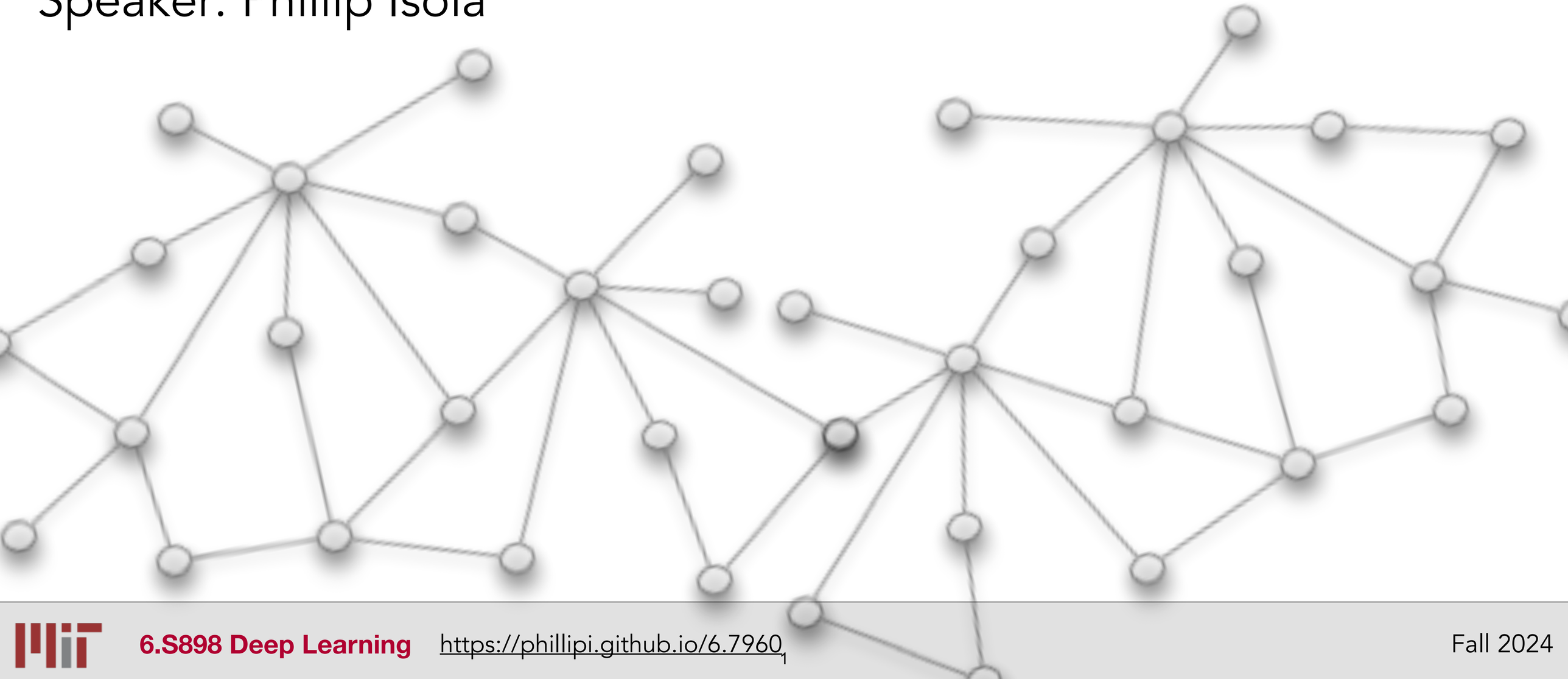
Lecture 5: Graph Neural Networks

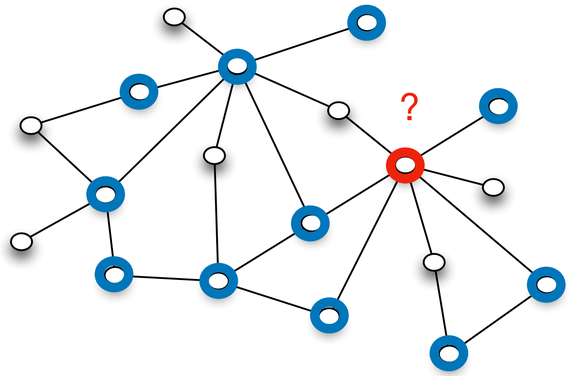
Speaker: Phillip Isola



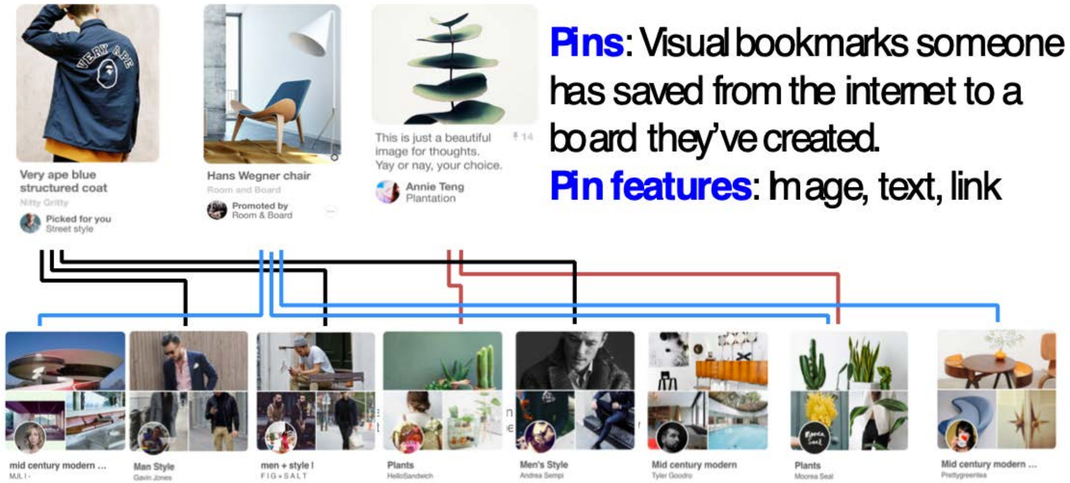
Roadmap

- Learning tasks with graphs
- Message passing GNNs
- Approximation Power

Prediction with graphs: examples



Node classification



Link Prediction

(e.g. Ying et al, 2018; illustration: J. Leskovec)

> concerned recommender systems, which are very naturally representable as a graph-structured task: with Pinterest being one of the most early adopters [18, 33]. GNNs have also been deployed for product recommendation at Amazon [12], E-commerce applications at Alibaba [32], engagement forecasting and friend ranking in Snapchat [22, 24], and most relevantly, they are powering traffic predictions within Baidu Maps [6].

Example: molecule property prediction

Graph
Molecule

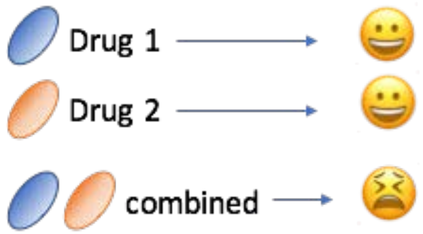
→

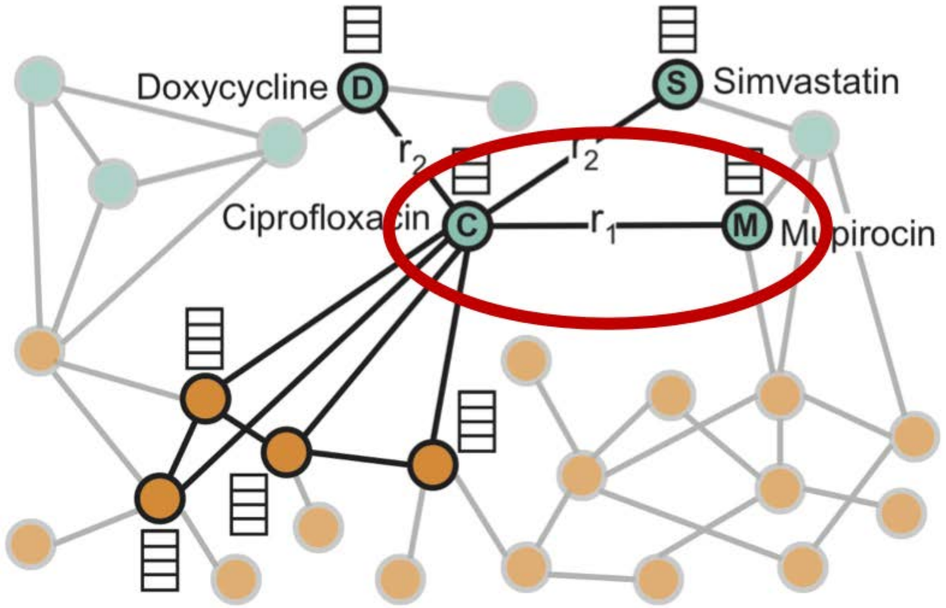
Property
Solubility
Toxicity
Drug efficacy
…

(Duvenaud et al, 2015, Stokes et al 2020,…)

On the cover: Antibiotic resistance is a pervasive public health problem, requiring the adoption of creative approaches to drug discovery. In this issue, ... Show more

Example: Polypharmacy side effects





Drugs

Proteins

Pair of Nodes
Drugs

→

Edge
Interaction type

(Zitnik et al, 2018)

