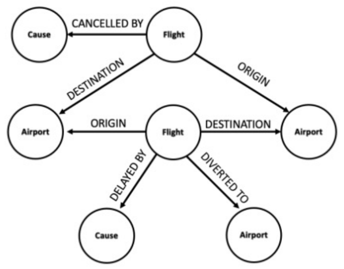
Graph neural networks

Based on slides from Jure Leskovec's CS244W

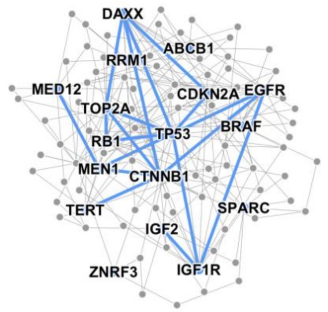
Many types of data are graphs



Event Graphs

Image credit: SalientNetworks

Computer Networks



Disease Pathways

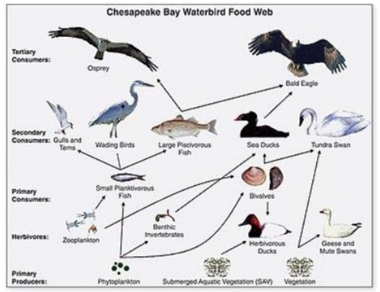


Image credit: Wikipedia

Food Webs

Image credit: Pinterest

Particle Networks

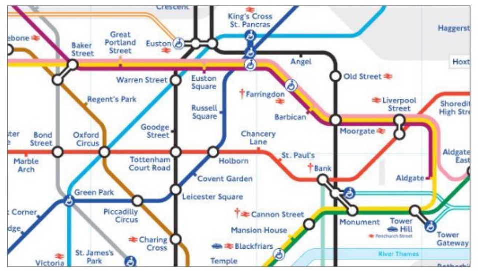


Image credit: visitlondon.com

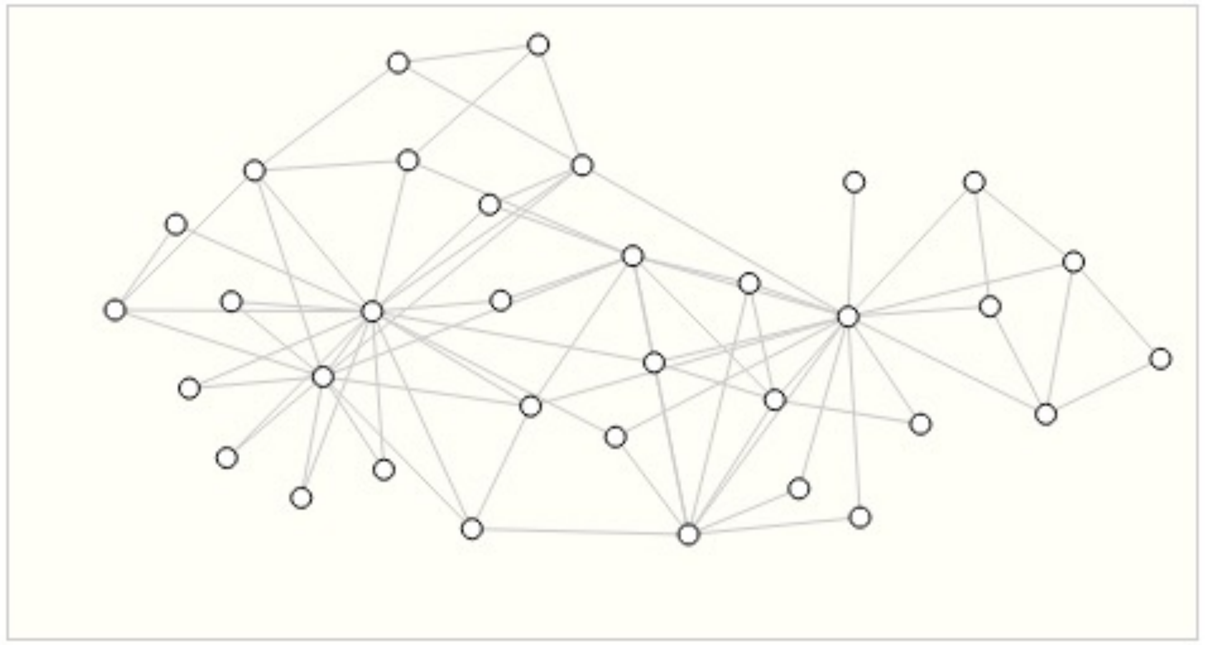
Underground Networks

Slide by Leskovec

GNN motivation

Main question:

How to utilize relational structure for better prediction?



Today: Modern ML toolbox

Modern DL toolbox is designed for simple sequences & grids

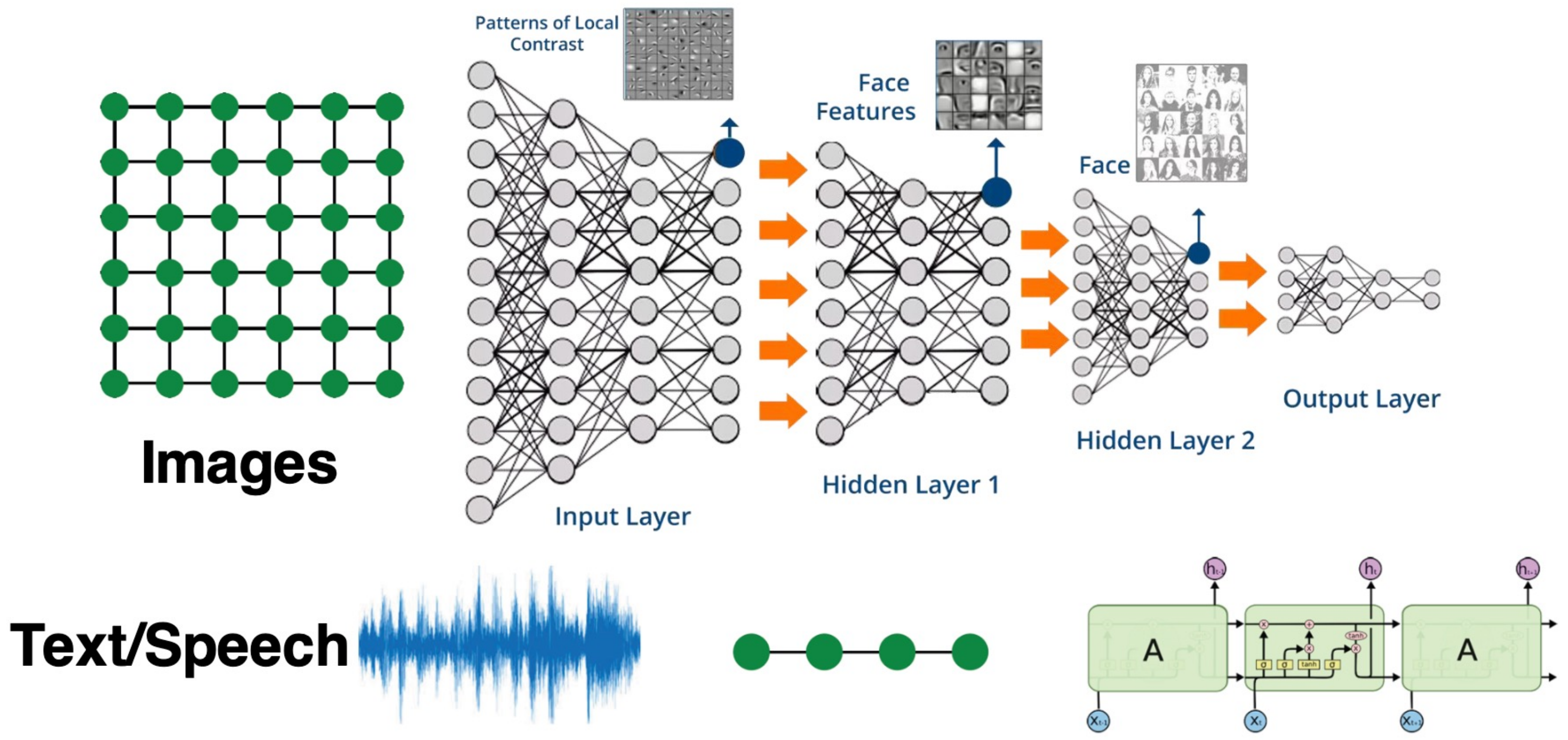
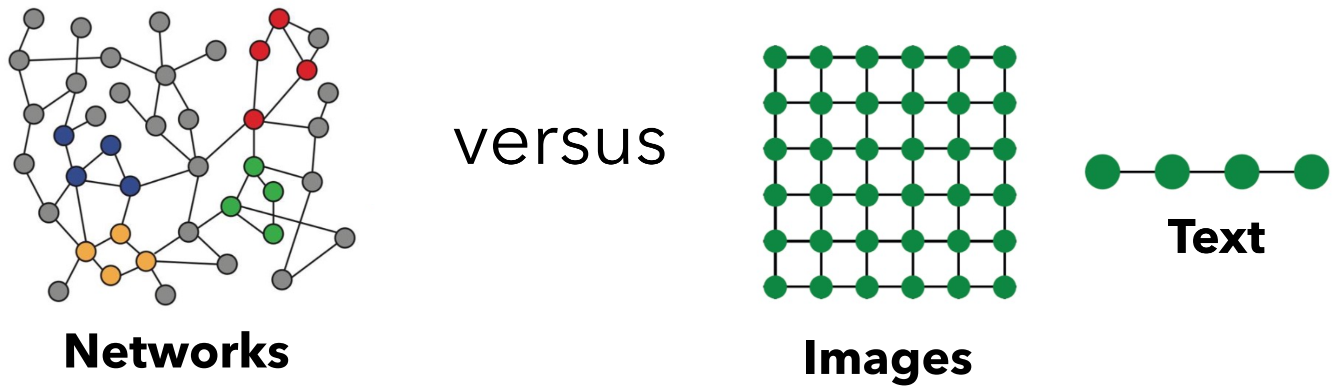


Figure by Leskovec

Why is graph deep learning hard?

Networks are complex

- Arbitrary size and complex topological structure



- No fixed node ordering or reference point
- Often dynamic and have multimodal features

Figure by Leskovec

Different types of tasks

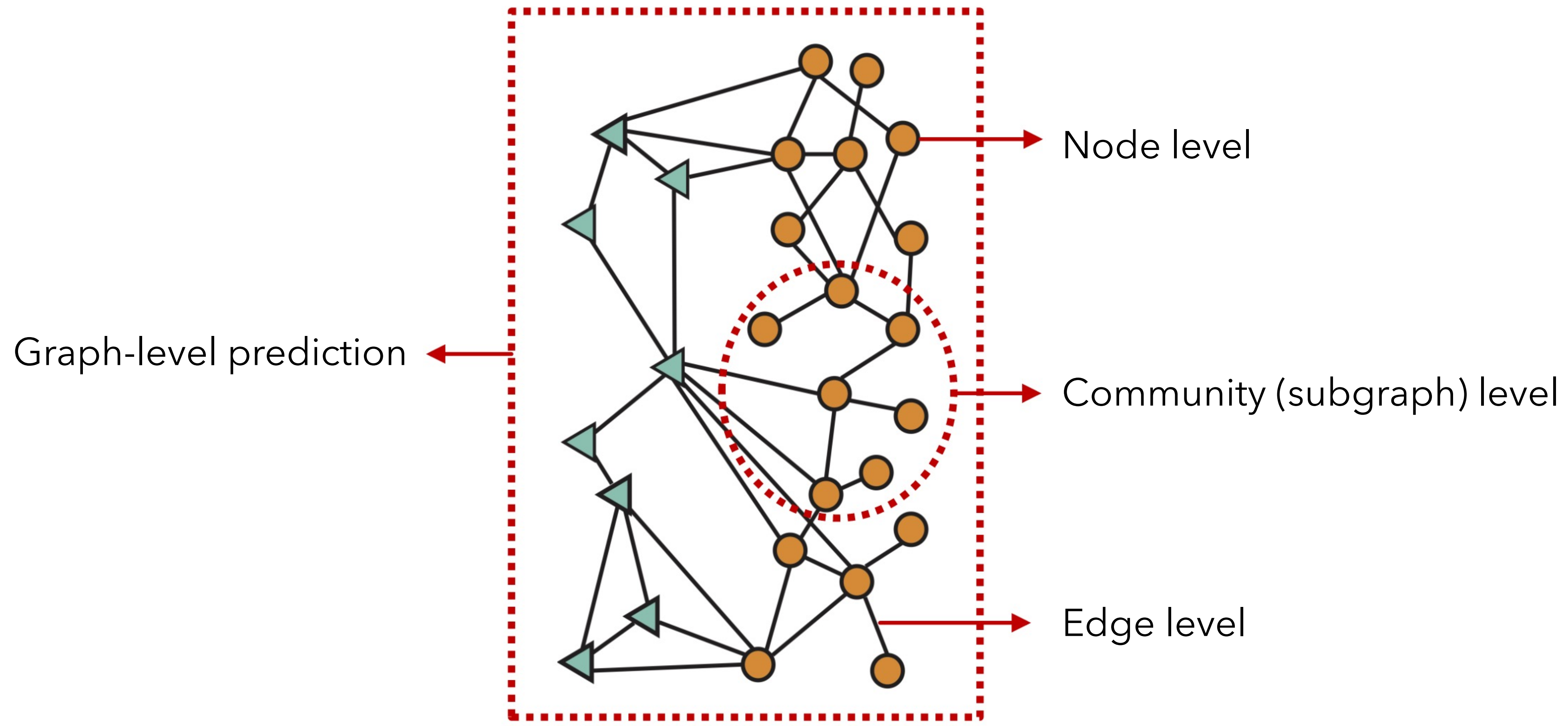
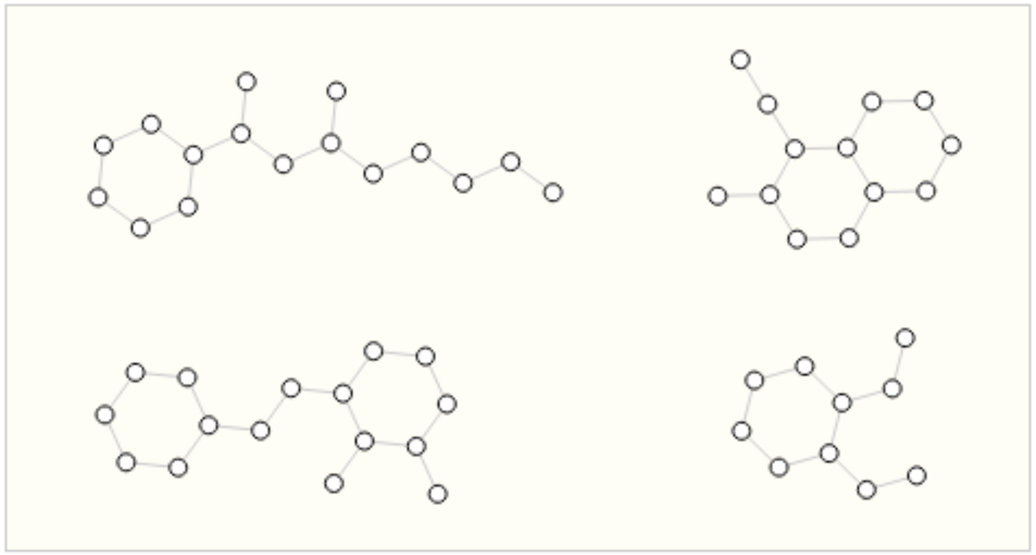
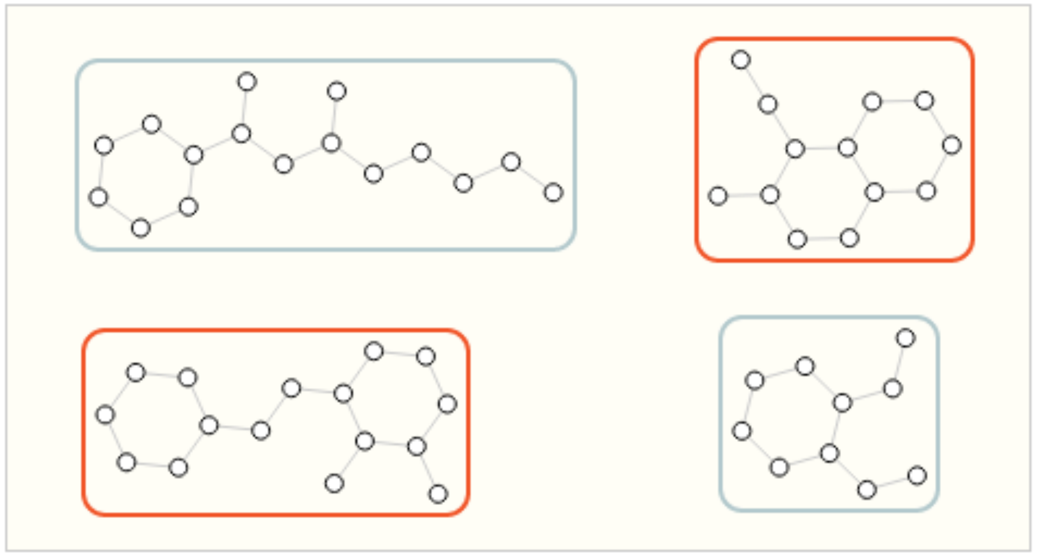


Figure by Leskovec

Prediction with graphs: Examples





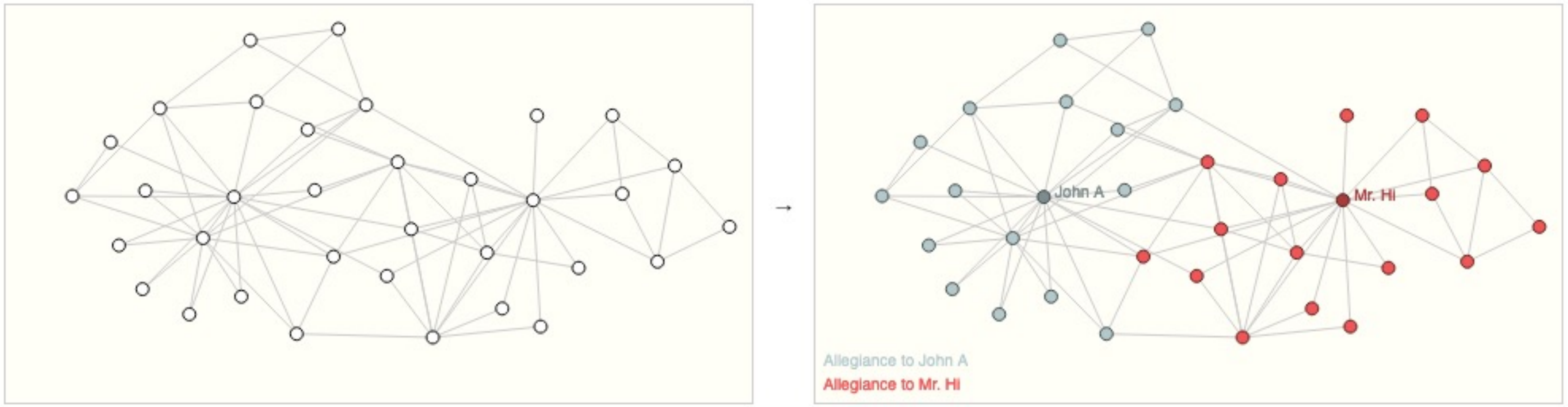
Graph-level tasks:

E.g., for a molecule represented as a graph, could predict:

- What the molecule smells like
- Whether it will bind to a receptor implicated in a disease

Figure by Sanchez-Lengeling et al. ['21]

Prediction with graphs: Examples

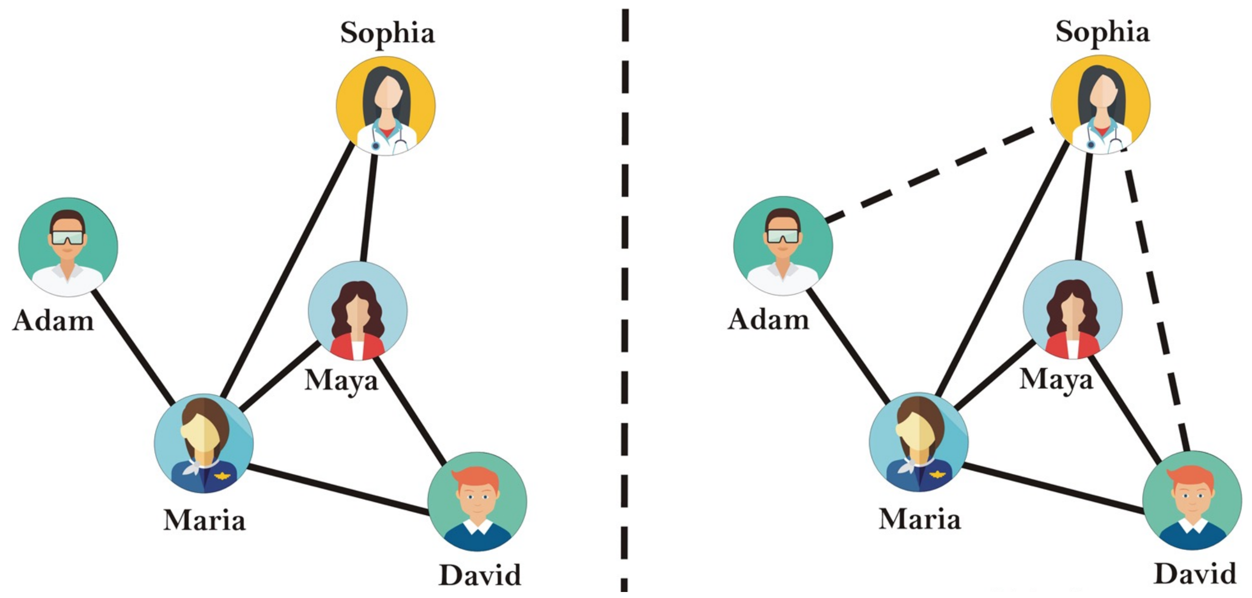


Node-level tasks:

E.g., political affiliations of users in a social network

Figure by Sanchez-Lengeling et al. ['21]

