Graph Neural Network

Part 2

Classical GNN Layers: GraphSAGE

- (2) GraphSAGE

$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}^{(l)} \cdot \mathrm{CONCAT}\left(\mathbf{h}_v^{(l-1)}, \mathrm{AGG}\left(\left\{\mathbf{h}_u^{(l-1)}, \forall u \in N(v)\right\}\right)\right)\right)$$

- How to write this as Message + Aggregation?
  - **Message** is computed within the $\mathrm{AGG}(\cdot)$
  - Two-stage aggregation
    - **Stage 1:** Aggregate from node neighbors

$$\mathbf{h}_{N(v)}^{(l)} \leftarrow \mathrm{AGG}\left(\left\{\mathbf{h}_u^{(l-1)}, \forall u \in N(v)\right\}\right)$$

    - **Stage 2:** Further aggregate over the node itself

$$\mathbf{h}_v^{(l)} \leftarrow \sigma\left(\mathbf{W}^{(l)} \cdot \mathrm{CONCAT}(\mathbf{h}_v^{(l-1)}, \mathbf{h}_{N(v)}^{(l)})\right)$$

GraphSAGE Neighbor Agg.

- **Mean:** Take a weighted average of neighbors

$$\text{AGG} = \underbrace{\boxed{\sum_{u \in N(v)}}}_{\text{Aggregation}} \frac{\mathbf{h}_u^{(l-1)}}{\boxed{|N(v)|}}$$

Aggregation

Message computation

- **Pool:** Transform neighbor vectors and apply symmetric vector function $\text{Mean}(\cdot)$ or $\text{Max}(\cdot)$

$$\text{AGG} = \boxed{\text{Mean}}(\{\boxed{\text{MLP}}(\mathbf{h}_u^{(l-1)}), \forall u \in N(v)\})$$

Aggregation Message computation

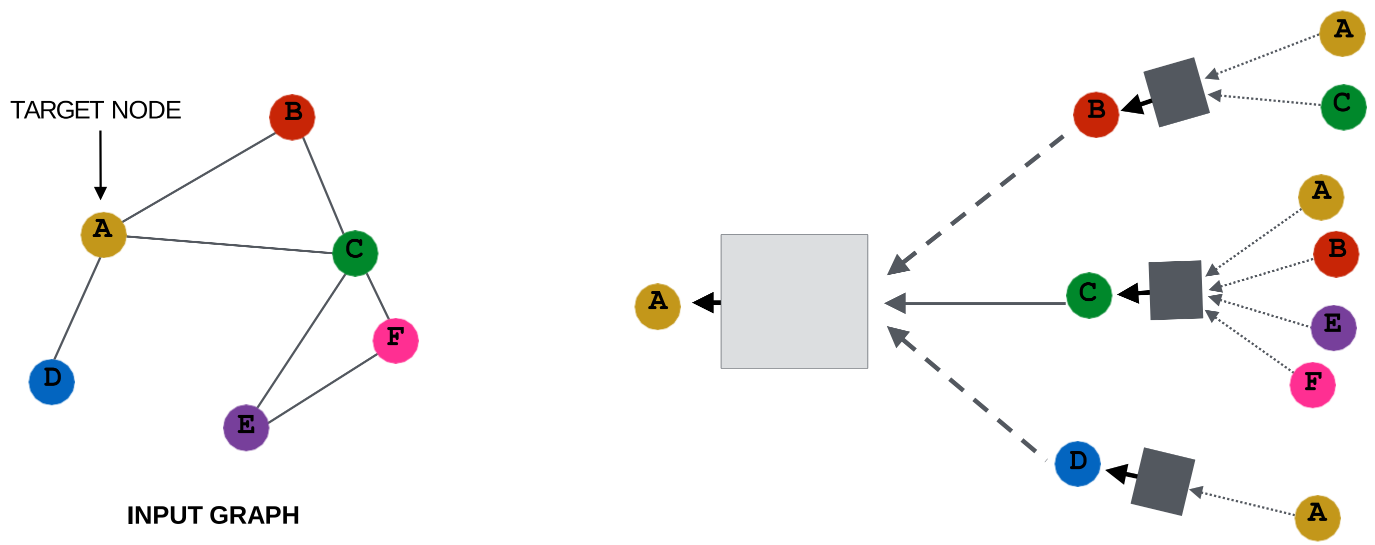
- **LSTM:** Apply LSTM to reshuffled of neighbors

$$\text{AGG} = \boxed{\text{LSTM}}([\mathbf{h}_u^{(l-1)}, \forall u \in \pi\big(N(v)\big)])$$

Aggregation

Node Neighorhood Sampling

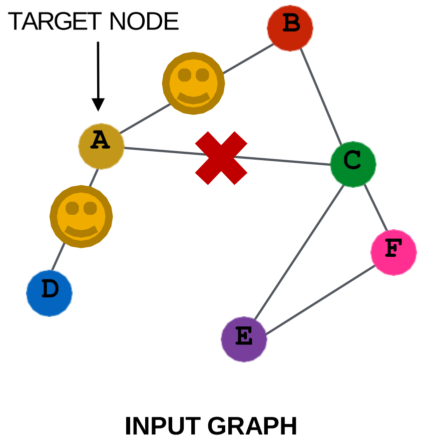
- **Previously:**
  - All the nodes are used for message passing

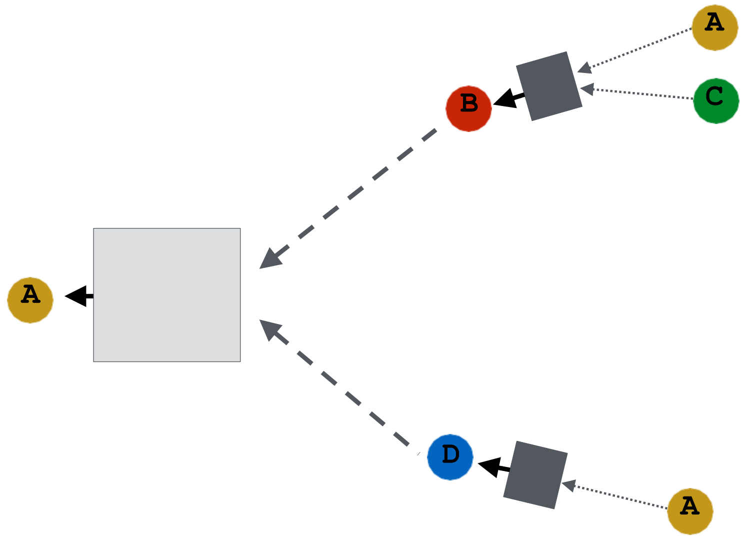


- **New idea:** (**Randomly**) sample a node's neighborhood for message passing

Neighorhood Sampling Example

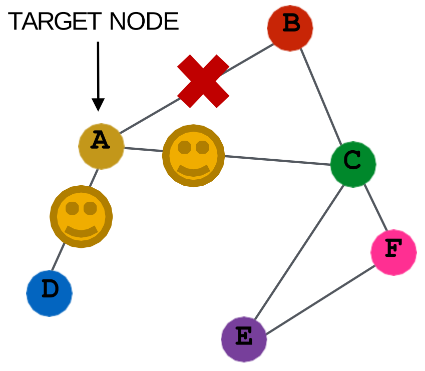
- **For example, we can randomly choose 2 neighbors to pass messages in a given layer**
  - Only nodes B and D will pass messages to A





