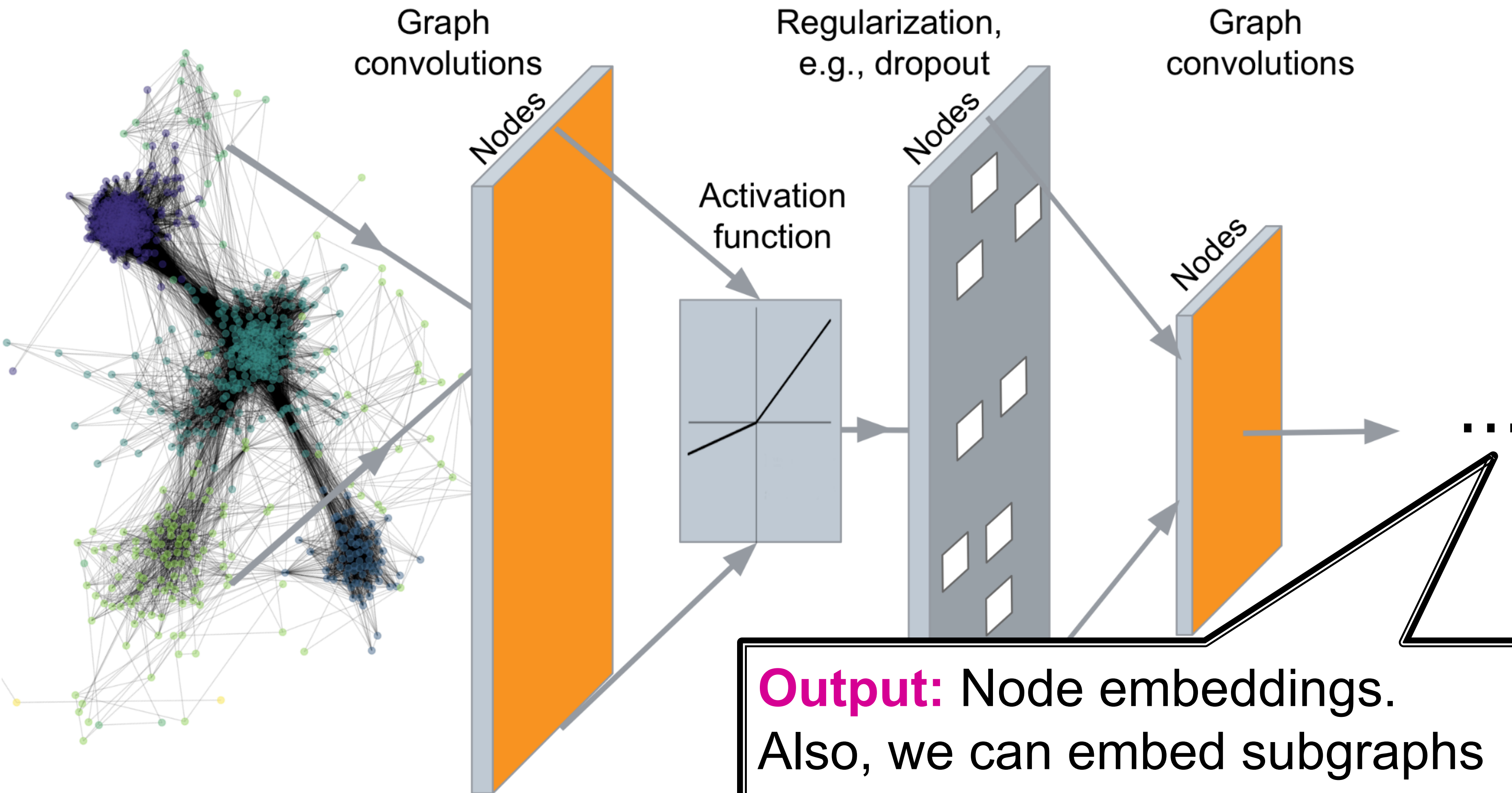
Stanford CS224W: GNN Augmentation and Training

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

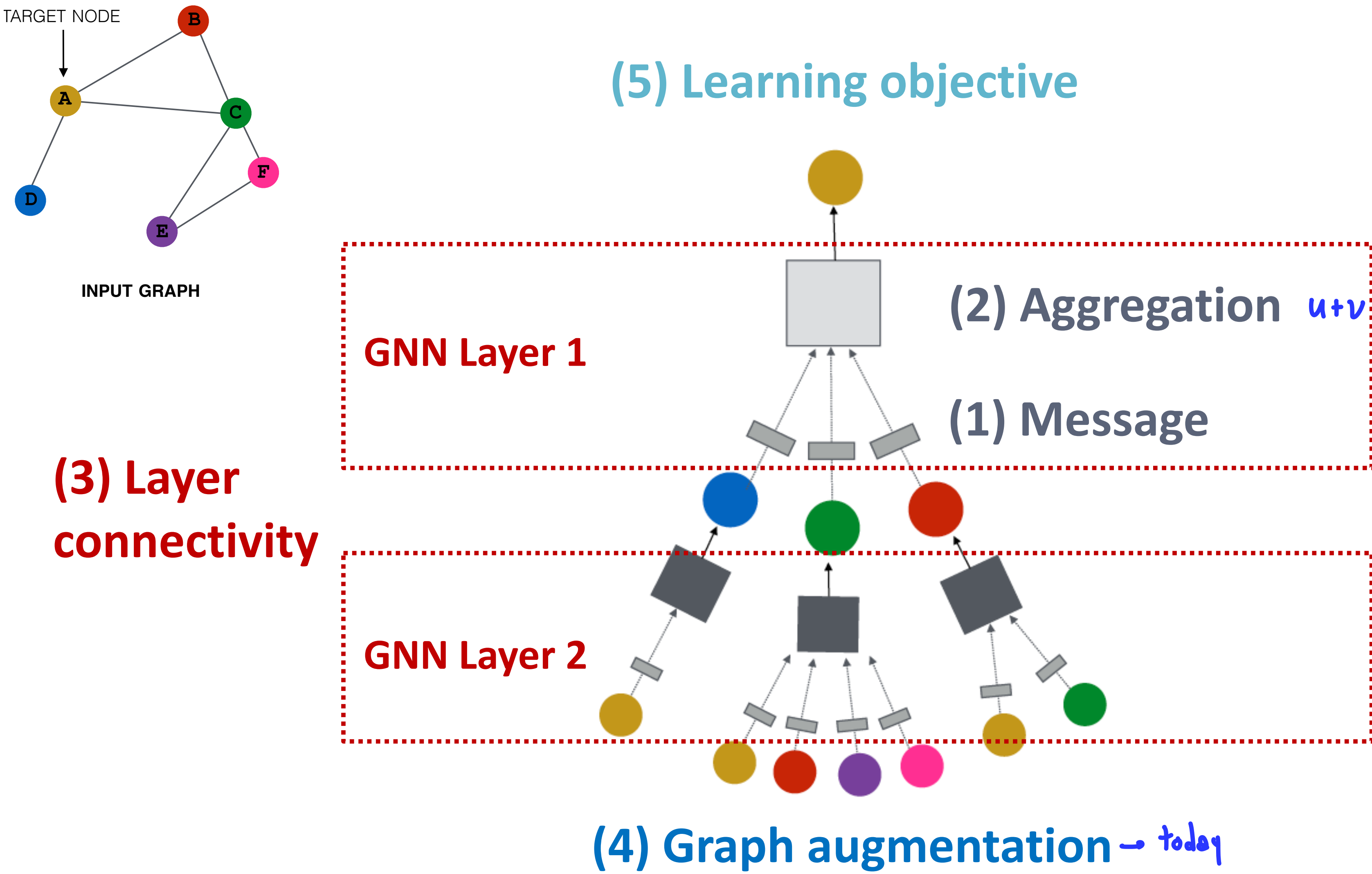
Recap: Deep Graph Encoders



Output: Node embeddings. Also, we can embed subgraphs and entire graphs

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

Recap: A General GNN Framework



Stanford CS224W: Graph Augmentation for GNNs

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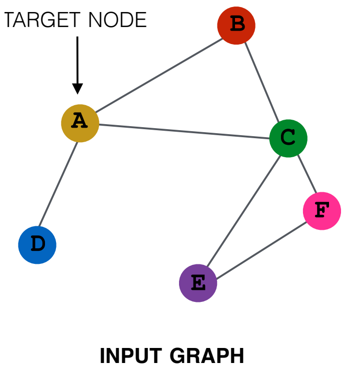
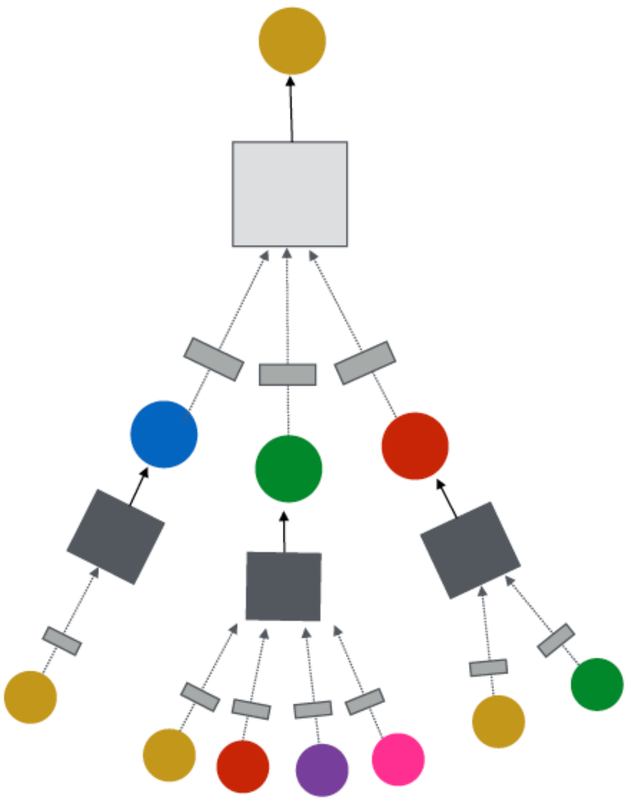
General GNN Framework



Idea: Raw input graph ≠ computational graph

- **Graph feature augmentation** ①
- **Graph structure augmentation** ②



(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
    ex. high deg. node
  - 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

for GNN has easier time to learn

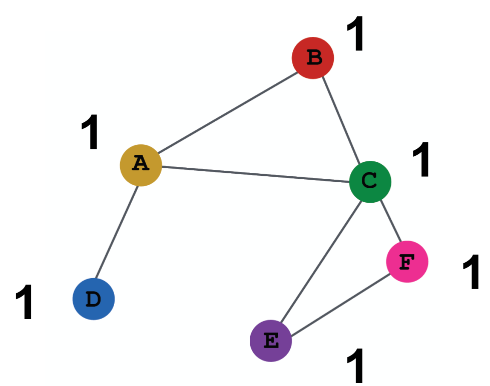
- **Graph Feature augmentation**
  - The input graph **lacks features** → **feature augmentation**
- **Graph Structure augmentation**
  - The graph is **too sparse** → **Add virtual nodes / edges**
  - The graph is **too dense** → **Sample neighbors when doing message passing**
  - The graph is **too 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**

all nodes have the same feature value of 1

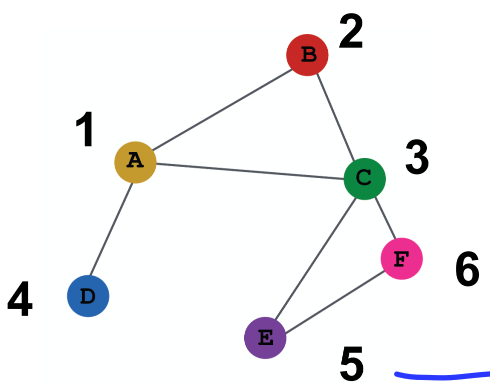


INPUT GRAPH

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** Expensive when $|V|$ large
  - These IDs are converted into **one-hot vectors**