Prediction with graphs: Examples



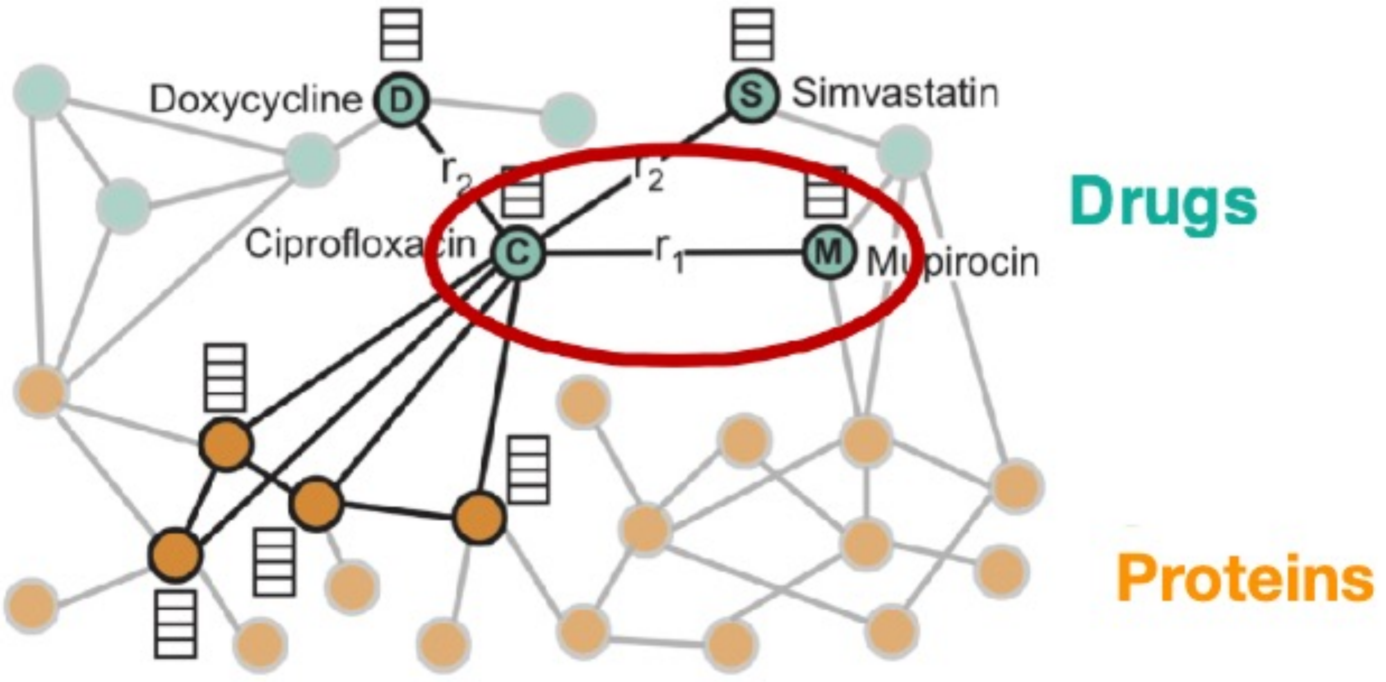
Edge-level tasks: E.g.:

- Suggesting new friends
- Recommendations on Amazon, Netflix, …

Figure by Ahmad et al. ['20]

Example: Polypharmacy side effects

Drug 1	😀
Drug 2	😀
Combined	😫



Nodes: Drugs
Edges: Interaction type

Figure by Zitnik et al. ['18]

Example: Traffic routing

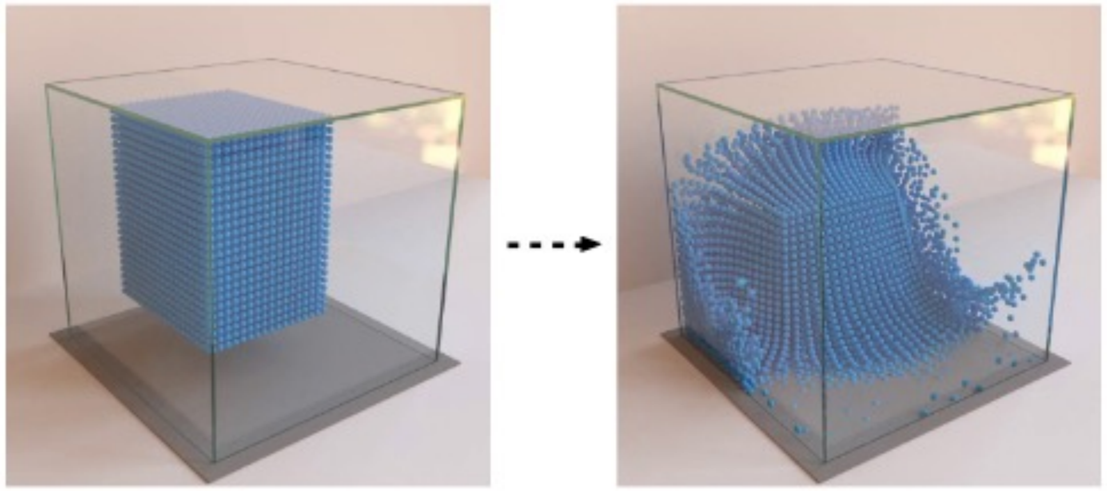
E.g., Google maps

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

Example: Learning to simulate physics

Nodes: Particles

Edges: Interaction between particles

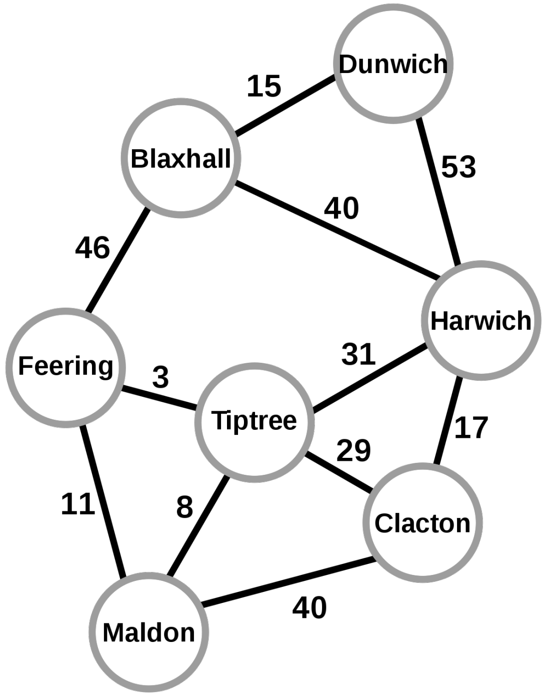


Goal: Predict how a graph will evolve over time

Sanchez-Gonzalez et al. ['20]

Example: Combinatorial optimization

Replace full algorithm or learn steps (e.g., branching decision)



$$\begin{array}{ll} \text{maximize} & \boldsymbol{c} \cdot \boldsymbol{z} \\ \text{subject to} & A\boldsymbol{z} \leq \boldsymbol{b} \\ & \boldsymbol{z} \in \mathbb{Z}^n \end{array}$$

Outline

1. Introduction
2. **Feature engineering for graphs**
3. GNN architecture
4. Training a GNN

Traditional ML pipeline

- Design features for nodes/links/graphs
- Obtain features for all training data

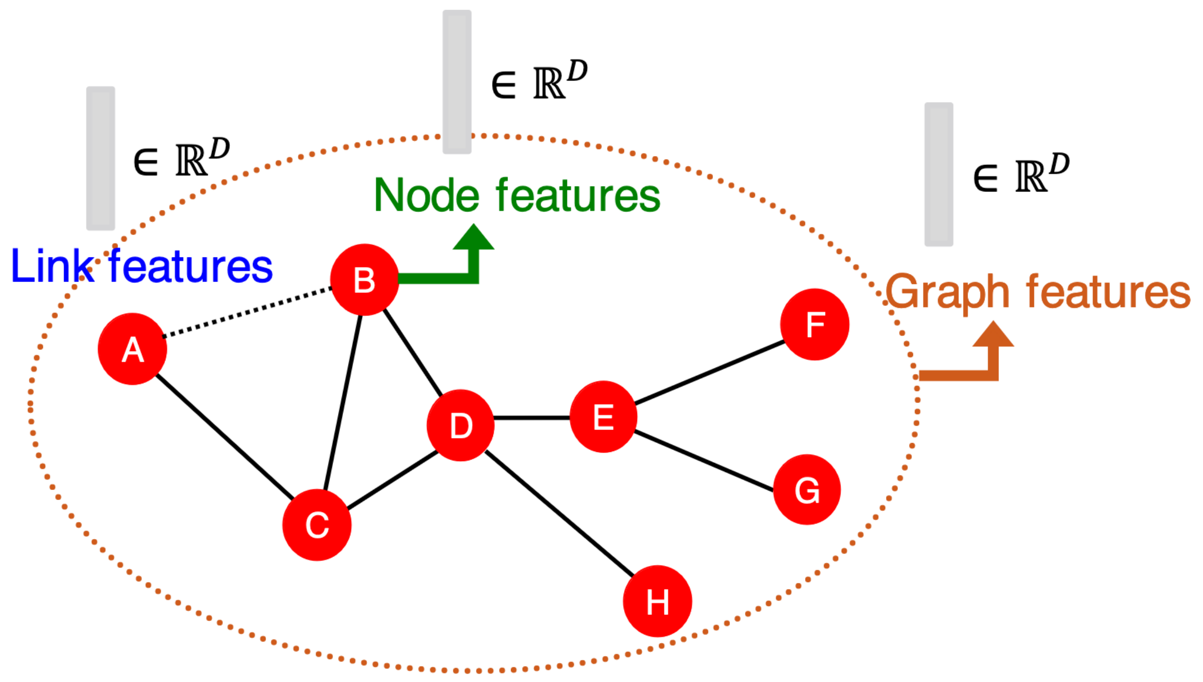
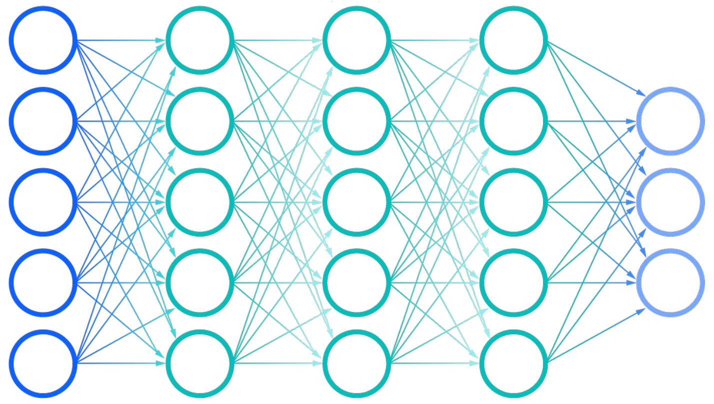


Figure by Leskovec

Traditional ML pipeline

Train an ML model:

- Logistic Regression, random forest, NN, etc.



Apply the model:

- Given new node/link/graph, obtain features and make prediction

Using effective features is key to achieving good performance

Figure by IBM

Different types of features

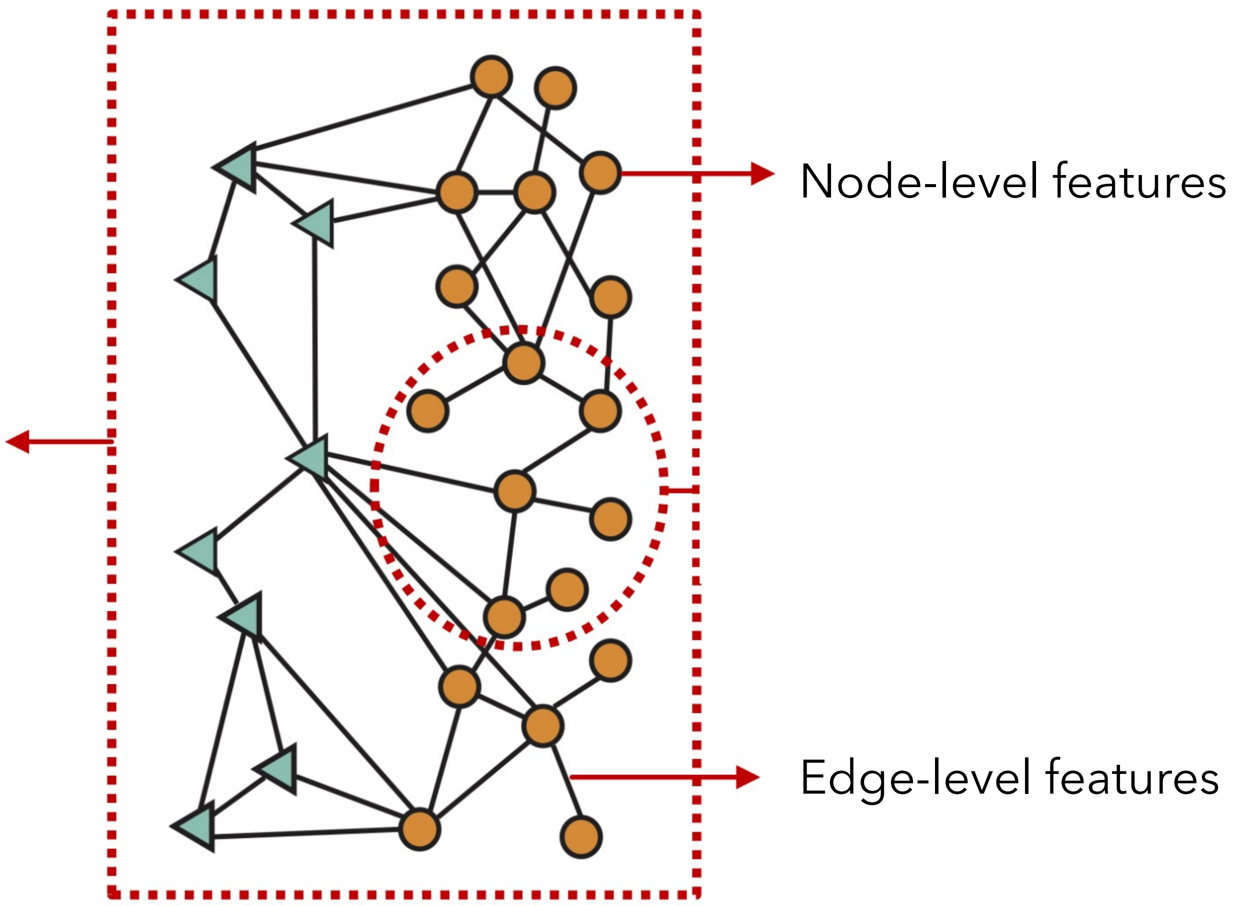


Figure by Leskovec

Outline

1. Introduction
2. Feature engineering for graphs
    a. **Node-level prediction**
    b. Edge-level prediction
3. GNN architecture
4. Training a GNN

Node-level features

Goal: Characterize structure and position of a node in network

Node degree, node centrality, clustering coefficient, graphlets

Node features

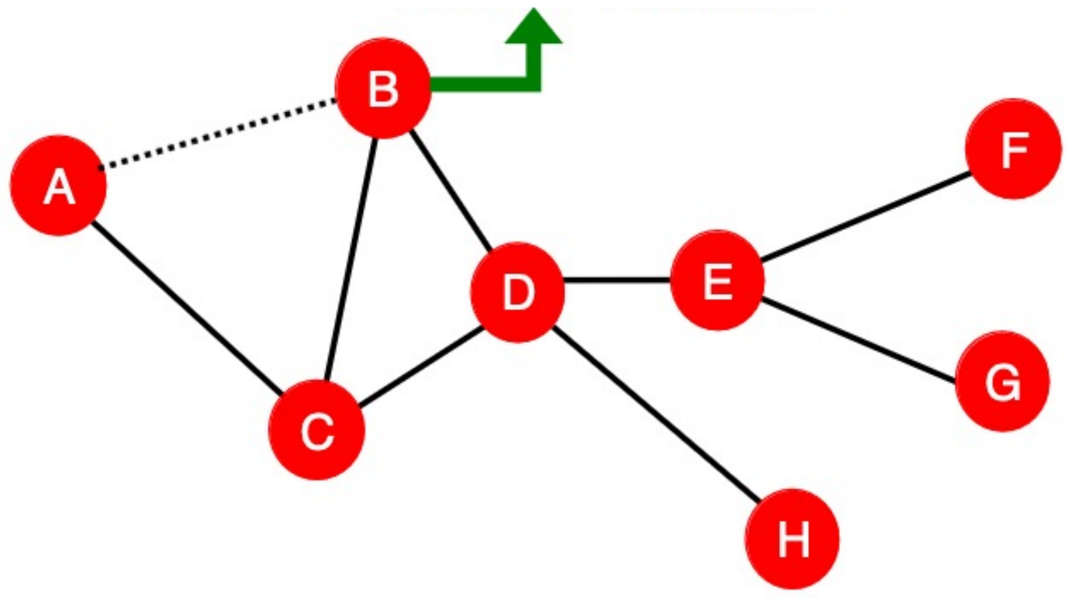
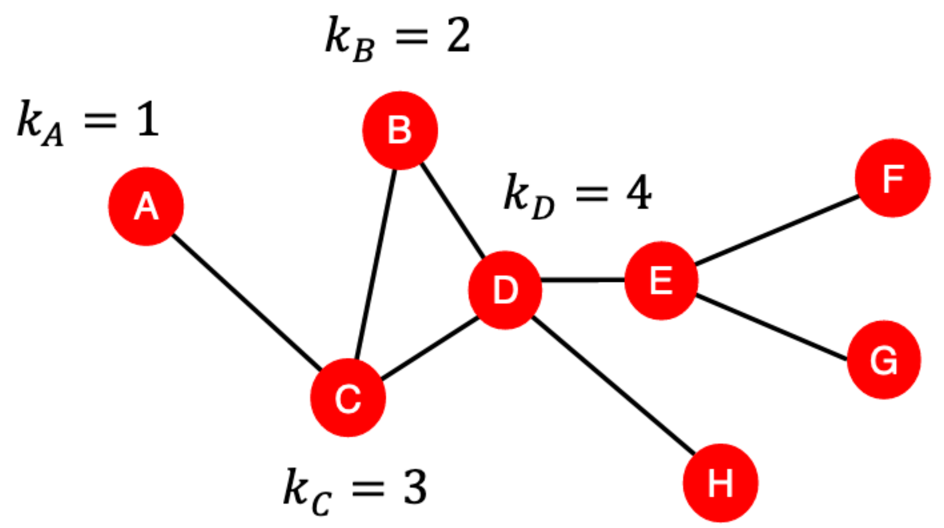


Figure by Leskovec

Node-level features: Degree

Degree k_v of node v = # neighboring nodes that the node has



Treats all neighboring nodes equally

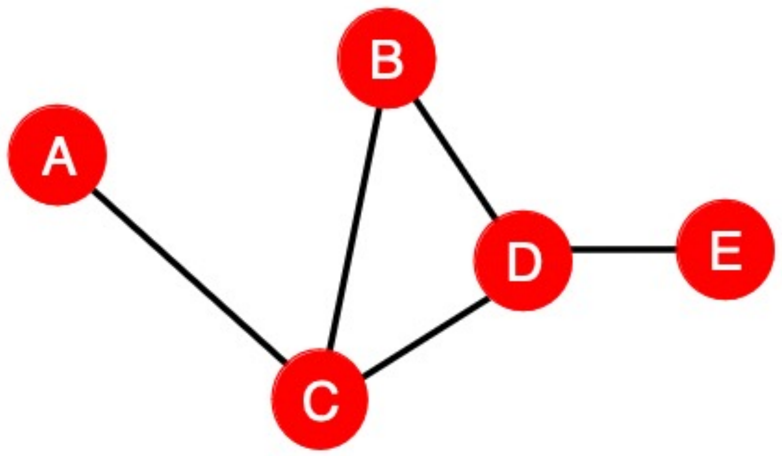
Node centrality takes the node importance in a graph into account

Figure by Leskovec

Node-level features: Centrality

E.g., betweenness centrality:

Node is important if it’s on many shortest paths between other nodes



Centrality $c_A = c_B = c_E = 0$

$c_C = 3$

- A-**C**-B
- A-**C**-D
- A-**C**-D-E

$c_D = 3$

- A-C-**D**-E
- B-**D**-E
- C-**D**-E

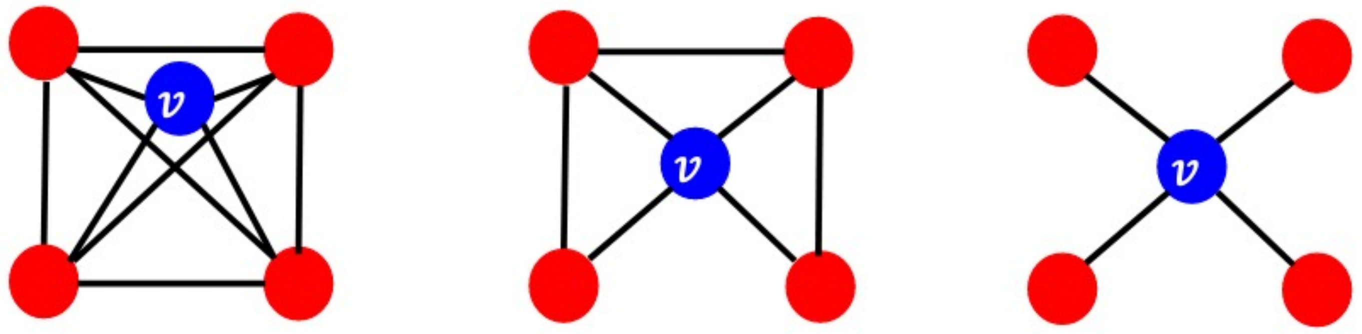
Figure by Leskovec

Node-level features: Clustering coeff.

