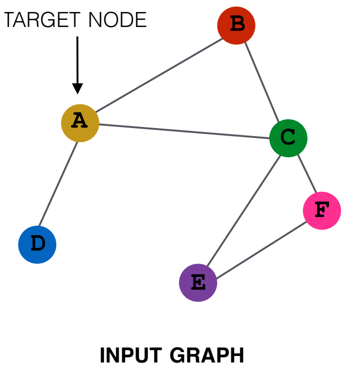
Stanford CS224W: GNN Augmentation and Training

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

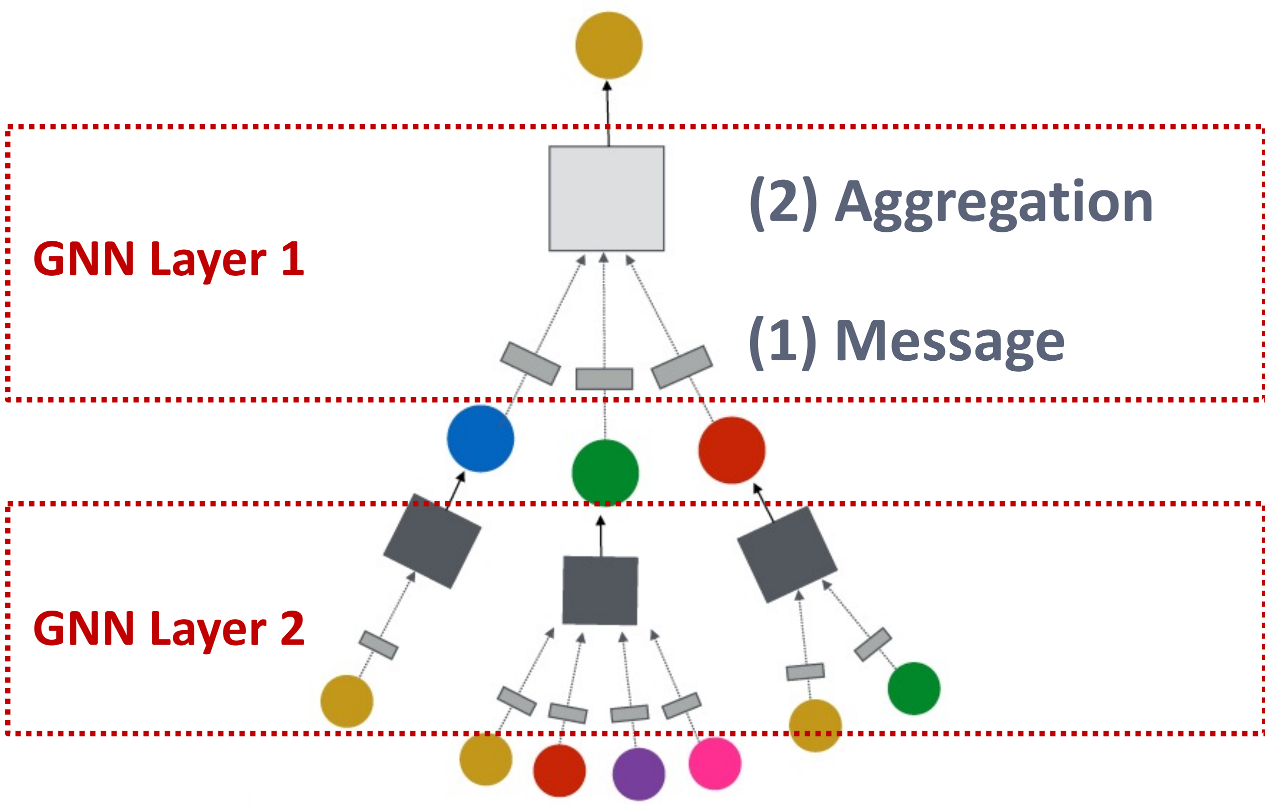
J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020

Recap: A General GNN Framework



(5) Learning objective

(3) Layer connectivity



(4) Graph augmentation

Stanford CS224W: Stacking Layers of a GNN

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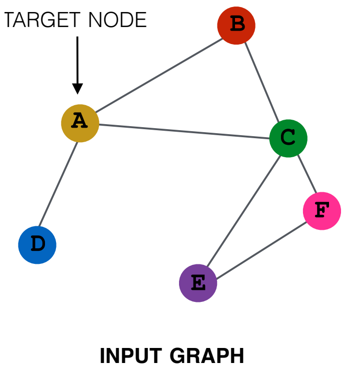
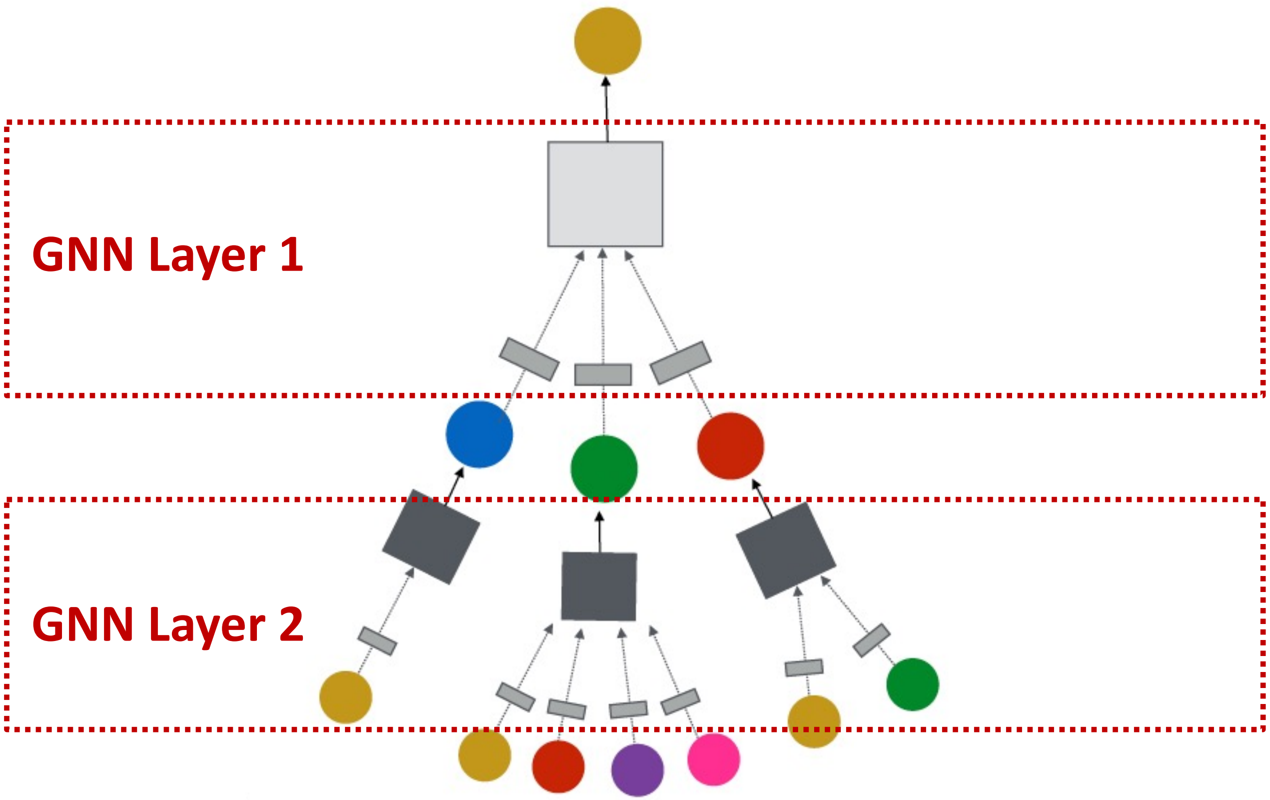
Stacking GNN Layers



How to connect GNN layers into a GNN?

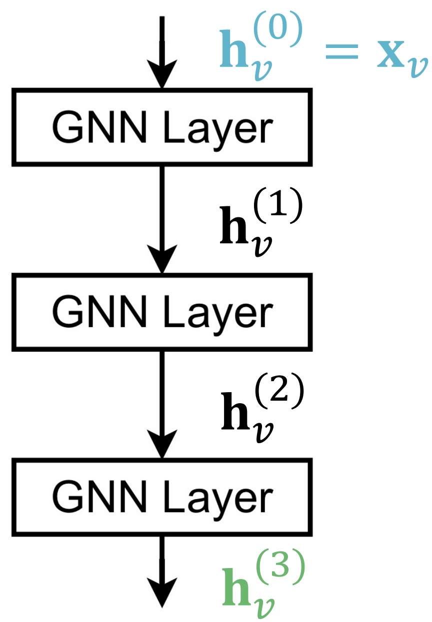
- **Stack layers sequentially**
- **Ways of adding skip connections**

(3) Layer connectivity



Stacking GNN Layers

- **How to construct a Graph Neural Network?**
  - **The standard way:** Stack GNN layers sequentially
  - **Input:** Initial raw node feature $\mathbf{x}_v$
  - **Output:** Node embeddings $\mathbf{h}_v^{(L)}$ after L GNN layers



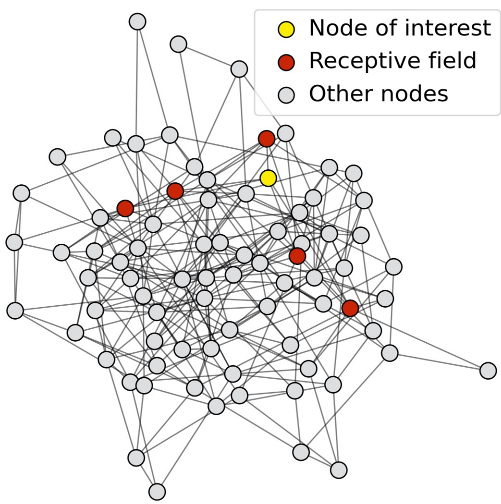
The Over-smoothing Problem

- **The Issue of stacking many GNN layers**
  - GNN suffers from **the over-smoothing problem**
- **The over-smoothing problem: all the node embeddings converge to the same value**
  - This is bad because we **want to use node embeddings to differentiate nodes**
- **Why does the over-smoothing problem happen?**

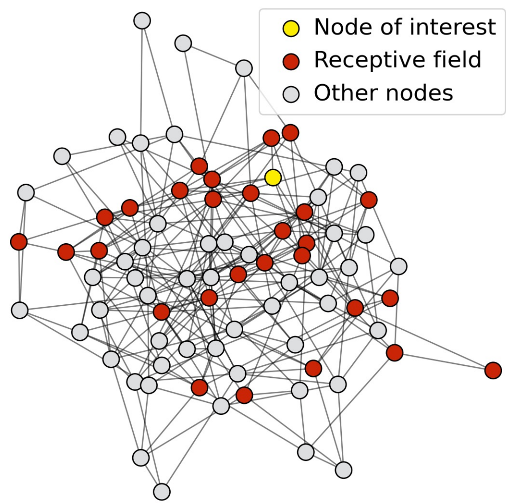
Receptive Field of a GNN

- **Receptive field:** the set of nodes that determine the embedding of a node of interest
  - **In a K-layer GNN, each node has a receptive field of K-hop neighborhood**

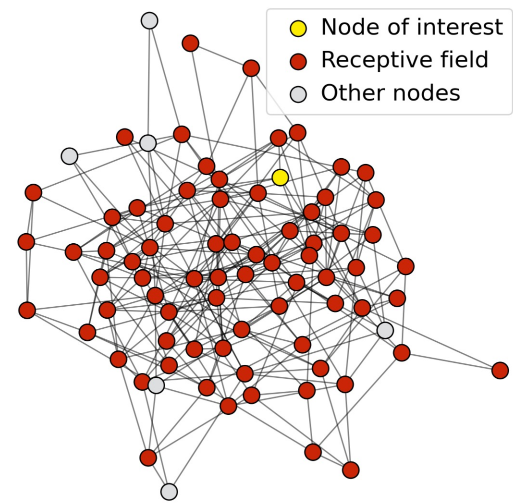
Receptive field for 1-layer GNN



Receptive field for 2-layer GNN



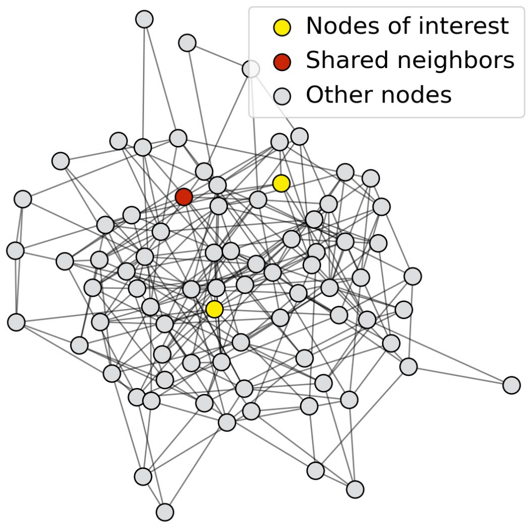
Receptive field for 3-layer GNN



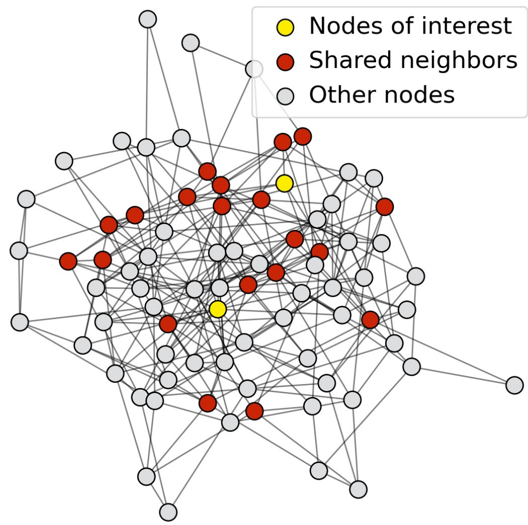
Receptive Field of a GNN

- **Receptive field overlap** for two nodes
  - **The shared neighbors quickly grows** when we increase the number of hops (num of GNN layers)

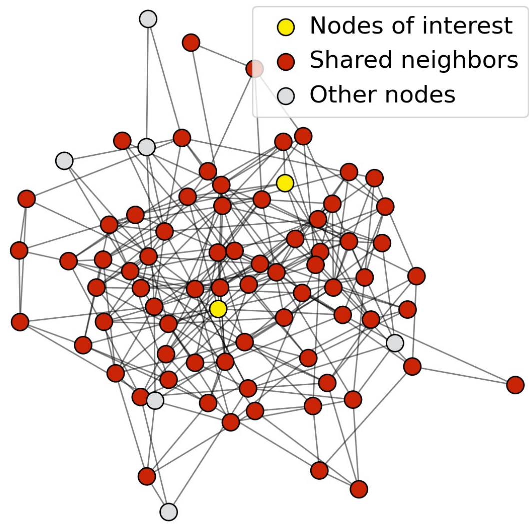
1-hop neighbor overlap
Only 1 node



2-hop neighbor overlap
About 20 nodes



3-hop neighbor overlap
Almost all the nodes!



Receptive Field & Over-smoothing

- We can explain over-smoothing via the notion of receptive field
  - We knew **the embedding of a node is determined by its** receptive field
    - If two nodes **have highly-overlapped receptive fields, then their embeddings are highly similar**
  - Stack many GNN layers → nodes will have highly-overlapped receptive fields → node embeddings will be highly similar → suffer from the over-smoothing problem
- Next: how do we overcome over-smoothing problem?