INPUT GRAPH

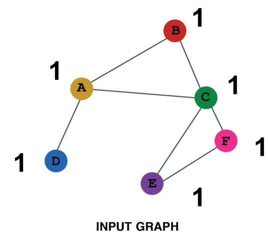
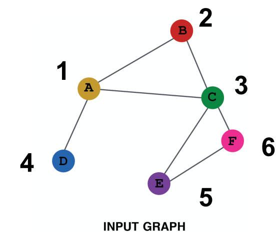
One-hot vector for node with ID=5

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**

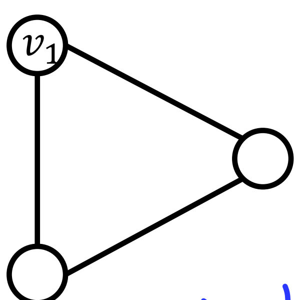
	Constant node feature 	**One-hot node feature** 
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a unique ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple 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 cheap	**High**. $O(\|V\|)$ dimensional feature, cannot apply to large graphs
Use cases	**Any graph, inductive settings** (generalize to new nodes)	all nodes/edges are known at training **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**

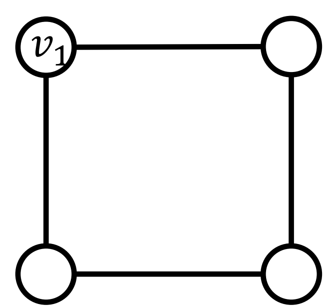
v_1 resides in a cycle with length 3



Both have deg. = 2

important in chemistry

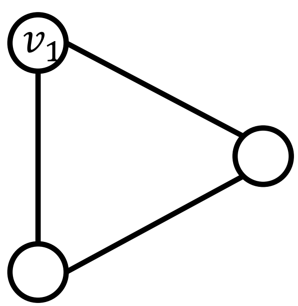
v_1 resides in a cycle with length 4



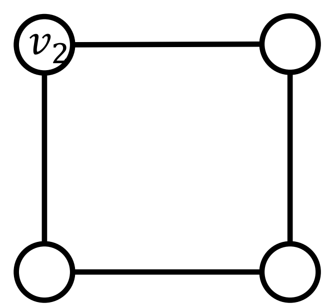
Feature Augmentation on Graphs

- 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

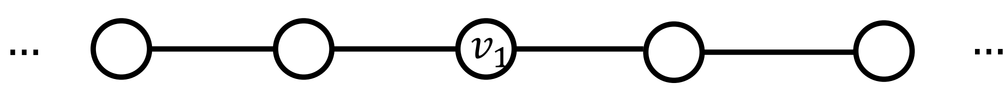
v_1 resides in a cycle with length 3



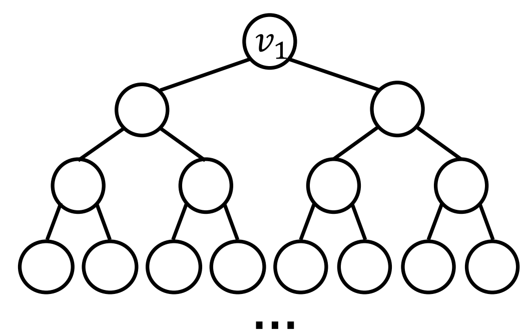
v_1 resides in a cycle with length 4



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:** create a feature vector for every node
  - We can use cycle count as augmented node features

We start from cycle with length 0

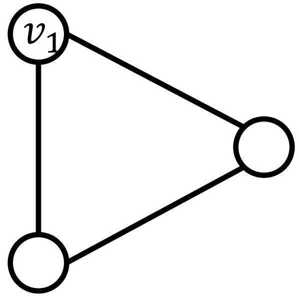
Augmented node feature for v_1

$$\begin{array}{cccccc} 0 & 1 & 2 & 3 & 4 & \\ \end{array}$$

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

self loop   reciprocated   triangle   square

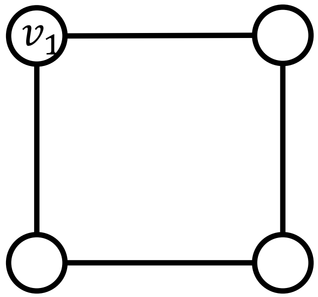
v_1 resides in a cycle with length 3



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?

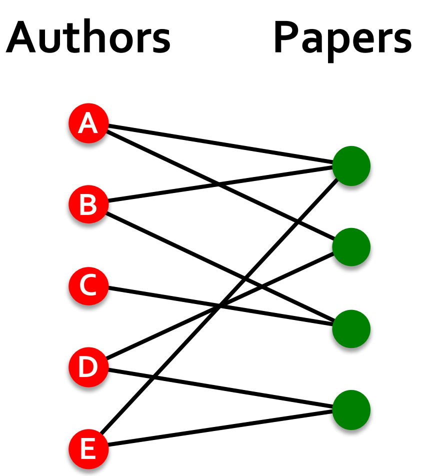
- **(2) Certain structures are hard to learn by GNN**
- Other commonly used augmented features:
  - **Node degree**
  - **Clustering coefficient** how many cycle of length 3? triangle counting
  - **PageRank**
  - **Centrality**
  - **...**
- Any **feature we have introduced in Lecture 2 can be used!**

Add Virtual Nodes / Edges

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

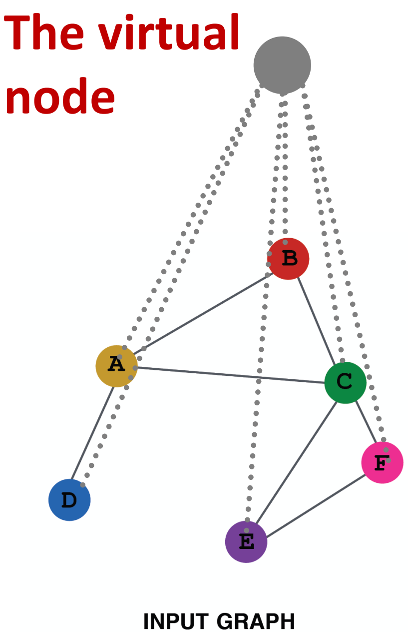
    2-hop neighbors

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



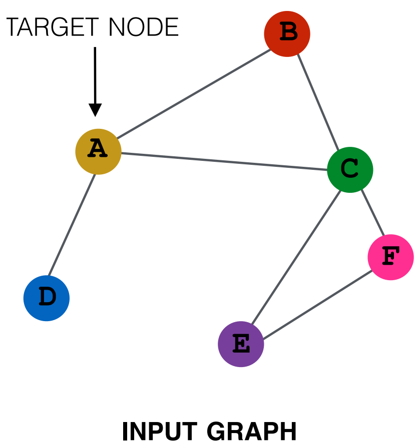
Add Virtual Nodes / Edges

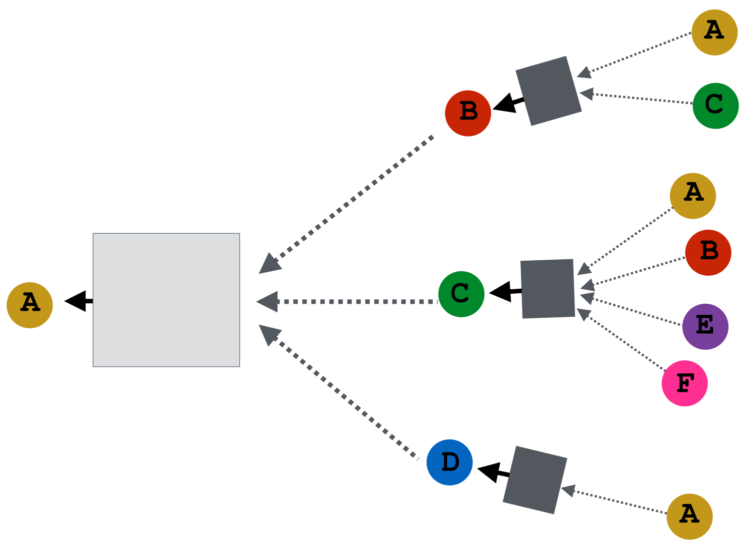
- **Motivation:** Augment sparse graphs
- **(2) Add virtual nodes**
  - The virtual node will connect to all the nodes in the graph
    - Suppose in a sparse graph, two nodes have shortest path distance of 10
    - After adding the virtual node, **all the nodes will have a distance of two**
      - **Node 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



