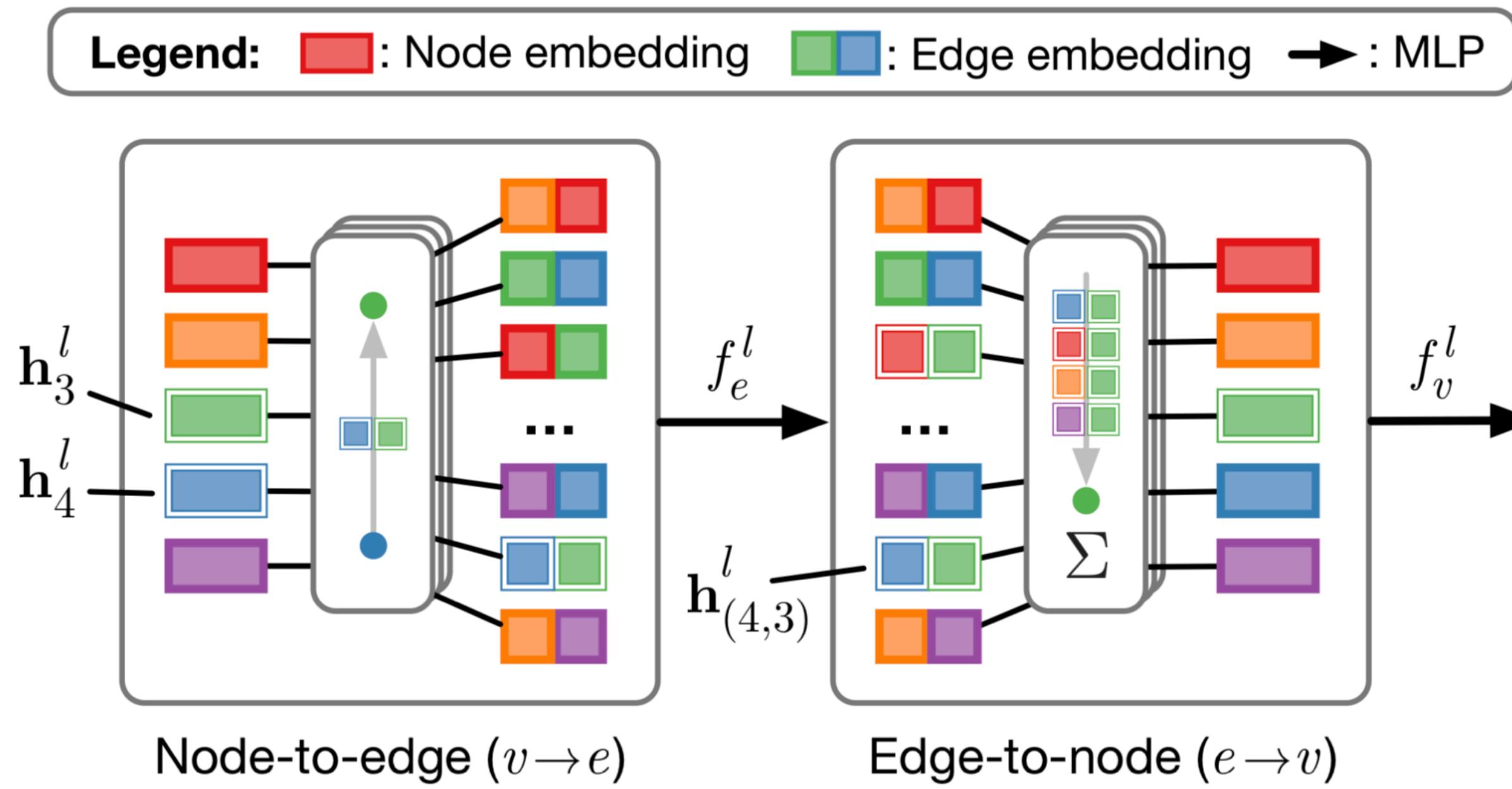
Pros:

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

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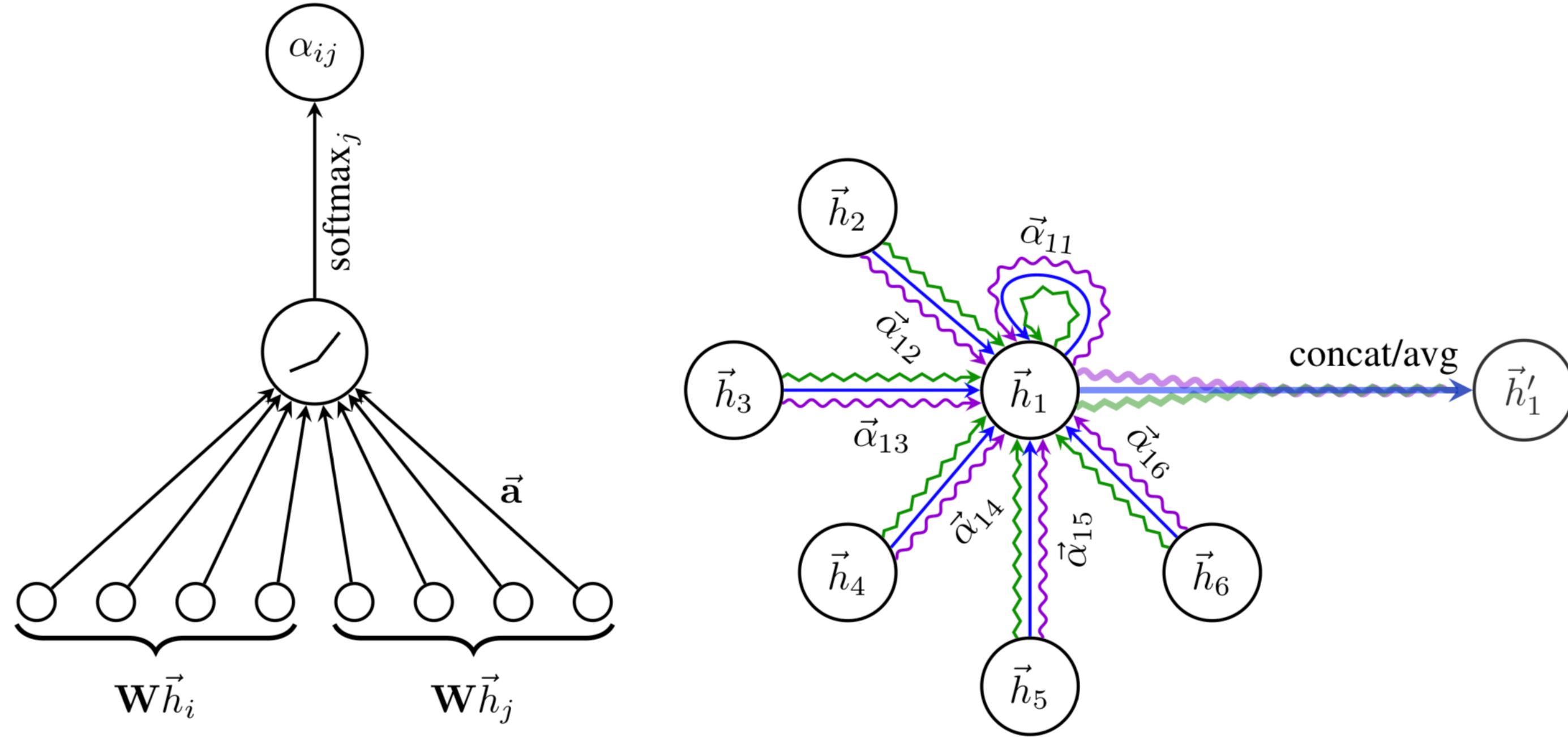
- Supports edge features
- More expressive than GCN
- As general as it gets (?)
- Supports sparse matrix ops

Cons:

- Need to store intermediate edge-based activations
- Difficult to implement with subsampling
→ In practice limited to small graphs

Graph neural networks with attention

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

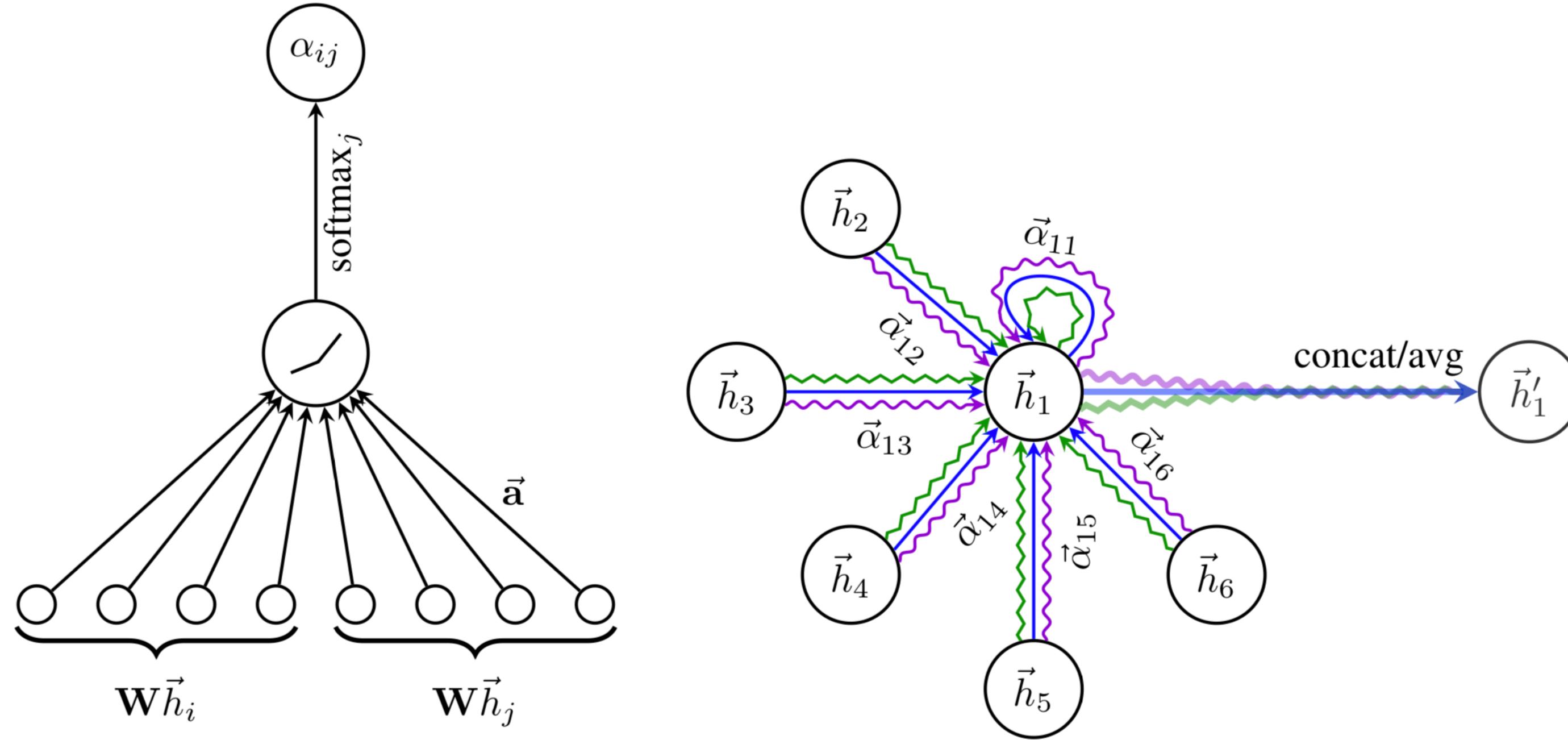


[Figure from Veličković et al. (ICLR 2018)]

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

Graph neural networks with attention

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



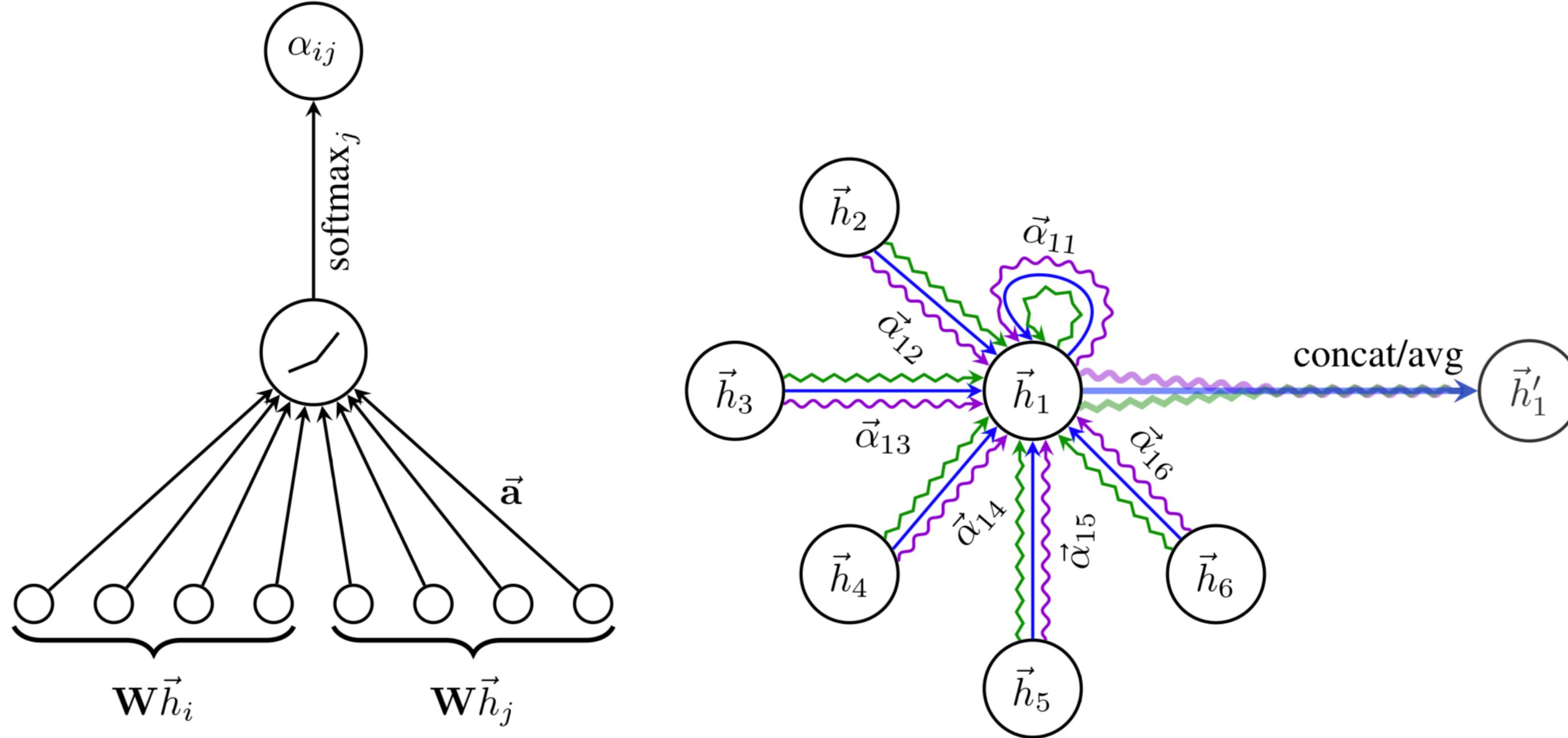
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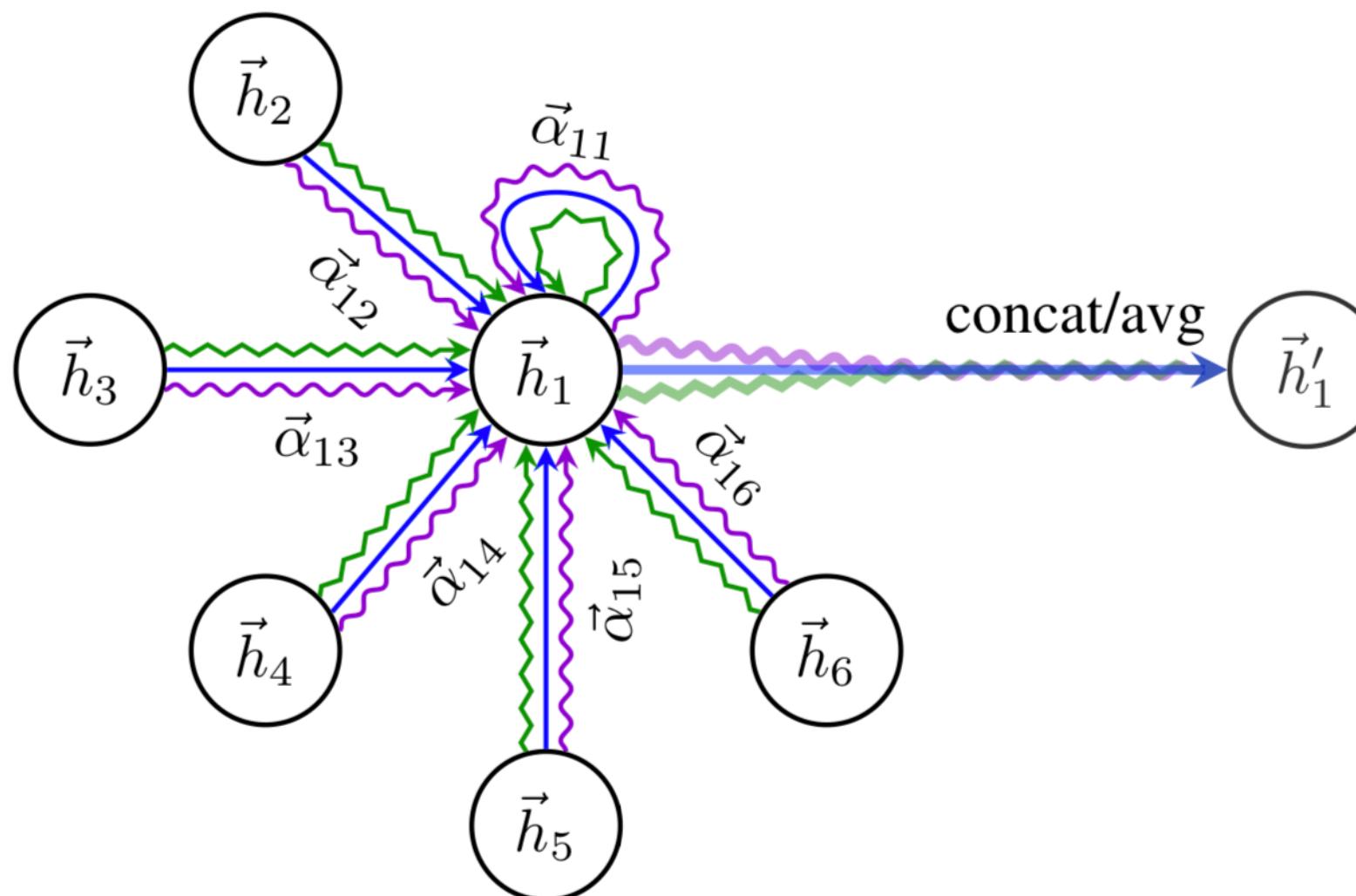
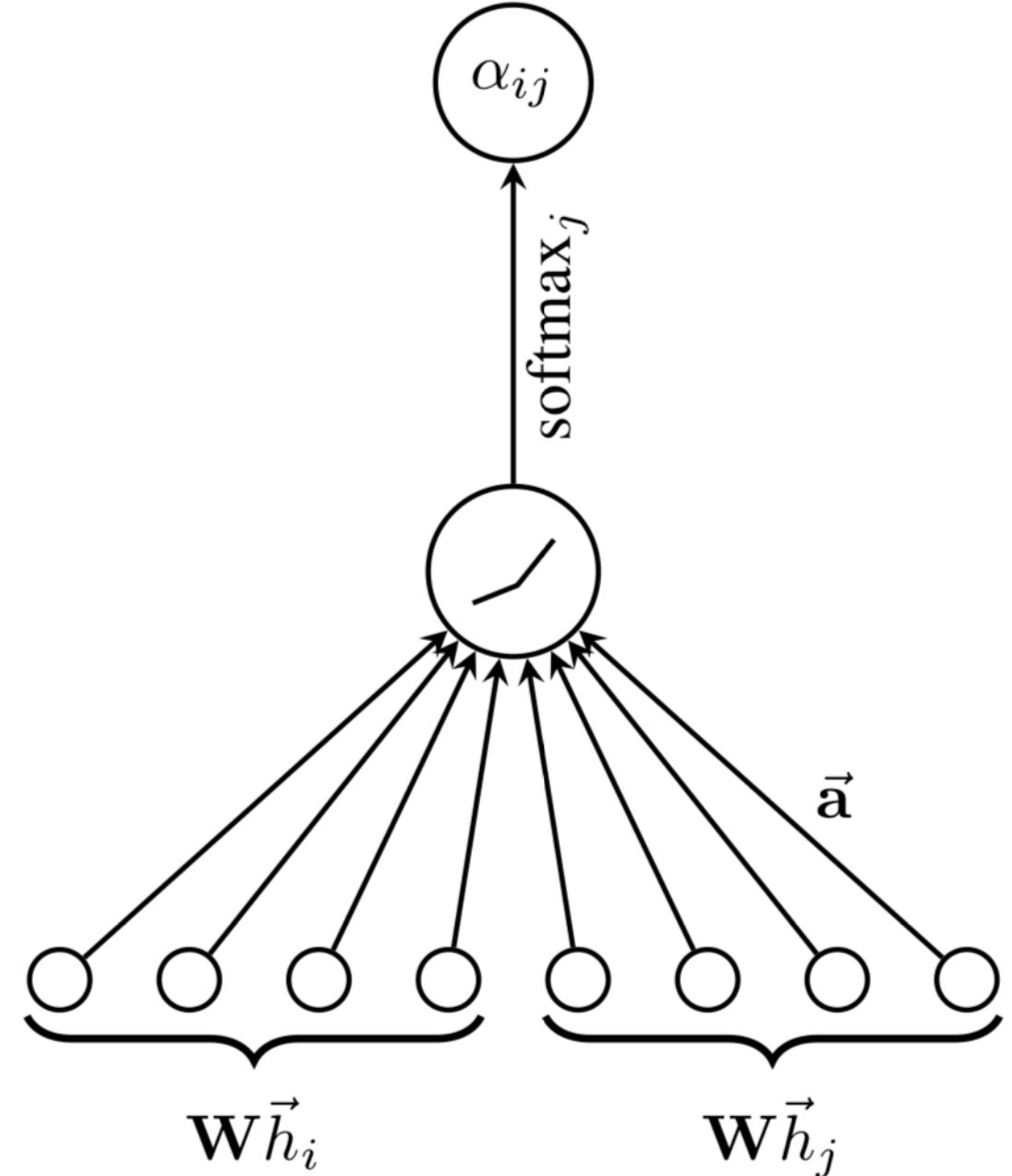
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Pros:

- 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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Pros:

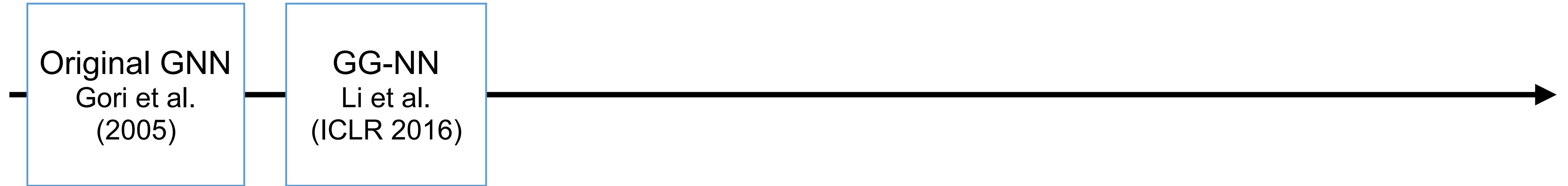
- No need to store intermediate edge-based activation vectors (when using dot-product attn.)
- Slower than GCNs but faster than GNNs with edge embeddings

Cons:

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

A brief history of graph neural nets

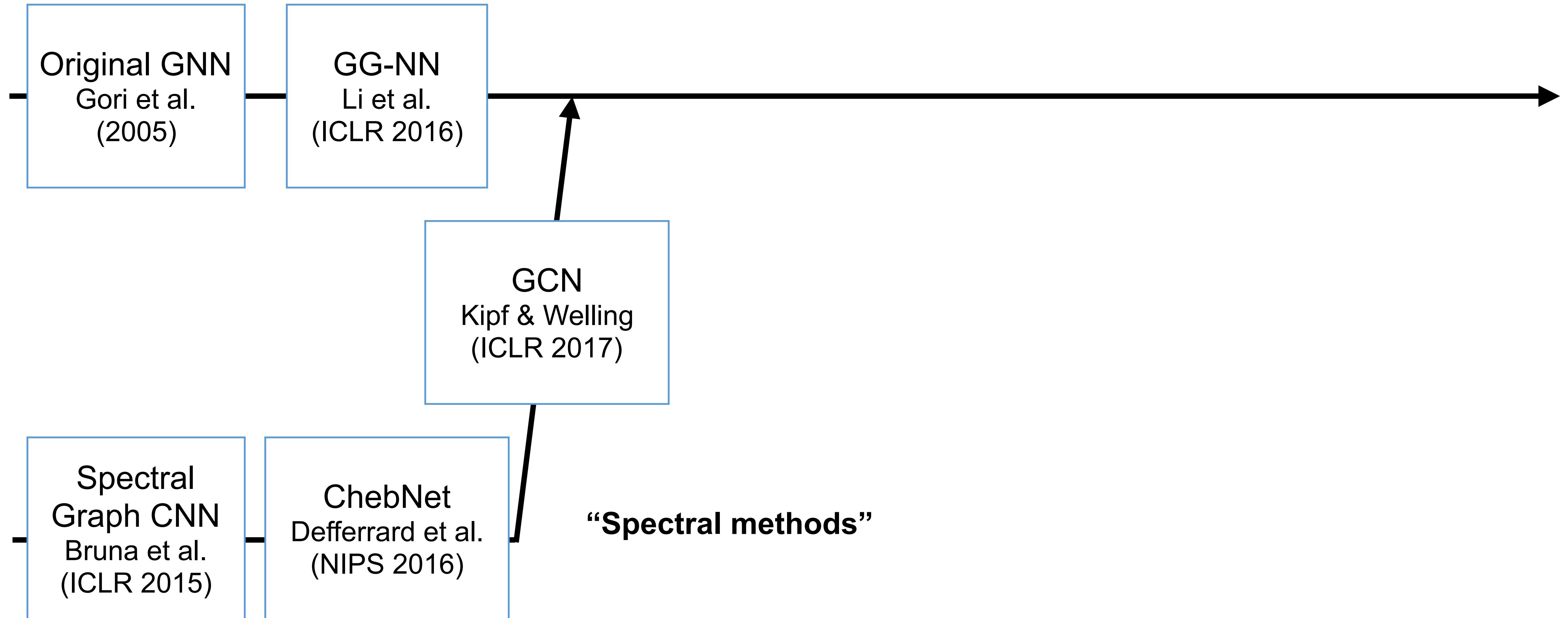
“Spatial methods”



(slide inspired by Marc Brockschmidt's talk on GNNs)