Design GNN Layer Connectivity

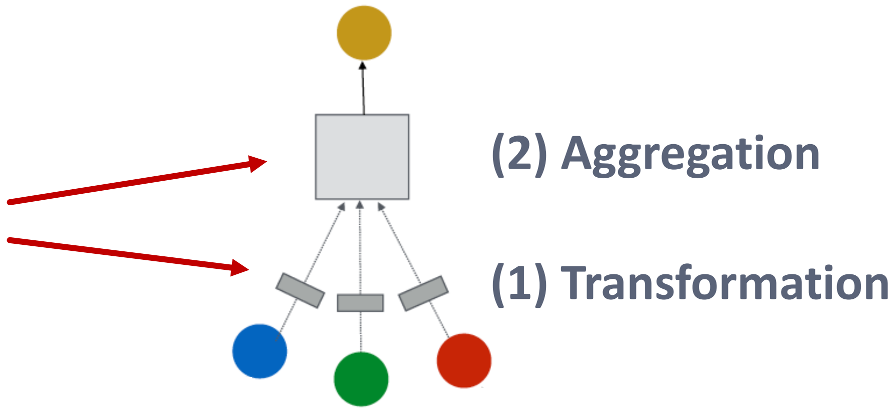
- **What do we learn from the over-smoothing problem?**
- **Lesson 1: Be cautious when adding GNN layers**
  - Unlike neural networks in other domains (CNN for image classification), **adding more GNN layers do not always help**
  - **Step 1: Analyze the necessary receptive field** to solve your problem. E.g., by computing the diameter of the graph
  - **Step 2:** Set number of GNN layers L to be a bit more than the receptive field we like. **Do not set L to be unnecessarily large**!

- **Question:** How to enhance the expressive power of a GNN, if the number of GNN layers is small?

Expressive Power for Shallow GNNs

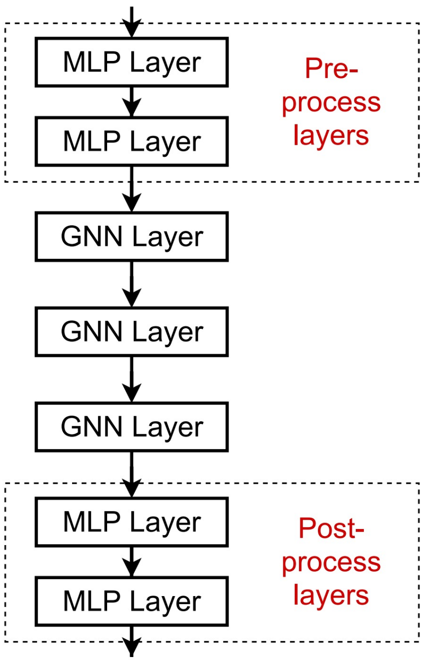
- **How to make a shallow GNN more expressive?**
- **Solution 1**: Increase the expressive power **within each GNN layer**
  - In our previous examples, each transformation or aggregation function only include one linear layer
  - We can **make aggregation / transformation become a deep neural network**!

If needed, each box could include a 3-layer MLP



Expressive Power for Shallow GNNs

- **How to make a shallow GNN more expressive?**
- **Solution 2:** Add layers that do not pass messages
  - A GNN does not necessarily only contain GNN layers
    - E.g., we can add **MLP layers** (applied to each node) before and after GNN layers, as **pre-process layers** and **post-process layers**



Pre-processing layers: Important when encoding node features is necessary.
E.g., when nodes represent images/text

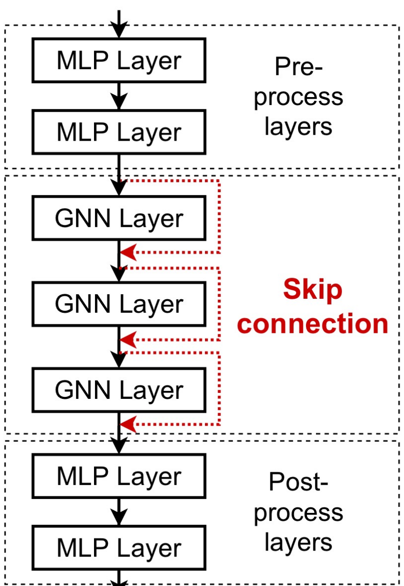
Post-processing layers: Important when reasoning / transformation over node embeddings are needed
E.g., graph classification, knowledge graphs

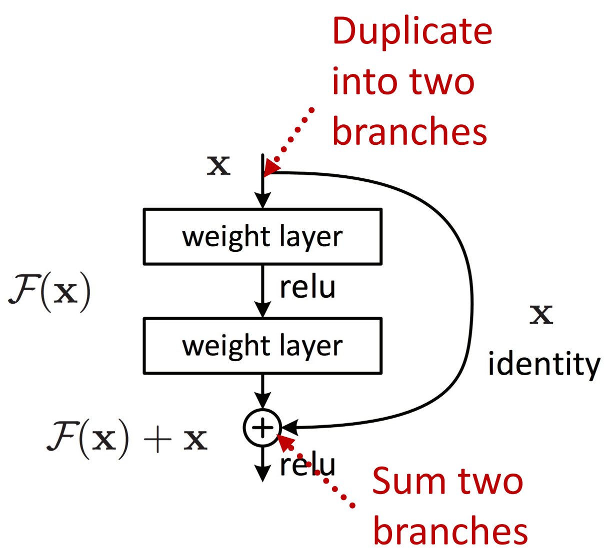
In practice, adding these layers works great!

He et al. [Deep Residual Learning for Image Recognition](), CVPR 2015

Design GNN Layer Connectivity

- **What if my problem still requires many GNN layers?**
- **Lesson 2: Add skip connections in GNNs**
  - **Observation from over-smoothing:** Node embeddings in earlier GNN layers can sometimes better differentiate nodes
  - **Solution:** We can increase the impact of earlier layers on the final node embeddings, **by adding shortcuts in GNN**





Idea of skip connections:

Before adding shortcuts:

$$\boldsymbol{F}(\mathbf{x})$$

After adding shortcuts:

$$\boldsymbol{F}(\mathbf{x}) + \mathbf{x}$$

Example: GCN with Skip Connections

- **A standard GCN layer**

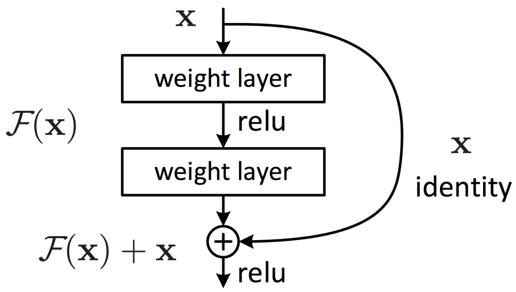
- $\mathbf{h}_v^{(l)} = \sigma\left(\boxed{\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}}\right)$

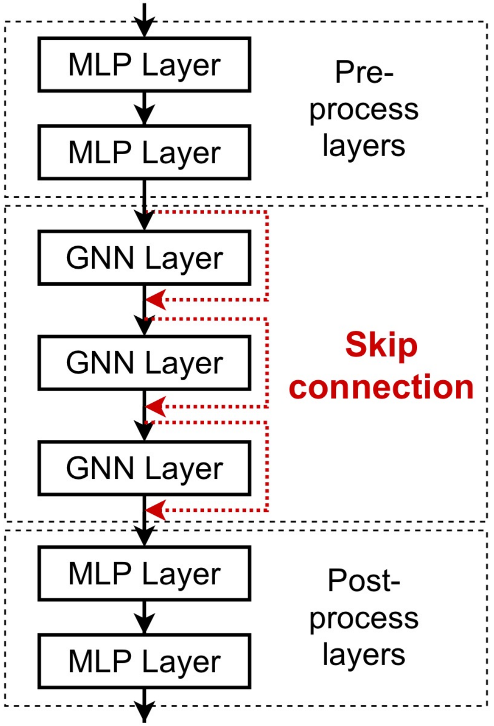
This is our $F(\mathbf{x})$

- **A GCN layer with skip connection**

- $\mathbf{h}_v^{(l)} = \sigma\left(\boxed{\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}} + \boxed{\mathbf{h}_v^{(l-1)}}\right)$

$F(\mathbf{x}) \quad + \quad \mathbf{x}$



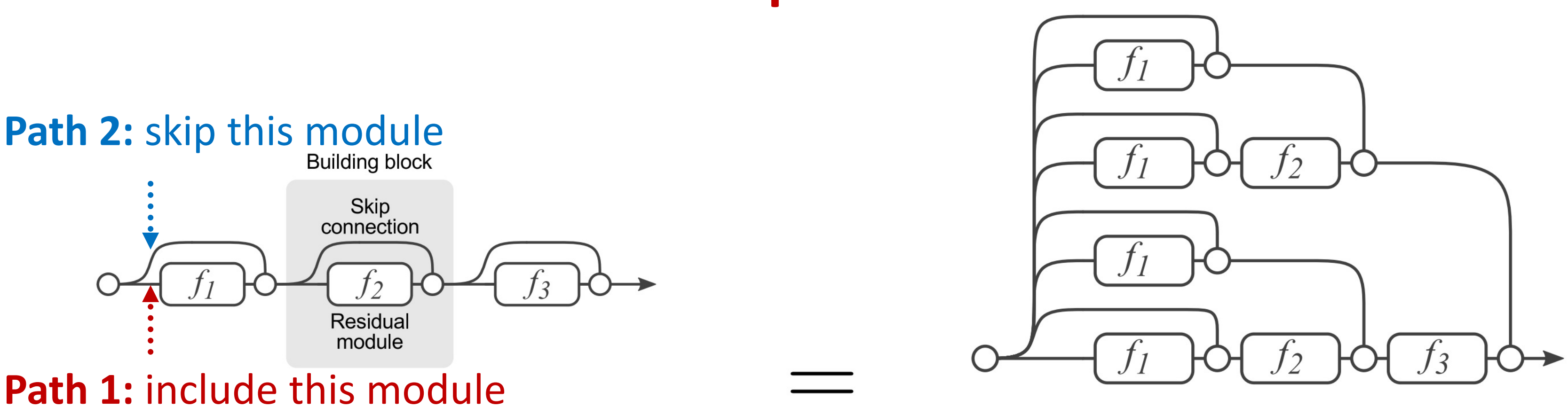


Idea of Skip Connections

- **Why do skip connections work?**
  - **Intuition:** Skip connections create **a mixture of models**
  - N skip connections → 2^N possible paths
  - Each path could have up to N modules
  - We automatically get **a mixture of shallow GNNs and deep GNNs**

All the possible paths:

$2 * 2 * 2 = 2^3 = 8$



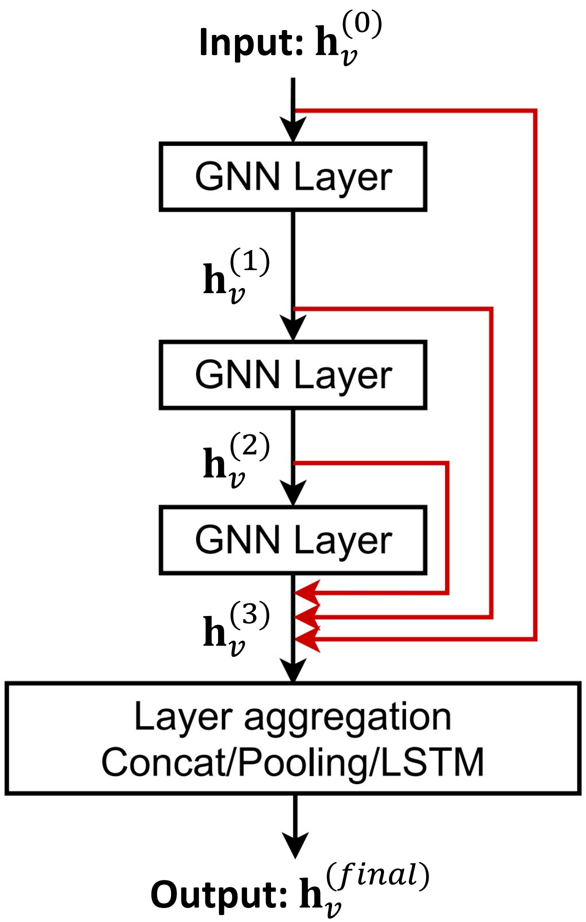
(a) Conventional 3-block residual network

(b) Unraveled view of (a)

Veit et al. Residual Networks Behave Like Ensembles of Relatively Shallow Networks, ArXiv 2016

Other Options of Skip Connections

- **Other options:** Directly skip to the last layer
  - The final layer directly **aggregates from the all the node embeddings** in the previous layers



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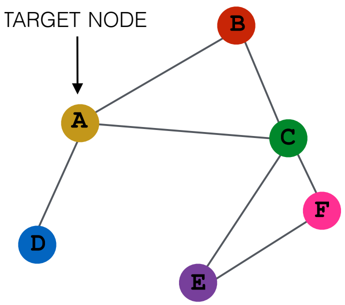
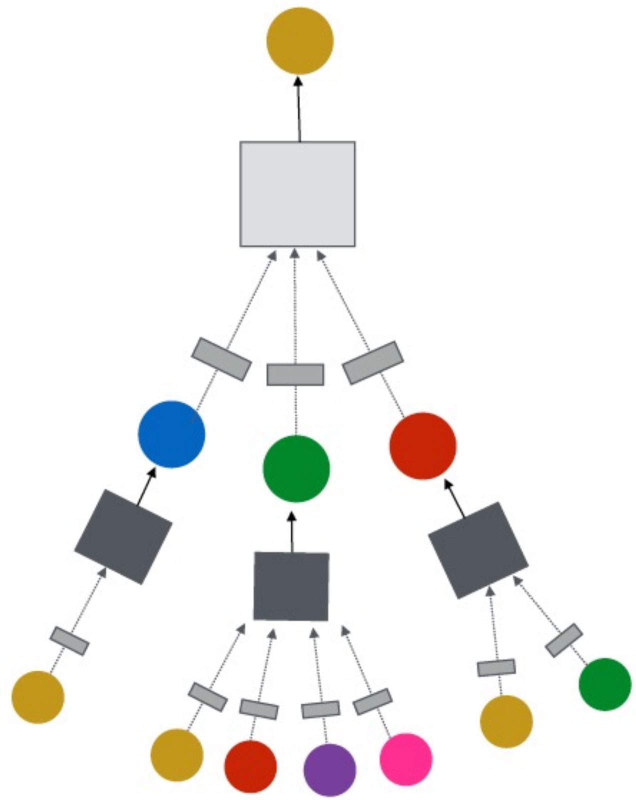
General GNN Framework



INPUT GRAPH

Idea: Raw input graph ≠ computational graph

- Graph feature augmentation
- Graph structure augmentation



(4) Graph augmentation

Why Augment Graphs

Our assumption so far has been

- **Raw input graph = computational graph**

Reasons for breaking this assumption

- **Features:**
  - The input graph **lacks features**
- **Graph structure:**
  - The graph is **too sparse** → inefficient message passing
  - The graph is **too dense** → message passing is too costly
  - The graph is **too large** → cannot fit the computational graph into a GPU
- It's **unlikely that the input graph happens to be the optimal computation graph** for embeddings

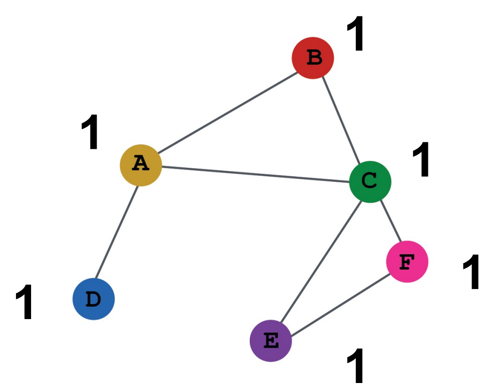
Graph Augmentation Approaches

- **Graph Feature augmentation**
  - The input graph **lacks features** → **feature augmentation**
- **Graph Structure augmentation**
  - The graph is **too sparse** → **Add virtual nodes / edges**
  - The graph is **too dense** → **Sample neighbors when doing message passing**
  - The graph is **too large** → **Sample subgraphs to compute embeddings**
    - Will cover later in lecture: Scaling up GNNs

Feature Augmentation on Graphs

Why do we need feature augmentation?