Neighorhood Sampling Example

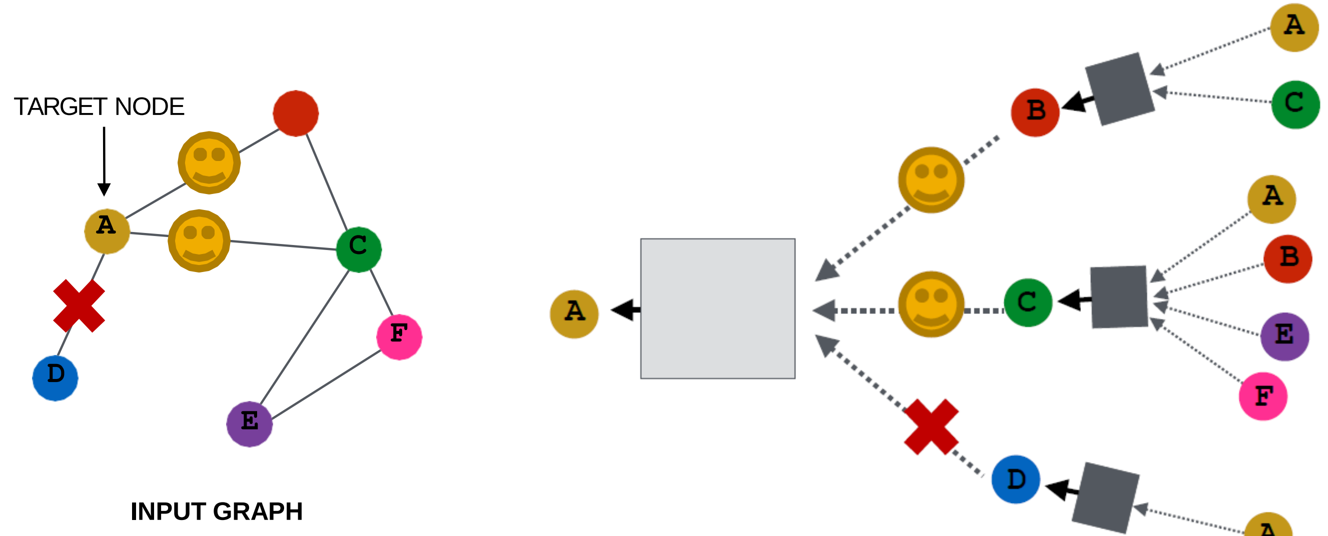
- **In the next layer when we compute the embeddings, we can sample different neighbors**
  - Only nodes C and D will pass messages to A



INPUT GRAPH

Neighorhood Sampling Example

- **In expectation, we get embeddings similar to the case where all the neighbors are used**
  - **Benefits:** Greatly **reduces** computational cost
  - And in practice it works great!



Acknowledgement: Jure Leskovec, Stanford University

GraphSAGE: L_2 Normalization

- **ℓ_2 Normalization:**
  - **Optional:** Apply ℓ_2 normalization to $\mathbf{h}_v^{(l)}$ at every layer
  - $\mathbf{h}_v^{(l)} \leftarrow \frac{\mathbf{h}_v^{(l)}}{\left\|\mathbf{h}_v^{(l)}\right\|_2} \; \forall v \in V$ where $\|u\|_2 = \sqrt{\sum_i u_i^2}$ (ℓ_2-norm)
  - Without ℓ_2 normalization, the embedding vectors have different scales (ℓ_2-norm) for vectors
  - In some cases (not always), normalization of embedding results in performance improvement
  - After ℓ_2 normalization, all vectors will have the same ℓ_2-norm

Classical GNN Layers: GAT(1)

- **(3) Graph Attention Networks**

$$\mathbf{h}_v^{(l)} = \sigma(\textstyle\sum_{u \in N(v)} \underbrace{\boxed{\alpha_{vu}}}_{\text{Attention weights}} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$

- **In GCN / GraphSAGE**
  - $\alpha_{vu} = \frac{1}{|N(v)|}$ is the **weighting factor (importance)** of node u's message to node v
  - $\Longrightarrow$ α_{vu} is defined **explicitly** based on the structural properties of the graph (node degree)
  - $\Longrightarrow$ All neighbors $u \in N(v)$ are equally important to node v

Classical GNN Layers: GAT(2)

- **(3) Graph Attention Networks**

$$\mathbf{h}_v^{(l)} = \sigma(\textstyle\sum_{u\in N(v)} \underbrace{\boxed{\alpha_{vu}}}_{\text{Attention weights}} \mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)})$$

Not all node's neighbors are equally important

- **Attention** is inspired by cognitive attention.
- The **attention** $\boldsymbol{\alpha_{vu}}$ focuses on the important parts of the input data and fades out the rest.
  - **Idea:** the NN should devote more computing power on that small but important part of the data.
  - Which part of the data is more important depends on the context and is learned through training.

Graph Attention Networks

Can we do better than simple neighborhood aggregation?

Can we let weighting factors α_{vu} to be learned?

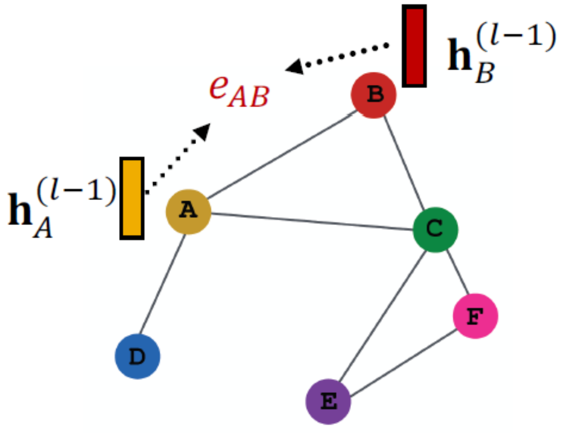
- **Goal:** Specify **arbitrary importance** to different neighbors of each node in the graph
- **Idea:** Compute embedding $\boldsymbol{h}_v^{(l)}$ of each node in the graph following an **attention strategy**:
  - Nodes attend over their neighborhoods' message
  - Implicitly specifying different weights to different nodes in a neighborhood

Attention Mechanism (1)

- Let α_{vu} be computed as a byproduct of an **attention mechanism $\boldsymbol{a}$:**
  - (1) Let a compute **attention coefficients $\boldsymbol{e_{vu}}$** across pairs of nodes u, v based on their messages:

$$e_{vu} = a(\mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}, \mathbf{W}^{(l)}\boldsymbol{h}_v^{(l-1)})$$

    - **$\boldsymbol{e_{vu}}$ indicates the importance of $\boldsymbol{u}'$s message to node $\boldsymbol{v}$**



$$e_{AB} = a(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)})$$

Attention Mechanism (2)

- **Normalize** e_{vu} into the **final attention weight** $\boldsymbol{\alpha_{vu}}$
  - Use the **softmax** function, so that $\sum_{u \in N(v)} \alpha_{vu} = 1$:

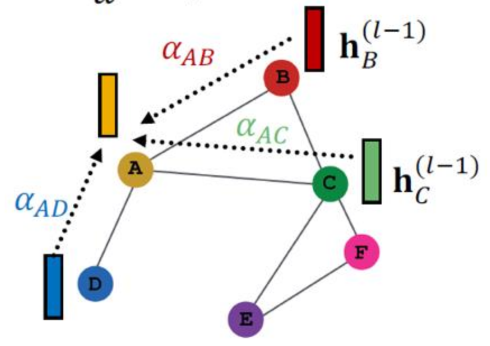
$$\alpha_{vu} = \frac{\exp(e_{vu})}{\sum_{k \in N(v)} \exp(e_{vk})}$$

- **Weighted sum** based on the **final attention weight** $\boldsymbol{\alpha_{vu}}$