Example: Predicting traffic times

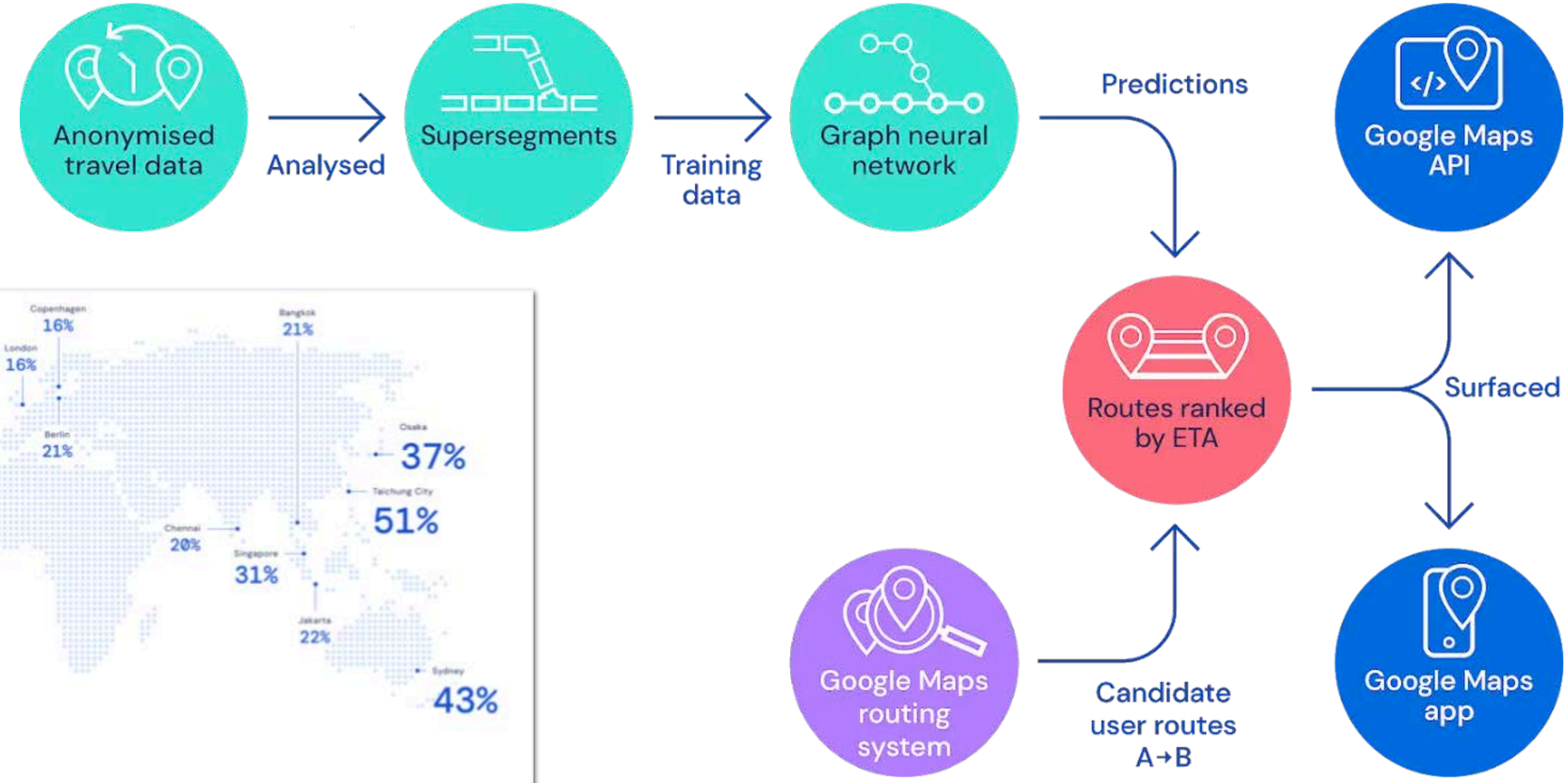
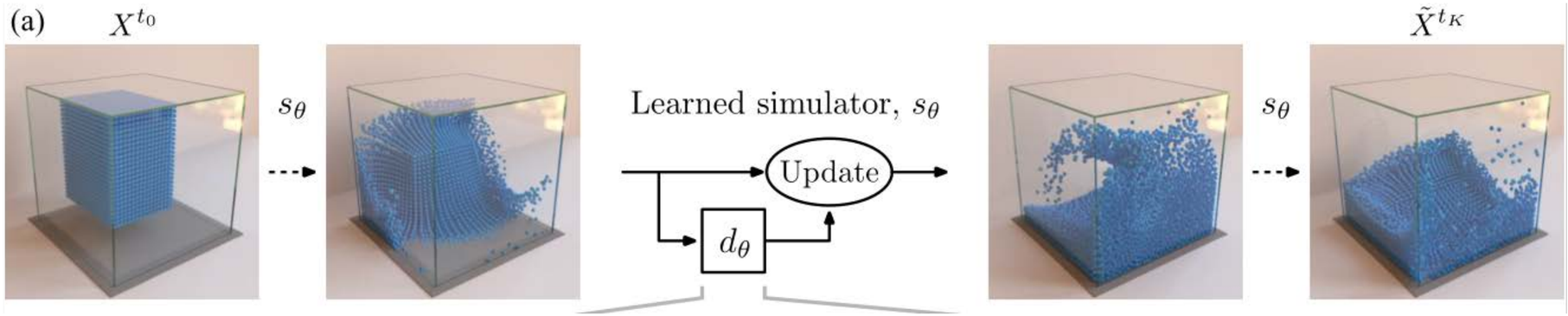


Figure 1: Google Maps estimated time-of-arrival (ETA) prediction improvements for several world regions, when using our deployed graph neural network-based estimator. Numbers represent relative reduction in negative ETA outcomes compared to the prior approach used in production. A negative ETA outcome occurs when the ETA error from the observed travel duration is over some threshold and acts as a

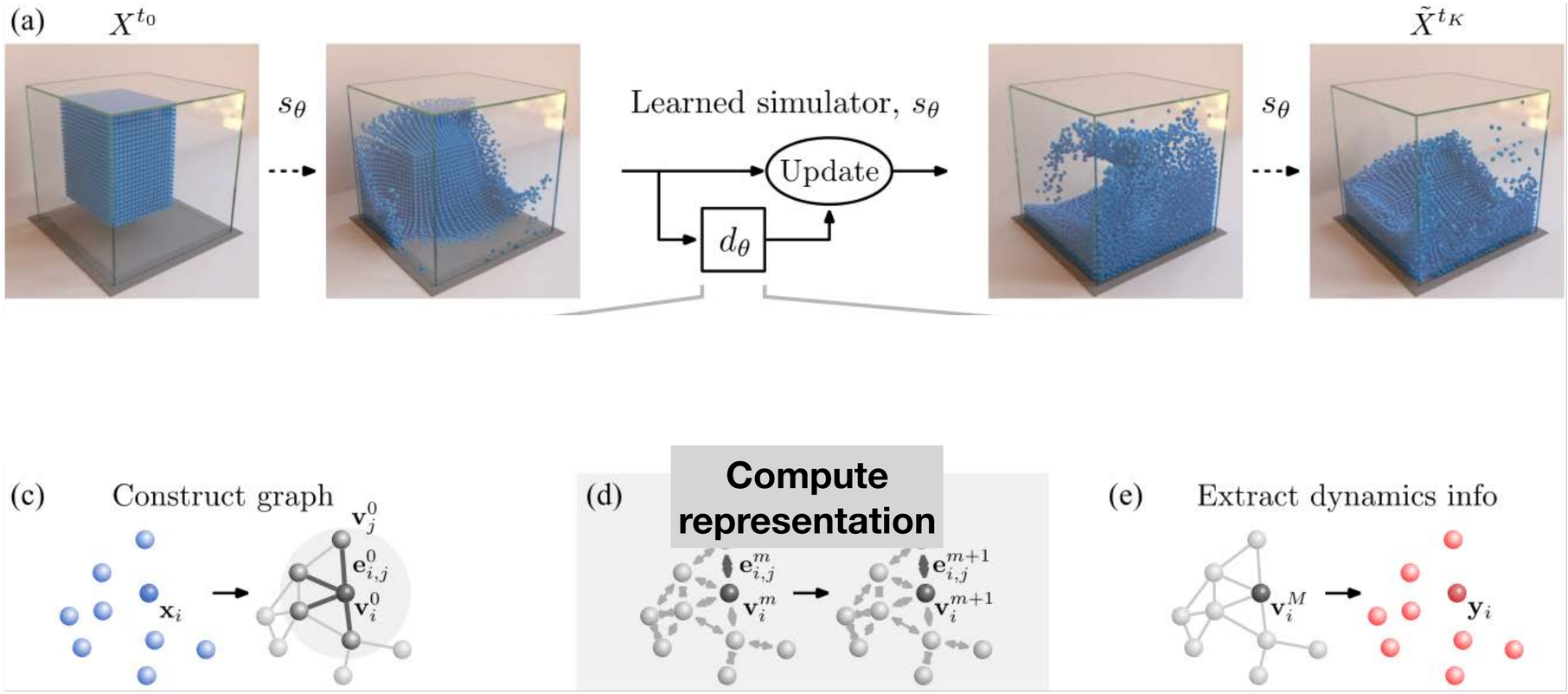
https://deepmind.com/blog/article/traffic-prediction-with-advanced-graph-neural-networks

Example: learning to simulate physics



(Sanchez-Gonzalez et al, 2020)

Example: learning to simulate physics



Collection of Nodes
Particles

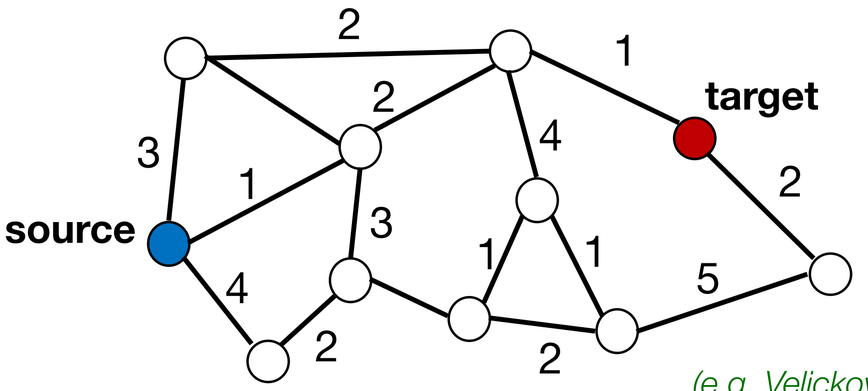
→

New state

(Sanchez-Gonzalez et al, 2020)

Example: (Combinatorial) Optimization

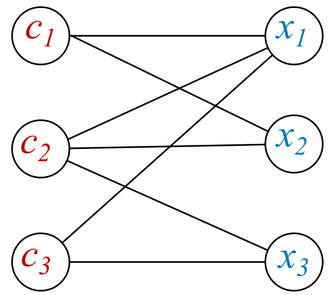
- replace full algorithm or
  learn steps (e.g. branching decision)



(e.g. Velickovic et al 2020)

"Neural Algorithmic Reasoning"

$$\min_x \; c^\top x$$
$$Ax \leq b$$
$$l \leq x \leq u$$
$$x \in \mathbb{Z}^p \times \mathbb{R}^{n-p}$$



constraints variables *(Gasse et al 2019)*

clauses variables *(Selsam et al 2018)*

Graph
Problem instance

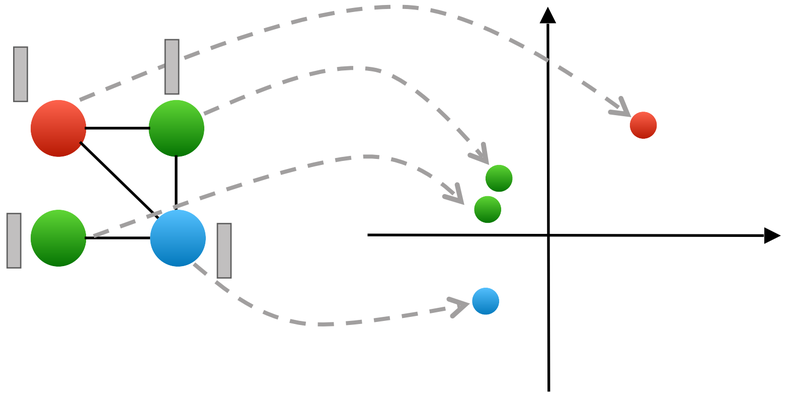
→

Solution / decision
Path
Branching variable
…

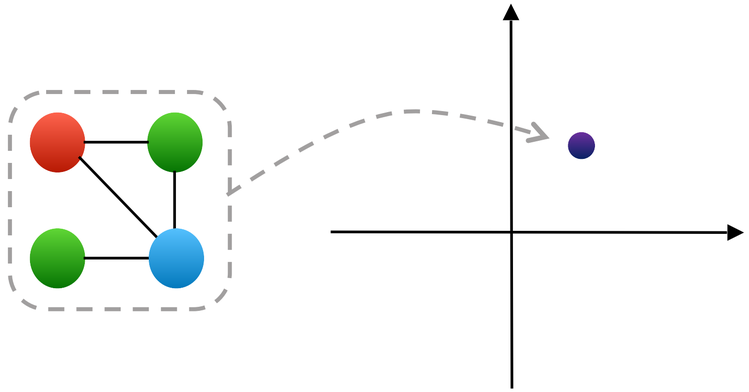
Two goals

Input: Graph + attribute vector for each node (adjacency matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$)

1. Node embeddings

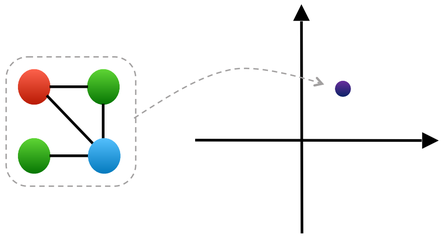


2. Graph embedding



GNNs: learn a **function** from graph/neighborhood + node/edge attributes to vector

Idea 1: fully-connected NN?