- **(1) Input graph does not have node features**
  - This is common when we only have the adj. matrix
- **Standard approaches:**
- **a) Assign constant values to nodes**

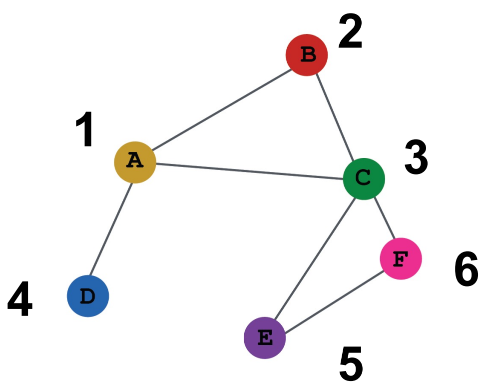


INPUT GRAPH

Feature Augmentation on Graphs

Why do we need feature augmentation?

- **(1) Input graph does not have node features**
  - This is common when we only have the adj. matrix
- **Standard approaches:**
- **b) Assign unique IDs to nodes**
  - These IDs are converted into **one-hot vectors**



INPUT GRAPH

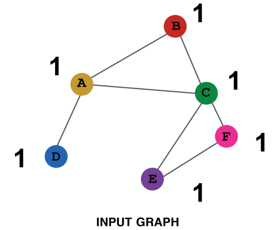
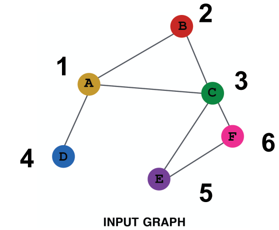
One-hot vector for node with ID=5

ID = 5

$$\underbrace{[0, 0, 0, 0, 1, 0]}_{\text{Total number of IDs = 6}}$$

Feature Augmentation on Graphs

- Feature augmentation: **constant** vs. **one-hot**

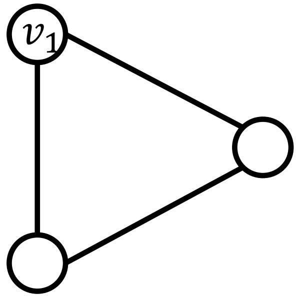
	Constant node feature 	**One-hot node feature** 
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a unique ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple to generalize to new nodes: we assign constant feature to them, then apply our GNN	**Low**. Cannot generalize to new nodes: new nodes introduce new IDs, GNN doesn't know how to embed unseen IDs
Computational cost	**Low**. Only 1 dimensional feature	**High**. $O(\|V\|)$ dimensional feature, cannot apply to large graphs
Use cases	**Any graph, inductive settings** (generalize to new nodes)	**Small graph, transductive settings** (no new nodes)

Feature Augmentation on Graphs

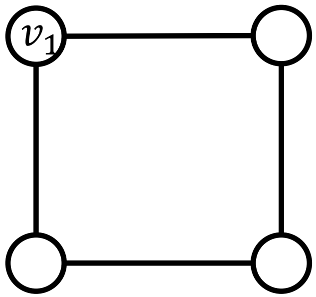
Why do we need feature augmentation?

- **(2) Certain structures are hard to learn by GNN**
- **Example:** Cycle count feature:
  - Can GNN learn the length of a cycle that v_1 resides in?
  - **Unfortunately, no**

v_1 resides in a cycle with length 3



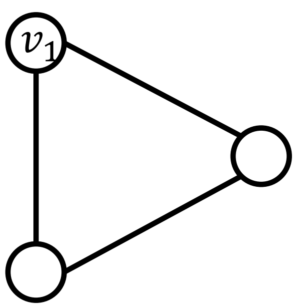
v_1 resides in a cycle with length 4



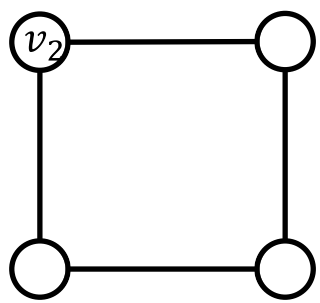
Feature Augmentation on Graphs

- v_1 **cannot differentiate which graph it resides in**
  - Because all the nodes in the graph have degree of 2
  - The computational graphs will be the same binary tree

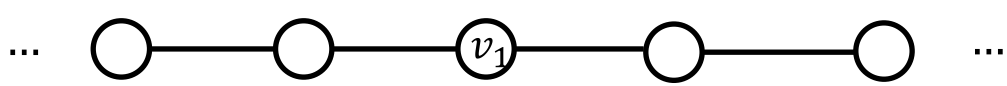
v_1 resides in a cycle with length 3



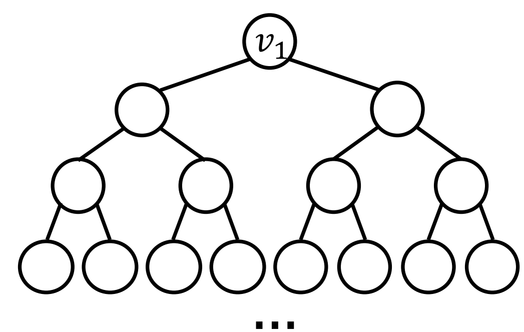
v_1 resides in a cycle with length 4



v_1 resides in a cycle with infinite length



The computational graphs for node v_1 are always the same



More about this topic later!

Feature Augmentation on Graphs

Why do we need feature augmentation?

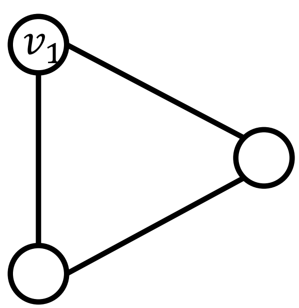
- **(2) Certain structures are hard to learn by GNN**
- **Solution:**
  - We can use cycle count as augmented node features

We start from cycle with length 0

Augmented node feature for v_1

[0, 0, 0, 1, 0, 0]

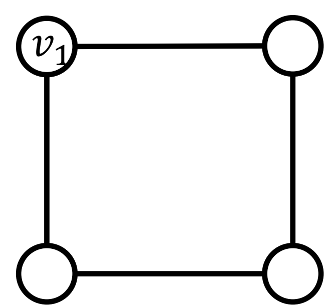
v_1 resides in a cycle with length 3



Augmented node feature for v_1

[0, 0, 0, 0, 1, 0]

v_1 resides in a cycle with length 4



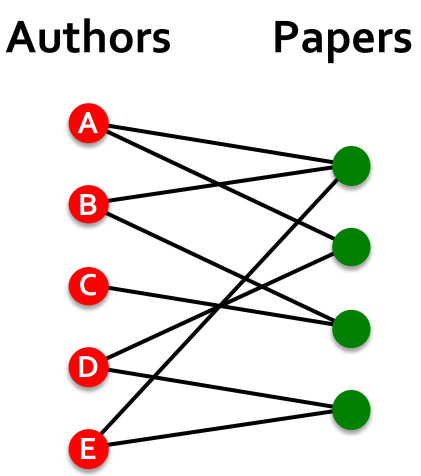
Feature Augmentation on Graphs

Why do we need feature augmentation?

- **(2) Certain structures are hard to learn by GNN**
- Other commonly used augmented features:
  - **Node degree**
  - **Clustering coefficient**
  - **PageRank**
  - **Centrality**
  - **…**
- Any **feature we have introduced in Lecture 2 can be used!**

Add Virtual Nodes / Edges

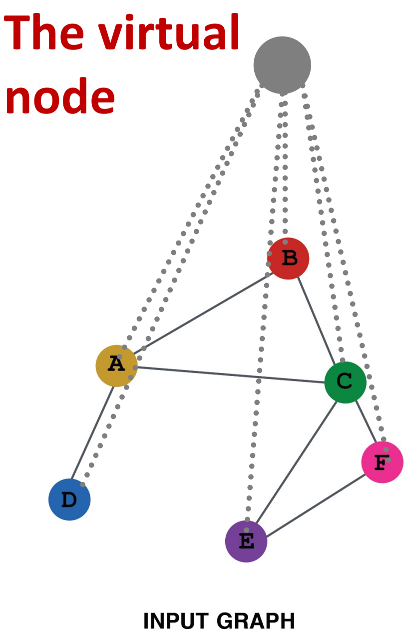
- **Motivation:** Augment sparse graphs
- **(1) Add virtual edges**
  - **Common approach:** Connect 2-hop neighbors via virtual edges
  - **Intuition:** Instead of using adj. matrix A for GNN computation, use $A + A^2$



- **Use cases:** Bipartite graphs
  - Author-to-papers (they authored)
  - 2-hop virtual edges make an author-author collaboration graph

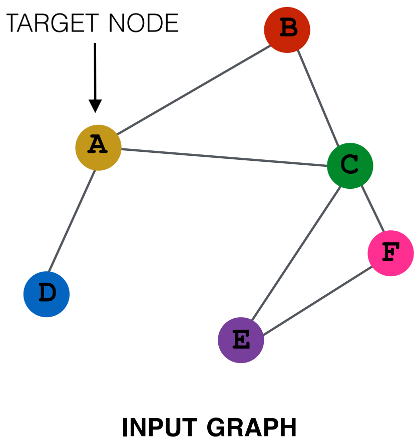
Add Virtual Nodes / Edges

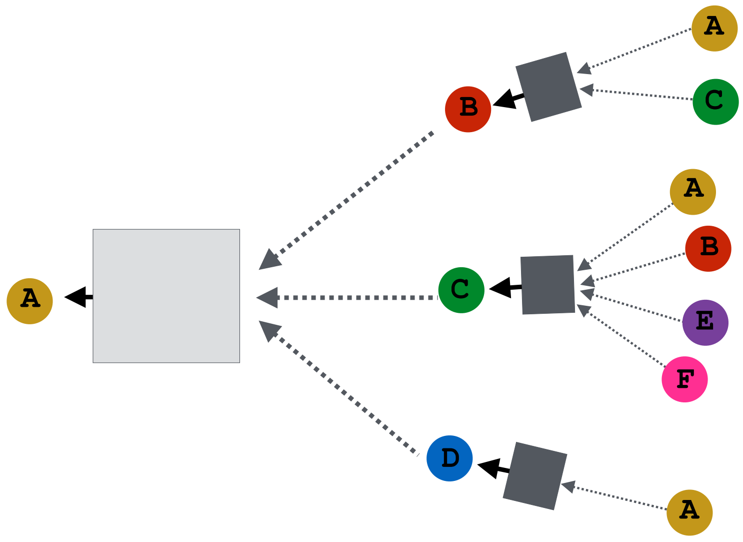
- **Motivation:** Augment sparse graphs
- **(2) Add virtual nodes**
  - The virtual node will connect to all the nodes in the graph
    - Suppose in a sparse graph, two nodes have shortest path distance of 10
    - After adding the virtual node, **all the nodes will have a distance of two**
      - **Node A – Virtual node – Node B**
  - **Benefits:** Greatly **improves message passing in sparse graphs**



Node Neighborhood Sampling

- **Previously:**
  - All the nodes are used for message passing

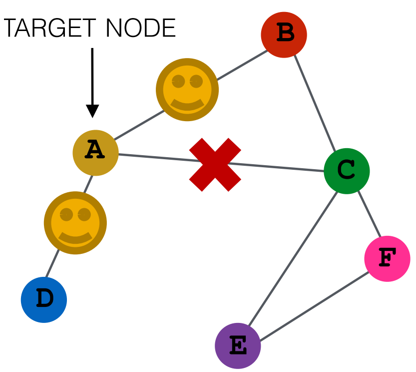




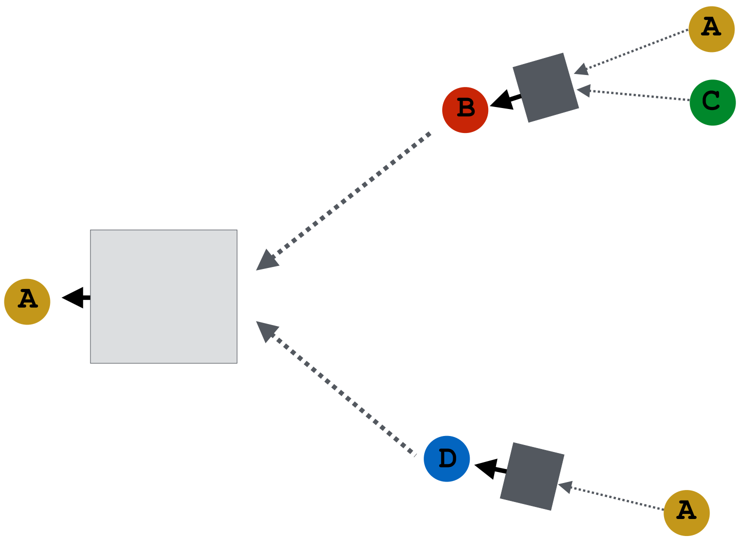
- **New idea:** (Randomly) sample a node's neighborhood for message passing

Neighborhood Sampling Example

- **For example, we can randomly choose 2 neighbors to pass messages in a given layer**
  - Only nodes B and D will pass messages to A

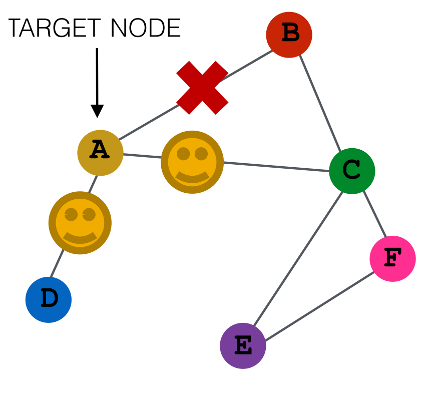


INPUT GRAPH

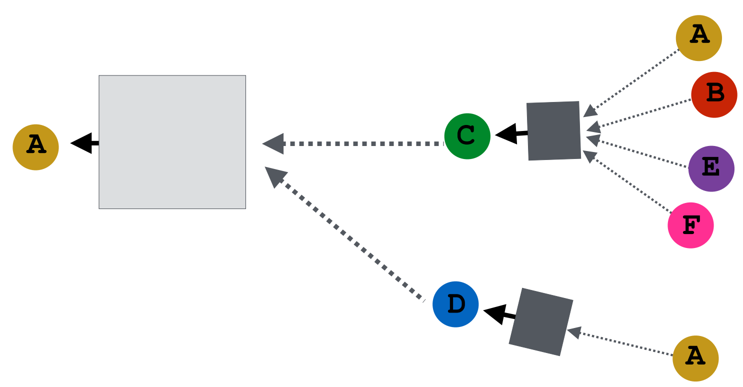


Neighborhood Sampling Example

- **In the next layer when we compute the embeddings, we can sample different neighbors**
  - Only nodes C and D will pass messages to A

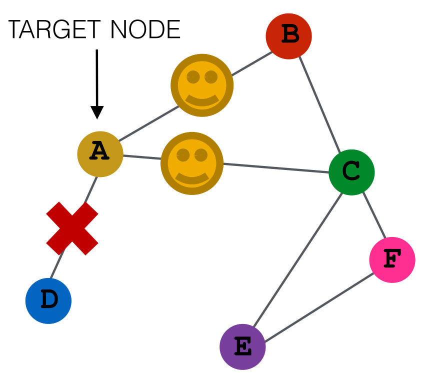


INPUT GRAPH

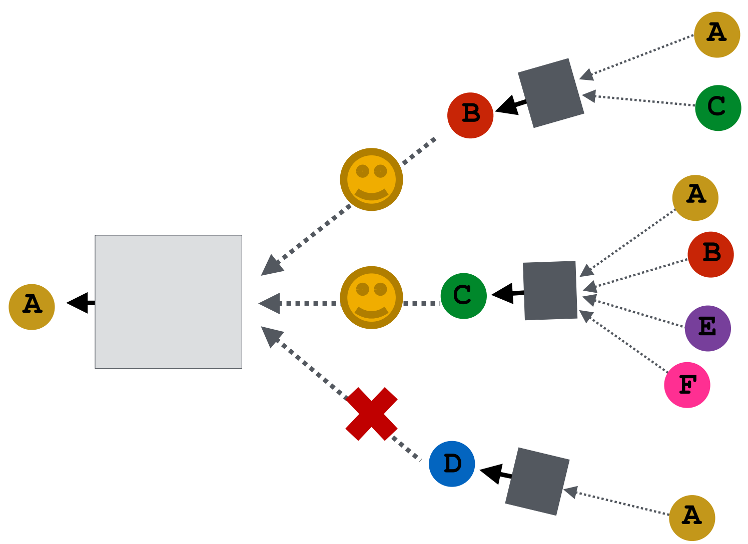


Neighborhood Sampling Example

- **In expectation, we get embeddings similar to the case where all the neighbors are used**
  - **Benefits:** Greatly reduces computational cost
    - **Allows for scaling to large graphs (more about this later)**
  - And in practice it works great!