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

Weighted sum using α_{AB}, α_{AC}, α_{AD}:

$$\mathbf{h}_A^{(l)} = \sigma(\alpha_{AB}\mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)} + \alpha_{AC}\mathbf{W}^{(l)}\mathbf{h}_C^{(l-1)} + \alpha_{AD}\mathbf{W}^{(l)}\mathbf{h}_D^{(l-1)})$$



- Parameters of a are trained jointly:
  - Learn the parameters together with weight matrices (i.e., other parameter of the neural net $\mathbf{W}^{(l)}$) in an end-to-end fashion

Attention Mechanism (4)

- **Multi-head attention:** Stabilizes the learning process of attention mechanism
  - **Create multiple attention scores** (each replica with a different set of parameters):

$$\mathbf{h}_v^{(l)}[1] = \sigma(\textstyle\sum_{u\in N(v)} \alpha_{vu}^{1} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$

$$\mathbf{h}_v^{(l)}[2] = \sigma(\textstyle\sum_{u\in N(v)} \alpha_{vu}^{2} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$

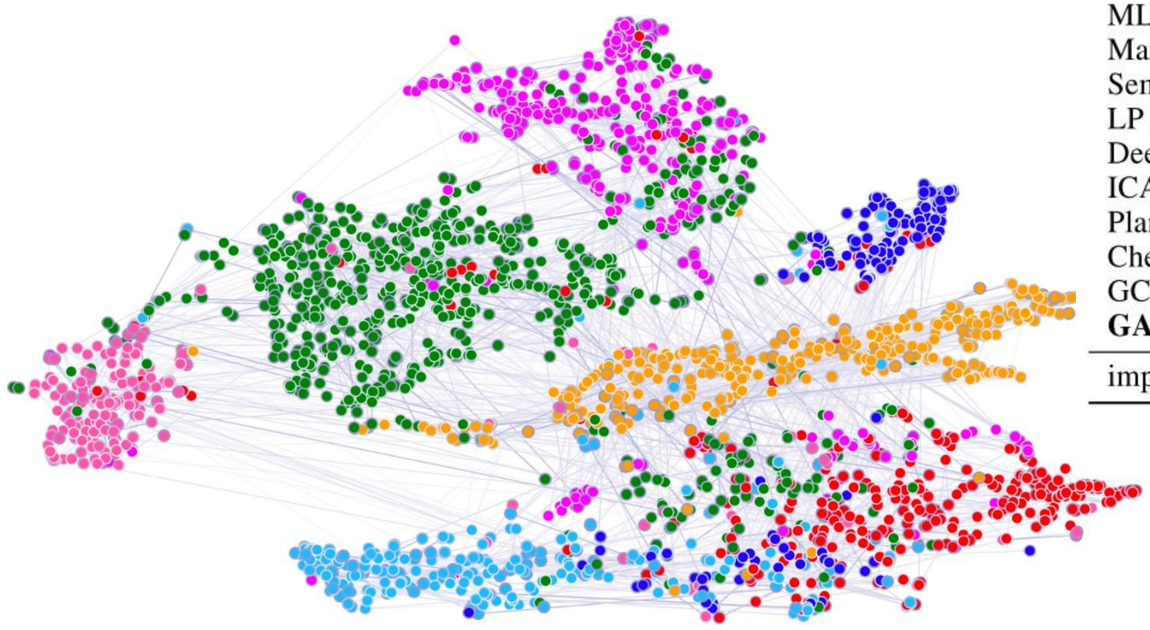
$$\mathbf{h}_v^{(l)}[3] = \sigma(\textstyle\sum_{u\in N(v)} \alpha_{vu}^{3} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$

  - **Outputs are aggregated:**
    - By concatenation or summation
    - $\mathbf{h}_v^{(l)} = \mathrm{AGG}(\mathbf{h}_v^{(l)}[1], \mathbf{h}_v^{(l)}[2], \mathbf{h}_v^{(l)}[3])$

Benefits of Attention Mechanism

- **Key benefit:** Allows for (implicitly) specifying **different importance values (α_{vu}) to different neighbors**
- **Computationally efficient**:
  - Computation of attentional coefficients can be parallelized across all edges of the graph
  - Aggregation may be parallelized across all nodes
- **Storage efficient**:
  - Sparse matrix operations do not require more than $O(V+E)$ entries to be stored
  - **Fixed** number of parameters, irrespective of graph size
- **Localized**:
  - Only **attends over local network neighborhoods**
- **Inductive capability**:
  - It is a shared *edge-wise* mechanism
  - It does not depend on the global graph structure

GAT: Cora Citation Net



Method	Cora
MLP	55.1%
ManiReg (Belkin et al., 2006)	59.5%
SemiEmb (Weston et al., 2012)	59.0%
LP (Zhu et al., 2003)	68.0%
DeepWalk (Perozzi et al., 2014)	67.2%
ICA (Lu & Getoor, 2003)	75.1%
Planetoid (Yang et al., 2016)	75.7%
Chebyshev (Defferrard et al., 2016)	81.2%
GCN (Kipf & Welling, 2017)	81.5%
GAT	**83.3%**
improvement w.r.t GCN	1.8%

Attention mechanism can be used with many different graph neural network models

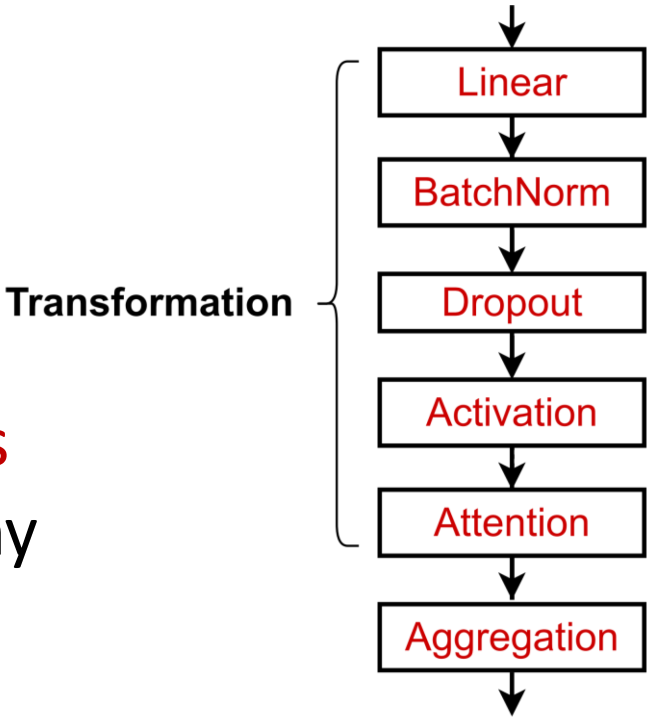
In many cases, attention leads to performance gains

- **t-SNE plot of GAT-based node embeddings:**
  - Node color: 7 publication classes
  - Edge thickness: Normalized attention coefficients between nodes i and j, across eight attention heads, $\sum_k(\alpha_{ij}^k + \alpha_{ji}^k)$

GNN Layer in Practice

- **In practice, these classic GNN layers are a great starting point**
  - We can often get better performance by considering a general GNN layer design
  - Concretely, we can include modern deep learning modules that proved to be useful in many domains