Captures topological properties of local neighborhood

Measures how connected v's neighboring nodes are

$$e_v = \frac{\#(\text{edges among neighboring nodes})}{\binom{k_v}{2}}$$



$e_v = 1$ $e_v = 0.5$ $e_v = 0$

$$\binom{k_v}{2} = \binom{4}{2} = 6$$

Figure by Leskovec

Outline

Edge-level features

E.g., local neighborhood overlap:

Captures # neighboring nodes shared between nodes u, v

Common neighbors: $|N(v_1) \cap N(v_2)|$

E.g., $|N(A) \cap N(B)| = |\{C\}| = 1$

Jaccard's coefficient: $\frac{|N(v_1) \cap N(v_2)|}{|N(v_1) \cup N(v_2)|}$

E.g., $\frac{|N(A) \cap N(B)|}{|N(A) \cup N(B)|} = \frac{|\{C\}|}{|\{C, D\}|} = \frac{1}{2}$

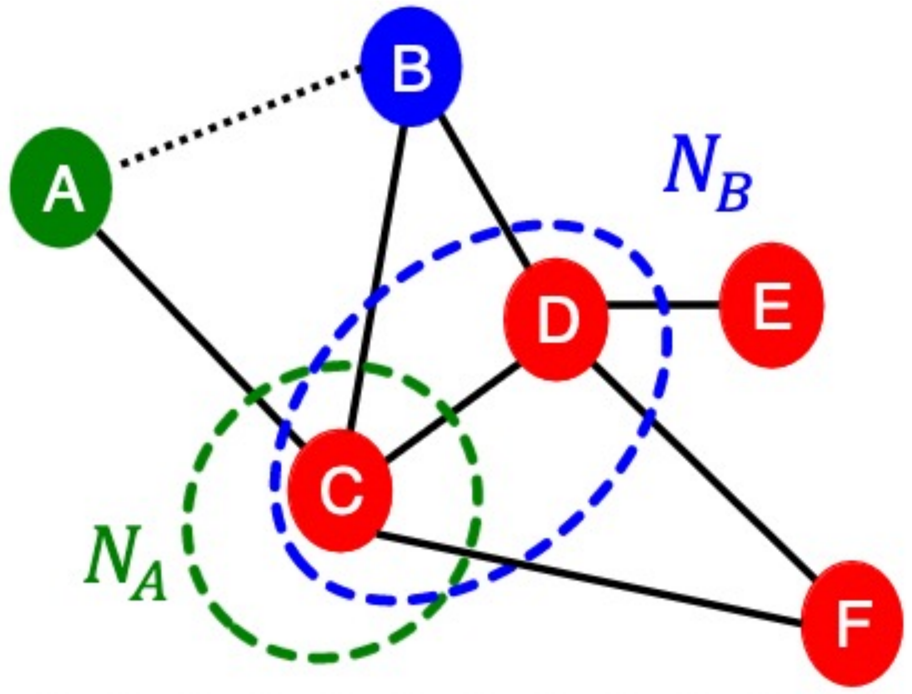


Figure by Leskovec

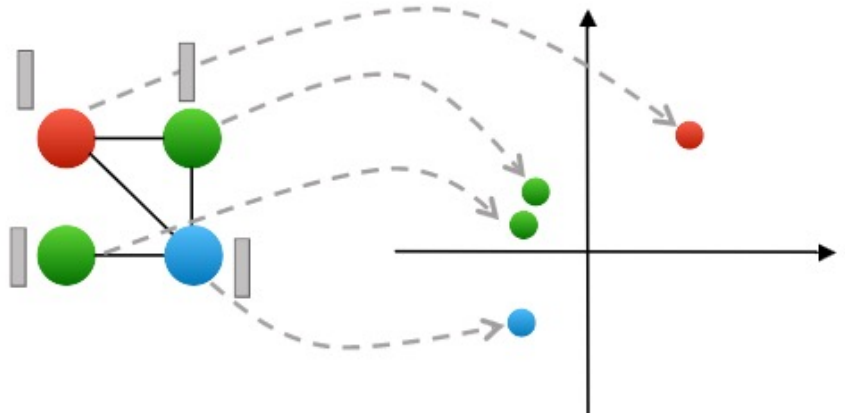
Outline

Setup

- V is the vertex set
- $\boldsymbol{A}$ is the adjacency matrix (assume binary)
- $\boldsymbol{X} \in \mathbb{R}^{|V| \times d}$ is a matrix of node features
- v: a node in V
- $N(v)$: the set of neighbors of v
- Node features:
  - Social networks: User profile, user image
  - Biological networks: Gene expression profiles, gene functional info

Two goals

1. Node embeddings



2. Graph embedding

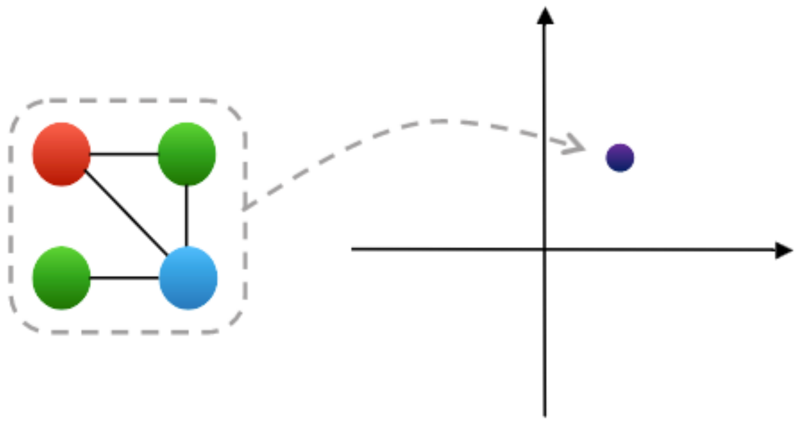
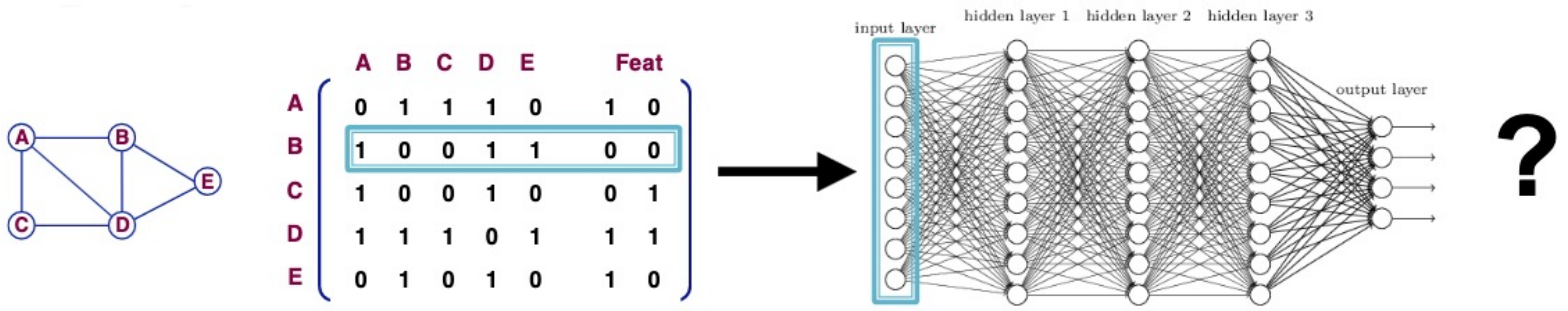


Figure by Jegelka

Idea 1: fully connected NN?

Idea: Join adjacency matrix & features, give as input to NN



$$\begin{array}{c|ccccc|cc} & A & B & C & D & E & \text{Feat} & \\ \hline A & 0 & 1 & 1 & 1 & 0 & 1 & 0 \\ B & \boxed{1} & 0 & 0 & 1 & 1 & 0 & 0 \\ C & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ D & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ E & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{array}$$

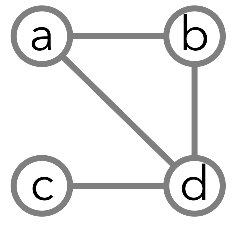
Issues:

- Huge input
- Doesn't generalize across graph size
- Sensitive to node ordering

Figure by Leskovec

Permutation invariance & equivariance

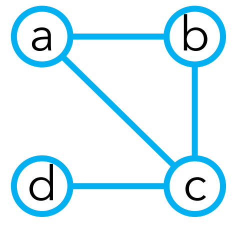
How to avoid sensitivity to node orderings?



$$A = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Permutation matrix

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$



$$PAP^T = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

We want either:

- **Permutation invariance**
  - Graph embedding
  - Output: single vector
  - $f(PAP^T, PX) = f(A, X)$
- **Permutation equivariance**
  - Node embedding
  - Output: vector per node
  - $f(PAP^T, PX) = Pf(A, X)$

Permutation invariance & equivariance

GNNs consist of permutation equivariant/invariant functions

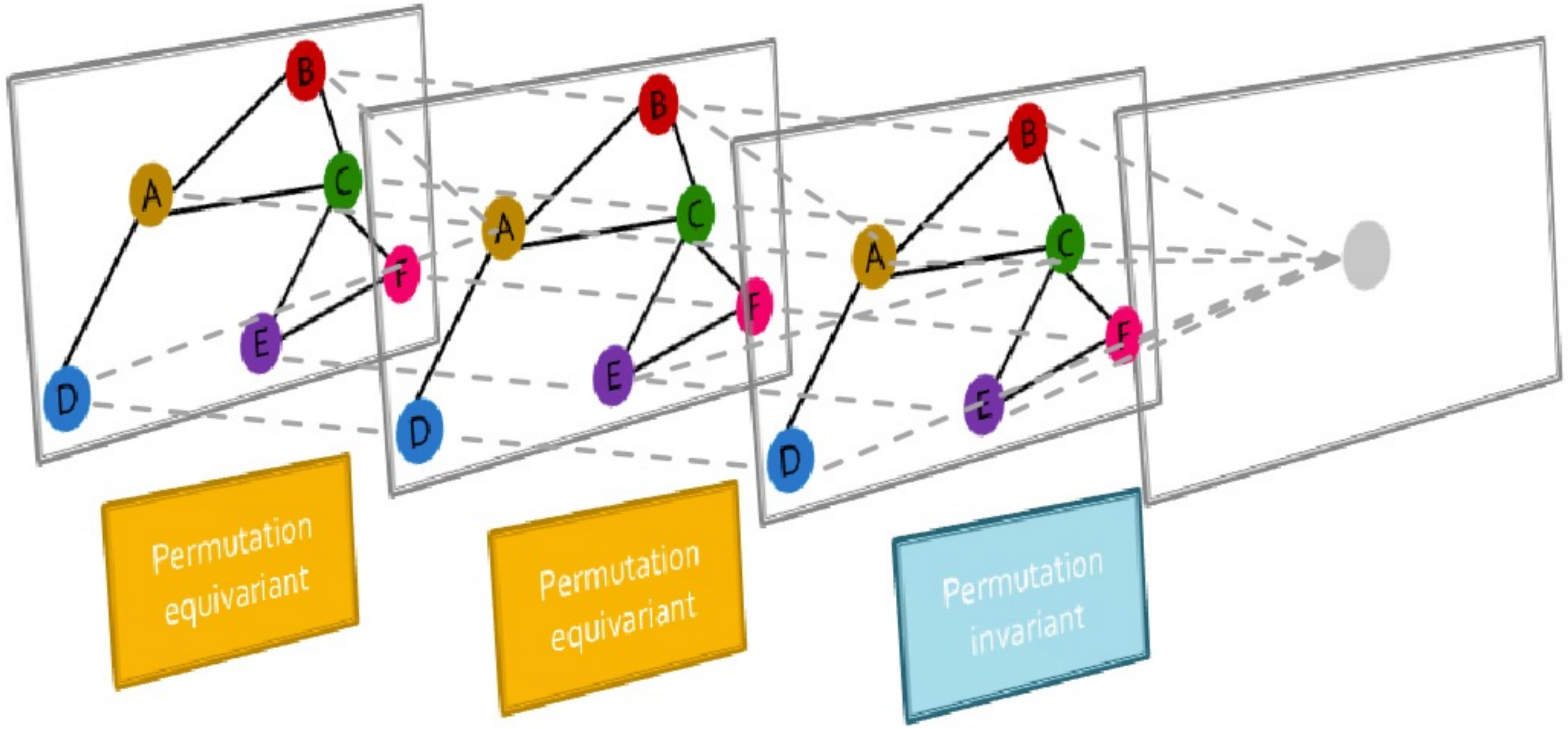


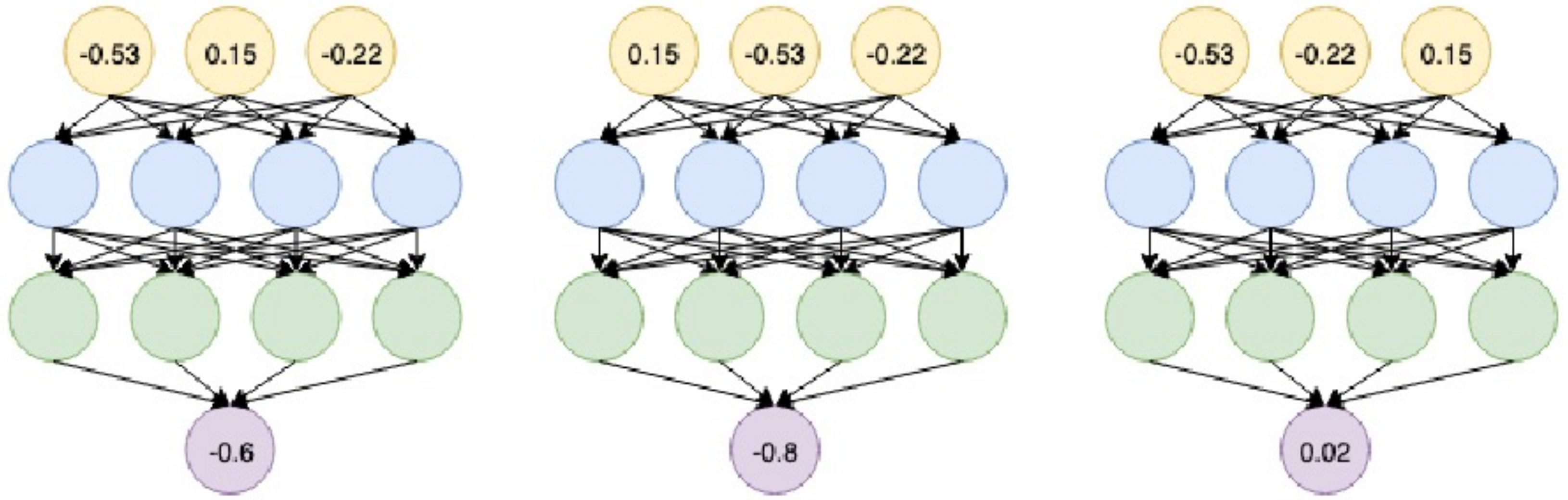
Figure by Bronstein, ICLR 2021 keynote

Permutation invariance & equivariance

Are other NN architectures permutation invariant / equivariant?

E.g., MLP

No.



Explains why naïve MLP approach fails for graphs

Graph neural networks

Idea:

1. Encode each node (node's neighborhood) with embedding
2. Aggregate set of node embeddings into graph embedding

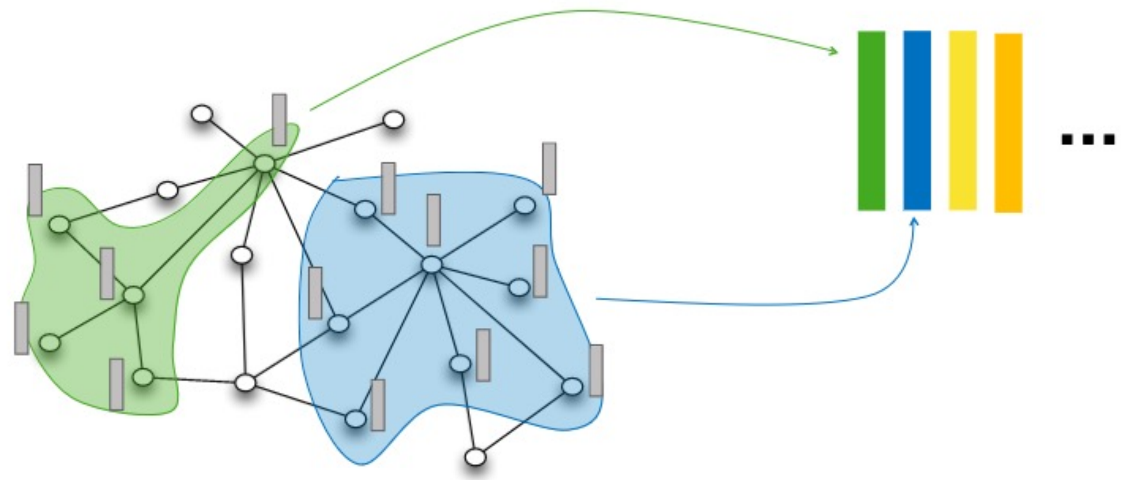
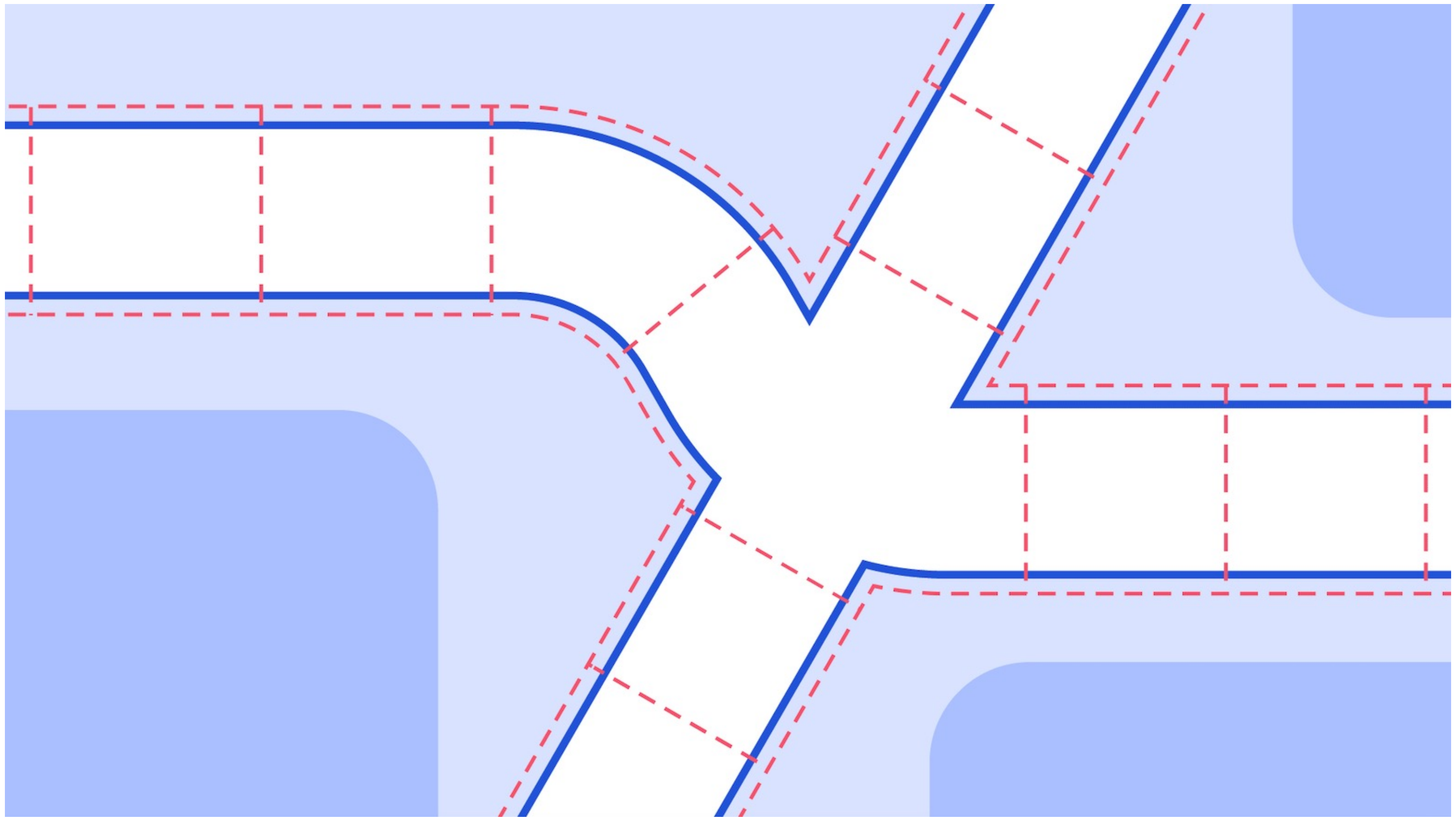


Figure by Jegelka

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



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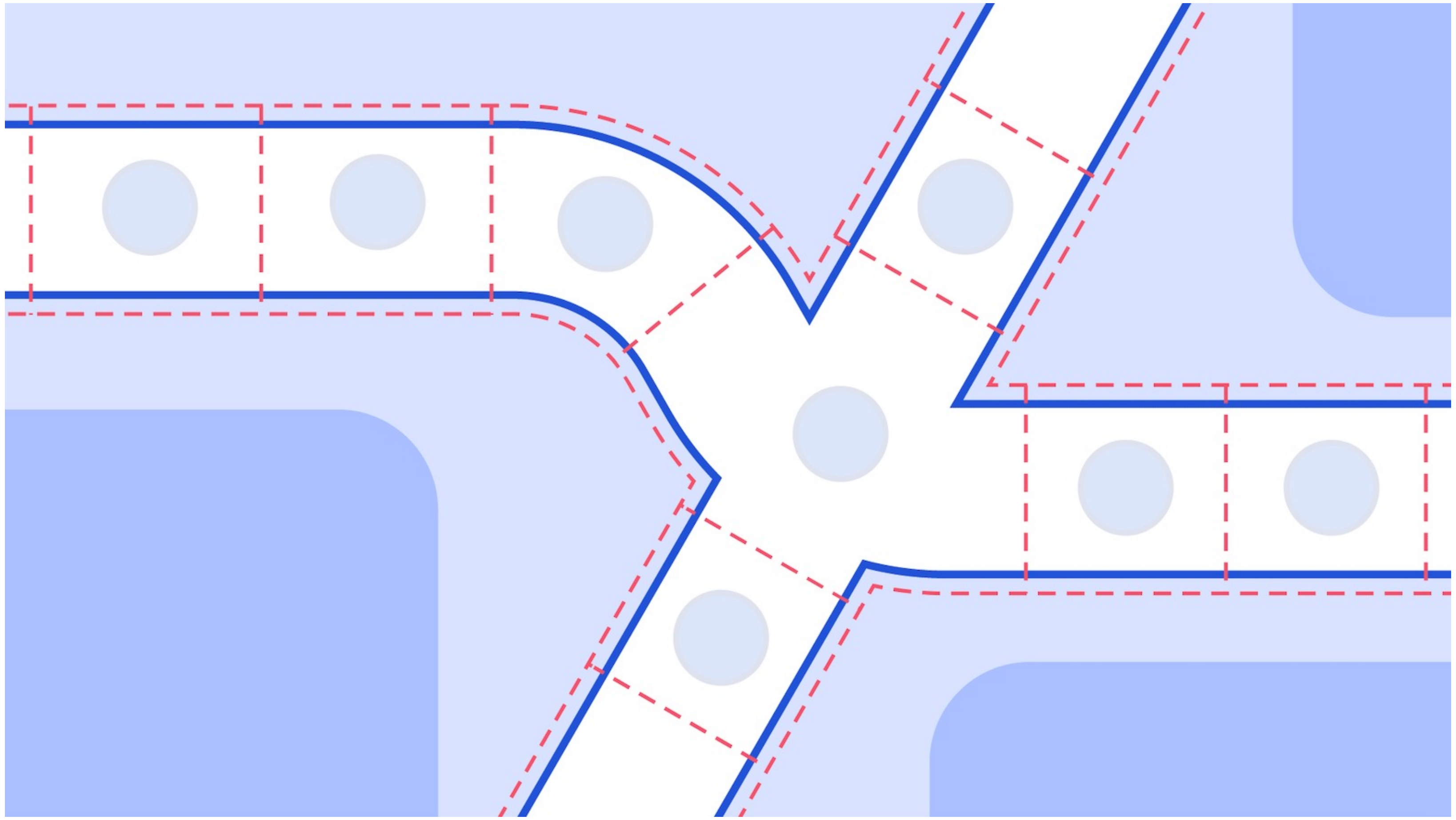