INPUT GRAPH



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CS224W: Machine Learning with Graphs

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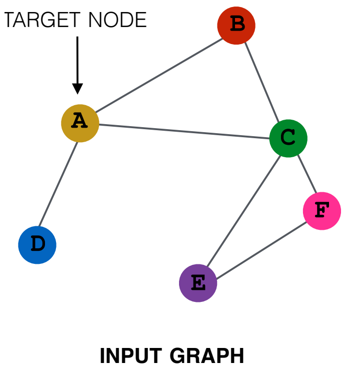
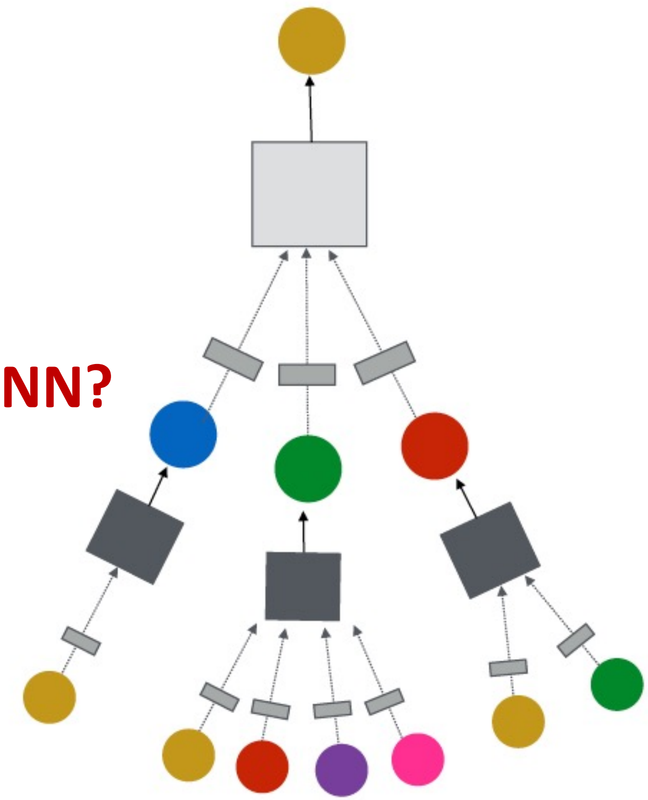
A General GNN Framework (4)



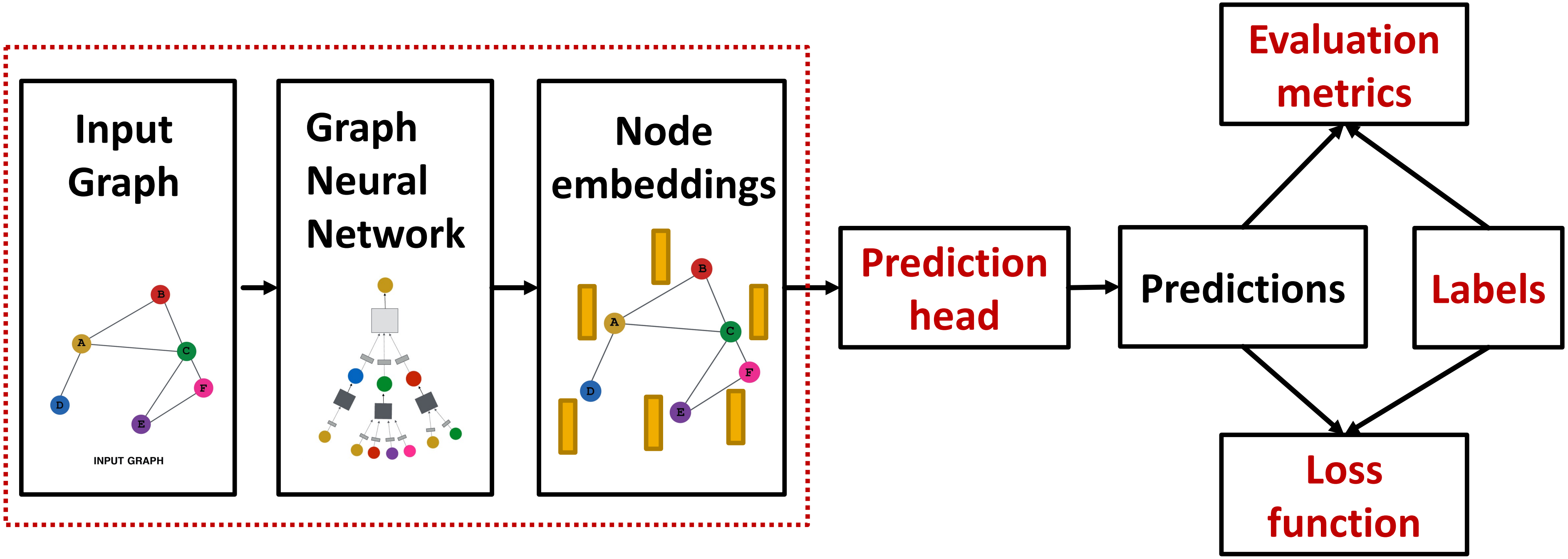
(5) Learning objective



Next: How do we train a GNN?

GNN Training Pipeline

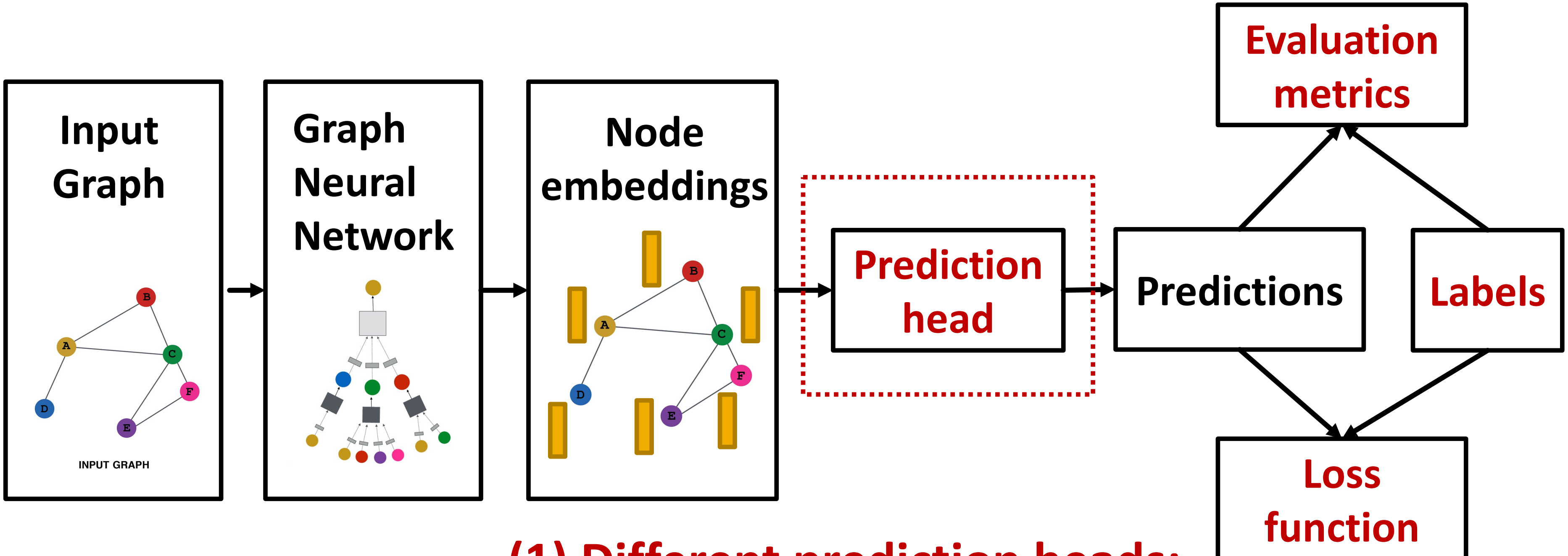
So far what we have covered



Output of a GNN: set of node embeddings

$$\{\mathbf{h}_v^{(L)}, \forall v \in G\}$$

GNN Training Pipeline (1)

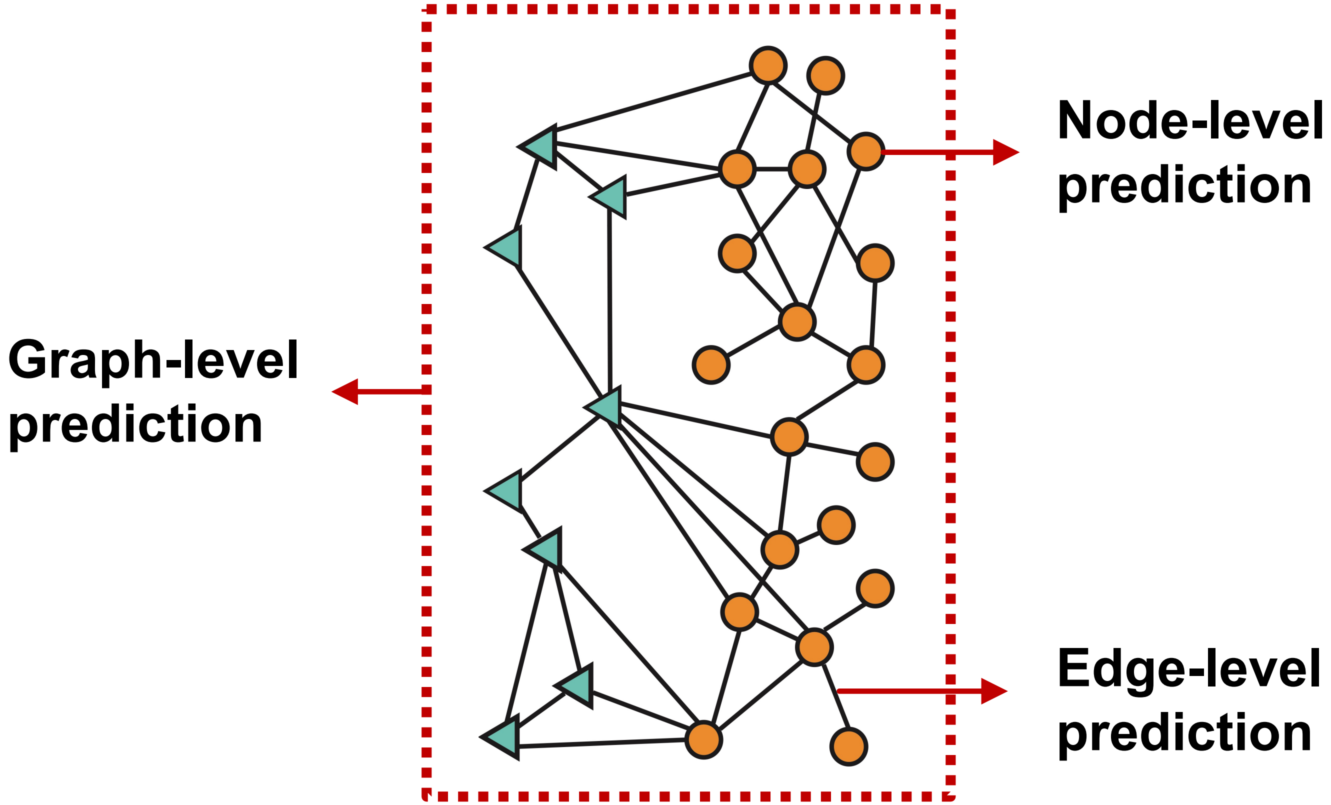


(1) Different prediction heads:

- Node-level tasks
- Edge-level tasks
- Graph-level tasks

GNN Prediction Heads

- **Idea:** Different task levels require different prediction heads

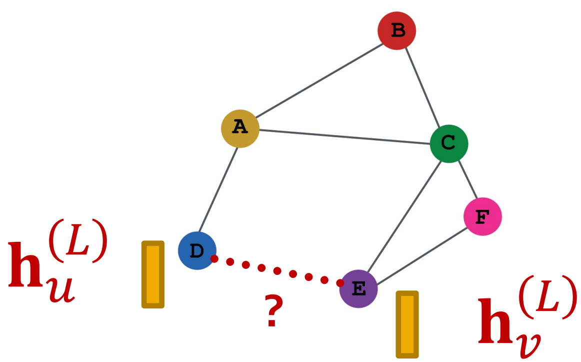


Prediction Heads: Node-level

- **Node-level prediction**: We can directly make prediction using node embeddings!
- After GNN computation, we have d-dim node embeddings: $\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\}$
- Suppose we want to make k-way prediction
  - Classification: classify among k categories
  - Regression: regress on k targets
- $\widehat{\boldsymbol{y}}_{\boldsymbol{v}} = \mathrm{Head}_{\mathrm{node}}(\mathbf{h}_v^{(L)}) = \mathbf{W}^{(H)}\mathbf{h}_v^{(L)}$
  - $\mathbf{W}^{(H)} \in \mathbb{R}^{k*d}$: We map node embeddings from $\mathbf{h}_v^{(L)} \in \mathbb{R}^d$ to $\widehat{\boldsymbol{y}}_v \in \mathbb{R}^k$ so that we can compute the loss

Prediction Heads: Edge-level

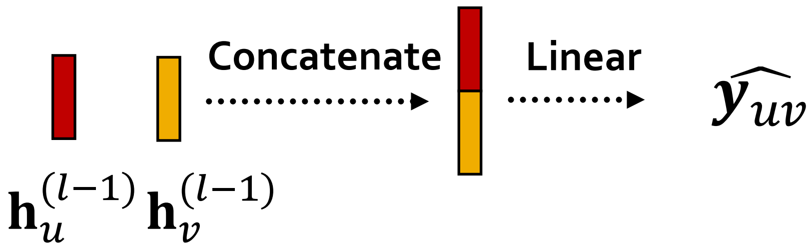
- **Edge-level prediction**: Make prediction using pairs of node embeddings
- Suppose we want to make k-way prediction
- $\widehat{\boldsymbol{y}}_{\boldsymbol{uv}} = \text{Head}_{\text{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$



- What are the options for $\text{Head}_{\text{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$?