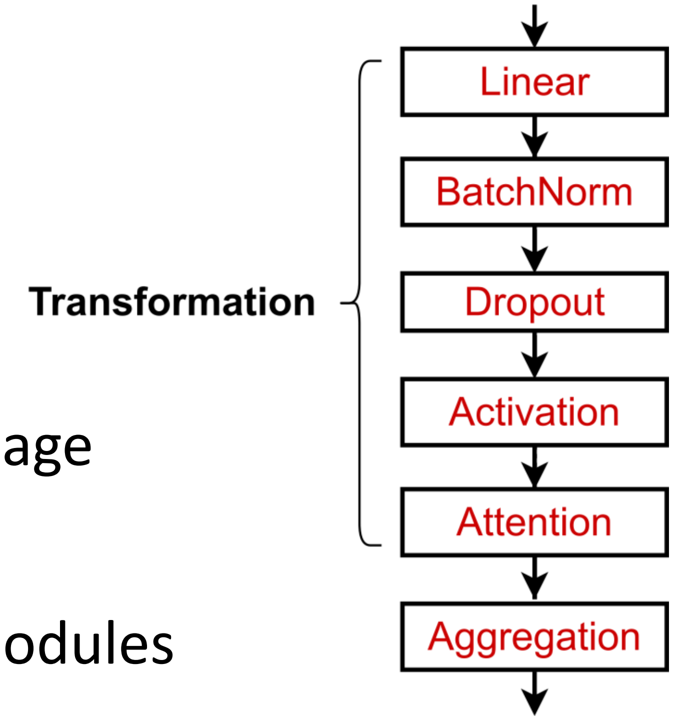
A suggested GNN Layer



GNN Layer in Practice

- **Many modern deep learning modules can be incorporated into a GNN layer**
  - **Batch Normalization:**
    - Stabilize neural network training
  - **Dropout:**
    - Prevent overfitting
  - **Attention/Gating:**
    - Control the importance of a message
  - **More:**
    - Any other useful deep learning modules

A suggested GNN Layer



Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift

Batch Normalization

- **Goal**: Stabilize neural networks training
- **Idea**: Given a batch of inputs (node embeddings)
  - Re-center the node embeddings into zero mean
  - Re-scale the variance into unit variance

Input: $\mathbf{X} \in \mathbb{R}^{N \times D}$
N node embeddings

Trainable Parameters:
$\boldsymbol{\gamma}, \boldsymbol{\beta} \in \mathbb{R}^{D}$

Output: $\mathbf{Y} \in \mathbb{R}^{N \times D}$
Normalized node embeddings

Step 1:
Compute the mean and variance over N embeddings

$$\boldsymbol{\mu}_j = \frac{1}{N}\sum_{i=1}^{N} \mathbf{X}_{i,j}$$

$$\boldsymbol{\sigma}_j^2 = \frac{1}{N}\sum_{i=1}^{N} \left(\mathbf{X}_{i,j} - \boldsymbol{\mu}_j\right)^2$$

Step 2:
Normalize the feature using computed mean and variance

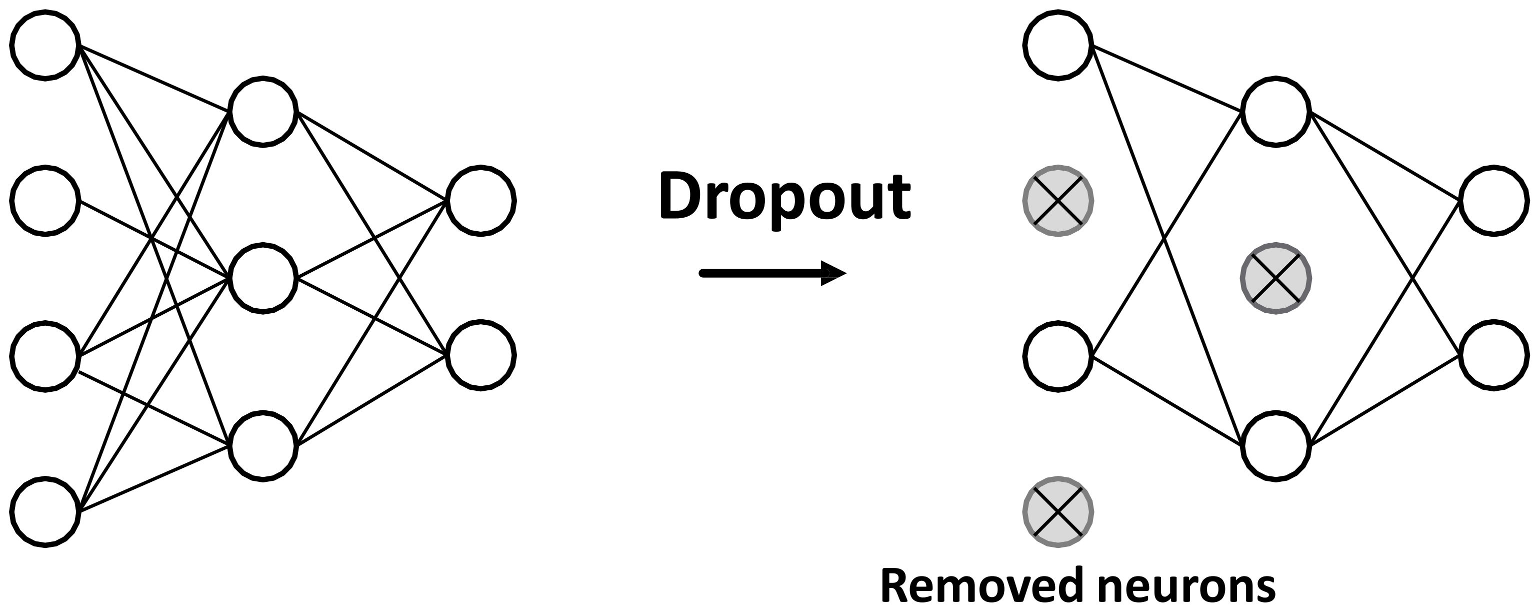
$$\widehat{\mathbf{X}}_{i,j} = \frac{\mathbf{X}_{i,j} - \boldsymbol{\mu}_j}{\sqrt{\boldsymbol{\sigma}_j^2 + \epsilon}}$$

$$\mathbf{Y}_{i,j} = \boldsymbol{\gamma}_j \widehat{\mathbf{X}}_{i,j} + \boldsymbol{\beta}_j$$