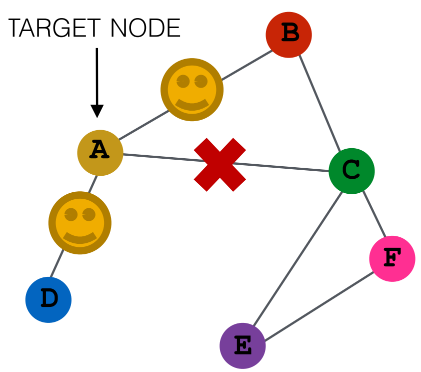


- **New idea:** (Randomly) sample a node's neighborhood for message passing

carefully select by heuristic

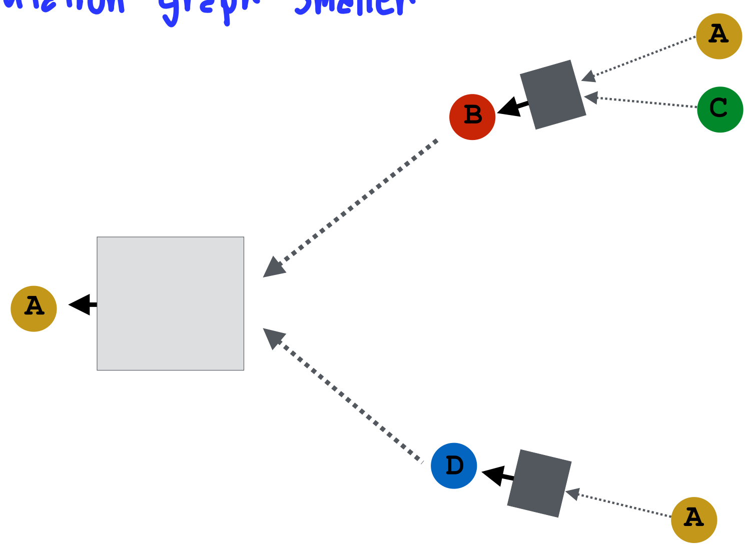
Neighborhood Sampling Example

- **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



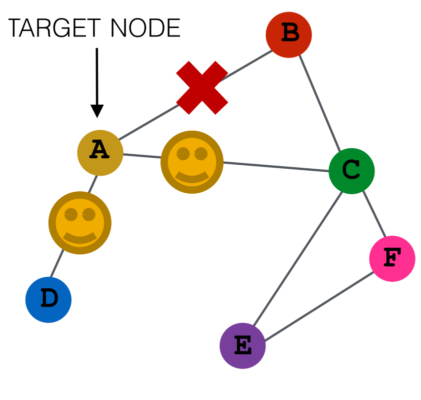
INPUT GRAPH

Computation graph smaller

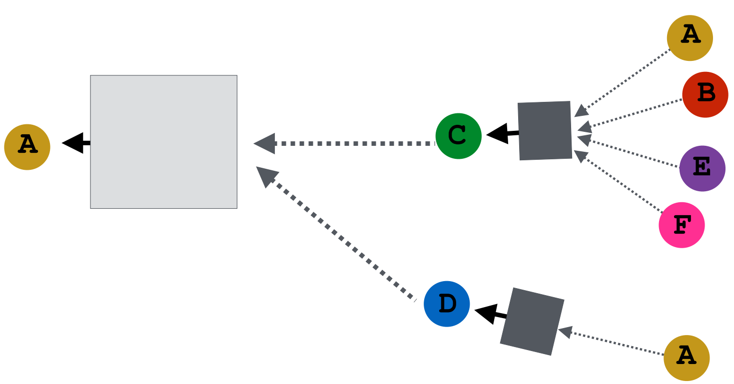


Neighborhood Sampling Example

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

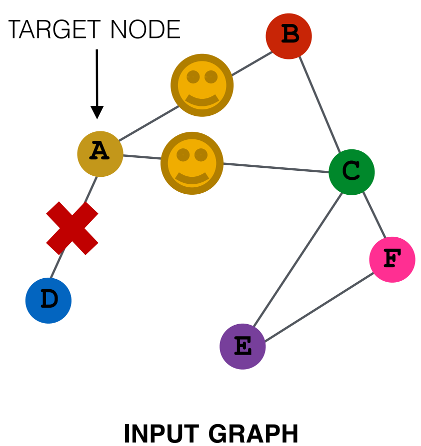


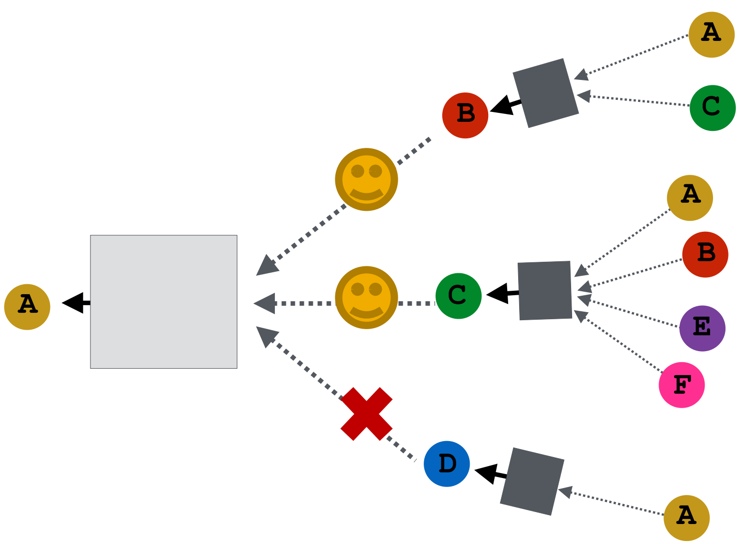
INPUT GRAPH



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!





So far:

- augmented feature vector / graph structure

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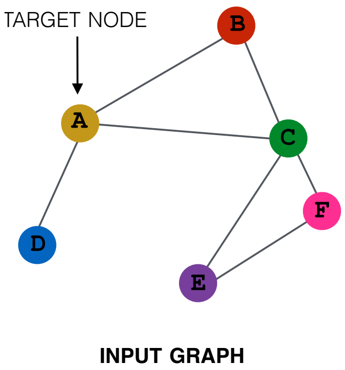
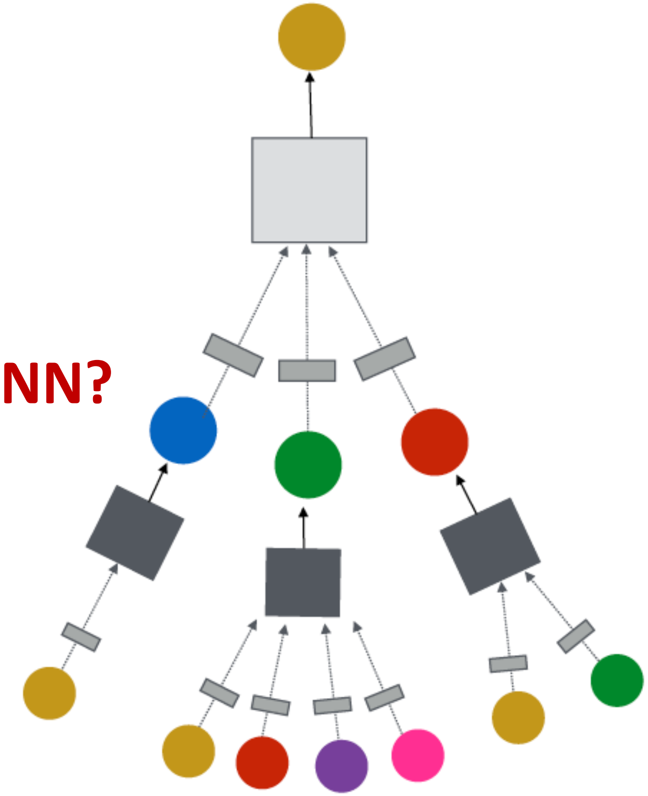
A General GNN Framework (4)



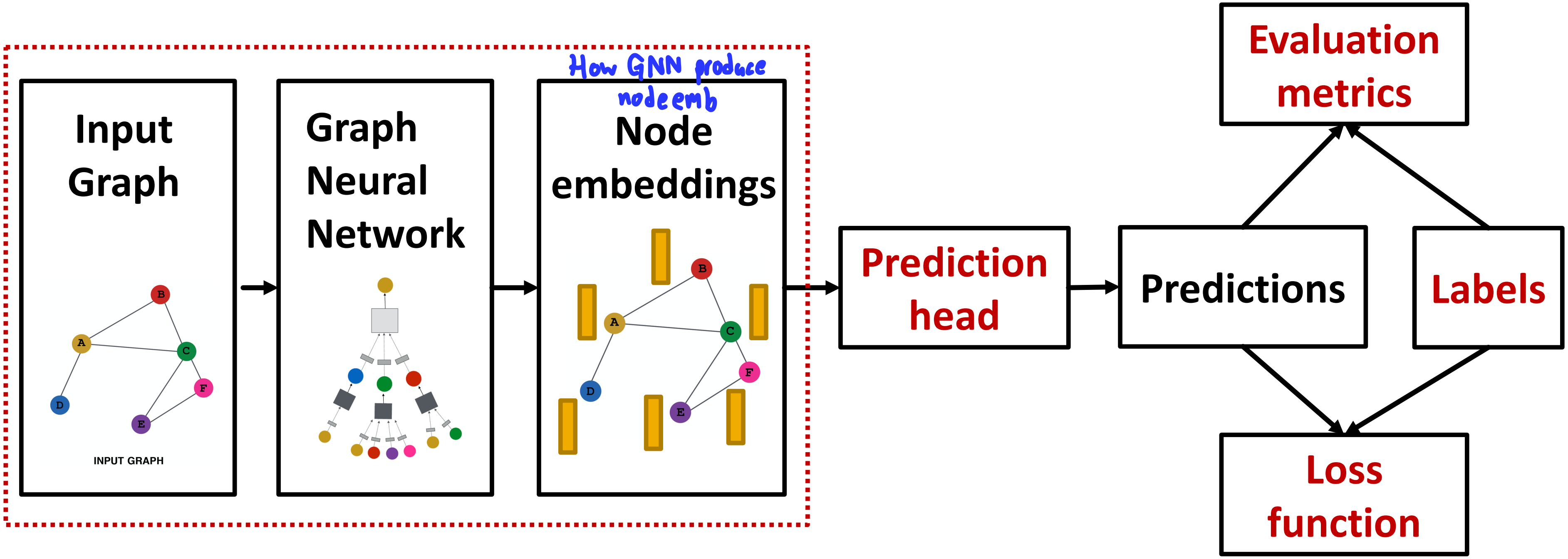
(5) Learning objective



Next: How do we train a GNN?

GNN Training Pipeline

So far what we have covered

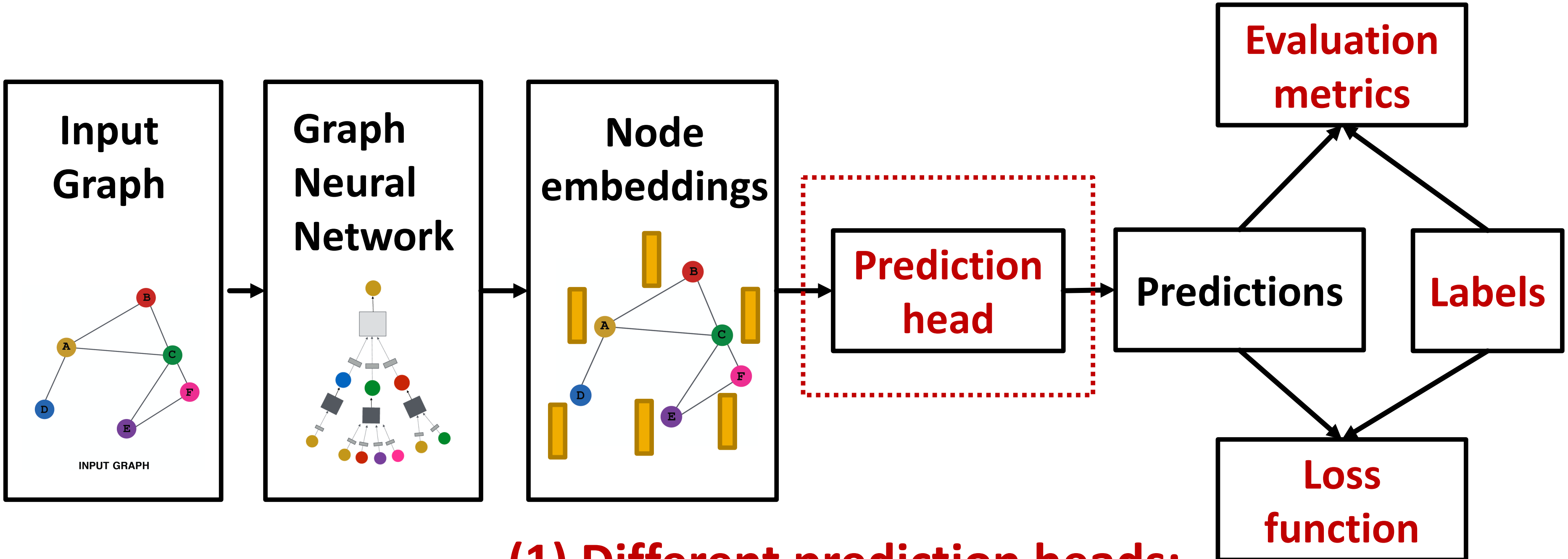


Output of a GNN: set of node embeddings

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

final layer L

GNN Training Pipeline (1)