A brief history of graph neural nets

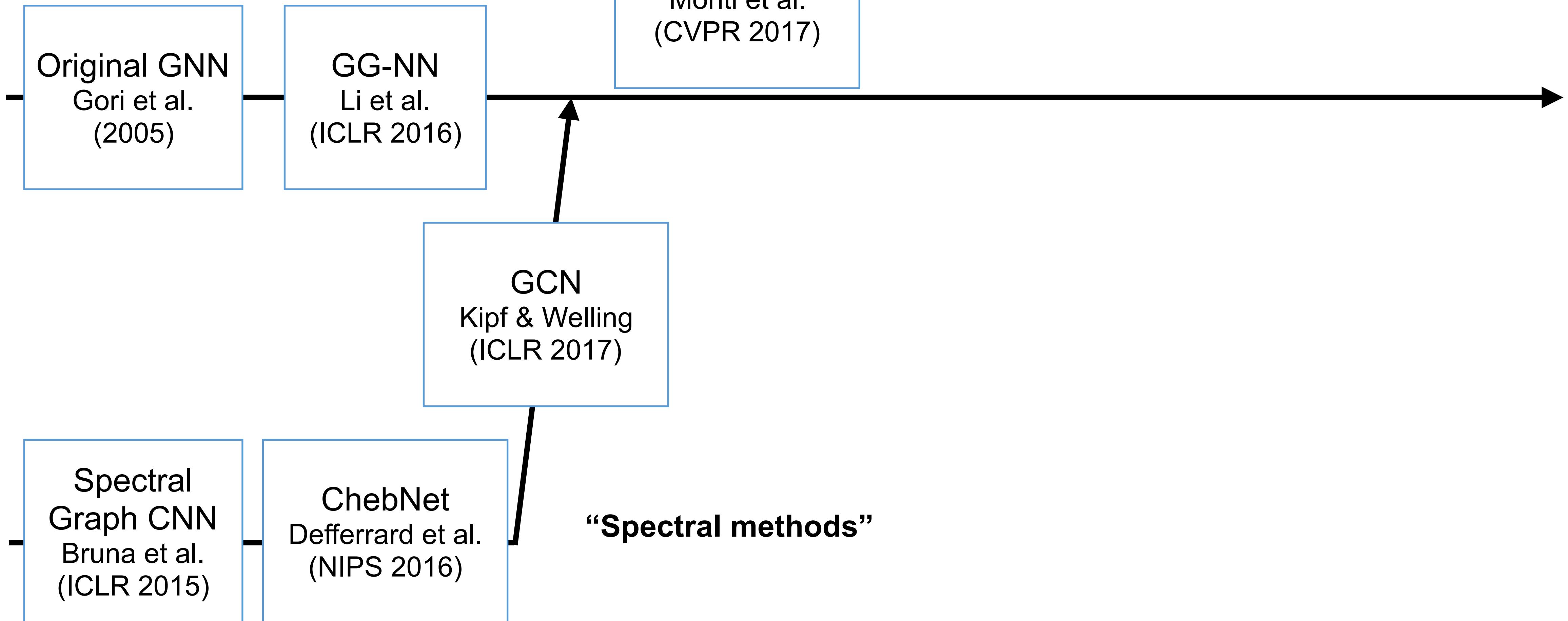
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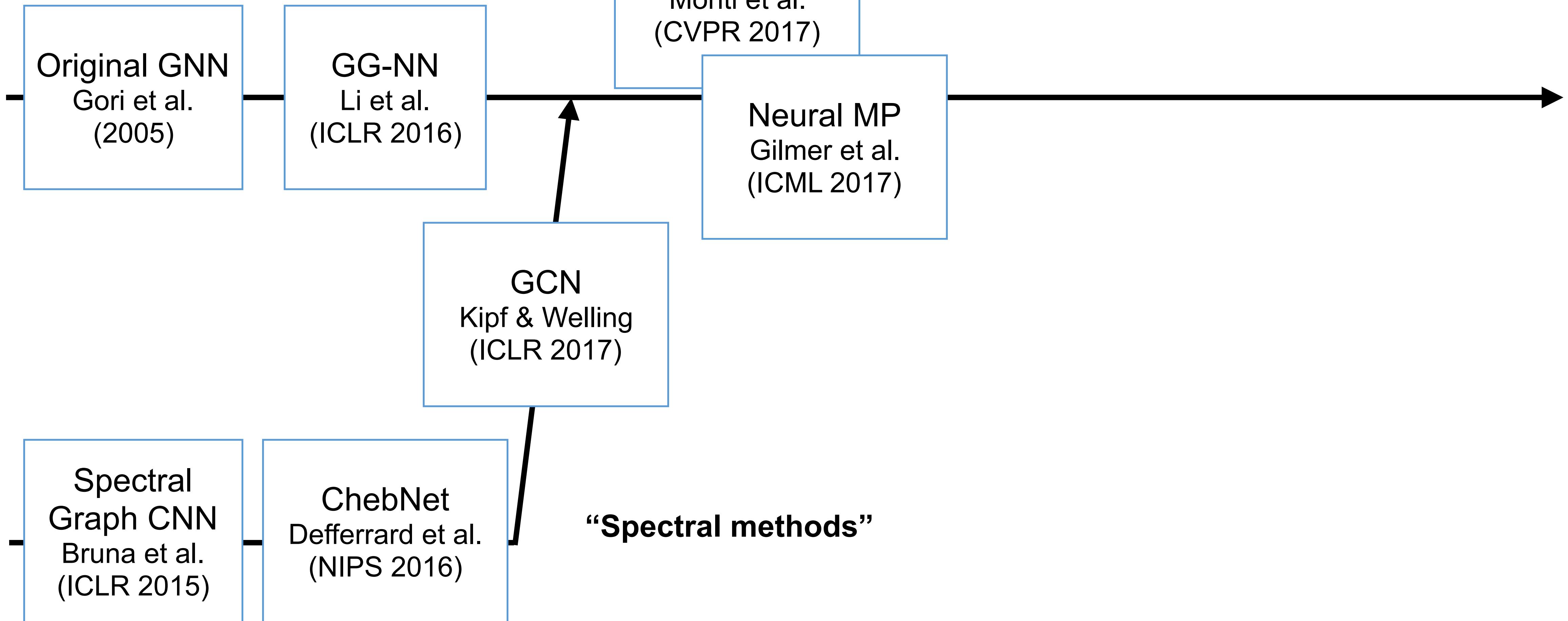
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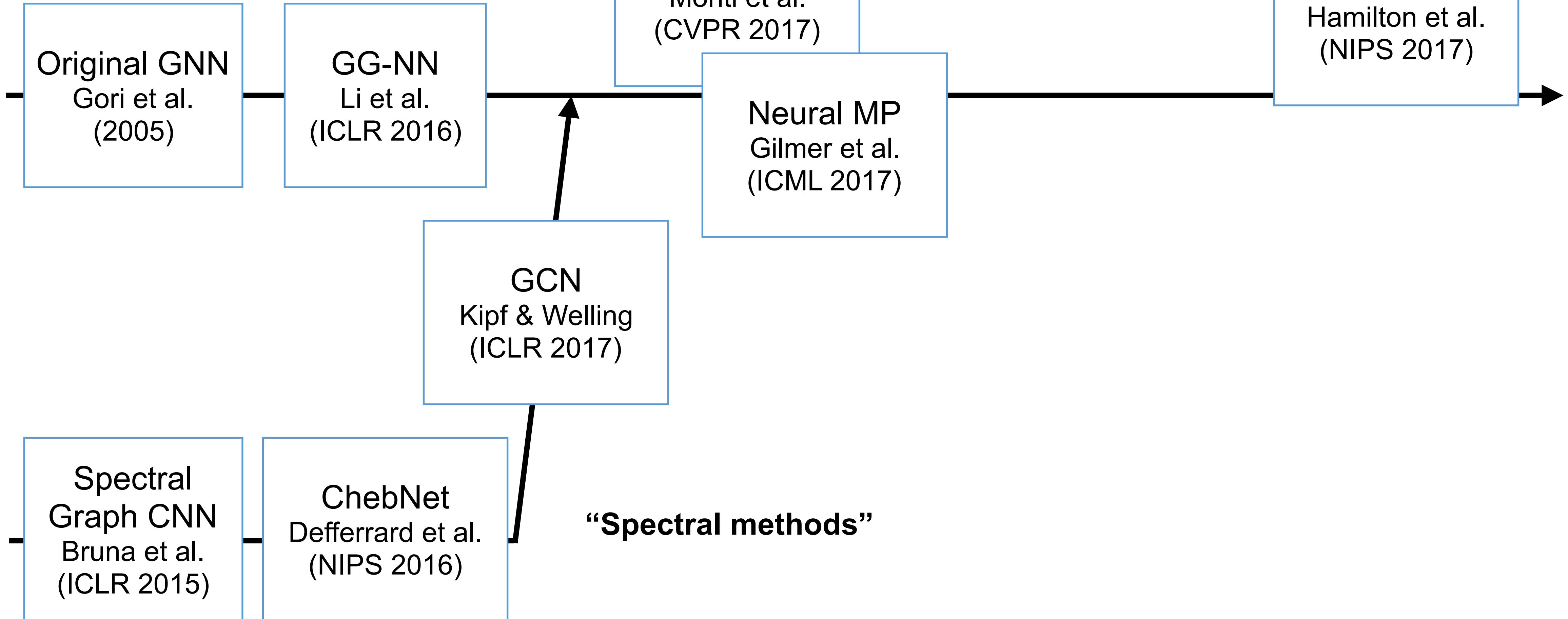
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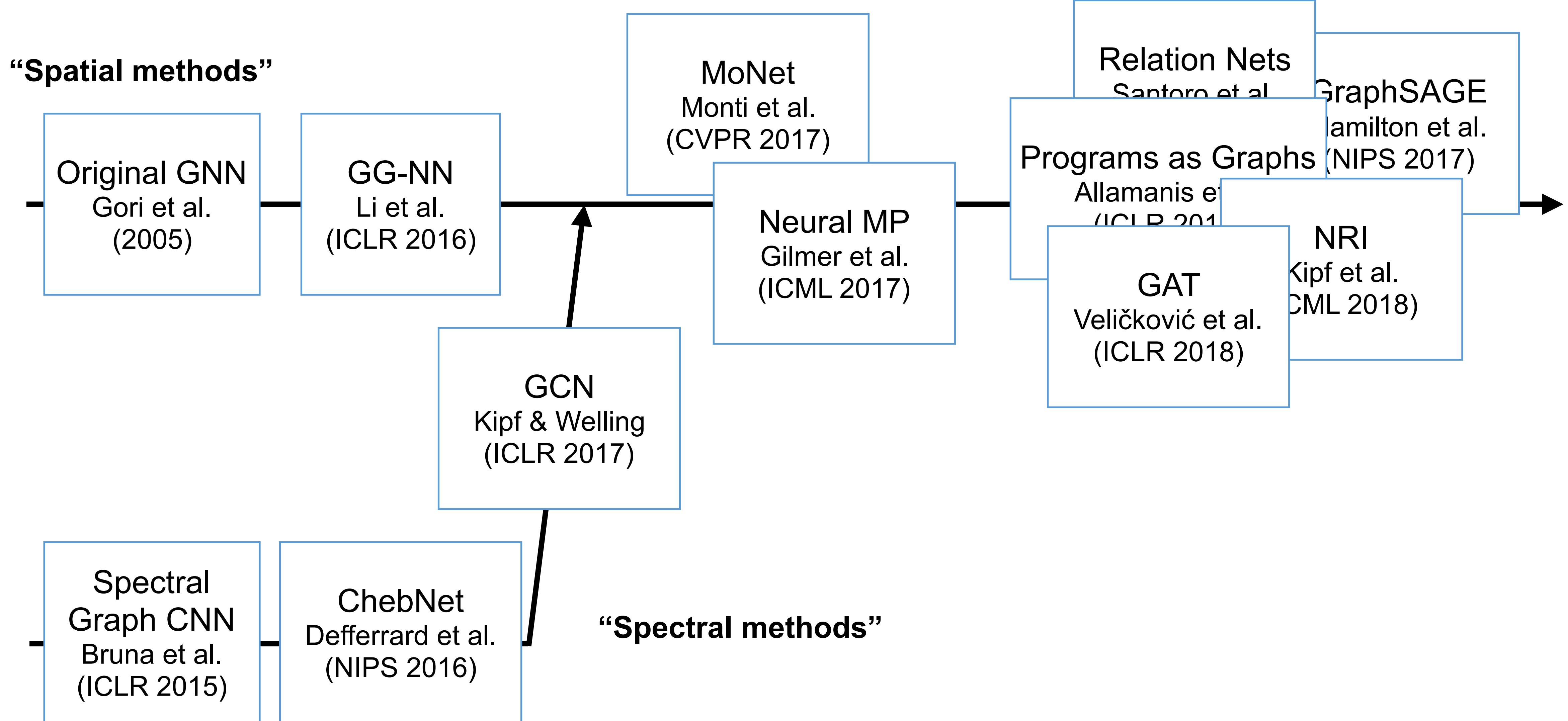
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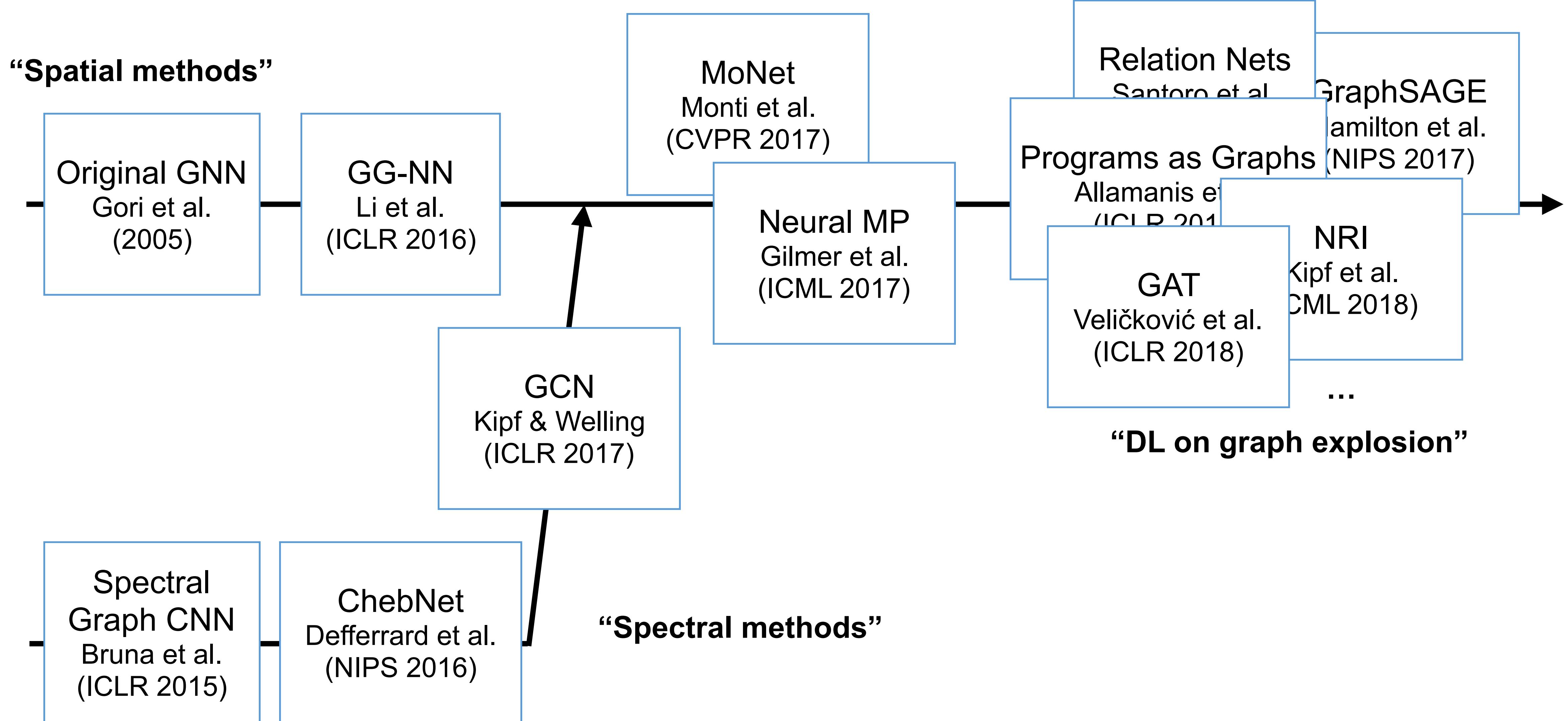
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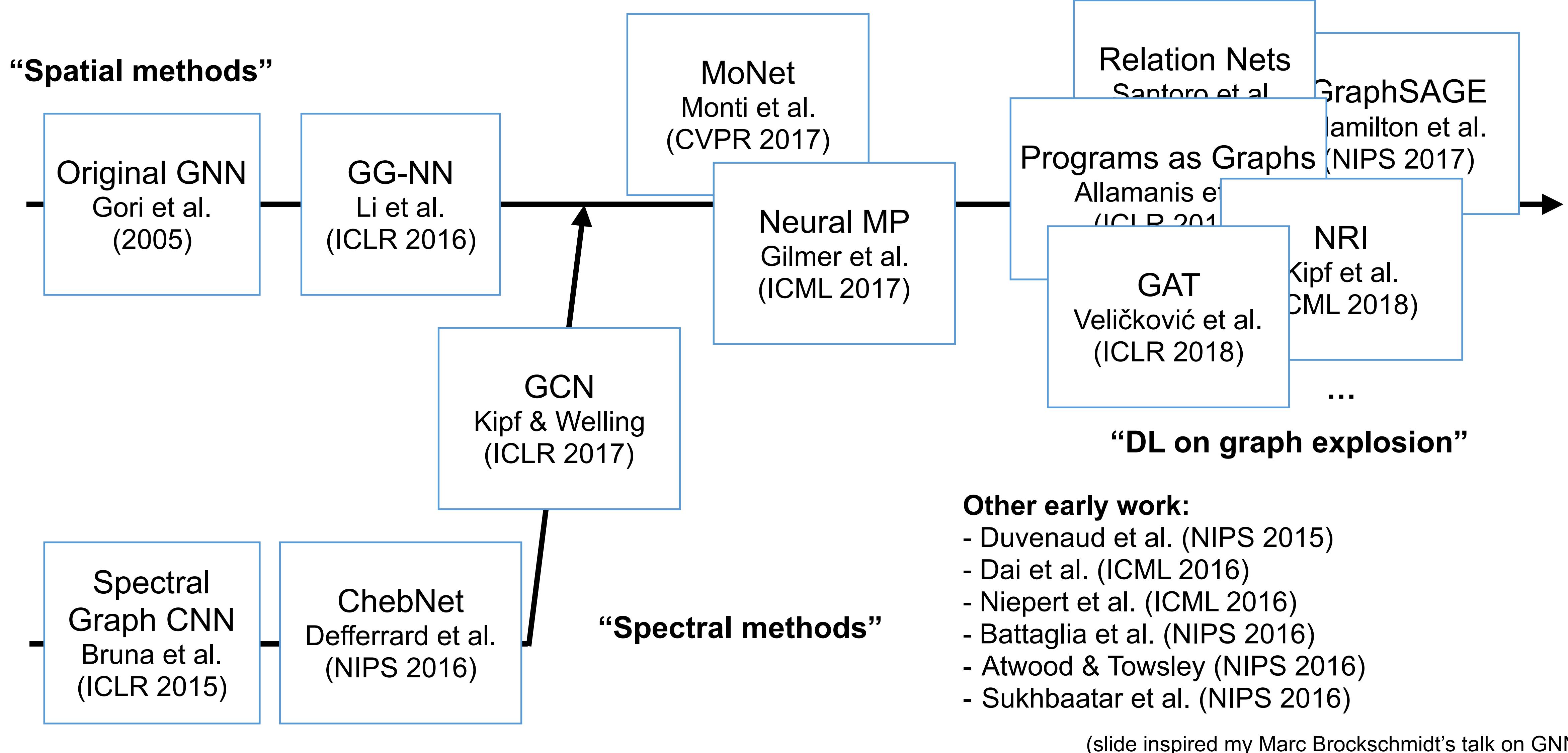
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A brief history of graph neural nets



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A brief history of graph neural nets



Part 2: Application to “classical” network problems

Node classification

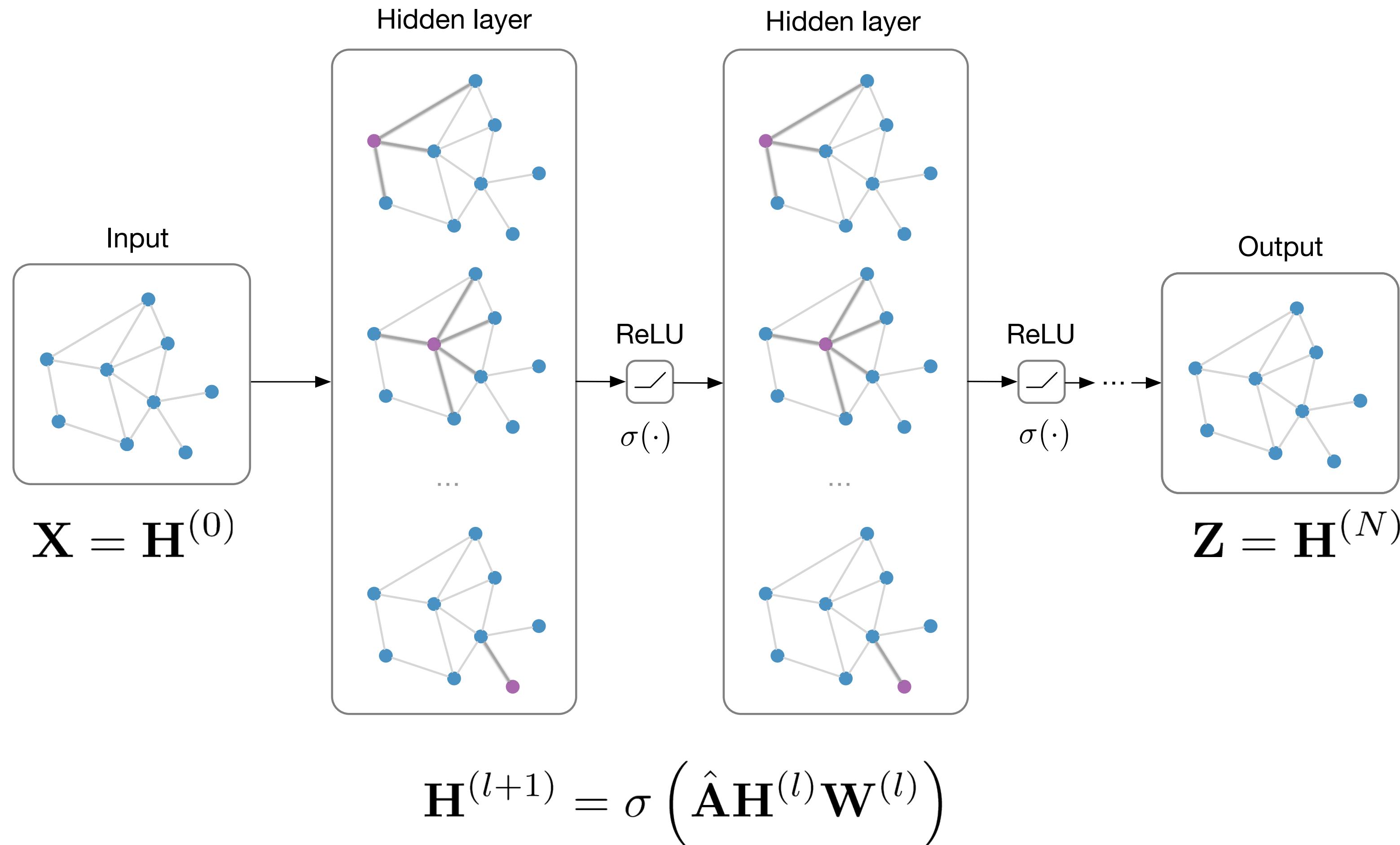
Graph classification

Link prediction



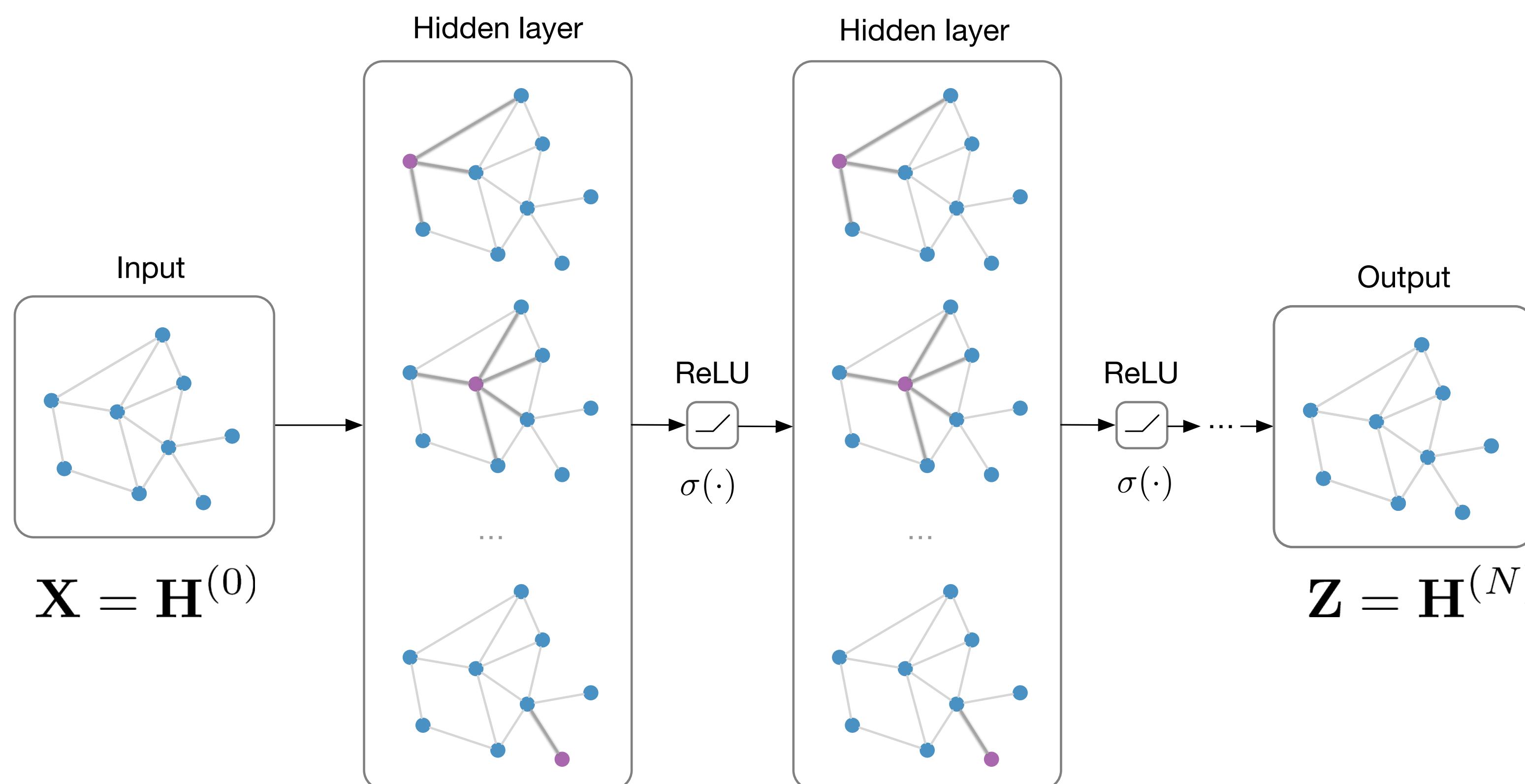
One fits all: Classification and link prediction with GNNs/GCNs