Dropout: A Simple Way to Prevent Neural Networks from Overfitting

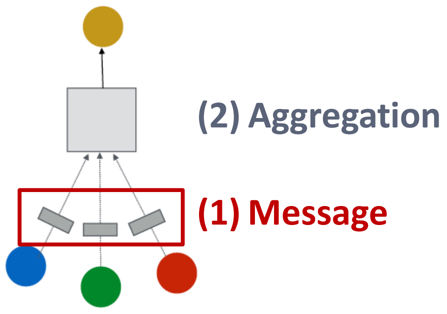
Dropout

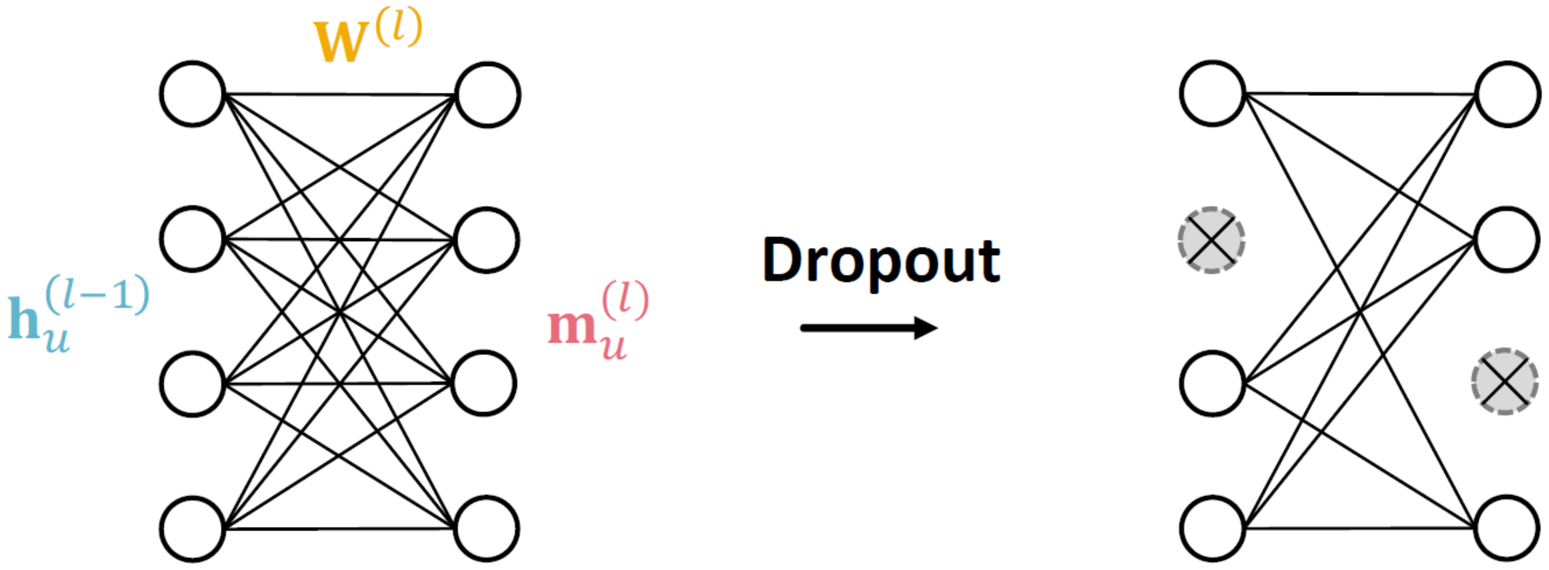
- **Goal**: Regularize a neural net to prevent overfitting.
- **Idea**:
  - **During training**: with some probability p, randomly set neurons to zero (turn off)
  - **During testing:** Use all the neurons for computation



Dropout for GNNs

- In GNN, Dropout is applied to **the linear layer in the message function**
  - **A simple message function with linear layer:** $\mathbf{m}_u^{(l)} = \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}$

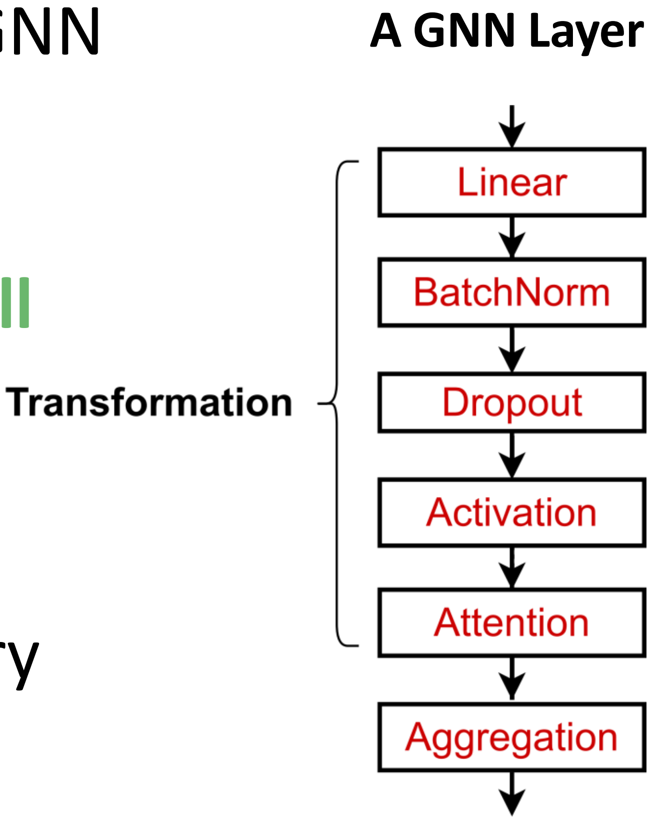




Visualization of a linear layer

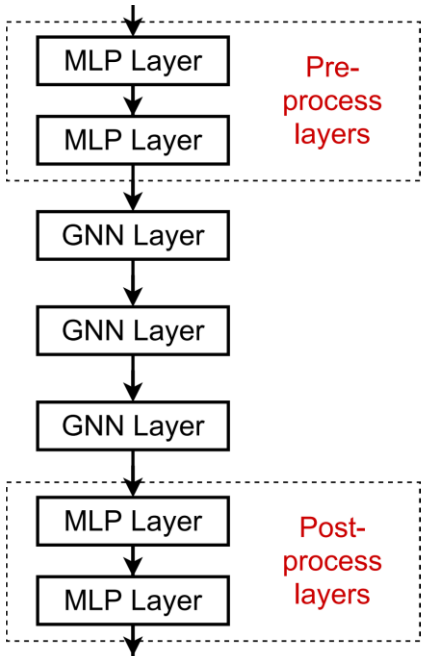
GNN Layer in Practice

- Summary: Modern deep learning **modules** can be included into a GNN layer for better performance
- Designing novel GNN layers is still an active research frontier!
- Suggested resources: You can explore diverse GNN designs or try out your own ideas in GraphGym



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**



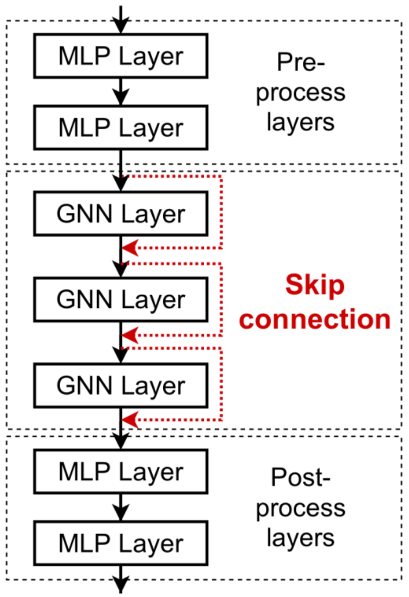
Pre-processing layers: Important when encoding node features is necessary.
E.g., when nodes represent images/text

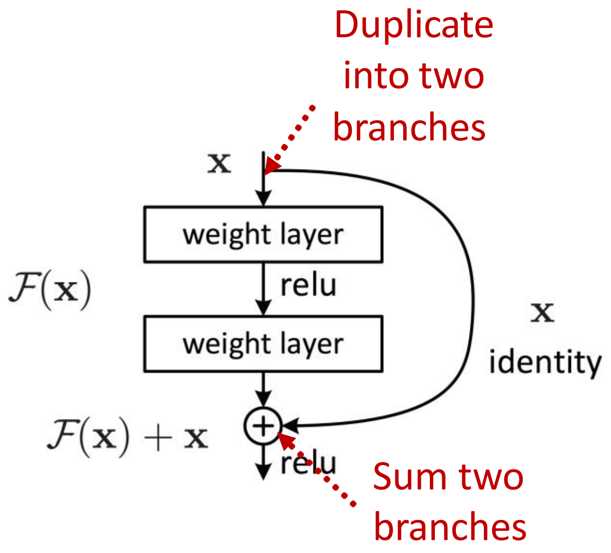
Post-processing layers: Important when reasoning / transformation over node embeddings are needed
E.g., graph classification, knowledge graphs

In practice, adding these layers works great!