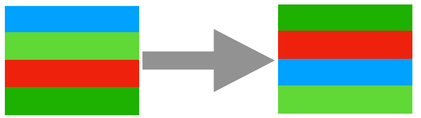


Idea 1: Use the adjacency matrix as input to a neural network

$$\mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix} \qquad \mathbf{PAP}^\top = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

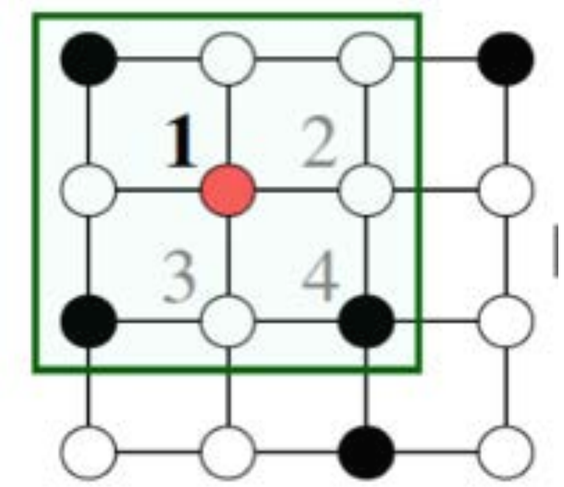
We want:

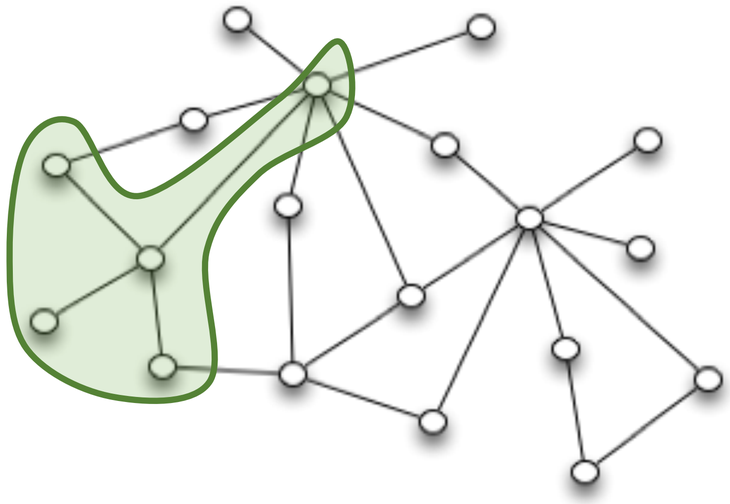
- **Permutation invariance (graph embedding)**:
  (output: single vector) and $f(\mathbf{PAP}^\top, \mathbf{PX}) = f(\mathbf{A}, \mathbf{X})$
- **Permutation equivariance (node embeddings)**:
  (output: one vector for each node) $f(\mathbf{PAP}^\top, \mathbf{PX}) = \mathbf{P}f(\mathbf{A}, \mathbf{X})$



Idea 2: Images are like graphs…

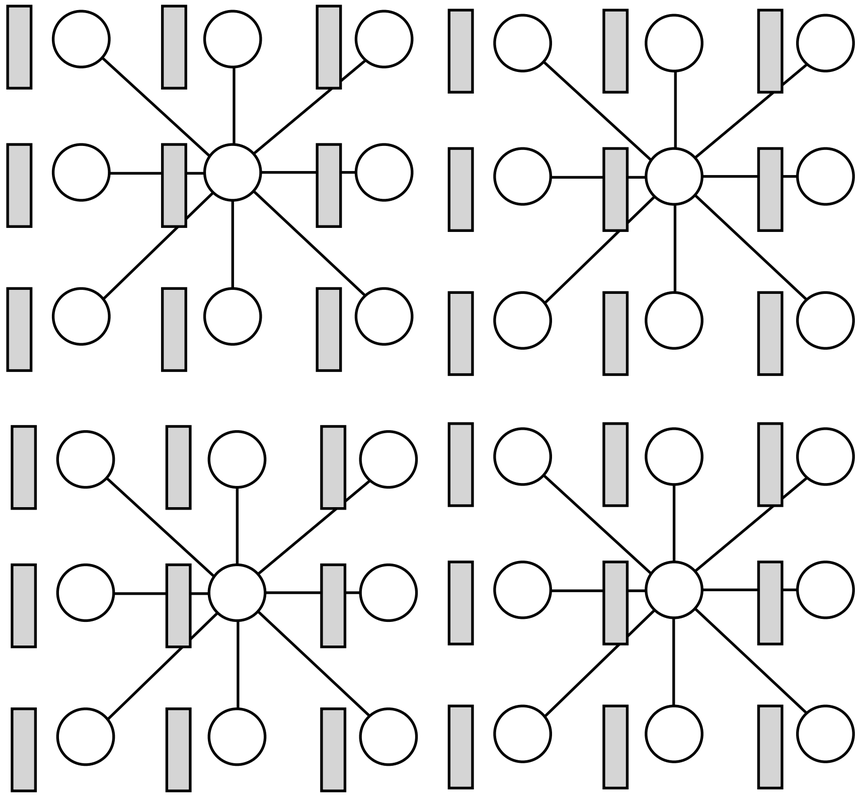
- Convolution? (local operator “encodes” local neighborhoods)





- What is different in a graph?
- Commonalities: local operations, globalize through depth, weight sharing, input can have varying size

A CNN is a GNN over a grid graph



Review questions:

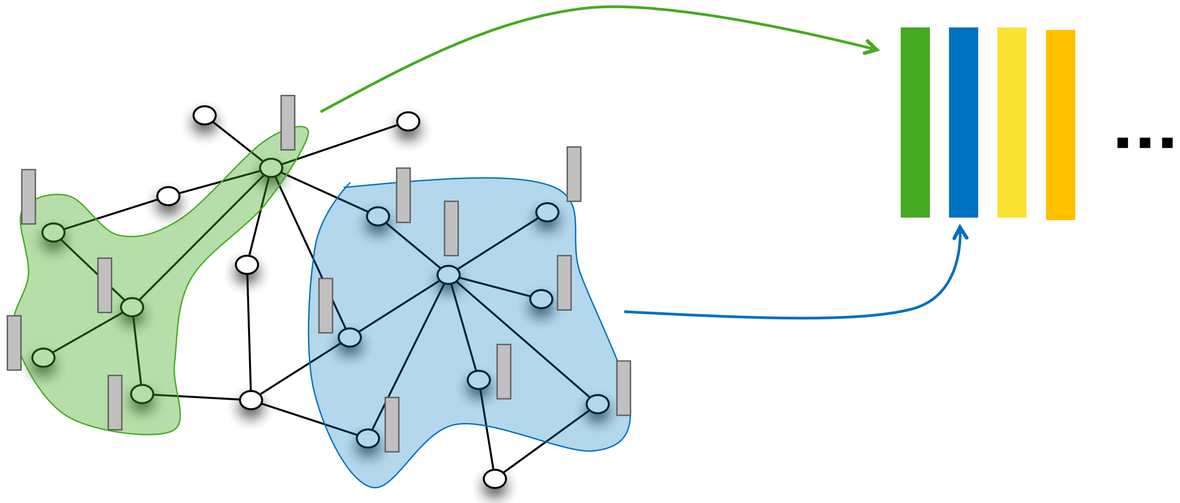
- What's the kernel size?
- What's the stride?

GNN's attribute vector per node == CNN's column of channels at each index in a feature map

Roadmap

- Learning tasks with graphs
- Message passing GNNs
- Approximation Power

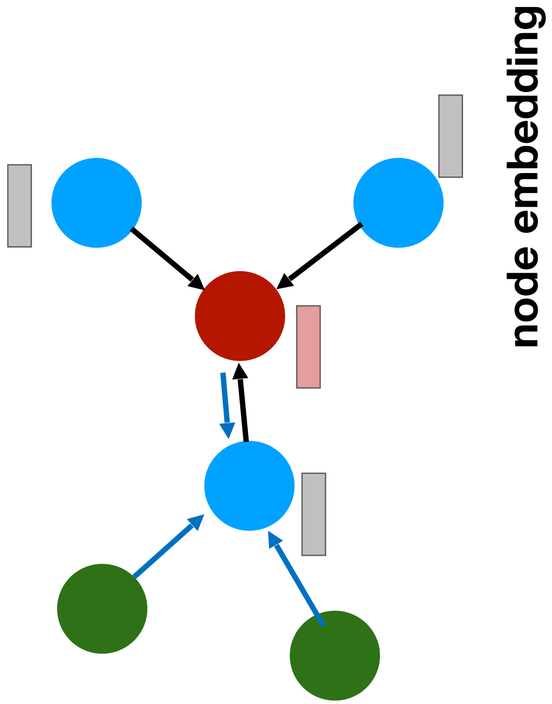
Graph neural networks



Idea:

1. Encode each node (based on message passing between nodes)
2. Aggregate *set* of node embeddings into a graph embedding

Encoding neighborhoods: general form



In each round *k*:

Aggregate information from neighbors

$$\mathbf{m}_{\mathcal{N}(v)}^{(k)} = \text{AGGREGATE}^{(k)}\left(\{\mathbf{h}_u^{(k-1)} : u \in \mathcal{N}(v)\}\right)$$

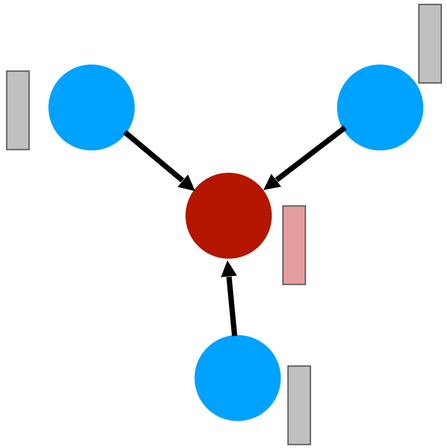
feature description of node u in round k-1

Update current node representation by incorporating messages from neighbors

$$\mathbf{h}_v^{(k)} = \text{UPDATE}^{(k)}\left(\mathbf{h}_v^{(k-1)}, \mathbf{m}_{\mathcal{N}(v)}^{(k)}\right)$$

(Merkwirth & Lengauer 2005; Scarselli et al 2009; Bruna et al 2014; Dai et al 2016; Battaglia et al., 2016; Defferrard et al., 2016; Duvenaud et al., 2015; Hamilton et al., 2017; Kearnes et al., 2016; Kipf & Welling, 2017; Gilmer et al 2017; Li et al., 2016; Velickovic et al., 2018; Verma & Zhang, 2018; Ying et al., 2018; Zhang et al., 2018; …)

What are the aggregation functions?