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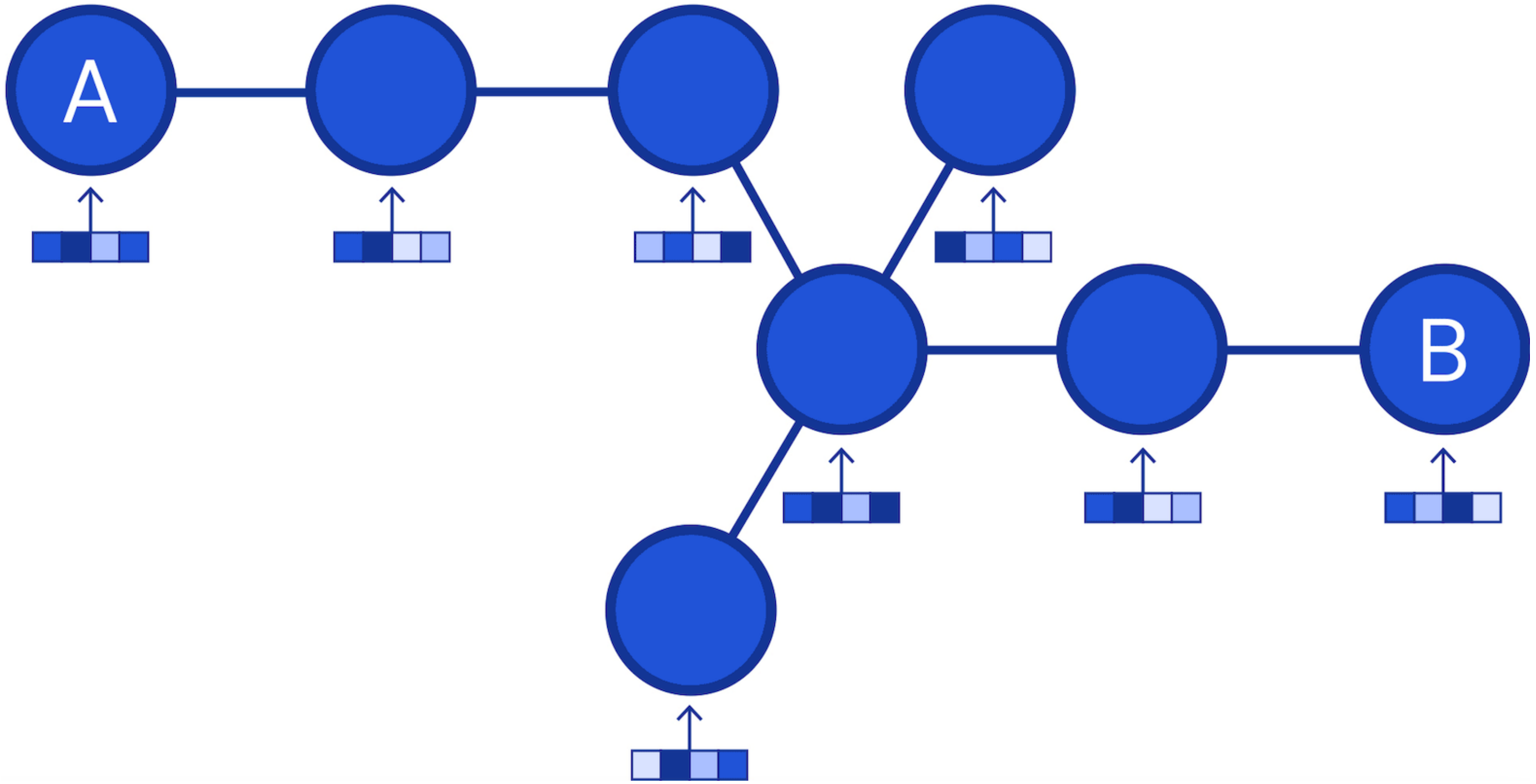

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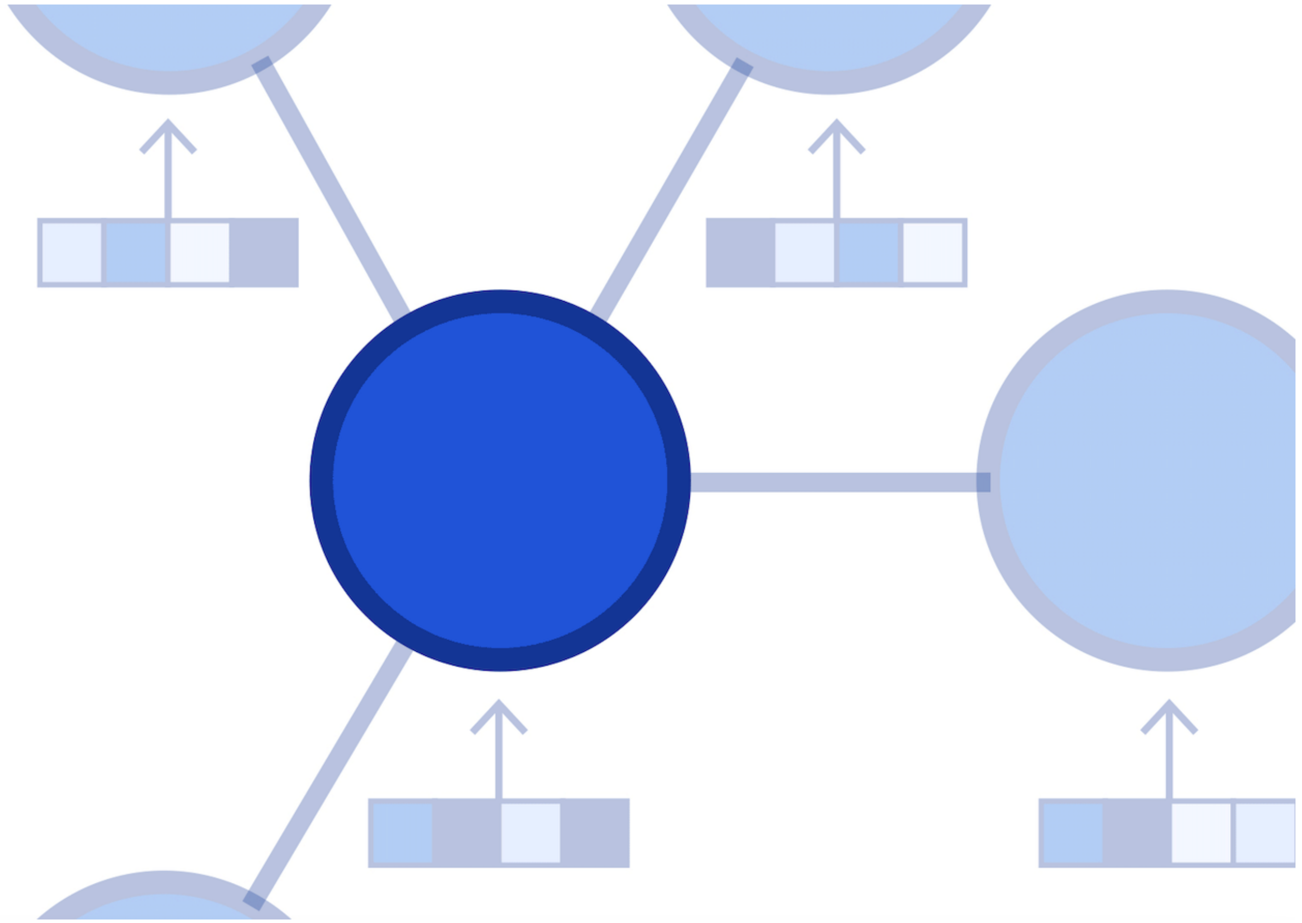

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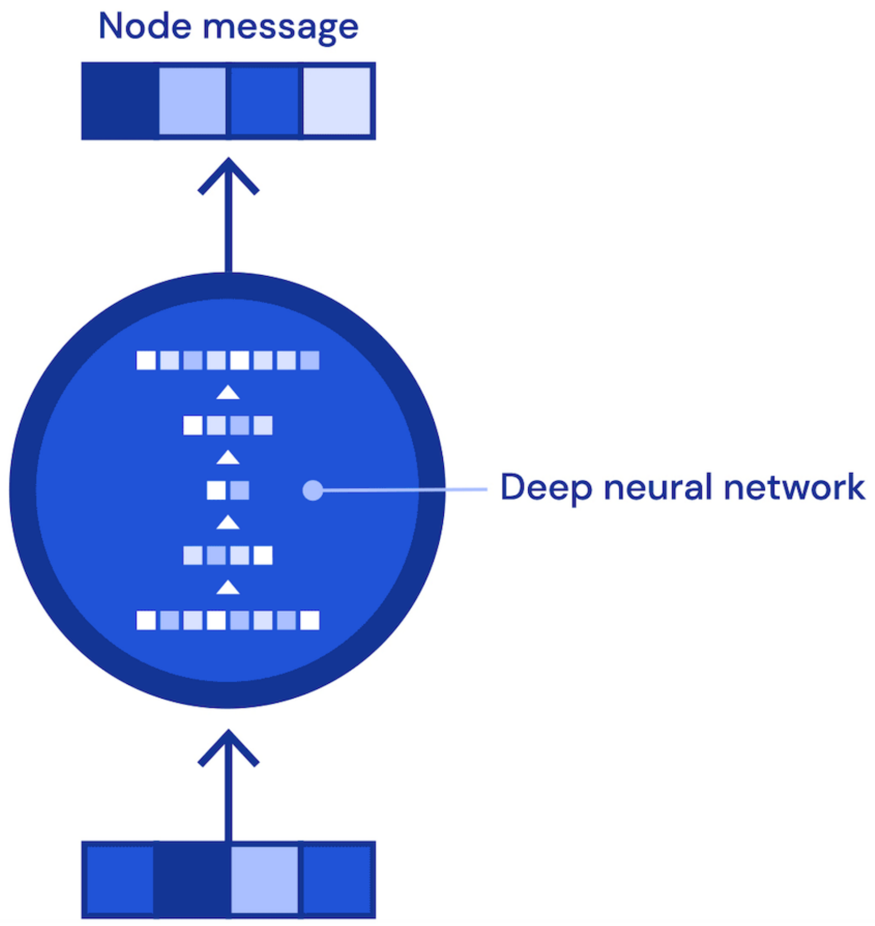

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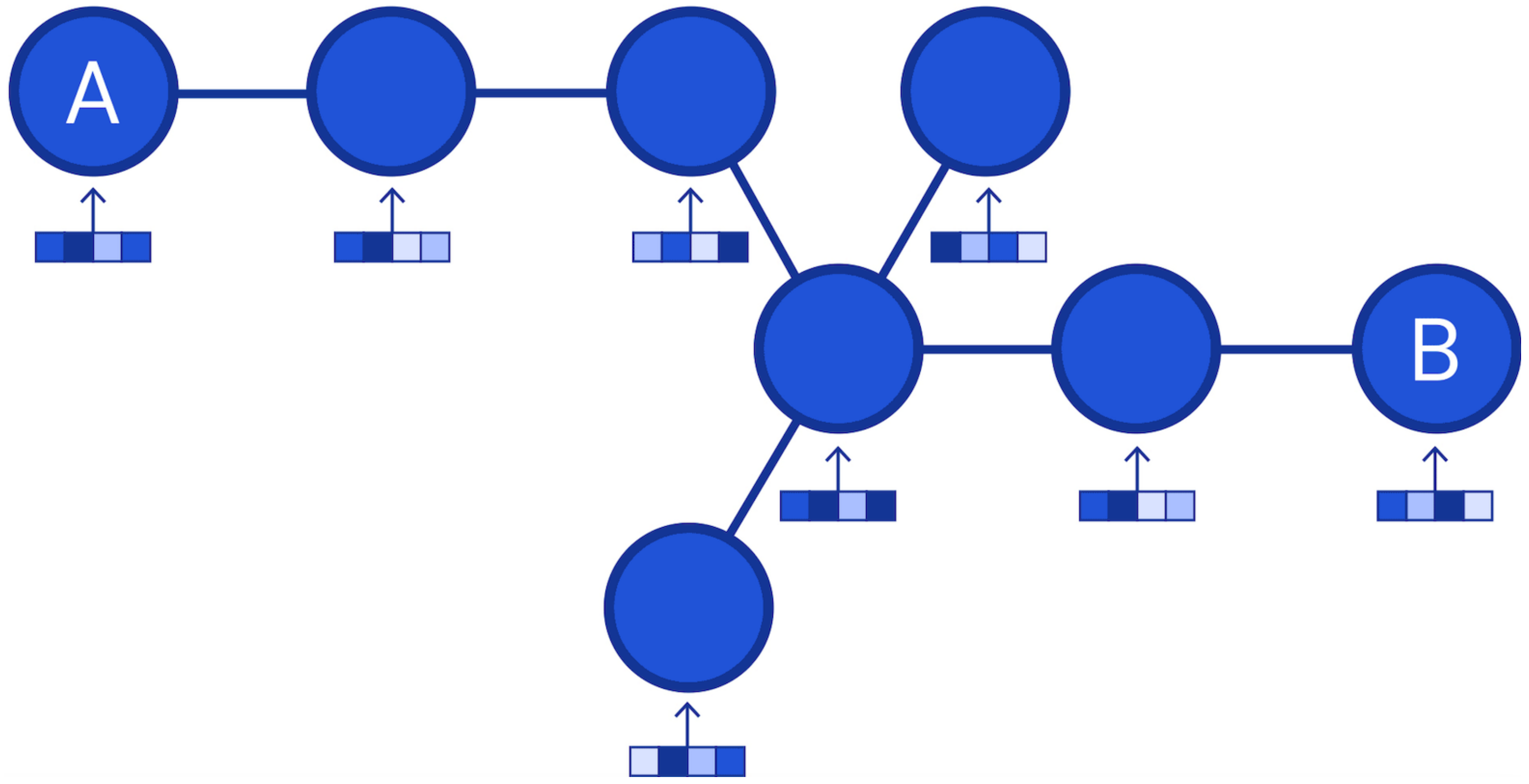

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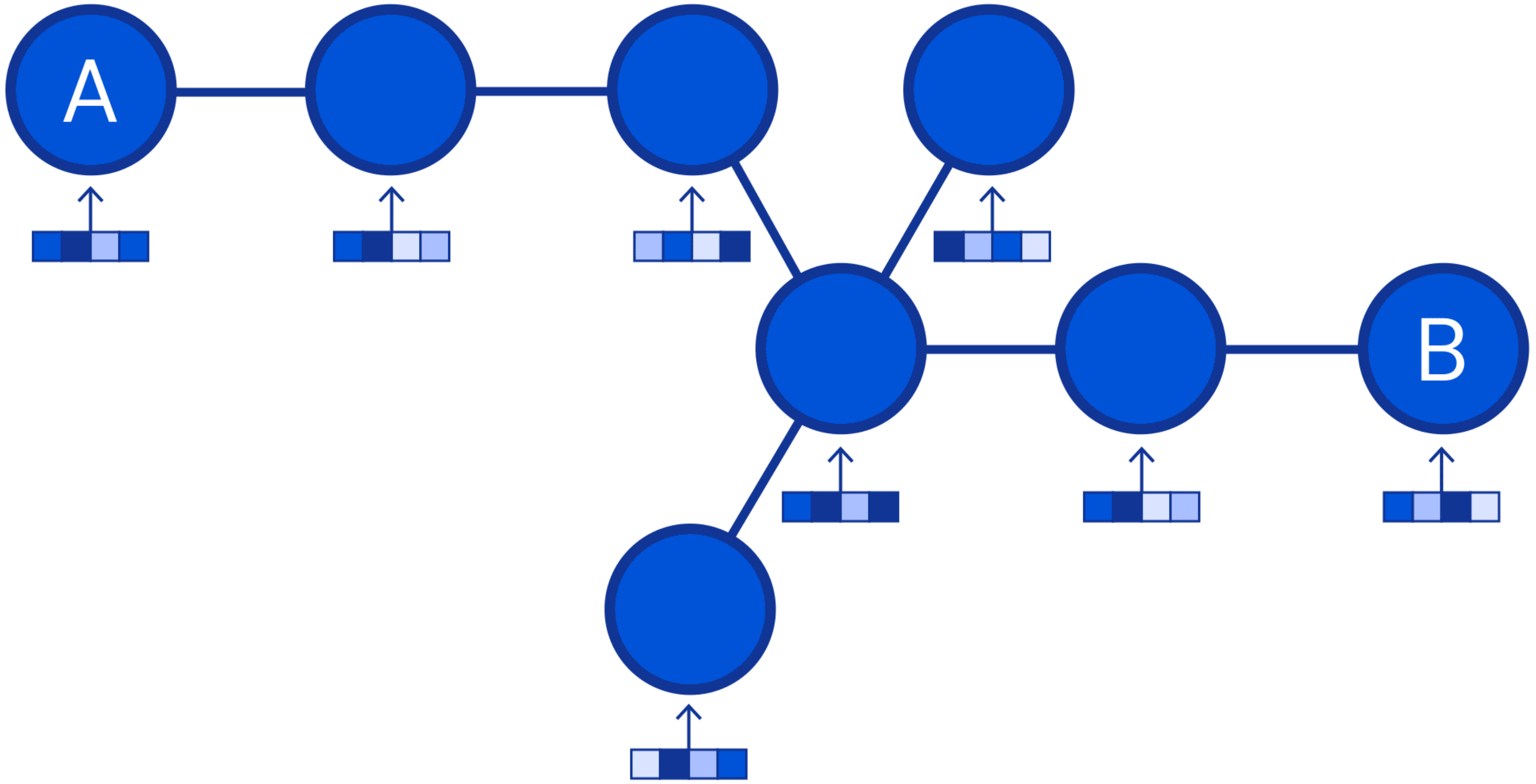


https://www.deepmind.com/blog/traffic-prediction-with-advanced-graph-neural-networks

Encoding neighborhoods: General form

$\boldsymbol{h}_u^{(0)} = \boldsymbol{x}_u$ (feature representation for node u)

In each round $k \in [K]$, for each node v:

1. **Aggregate** over neighbors

$$\boldsymbol{m}_{\underbrace{N(v)}_{\text{Neighborhood of } v}}^{(k)} = \mathrm{AGGREGATE}^{(k)}\left(\left\{\boldsymbol{h}_u^{(k-1)} : u \in N(v)\right\}\right)$$

Figure by Jegelka

Encoding neighborhoods: General form

$\boldsymbol{h}_u^{(0)} = \boldsymbol{x}_u$ (feature representation for node u)

In each round $k \in [K]$, for each node v:

1. **Aggregate** over neighbors
$$\boldsymbol{m}_{N(v)}^{(k)} = \mathrm{AGGREGATE}^{(k)}\left(\left\{\boldsymbol{h}_u^{(k-1)} : u \in N(v)\right\}\right)$$
2. **Update** current node representation
$$\boldsymbol{h}_v^{(k)} = \mathrm{COMBINE}^{(k)}\left(\boldsymbol{h}_v^{(k-1)}, \boldsymbol{m}_{N(v)}^{(k)}\right)$$

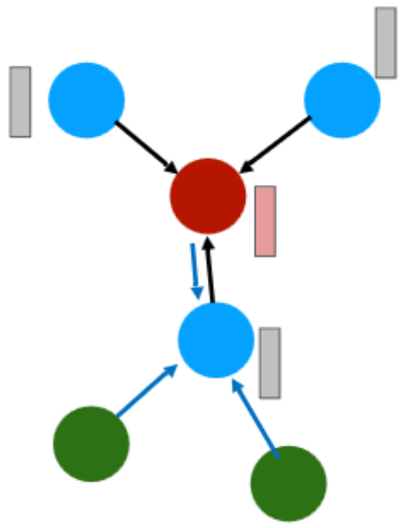
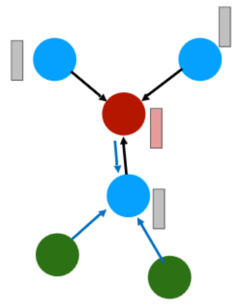


Figure by Jegelka

The basic GNN

[Merkwirth and Lengauer ‘05; Scarselli et al. ‘09]



$$\boldsymbol{m}_{N(v)} = \text{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \sum_{u \in N(v)} \boldsymbol{h}_u$$

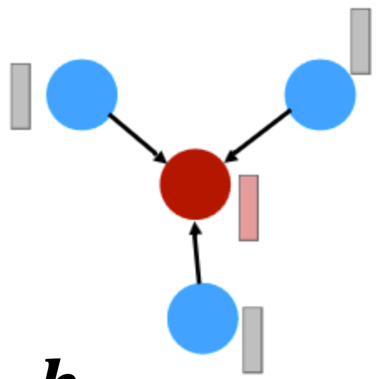
$$\text{COMBINE}(\boldsymbol{h}_v, \boldsymbol{m}_{N(v)}) = \underline{\sigma}(\underline{W_{\text{self}}}\boldsymbol{h}_v + \underline{W_{\text{neigh}}}\boldsymbol{m}_{N(v)} + \underline{\boldsymbol{b}})$$

Trainable parameters

Non-linearity (e.g., tanh or ReLU)

Figure by Jegelka

Aggregation functions



$$\boldsymbol{m}_{N(v)} = \text{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \underbrace{\sum_{u \in N(v)} \boldsymbol{h}_u}_{\boxed{\text{Unstable, highly sensitive to node degrees}}}$$

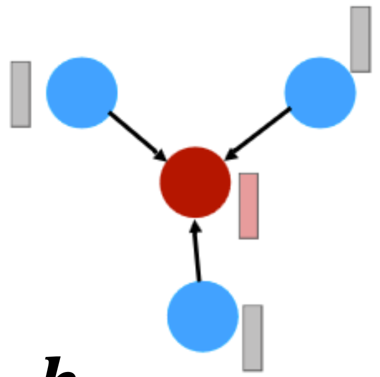
Instead, take averages, e.g.:

- $\boldsymbol{m}_{N(v)} = \frac{1}{|N(v)|} \sum_{u \in N(v)} \boldsymbol{h}_u$ [Merkwirth & Lengauer '05, Scarselli et al. '09]
- $\boldsymbol{m}_{N(v)} = \sum_{u \in N(v)} \frac{1}{\sqrt{|N(u)||N(v)|}} \boldsymbol{h}_u$ [Kipf & Welling '16, Hamilton et al. '17]

Can we do more to improve?