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**




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

Idea of skip connections:
Before adding shortcuts:

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

After adding shortcuts:

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

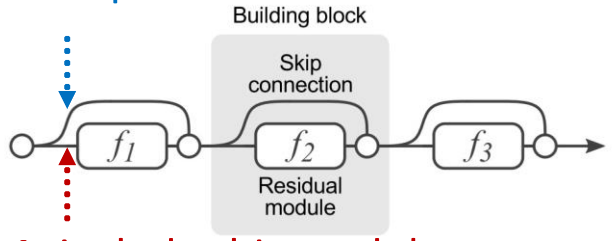
Skip Connections

- **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:

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

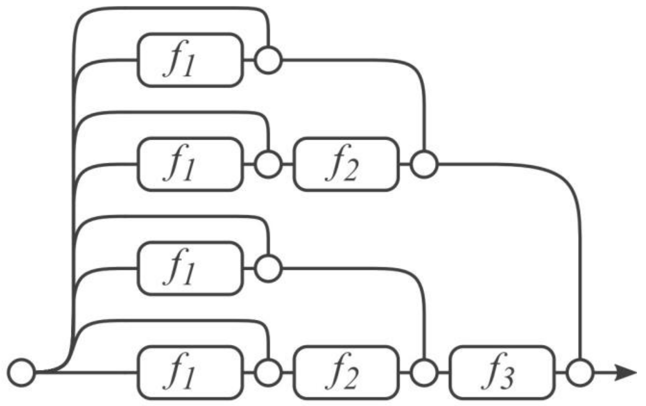
Path 2: skip this module



Path 1: include this module

(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

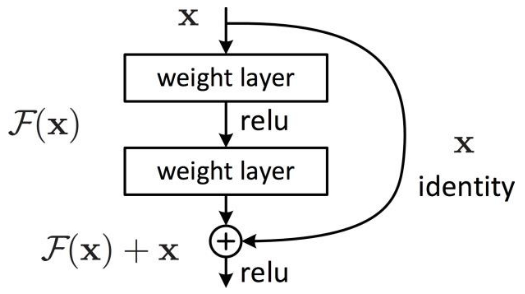
GCN with Skip Connections

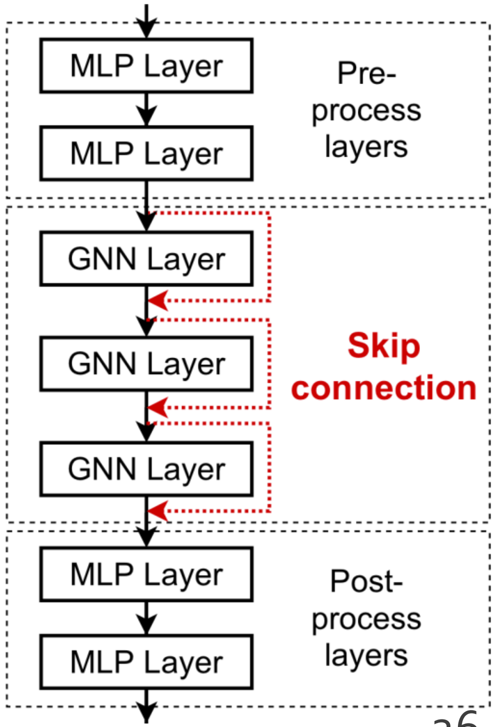
- **A standard GCN layer**

- $$\mathbf{h}_v^{(l)} = \sigma\left(\underbrace{\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}}_{\text{This is our } F(\mathbf{x})}\right)$$