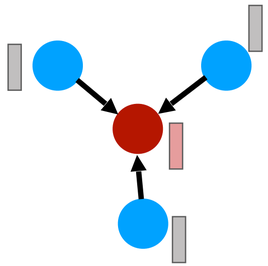
$$\mathbf{m}_{\mathcal{N}(v)}^{(k)} = \text{AGGREGATE}^{(k)}\left(\{\mathbf{h}_u^{(k-1)} : u \in \mathcal{N}(v)\}\right)$$

$$= \bigoplus_{u \in \mathcal{N}(v)} \psi^{(k)}\left(\mathbf{h}_u^{(k-1)}, \mathbf{h}_v^{(k-1)}\right)$$

$$\mathbf{h}_v^{(k)} = \text{UPDATE}^{(k)}\left(\mathbf{h}_v^{(k-1)}, \mathbf{m}_{\mathcal{N}(v)}^{(k)}\right)$$

$\mathcal{N}(v) = \{u \mid \exists (u, v) \in E(\mathcal{G})\}$ node's neighborhood

What are the aggregation functions?



Aggregate: permutation invariant, multi-set function

- Sum, average, …

$$\mathbf{m}_{\mathcal{N}(v)} = \frac{1}{|\mathcal{N}(v)|} \sum_{u \in \mathcal{N}(v)} \mathbf{h}_u$$

(Merkwirth & Lengauer 2005, Scarselli et al 2009)

$$\mathbf{m}_{\mathcal{N}(v)} = \sum_{u \in \mathcal{N}(v)} \frac{\mathbf{h}_u}{\sqrt{|\mathcal{N}(v)||\mathcal{N}(u)|}}$$

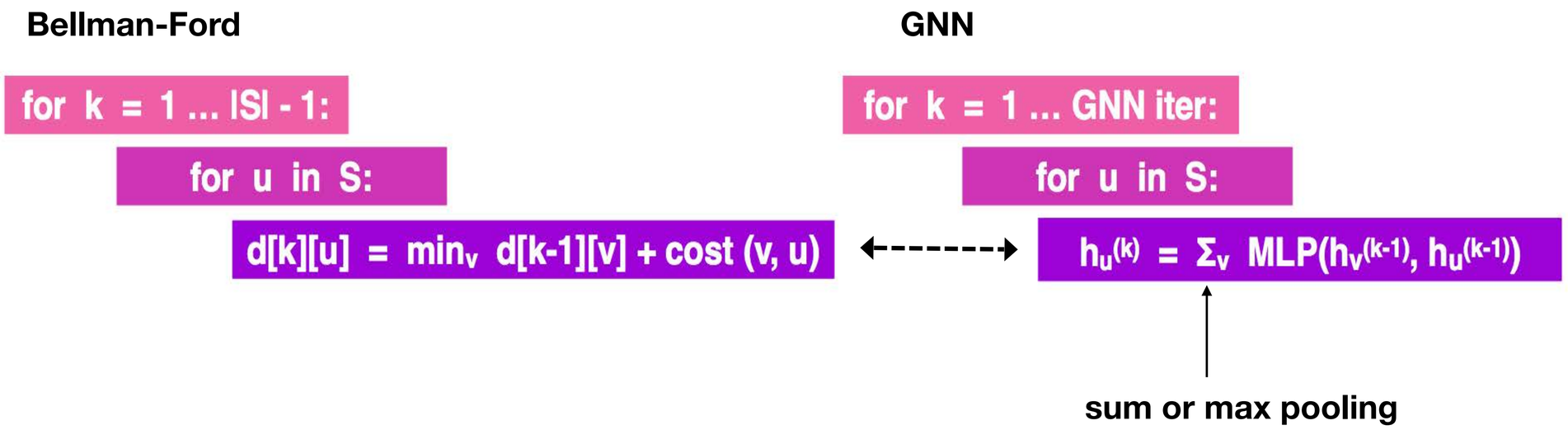
(Kipf & Welling 2016, Hamilton et al 2017)

- Min / max *(coordinate-wise)*

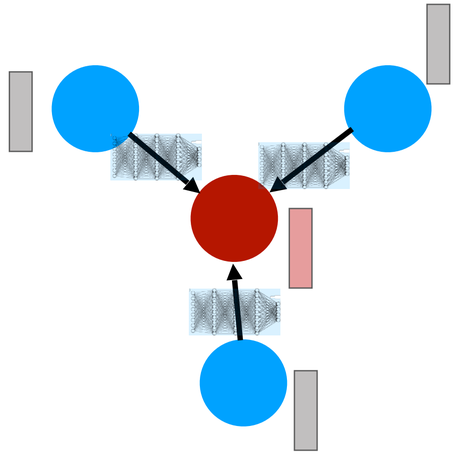
$$\mathbf{m}_{\mathcal{N}(v)} = \max \left\{ \mathbf{h}_u^{(k-1)} : u \in \mathcal{N}(v) \right.$$

Can implement e.g. shortest path: $d_v^{(k)} = \min_{u \in \mathcal{N}(v)} d_u^{(k-1)} + \text{cost}(u, v)$

Learning a shortest path algorithm



Aggregation functions and updates



Aggregate: General form *(universal approximation of multi-set functions)*: *(Zaheer et al 2017, Qi et al 2017, Xu et al 2019)*

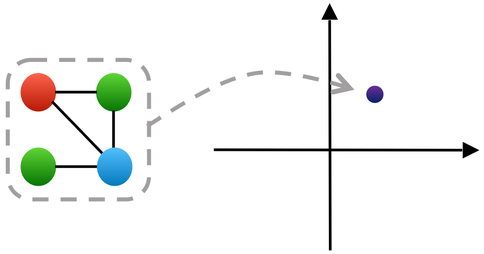
$$\mathbf{m}_{\mathcal{N}(v)} = \mathrm{MLP}_2\Big(\sum_{u \in \mathcal{N}(v)} \mathrm{MLP}_1(\mathbf{h}_u, \mathbf{h}_v)\Big)$$

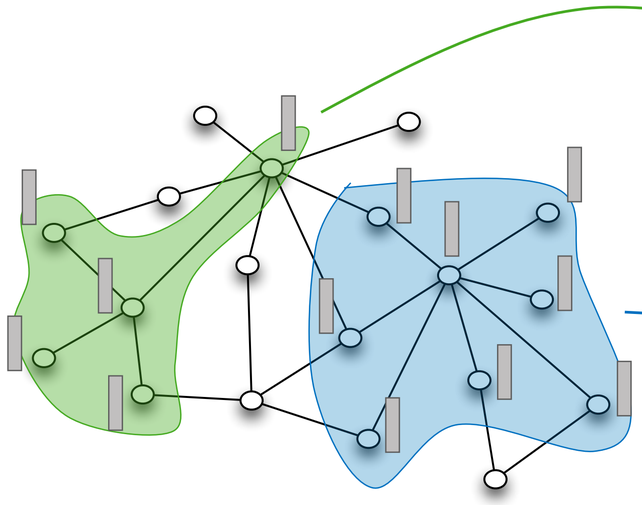
Learned aggregation function

Update: e.g. $\mathbf{h}_v^{(k)} = \sigma(\mathbf{W}_{\text{self}}\mathbf{h}_v^{(k-1)} + \mathbf{W}_{\text{neigh}}\mathbf{m}_{\mathcal{N}(v)}^{(k)} + b)$

learned

Graph embeddings





$$\mathbf{h}_{\mathcal{G}}$$

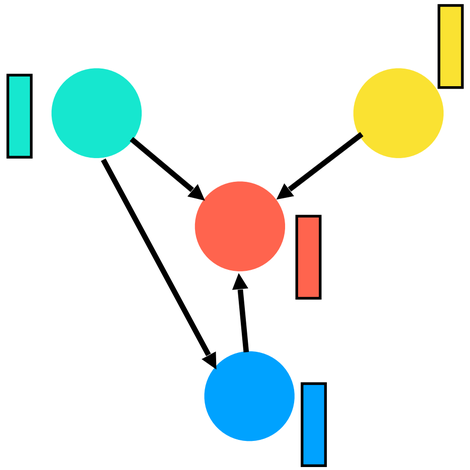
$$\mathbf{h}_{\mathcal{G}} = \text{READOUT}\left(\{\mathbf{h}_v^{(K)} : v \in \mathcal{G}\}\right)$$

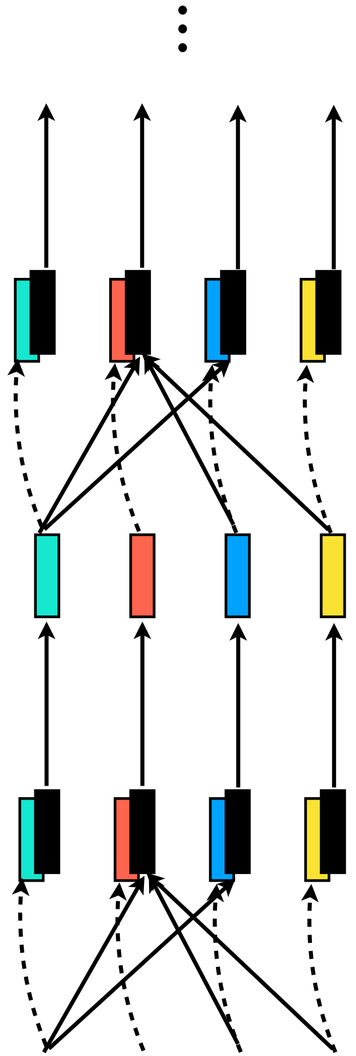
pooling operation (just like AGGREGATE)

Idea:

1. Encode each node (based on message passing between nodes)
2. **Aggregate *set* of node embeddings into a graph embedding**