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



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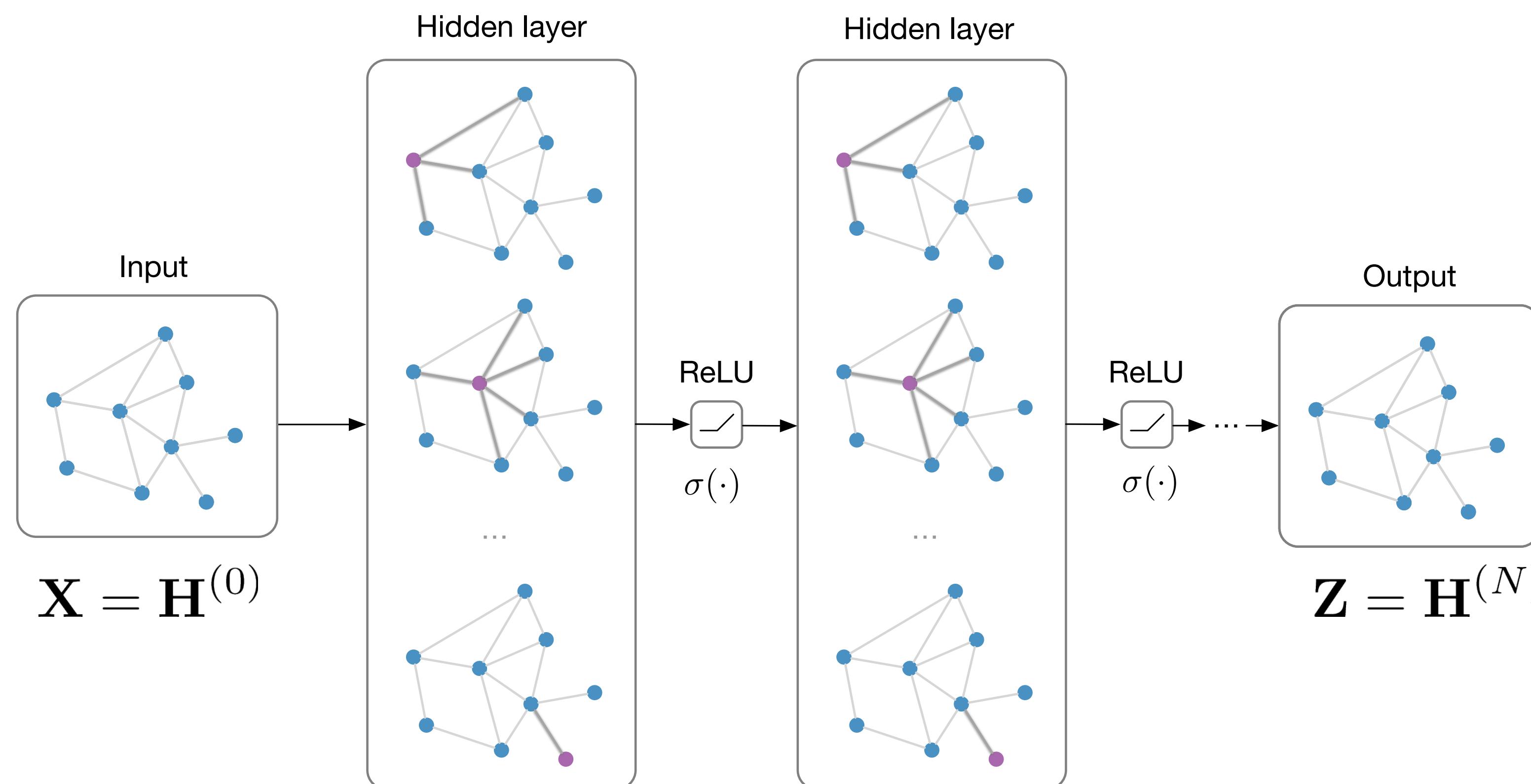


$$\mathbf{H}^{(l+1)} = \sigma \left(\hat{\mathbf{A}} \mathbf{H}^{(l)} \mathbf{W}^{(l)} \right)$$

Node classification:
softmax(\mathbf{z}_n)
e.g. Kipf & Welling (ICLR 2017)

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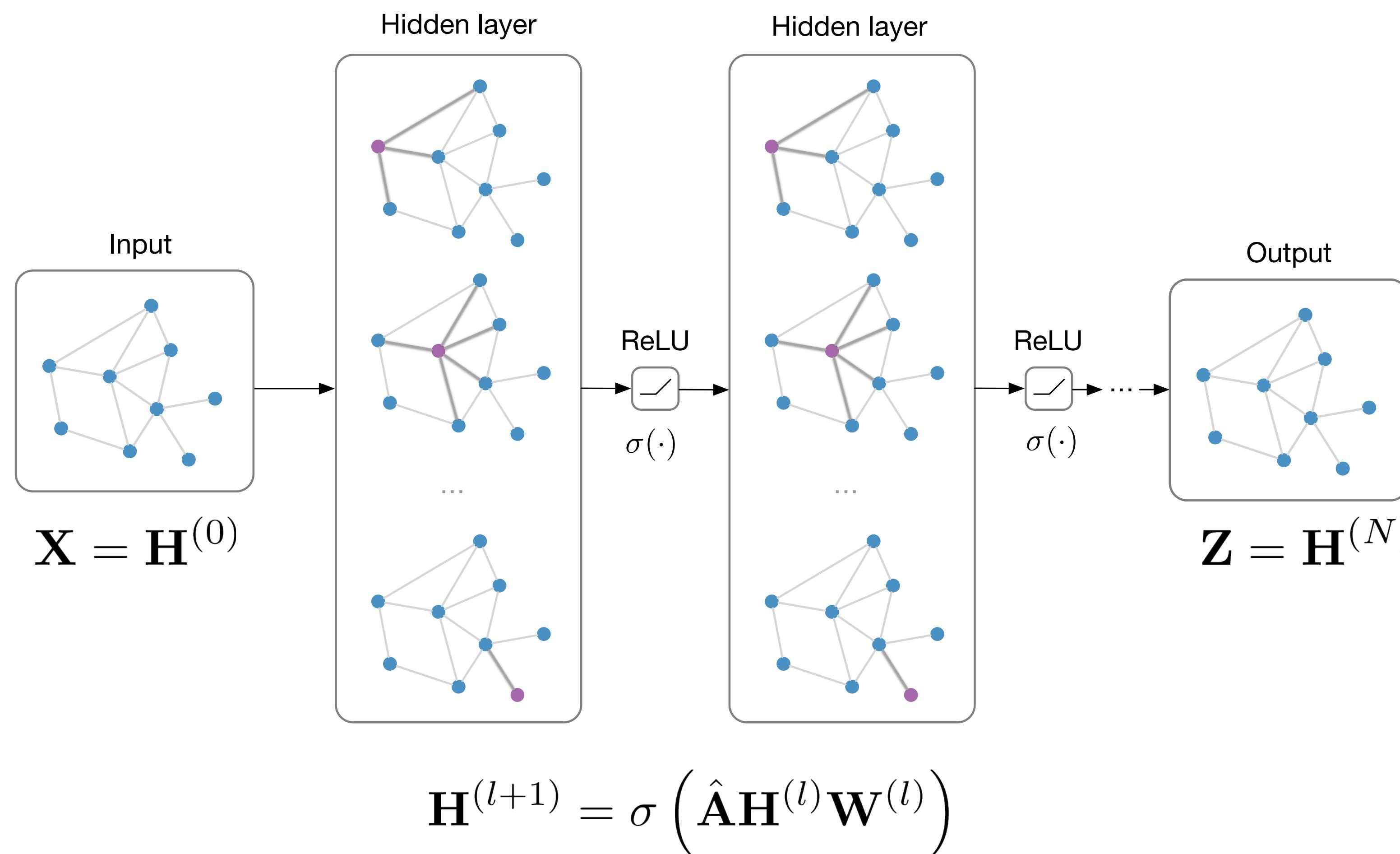


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- Node classification:**
 $\text{softmax}(\mathbf{z}_n)$
e.g. Kipf & Welling (ICLR 2017)
- Graph classification:**
 $\text{softmax}(\sum_n \mathbf{z}_n)$
e.g. Duvenaud et al. (NIPS 2015)

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Link prediction:

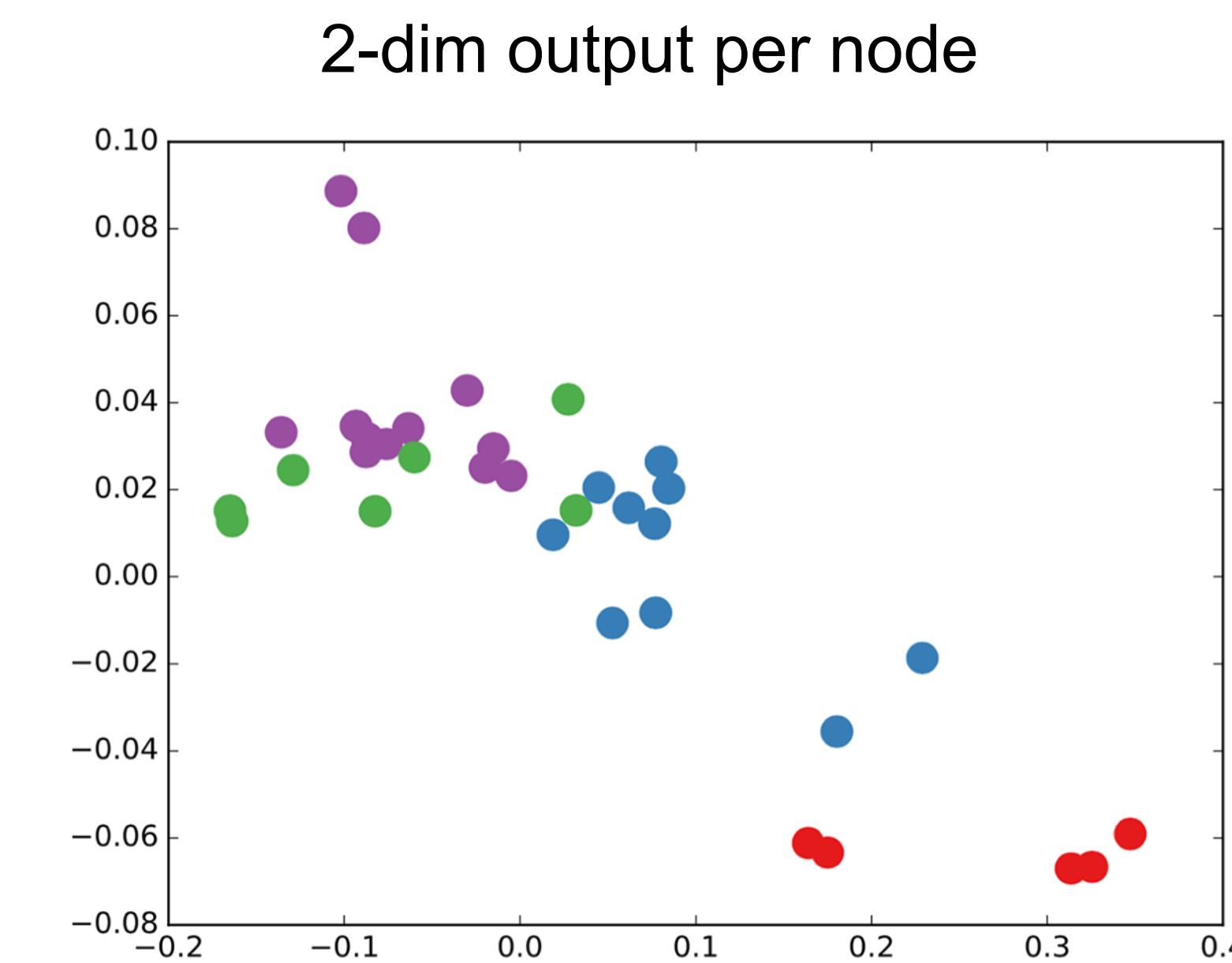
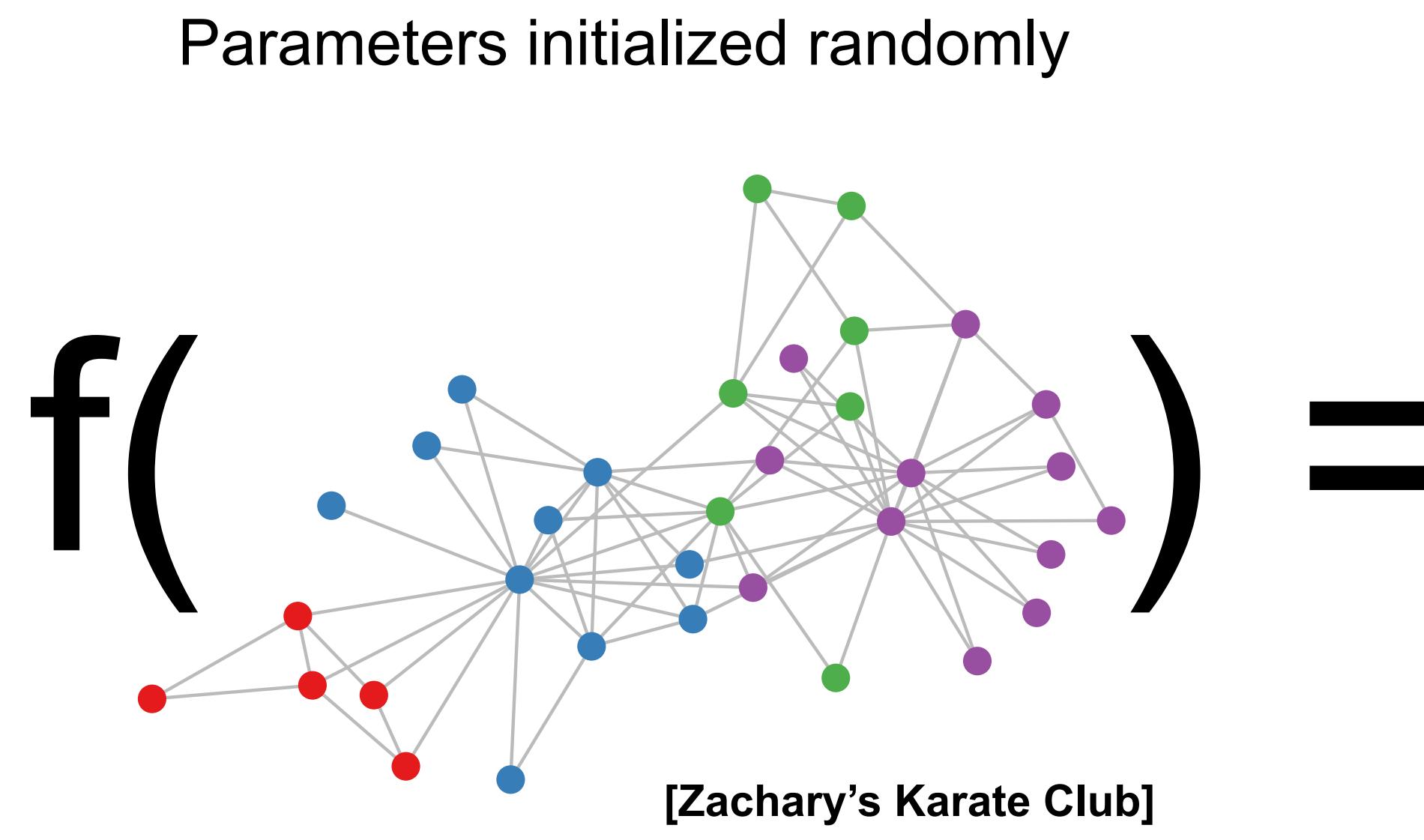
$$p(A_{ij}) = \sigma(\mathbf{z}_i^T \mathbf{z}_j)$$

Kipf & Welling (NIPS BDL 2016)

“Graph Auto-Encoders”

What do learned representations look like?

Forward pass through **untrained** 3-layer GCN model



Semi-supervised classification on graphs

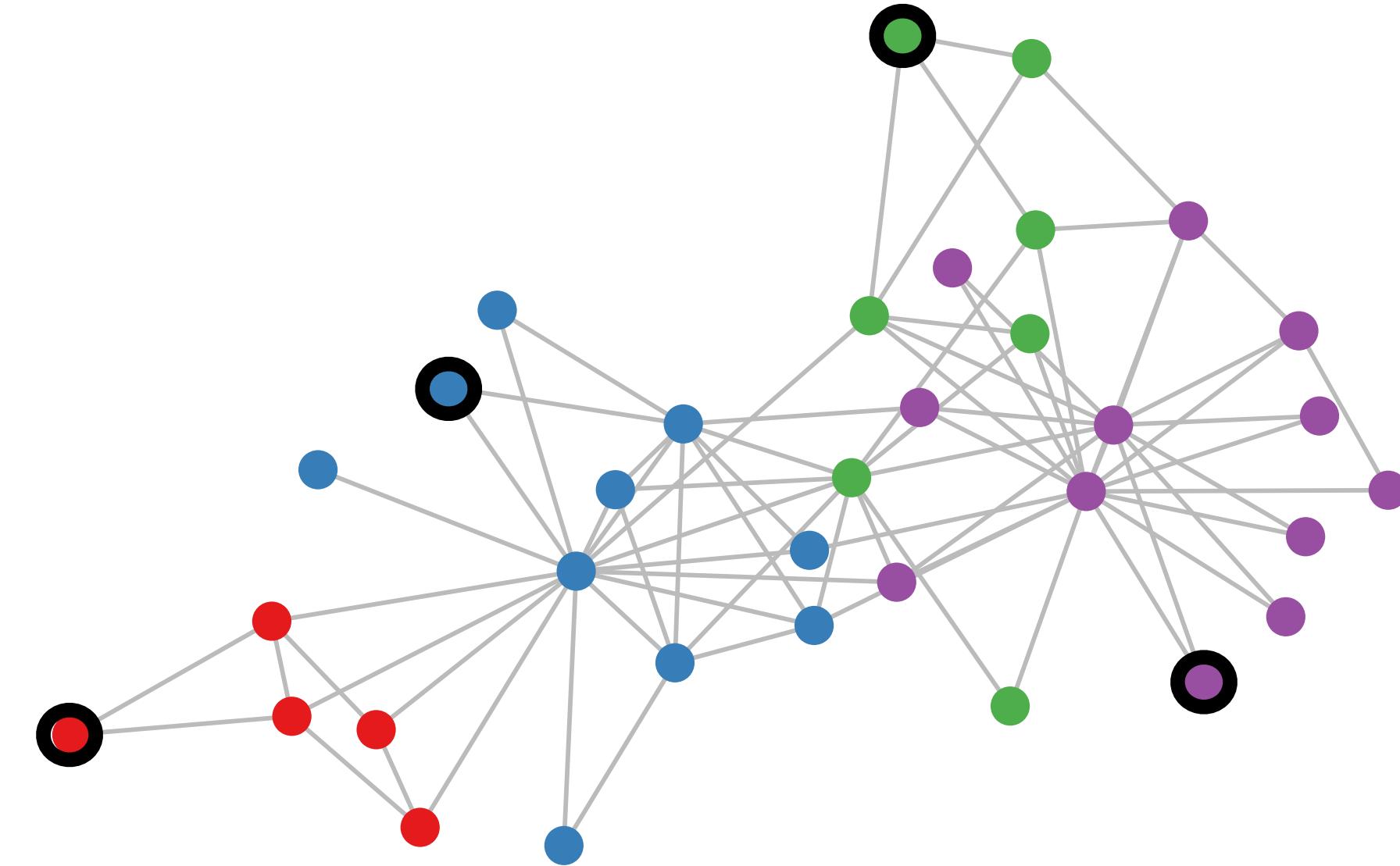
Setting:

Some nodes are labeled (black circle)

All other nodes are unlabeled

Task:

Predict node label of unlabeled nodes



Semi-supervised classification on graphs

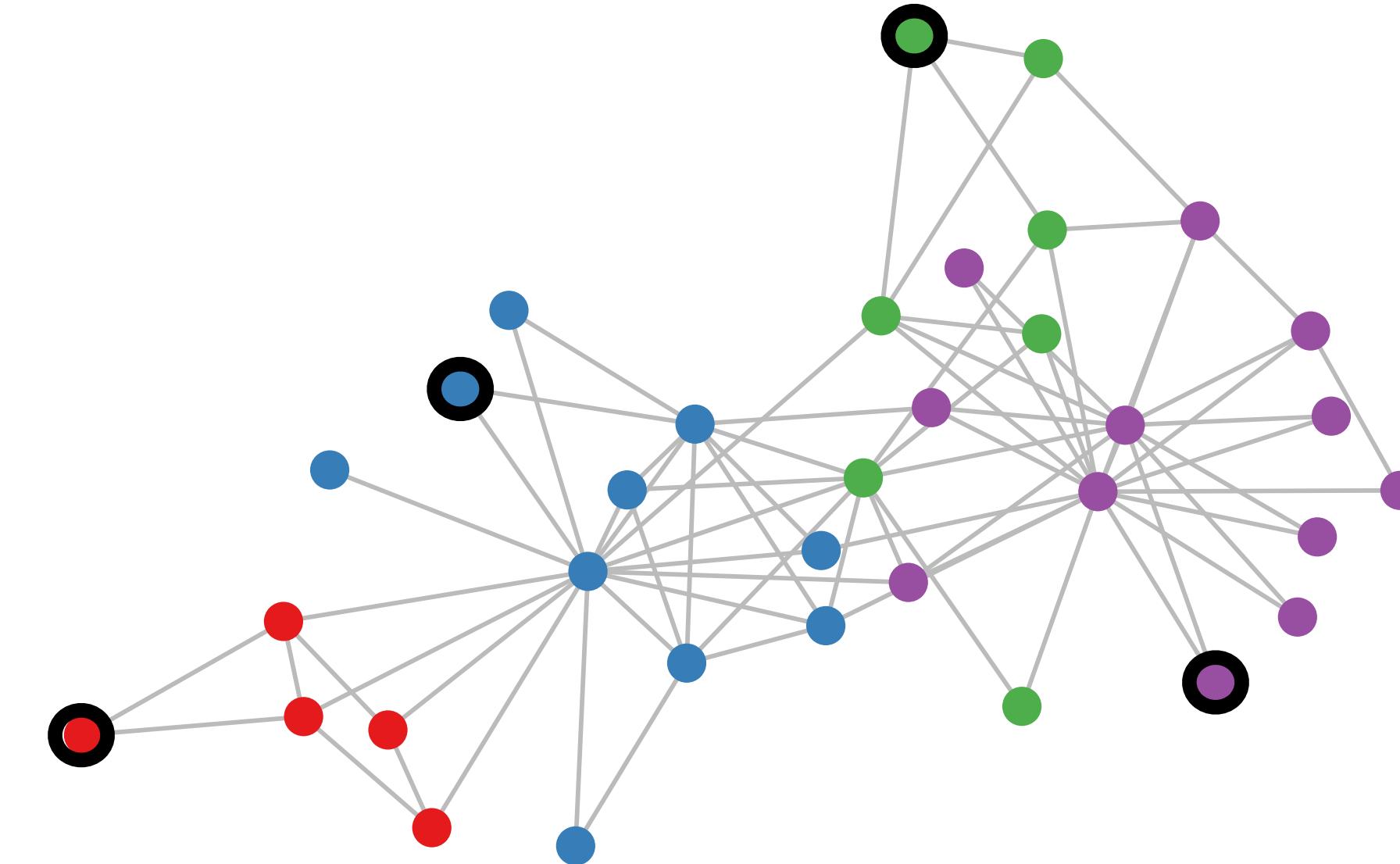
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Evaluate loss on labeled nodes only:

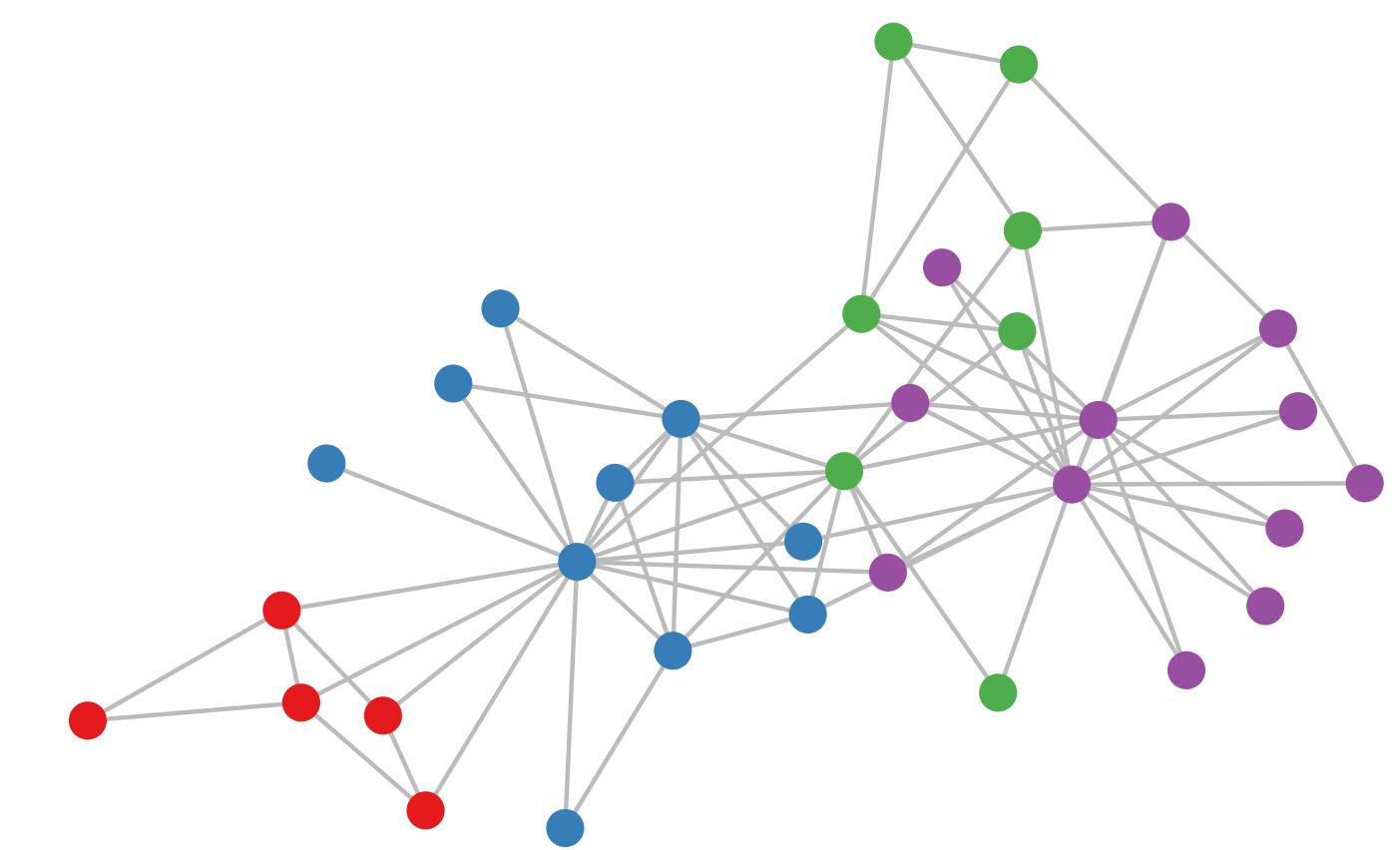
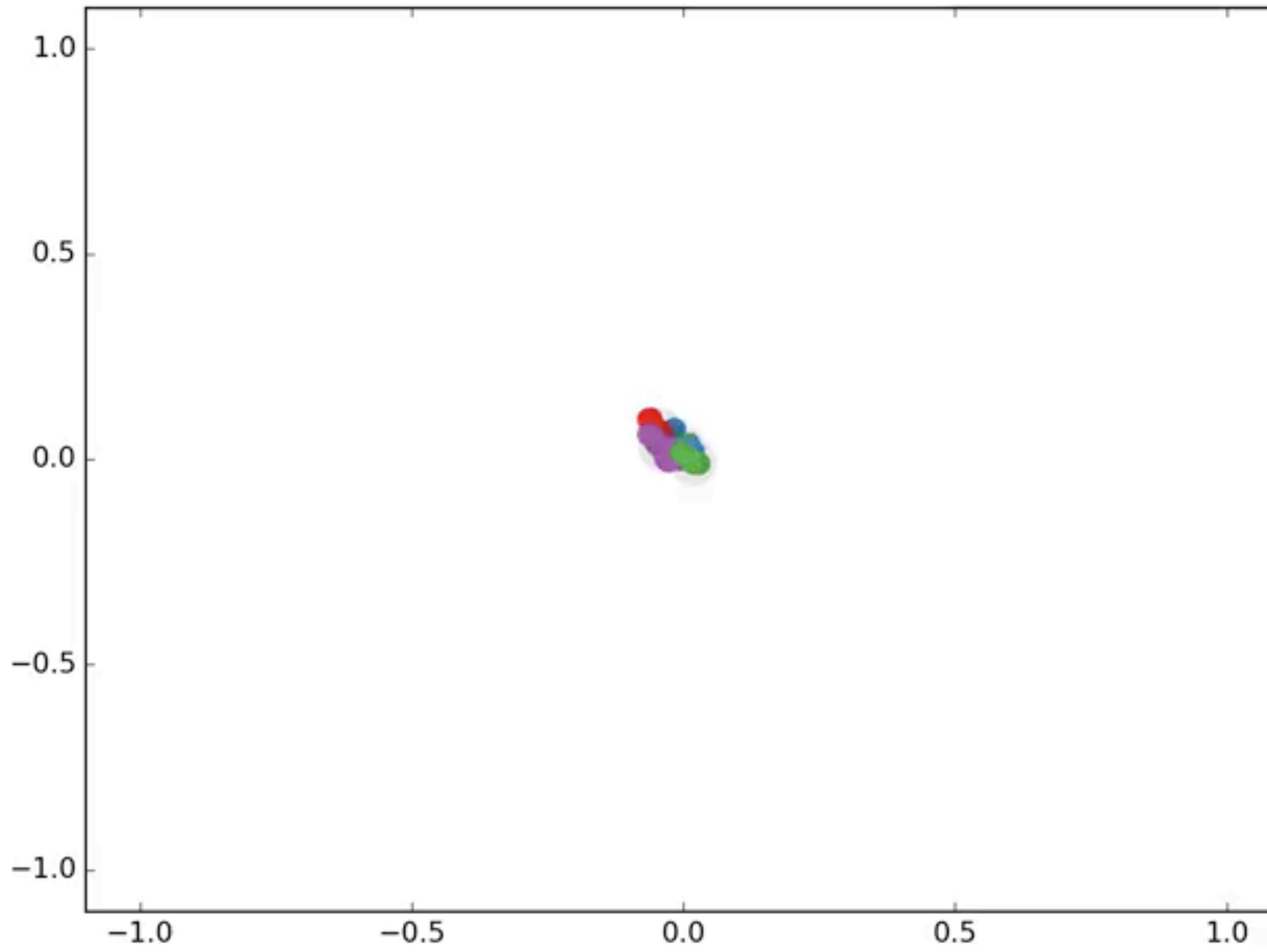
$$\mathcal{L} = - \sum_{l \in \mathcal{Y}_L} \sum_{f=1}^F Y_{lf} \ln Z_{lf}$$