- **A GCN layer with skip connection**

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

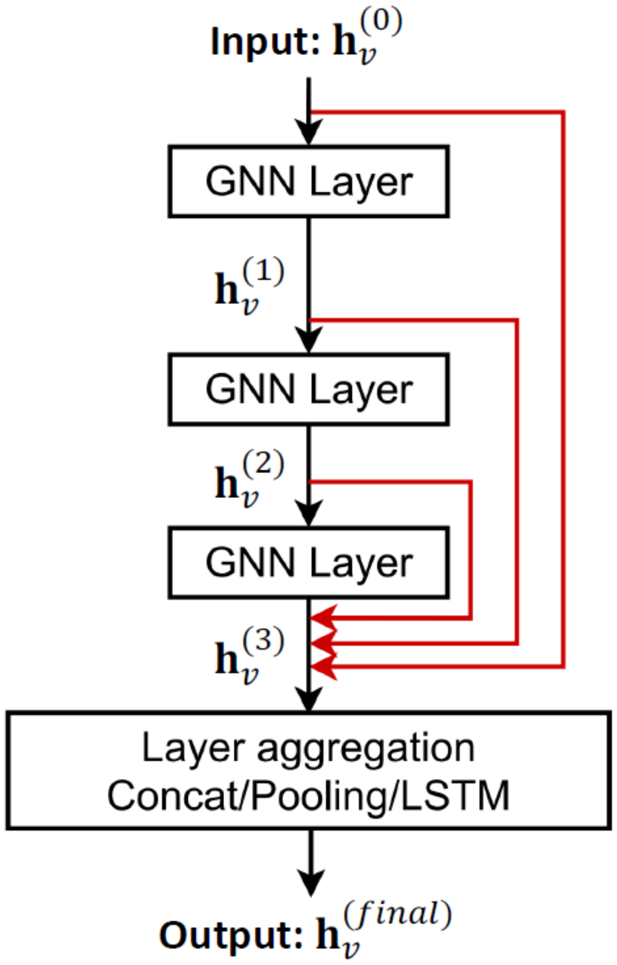




Representation learning on graphs with jumping knowledge networks

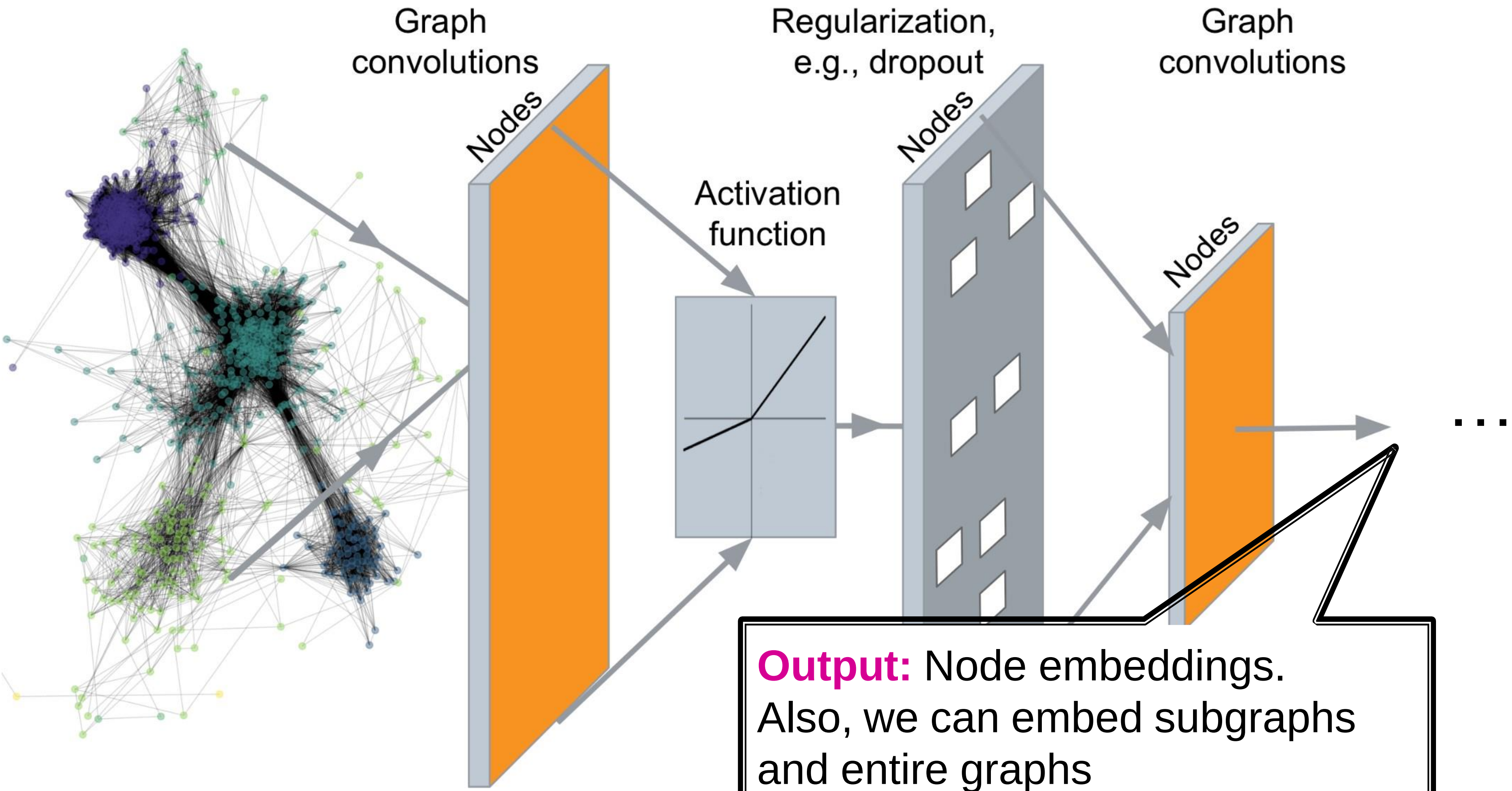
Other Skip Connections

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



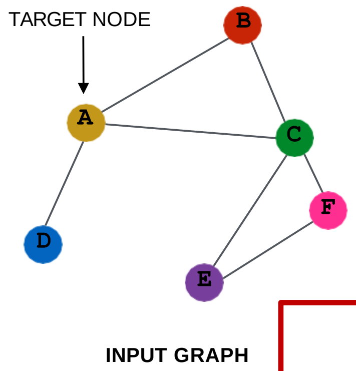
Graph Augmentation

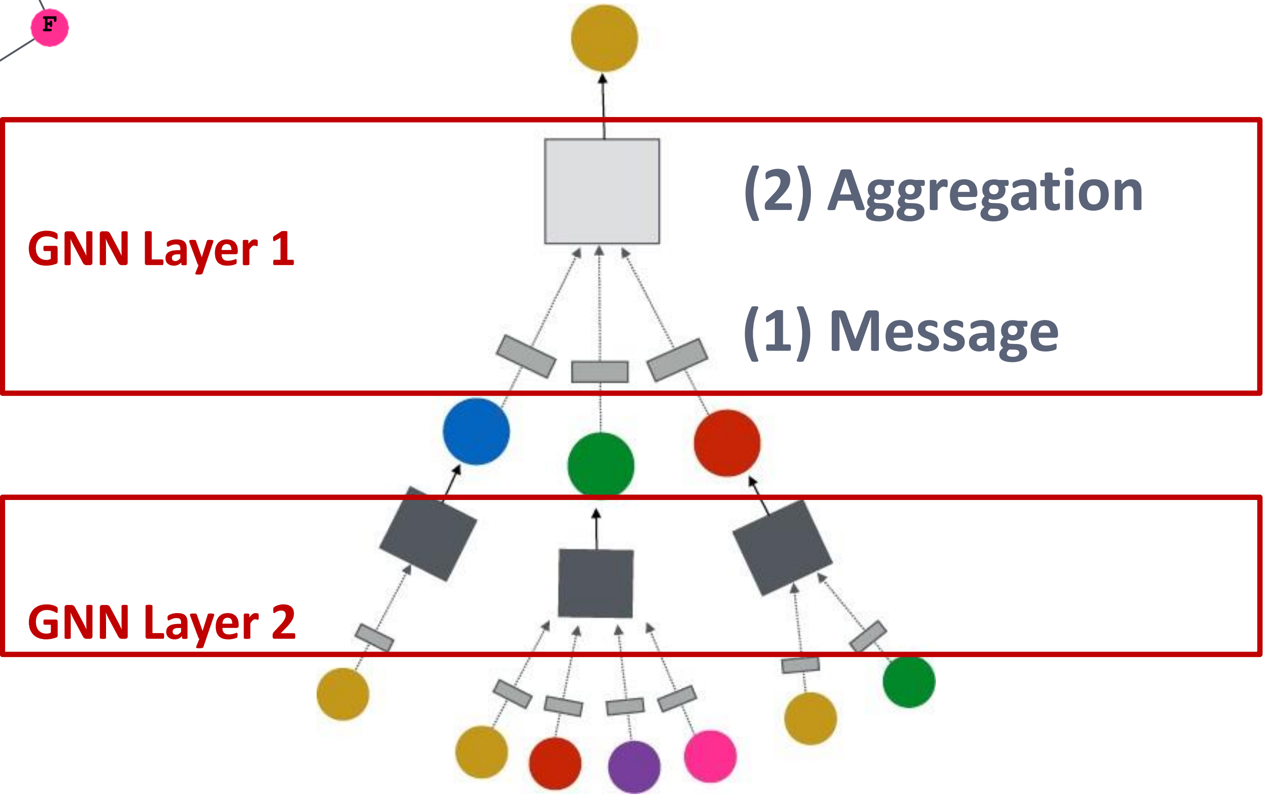
Recap: Deep Graph Encoders



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

Recap: GNN Framework





(5) Learning objective

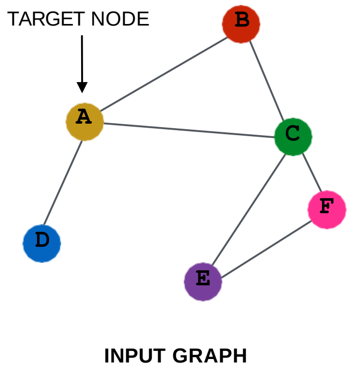
(3) Layer connectivity

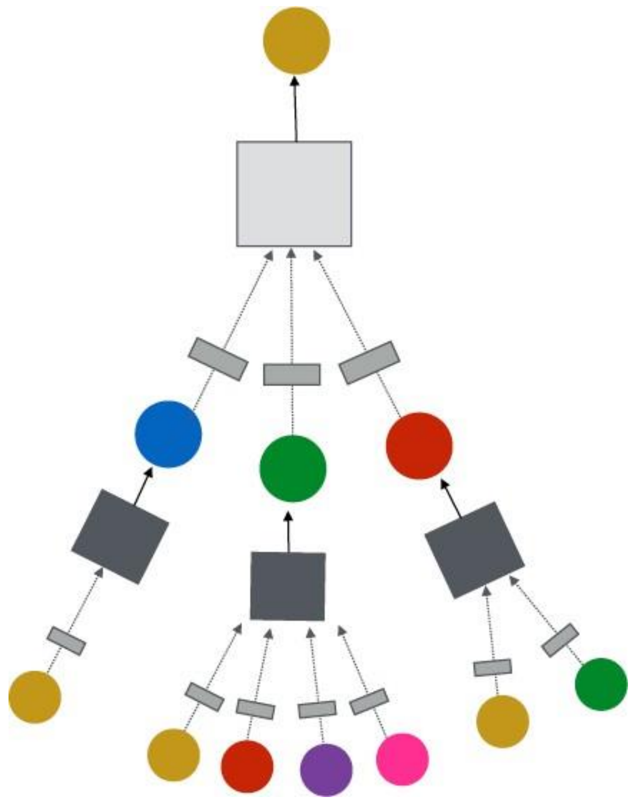
(4) Graph augmentation

GNN Framework

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

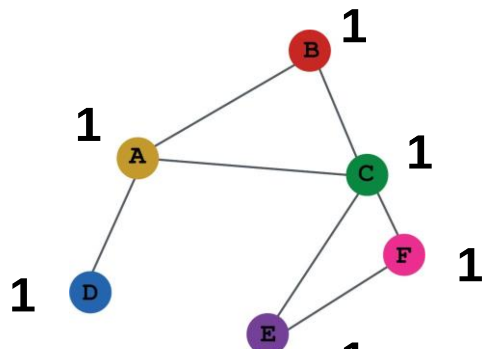
Graph Augmentation Approaches

- **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**

Features Augmentation on Graphs

When might 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**

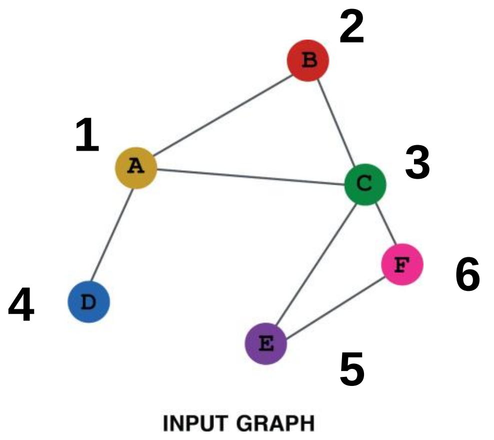


INPUT GRAPH

Features Augmentation on Graphs

When might 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**



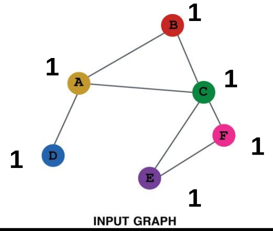
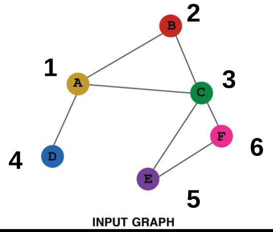
One-hot vector for node with ID=5

ID = 5

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

Features Augmentation on Graphs

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

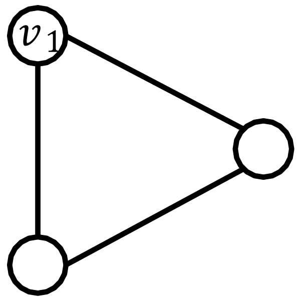
	Constant node feature 	**One-hot node feature** 
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a unique ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple 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)

Features Augmentation on Graphs

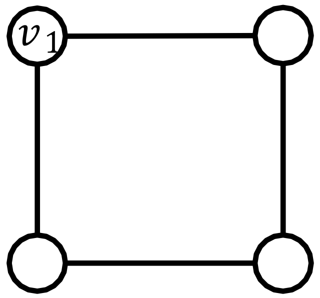