Prediction Heads: Edge-level

- **Options for** $\text{Head}_{\text{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$:
- **(1) Concatenation + Linear**
  - We have seen this in graph attention



  - $\widehat{\boldsymbol{y}}_{\boldsymbol{uv}} = \text{Linear}(\text{Concat}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}))$
  - Here $\text{Linear}(\cdot)$ will map $2d$-dimensional embeddings (since we concatenated embeddings) to k-dim embeddings (k-way prediction)

Prediction Heads: Edge-level

- **Options for** $\text{Head}_{\text{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$:
- **(2) Dot product**
  - $\widehat{\boldsymbol{y}}_{\boldsymbol{uv}} = (\mathbf{h}_u^{(L)})^T \mathbf{h}_v^{(L)}$
  - **This approach only applies to 1-way prediction** (e.g., link prediction: predict the existence of an edge)
  - **Applying to $\boldsymbol{k}$-way prediction:**
    - Similar to **multi-head attention**: $\mathbf{W}^{(1)}, \dots, \mathbf{W}^{(k)}$ trainable

$$\widehat{\boldsymbol{y}}_{\boldsymbol{uv}}^{(\mathbf{1})} = (\mathbf{h}_u^{(L)})^T \mathbf{W}^{(1)} \mathbf{h}_v^{(L)}$$

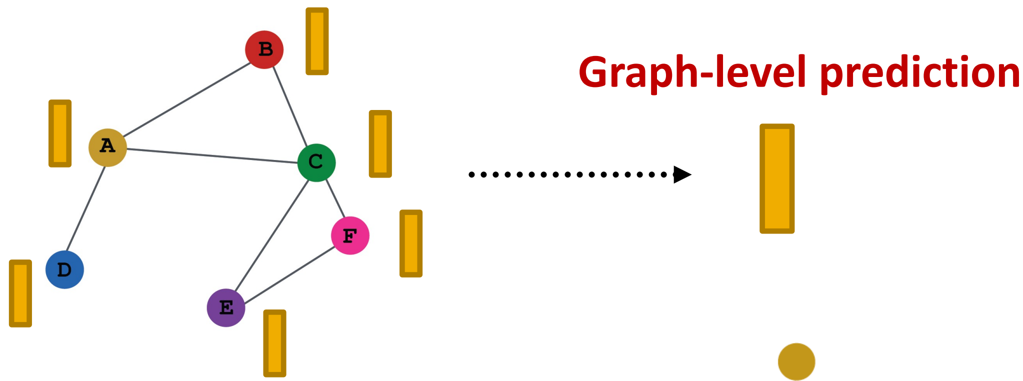
$$\dots$$

$$\widehat{\boldsymbol{y}}_{\boldsymbol{uv}}^{(\boldsymbol{k})} = (\mathbf{h}_u^{(L)})^T \mathbf{W}^{(k)} \mathbf{h}_v^{(L)}$$

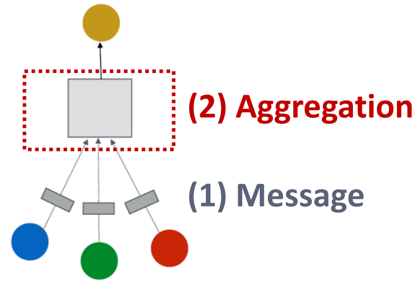
$$\widehat{\boldsymbol{y}}_{uv} = \text{Concat}(\widehat{\boldsymbol{y}}_{\boldsymbol{uv}}^{(\mathbf{1})}, \dots, \widehat{\boldsymbol{y}}_{\boldsymbol{uv}}^{(\boldsymbol{k})}) \in \mathbb{R}^k$$

Prediction Heads: Graph-level

- **Graph-level prediction**: Make prediction using all the node embeddings in our graph
- Suppose we want to make k-way prediction
- $\hat{\boldsymbol{y}}_G = \text{Head}_{\text{graph}}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\})$



- $\text{Head}_{\text{graph}}(\cdot)$ is similar to $\text{AGG}(\cdot)$ in a GNN layer!



K. Xu*, W. Hu*, J. Leskovec, S. Jegelka. How Powerful Are Graph Neural Networks, ICLR 2019

Prediction Heads: Graph-level

- Options for $\mathrm{Head}_{\mathrm{graph}}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\})$
- **(1) Global mean pooling**

$$\widehat{\boldsymbol{y}}_G = \mathrm{Mean}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\})$$

- **(2) Global max pooling**

$$\widehat{\boldsymbol{y}}_G = \mathrm{Max}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\})$$

- **(3) Global sum pooling**

$$\widehat{\boldsymbol{y}}_G = \mathrm{Sum}(\{\mathbf{h}_v^{(L)} \in \mathbb{R}^d, \forall v \in G\})$$

- These options work great for small graphs
- **Can we do better for large graphs?**

Issue of Global Pooling

- **Issue:** Global pooling over a (large) graph will lose information
- **Toy example:** we use 1-dim node embeddings
  - Node embeddings for G_1: $\{-1, -2, 0, 1, 2\}$
  - Node embeddings for G_2: $\{-10, -20, 0, 10, 20\}$
  - Clearly G_1 and G_2 have very different node embeddings → Their structures should be different
- **If we do global sum pooling:**
  - **Prediction for** G_1: $\hat{y}_G = \text{Sum}(\{-1, -2, 0, 1, 2\}) = 0$
  - **Prediction for** G_2: $\hat{y}_G = \text{Sum}(\{-10, -20, 0, 10, 20\}) = 0$
  - We cannot differentiate G_1 and G_2!

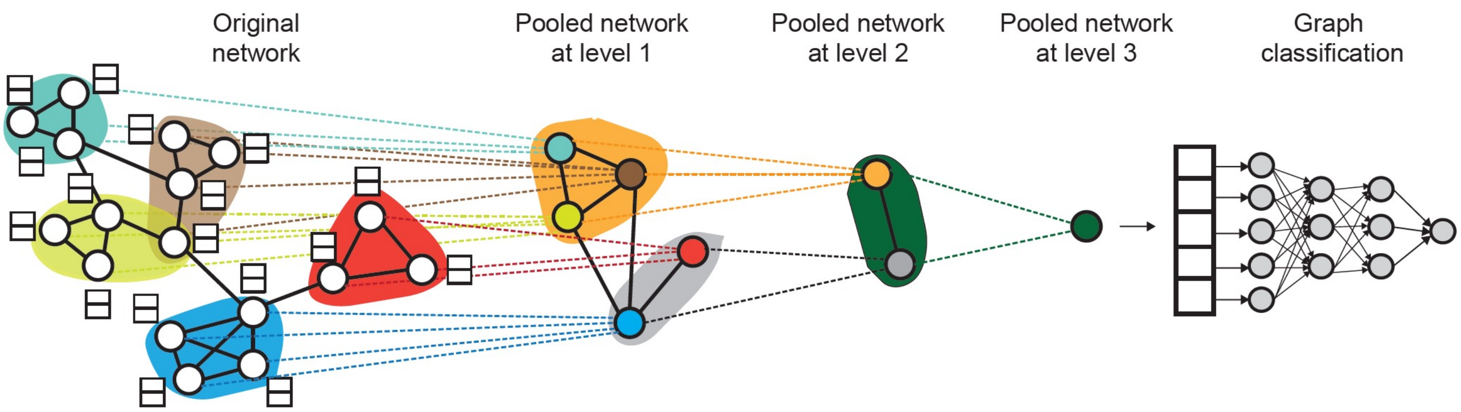
Hierarchical Global Pooling

- **A solution:** Let's aggregate all the node embeddings **hierarchically**
  - **Toy example:** We will aggregate via $\mathrm{ReLU}\big(\mathrm{Sum}(\cdot)\big)$
    - We first separately aggregate the first 2 nodes and last 3 nodes
    - Then we aggregate again to make the 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:** $\hat{y}_G = \mathrm{ReLU}\big(\mathrm{Sum}(\{y_a, y_b\})\big) = \mathbf{3}$
  - 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:** $\hat{y}_G = \mathrm{ReLU}\big(\mathrm{Sum}(\{y_a, y_b\})\big) = \mathbf{30}$

Now we can differentiate G_1 and G_2 !

Hierarchical Pooling In Practice

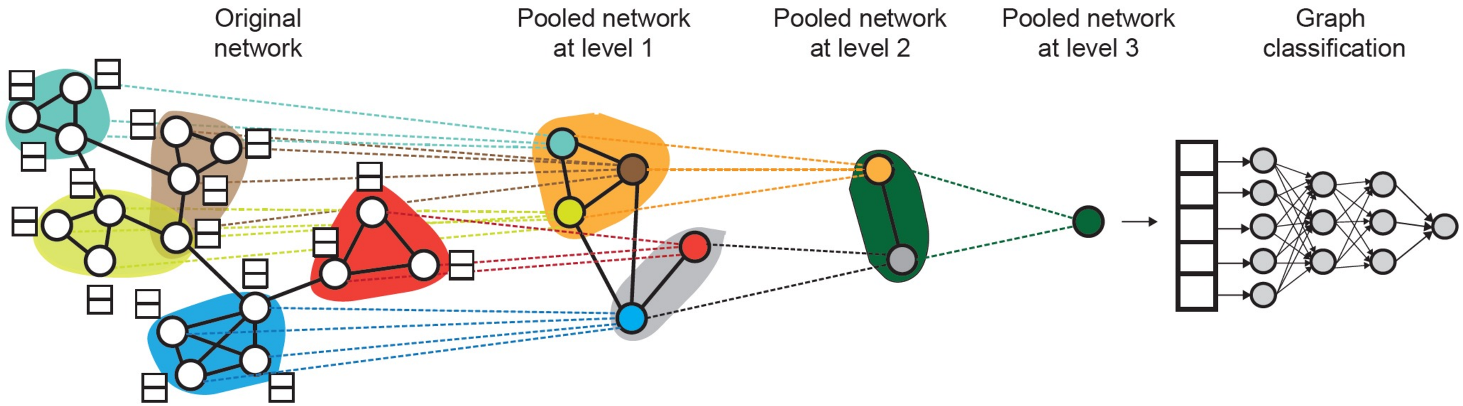
- **DiffPool idea:**
  - **Hierarchically pool node embeddings**



  - **Leverage 2 independent GNNs at each level**
    - **GNN A:** Compute node embeddings
    - **GNN B:** Compute the cluster that a node belongs to
  - **GNNs A and B at each level can be executed in parallel**

Hierarchical Pooling In Practice

- **DiffPool idea:**



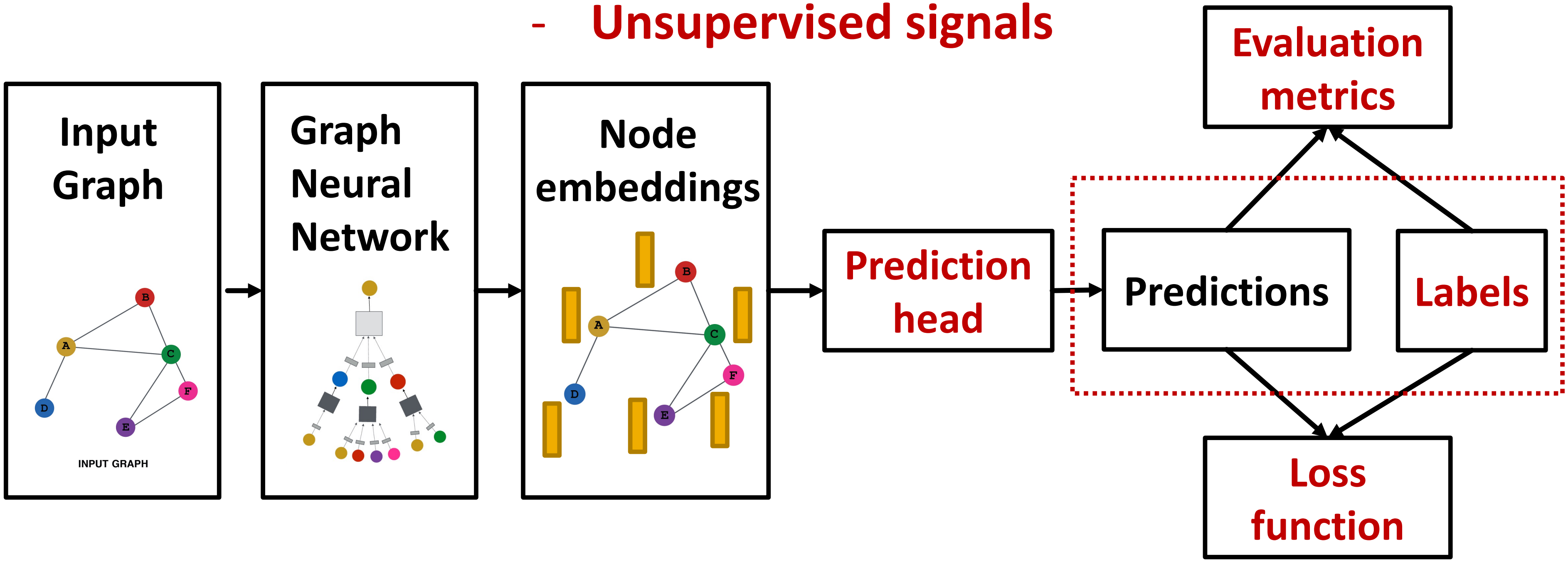
  - **For each Pooling layer**
    - Use clustering assignments from **GNN B** to aggregate node embeddings generated by **GNN A**
    - Create a **single new node** for each cluster, maintaining edges between clusters to generated a new **pooled** network
  - **Jointly train GNN A and GNN B**

Stanford CS224W: Training Graph Neural Networks

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

GNN Training Pipeline (2)

(2) Where does ground-truth come from?
- **Supervised labels**
- **Unsupervised signals**



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: predict if two nodes are connected
- **Sometimes the differences are blurry**
  - We still have "supervision" in unsupervised learning
    - E.g., train a GNN to predict node clustering coefficient
  - An alternative name for "**unsupervised**" is "**self-supervised**"

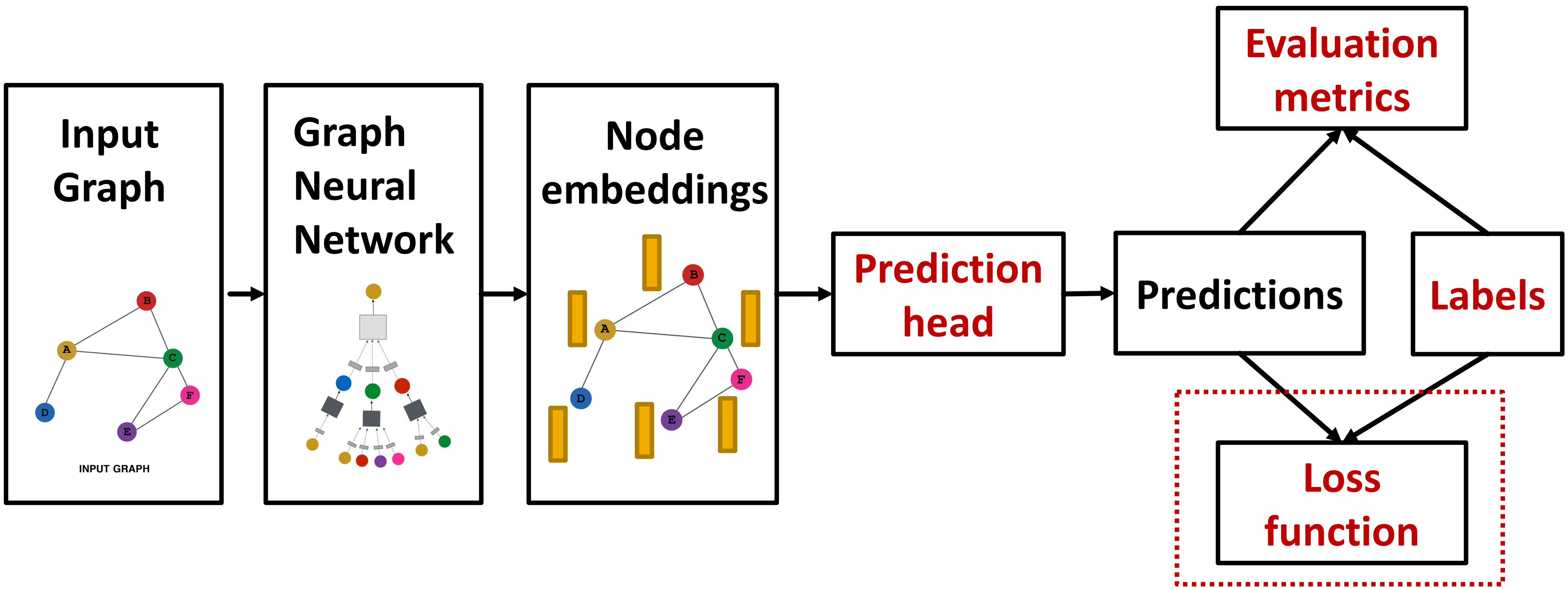
Supervised Labels on Graphs

- **Supervised labels come from the specific use cases**. For example:
  - **Node labels y_v:** in a citation network, which subject area does a node belong to
  - **Edge labels y_{uv}:** in a transaction network, whether an edge is fraudulent
  - **Graph labels y_G:** among molecular graphs, the drug likeness of graphs
- **Advice:** Reduce your task to node / edge / graph labels, since they are easy to work with
  - **E.g.,** we knew some nodes form a cluster. We can treat the cluster that a node belongs to as a **node label**