\mathcal{Y}_L set of labeled node indices

\mathbf{Y} label matrix

\mathbf{Z} GCN output (after softmax)

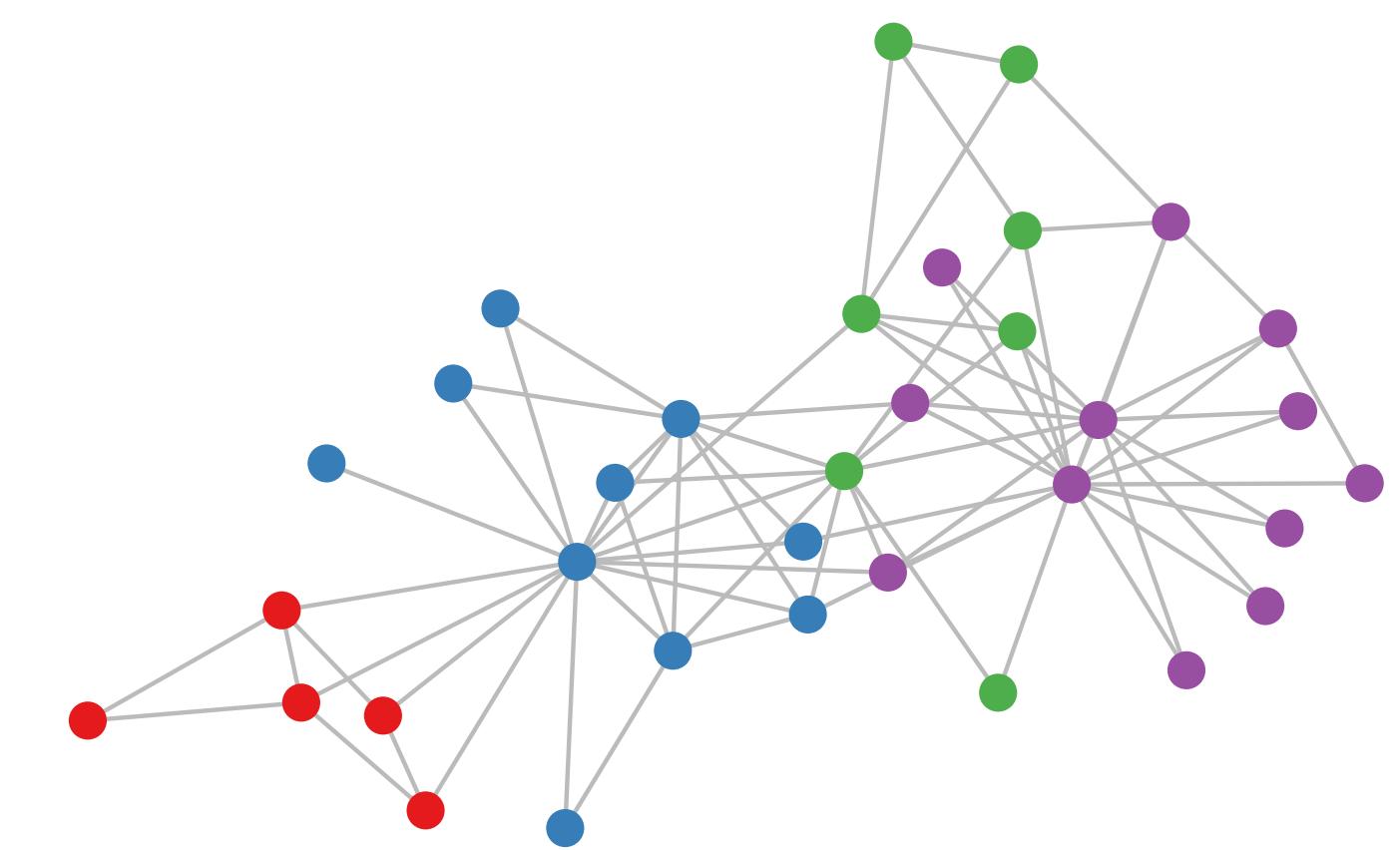
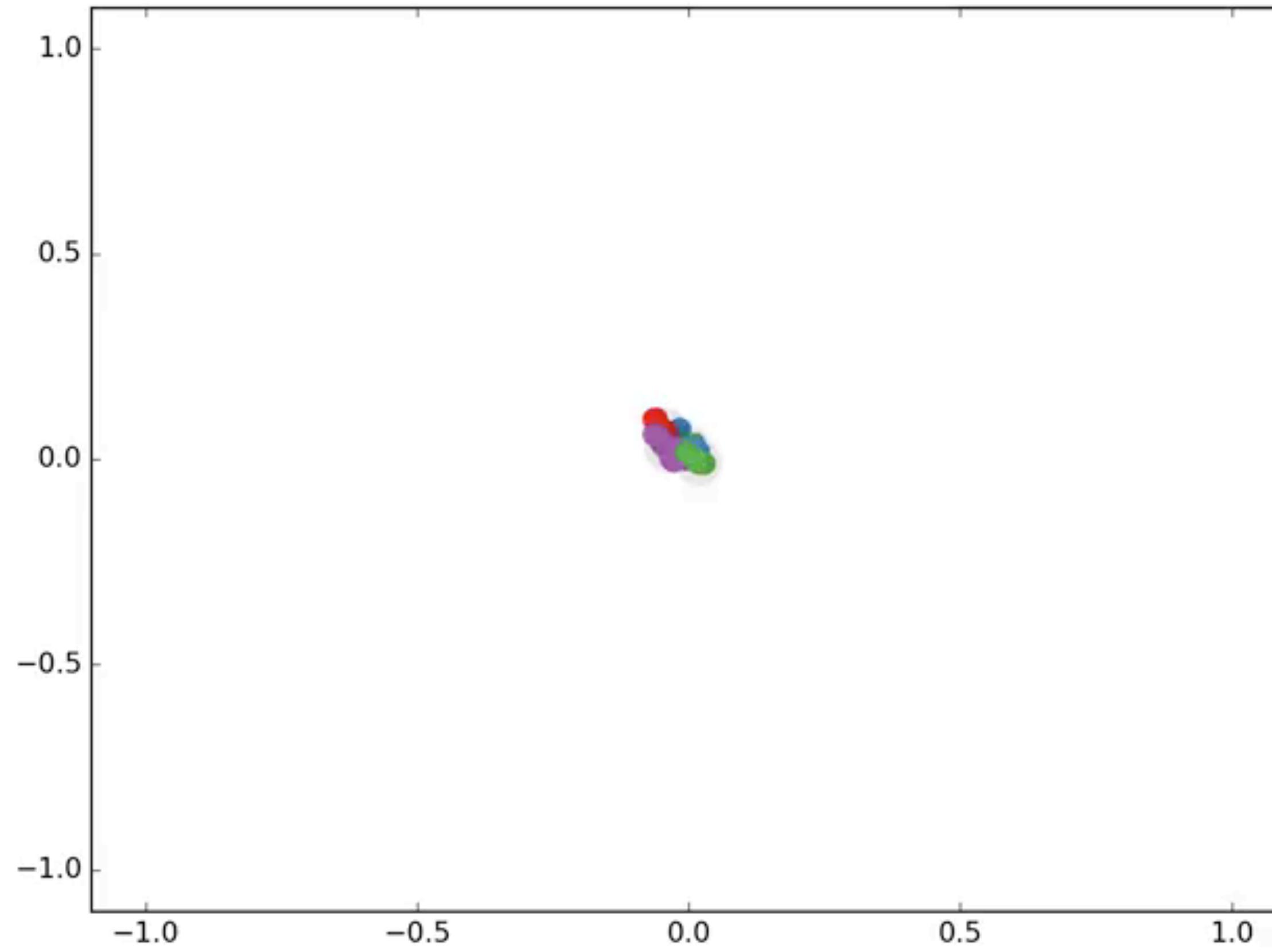
Toy example (semi-supervised learning)



Video also available here:

<http://tkipf.github.io/graph-convolutional-networks>

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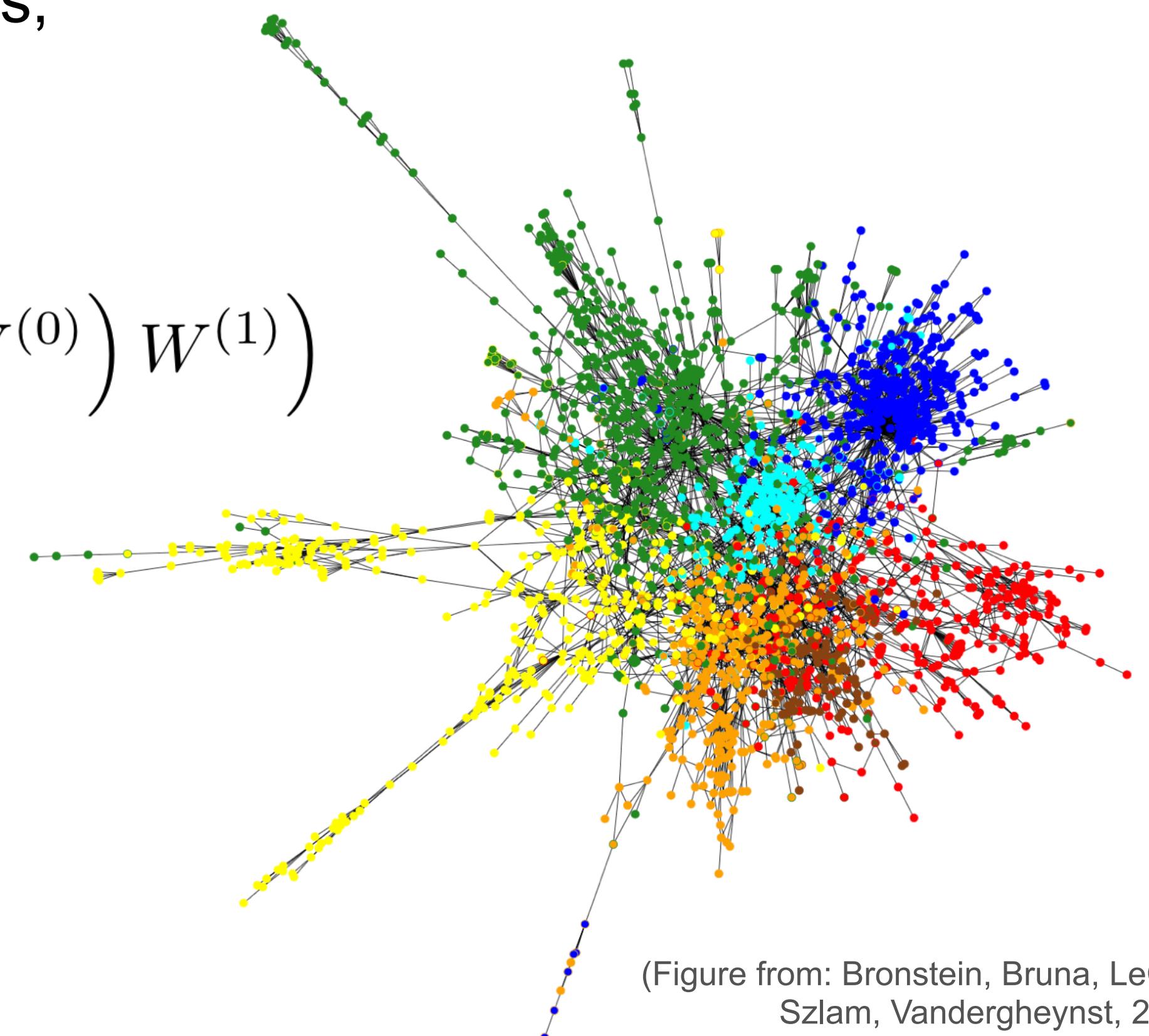
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Application: Classification on citation networks

Input: Citation networks (nodes are papers, edges are citation links,
optionally bag-of-words features on nodes)

Target: Paper category (e.g. stat.ML, cs.LG, ...)

Model: 2-layer GCN $Z = f(X, A) = \text{softmax}\left(\hat{A} \text{ReLU}\left(\hat{A}XW^{(0)}\right) W^{(1)}\right)$



Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017

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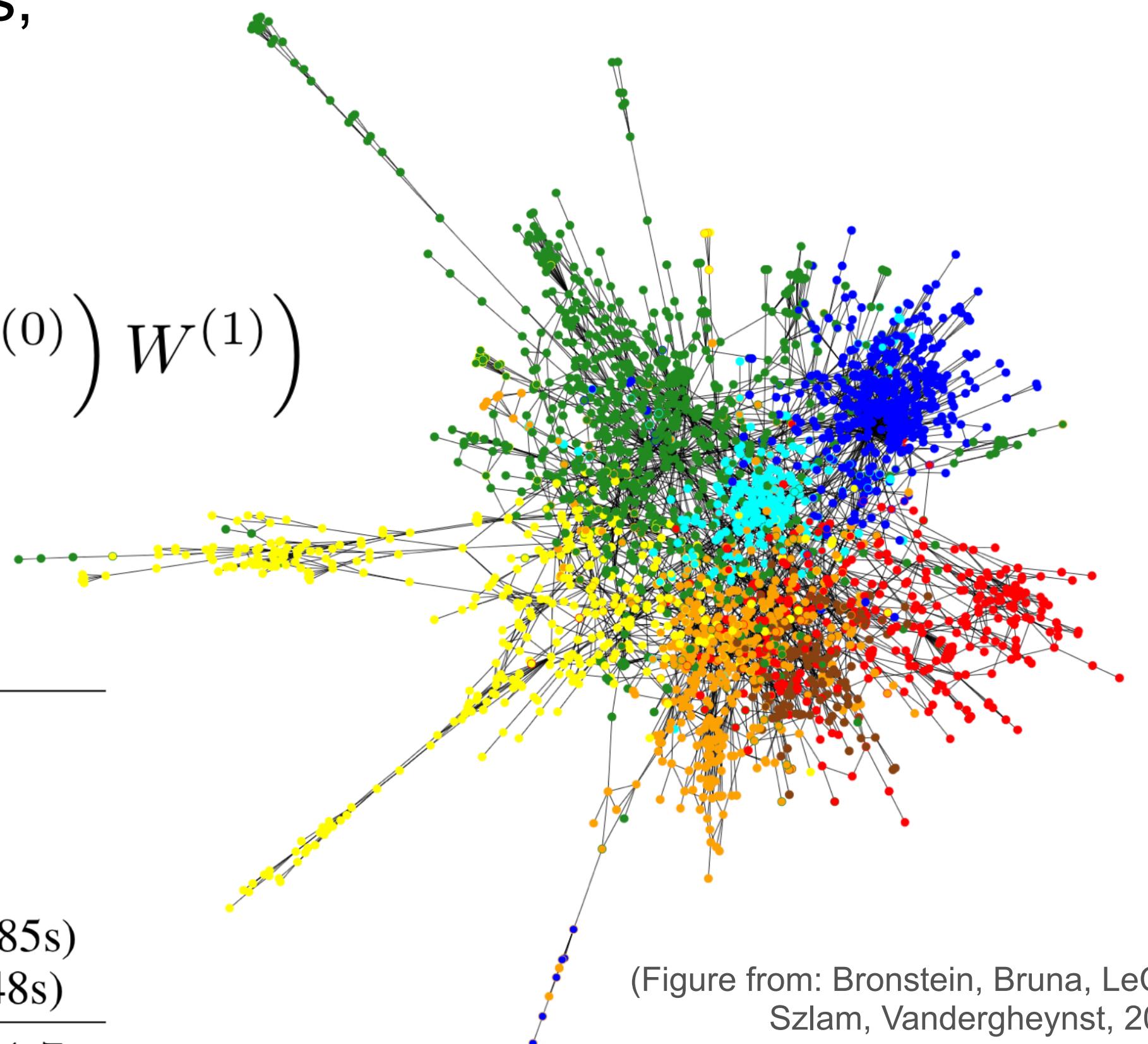
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Classification results (accuracy)

Method	Citeseer	Cora	Pubmed	NELL
ManiReg [3]	60.1	59.5	70.7	21.8
SemiEmb [24]	59.6	59.0	71.1	26.7
LP [27]	45.3	68.0	63.0	26.5
DeepWalk [18]	43.2	67.2	65.3	58.1
Planetoid* [25]	64.7 (26s)	75.7 (13s)	77.2 (25s)	61.9 (185s)
GCN (this paper)	70.3 (7s)	81.5 (4s)	79.0 (38s)	66.0 (48s)
GCN (rand. splits)	67.9 ± 0.5	80.1 ± 0.5	78.9 ± 0.7	58.4 ± 1.7

no input features



Kipf & Welling, Semi-Supervised Classification with Graph Convolutional Networks, ICLR 2017

Part 3: Emerging research directions for structured deep models

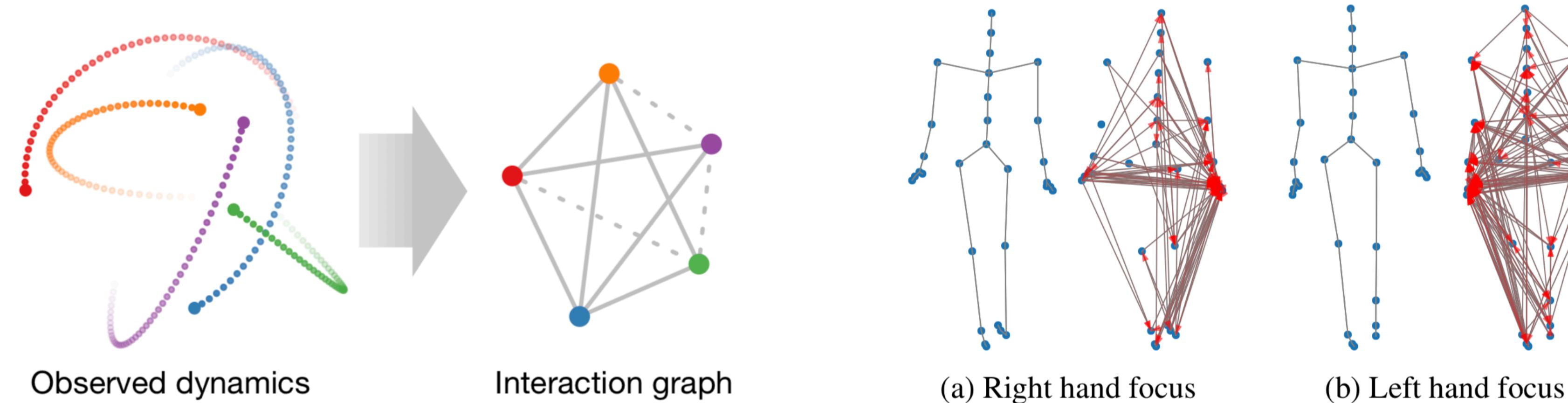
Latent graph inference

Deep generative models for graphs

Latent graph inference

Neural Relational Inference for Interacting Systems

Thomas Kipf^{* 1} Ethan Fetaya^{* 2 3} Kuan-Chieh Wang^{2 3} Max Welling^{1 4} Richard Zemel^{2 3 4}

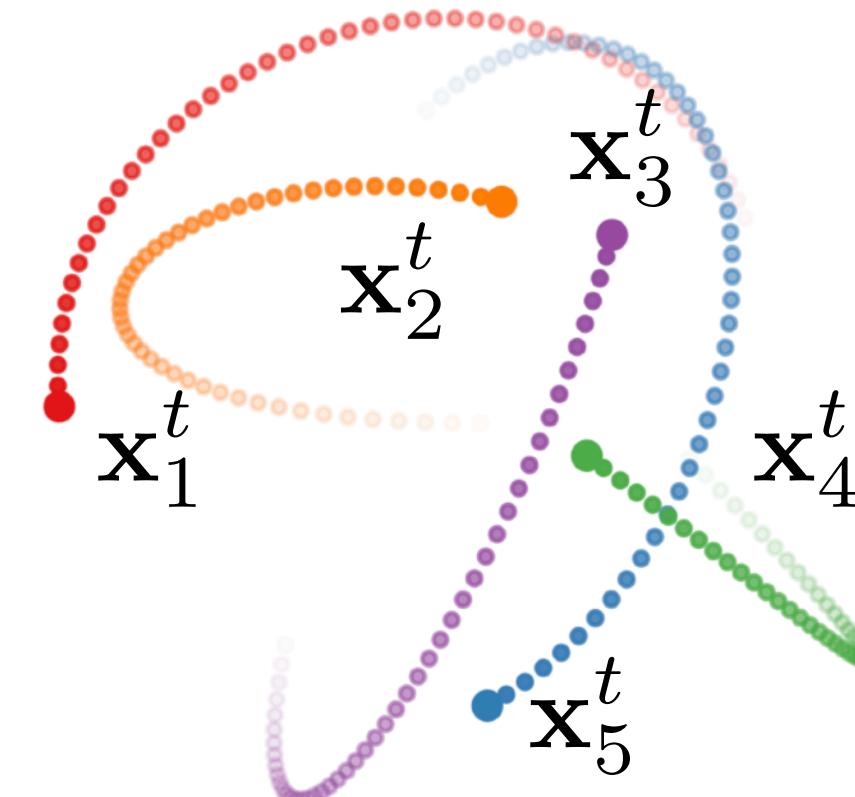


To be presented at ICML 2018!

Motivation: Learning physical dynamics

Need to model **interactions** and their **effect on dynamics**

Simple example:



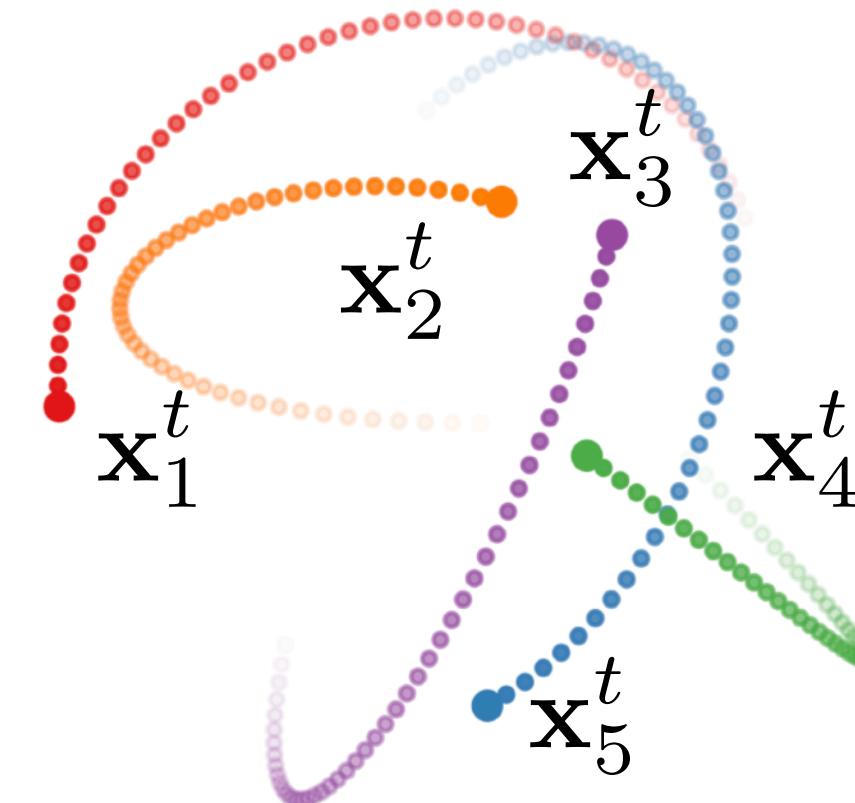
Observed dynamics

- 5 particles + their trajectories \mathbf{x}_i^t
- Concatenate feature vectors
$$\mathbf{x}^t = [\mathbf{x}_1^t, \mathbf{x}_2^t, \dots, \mathbf{x}_5^t]$$
- Feed into neural net
$$\mathbf{x}^{t+1} = \text{MLP}(\mathbf{x}^t) \text{ (or RNN)}$$

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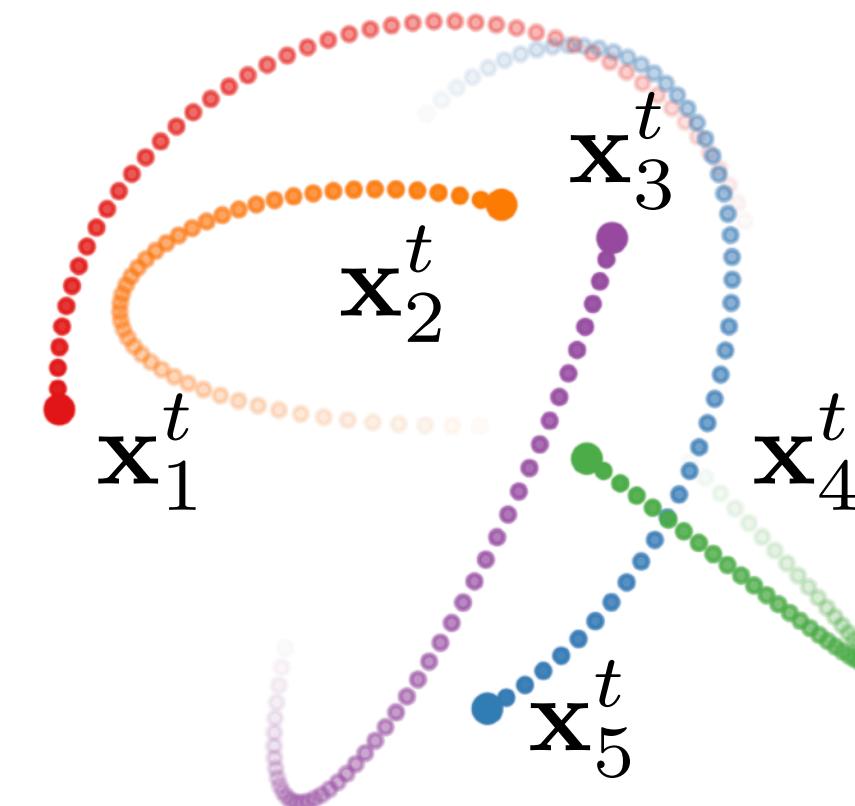
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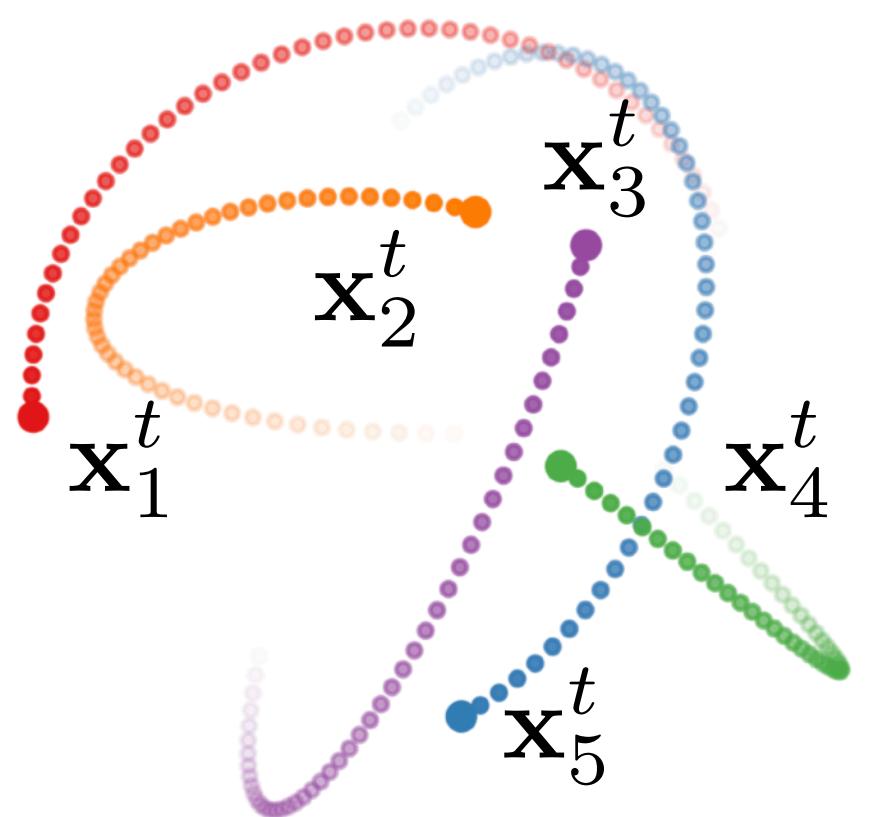
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- Done?