Figure by Jegelka

Aggregation functions



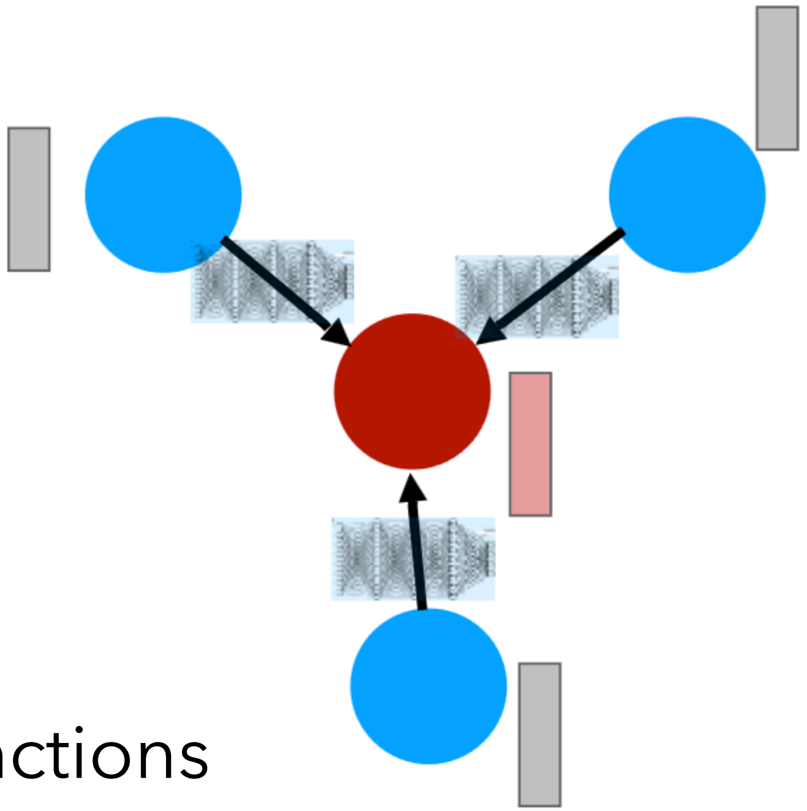
$$\boldsymbol{m}_{N(v)} = \text{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \underbrace{\sum_{u \in N(v)} \boldsymbol{h}_u}_{\text{Unstable, highly sensitive to node degrees}}$$

Should be a permutation invariant, multi-set function

Figure by Jegelka

Aggregation functions

$$\boldsymbol{m}_{N(v)} = \mathrm{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\})$$
$$= \mathrm{MLP}_2\left(\sum_{u \in N(v)} \mathrm{MLP}_1(\boldsymbol{h}_u, \boldsymbol{h}_v)\right)$$



Universal approximation of multi-set functions

[Zaheer et al. '17, Qi et al. '17, Xu et al. '19]

$$\mathrm{COMBINE}\left(\boldsymbol{h}_v, \boldsymbol{m}_{N(v)}\right) = \sigma\left(W_{\mathrm{self}} \boldsymbol{h}_v + W_{\mathrm{neigh}} \boldsymbol{m}_{N(v)} + \boldsymbol{b}\right)$$

Figure by Jegelka

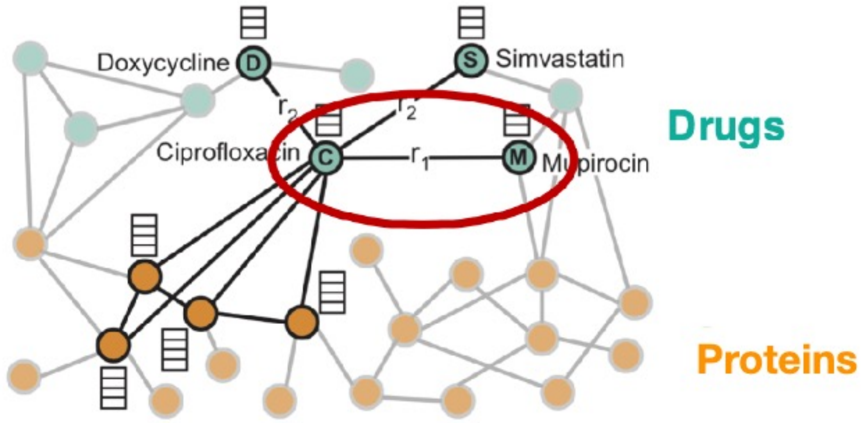
Generalizations

- Use edge attributes/features in aggregation

$$m_{N(v)} = \mathrm{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \sum_{u \in N(v)} \mathrm{MLP}(\boldsymbol{h}_u, \boldsymbol{h}_v, w_{uv})$$

- Different aggregations for different types of edges

E.g., Zitnik et al. ['18]

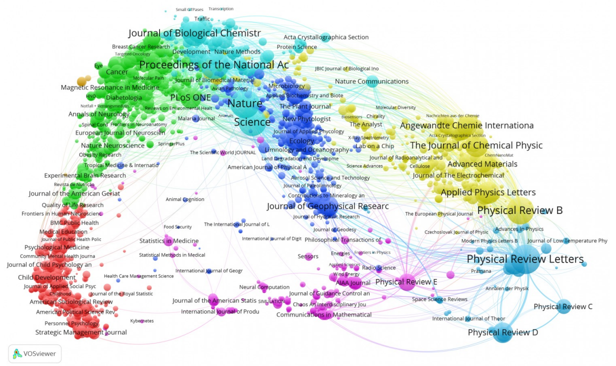


Generalizations

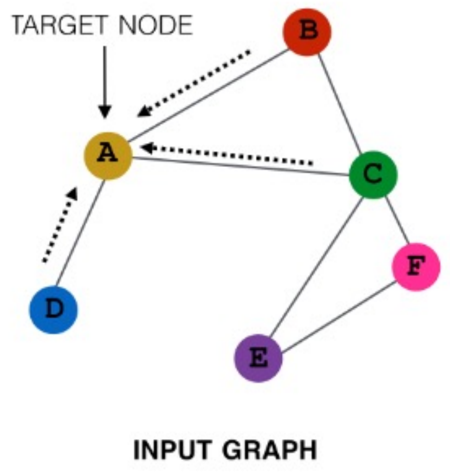
Attention [Velickovic et al. '18]:

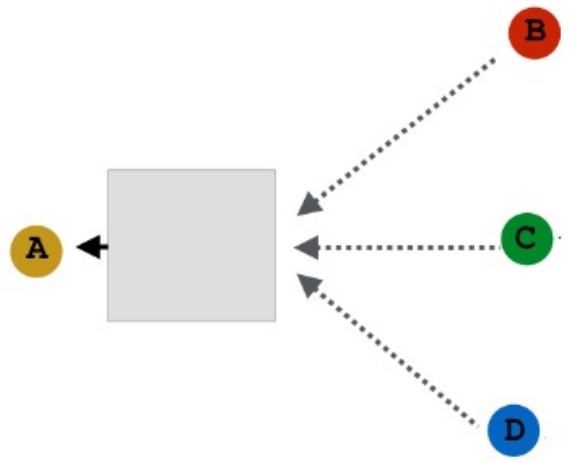
$$m_{N(v)} = \text{AGGREGATE}(\{\boldsymbol{h}_u : u \in N(v)\}) = \sum_{u \in N(v)} \alpha_{v,u} \boldsymbol{h}_u$$

- Useful when some neighbors might be more/less informative
- E.g., classifying papers by topic based on citation networks
  - Some papers that span topical boundaries, highly-cited across fields
  - GNN should learn to ignore uninformative neighbors



Node embeddings unrolled

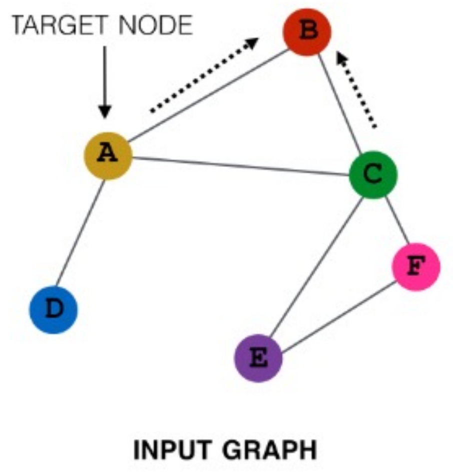


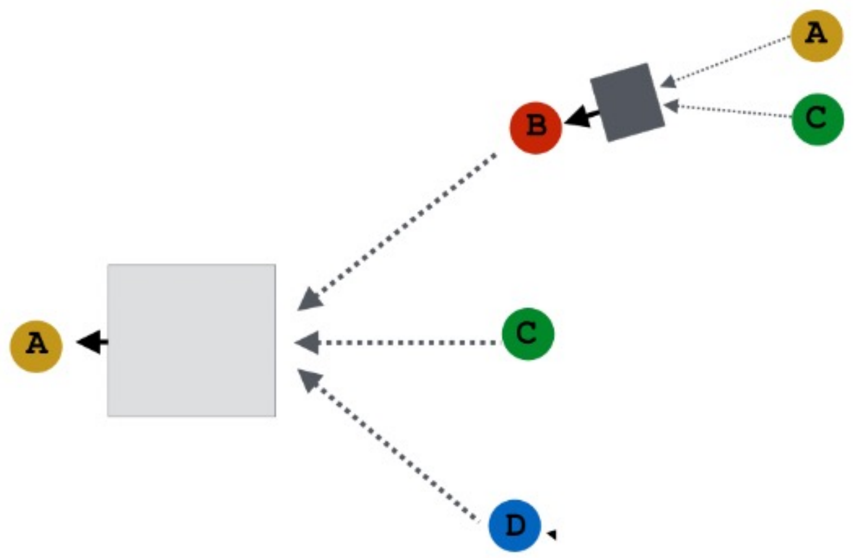


Grey boxes: aggregation functions that we learn

Figures by Leskovec

Node embeddings unrolled

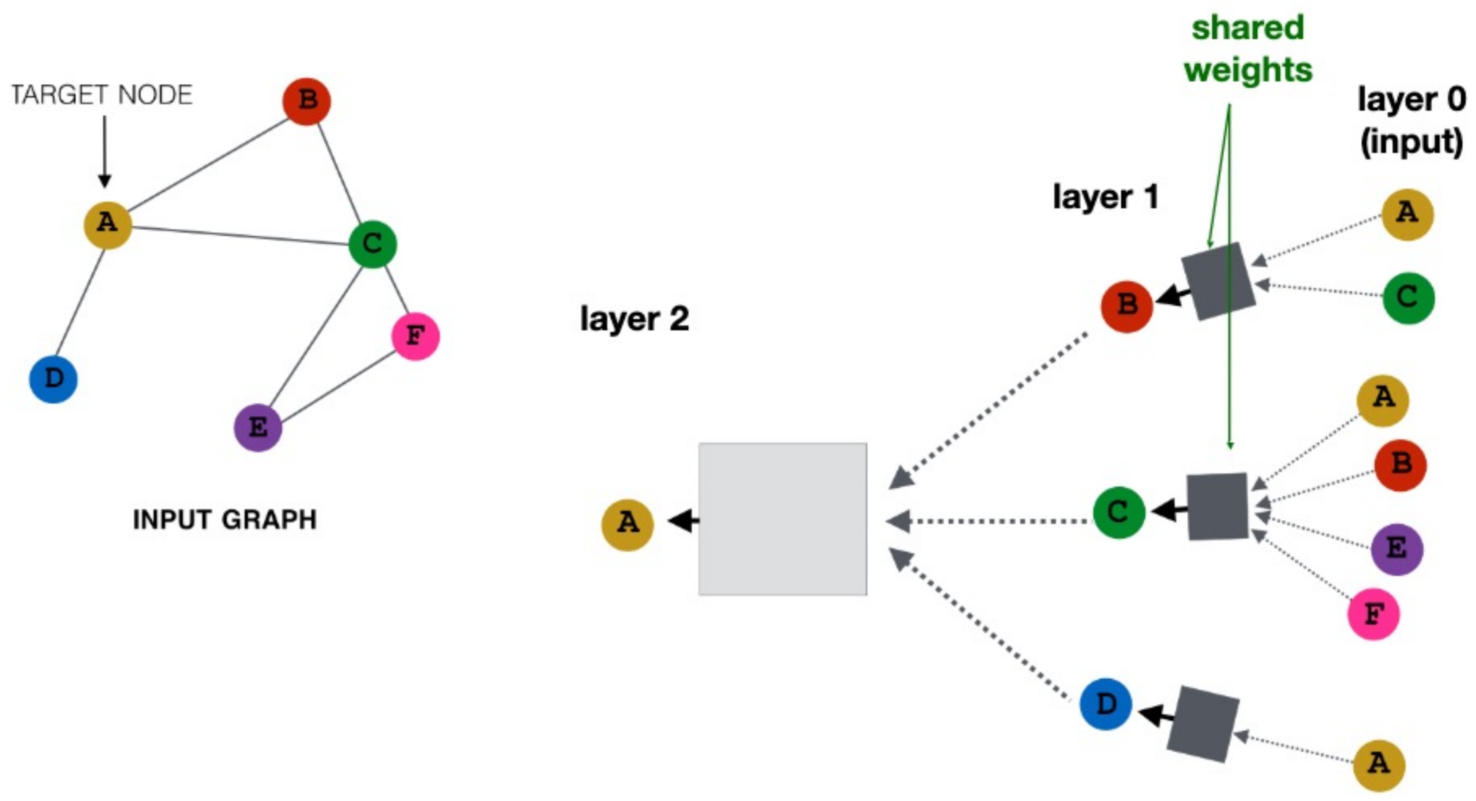




Grey boxes: aggregation functions that we learn

Figures by Leskovec

Node embeddings unrolled

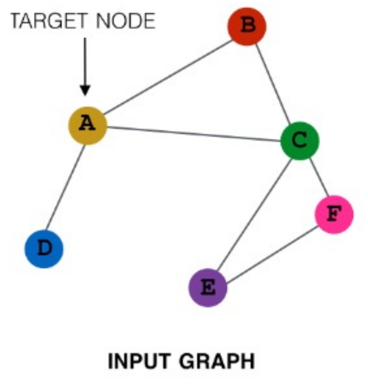


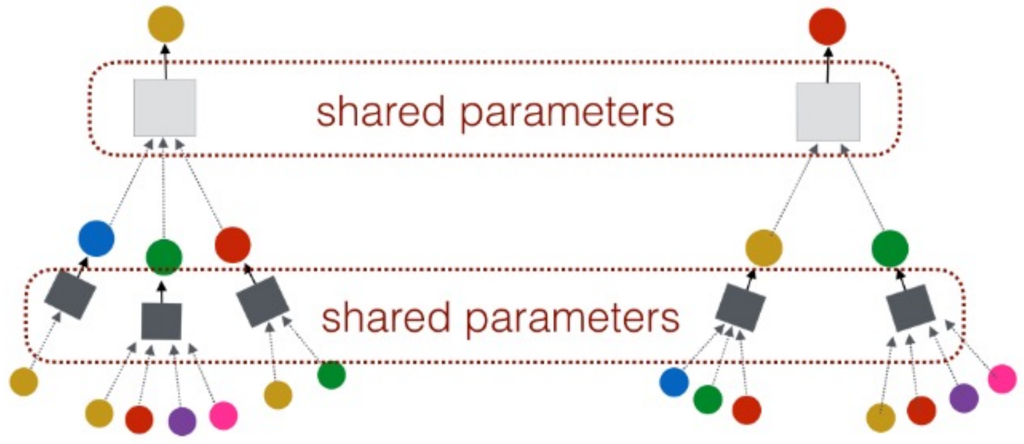
Grey boxes: aggregation functions that we learn

Figures by Leskovec

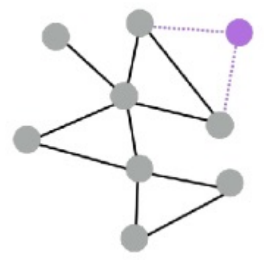
Weight sharing

Use the same aggregation functions for all nodes





Can generate encodings for previously unseen nodes & graphs!