Unsupervised Signals on Graphs

- **The problem:** sometimes **we only have a graph, without any external labels**
- **The solution:** "self-supervised learning", we can find supervision signals within the graph.
  - For example, we can **let GNN predict the following:**
  - **Node-level y_v.** Node statistics: such as clustering coefficient, PageRank, …
  - **Edge-level y_{uv}.** Link prediction: hide the edge between two nodes, predict if there should be a link
  - **Graph-level y_G.** Graph statistics: for example, predict if two graphs are isomorphic
  - **These tasks do not require any external labels!**

GNN Training Pipeline (3)



(3) How do we compute the final loss?
- **Classification loss**
- **Regression loss**

Settings for GNN Training

- **The setting:** We have N data points
  - Each data point can be a node/edge/graph
  - **Node-level**: prediction $\widehat{\boldsymbol{y}}_v^{(i)}$, label $\boldsymbol{y}_v^{(i)}$
  - **Edge-level**: prediction $\widehat{\boldsymbol{y}}_{uv}^{(i)}$, label $\boldsymbol{y}_{uv}^{(i)}$
  - **Graph-level**: prediction $\widehat{\boldsymbol{y}}_G^{(i)}$, label $\boldsymbol{y}_G^{(i)}$
  - We will use prediction $\widehat{\boldsymbol{y}}^{(i)}$, label $\boldsymbol{y}^{(i)}$ to refer **predictions at all levels**

Classification or Regression

- **Classification**: labels $\boldsymbol{y}^{(i)}$ with discrete value
  - E.g., Node classification: which category does a node belong to
- **Regression**: labels $\boldsymbol{y}^{(i)}$ with continuous value
  - E.g., predict the drug likeness of a molecular graph
- GNNs can be applied to both settings
- **Differences: loss function & evaluation metrics**

Classification Loss

- As discussed in lecture 6, **cross entropy (CE)** is a very common loss function in classification
- K-way prediction for i-th data point:

$$\mathrm{CE}\left(\underbrace{\boldsymbol{y}^{(i)}}_{\text{Label}}, \underbrace{\widehat{\boldsymbol{y}}^{(i)}}_{\text{Prediction}}\right) = -\sum_{j=1}^{K} \boldsymbol{y}_j^{(i)} \log\left(\widehat{\boldsymbol{y}}_j^{(i)}\right)$$

i-th data point

j-th class

where:

E.g.

0	0	1	0	0

$\boldsymbol{y}^{(i)} \in \mathbb{R}^K$ = one-hot label encoding

$\widehat{\boldsymbol{y}}^{(i)} \in \mathbb{R}^K$ = prediction after $\mathrm{Softmax}(\cdot)$

E.g.

0.1	0.3	0.4	0.1	0.1

- Total loss over all N training examples

$$\mathrm{Loss} = \sum_{i=1}^{N} \mathrm{CE}\left(\boldsymbol{y}^{(i)}, \widehat{\boldsymbol{y}}^{(i)}\right)$$

Regression Loss

- For regression tasks we often use **Mean Squared Error (MSE)** a.k.a. **L2 loss**
- K-way regression for data point (i):

$$\mathrm{MSE}\left(\boldsymbol{y}^{(i)}, \widehat{\boldsymbol{y}}^{(i)}\right) = \sum_{j=1}^{K} \left(\boldsymbol{y}_j^{(i)} - \widehat{\boldsymbol{y}}_{\boxed{j}}^{\boxed{(i)}}\right)^2$$

***i*-th data point**

***j*-th target**

where:

E.g.

1.4	2.3	1.0	0.5	0.6

$\boldsymbol{y}^{(i)} \in \mathbb{R}^k$ = Real valued vector of targets

$\widehat{\boldsymbol{y}}^{(i)} \in \mathbb{R}^k$ = Real valued vector of predictions

E.g.

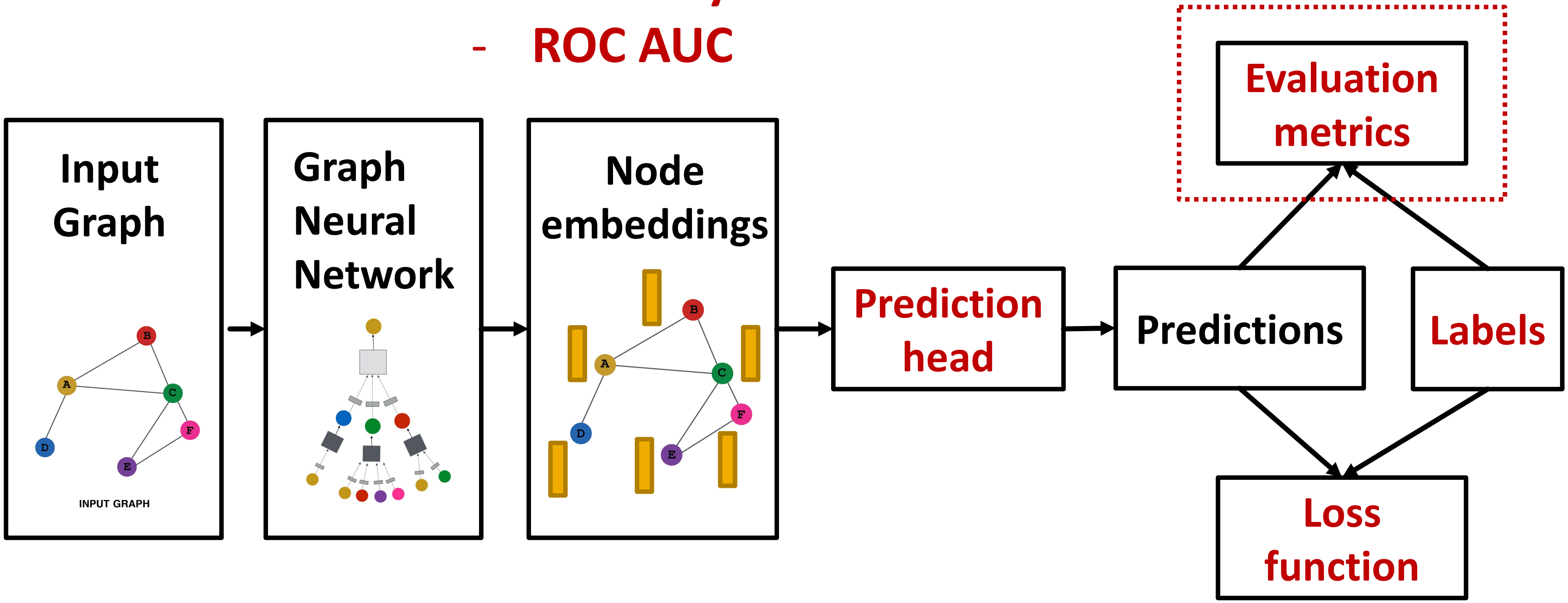
0.9	2.8	2.0	0.3	0.8

- Total loss over all N training examples

$$\mathrm{Loss} = \sum_{i=1}^{N} \mathrm{MSE}\left(\boldsymbol{y}^{(i)}, \widehat{\boldsymbol{y}}^{(i)}\right)$$

GNN Training Pipeline (4)

(4) How do we measure the success of a GNN?
- **Accuracy**
- **ROC AUC**



Evaluation Metrics: Regression

- **We use standard evaluation metrics for GNN**
  - (Content below can be found in any ML course)
  - In practice we will use sklearn for implementation
  - Suppose we make predictions for N data points
- **Evaluate regression tasks on graphs:**
  - **Root mean square error (RMSE)**

$$\sqrt{\sum_{i=1}^{N} \frac{(\boldsymbol{y}^{(i)} - \widehat{\boldsymbol{y}}^{(i)})^2}{N}}$$

  - **Mean absolute error (MAE)**

$$\frac{\sum_{i=1}^{N} \left| \boldsymbol{y}^{(i)} - \widehat{\boldsymbol{y}}^{(i)} \right|}{N}$$

Evaluation Metrics: Classification

- **Evaluate classification tasks on graphs:**
- **(1) Multi-class classification**
  - **We simply report the accuracy**

$$\frac{1\left[\operatorname{argmax}\left(\widehat{\boldsymbol{y}}^{(i)}\right) = \boldsymbol{y}^{(i)}\right]}{N}$$

- **(2) Binary classification**
  - Metrics sensitive to classification threshold
    - **Accuracy**
    - **Precision / Recall**
    - If the range of prediction is $[0,1]$, we will use 0.5 as threshold
  - Metric Agnostic to classification threshold
    - **ROC AUC**

Metrics for Binary Classification

- **Accuracy:**

$$\frac{\mathrm{TP}+\mathrm{TN}}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}}=\frac{\mathrm{TP}+\mathrm{TN}}{|\mathrm{Dataset}|}$$

- **Precision (P):**

$$\frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FP}}$$

- **Recall (R):**

$$\frac{\mathrm{TP}}{\mathrm{TP}+\mathrm{FN}}$$

- **F1-Score:**

$$\frac{2\mathrm{P}*\mathrm{R}}{\mathrm{P}+\mathrm{R}}$$

Confusion matrix

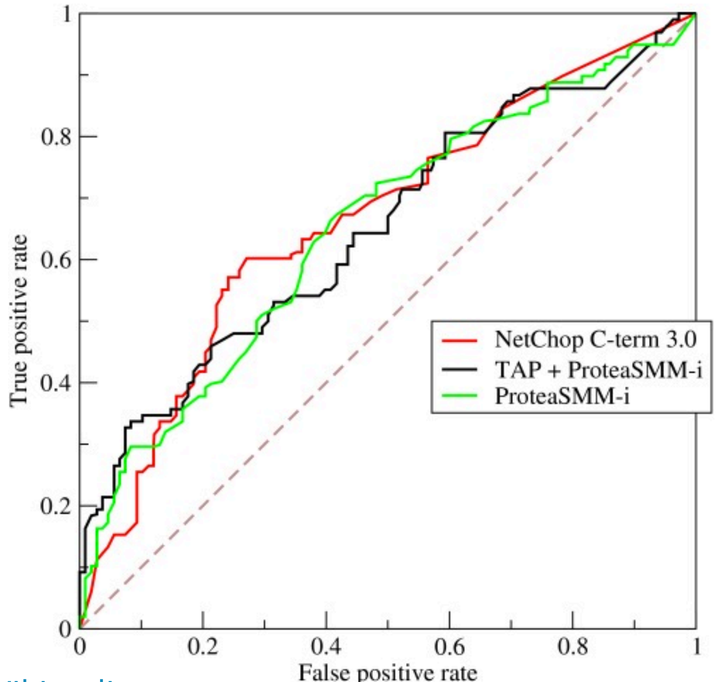
	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

[Sklearn Classification Report]

(4) Evaluation Metrics

- **ROC Curve:** Captures the tradeoff in TPR and FPR **as the classification threshold is varied for a binary classifier.**

TPR



FPR

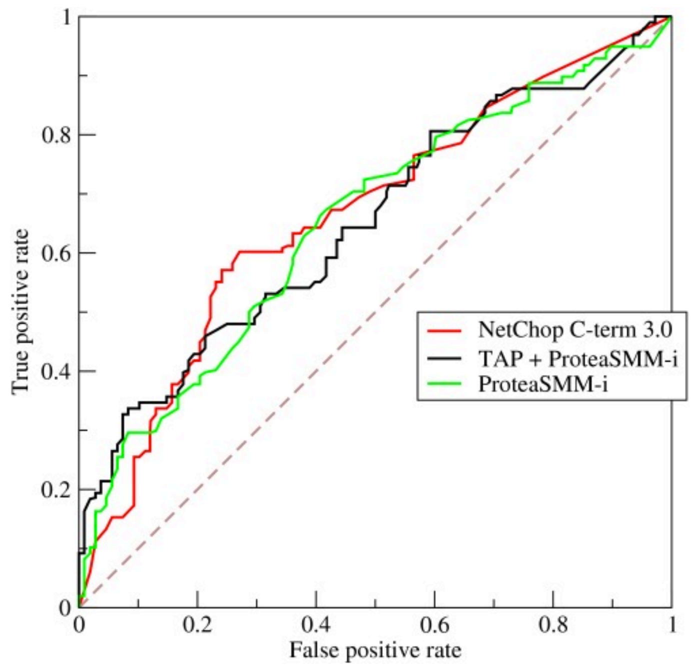
Image Credit: Wikipedia

$$\text{TPR} = \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

Note: the dashed line represents **performance of a random classifier**

(4) Evaluation Metrics



Content Credit: [Wikipedia]

- **ROC AUC:** **Area under the ROC Curve.**
- **Intuition:** The probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one

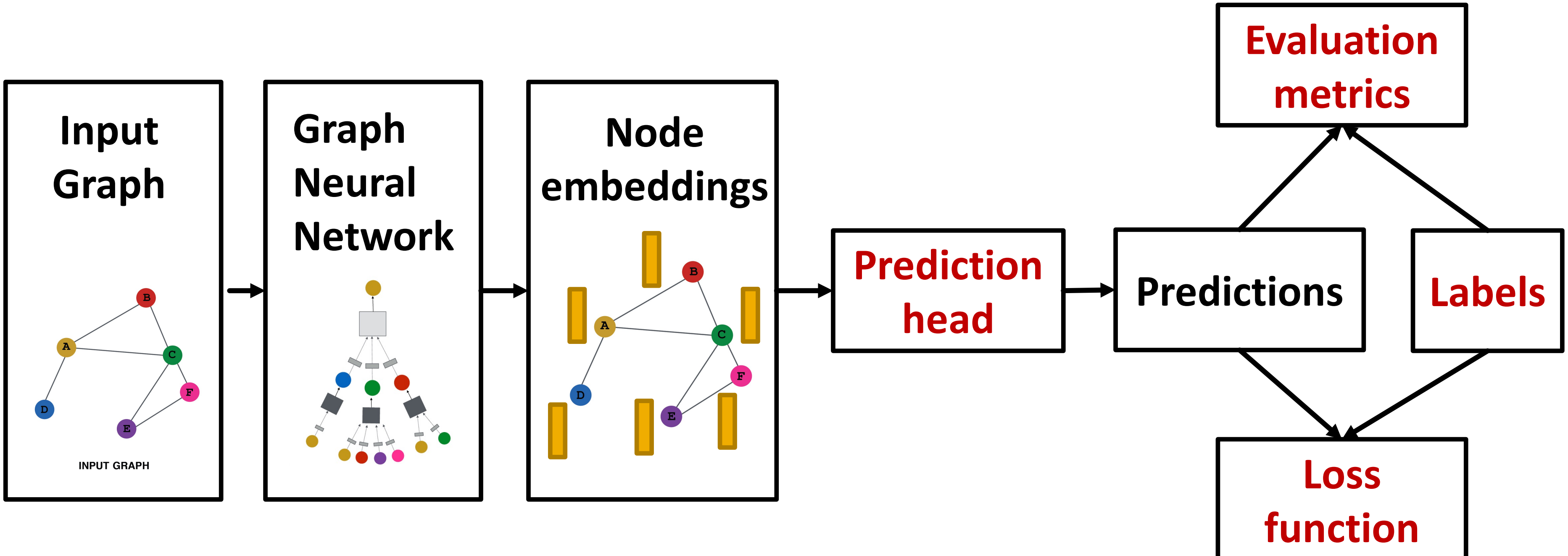
Stanford CS224W: Setting-up GNN Prediction Tasks

CS224W: Machine Learning with Graphs

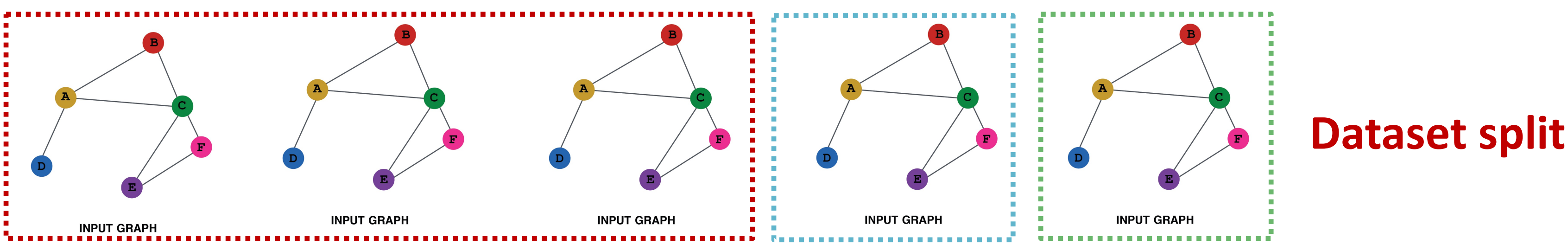
Jure Leskovec, Stanford University

http://cs224w.stanford.edu

GNN Training Pipeline (5)



(5) How do we split our dataset into train / validation / test set?