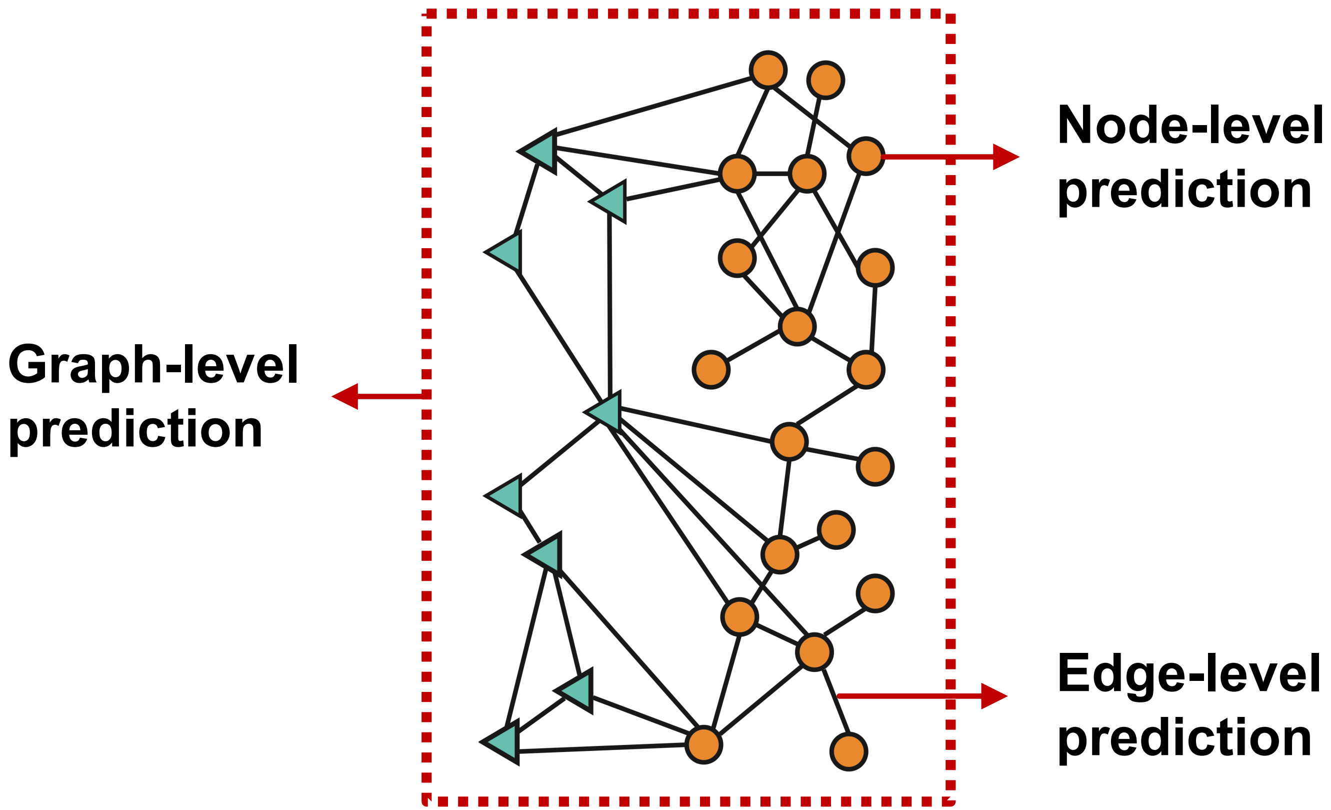


(1) Different prediction heads:

- 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
- $\overset{\text{output}}{\widehat{\boldsymbol{y}}_v} = \text{Head}_{\text{node}}(\mathbf{h}_v^{(L)}) = \mathbf{W}^{(H)}\mathbf{h}_v^{(L)}$ final emb.

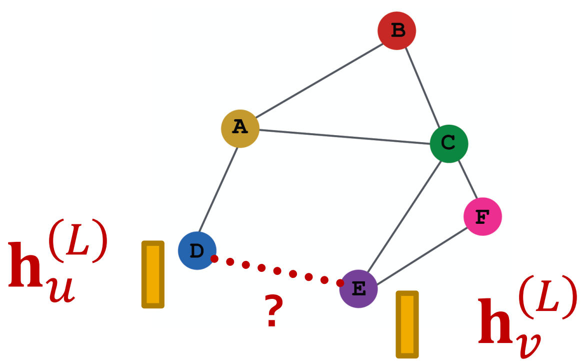
  hat symbol = predicted values

  - $\mathbf{W}^{(H)} \in \mathbb{R}^{k*d}$: 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

    emb. space $\longrightarrow$ prediction space

Prediction Heads: Edge-level

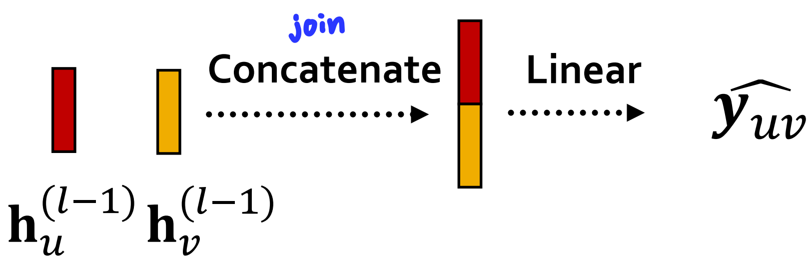
- **Edge-level prediction**: Make prediction using pairs of node embeddings
- Suppose we want to make k-way prediction
- $\hat{\boldsymbol{y}}_{\boldsymbol{uv}} = \mathrm{Head}_{\mathrm{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$



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

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 GAT



  - $\widehat{\boldsymbol{y}}_{\boldsymbol{uv}} = \text{Linear}(\text{Concat}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)}))$
  - 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** $\mathrm{Head}_{\mathrm{edge}}(\mathbf{h}_u^{(L)}, \mathbf{h}_v^{(L)})$:
- **(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)
    binary
  - **Applying to k-way prediction:**
    - Similar to **multi-head attention**: $\mathbf{W}^{(1)}, \ldots, \mathbf{W}^{(k)}$ trainable

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

trainable

$$\ldots$$

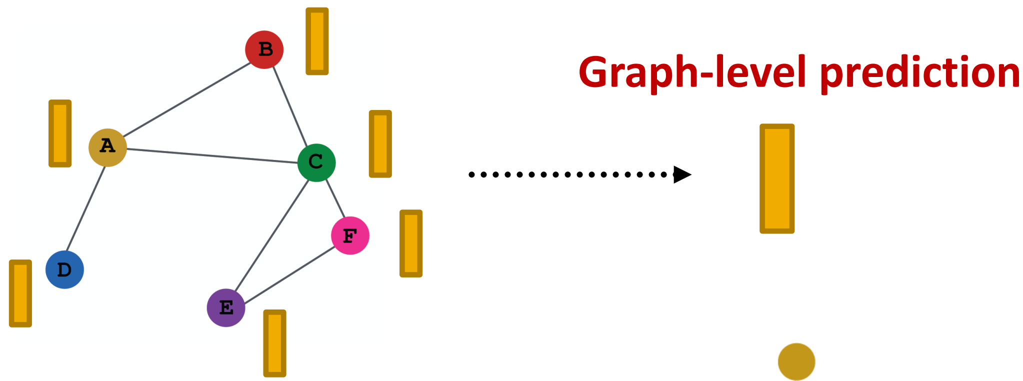
$$\widehat{\boldsymbol{y}}_{\boldsymbol{uv}}^{(k)} = (\mathbf{h}_u^{(L)})^T \mathbf{W}^{(k)} \mathbf{h}_v^{(L)}$$

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

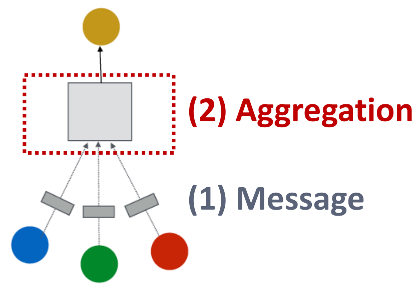
Prediction Heads: Graph-level

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

aggregate



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



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** |V| not play a role, compare graphs with diff. size ✓

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

- **(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** really wanna understand how many nodes are there in the graph & structure of the graph ✓

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

- 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: 1 2 3 4 5
  - Node embeddings for G_1: $\{-1, -2, 0, 1, 2\}$
  - node: 1 2 3 4 5
  - 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: $\hat{y}_G = \mathrm{Sum}(\{-1, -2, 0, 1, 2\}) = 0$
  - **Prediction for** G_2: $\hat{y}_G = \mathrm{Sum}(\{-10, -20, 0, 10, 20\}) = 0$
  - 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 $\mathrm{ReLU}(\mathrm{Sum}(\cdot))$
    - How do we design?
    - 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**: $\hat{y}_a = \mathrm{ReLU}(\mathrm{Sum}(\{-1, -2\})) = 0$, $\hat{y}_b = \mathrm{ReLU}(\mathrm{Sum}(\{0,1,2\})) = 3$
    - **Round 2:** $\hat{y}_G = \mathrm{ReLU}(\mathrm{Sum}(\{y_a, y_b\})) = \mathbf{3}$
  - G_2 node embeddings: $\{-10, -20, 0, 10, 20\}$
    - **Round 1**: $\hat{y}_a = \mathrm{ReLU}(\mathrm{Sum}(\{-10, -20\})) = 0$, $\hat{y}_b = \mathrm{ReLU}(\mathrm{Sum}(\{0,10,20\})) = 30$
    - **Round 2:** $\hat{y}_G = \mathrm{ReLU}(\mathrm{Sum}(\{y_a, y_b\})) = \mathbf{30}$

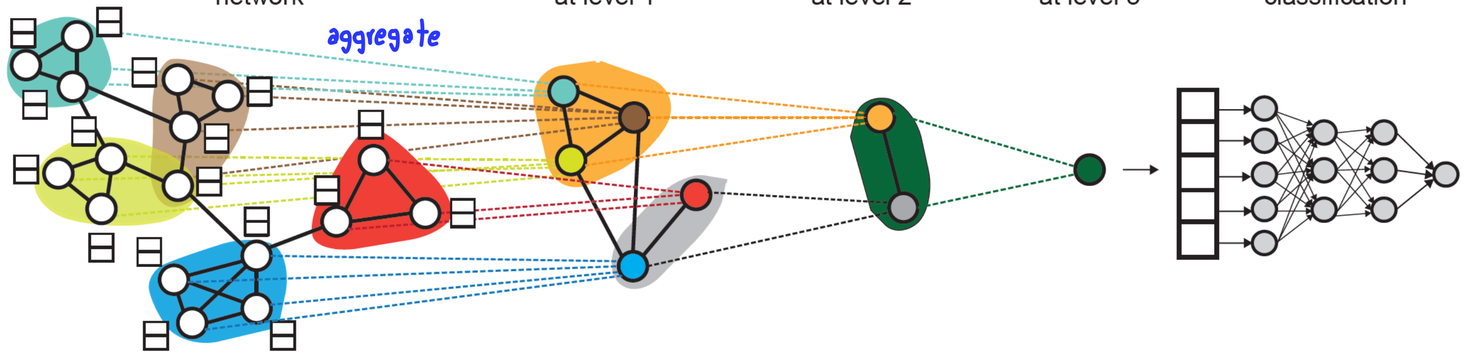
Now we can differentiate G_1 and G_2 !