When might we need feature augmentation?

- **(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



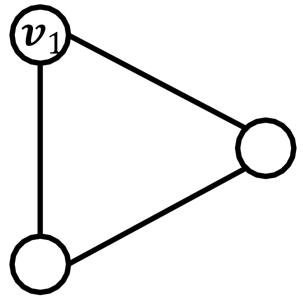
v_1 resides in a cycle with length 4



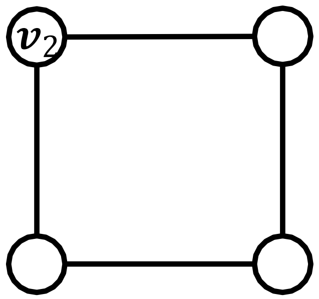
Features Augmentation on Graphs

- **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

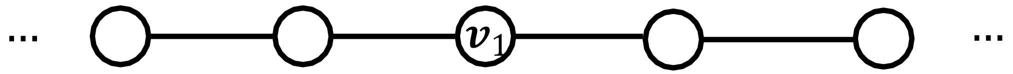
$v_!$ resides in a cycle with length 3



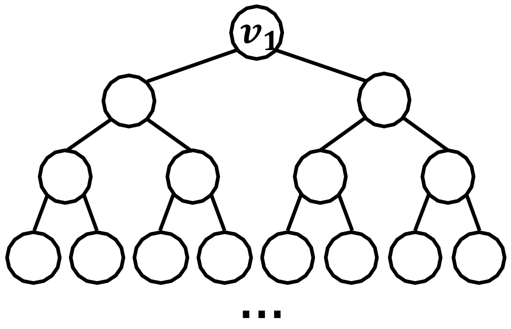
$v_!$ resides in a cycle with length 4



$v_!$ resides in a cycle with infinite length



The computational graphs for node v_1 are always the same



Features Augmentation on Graphs

When might we need feature augmentation?

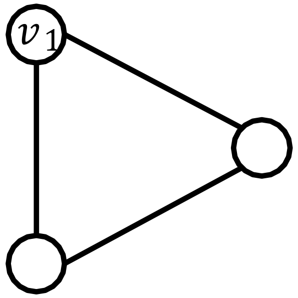
- **(2) Certain structures are hard to learn by GNN**
- Solution: We can use cycle count as augmented node features

We start from cycle with length 0

Augmented node feature for v_1

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

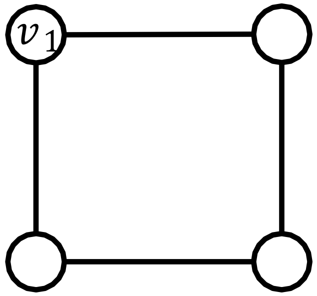
v_1 resides in a cycle with length 3



Augmented node feature for v_1

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

v_1 resides in a cycle with length 4



Features Augmentation on Graphs

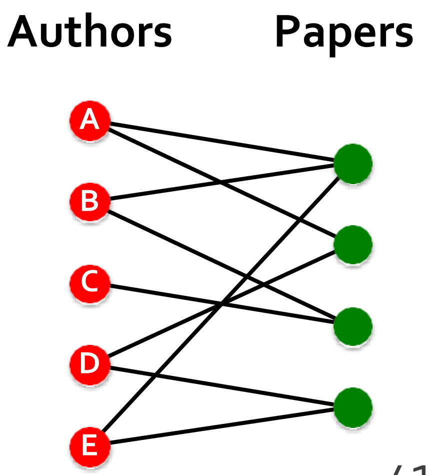
When might we need feature augmentation?

- **(2) Certain structures are hard to learn by GNN**
- Other commonly used augmented features:
  - **Node degree**
  - **Clustering coefficient**
  - **Centrality**
  - **…**

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 $A + A^2$

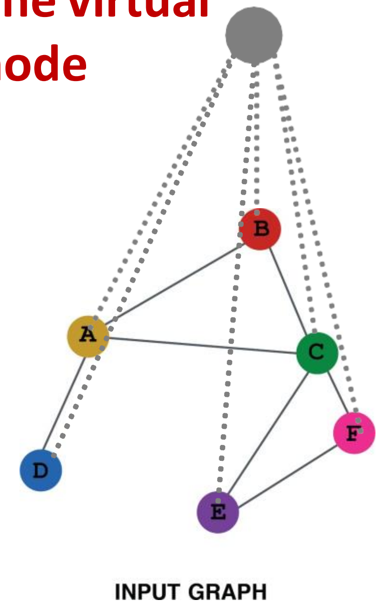
- **Use cases:** Bipartite graphs
  - Author-to-papers (they authored)
  - 2-hop virtual edges make an author-author collaboration graph



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**

The virtual node


B
A
C
F
D
E
INPUT GRAPH