Figures by Leskovec

Outline

GNN Pipeline

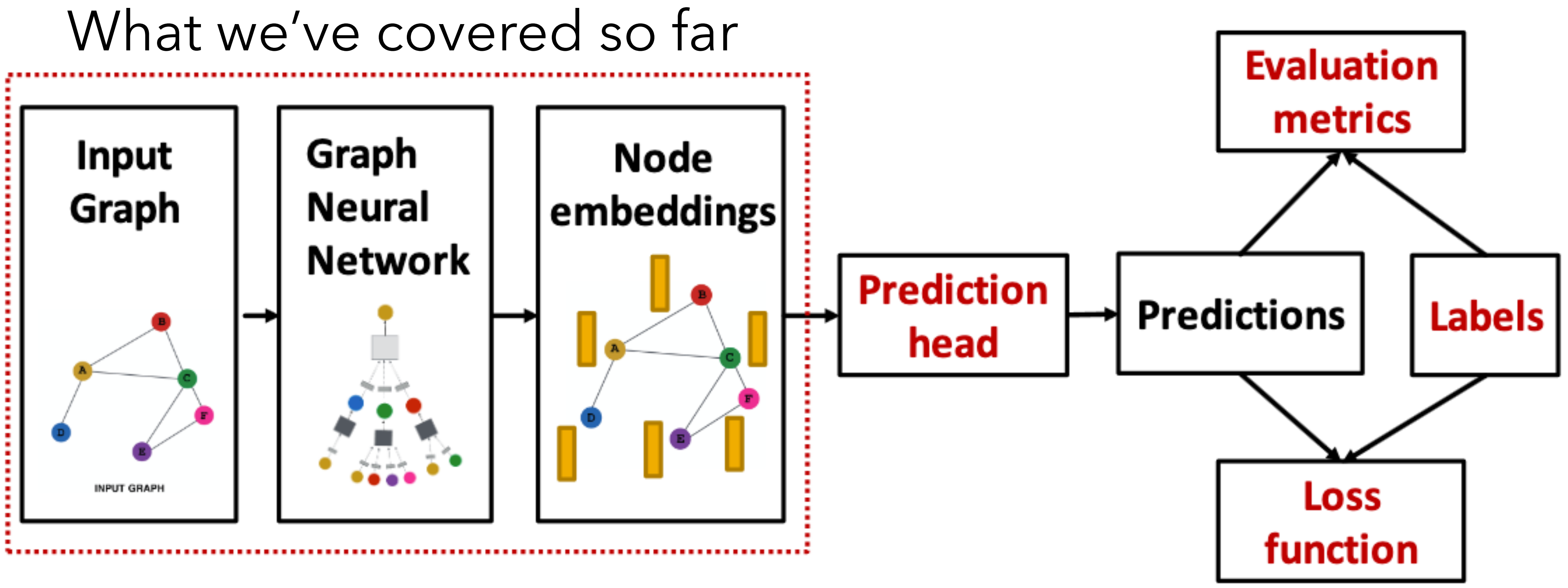


Figure by Leskovec

Prediction heads

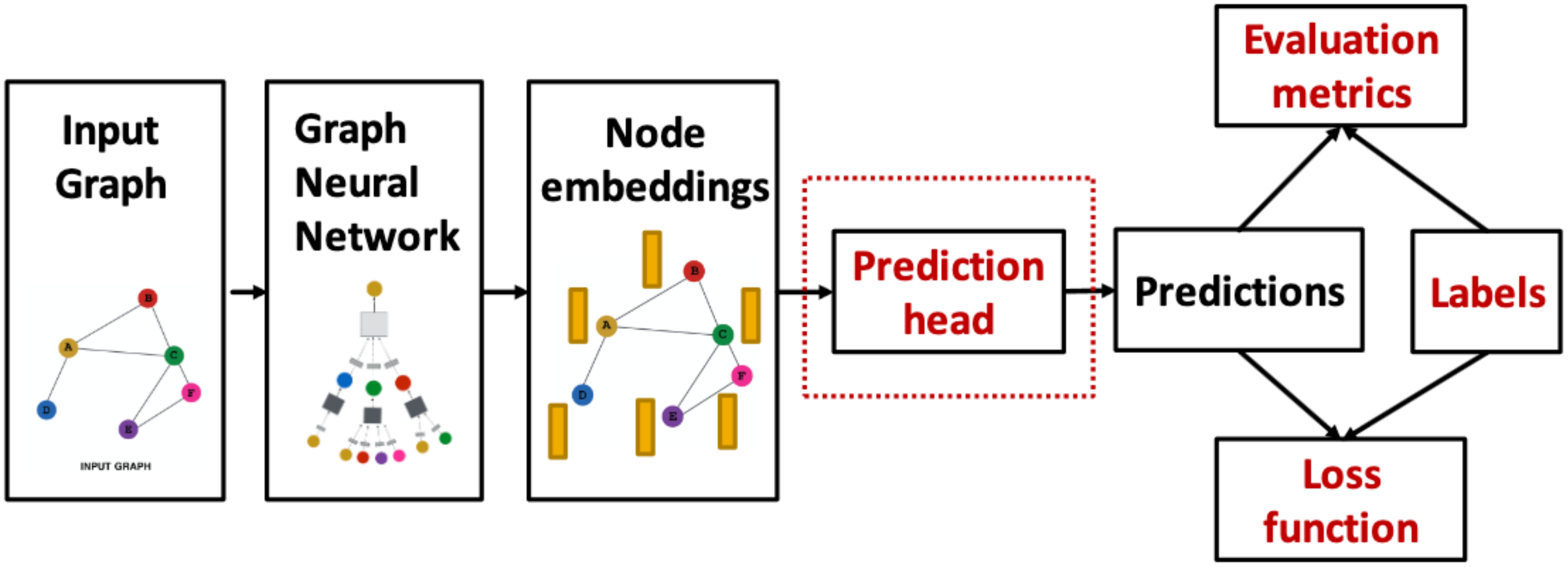


Figure by Leskovec

Prediction heads

Different task levels require different prediction heads

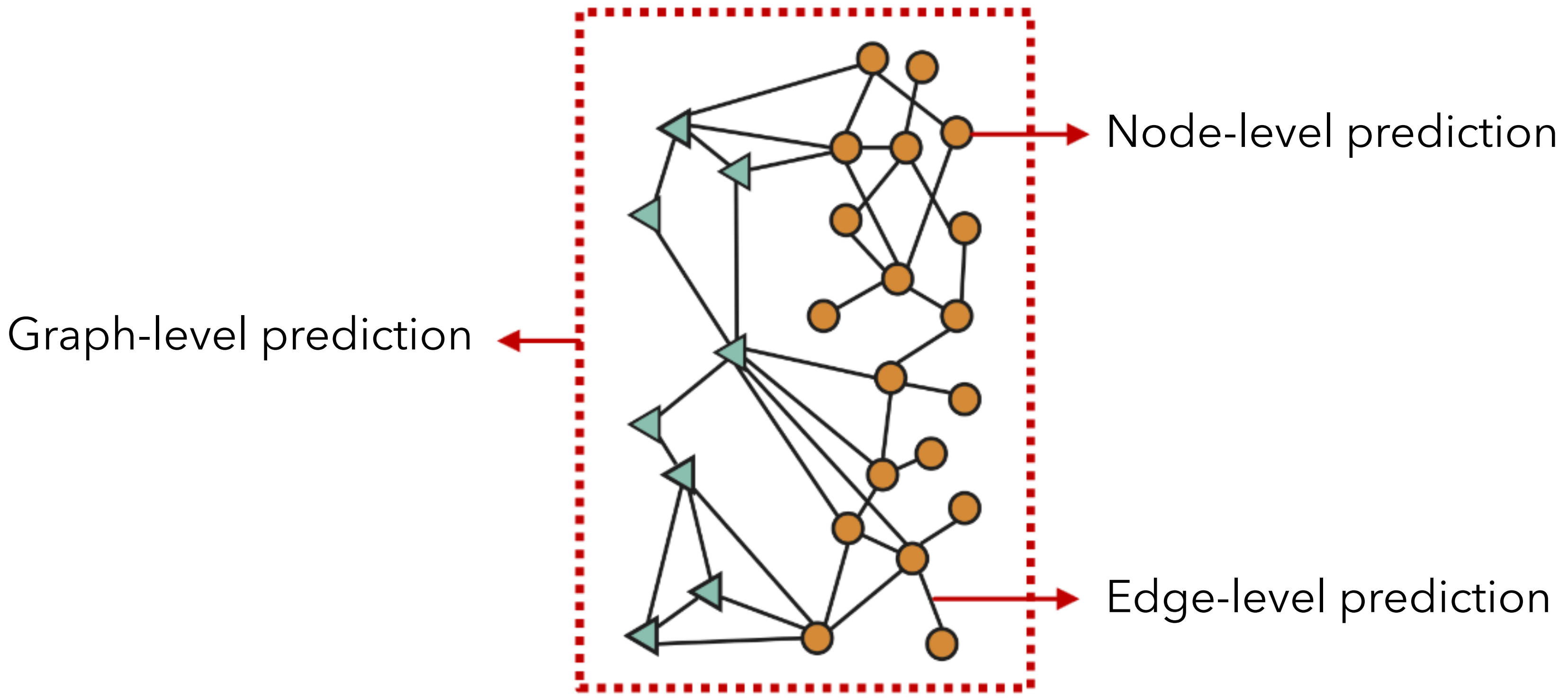


Figure by Leskovec

Prediction heads: Node-level

After GNN computation, we have node embeddings

$$\left\{\boldsymbol{h}_v^{(K)} \in \mathbb{R}^d, \forall v \in V\right\}$$

Suppose we want to make k-way predictions

- Classification: classify among k categories
- Regression: regress on k targets

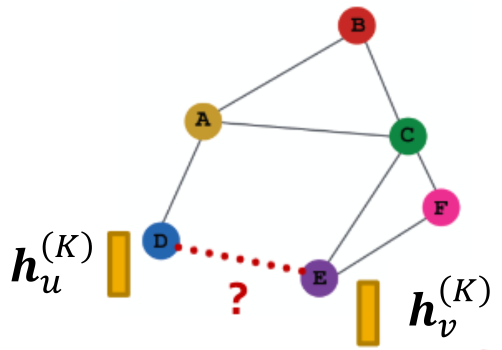
$$\widehat{\boldsymbol{y}}_v = \mathrm{Head}_{\mathrm{node}}\left(\boldsymbol{h}_v^{(K)}\right) = W^{(H)}\boldsymbol{h}_v^{(K)}$$

- $W^{(H)} \in \mathbb{R}^{d\times k}$ so $\widehat{\boldsymbol{y}}_v \in \mathbb{R}^k$

Prediction heads: Edge-level

Suppose we want to make k-way predictions

$$\widehat{\boldsymbol{y}}_{uv} = \text{Head}_{\text{edge}}\left(\boldsymbol{h}_u^{(K)}, \boldsymbol{h}_v^{(K)}\right)$$



$$\widehat{\boldsymbol{y}}_{uv} = \text{Linear}\left(\text{Concatenate}\left(\boldsymbol{h}_u^{(K)}, \boldsymbol{h}_v^{(K)}\right)\right)$$

Linear maps $2d$-dimensional embedding to k-way embedding

Similar to multi-head attention:

$$\widehat{\boldsymbol{y}}_{uv}[1] = \boldsymbol{h}_u^{(K)} W^{(1)} \boldsymbol{h}_v^{(K)}$$

$$\vdots$$

$$\widehat{\boldsymbol{y}}_{uv}[k] = \boldsymbol{h}_u^{(K)} W^{(k)} \boldsymbol{h}_v^{(K)}$$

Prediction heads: Graph-level

Graph-level prediction:

Make prediction using all node embeddings

$$\hat{\boldsymbol{y}}_G = \mathrm{HEAD}_{\mathrm{graph}}\left(\left\{\boldsymbol{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\right\}\right)$$

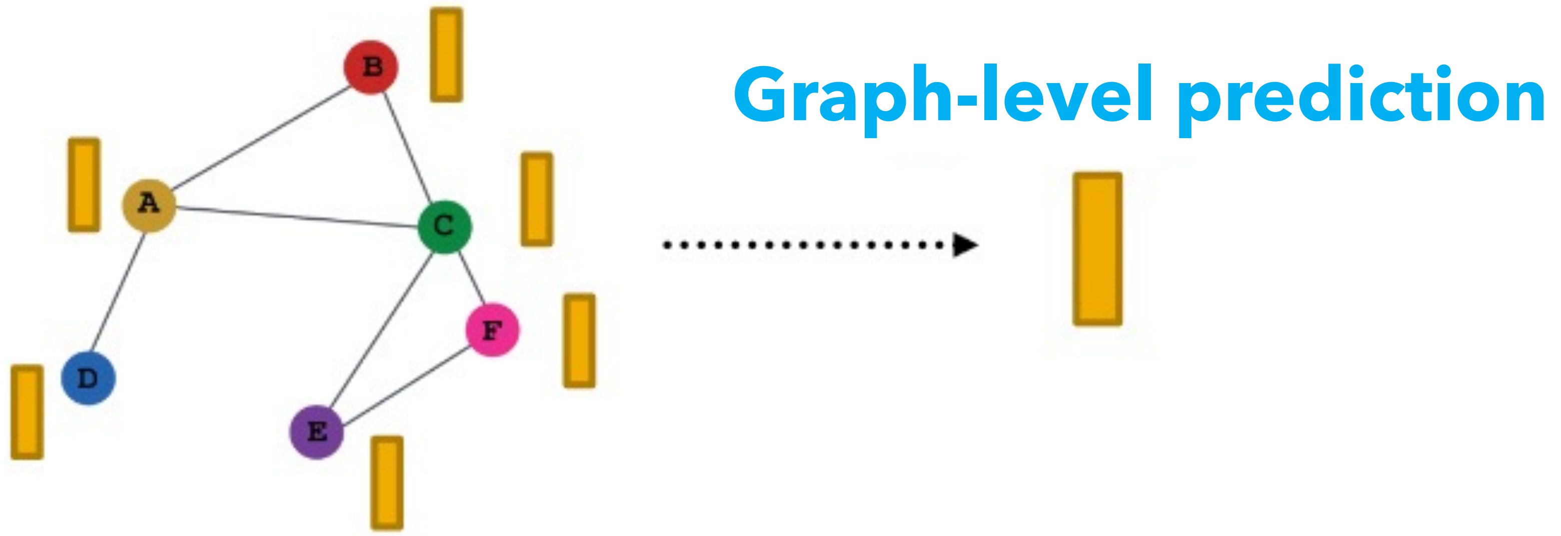


Figure by Leskovec

Prediction heads: Graph-level

Options for $\mathrm{HEAD}_{\mathrm{graph}}\left(\left\{\boldsymbol{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\right\}\right)$:

- Global **mean** pooling $\widehat{\boldsymbol{y}}_G = \mathbf{Mean}\left(\left\{\boldsymbol{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\right\}\right)$
- Global **max** pooling $\widehat{\boldsymbol{y}}_G = \mathbf{Max}\left(\left\{\boldsymbol{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\right\}\right)$
- Global **sum** pooling $\widehat{\boldsymbol{y}}_G = \mathbf{Sum}\left(\left\{\boldsymbol{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\right\}\right)$

Work well for **small** graphs

What about large graphs?

Issue of global pooling

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

Toy example with 1-dim node embeddings:

- Node embeddings for G_1: $\{-1, -2, 0, 1, 2\}$
- Node embeddings for G_2: $\{-10, -20, 0, 10, 20\}$
- If we do global sum pooling:
  - Prediction for G_1: $\hat{y}_{G_1} = \mathrm{Sum}(\{-1, -2, 0, 1, 2\}) = 0$
  - Prediction for G_2: $\hat{y}_{G_2} = \mathrm{Sum}(\{-10, -20, 0, 10, 20\}) = 0$
  - **Cannot differentiate between G_1 and G_2!**

Hierarchical global pooling

- **A solution:** Aggregate all node embeddings **hierarchically**
- **Toy example**: Aggregate via ReLU(Sum(·))
  - First separately aggregate the first 2 nodes and the last 3 nodes
  - Then aggregate again to make final prediction
- G_1 node embeddings: $\{-1, -2, 0, 1, 2\}$
  - **Round 1**: $\hat{y}_a = \mathrm{ReLU}\big(\mathrm{Sum}(\{-1, -2\})\big) = 0,$

    $\hat{y}_b = \mathrm{ReLU}\big(\mathrm{Sum}(\{0, 1, 2\})\big) = 3$
  - **Round 2**: $\hat{y}_{G_1} = \mathrm{ReLU}\big(\mathrm{Sum}(\{\hat{y}_a, \hat{y}_b\})\big) = 3$

Hierarchical global pooling

- **A solution:** Aggregate all node embeddings **hierarchically**
- **Toy example**: Aggregate via ReLU(Sum(·))
  - First separately aggregate the first 2 nodes and the last 3 nodes
  - Then aggregate again to make final prediction
- G_1 node embeddings: $\{-1, -2, 0, 1, 2\}$, $\hat{y}_{G_1} = 3$
- G_2 node embeddings: $\{-10, -20, 0, 10, 20\}$
  - **Round 1**: $\hat{y}_a = \mathrm{ReLU}\big(\mathrm{Sum}(\{-10, -20\})\big) = 0$,
    $\hat{y}_b = \mathrm{ReLU}\big(\mathrm{Sum}(\{0, 10, 20\})\big) = 30$
  - **Round 2**: $\hat{y}_{G_2} = \mathrm{ReLU}\big(\mathrm{Sum}(\{\hat{y}_a, \hat{y}_b\})\big) = 30$

Can differentiate between $\boldsymbol{G_1}$ and $\boldsymbol{G_2}$

Hierarchical pooling in practice

DiffPool idea: Hierarchically pool node embeddings

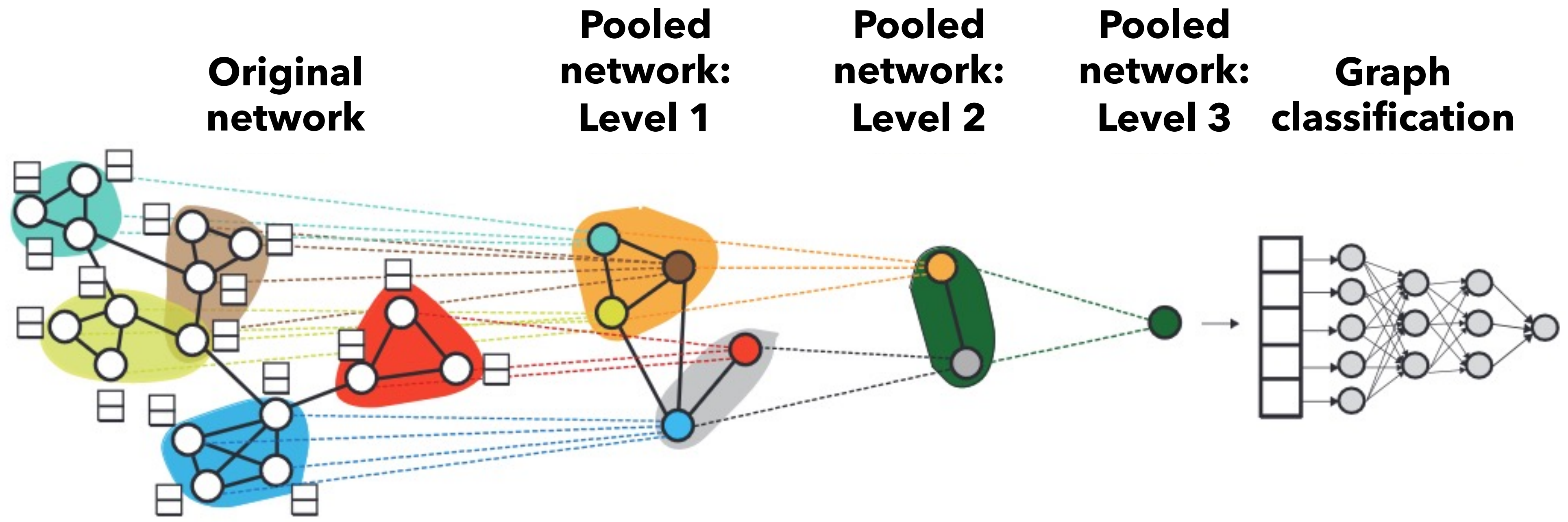


Figure by Ying et al. NeurIPS'18

Hierarchical pooling in practice

Leverage 2 independent GNNs at each level

- **GNN A:** Compute node embeddings
- **GNN B:** Compute the cluster that a node belongs to

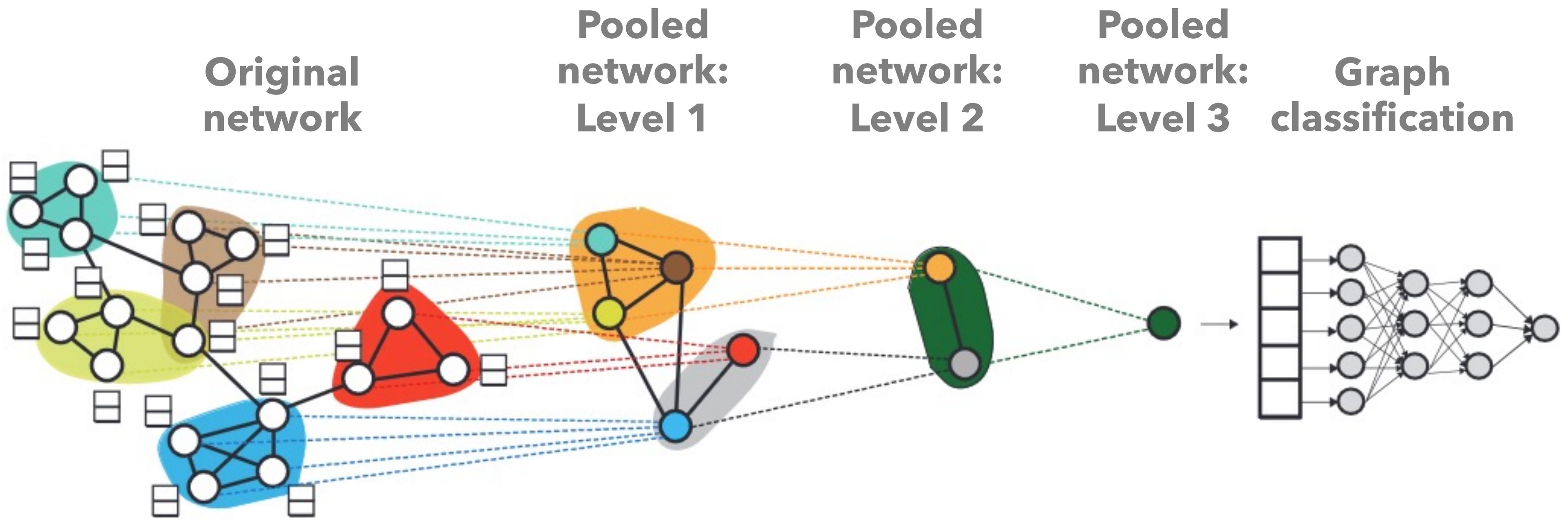


Figure by Ying et al. NeurIPS'18

GNN Pipeline

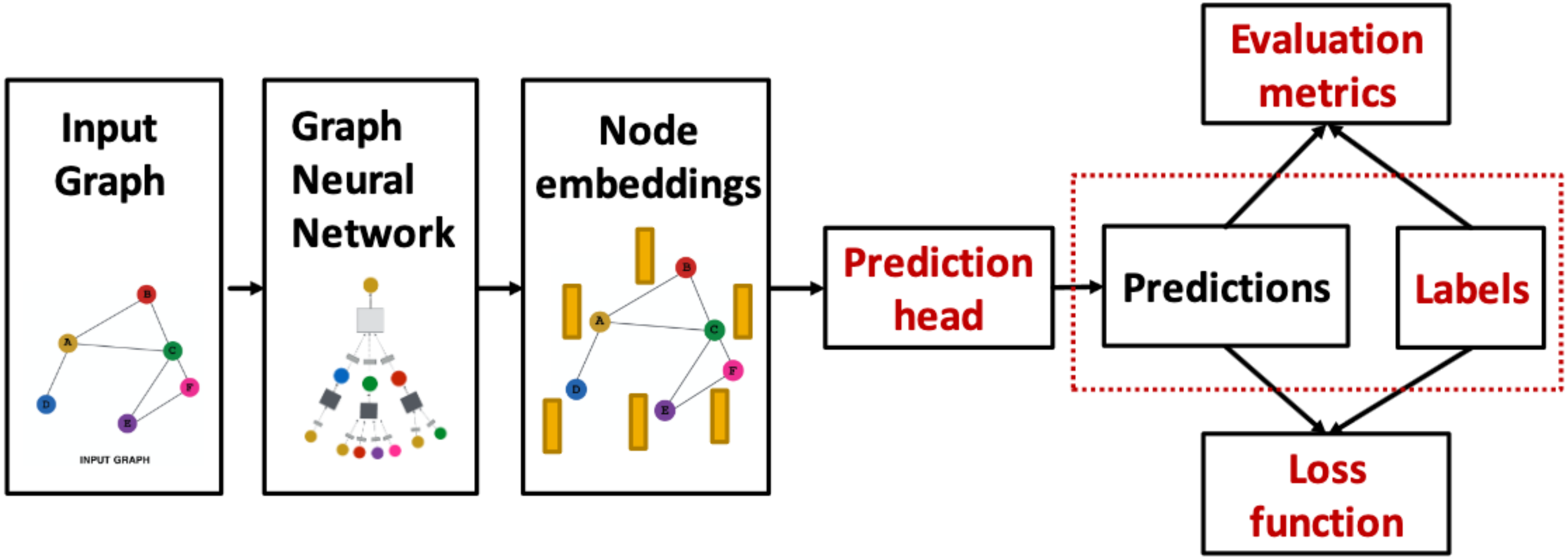


Figure by Leskovec

Supervised vs unsupervised

Supervised learning on graphs

- Labels come from external sources
- E.g., predict drug likeness of a molecular graph