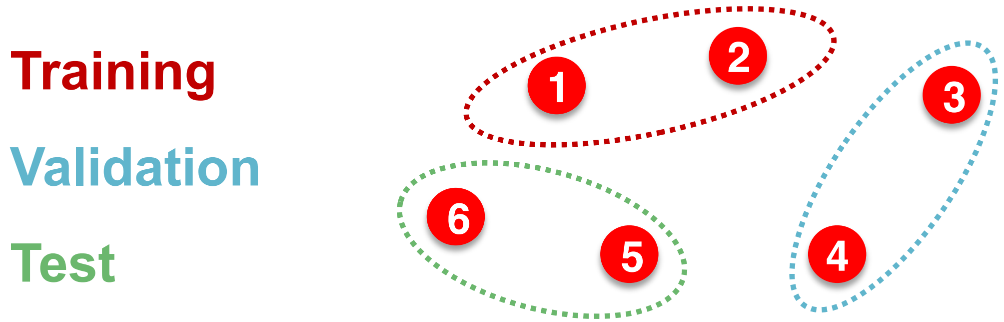


Dataset Split: Fixed / Random Split

- **Fixed split:** We will split our dataset **once**
  - **Training set**: used for optimizing GNN parameters
  - **Validation set**: develop model/hyperparameters
  - **Test set**: held out until we report final performance
- **A concern:** sometimes we cannot guarantee that the test set will really be held out
- **Random split:** we will **randomly split** our dataset into training / validation / test
  - We report **average performance over different random seeds**

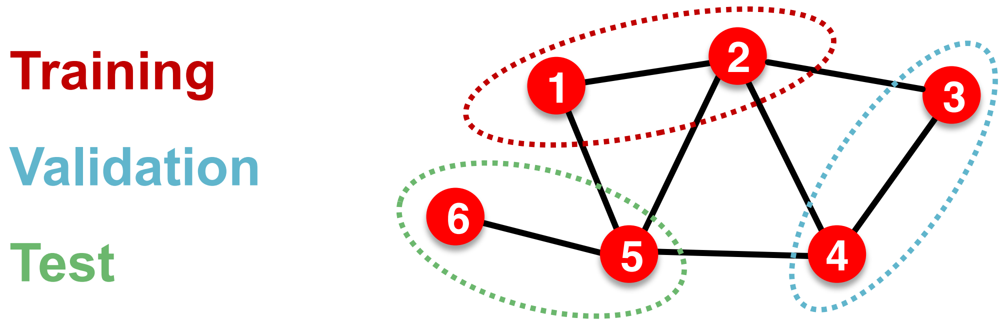
Why Splitting Graphs is Special

- **Suppose we want to split an image dataset**
  - **Image classification: Each data point is an image**
  - Here **data points are independent**
    - **Image 5 will not affect our prediction on image 1**



Why Splitting Graphs is Special

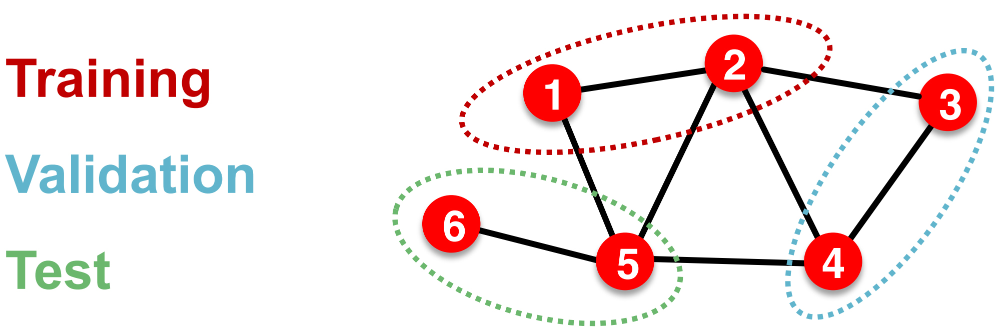
- **Splitting a graph dataset is different!**
  - **Node classification: Each data point is a node**
  - Here **data points are NOT independent**
    - **Node 5 will affect our prediction on node 1,** because it will participate in message passing → affect node 1's embedding



- **What are our options?**

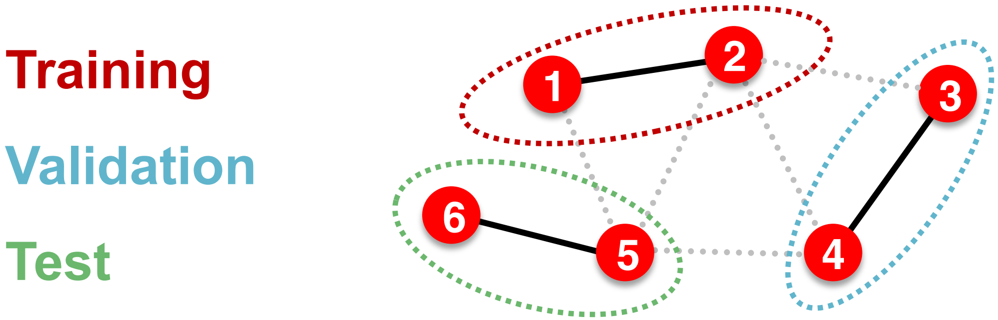
Why Splitting Graphs is Special

- **Solution 1 (Transductive setting): The input graph can be observed in all the dataset splits (training, validation and test set).**
- **We will only split the (node) labels**
  - **At training time**, we compute embeddings **using the entire graph**, and train **using node 1&2's labels**
  - **At validation time**, we compute embeddings **using the entire graph**, and **evaluate on node 3&4's labels**



Why Splitting Graphs is Special

- **Solution 2 (Inductive setting): We break the edges between splits to get multiple graphs**
  - **Now we have 3 graphs that are independent. Node 5 will not affect our prediction on node 1 any more**
  - **At training time**, we compute embeddings **using the graph over node 1&2**, and train **using node 1&2's labels**
  - **At validation time**, we compute embeddings **using the graph over node 3&4**, and **evaluate on node 3&4's labels**

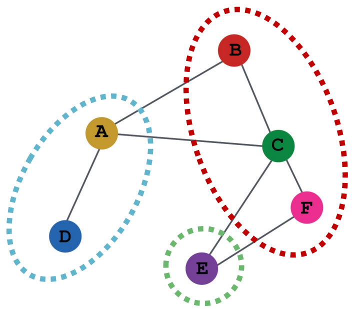


Transductive / Inductive Settings

- **Transductive setting:** training / validation / test sets are **on the same graph**
  - The **dataset consists of one graph**
  - **The entire graph can be observed in all dataset splits, we only split the labels**
  - Only applicable to **node / edge** prediction tasks
- **Inductive setting:** training / validation / test sets are **on different graphs**
  - The **dataset consists of multiple graphs**
  - Each split can **only observe the graph(s) within the split**. A successful model should **generalize to unseen graphs**
  - Applicable to **node / edge / graph** tasks

Example: Node Classification

- **Transductive** node classification
  - **All the splits can observe the entire graph structure**, but can only observe the labels of their respective nodes

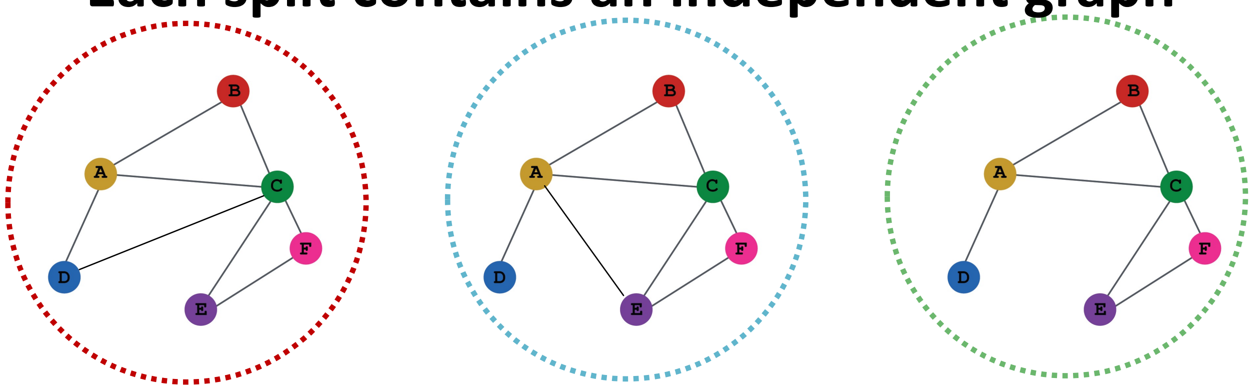


Training

Validation

Test

- **Inductive** node classification
  - Suppose we have a dataset of 3 graphs
  - **Each split contains an independent graph**



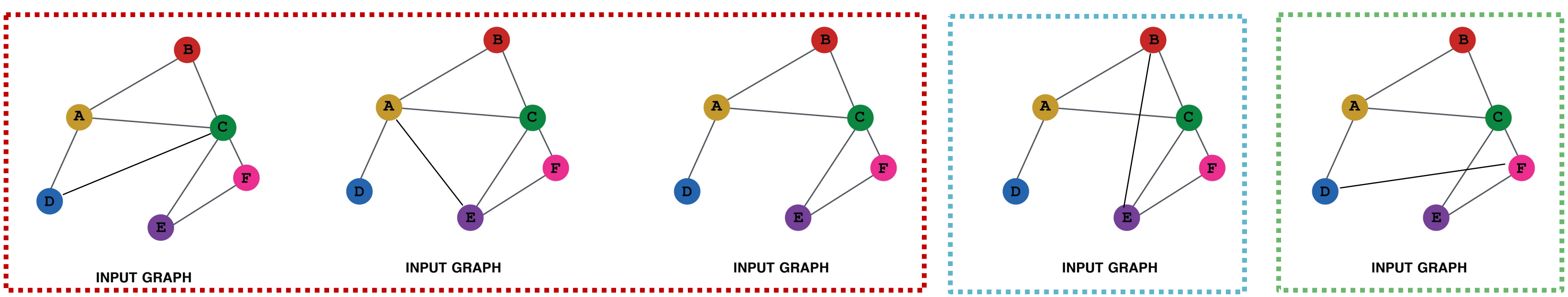
Training

Validation

Test

Example: Graph Classification

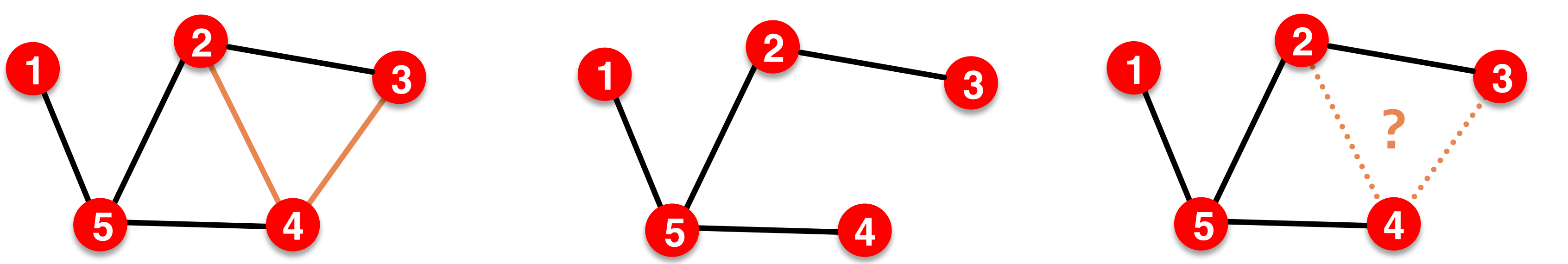
- Only the **inductive setting** is well defined for **graph classification**
  - Because **we have to test on unseen graphs**
  - Suppose we have a dataset of 5 graphs. Each split will contain independent graph(s).



Training **Validation** **Test**

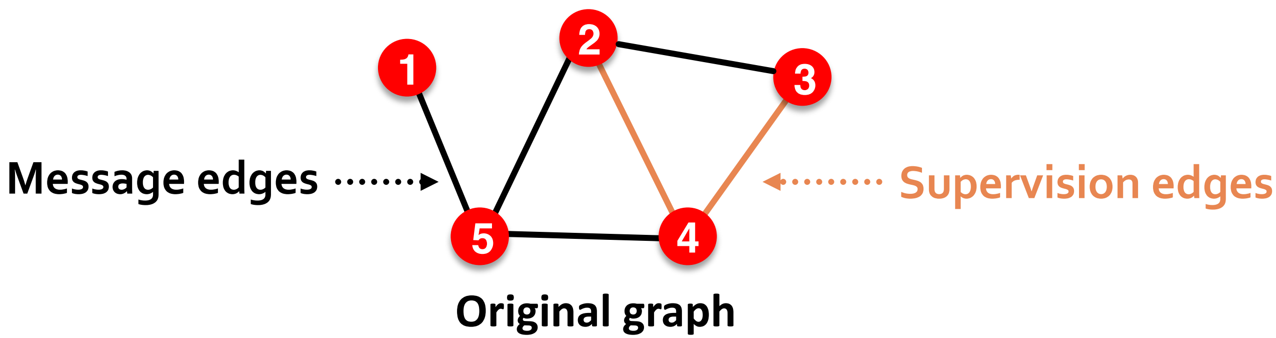
Example: Link Prediction

- **Goal of link prediction: predict missing edges**
- **Setting up link prediction is tricky:**
  - Link prediction is an unsupervised / self-supervised task. We need to **create the labels** and **dataset splits** on our own
  - Concretely, we need to **hide some edges from the GNN** and the **let the GNN predict if the edges exist**



Original graph **Input graph to GNN** **Predictions made by GNN**

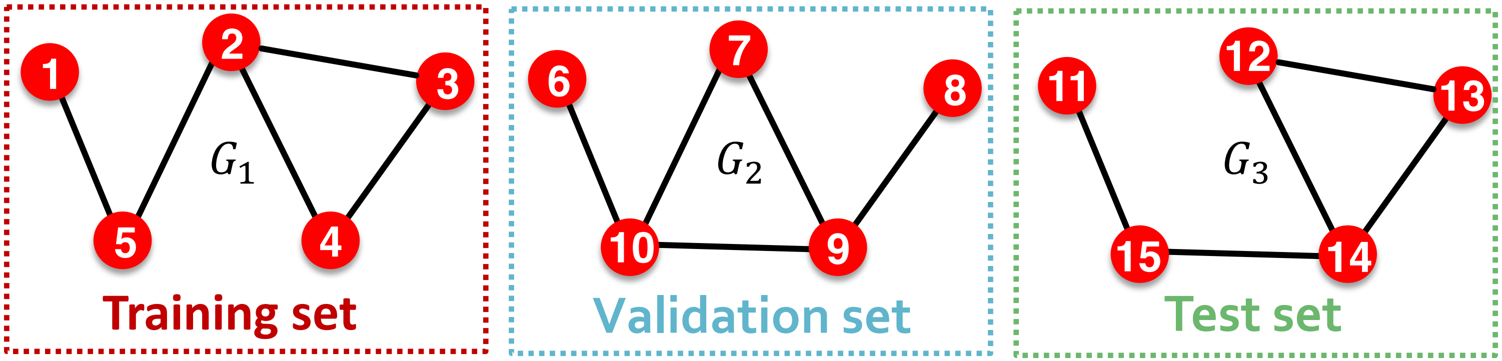
Setting up Link Prediction



- For link prediction, we will split edges twice
- **Step 1:** Assign 2 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 are used as supervision for edge predictions made by the model, will not be fed into GNN!