Ying et al. Hierarchical Graph Representation Learning with Differentiable Pooling, NeurIPS 2018

Hierarchical Pooling In Practice

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

Apply graph partioning / clustering
commu. dectection
Identify cluster



community structure

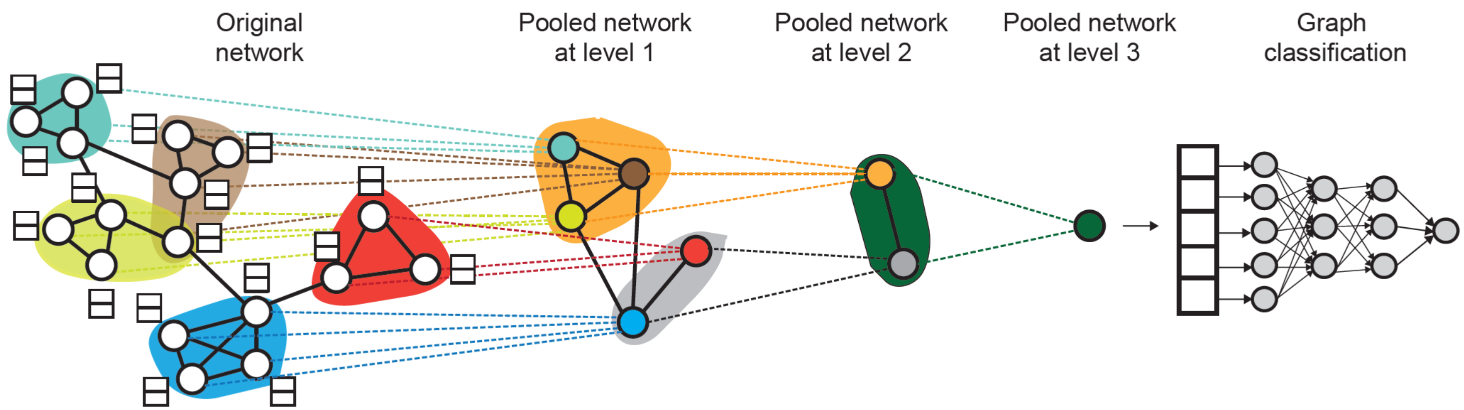
  - **Leverage 2 independent GNNs at each level**
    - **GNN A:** Compute node embeddings
    - **GNN B:** Compute the cluster that a node belongs to

cluster + aggregate

  - **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**

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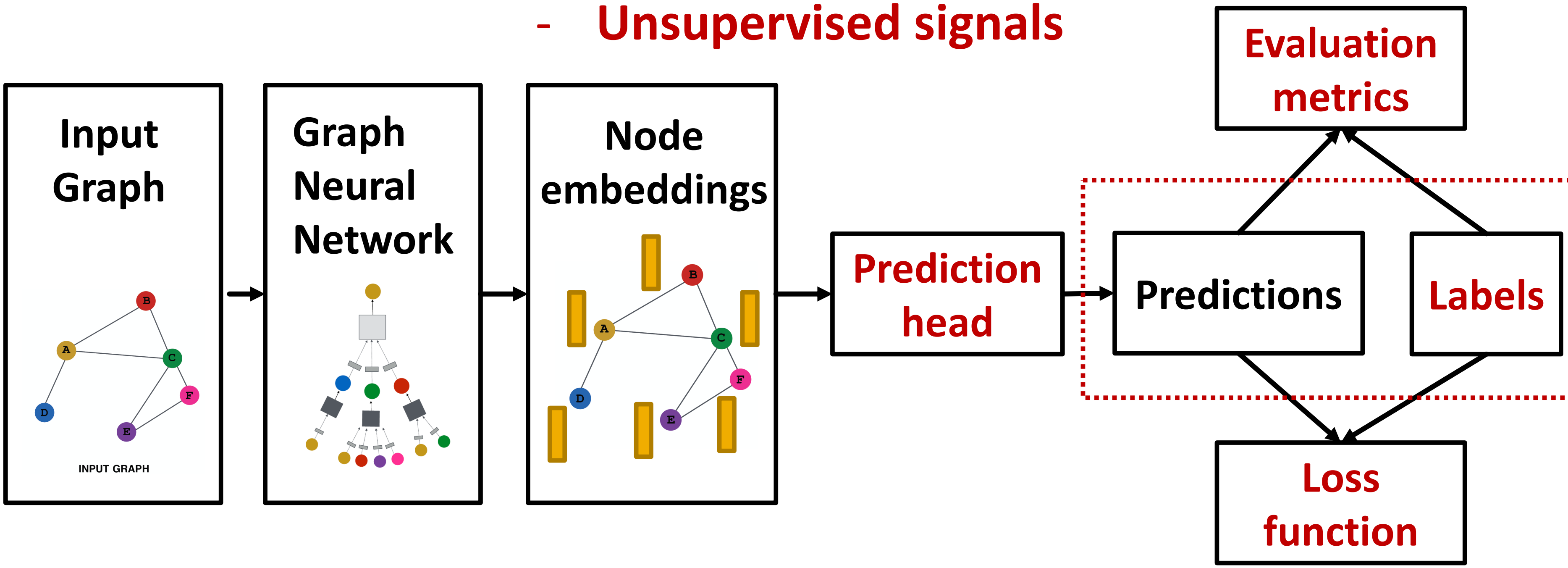
GNN Training Pipeline (2)

(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**
  - sometimes external / internal
  - We still have "supervision" in unsupervised learning
    - E.g., train a GNN to predict node clustering coefficient → internal
  - An alternative name for "**unsupervised**" is "**self-supervised**"

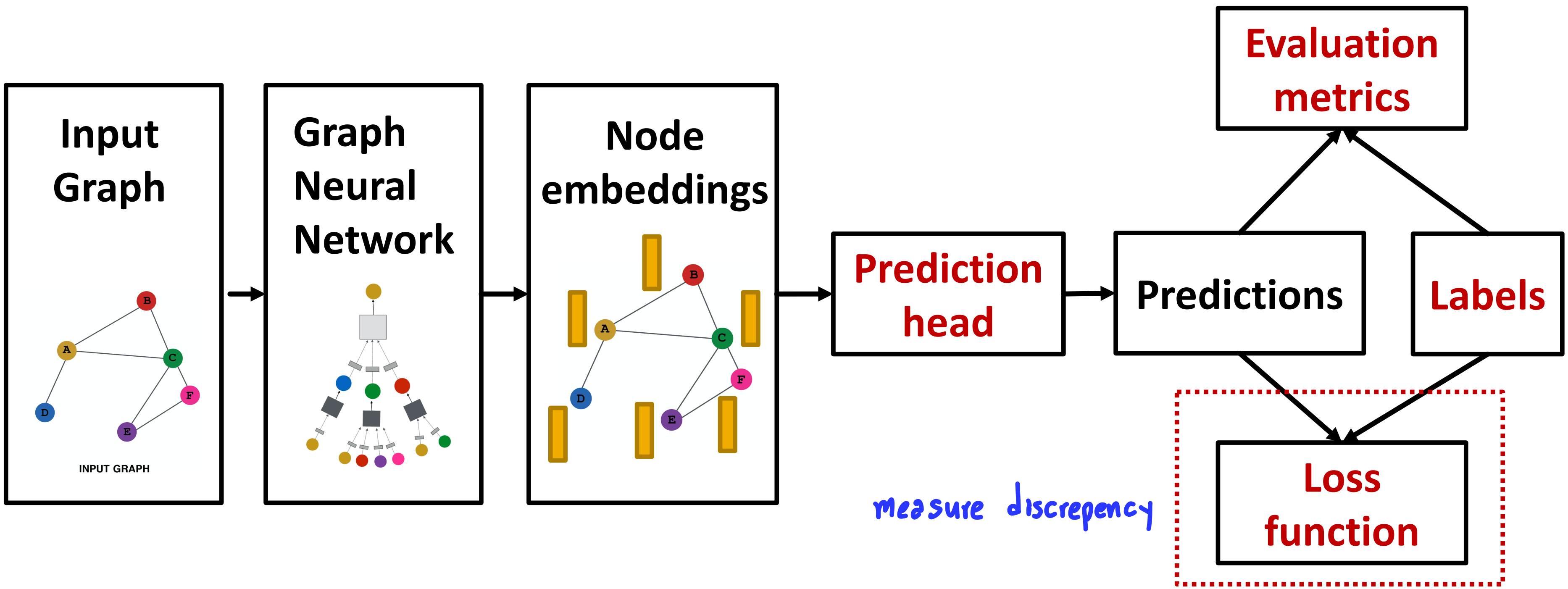
Supervised Labels on Graphs

- **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 (external labels)
  - **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 จะอ้างอิงจากงาน คนอื่นได้
  - **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:

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

***i*-th data point**

***j*-th class**

log (ใกล้ 0) = high negative

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):

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

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

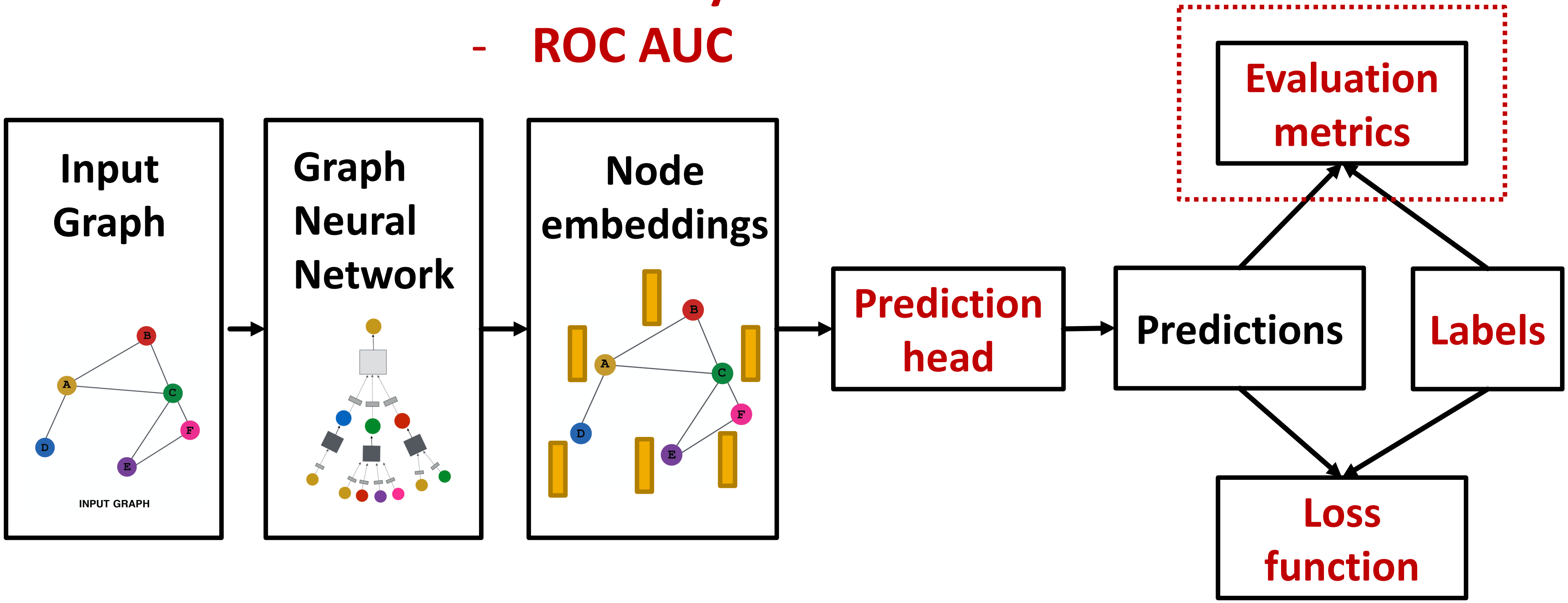
- Total loss over all N training examples

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

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

classification acc.