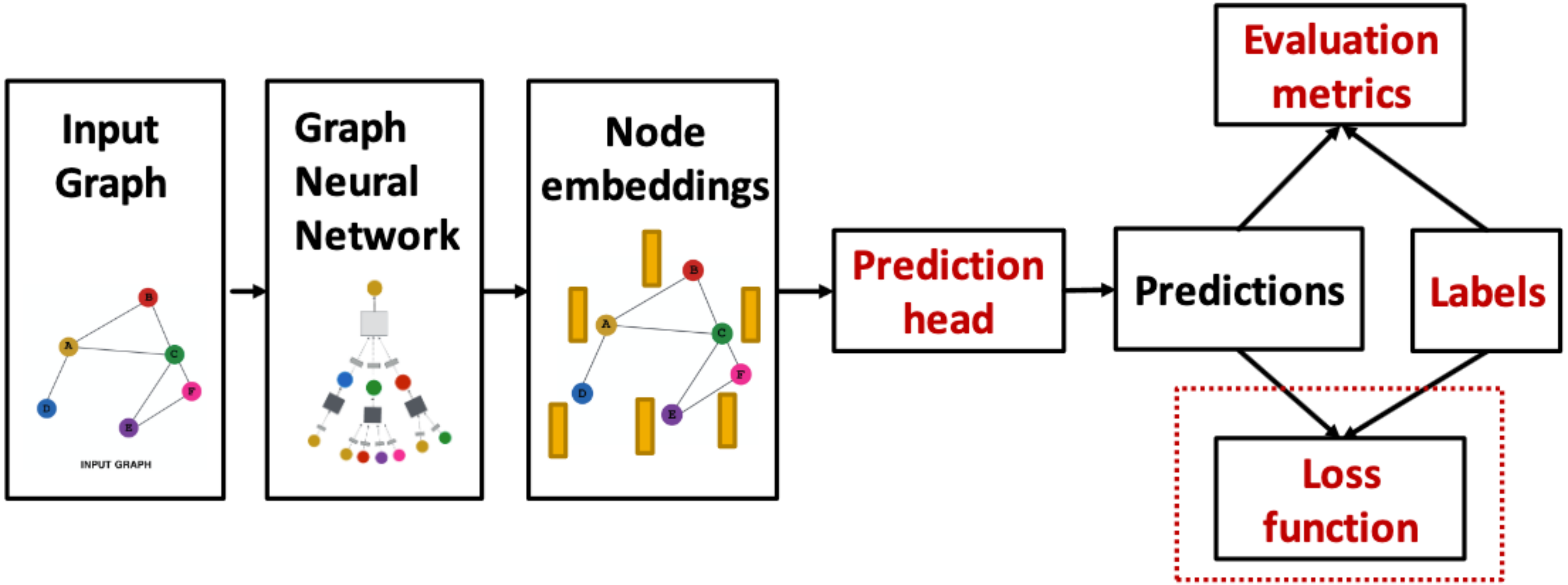
Unsupervised learning on graphs

- Signals come from graphs themselves
- E.g., link prediction: delete edges, predict if 2 nodes are connected

Sometimes the differences are blurry

- We still have "supervision" in unsupervised learning
- Alternative name for "unsupervised" is "**self-supervised**"

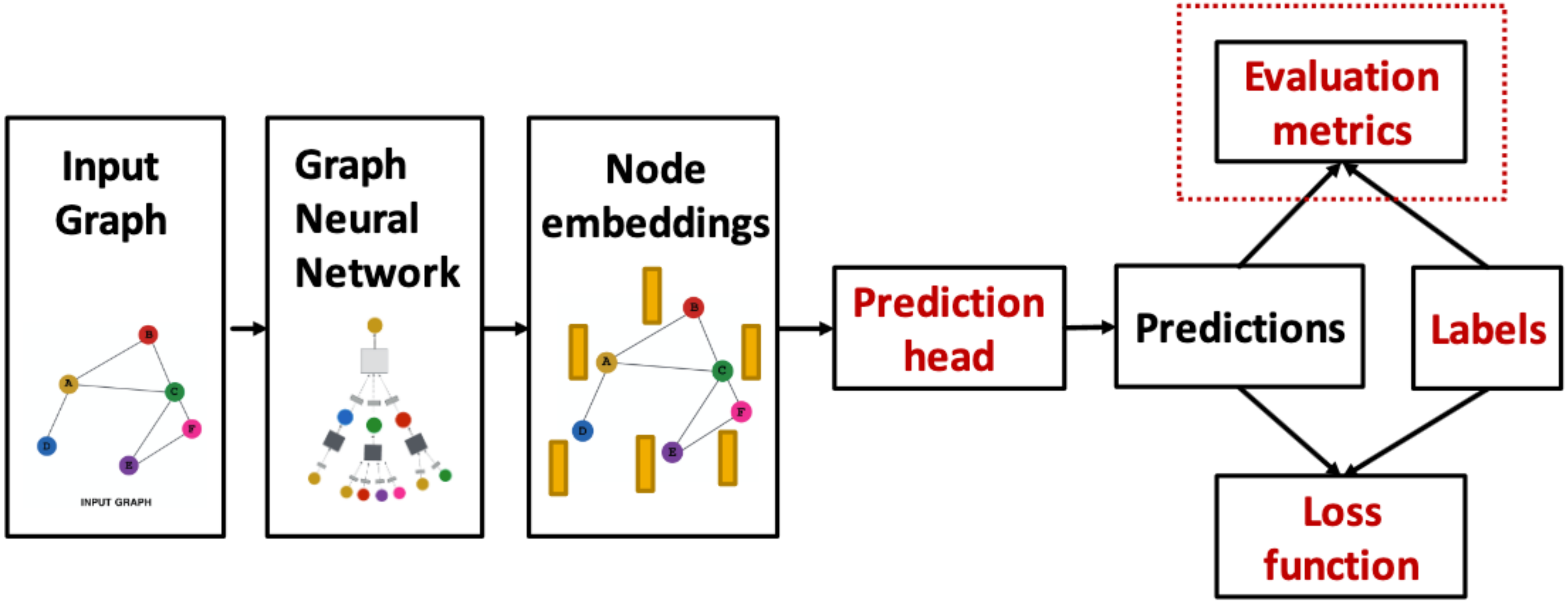
GNN pipeline



E.g., cross entropy for **classification**, MSE for **regression**

Figure by Leskovec

Loss functions



E.g., accuracy: $\frac{1}{N}\sum_{i=1}^{N} \mathbf{1}_{\{y_i \neq \hat{y}_i\}}$

Outline

Training, validation, and test sets

Training set: used for optimizing GNN parameters

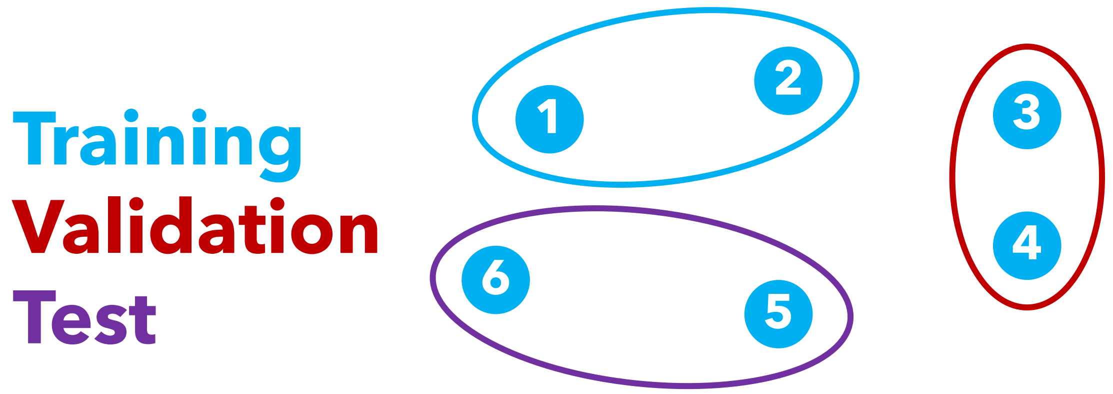
Validation set: develop model/hyperparameters

Test set: held out until we report final performance

Why graphs are special

Suppose we want to split an image dataset

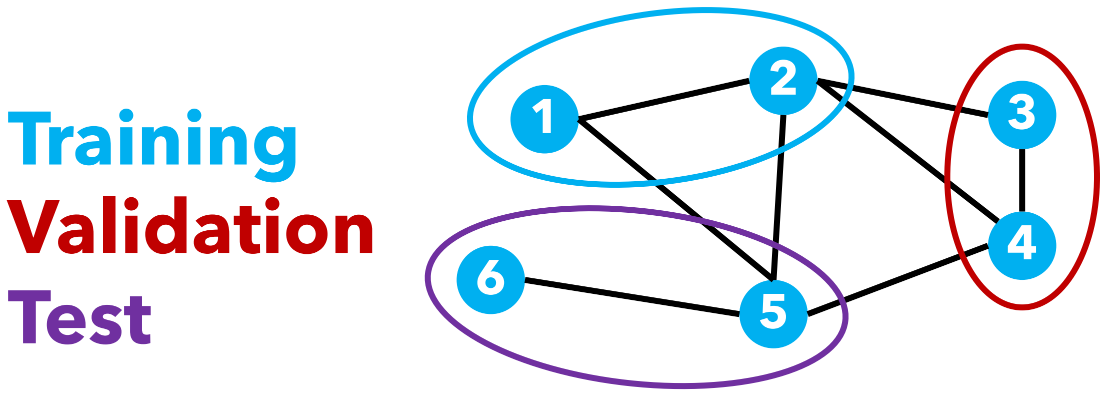
- Each data point is an image
- Data points are independent
- Image 5 will not affect our prediction on image 1



Why graphs are special

Splitting a graph dataset is different

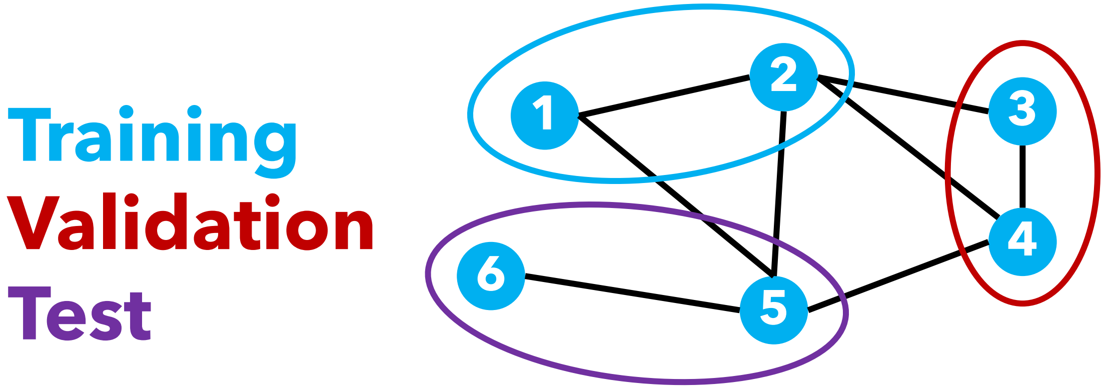
- Node classification: Each data point is a node
- Data points are NOT independent
  - Node 5 will affect our prediction on node 1 due to message passing



Transductive learning

Solution 1 (Transductive setting):

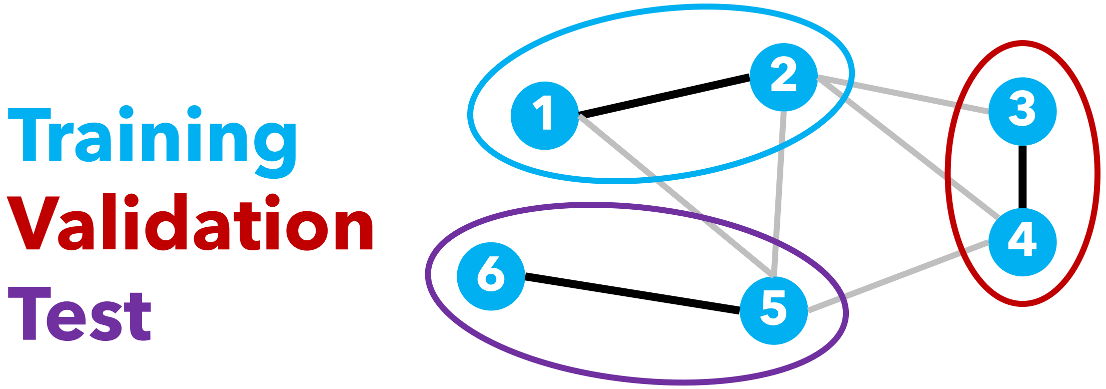
- Input graph can be observed in all the dataset splits
  - Training, validation and test set
- Only split the (node) labels
- Training: compute embeddings using entire graph
  - Train using node 1&2's labels
- Validation: compute embeddings using entire graph
  - Evaluate on node 3&4's labels



Inductive learning

Solution 2 (Inductive setting):

- Break the edges between splits to get multiple graphs
- 3 graphs are independent: node 5 won't affect prediction on node 1
- Training: compute embeddings using graph over node 1&2
    - Train using node 1&2's labels
- Validation: compute embeddings using the graph over node 3&4
    - Evaluate on node 3&4's labels



Transductive vs inductive

Transductive setting:

- Training / validation / test sets are on the same graph
- Dataset consists of one graph
- Entire graph can be observed in all dataset splits: only split labels
- Only applicable to node / edge prediction tasks

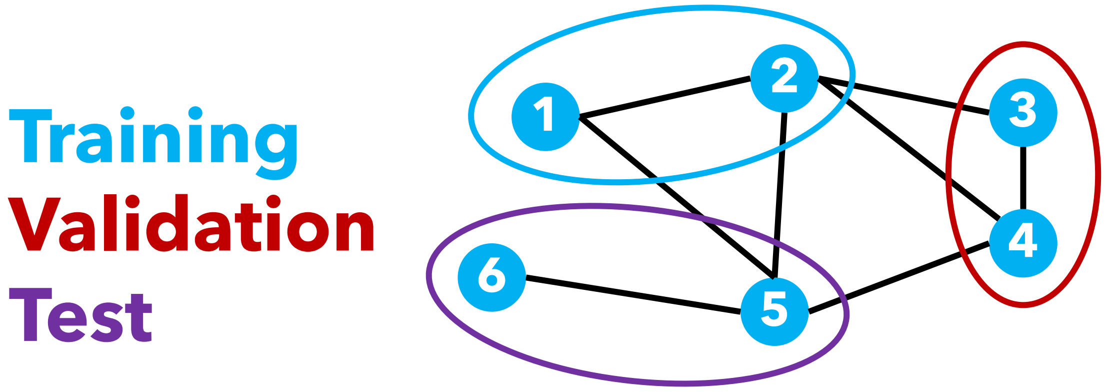
Inductive setting:

- Training / validation / test sets are on different graphs
- Dataset consists of multiple graphs
- Each split can only observe the graph(s) within the split
- Successful model should generalize to unseen graphs
- Applicable to node / edge / graph tasks

Example: Node classification

Transductive setting:

- All splits can observe the entire graph structure
- Can only observe the labels of their respective nodes

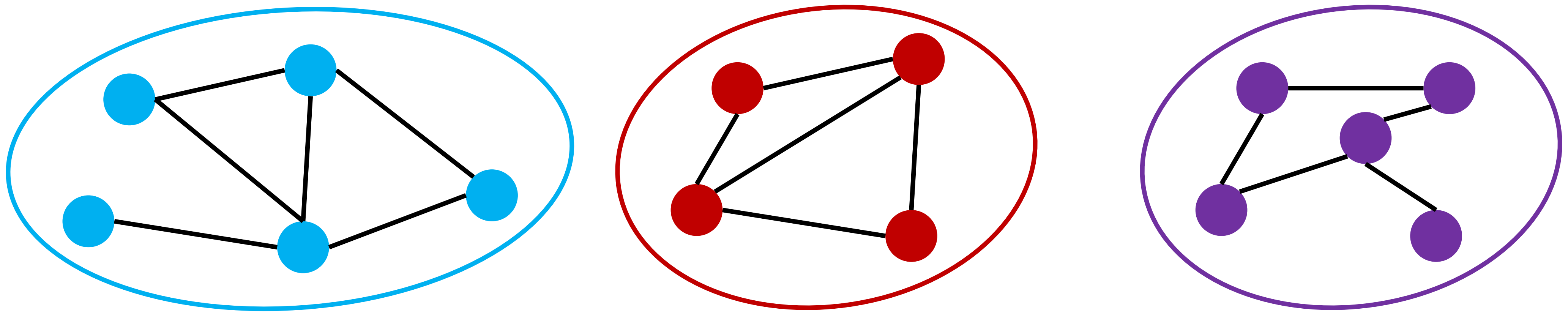


Example: Node classification

Inductive setting:

- Suppose have a dataset of 3 graphs
- Each split contains a different graph

Training
Validation
Test



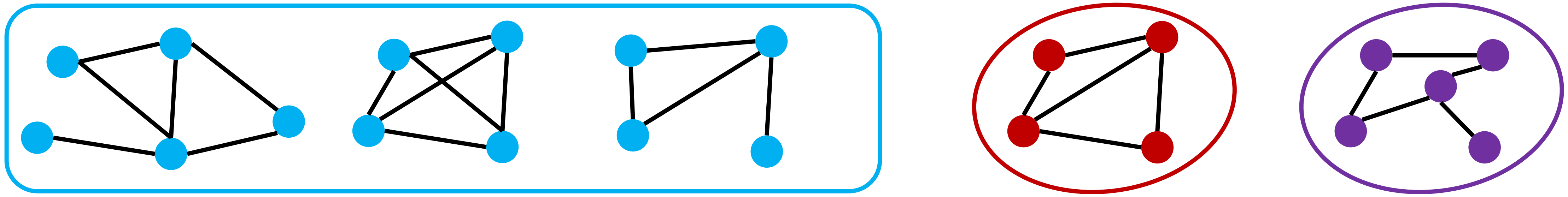
Example: Graph classification

Only the inductive setting is well defined for graph classification

- Have to test on unseen graphs
- Suppose we have a dataset of 5 graphs

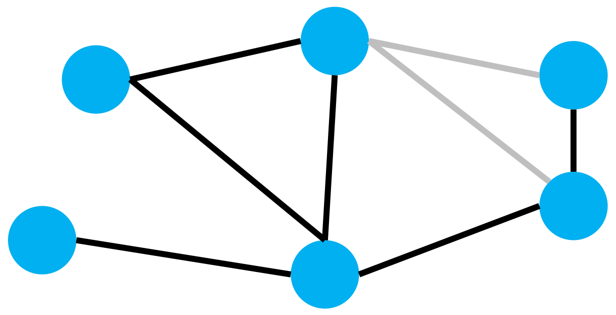
  Each split will contain independent graph(s)

Training
Validation
Test

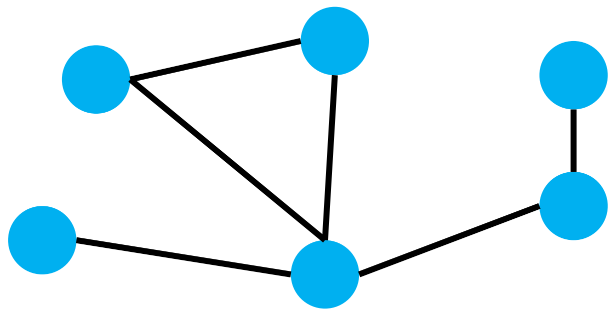


Example: Link prediction

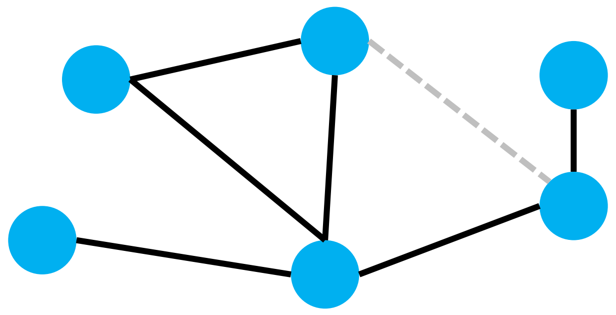
- **Goal:** predict missing edges
- Link prediction is an unsupervised / self-supervised task
- Need to hide some edges from the GNN
    - Let the GNN predict if the edges exist



Original graph



Input to GNN

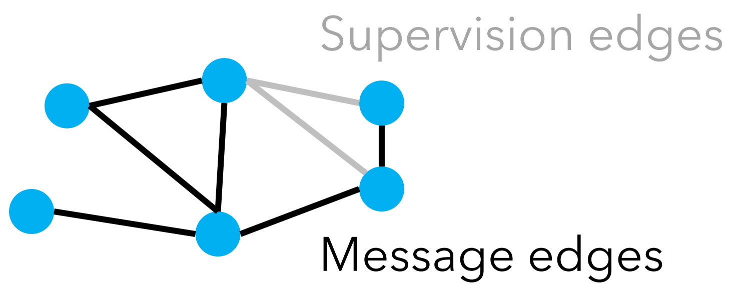


Predictions made by GNN

Setting up link prediction

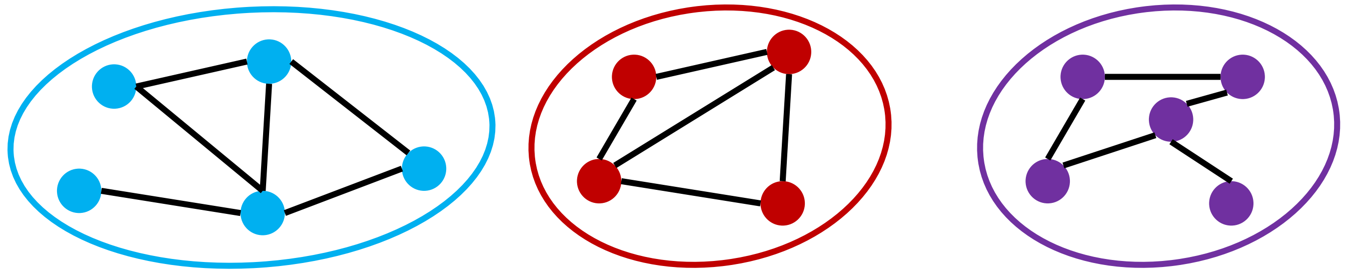
- For link prediction, we'll **split edges twice**
- Step 1: Assign **two types** of edges in the original graph
  - Message edges: Used for GNN message passing
  - Supervision edges: Use for computing objectives
- After step 1:
  - Only message edges will remain in the graph
  - Supervision edges used as supervision for model's predictions

    Will not be fed into GNN!