Works (somewhat), but we can do a lot better.

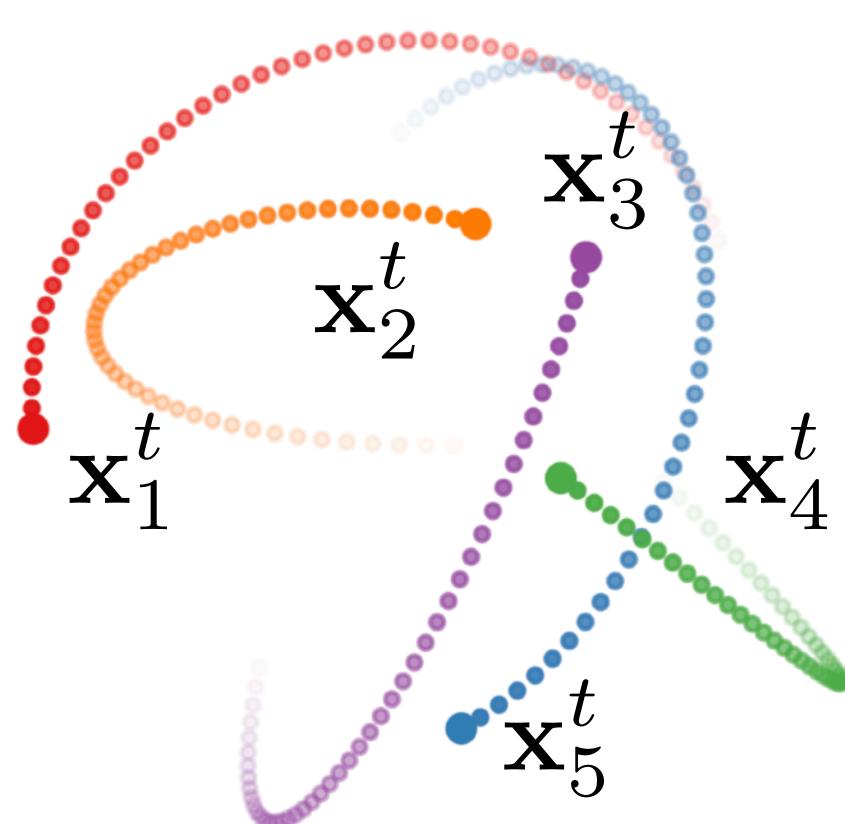
A naïve model of Intuitive Physics

Problems:



Observed dynamics

A naïve model of Intuitive Physics

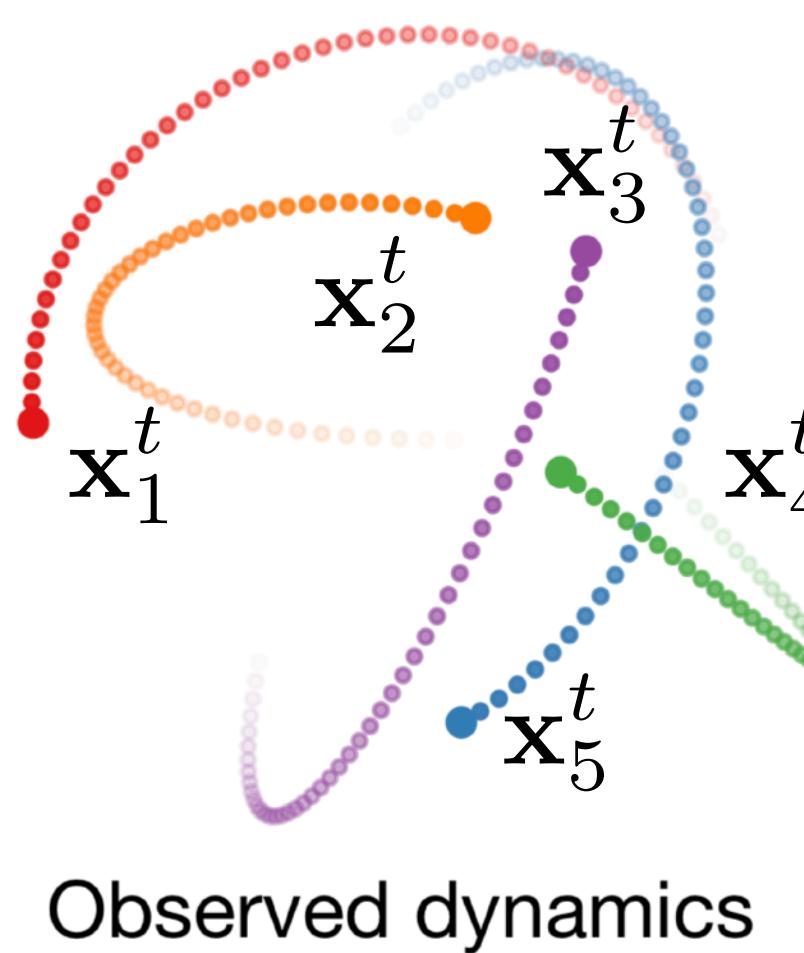


Observed dynamics

Problems:

- Arbitrary ordering of nodes
→ Need permutation equivariance

A naïve model of Intuitive Physics

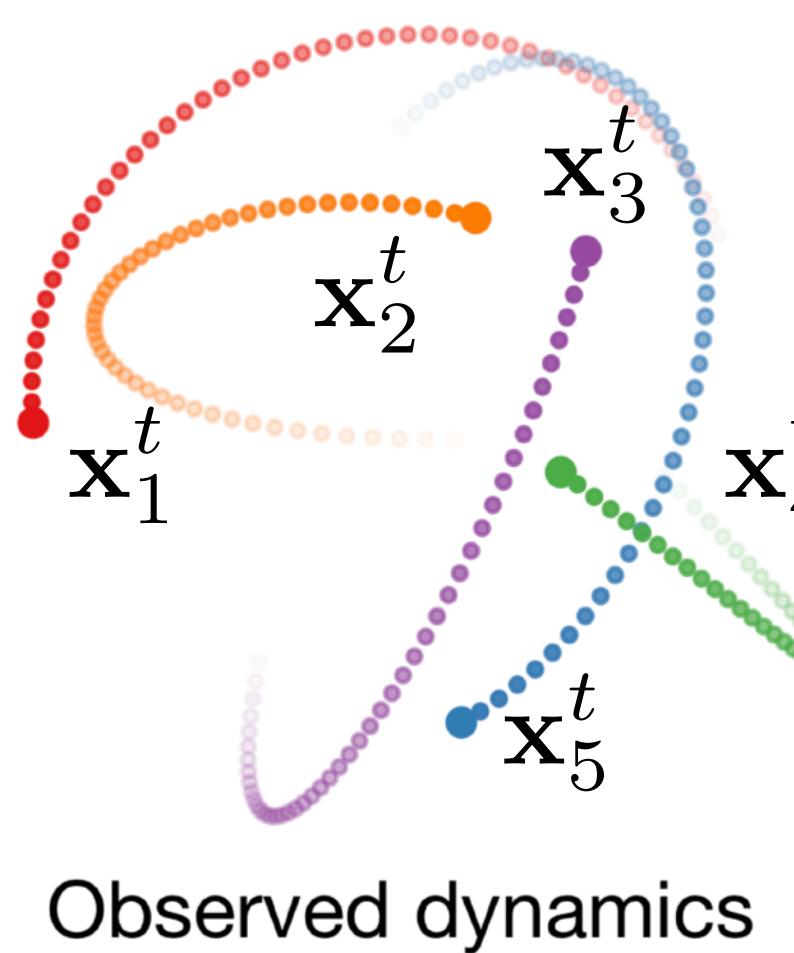


Observed dynamics

Problems:

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- Model doesn't know about **structure** of interactions
 - For many fundamental physical systems, interactions are **pairwise**

A naïve model of Intuitive Physics

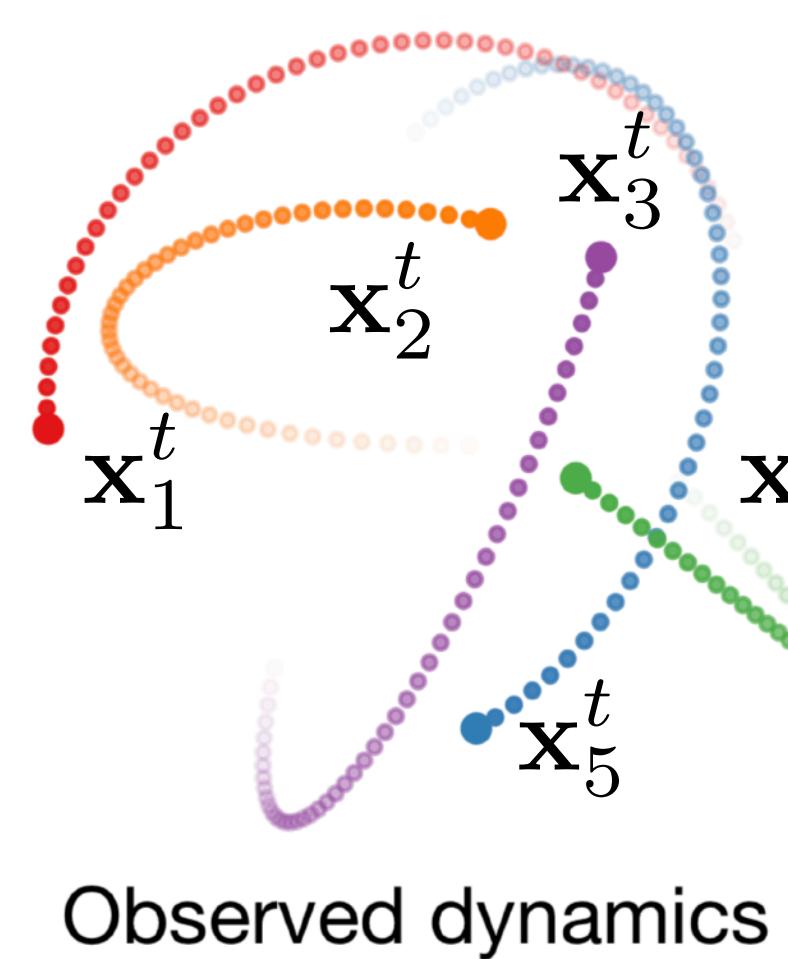


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Structured neural models to the rescue!

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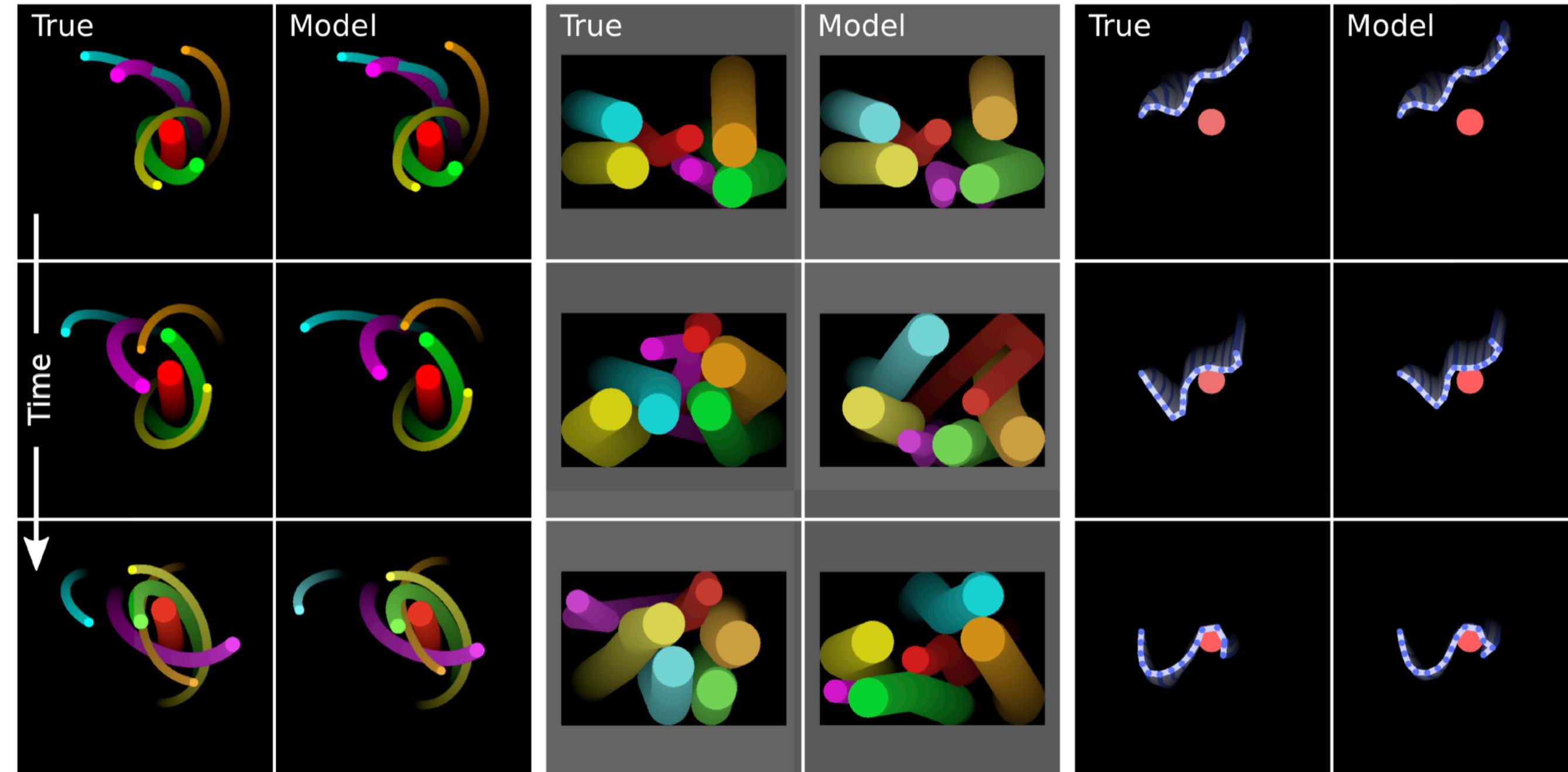
Structured neural models to the rescue!

Graph Neural Networks (GNNs) are an ideal candidate.

GNNs for interacting systems

Using GNNs, we can learn to model physical dynamics of interacting systems with very high precision

if we know about the underlying **structure** of the interactions and their **types** (should there be different types)



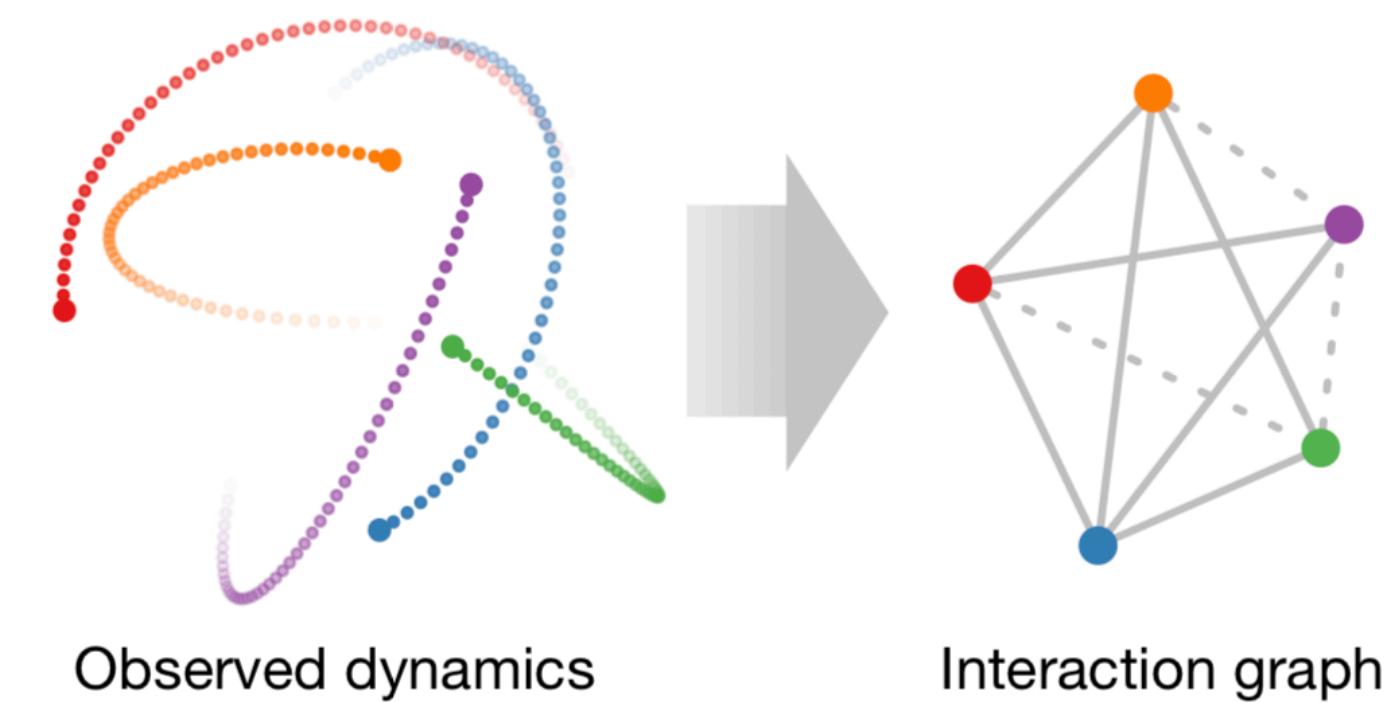
Battaglia et al., (NIPS 2016)

Neural Relational Inference for Interacting Systems

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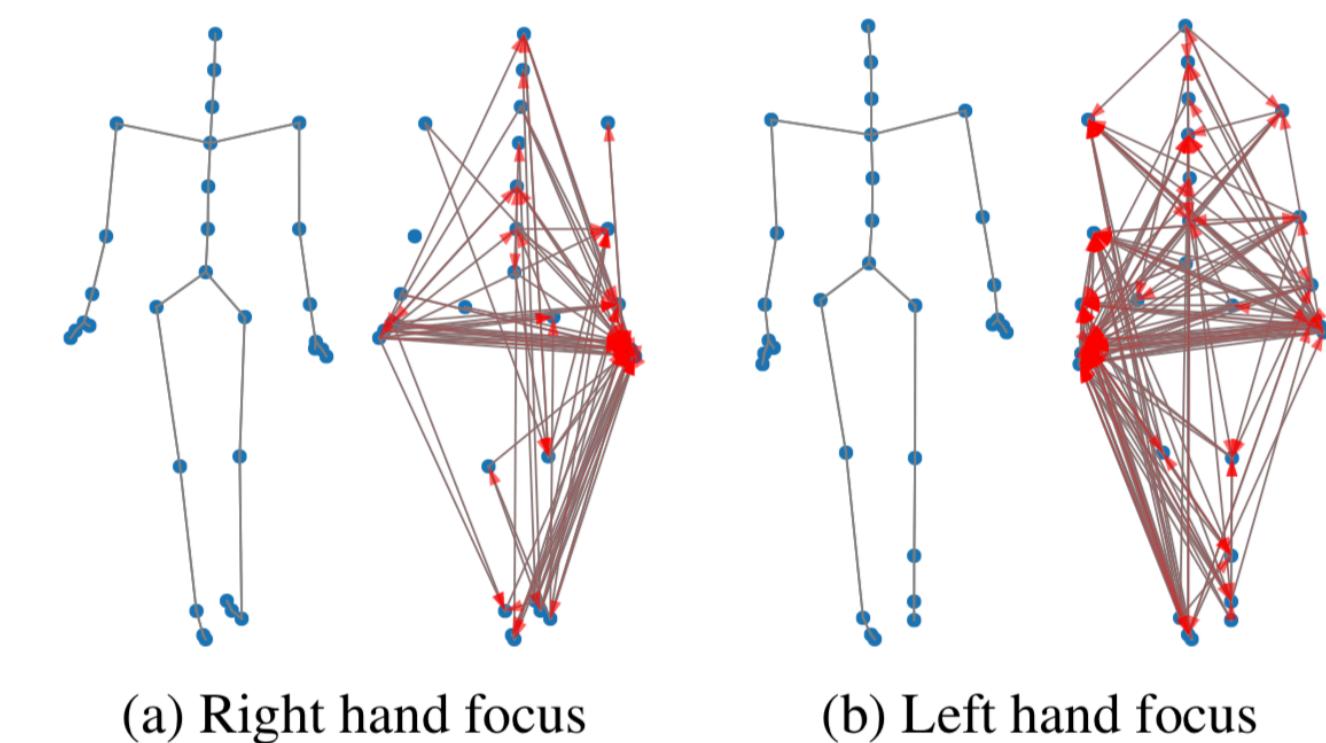
Our work (ICML 2018):

1. Learn dynamics of interacting system **without** knowing structure of interactions
2. Infer **latent interaction graph** (plus edge types) using a VAE
3. Applications for **physical systems, motion capture data and multi-agent systems**

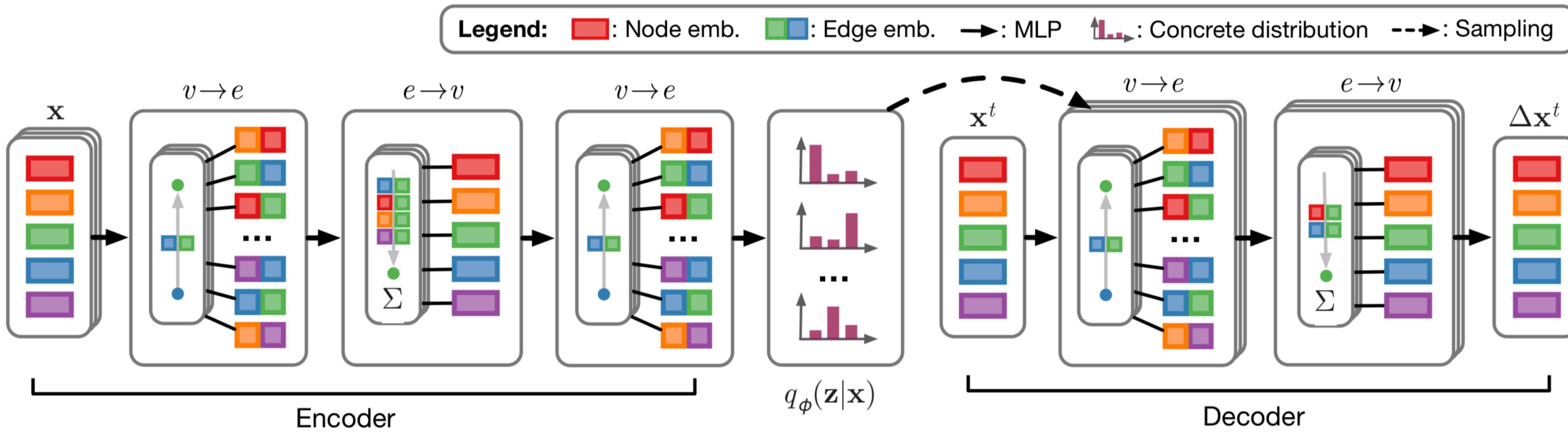


Observed dynamics

Interaction graph



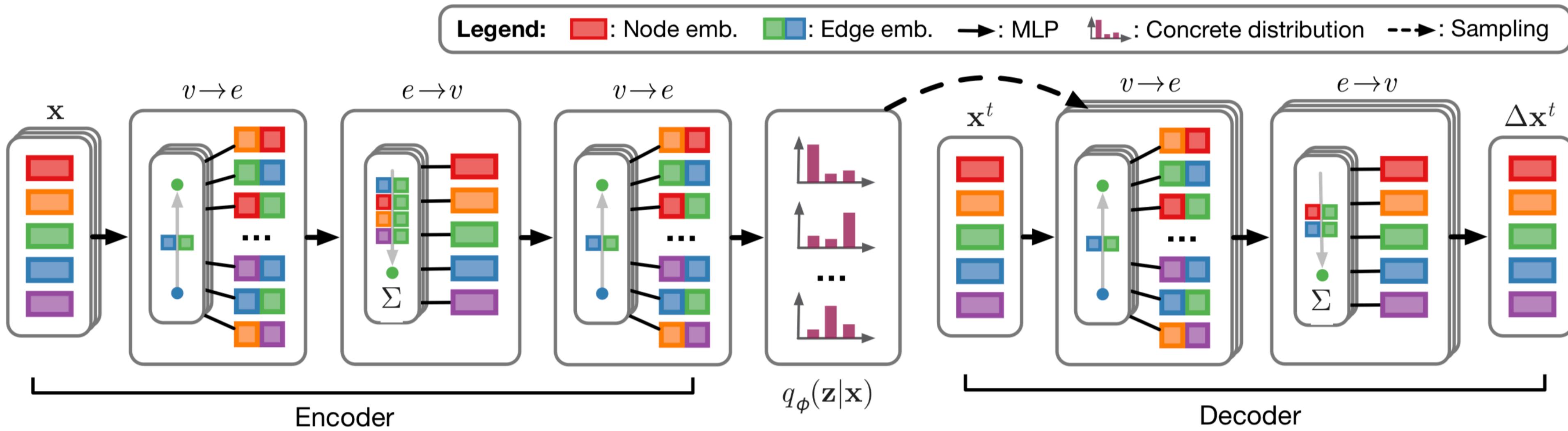
Neural Relational Inference - Model overview



Model: Variational auto-encoder with (discrete) edge types as discrete latent variables

Encoder and decoder are GNN-based!