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

should be balanced class

ex. $\overset{T}{50}/\overset{F}{50}$

- **(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:**

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

harmonic mean

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)

P

R

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.**

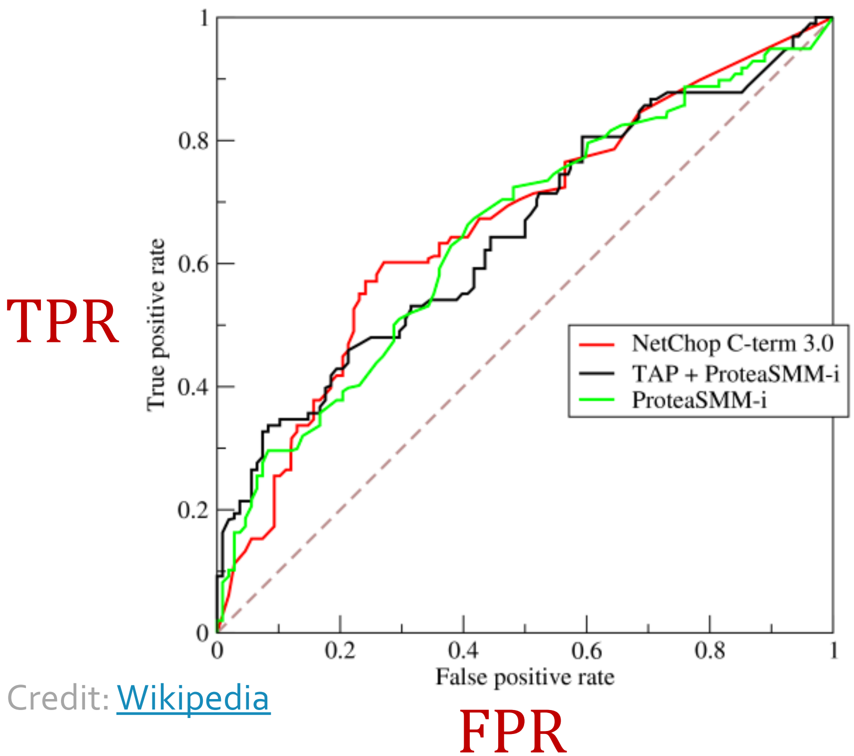


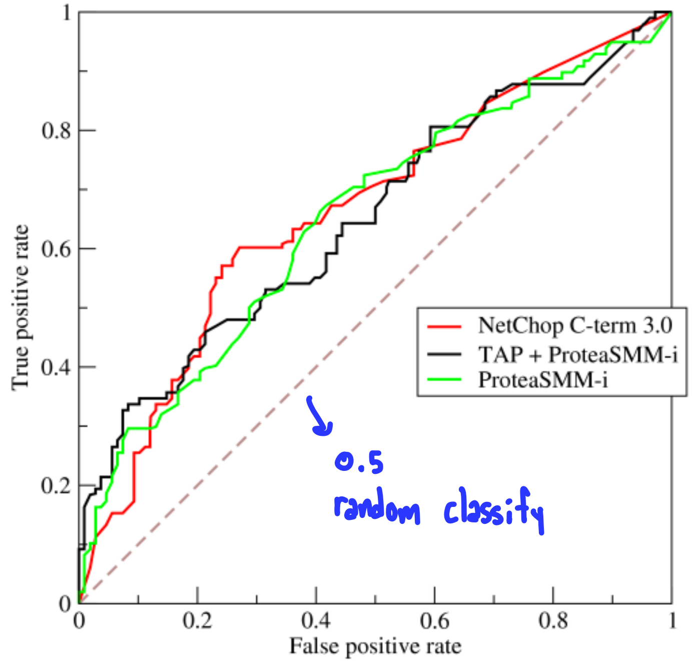
Image Credit: [Wikipedia]

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

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

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

(4) Evaluation Metrics



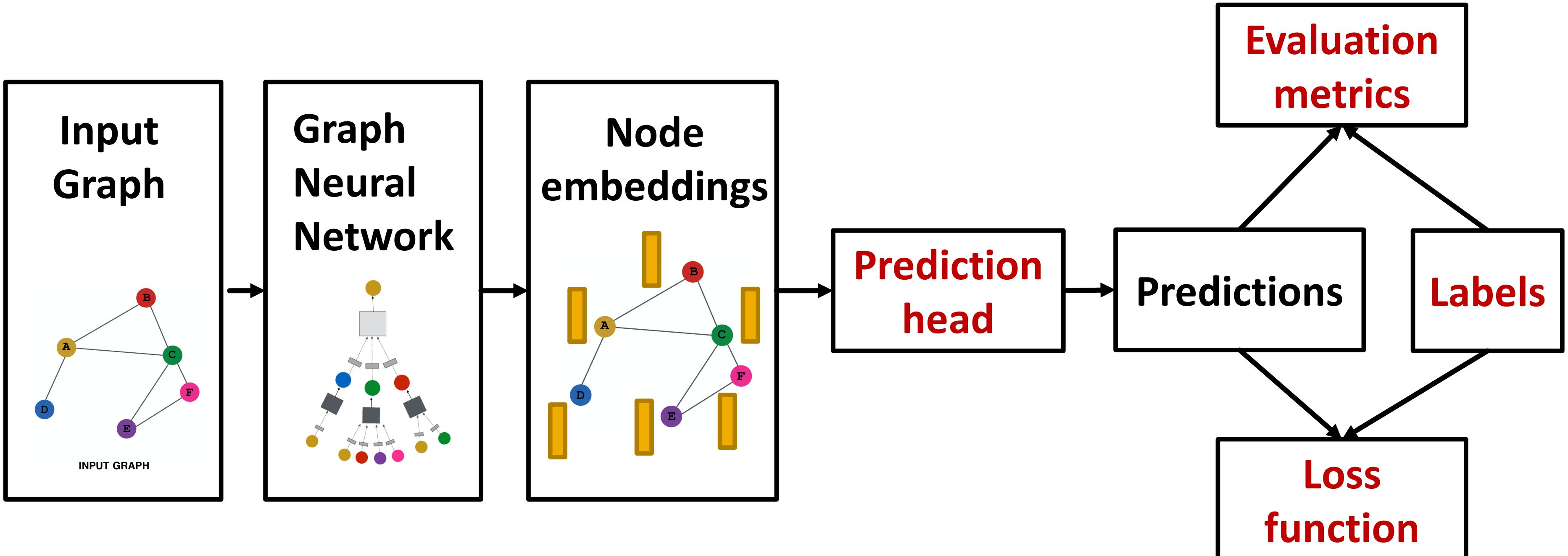
Content Credit: [Wikipedia]

- **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

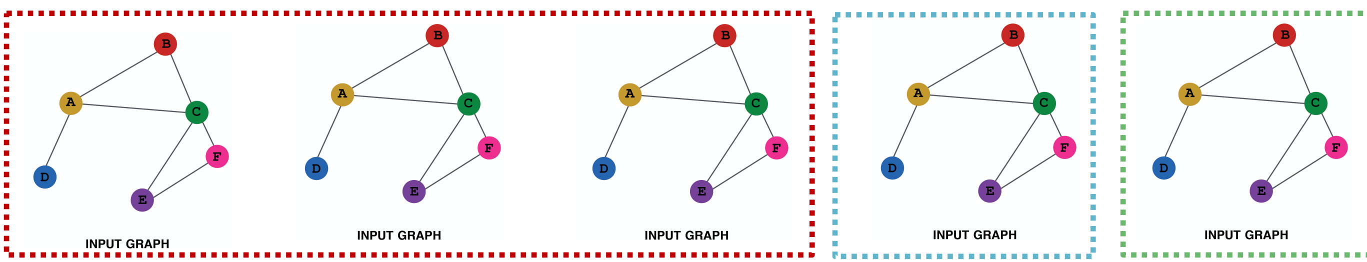
Stanford CS224W: Setting-up GNN Prediction Tasks

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?



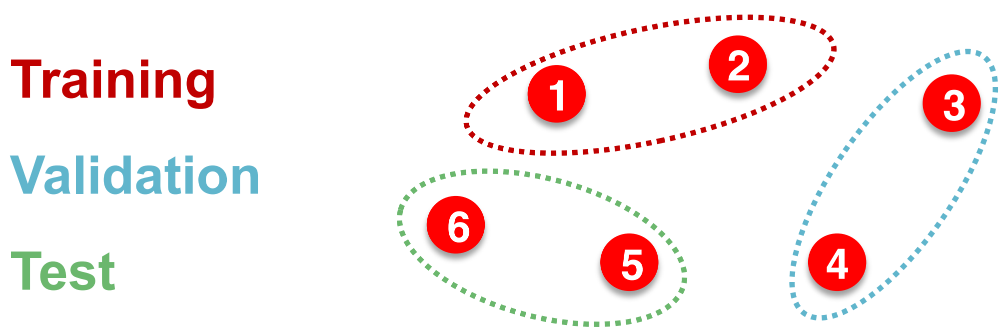
Dataset split

Dataset Split: Fixed / Random Split

- **Fixed split:** We will split our dataset **once**
  - 3 disjoint indep. pieces
  - **Training set**: used for optimizing GNN parameters
  - **Validation set**: develop model/hyperparameters tune
  - **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**

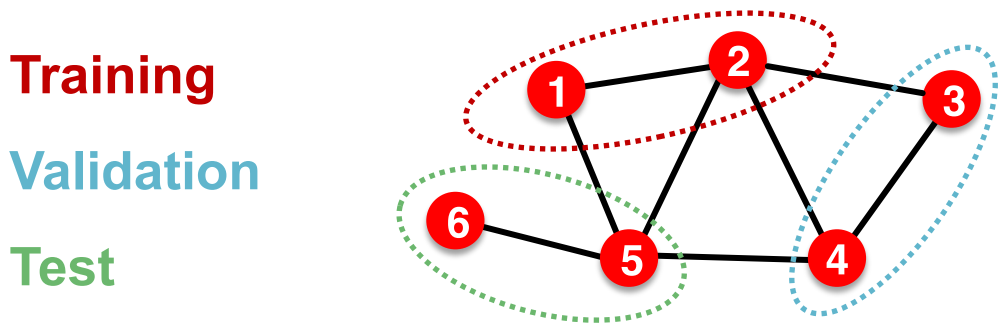
Why Splitting Graphs is Special

- Suppose we want to split an image dataset no leakage
  - **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** (dependent)
    - **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**