GNNs unrolled

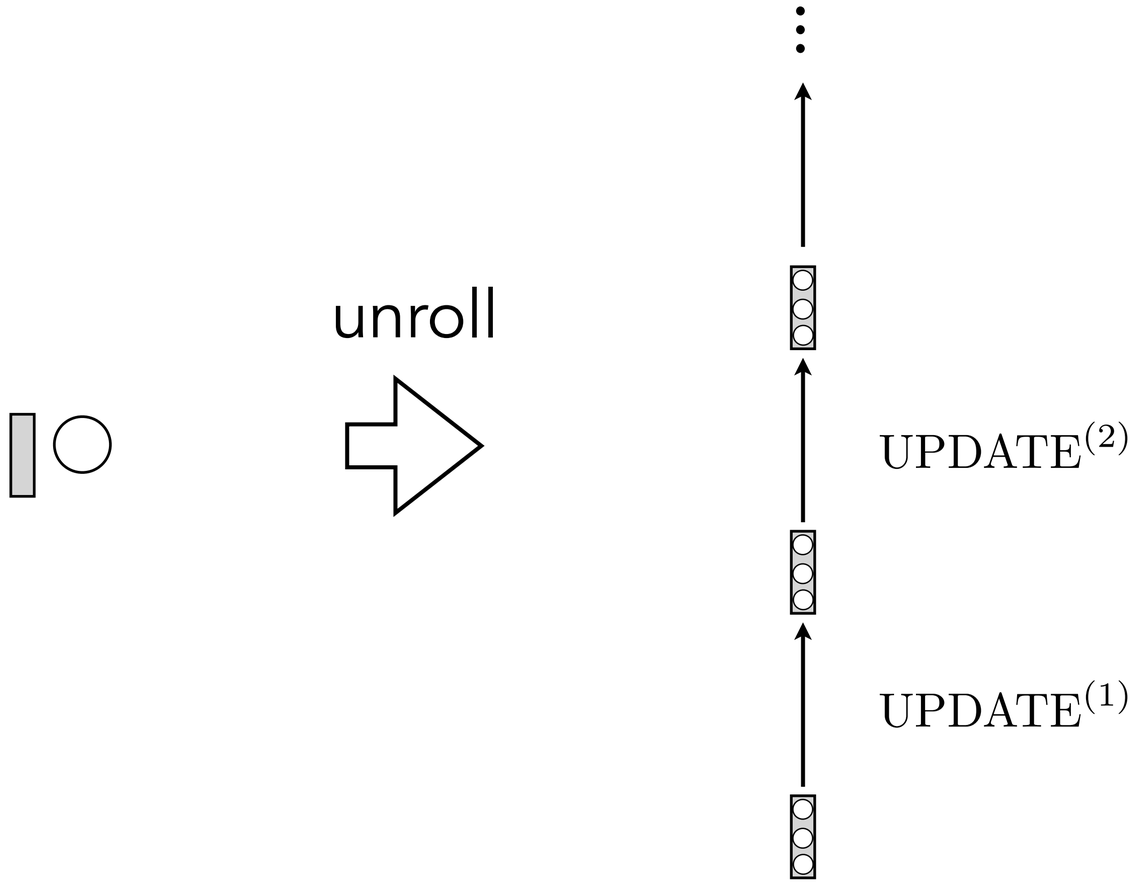




- Like an MLP, but nodes are vectors rather than scalars, edges are potentially complex functions (e.g., an edge can be an MLP)
- Each iteration of GNN message passing is a layer
  - AGGREGATE is akin to a linear layer
  - UPDATE is akin to a pointwise layer

What is the graph for an MLP?

An MLP is a GNN over single node



Update:

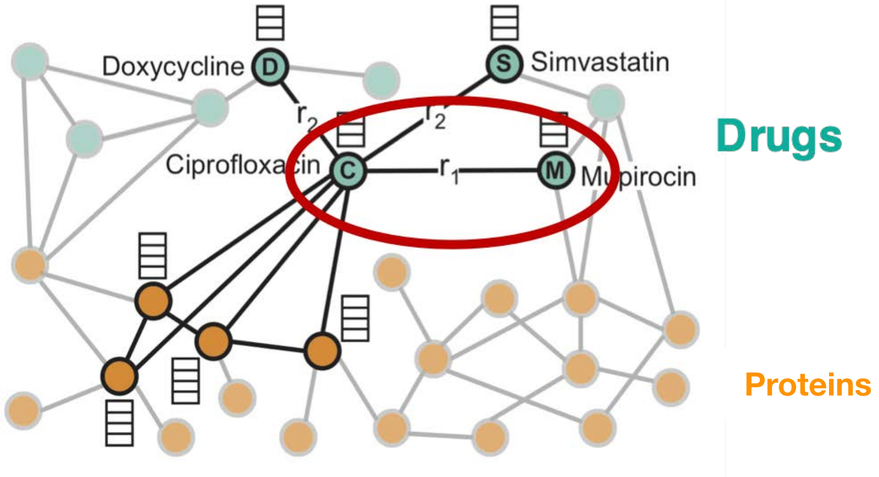
$$\mathbf{h}_v^{(k)} = \sigma(\mathbf{W}_{\text{self}}\mathbf{h}_v^{(k-1)} + \mathbf{W}_{\text{neigh}}\mathbf{m}_{\mathcal{N}(v)}^{(k)} + b)$$

Generalizations

- Use **edge attributes** / features in aggregation

$$\mathbf{m}_{\mathcal{N}(v)} = \sum_{u \in \mathcal{N}(v)} \text{MLP}^{(k)}(\mathbf{h}_u^{(k-1)}, \mathbf{h}_v^{(k-1)}, \mathbf{w}_{uv})$$

- **Multi-relational**: multiple "channels" *different aggregations for different types of edges*



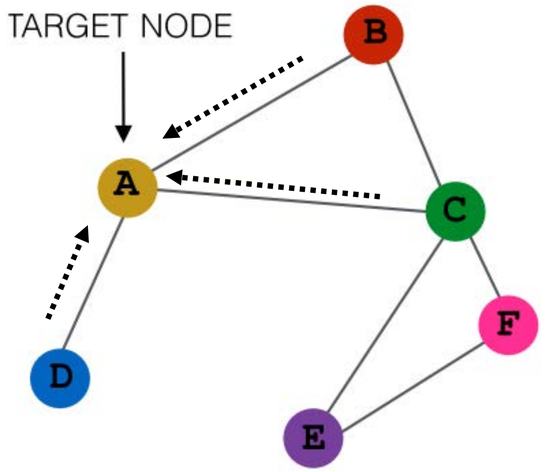
(Zitnik et al, 2018)

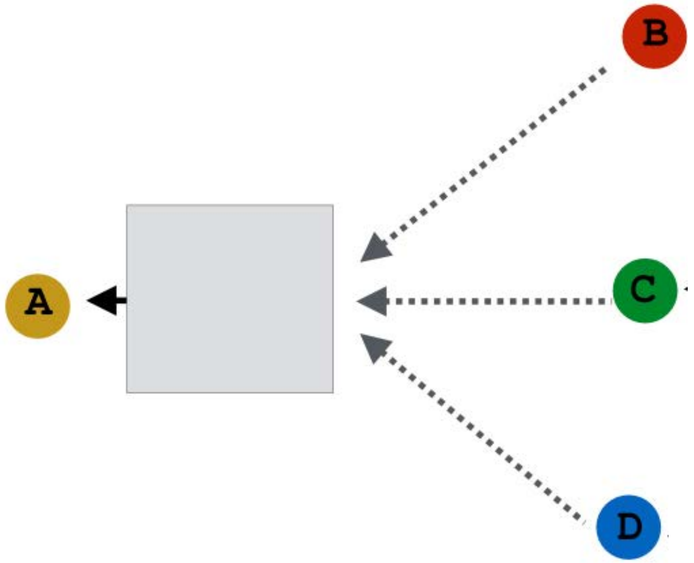
- **Attention** *(Velickovic et al 2018)*:

$$\mathbf{m}_{\mathcal{N}(v)} = \sum_{u \in \mathcal{N}(v)} \alpha_{v,u} \mathbf{h}_u$$

- Janossy pooling *(Murphy et al 2018)*
  permutation-sensitive *function averaged over permutations*

Node embeddings: tree view

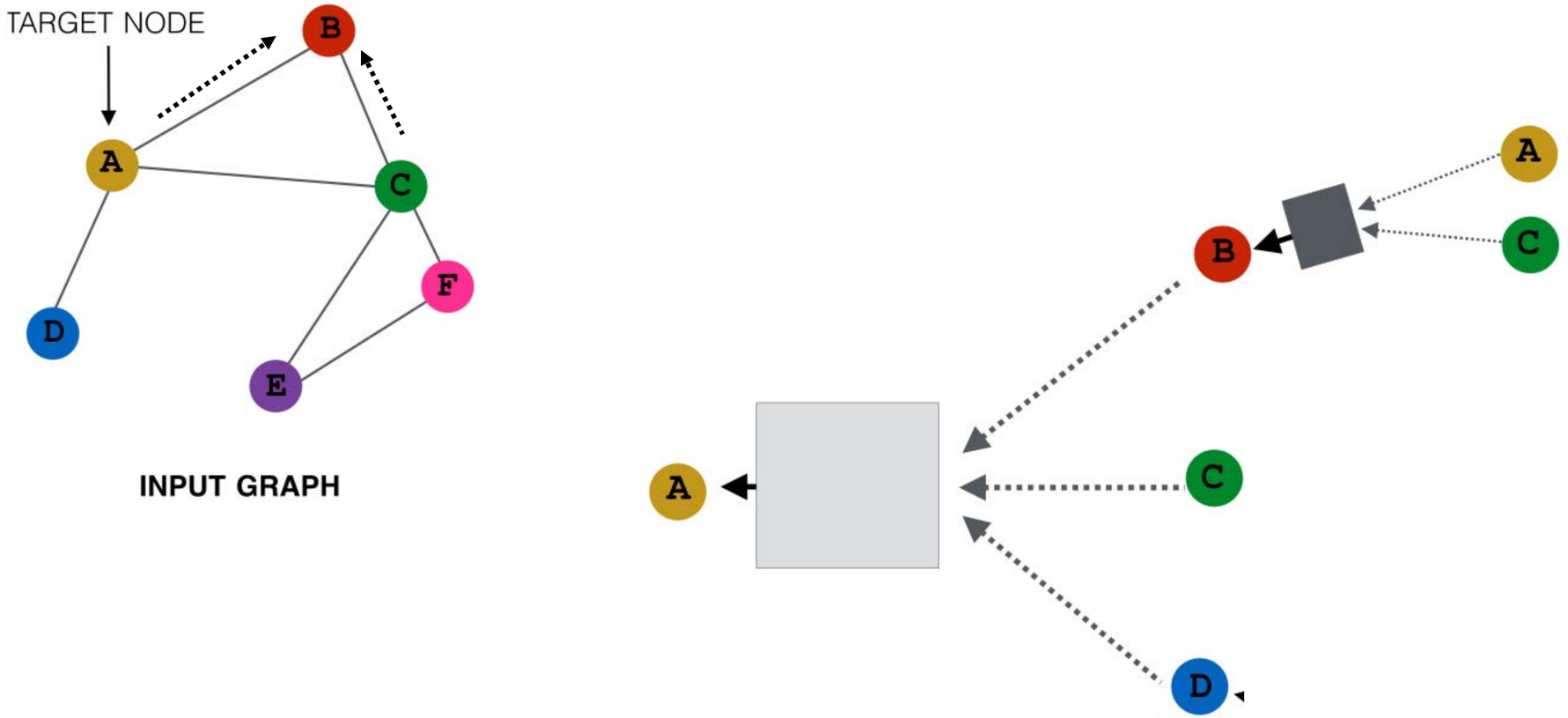




grey boxes: aggregation functions that we learn

(illustrations: J. Leskovec)