Setting up link prediction

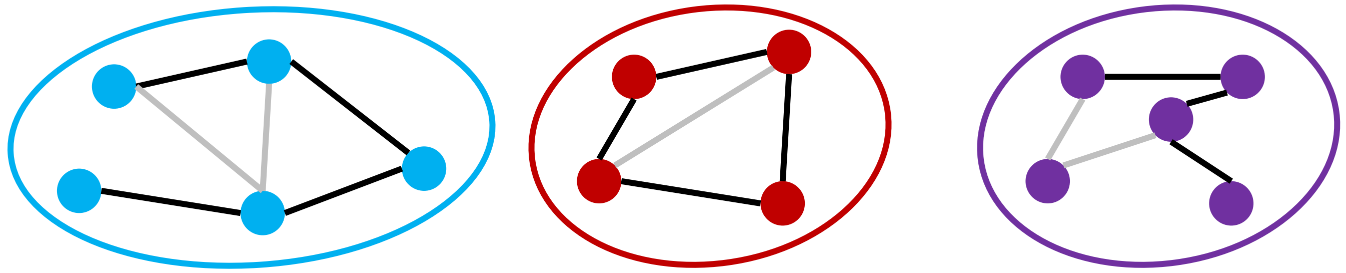
- Step 2: Split edges into train / validation / test
- Option 1: **Inductive** link prediction split
  - Suppose we have a dataset of 3 graphs
  - Each inductive split will contain an independent graph



Training
Validation
Test

Setting up link prediction

- Step 2: Split edges into train / validation / test
- Option 1: **Inductive** link prediction split
  - Suppose we have a dataset of 3 graphs
  - Each inductive split will contain an independent graph
  - In train/val/test set, each graph will have 2 types of edges:
    - Message edges
    - Supervision edges (not the input to GNN)

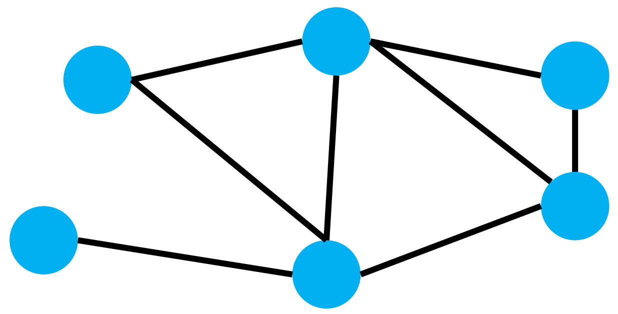


Training
Validation
Test

Setting up link prediction

Option 2: **Transductive** link prediction split:

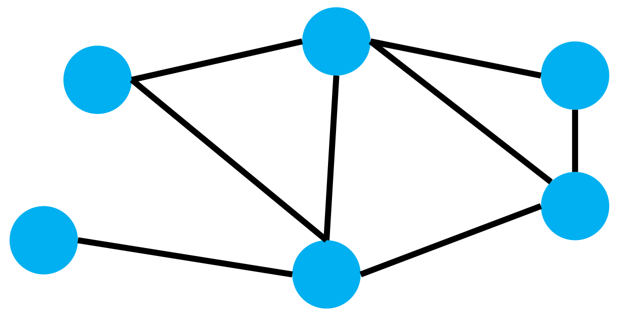
- Default setting when people talk about link prediction
- Suppose we have a dataset of 1 graph



Setting up link prediction

Option 2: **Transductive** link prediction split:

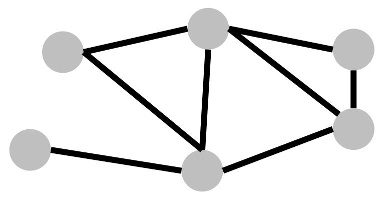
- Entire graph can be observed in all dataset splits
- Need to hold out validation / test edges
- To train, must hold out supervision edges for the training set

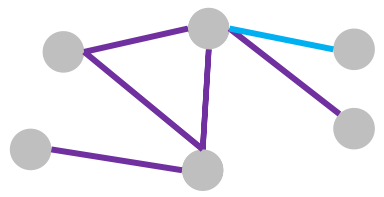


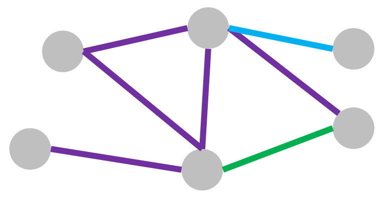
Setting up link prediction

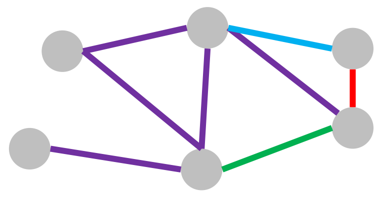
Option 2: **Transductive** link prediction split

Original graph









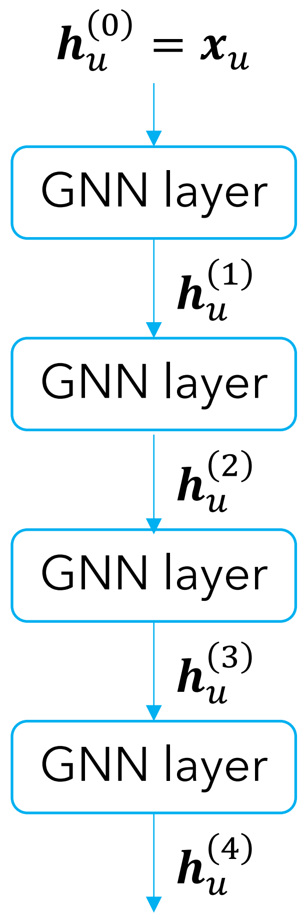
(1) At training time:
Use **training message** edges to predict **training supervision** edges

(2) At validation time:
Use **training message** + **supervision** edges to predict **validation** edges

(3) At test time:
Use **training message** + **supervision** edges and **validation** edges to predict **test** edges

Outline

Over-smoothing problem



Issue with stacking many GNN layers:
GNN suffers from the *over-smoothing problem*

The **over-smoothing problem**:
All node embeddings converge to same value

Bad bc want to use embeddings to differentiate nodes

Why does the over-smoothing problem happen?

Receptive field of a GNN

- Receptive field:
  Set of nodes that determine embedding of node of interest
- K-layer GNN: node's receptive field is its K-hop neighborhood

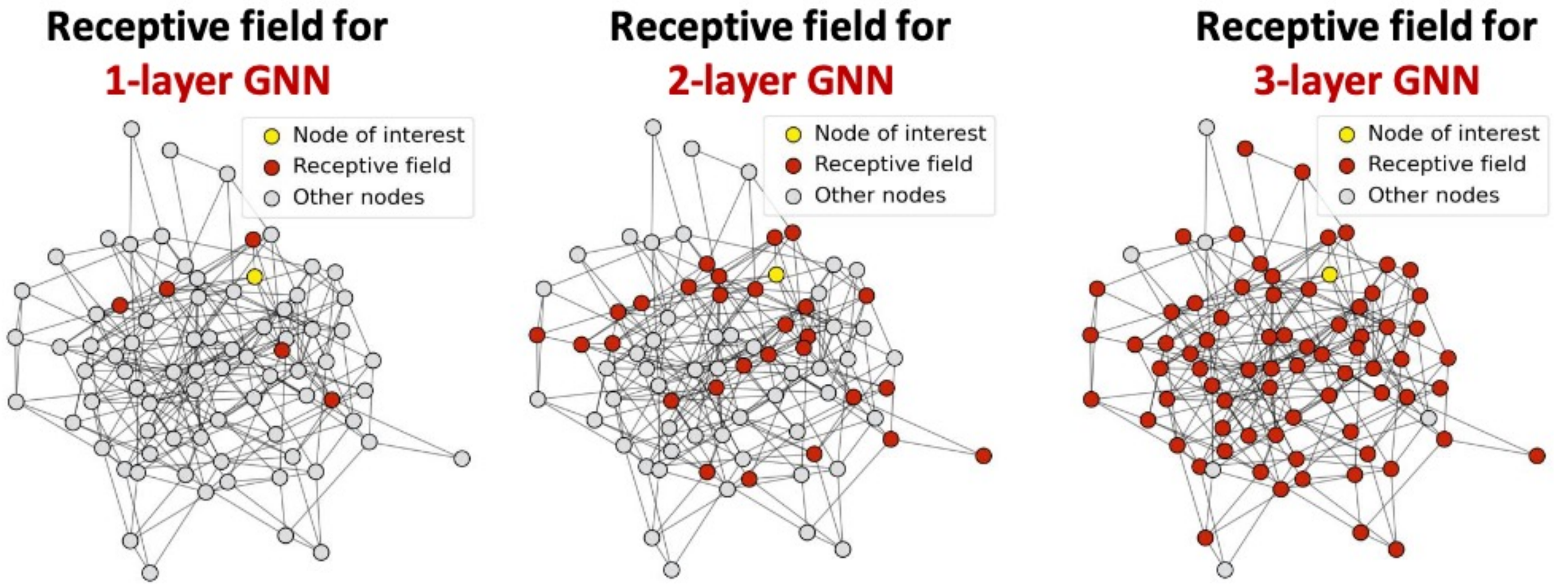


Figure by Leskovec

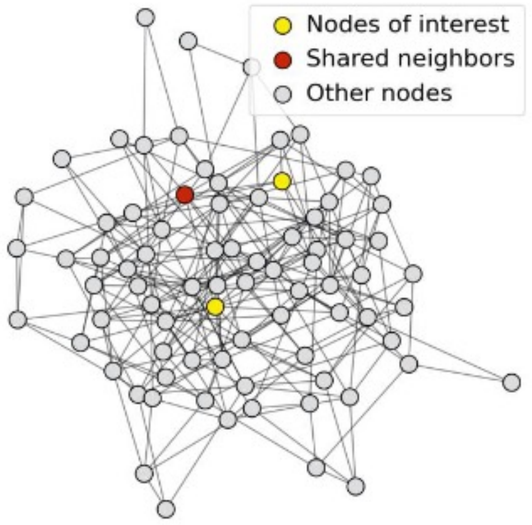
Receptive field of a GNN

Receptive field **overlap** for two nodes

- Shared neighbors quickly grows when we increase # GNN layers

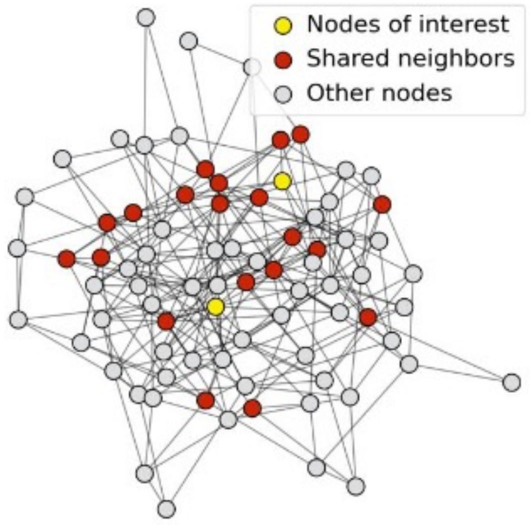
1-hop neighbor overlap

Only 1 node



2-hop neighbor overlap

About 20 nodes



3-hop neighbor overlap

Almost all the nodes!

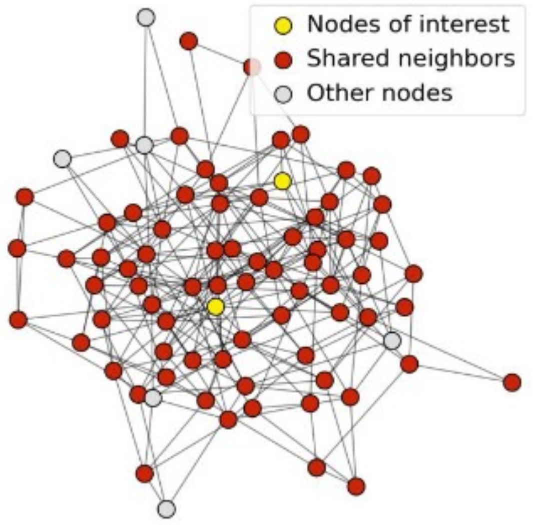


Figure by Leskovec

Receptive field and oversmoothing

Can explain over-smoothing via **receptive fields**

Embedding of a node is determined by its receptive field

- Nodes have very overlapped receptive fields ⇒ similar embeddings
- Stack many GNN layers

  → nodes will have highly-overlapped receptive fields

  → node embeddings will be highly similar

  → suffer from the over-smoothing problem

How to overcome over-smoothing problem?

Design GNN layer connectivity

Lesson: Be cautious when adding GNN layers

Adding GNN layers doesn’t always help, unlike NNs in other domains

Step 1: Analyze necessary receptive field to solve problem

E.g., by computing graph’s diameter

Step 2: Set # GNN layers to be a bit more than receptive field

Skip connections

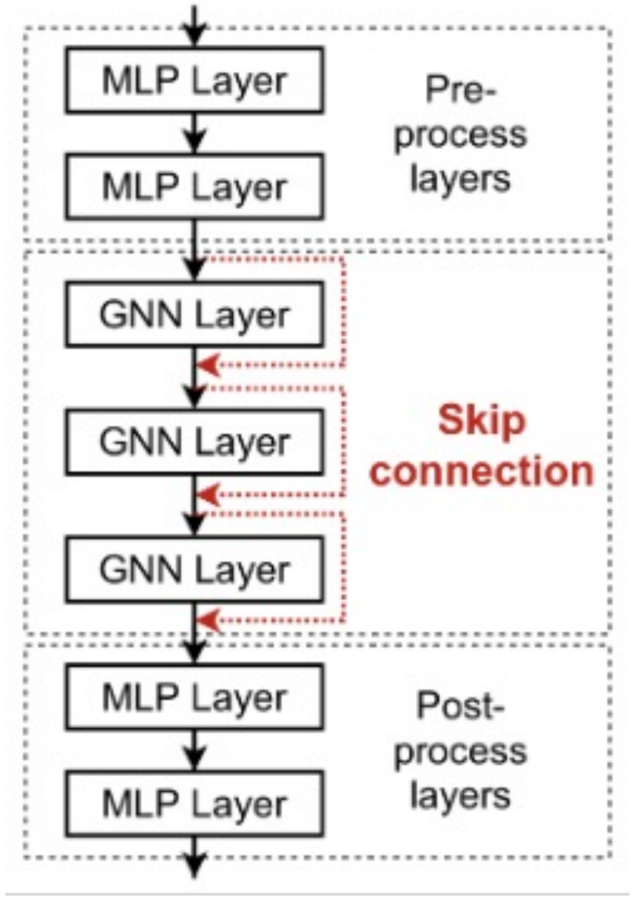
What if my problem still requires many GNN layers?

Observation:

Embeddings in early layers can better differentiate nodes

Solution: add **shortcuts** in GNN (skip connections)

Skip connections



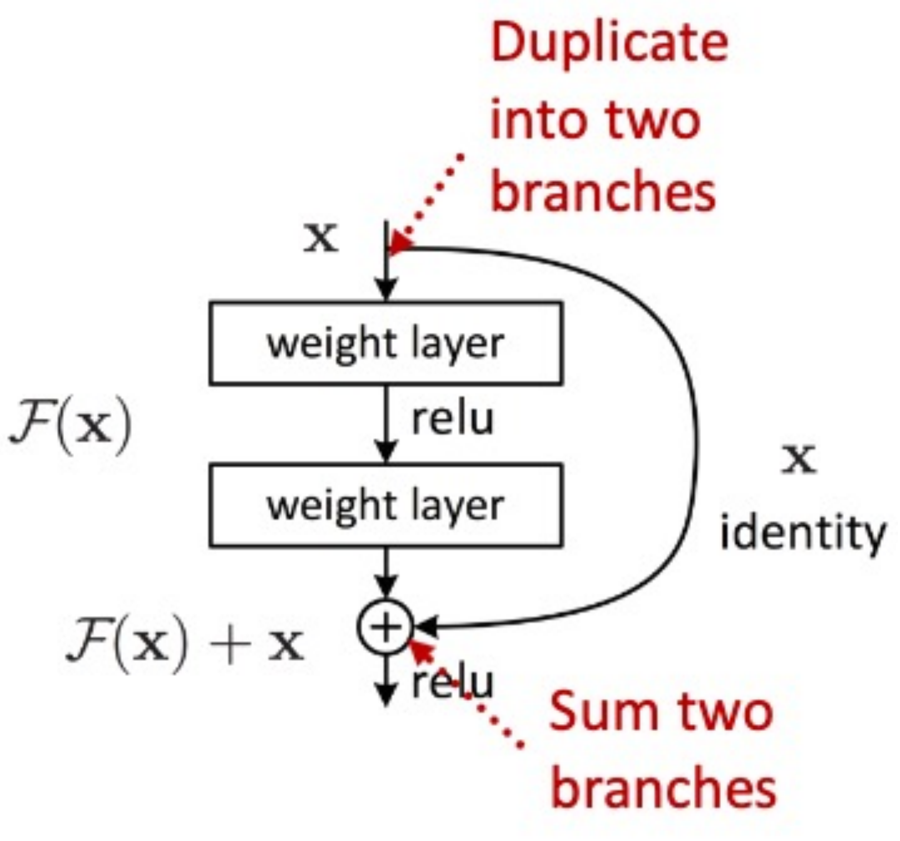

Duplicate into two branches
$\mathbf{x}$
weight layer
relu
weight layer
$\mathcal{F}(\mathbf{x})$
$\mathbf{x}$
identity
$\mathcal{F}(\mathbf{x}) + \mathbf{x}$
relu
Sum two branches

Figure by Leskovec

Outline

1. Introduction
2. Feature engineering for graphs
3. GNN architecture
4. Training a GNN
    a. GNN pipeline
    b. Train/validation/test splits
    c. Skip connections
    d. Graph manipulations

Node feature augmentation

Useful if, e.g., input graph does not have node features

- Common when we only have the adj. matrix

Standard approach: assign unique IDs to nodes

- 👍 High expressive power
- 👎 Can't generalize to new nodes
- 👎 High computational cost (many features)

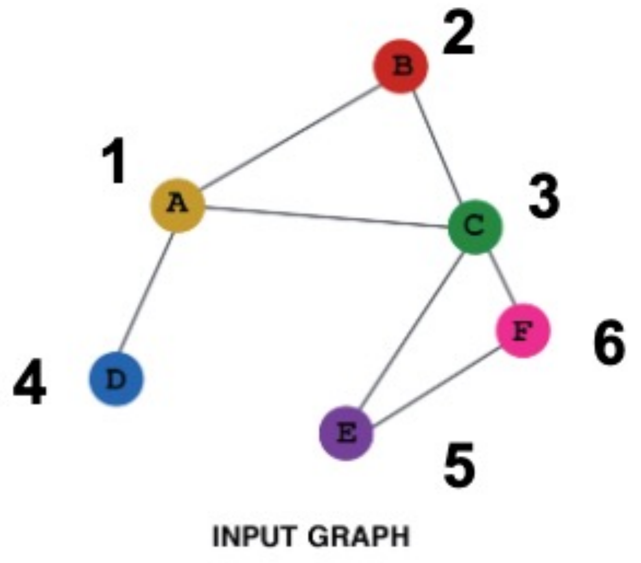
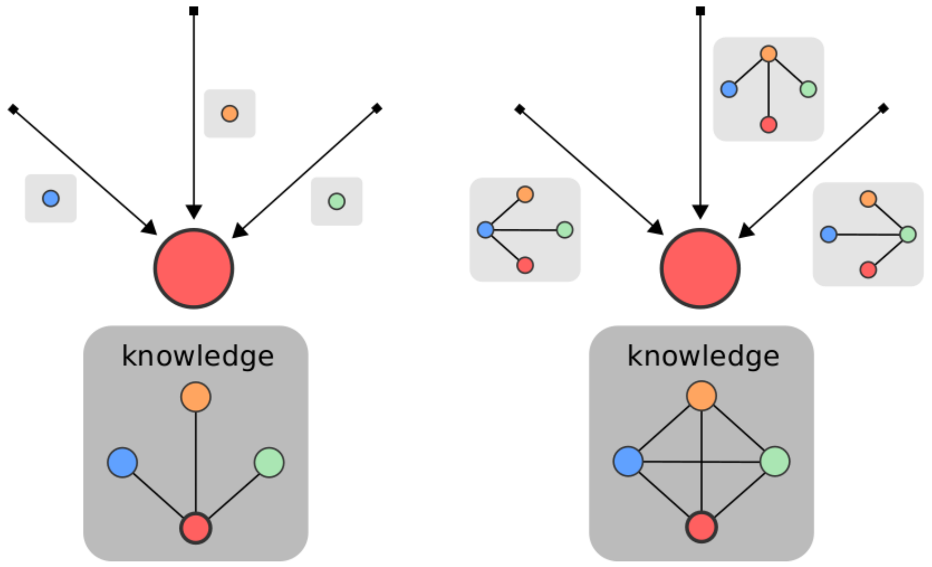


Figure by Leskovec

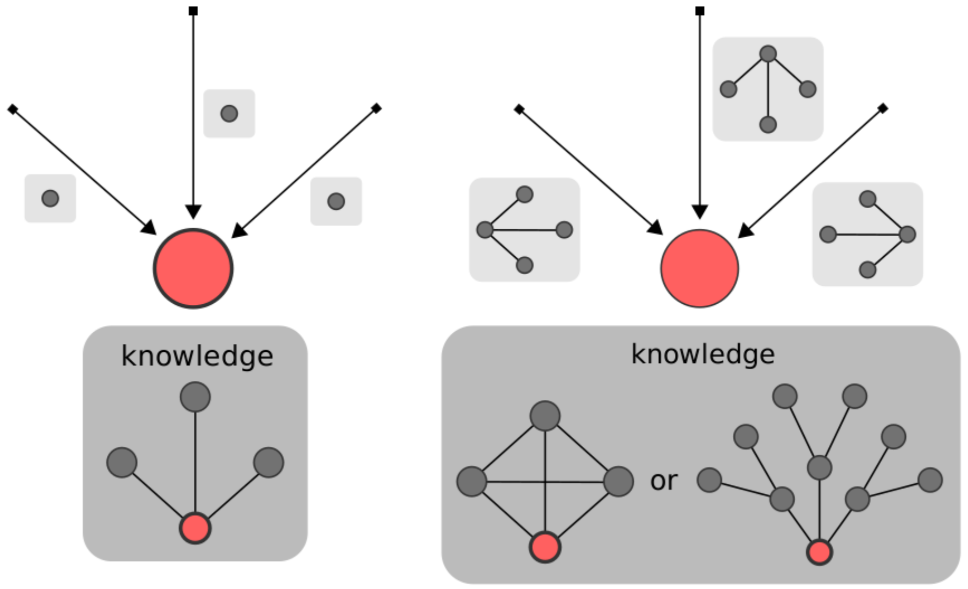
Why do we need feature augmentation?

Certain structures are hard to learn by GNN

E.g., cycle count



Nodes **can** distinguish each other



Nodes **can't** distinguish each other

https://andreasloukas.blog/2019/12/27/what-gnn-can-and-cannot-learn/

Outline

Papers we'll read

Veličković, Petar, et al. "Neural execution of graph algorithms." *ICLR*. 2020.

- GNNs don't work off-the-shelf for combinatorial tasks
- How to **align** GNN architectures to these tasks

Cappart, Quentin, et al. "Combinatorial optimization and reasoning with GNNs." *arXiv*.

- **Broad overview** of the field; current & future directions