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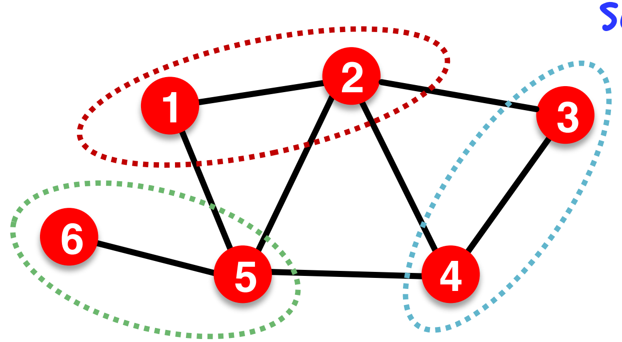
Training

Validation

Test



Semi-supervised setting

Given:
- graph
- edges
- node features

but labels of node are only subset of node labels

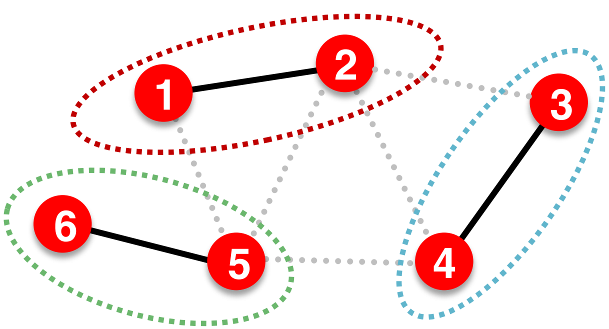
Why Splitting Graphs is Special

- **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**

Training

Validation

Test



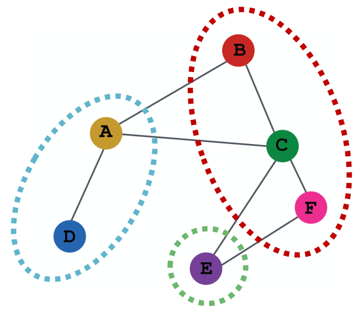
Drawbrack is throw away some graph information

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



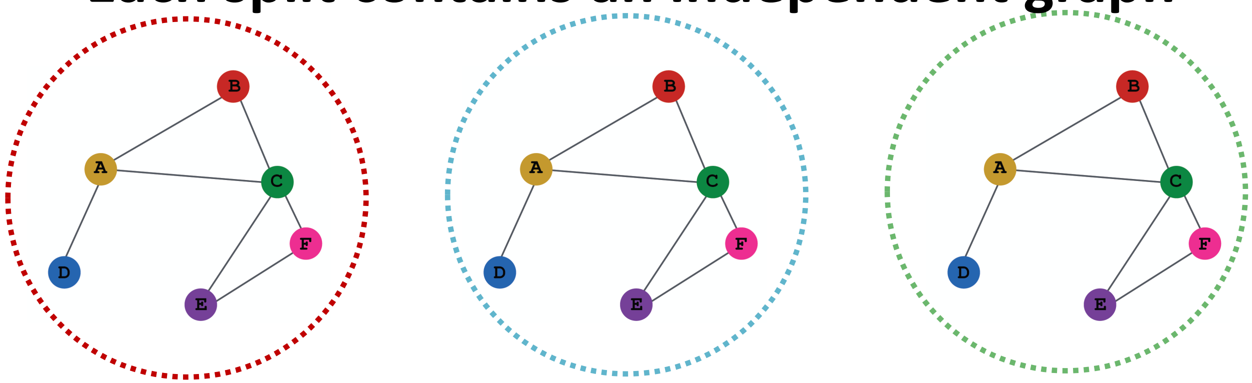
Training

Validation

Test

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

create multiple graph by dropping/cutting the edges



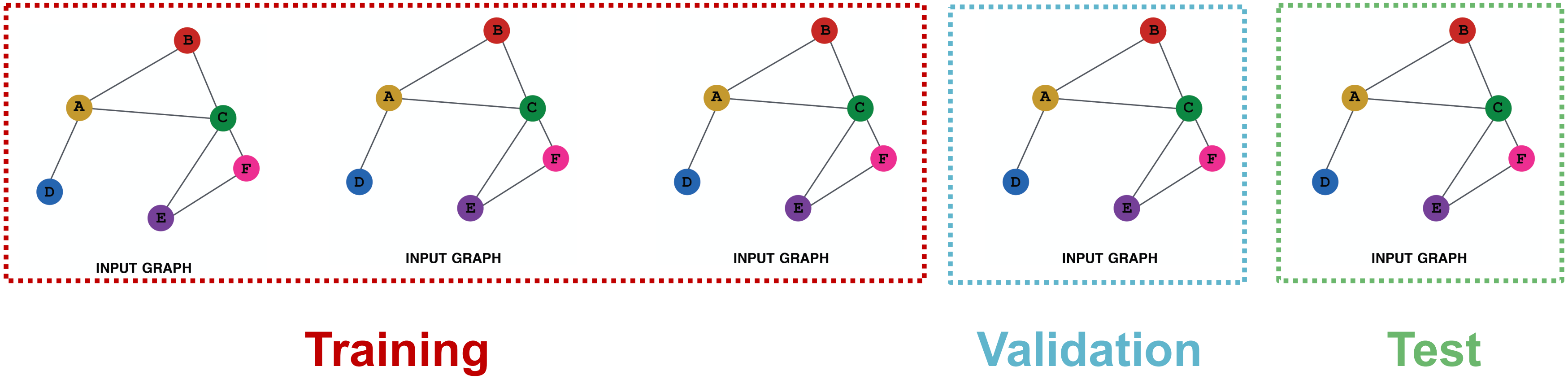
Training

Validation

Test

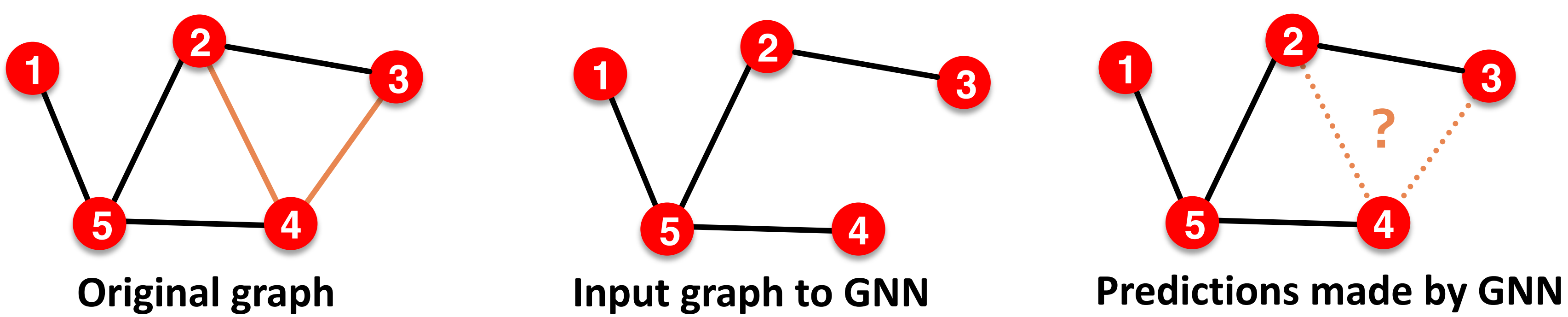
Example: Graph Classification

- 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).

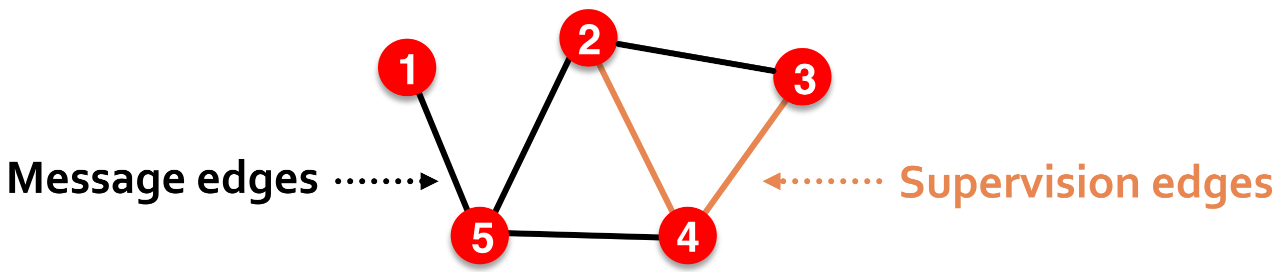


Example: Link Prediction trickiest!

- **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**



Setting up Link Prediction

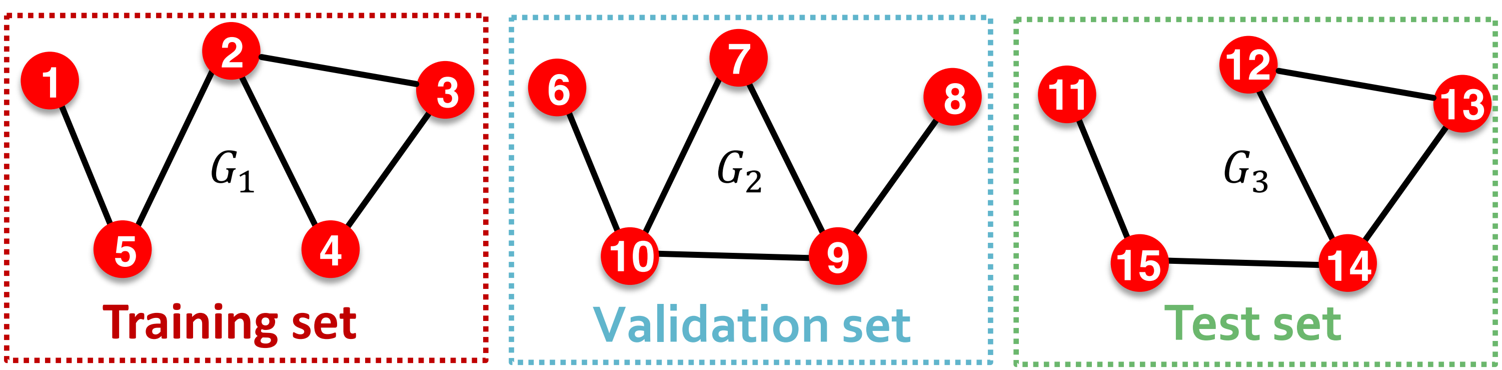


Original graph

- 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 loss function
  - 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!