Node embeddings: tree view



grey boxes: aggregation functions that we learn

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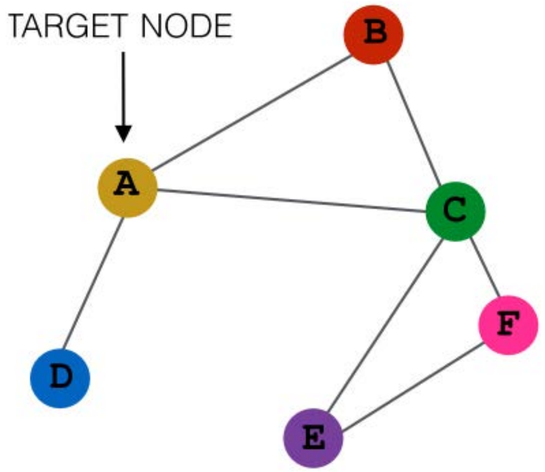
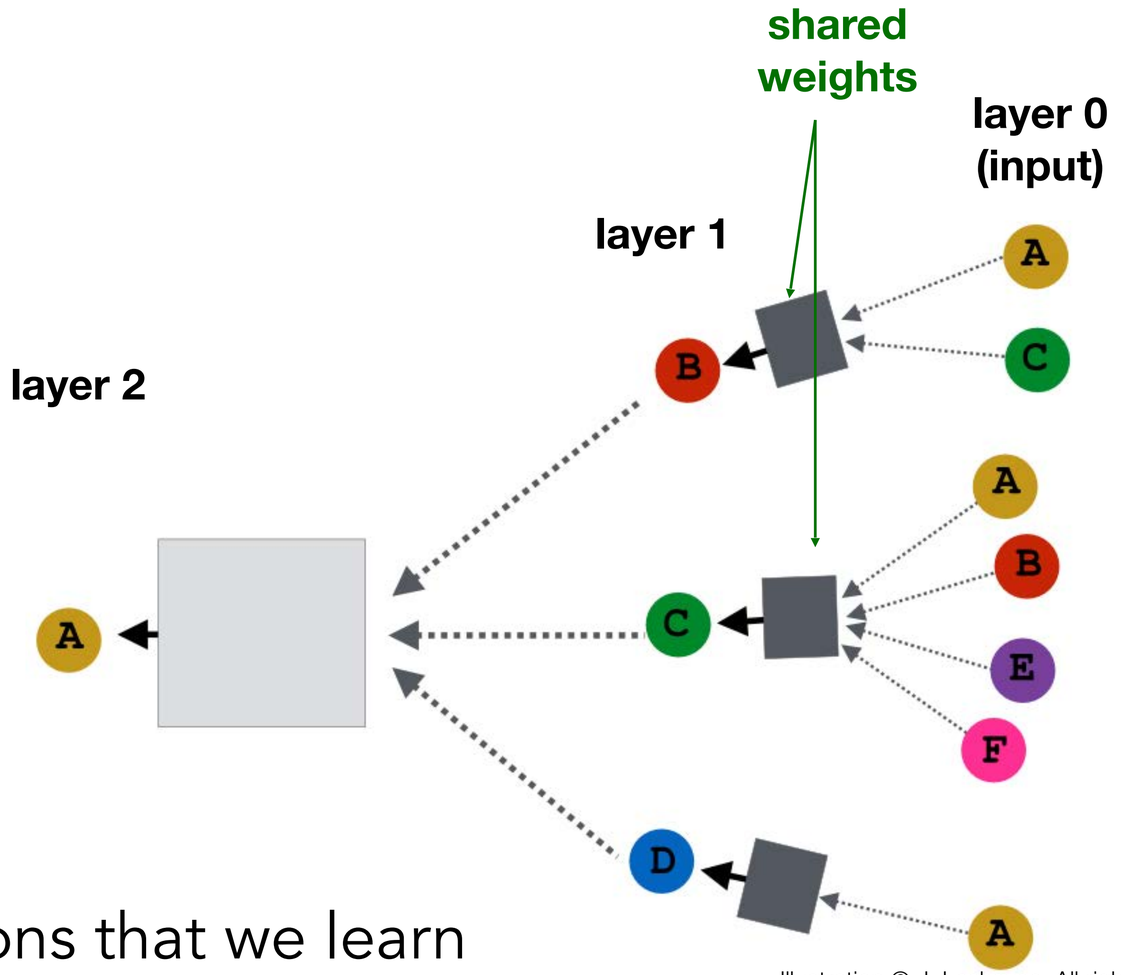
Node embeddings: tree view



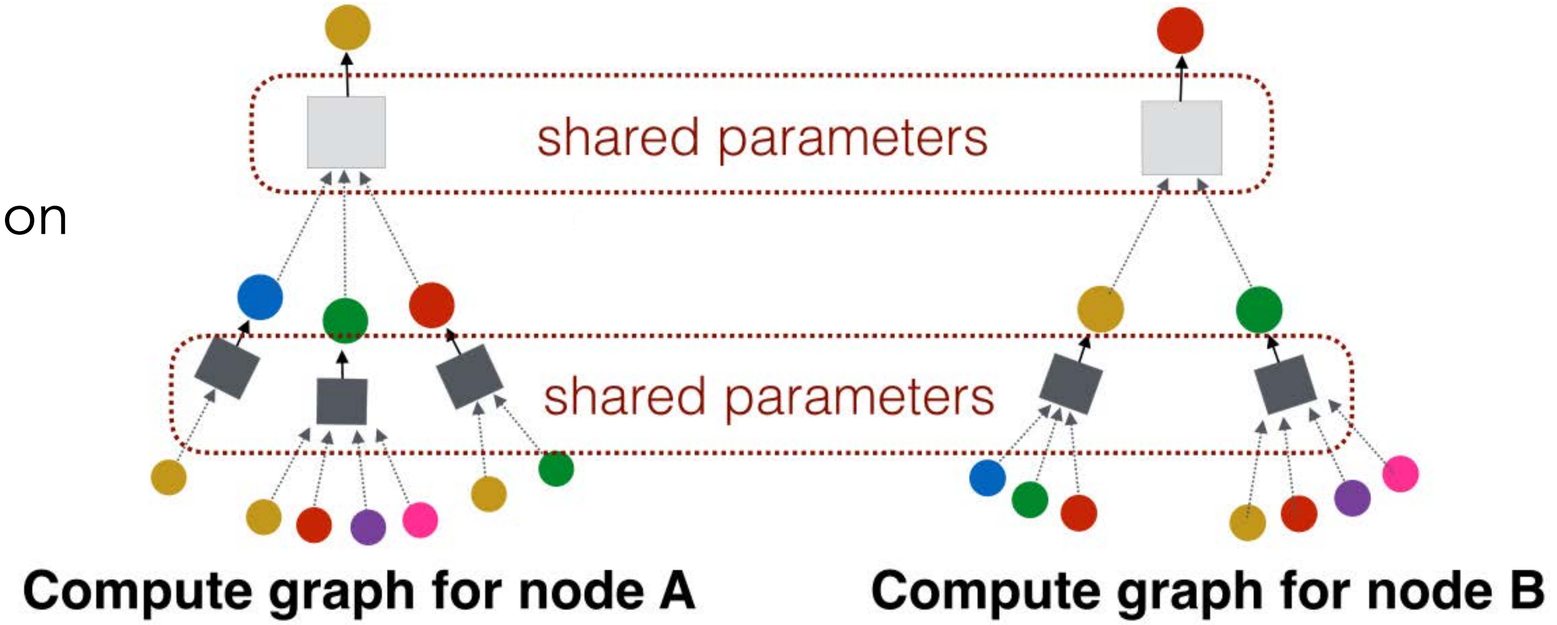


grey boxes: aggregation functions that we learn

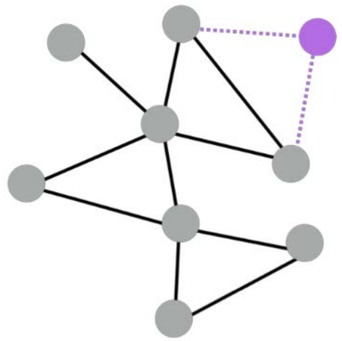
(illustrations: J. Leskovec)

Weight sharing

- We use the same aggregation functions for all nodes.



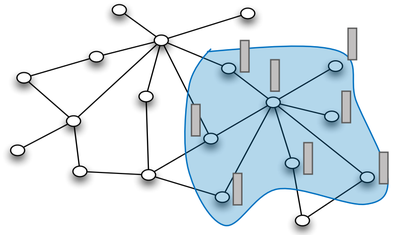
- So we can generate encodings for previously unseen nodes & graphs too!
  (dynamic graphs, different molecules, …)



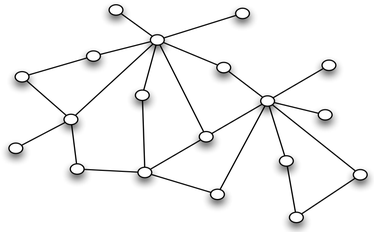
Illustrations: J. Leskovec

Training a GNN

- **What is a data point?**



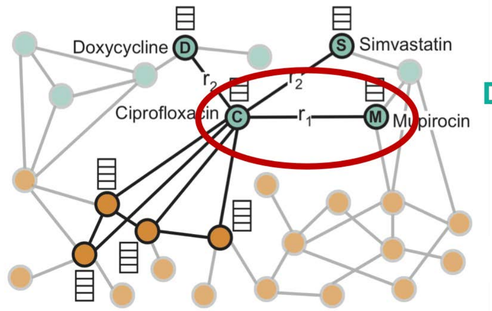
{node, label} pairs



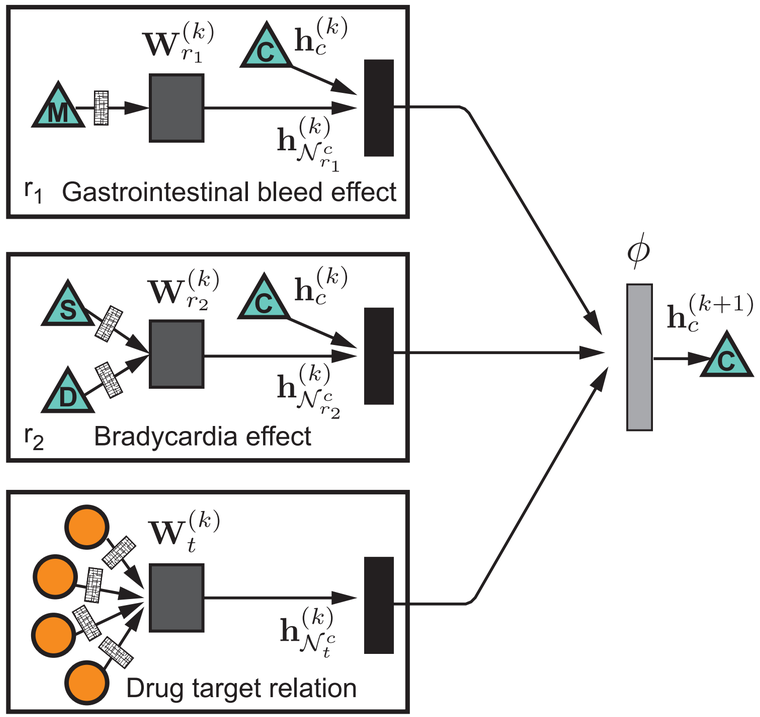
{graph, label} pairs

- **What to specify?**
  - Aggregate, updates and readout functions
  - Loss function on prediction
- **Train** with SGD

Example architecture 1: polypharmacy



- Different types of edges: drug-drug, drug-protein, protein-protein



$$\mathbf{h}_v^{(k+1)} = \mathrm{ReLU}\left(\sum_r \sum_{u \in \mathcal{N}_r(v)} c^{vu} \mathbf{W}_r^{(k)} \mathbf{h}_u^{(k)} + c_r^v \mathbf{h}_v^{(k)}\right)$$