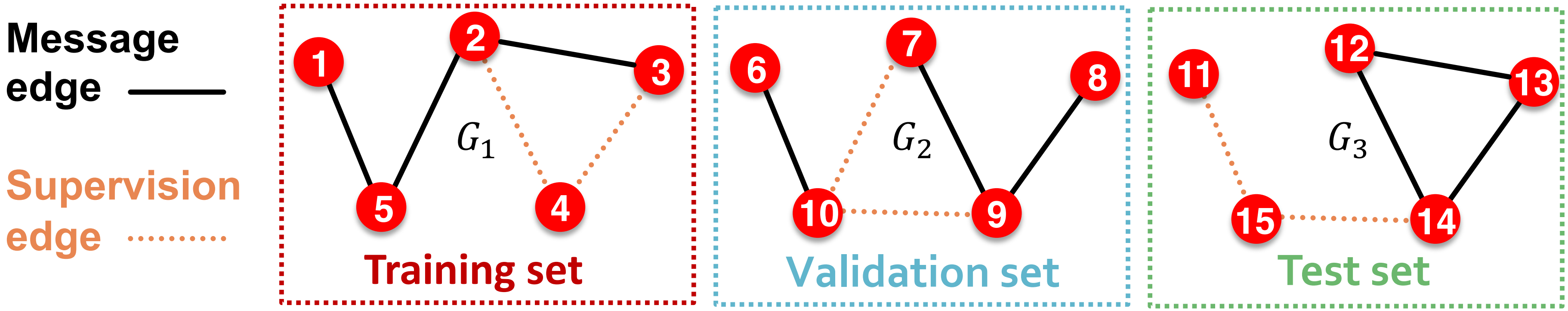
Setting up Link Prediction

- **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**



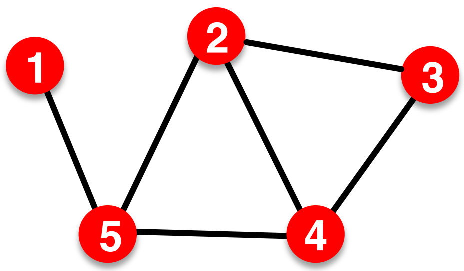
Setting up Link Prediction

- **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** or **val** or **test** set, **each graph will have 2 types of edges: message edges** + **supervision edges**
    - **Supervision edges** are not the input to GNN



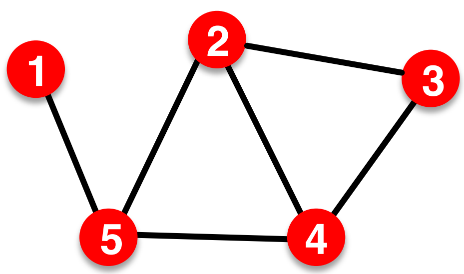
Setting up Link Prediction

- **Option 2: Transductive link prediction split:**
  - **This is the default setting when people talk about link prediction**
  - **Suppose we have a dataset of 1 graph**



Setting up Link Prediction

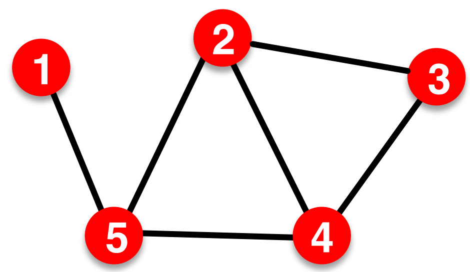
- **Option 2: Transductive link prediction split:**
  - **By definition of "transductive", the entire graph can be observed in all dataset splits**
    - **But since edges are both part of graph structure and the supervision, we need to hold out validation / test edges**
    - **To train the training set, we further need to hold out supervision edges for the training set**



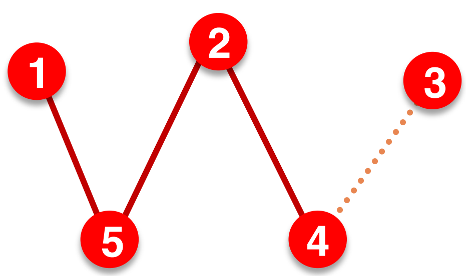
- **Next:** we will show the exact settings

Setting up Link Prediction

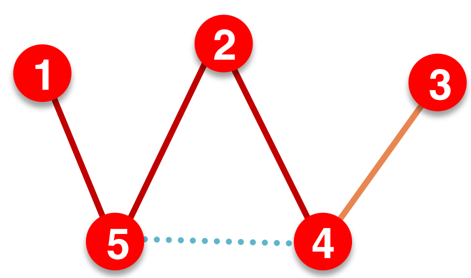
- **Option 2: Transductive link prediction split:**



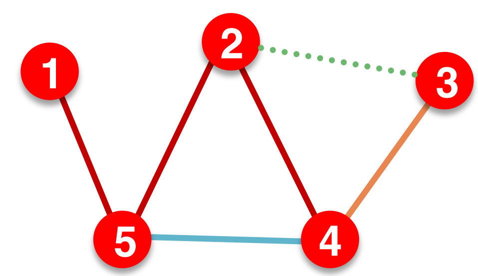
The original graph



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



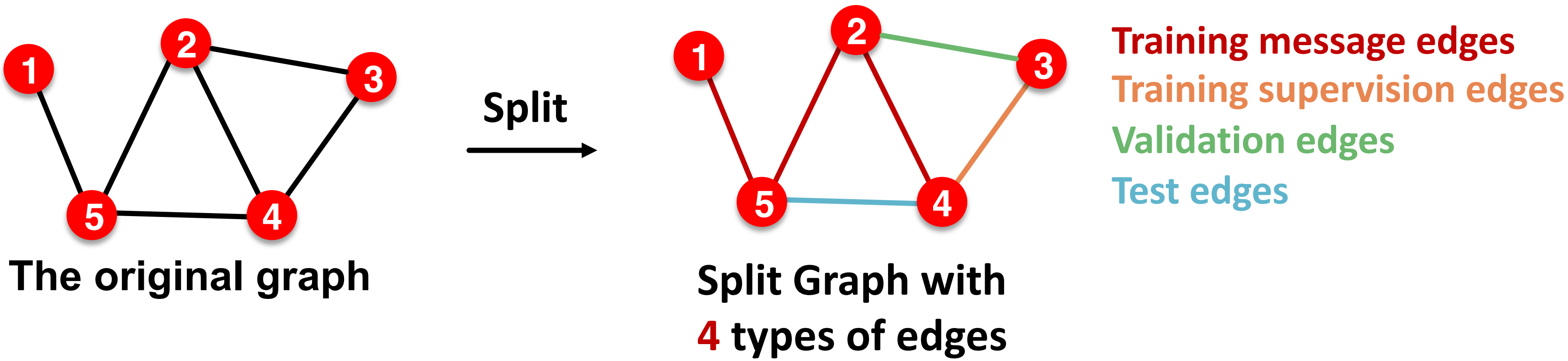
(2) At validation time:
Use **training message edges & training supervision edges** to predict **validation edges**



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

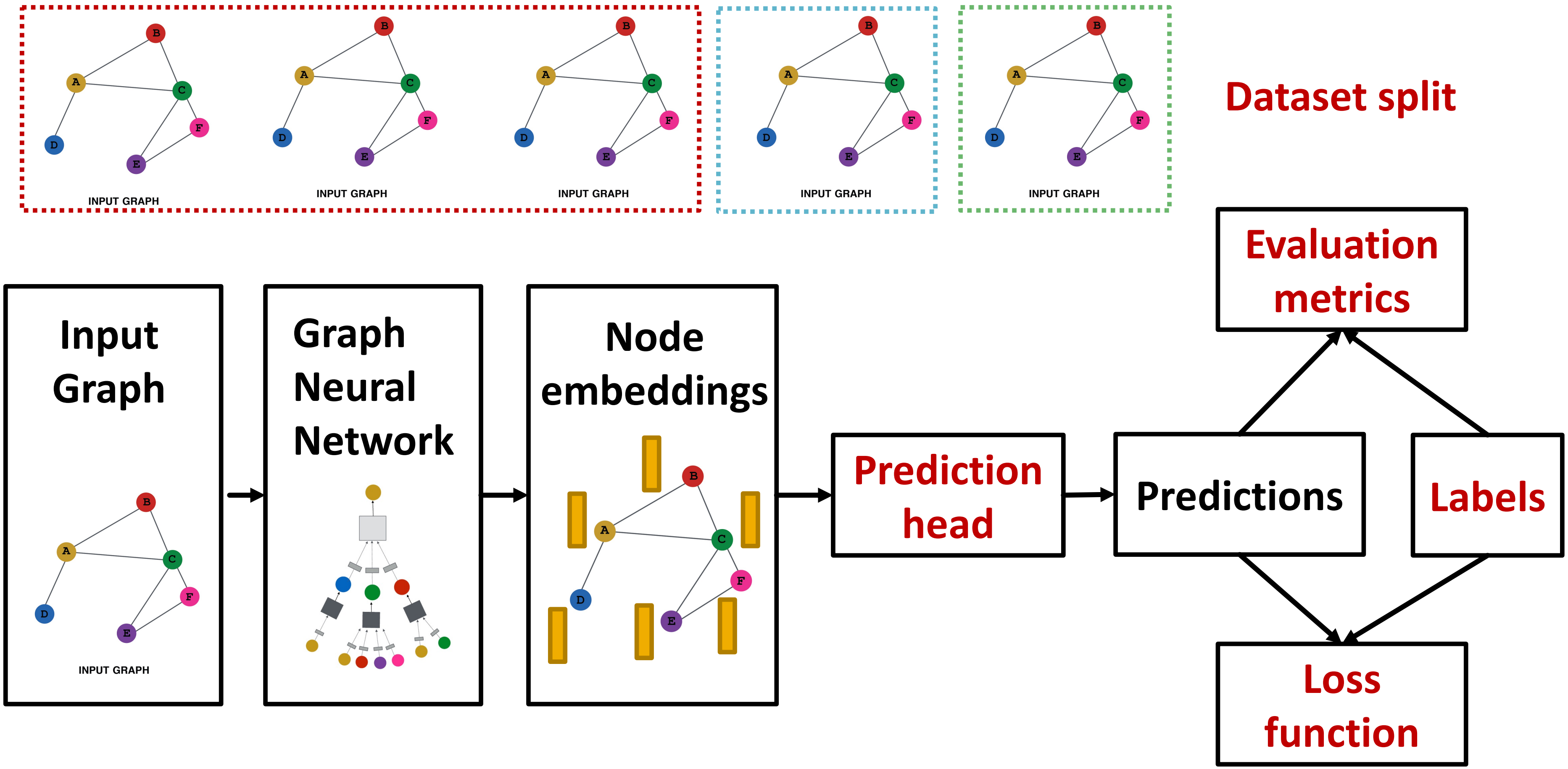
Setting up Link Prediction

- **Summary: Transductive link prediction split:**



- **Note:** Link prediction settings are tricky and complex. You may find papers do link prediction differently.
- Luckily, we have full support in **PyG and** [**GraphGym**]

GNN Training Pipeline



Implementation resources:

DeepSNAP provides core modules for this pipeline

GraphGym further implements the full pipeline to facilitate GNN design

Summary of the Lecture

- **We introduce a general GNN framework:**
  - **GNN Layer**:
    - Transformation + Aggregation
    - Classic GNN layers: GCN, GraphSAGE, GAT
  - **Layer connectivity**:
    - The over-smoothing problem
    - Solution: skip connections
  - **Graph Augmentation:**
    - Feature augmentation
    - Structure augmentation
  - **Learning Objectives**
    - The full training pipeline of a GNN

Stanford CS224W: When Things Don't Go As Planned

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

General Tips

- **Data preprocessing is important:**
  - Node attributes can vary a lot!
    - E.g. probability ranges $(0,1)$, but some inputs could have much larger range, say $(-1000, 1000)$
  - Use normalization
- **Optimizer:**
    - ADAM is relatively robust to learning rate
- **Activation function**
  - ReLU activation function often works well
  - Other alternatives: LeakyReLU, SWISH, rational activation
  - No activation function at your output layer:
- **Include bias term in every layer**
- **Embedding dimensions:**
  - 32, 64 and 128 are often good starting points

Debugging Deep Networks

- **Debug issues:** Loss/accuracy not converging during training
  - Check pipeline (e.g. in PyTorch we need zero_grad)
  - Adjust hyperparameters such as learning rate
  - Pay attention to weight parameter initialization
- **Important for model development:**
  - **Overfit on (part of) training data:**
    - With a small training dataset, loss should be essentially close to 0, with an expressive neural network
    - If neural network cannot overfit a single data point, something is wrong
  - **Scrutinize loss function!**
  - **Scrutinize visualizations!**

Resources on Graph Neural Networks

GraphGym:
Easy and flexible implementation support based on PyTorch Geometric

PyG **DGL** **GraphNets**

GNN framework:
Implements a variety of GNN architectures

PyTorch TensorFlow

Auto-differentiation framework

Resources on Graph Neural Networks

Tutorials and overviews:
- Relational inductive biases and graph networks (Battaglia et al., 2018)
- Representation learning on graphs: Methods and applications (Hamilton et al., 2017)

Attention-based neighborhood aggregation:
- Graph attention networks (Hoshen, 2017; Velickovic et al., 2018; Liu et al., 2018)

Embedding entire graphs:
- Graph neural nets with edge embeddings (Battaglia et al., 2016; Gilmer et. al., 2017)
- Embedding entire graphs (Duvenaud et al., 2015; Dai et al., 2016; Li et al., 2018) and graph pooling (Ying et al., 2018, Zhang et al., 2018)
- Graph generation and relational inference (You et al., 2018; Kipf et al., 2018)
- How powerful are graph neural networks(Xu et al., 2017)

Embedding nodes:
- Varying neighborhood: Jumping knowledge networks (Xu et al., 2018), GeniePath (Liu et al., 2018)
- Position-aware GNN (You et al. 2019)

Spectral approaches to graph neural networks:
- Spectral graph CNN & ChebNet (Bruna et al., 2015; Defferrard et al., 2016)
- Geometric deep learning (Bronstein et al., 2017; Monti et al., 2017)

Other GNN techniques:
- Pre-training Graph Neural Networks (Hu et al., 2019)
- GNNExplainer: Generating Explanations for Graph Neural Networks (Ying et al., 2019)