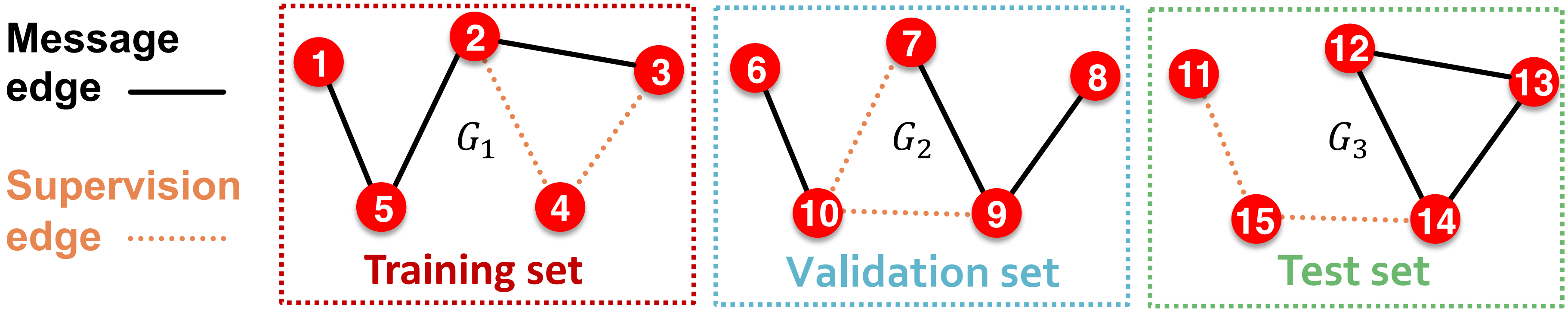
Setting up Link Prediction

- 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



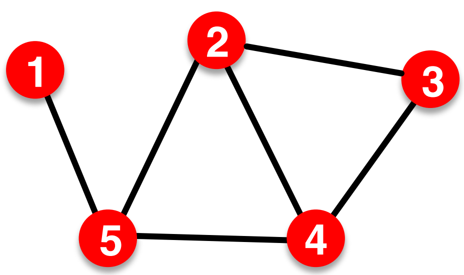
Setting up Link Prediction

- **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



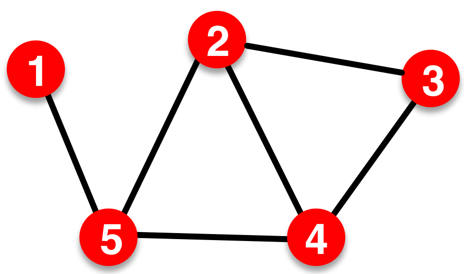
Setting up Link Prediction

- **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

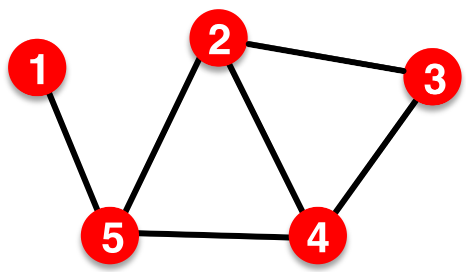
- **Option 2: Transductive link prediction split:**
  - **By definition of "transductive", the entire graph can be observed in all dataset splits**
    - **But since edges are both part of graph structure and the supervision, we need to hold out validation / test edges**
    - **To train the training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



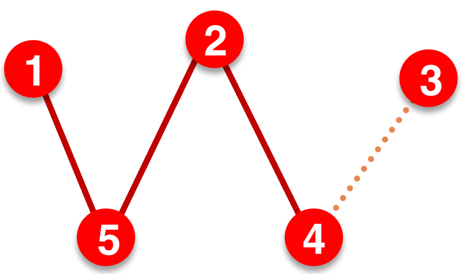
- **Next:** we will show the exact settings

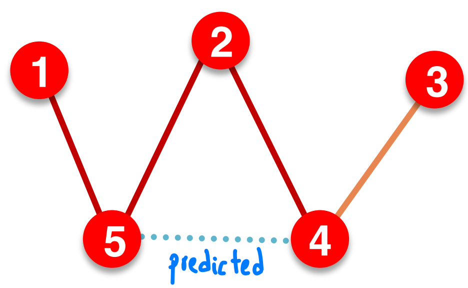
Setting up Link Prediction

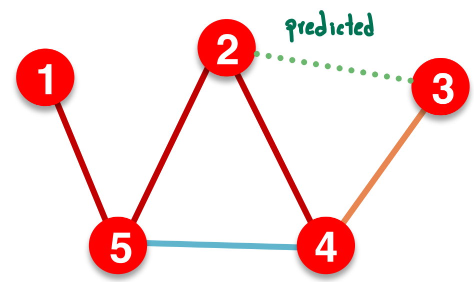
- **Option 2: Transductive link prediction split:**



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**

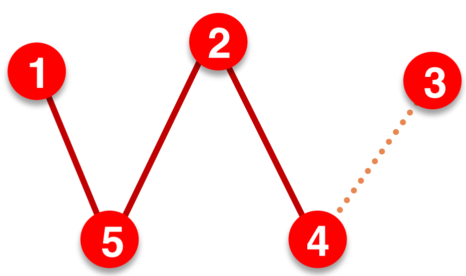
(3) At test time:
Use **training message edges & training supervision edges & validation edges** to predict **test edges**

Setting up Link Prediction

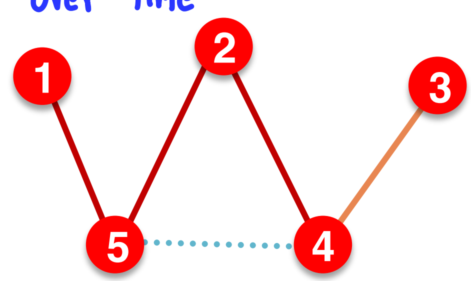
- ## Option 2: Transductive link prediction split:

Why do we use growing number of edges?
After training, supervision edges are known to GNN.
Therefore, an ideal model should use supervision edges in message passing at validation time.
The same applies to the test time.

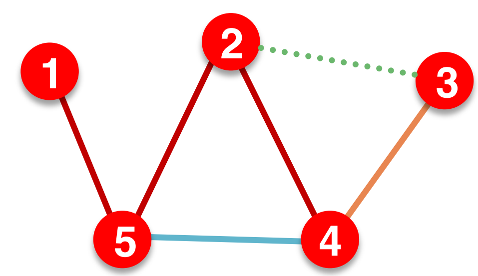
evolving over time



(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**



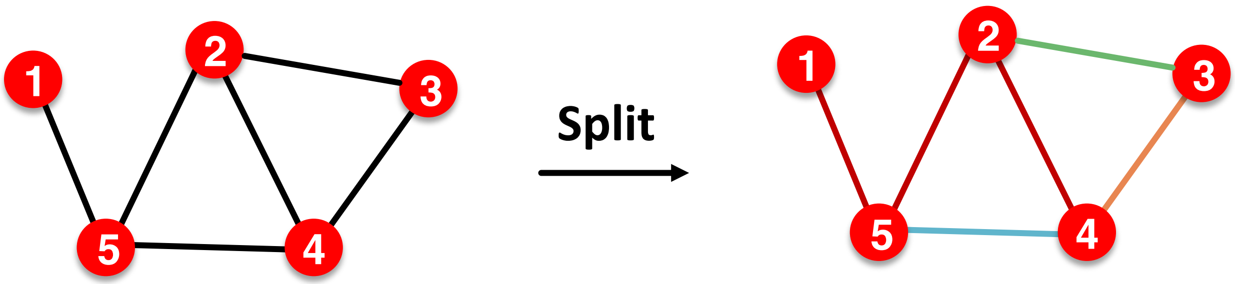
(3) At test time:
Use **training message edges & training supervision edges & validation edges** to predict **test edges**

Setting up Link Prediction

tricky

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

4 types of edges



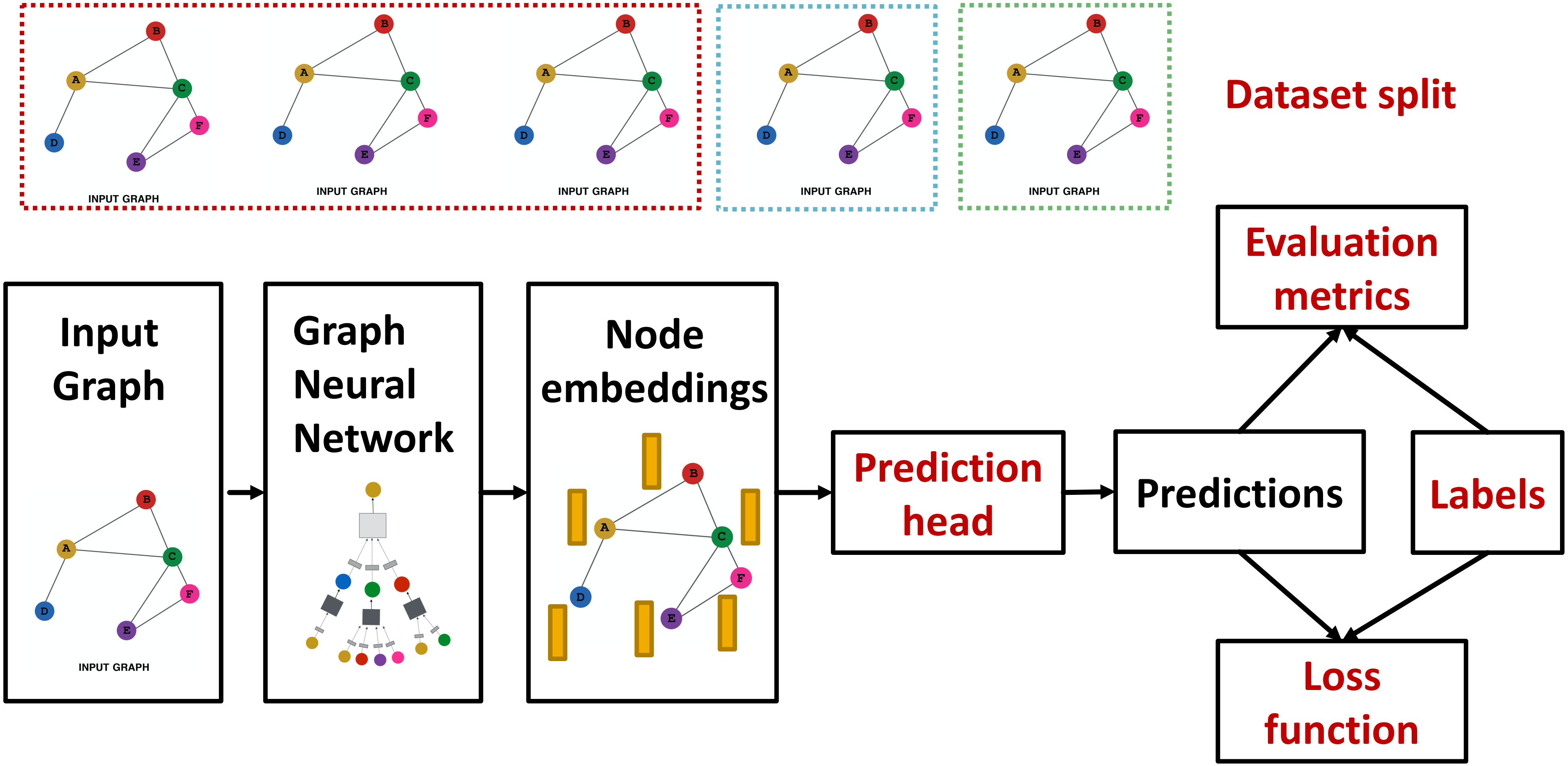
The original graph

Split Graph with 4 types of edges

1. Training message edges
2. Training supervision edges
3. Validation edges
4. Test edges

- **Note:** Link prediction settings are tricky and complex. You may find papers do link prediction differently. But if you follow our reasoning steps, **this should be the right way to implement link prediction**
- Luckily, we have full support in DeepSNAP **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 perspective for GNNs**
  - **GNN Layer**:
    - Transformation + Aggregation
    - Classic GNN layers: GCN, GraphSAGE, GAT
  - **Layer connectivity**:
    - The over-smoothing problem
    - Solution: skip connections

lect. 7

  - **Graph Augmentation:**
    - Feature augmentation
    - Structure augmentation
  - **Learning Objectives**
    - The full training pipeline of a GNN

lect. 8