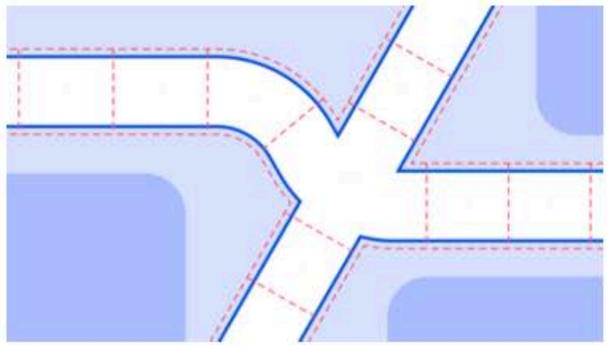
separate aggregation per edge type r, then sum them up

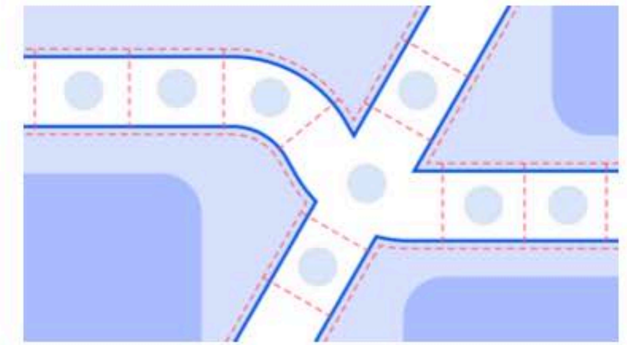
Modeling Polypharmacy Side Effects with Graph Convolutional Networks

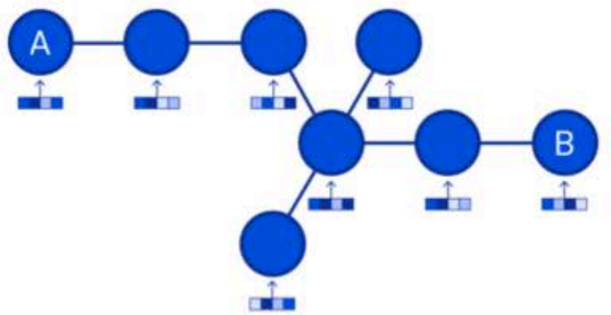
Marinka Zitnik [1], Monica Agrawal [1] and Jure Leskovec [1,2,*]

Example architecture 2: Google Maps

- segments *v* (50-100m), supersegments *u* (ca 20 segments);
  input features: historical travel times, road type, traffic pattern at prediction time
- 3 aggregation/update operations: $\mathbf{h}_v$'s (using adjacent edges $\mathbf{h}_e$, $\mathbf{h}_u$),
  edges $\mathbf{h}_e$ (using adjacent segments $\mathbf{h}_v$ and $\mathbf{h}_u$),
  $\mathbf{h}_u$ (using segments $\mathbf{h}_v$ and edges $\mathbf{h}_e$ in supersegment)
- combination of pooling operations for each aggregation
- linear combination of losses per time horizon (segment travel time, super segment time, cumulative segment time, self-supervised / generative loss)

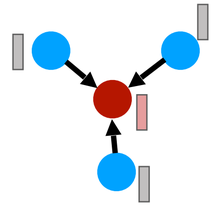






(Derrow-Pinion et al., ETA Prediction with Graph Neural Networks in Google Maps, CIKM 2021)

Many connections

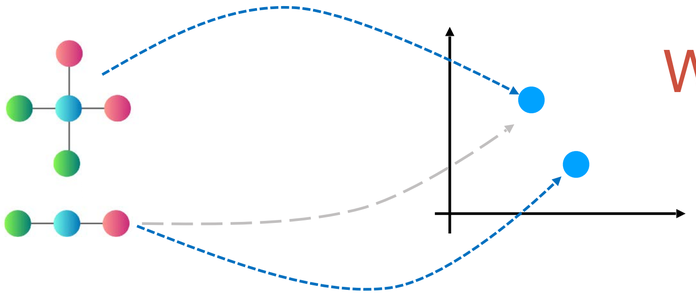


- **Graph signal processing and convolutions**
- **Inference in graphical models** *(Dai et al 2016)*
  - Node embeddings = latent variables
  - Given node features and graph, infer latent variables
  - “Neural message passing”
- **Distributed / Local algorithms** *(Sato et al 2019, Loukas 2020)*
  - Bounds for detection, verification, computation with GNNs
- **Random walks** *(Xu et al 2018)*
  - Oversmoothing, graph structure and depth
  - (Adaptive) skip connections
- **Graph isomorphism testing** *(Morris et al 2019, Xu et al 2019)*

Roadmap

- Learning tasks with graphs
- Message passing GNNs
- Approximation Power

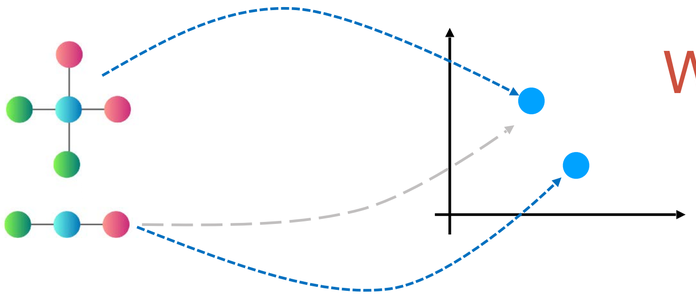
Which functions can GNNs approximate?



Which graphs can GNNs distinguish?

$$f(G) \neq f(G')?$$

Which functions can GNNs approximate?



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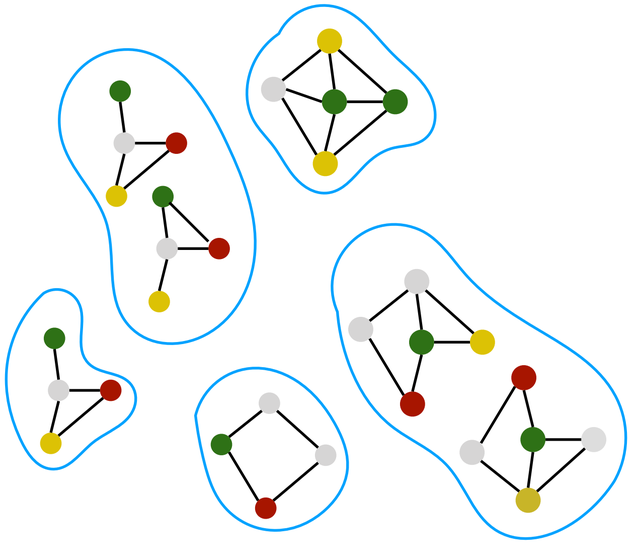


Distinction implies function approximation

for node and graph predictions

(Symmetric Stone-Weierstrass theorem)

(Azizian & Lelarge 21, Chen-Villar-Chen-Bruna 19, Keriven & Peyré 19, Maron-Fetaya-Segol-Lipman 19)

$$(G, G') \in \rho(\mathcal{F}) \;\Leftrightarrow$$

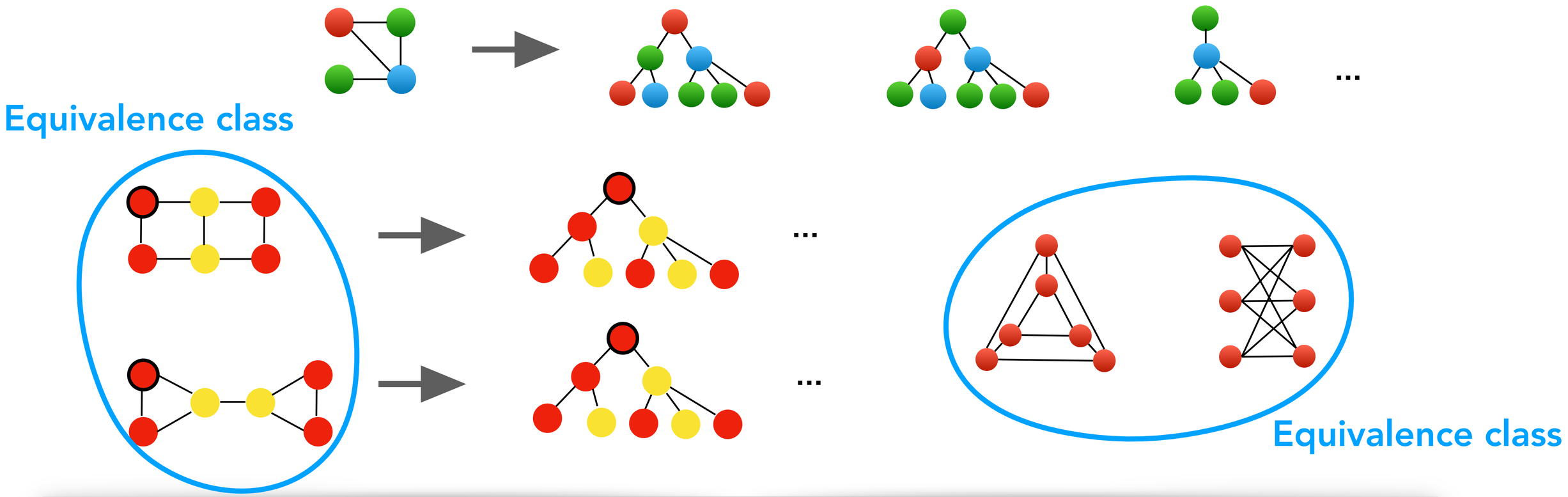
$$\forall F \in \mathcal{F},\; F(G) = F(G')$$

Theorem.

If function H on a compact domain does not assign different labels to graphs in one equivalence class, then it can be approximated by message passing GNNs:

$$\forall \epsilon > 0,\;\; \exists F \in \mathcal{F}^{\mathrm{GNN}} \;:\; \sup_{G \in K} \|H(G) - F(G)\| \leq \epsilon$$

Discriminative Power



Theorem *(Morris-Ritzert-Fey-Hamilton-Lenssen-Rattan-Grohe 19, Xu-Hu-Leskovec-Jegelka 19)*
Any GNN can at best distinguish the same graphs as the 1-dim WL algorithm.

Color refinement / Weisfeiler-Leman algorithm

(Morgan 65, Weisfeiler & Leman 68)

coloring $c^{(t)} : V(G) \to \Sigma$

$$c^{(t)}(v) = \mathrm{Hash}\left(c^{(t-1)}(v),\, c^{(t-1)}(u) \mid u \in \mathcal{N}(v)\right)$$

isomorphism test: $\{c^{(t_\infty)}(v) | v \in V(G)\} \neq \{c^{(t_\infty)}(v') | v' \in V(G')\}?$

Color refinement / Weisfeiler-Leman algorithm

(Morgan 65, Weisfeiler & Leman 68)

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$$c^{(t)}(v) = \mathrm{Hash}\Big(c^{(t-1)}(v),\, c^{(t-1)}(u) \mid u \in \mathcal{N}(v)\Big)$$

vs GNN: $$\mathbf{h}_v^{(t)} = f_{\mathrm{Update}}\Big(\mathbf{h}_v^{(t-1)},\, f_{\mathrm{Agg}}\big(\{\mathbf{h}_u^{(t-1)} \mid u \in \mathcal{N}(v)\}\big)\Big)$$

Color refinement / Weisfeiler-Leman algorithm

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Theorem *(Morris-Ritzert-Fey-Hamilton-Lenssen-Rattan-Grohe 19, Xu-Hu-Leskovec-J 19)*
Any GNN can at best distinguish the same graphs as the 1-dim WL algorithm.
For any n, there exists a GNN such that for any t, $c^{(t)} \equiv h^{(t)}$.