Neural Relational Inference - Model overview



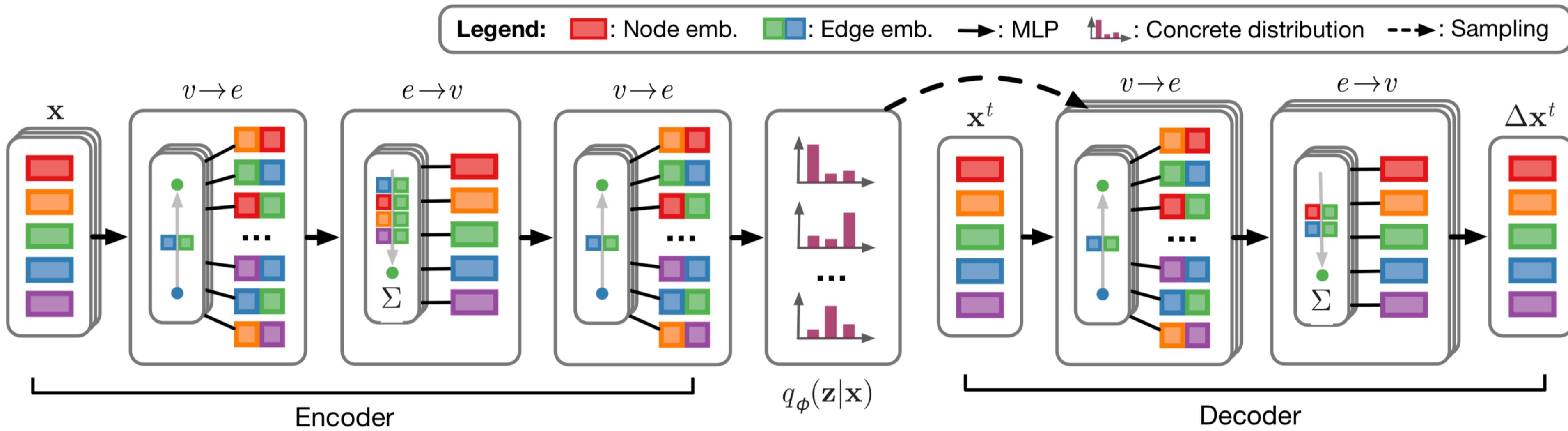
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Encoder and decoder are GNN-based!

Main intuition:

- Encoder **generates hypothesis** on how the system interacts
- Decoder **learns a dynamical model** constrained by the encoder's “interaction hypothesis”

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- Encoder **generates hypothesis** on how the system interacts
- Decoder **learns a dynamical model** constrained by the encoder's "interaction hypothesis"

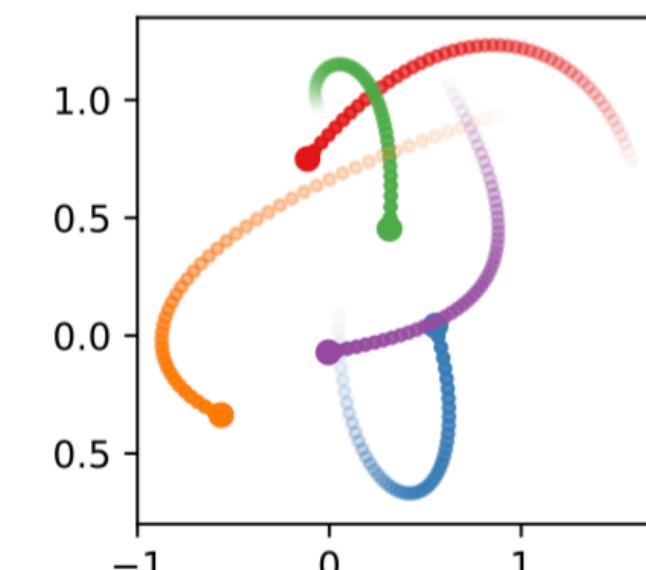
Trained jointly using **Gumbel softmax trick** as straight-through gradient estimator

Yang et al. (ICLR 2017), Maddison et al. (ICLR 2017)

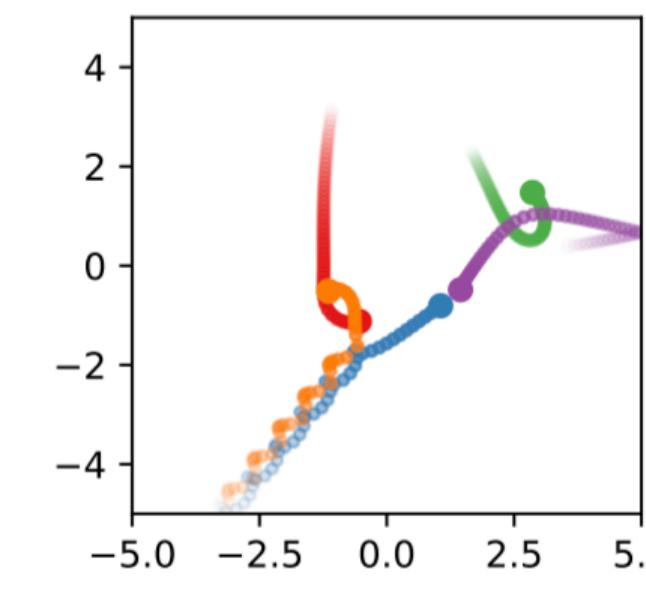
Learning latent interaction graphs

Table 1. Accuracy (in %) of unsupervised interaction recovery.

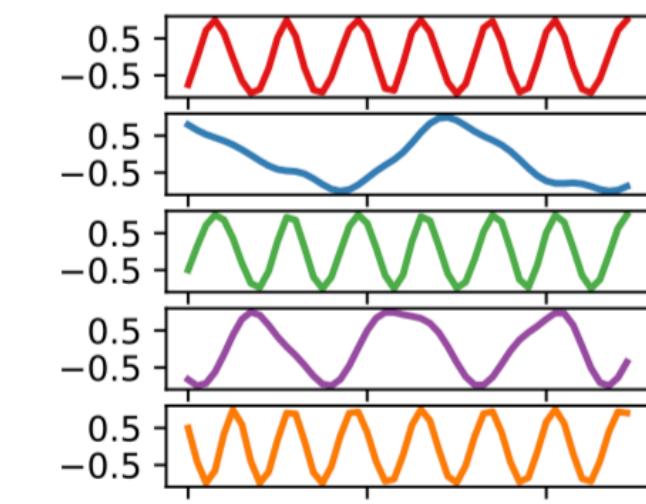
Model	Springs	Charged	Kuramoto
5 objects			
Corr. (path)	52.4	55.8	62.8
Corr. (LSTM)	55.0	61.8	55.9
NRI (sim.)	99.9	59.1	—
NRI (learned)	99.8	82.6	96.0
Supervised	99.9	96.3	99.8
10 objects			
Corr. (path)	50.4	51.4	59.3
Corr. (LSTM)	51.0	52.9	53.9
NRI (sim.)	98.2	53.9	—
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Springs (2D)



Charged (2D)

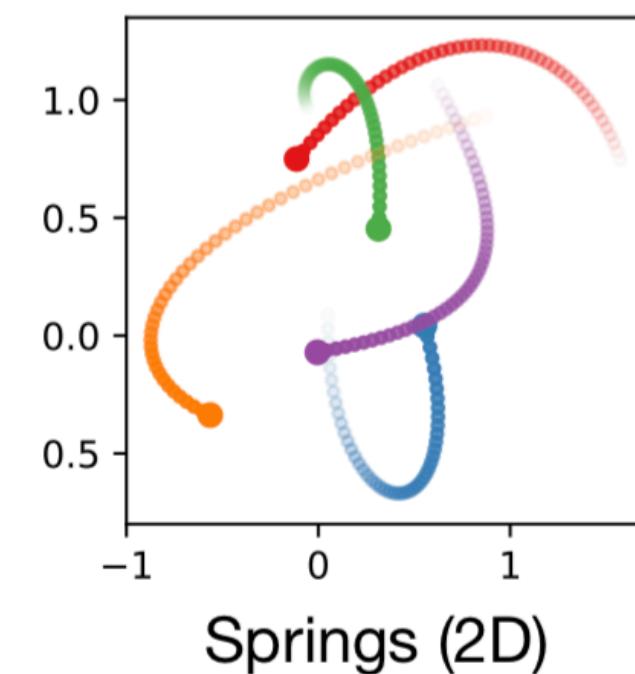


Kuramoto (1D)

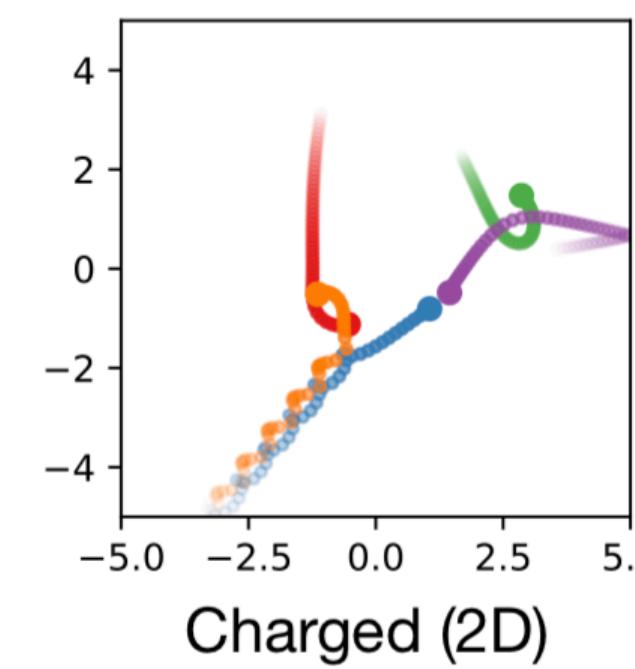
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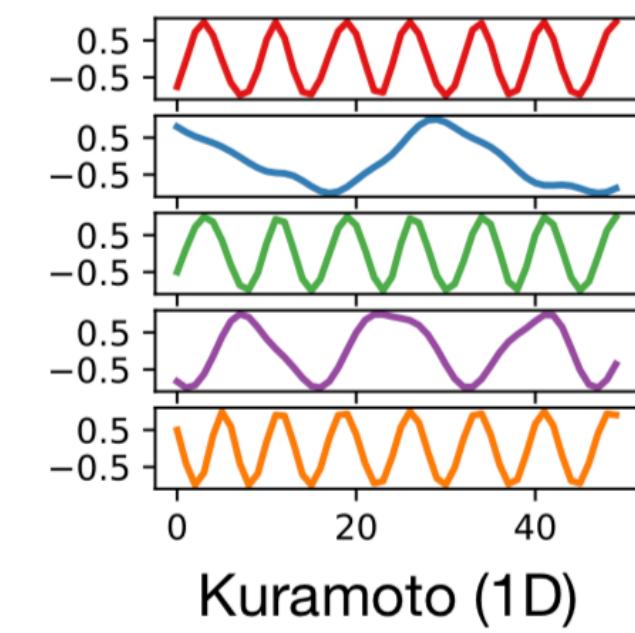
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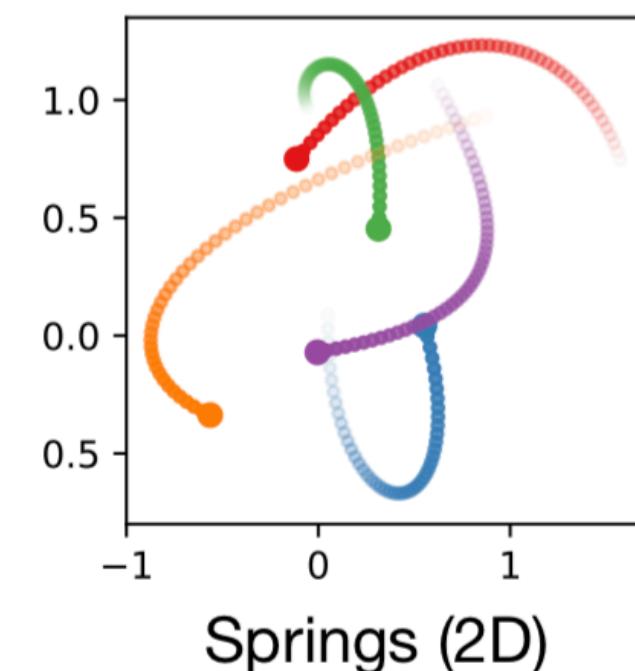
Kuramoto (1D)

**NRI can learn to discover
ground-truth relations
with very high accuracy!**

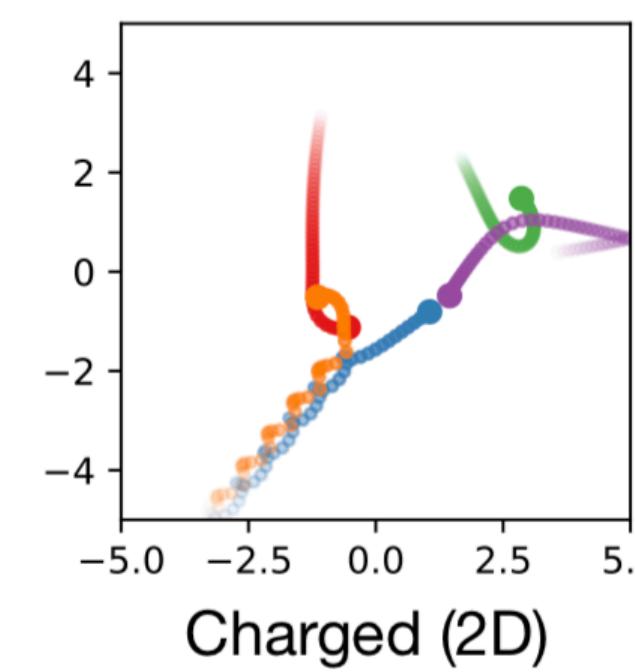
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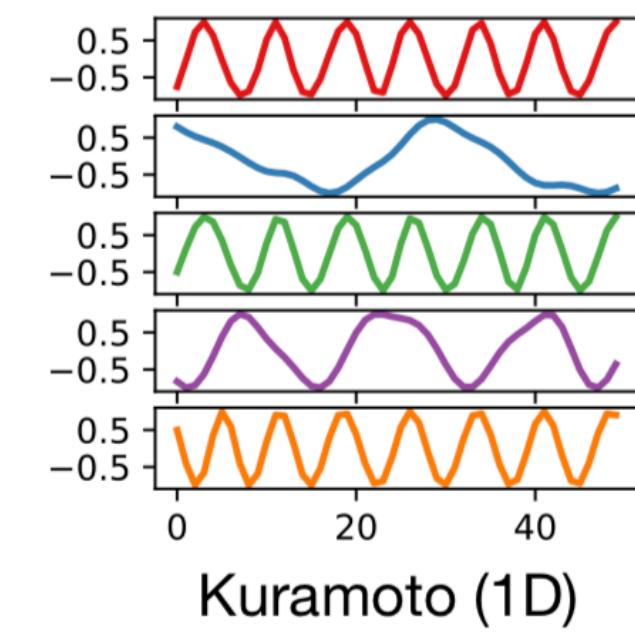
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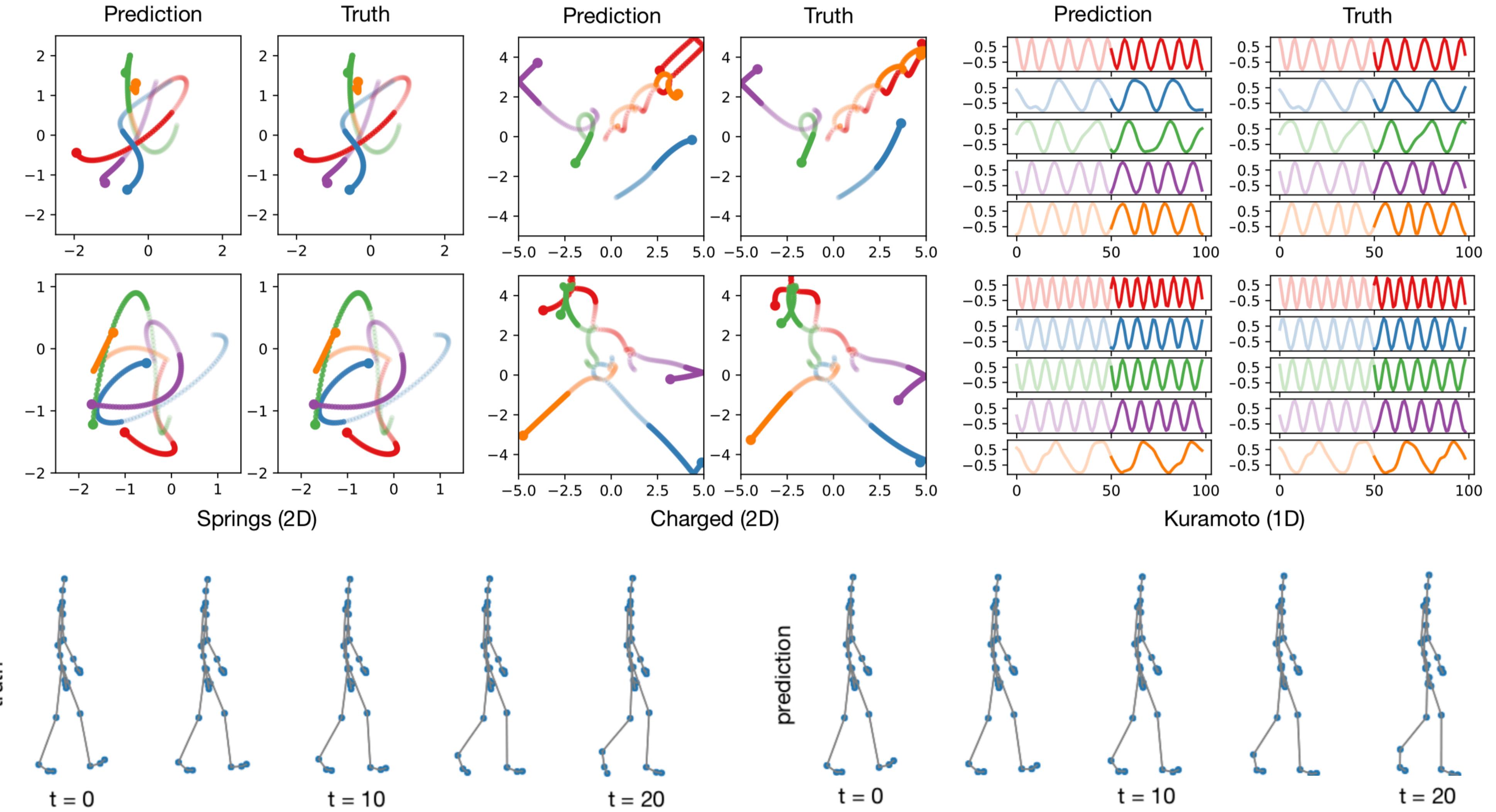
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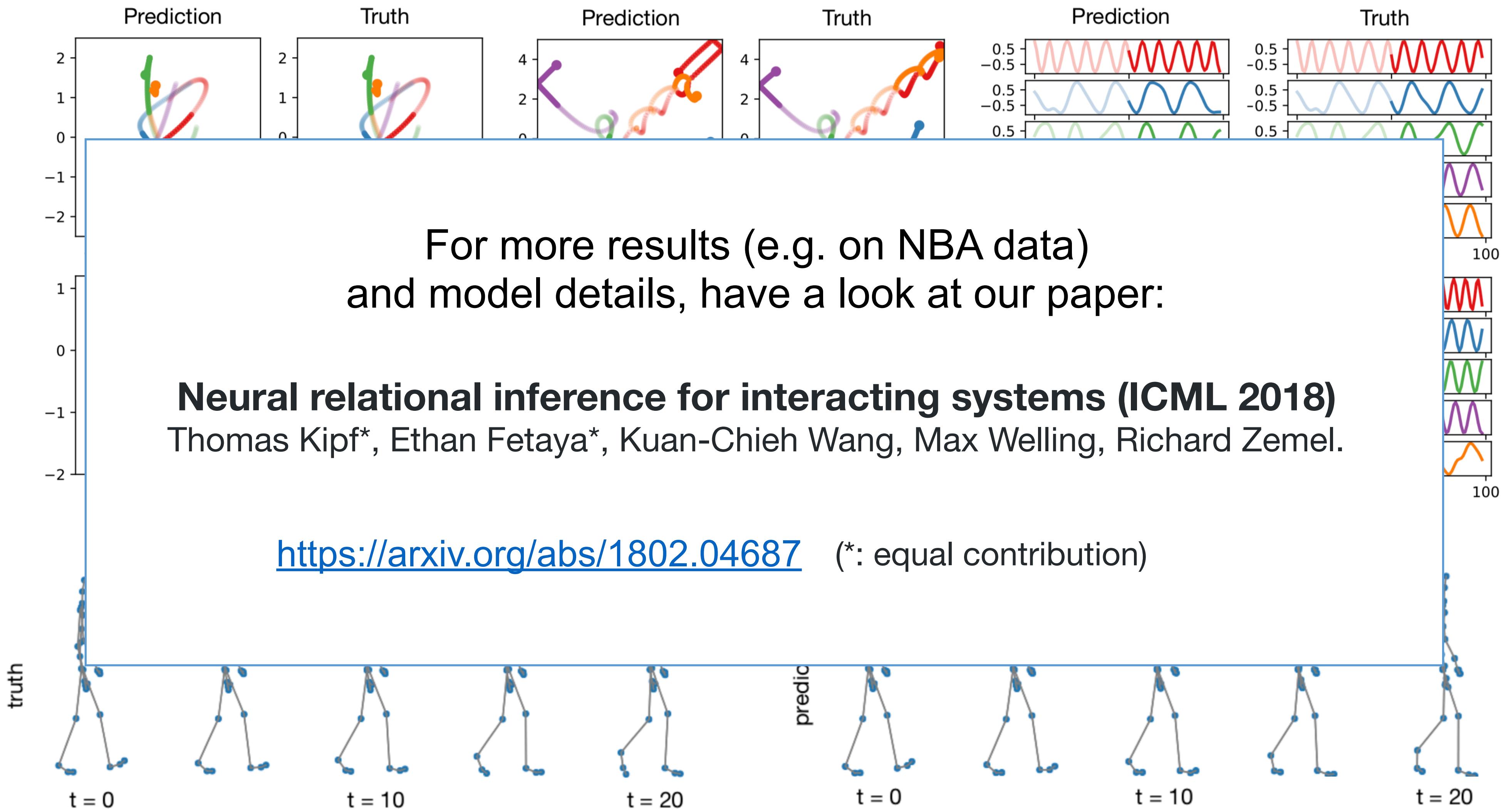
Potential applications:

- Inference of causal relations
- Discovering protein interaction networks
- Program induction
(with programs as graphs)

Qualitative results



Qualitative results



Deep generative models of graphs

MolGAN: An implicit generative model for small molecular graphs

Nicola De Cao¹ Thomas Kipf¹

Abstract

Deep generative models for graph-structured data offer a new angle on the problem of chemical synthesis: by optimizing differentiable models that directly generate molecular graphs, it is possible to side-step expensive search procedures in the discrete and vast space of chemical structures. We introduce MolGAN, an implicit, likelihood-free generative model for small molecular graphs that circumvents the need for expensive graph matching procedures or node ordering heuristics of previous likelihood-based methods. Our method adapts generative adversarial networks (GANs) to operate directly on graph-structured

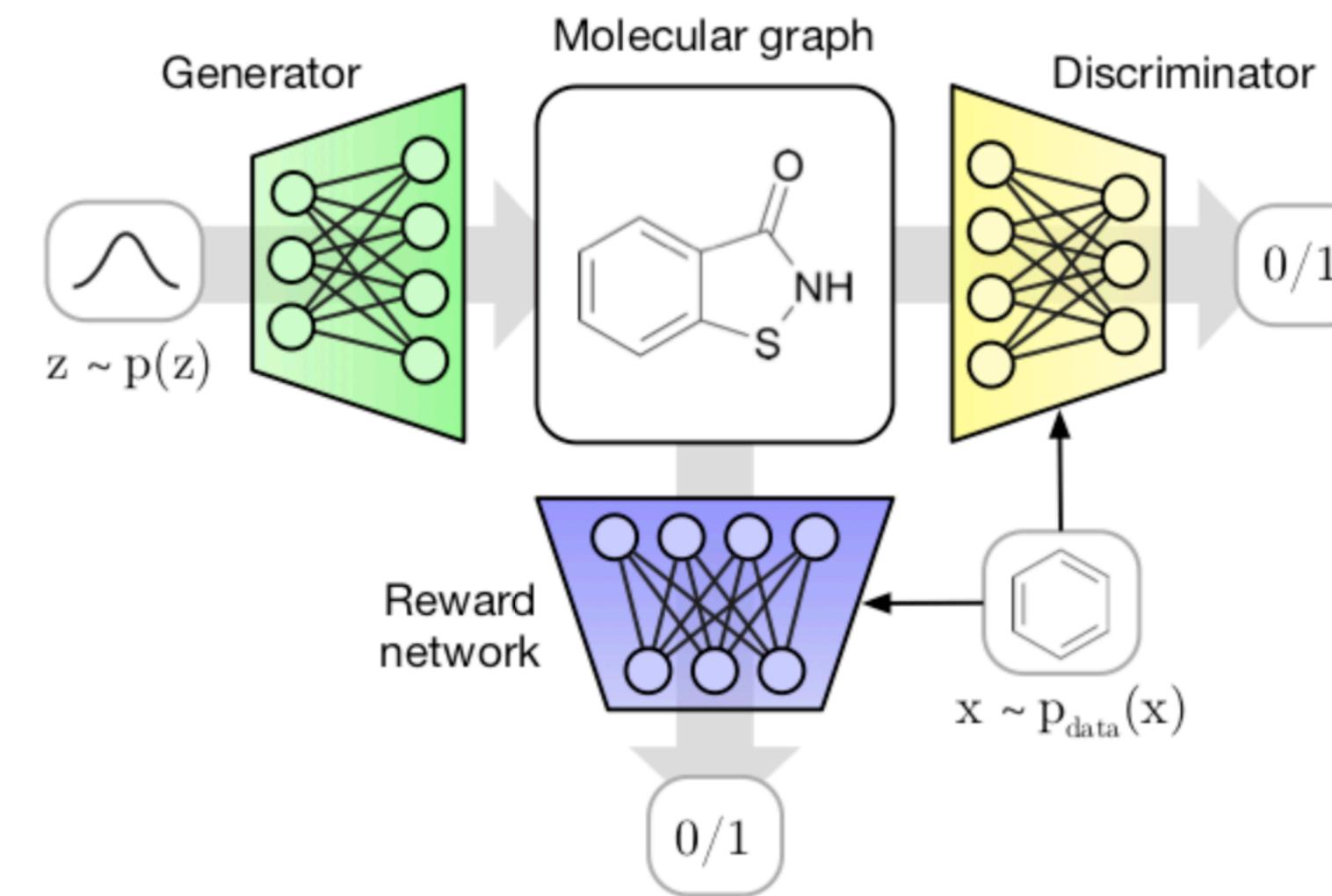


Figure 1. Schema of MolGAN. A vector z is sampled from a prior



With Nicola De Cao

(Under review at
ICML TADGM Workshop)

arXiv version:
<https://arxiv.org/abs/1805.11973>

Likelihood-based (deep) graph generation

Version 1: Generate graph (or predict new links) between known entities

Graph-based autoencoders:

- Encoder: GNN/GCN
- Decoder: Pairwise scoring function

$$p(A_{ij}) = f(\mathbf{z}_i, \mathbf{z}_j)$$

e.g. $p(A_{ij}) = \sigma(\mathbf{z}_i^T \mathbf{z}_j)$



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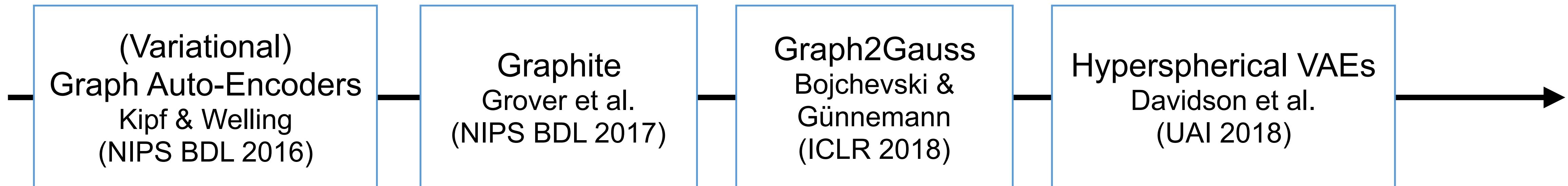
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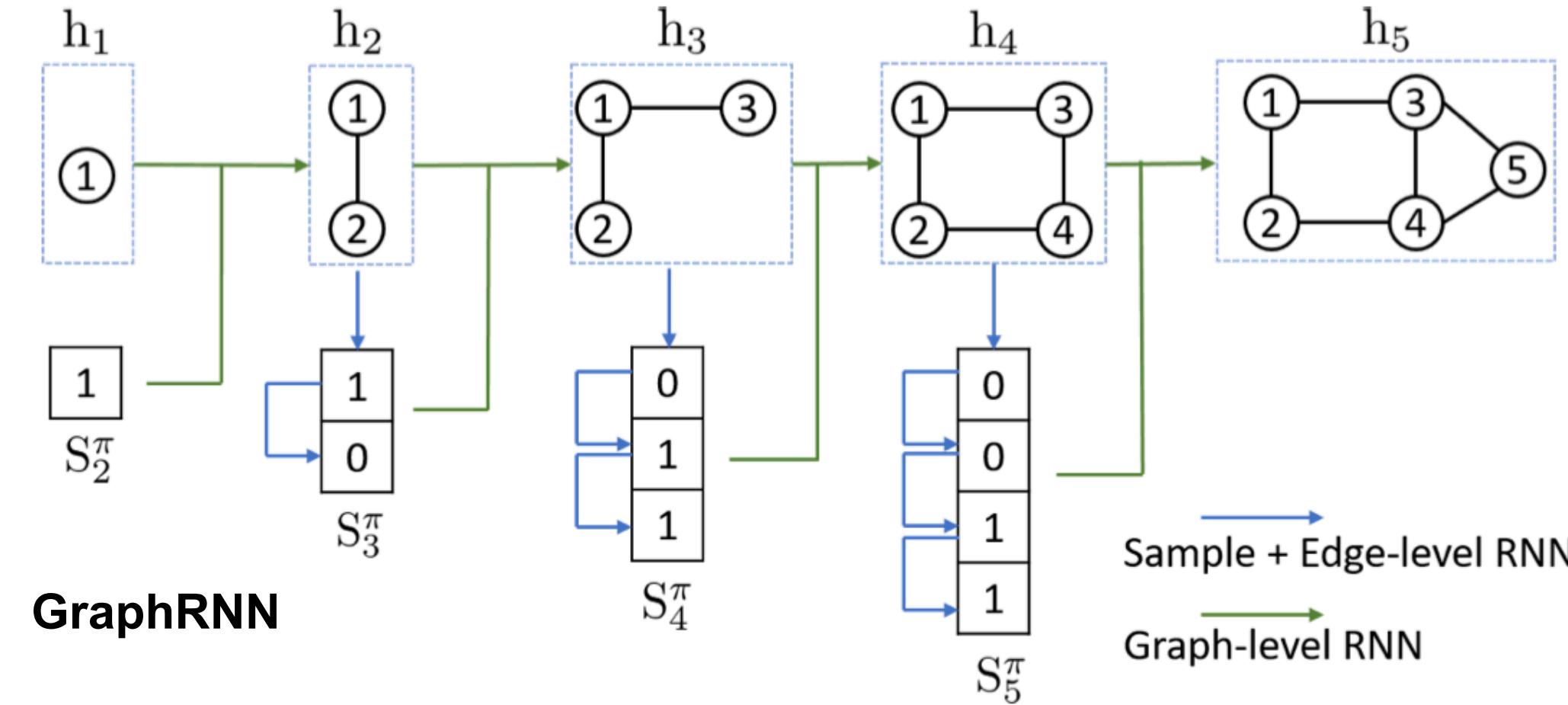
(Incomplete) History:



Likelihood-based (deep) graph generation

Version 2: Generate graphs from scratch (single embedding vector)

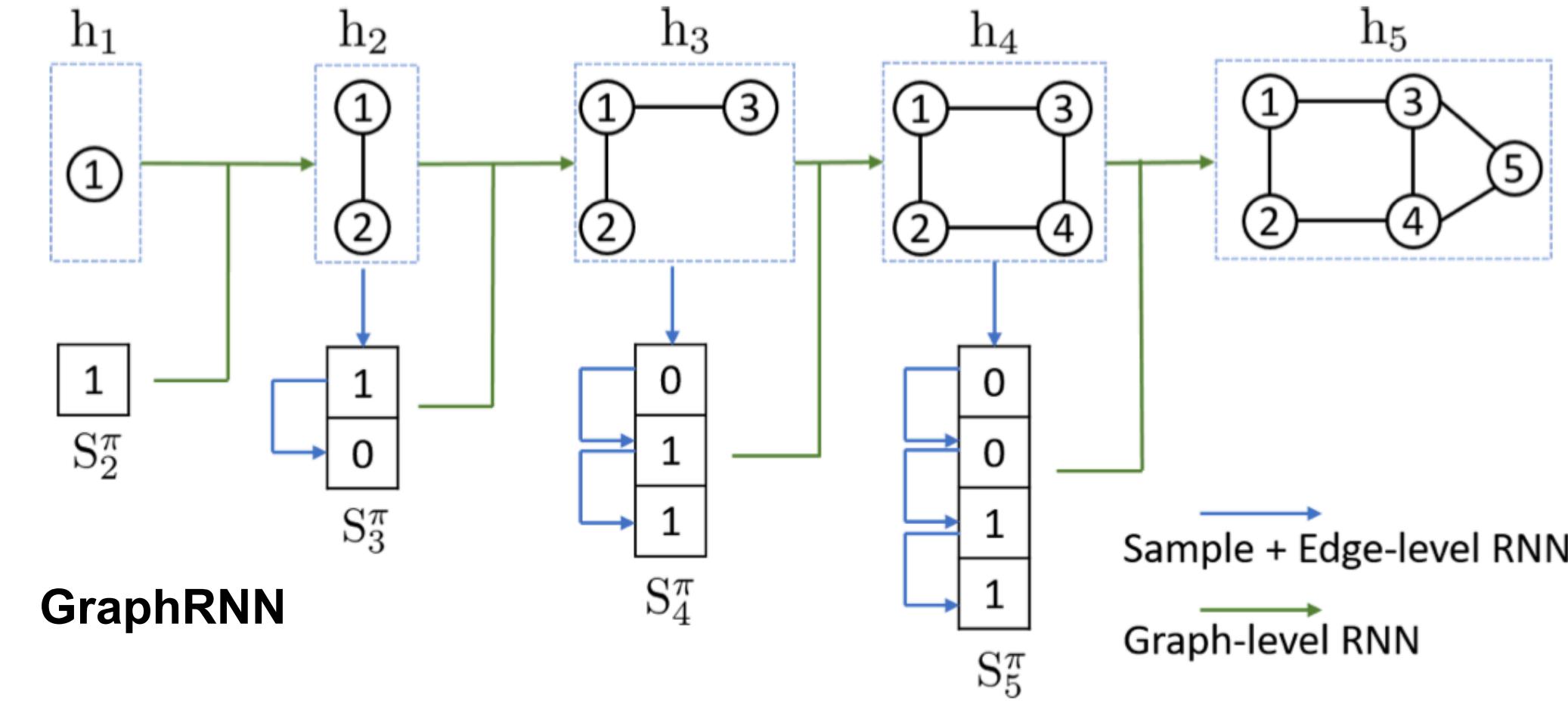
Sequentially:



Likelihood-based (deep) graph generation

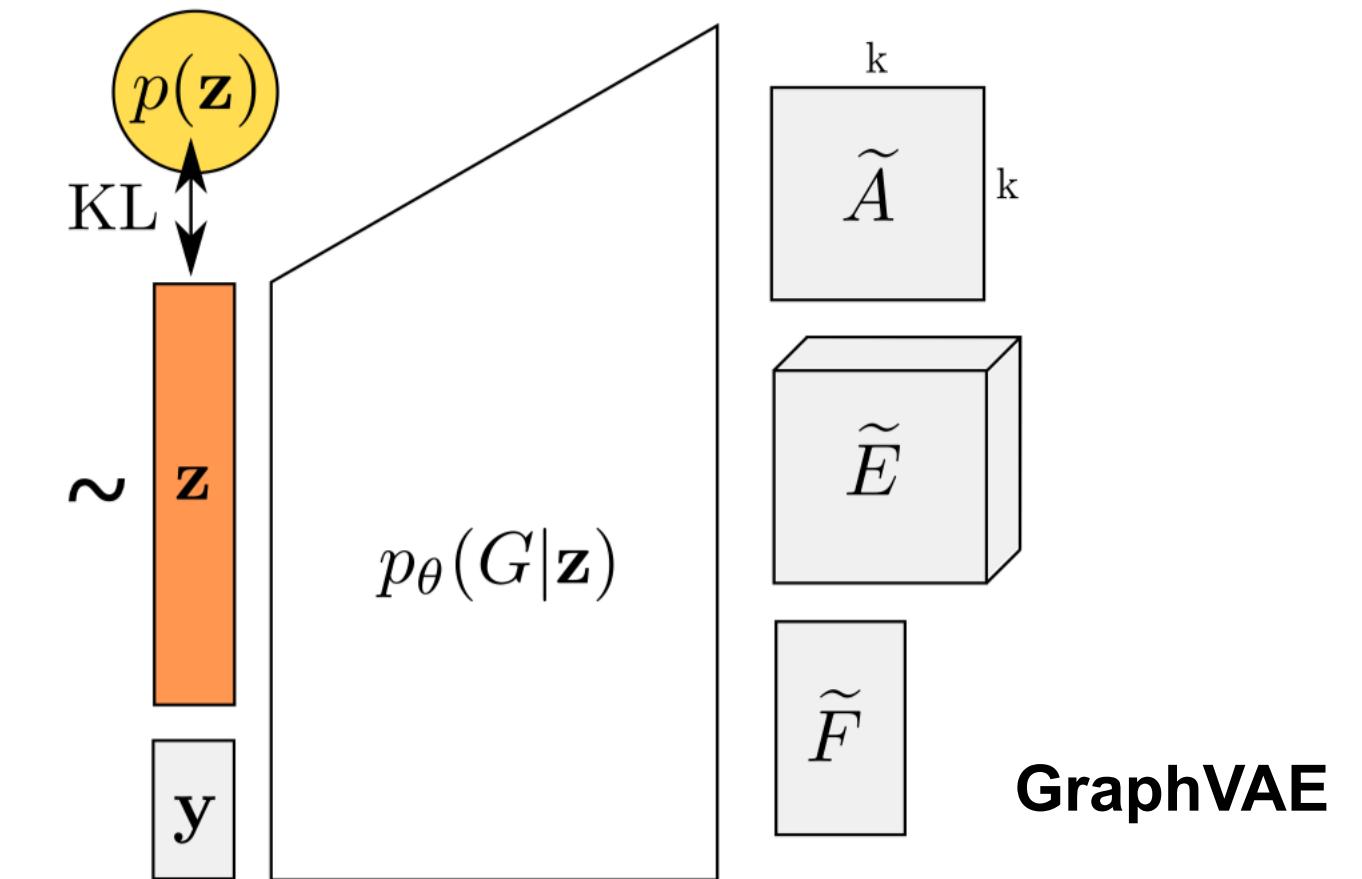
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Sequentially:



GraphRNN

Or in a single step:



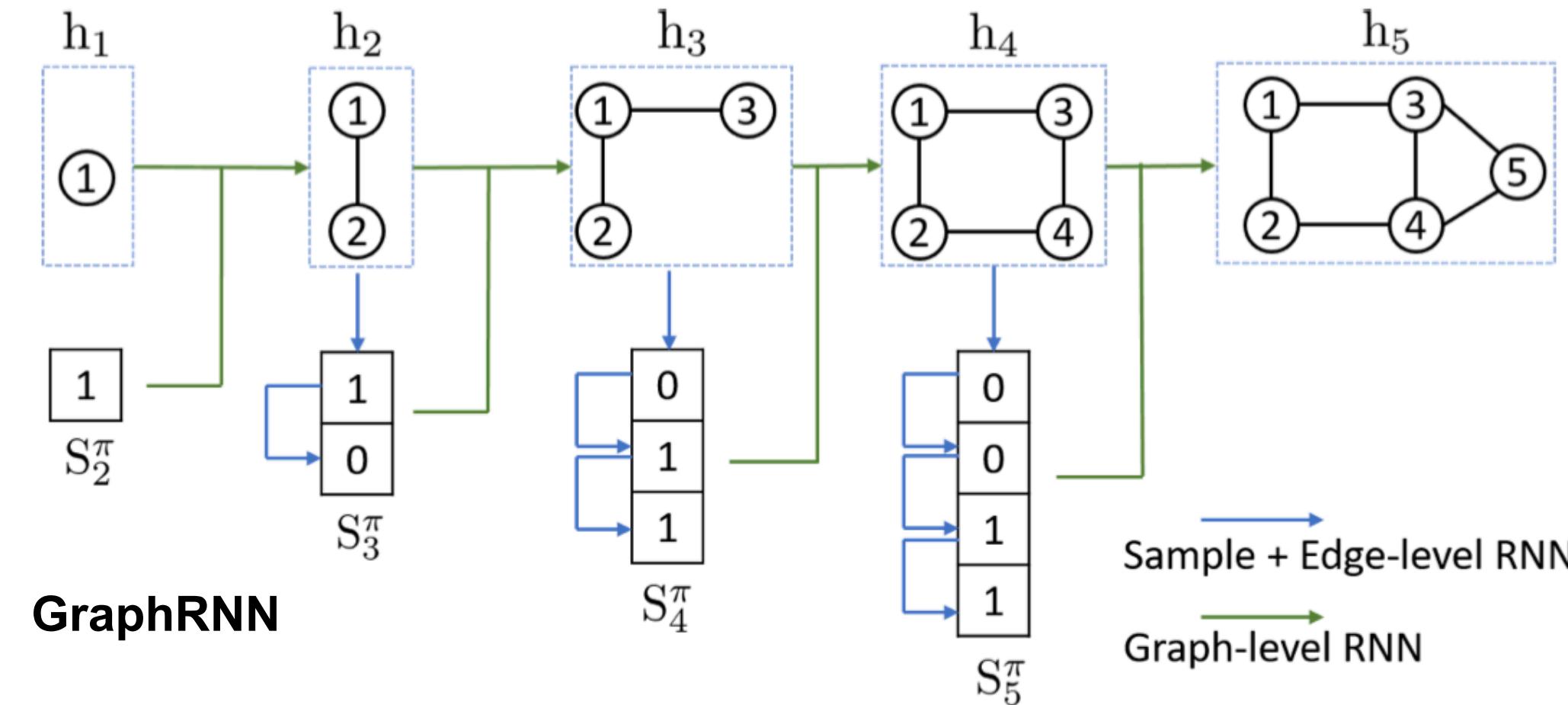
GraphVAE

Likelihood-based (deep) graph generation

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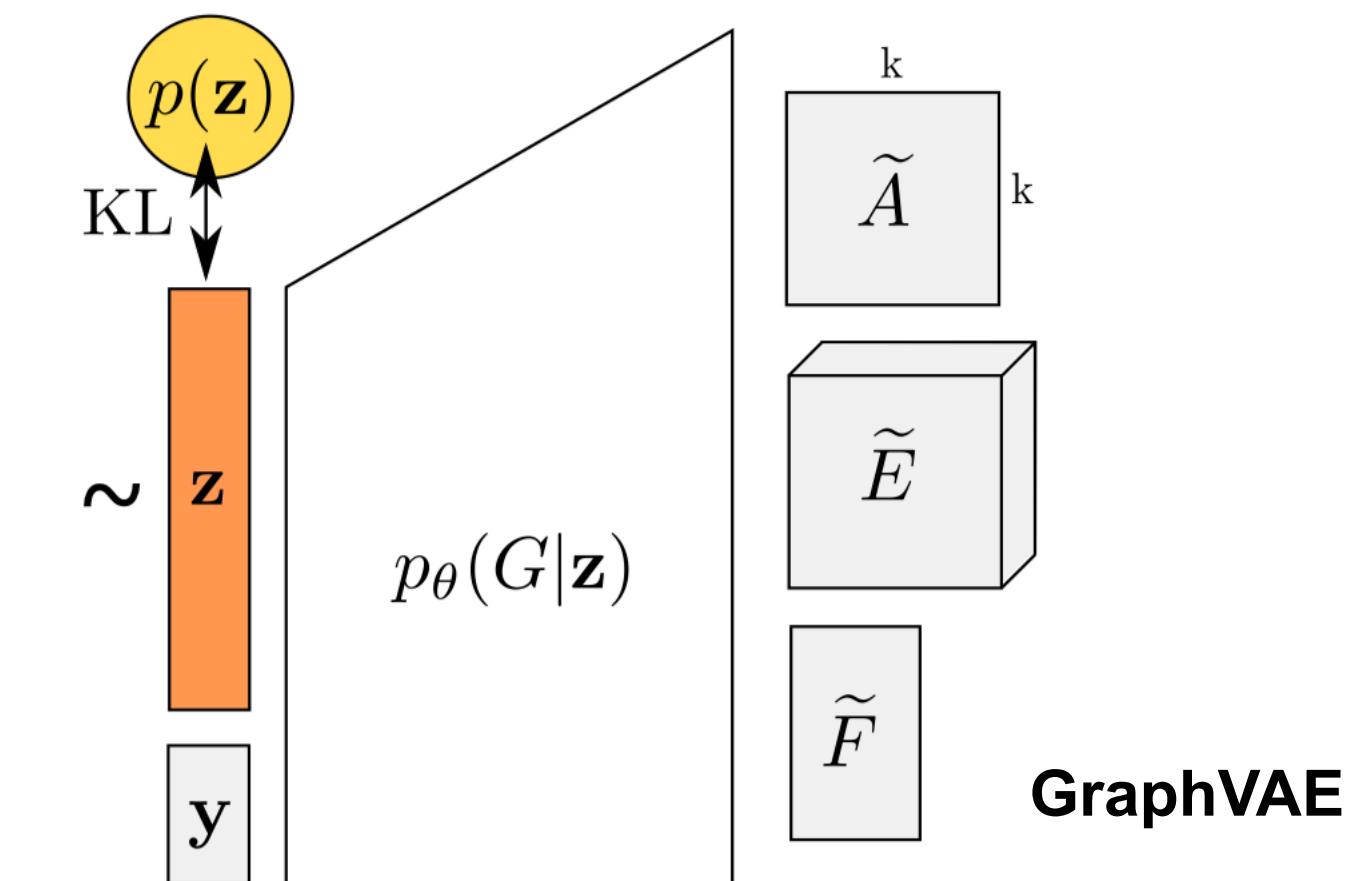


Learning Graphical
State Transitions
Johnson
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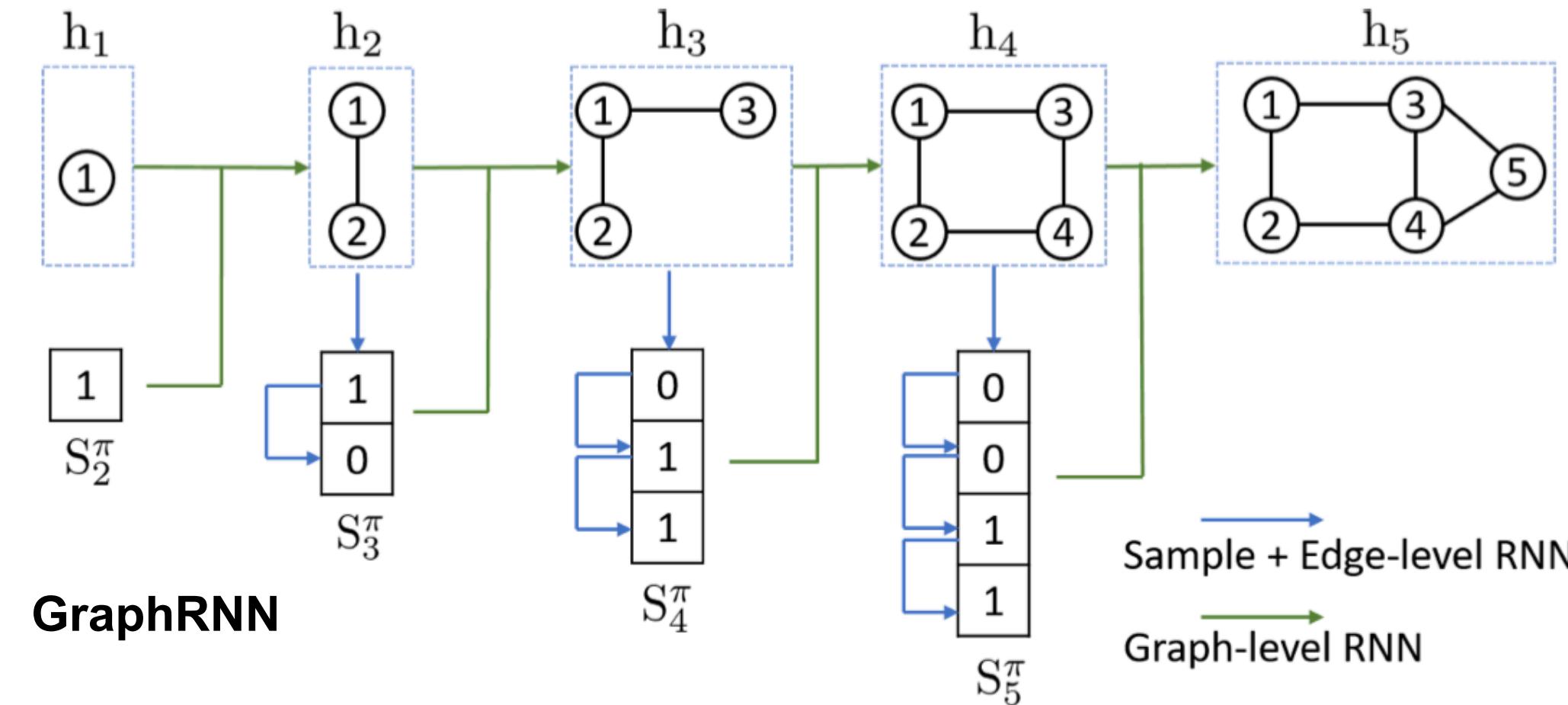


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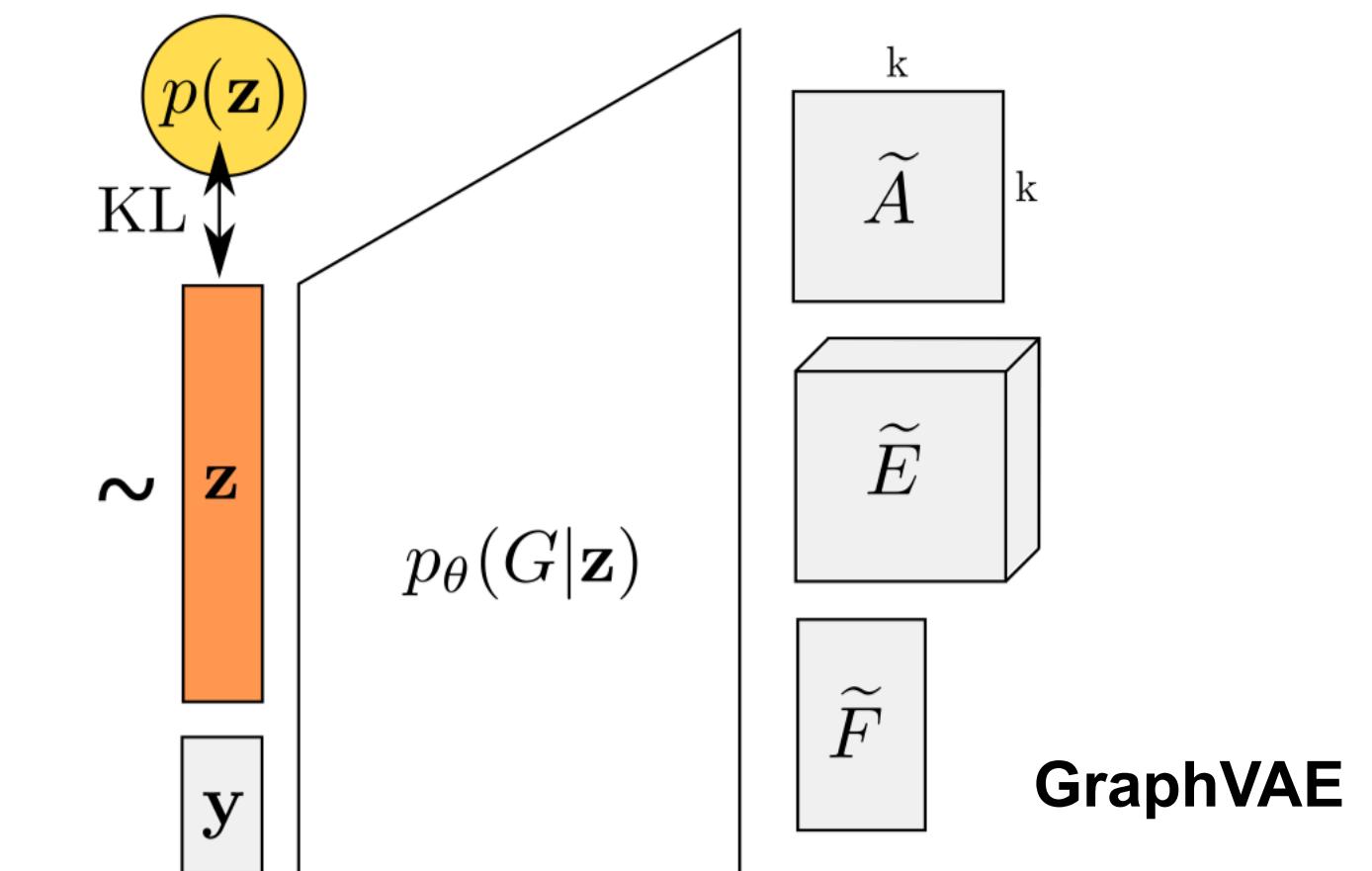
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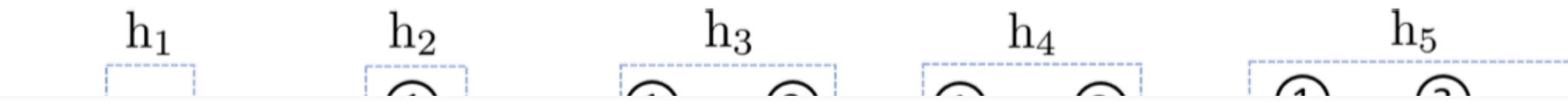
Both 1-2 times rejected... Seems to be hard to get these ideas published!

Likelihood-based (deep) graph generation

Version 2: Generate graphs from scratch (single embedding vector)

Or in a single step:

Sequentially:



Problem:

Need to define some node ordering or
perform (expensive) graph matching

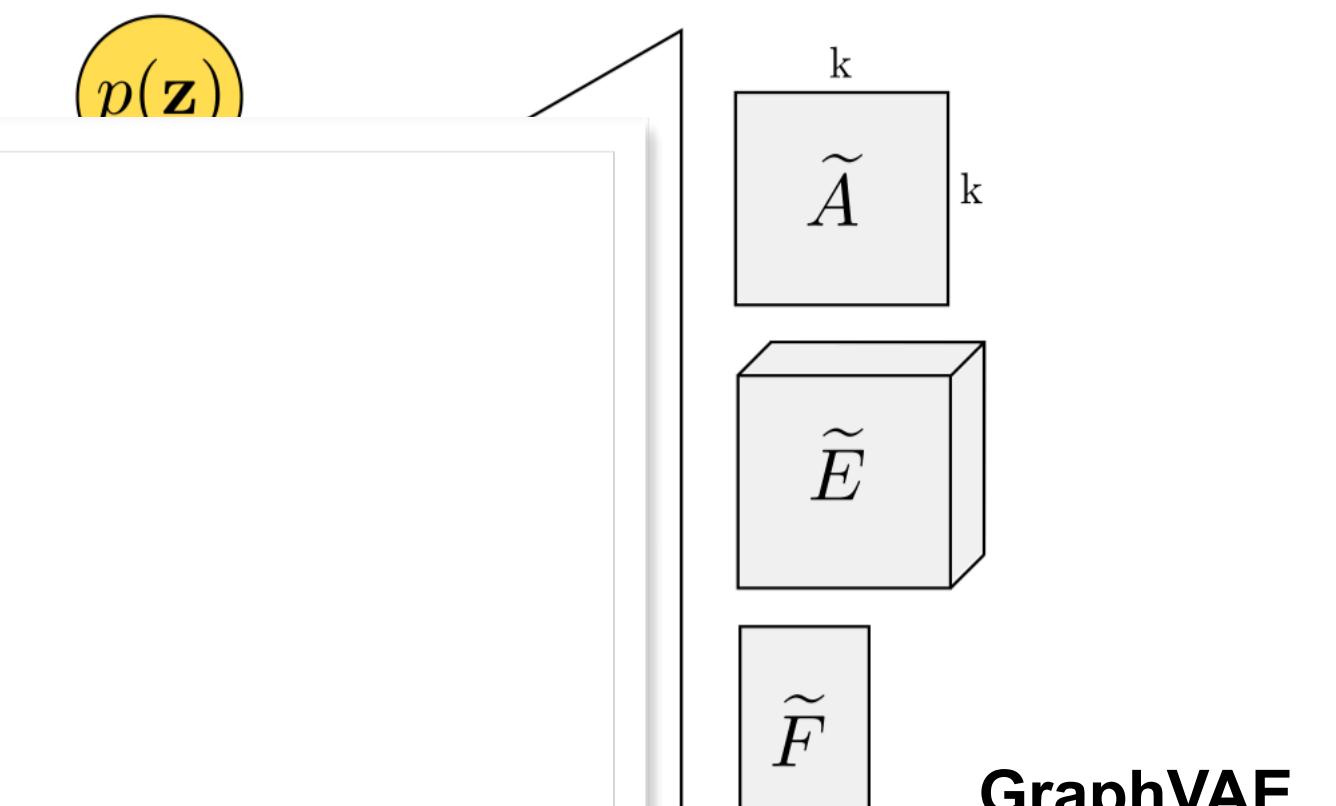
(evaluating all possible permutations is too expensive)

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State Transitions
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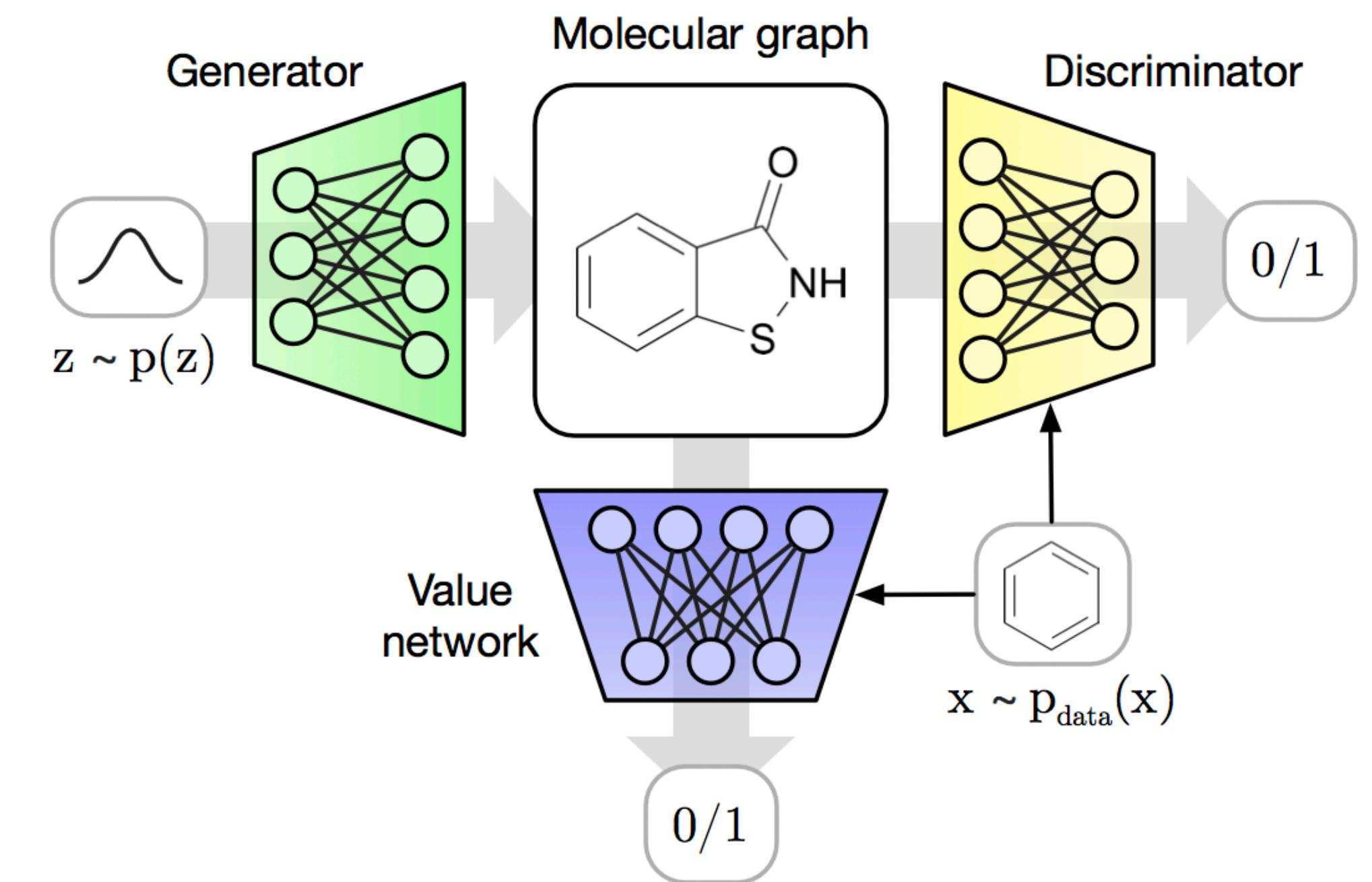
MolGAN model

Implicit models offer promising alternative:
No graph matching / fixed ordering needed!

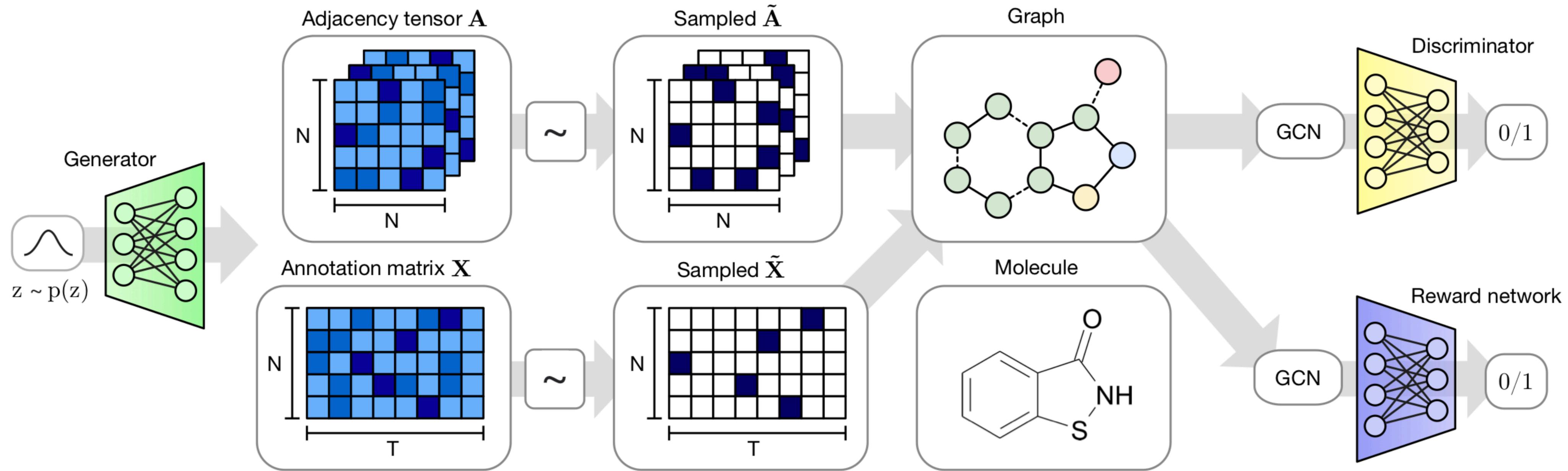
In practice: Use **GANs** and/or **RL**

MolGAN:

- Couple graph generator to a **discriminator** and a **value network**
- Train discriminator via GAN objective
- Train value net via RL objective
- Generator is trained jointly



MolGAN model architecture

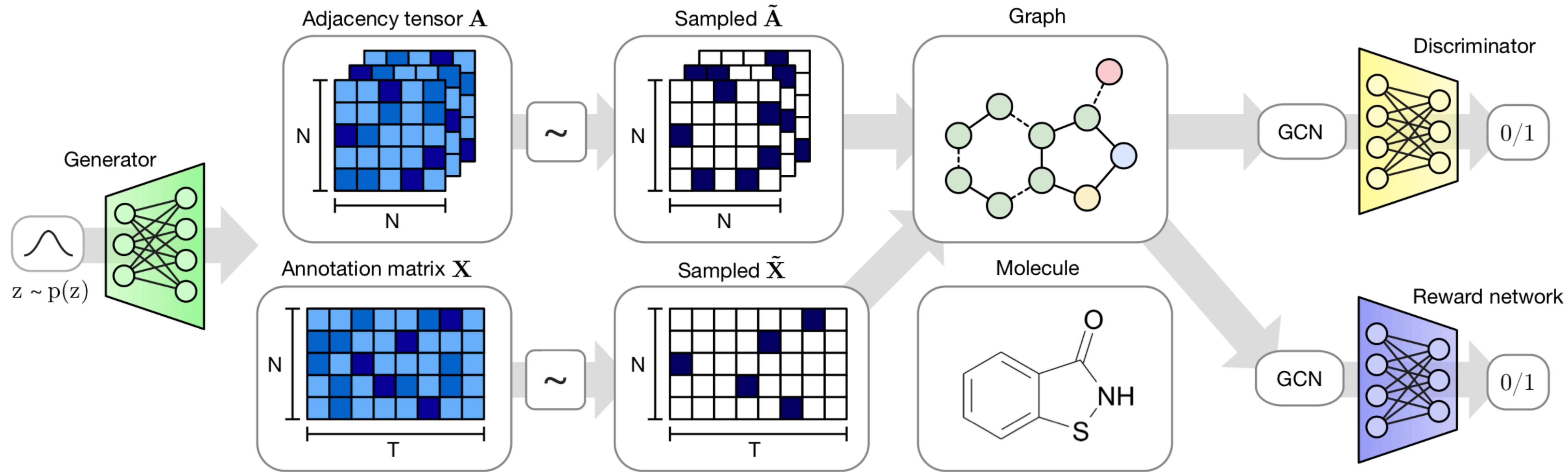


Generator: MLP to predict graph at once

Discriminator / value net: GNN/GCN
(with support for multiple edge types)

$$\left\{ \begin{array}{l} \mathbf{h}'^{(\ell+1)}_i = f_s(\mathbf{h}_i^{(\ell)}, \mathbf{x}_i) + \sum_{j=1}^N \sum_{y=1}^Y \frac{A_{ijy}}{|\mathcal{N}_i|} f_y(\mathbf{h}_j^{(\ell)}, \mathbf{x}_i) \\ \mathbf{h}_i^{(\ell+1)} = \tanh(\mathbf{h}'^{(\ell+1)}_i), \end{array} \right.$$

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+ gated global pooling

Li et al., (ICLR 2016)

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$$\mathbf{h}'_{\mathcal{G}} = \sum_{v \in \mathcal{V}} \sigma(i(\mathbf{h}_v^{(L)}, \mathbf{x}_v)) \odot \tanh(j(\mathbf{h}_v^{(L)}, \mathbf{x}_v))$$

Chemical synthesis results

ORGAN: GAN-based sequence generation model, Guimaraes et al. (2017)

Objective	Algorithm	Valid (%)	Unique (%)	Time (h)	Diversity	Druglikeness	Synthesizability	Solubility
Druglikeness	ORGAN	88.2	-	-	0.55	0.52	0.32	0.35
	OR(W)GAN	85.0	8.2*	10.06*	0.95	0.60	0.54	0.47
	Naive RL	97.1	-	-	0.80	0.57	0.53	0.50
	MolGAN	99.9	2.0	1.66	0.95	0.61	0.68	0.52
	MolGAN (QM9)	100.0	2.2	4.12	0.97	0.62	0.59	0.53
Synthesizability	ORGAN	96.5	-	-	0.92	0.51	0.83	0.45
	OR(W)GAN	97.6	30.7*	9.60*	1.00	0.20	0.75	0.84
	Naive RL	97.7	-	-	0.96	0.52	0.83	0.46
	MolGAN	99.4	2.1	1.04	0.75	0.52	0.90	0.67
	MolGAN (QM9)	100.0	2.1	2.49	0.95	0.53	0.95	0.68
Solubility	ORGAN	94.7	54.3*	8.65*	0.76	0.50	0.63	0.55
	OR(W)GAN	94.1	20.8*	9.21*	0.90	0.42	0.66	0.54
	Naive RL	92.7	-	-	0.75	0.49	0.70	0.78
	MolGAN	99.8	2.3	0.58	0.97	0.45	0.42	0.86
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Conclusions

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Relational reasoning

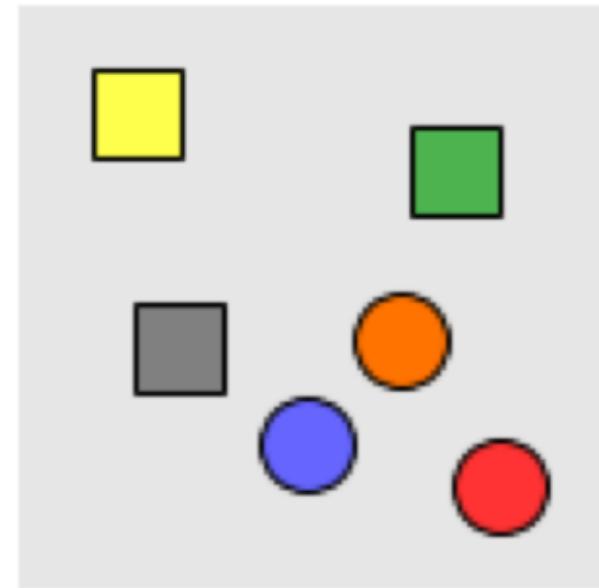


[Santoro et al., NIPS 2017]

Conclusions

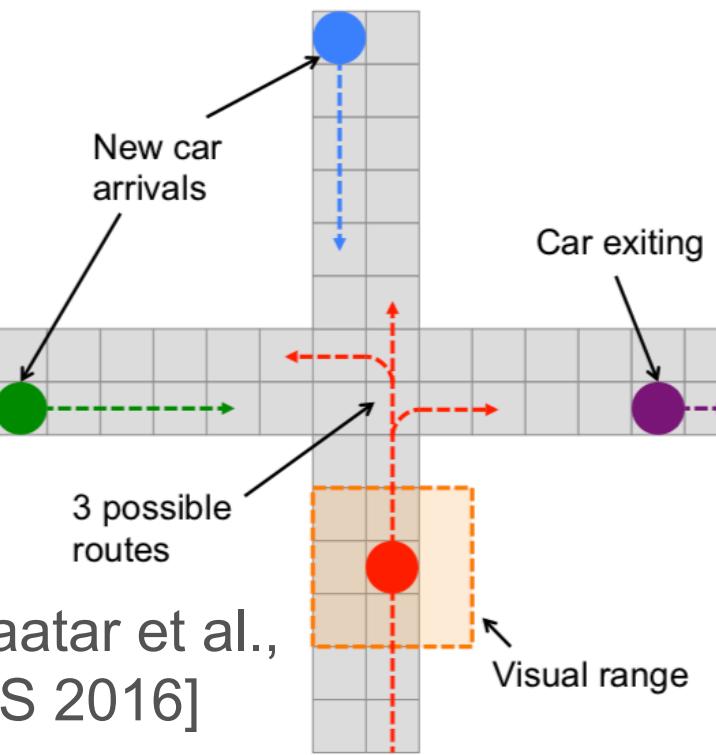
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Multi-Agent RL

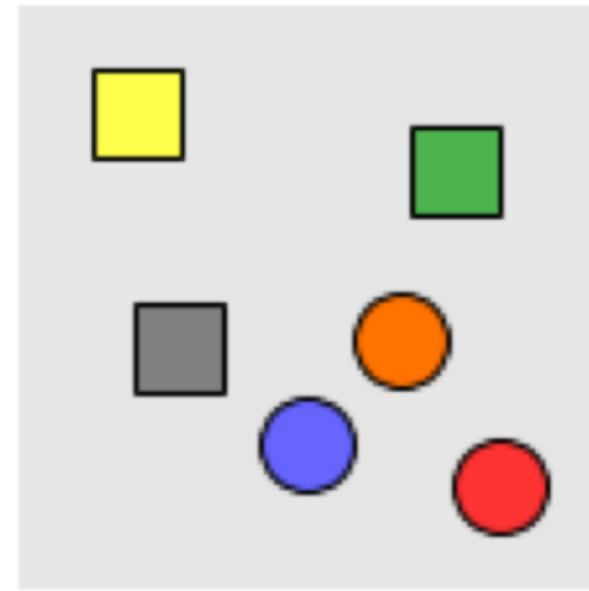


[Sukhbaatar et al.,
NIPS 2016]

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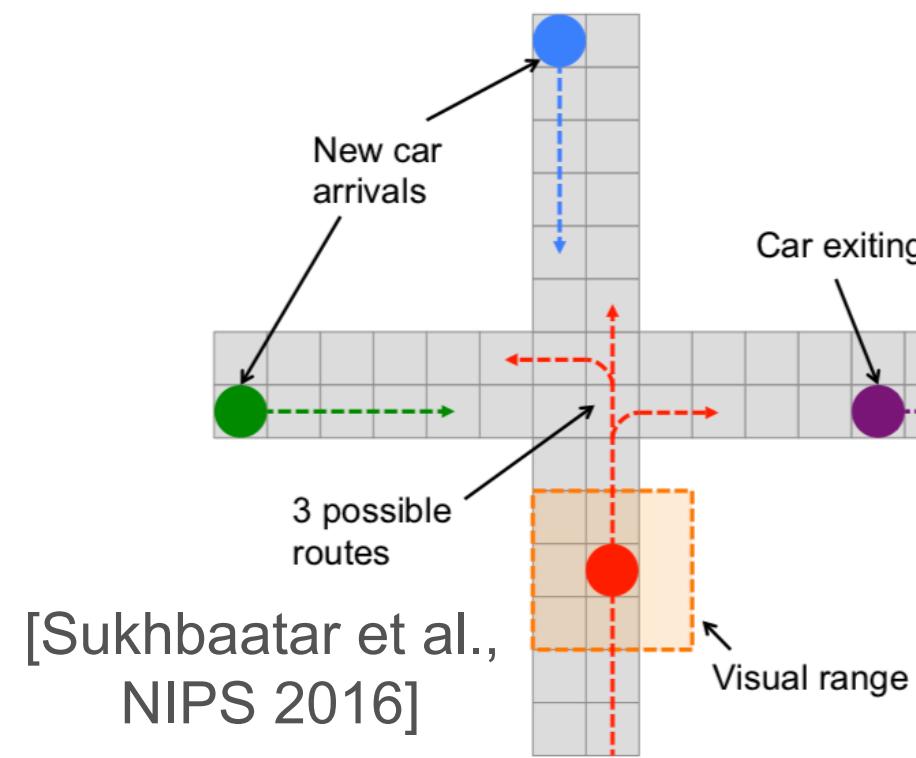
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GCN for recommendation on 16 billion edge graph!



Pinterest



Source pin

[Leskovec lab, Stanford]



SUCCESSFUL
RECOMMENDATION

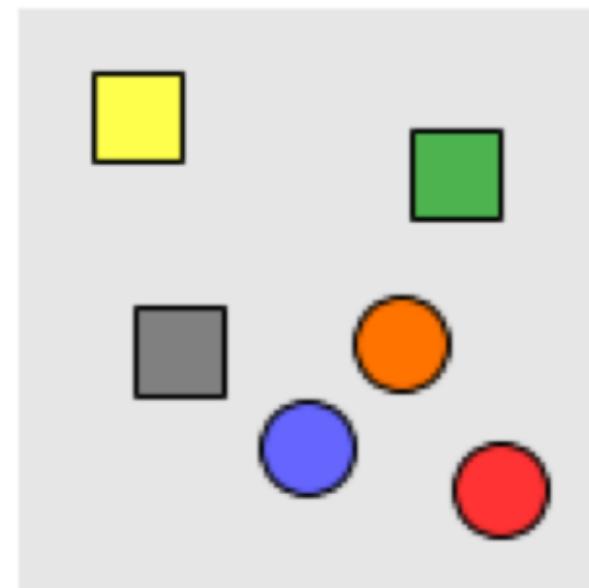


BAD RECOMMENDATION

Conclusions

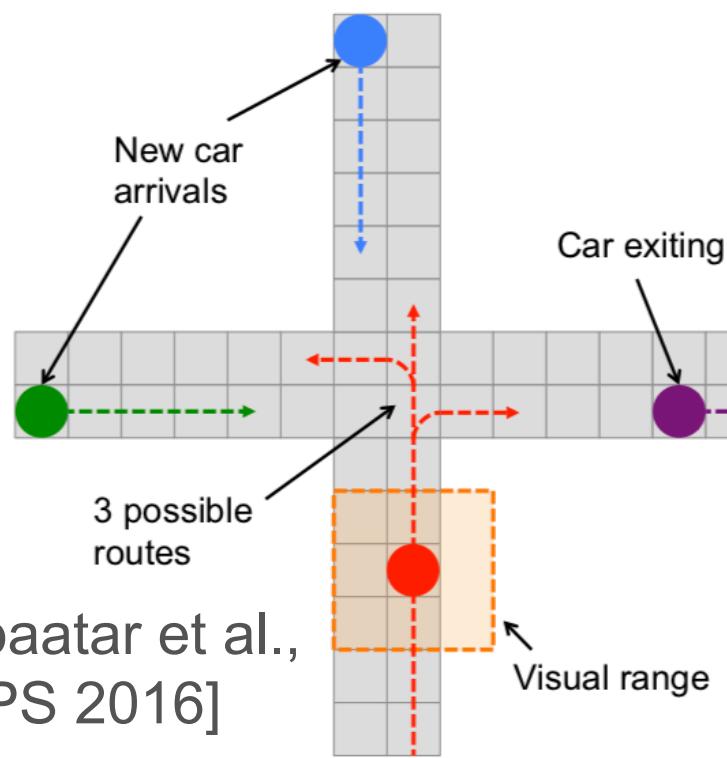
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SUCCESSFUL
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BAD RECOMMENDATION

Finding bugs in code

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    var buffer = EnsureTempBuffer( length );  
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[Allamanis et al., ICLR 2018]

Conclusions

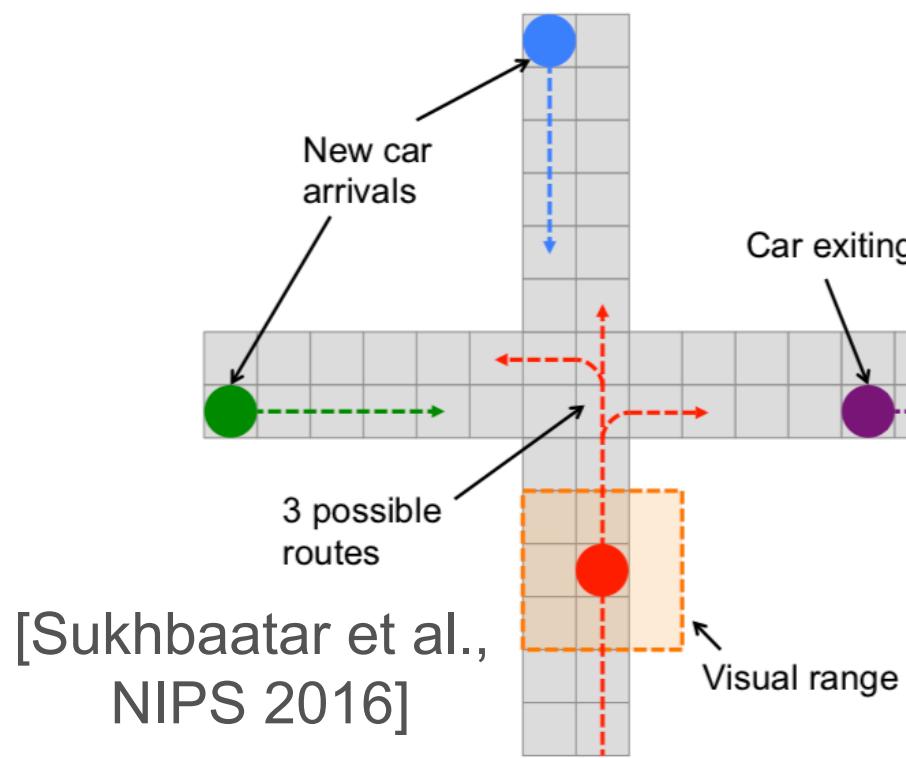
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SUCCESSFUL
RECOMMENDATION



BAD RECOMMENDATION

Some open problems:

- Theory
- Scalable, stable generative models
- Learning on large, evolving data
- Multi-modal and cross-modal learning (e.g. sequence2graph etc.)

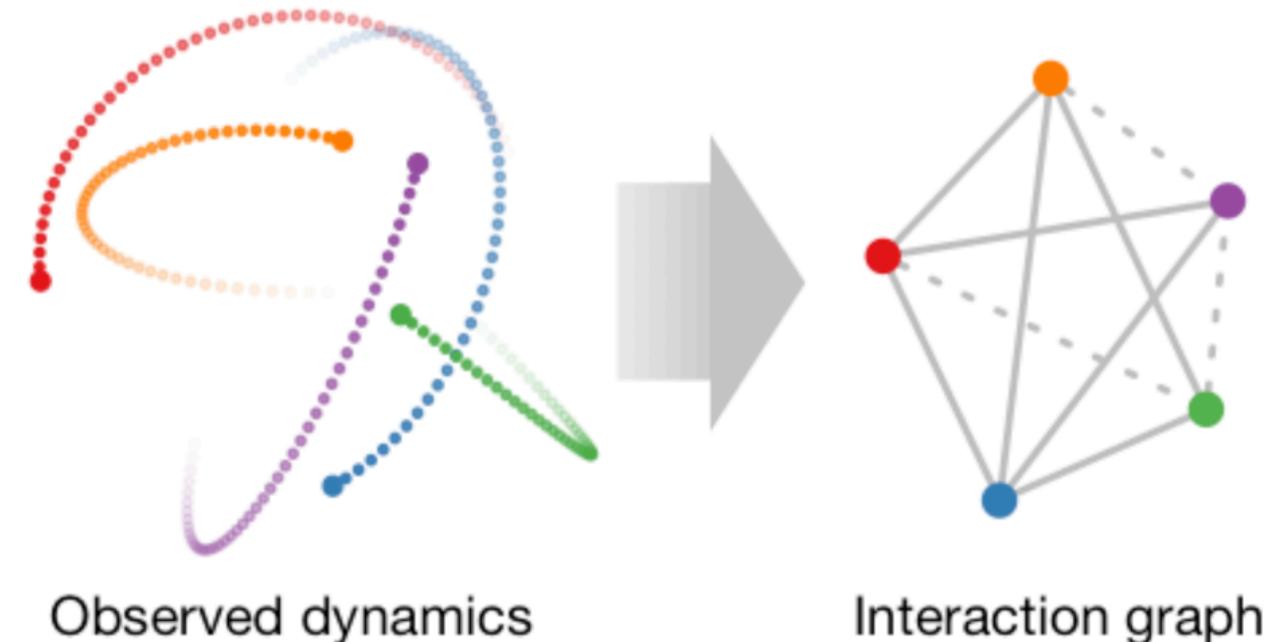
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[Allamanis et al., ICLR 2018]

Further reading

Have a look at our ICML paper for an overview of recent work in the field:



Neural relational inference for interacting systems (ICML 2018)

Thomas Kipf*, Ethan Fetaya*, Kuan-Chieh Wang, Max Welling, Richard Zemel.

<https://arxiv.org/abs/1802.04687> (*: equal contribution)

Code on Github:

<http://github.com/ethanfetaya/nri>

Other material:

Blog post on Graph Convolutional Networks:

<http://tkipf.github.io/graph-convolutional-networks>

GCN code on Github:

<http://github.com/tkipf/gcn>

Get in touch:

- E-Mail: t.n.kipf@uva.nl
- Twitter: [@thomaskipf](https://twitter.com/thomaskipf)
- Web: tkipf.github.io



Project supported by SAP