How could we ensure that the aggregation is injective?

- Any (multi-)set function can be represented with nonlinear functions g_1, g_2 as:

$$f_{\text{Agg}}(S) = g_1 \quad \sum_{\mathbf{h} \in S} g_2(\mathbf{h}) \Bigg)$$

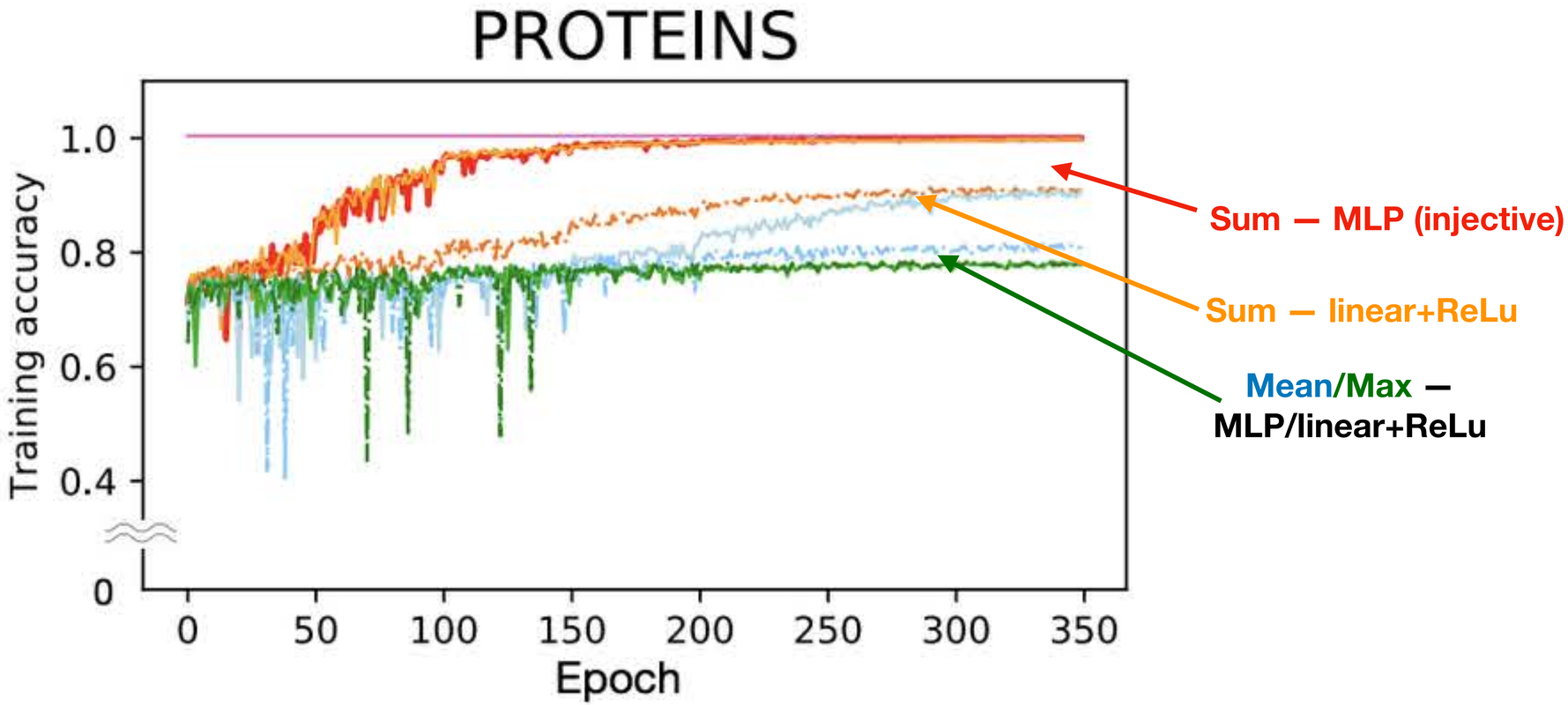
- We can universally approximate g_1 and g_2 by MLPs! (see a few slides ago)

$$\mathbf{m}_{\mathcal{N}(v)}^{(k)} = \text{MLP}_2 \sum_{u \in \mathcal{N}(v)} \text{MLP}_1(\mathbf{h}_u^{(k-1)})$$

Does this make a difference in practice?

- vary g and pooling operation

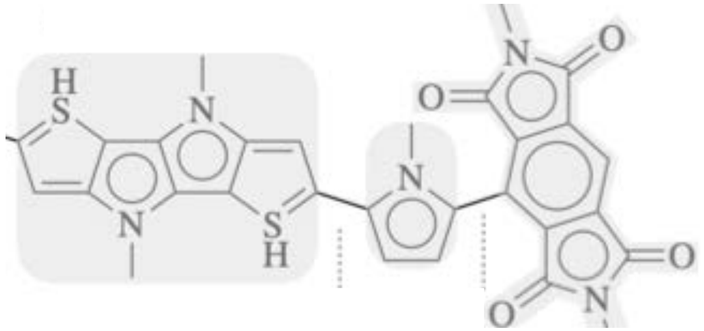
$$f_{\text{Agg}}(S) = g_1 \left(\sum_{\mathbf{h} \in S} g_2(\mathbf{h}) \right)$$



Learning structural graph properties

Can GNNs compute:

- the length of the shortest / longest cycle?
- diameter of the graph?
- the number of occurrences of a motif?



Lemma *(Garg et al 2020, Chen et al 2020)*

No! Message Passing GNNs (as discussed here) cannot compute these in general.

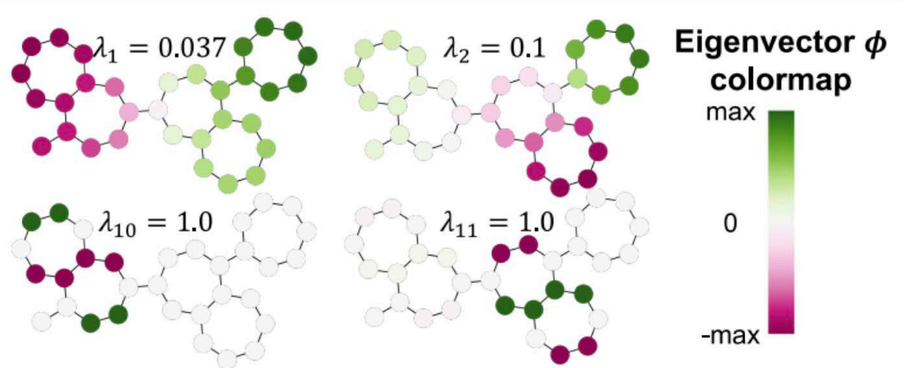
Improving discriminative power

- **Positional encodings**
  - Add node input features that encode "position" in the graph
- For instance: eigenvectors of the graph Laplacian (or its normalized versions)

$$L = D - A$$

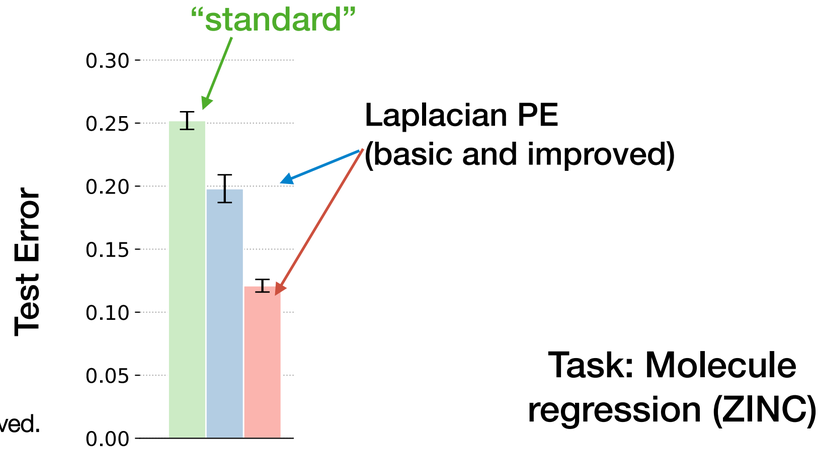
Diagonal matrix with node degrees

Adjacency matrix



(Kreuzer, Beaini, Hamilton, Létourneau, Tossou 2021)

- adds global structural information
- Challenge: ambiguities (sign flips, eigenvalue multiplicities)

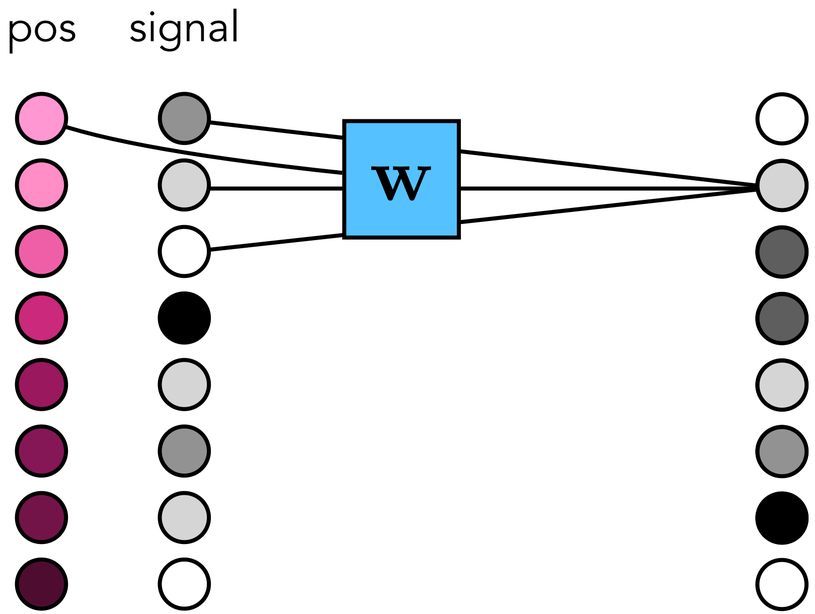


from: Lim-Robinson-Zhao-Smidt-Sra-Maron-J 22

Call back to CNNs:
What if you *don't* want to be shift invariant?

1. Use an architecture that is not shift invariant (e.g., MLP)

2. Add location information to the *input* to the convolutional filters — this is called **positional encoding**



Summary

- Encodes graph structure and node/edge attributes
- Important: permutation invariance/equivariance

- Main idea: **message passing** and **aggregations**
- **Can take graphs of varying size and structure** (similar to CNNs)
- Connections: graph signal processing, graphical models, distributed computing, isomorphism testing, …

- Representational enhancements: higher-order, node IDs/augmentation

Appendix

- Graph Laplacian (unnormalized): degree matrix D - adjacency matrix A

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

$$\mathbf{D}_{ii} = \deg(v_i) \text{ or } \sum_{(v_i, v_j) \in E} w_{ij} \quad \text{and} \quad \mathbf{D}_{ij} = 0 \text{ for } i \neq j$$

- normalized: $\mathbf{I} - \mathbf{D}^{-1}\mathbf{A}$ or $\mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$

6.7960 Deep Learning
Fall 2024