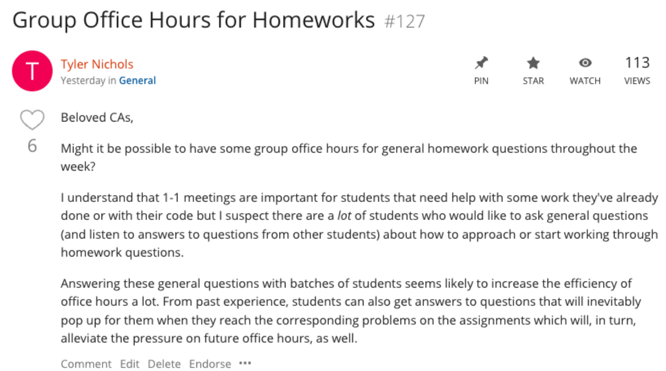
Stanford CS224W: A General Perspective on Graph Neural Networks

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

Announcements

- Colab 1 due this Thursday
- Colab 2 out on Thursday (same day)
- Thank you for the suggestion for in-person & group office hours!



Group Office Hours for Homeworks #127

Tyler Nichols
Yesterday in General

PIN STAR WATCH 113 VIEWS

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Beloved CAs,

Might it be possible to have some group office hours for general homework questions throughout the week?

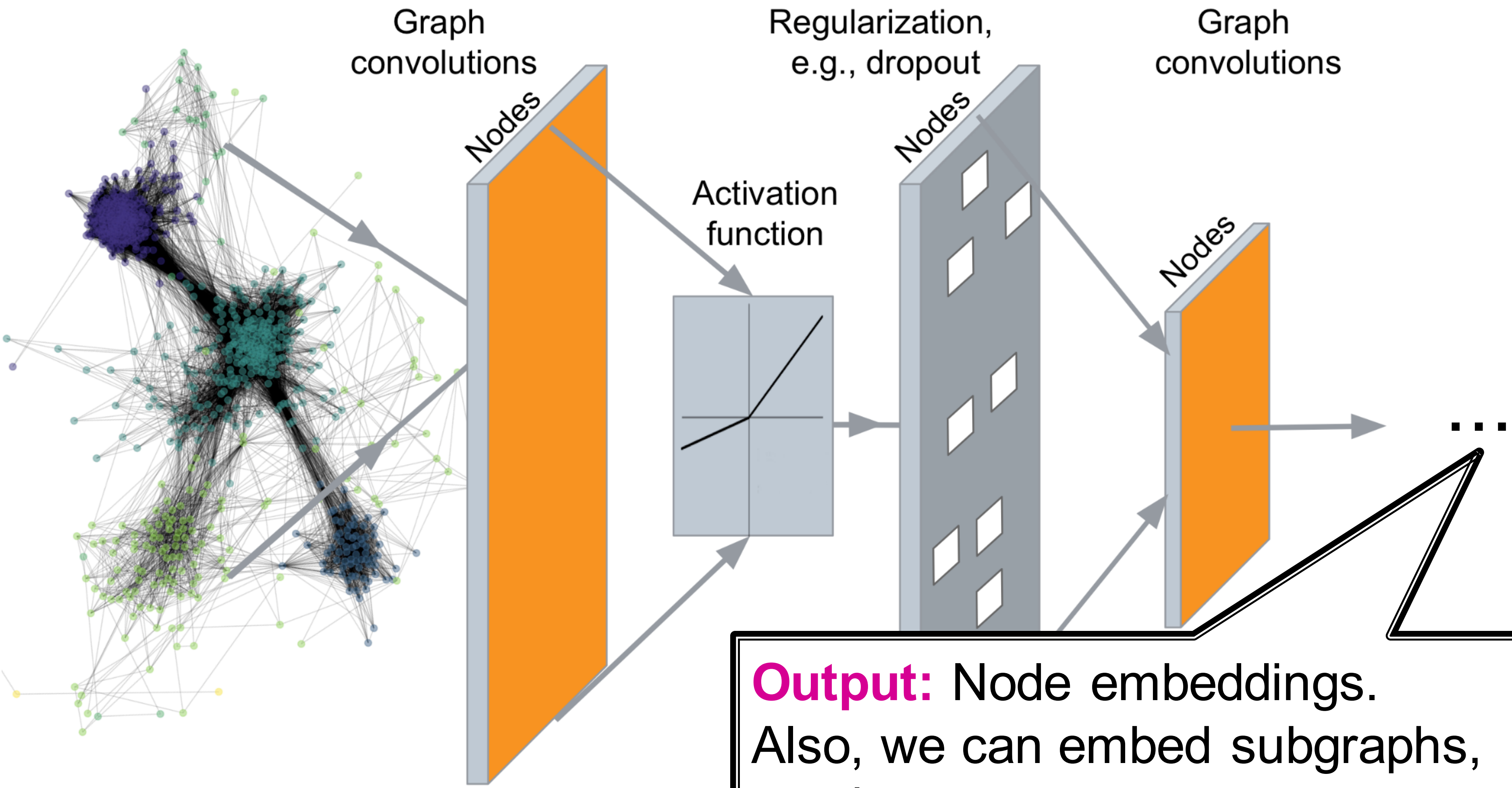
I understand that 1-1 meetings are important for students that need help with some work they've already done or with their code but I suspect there are a *lot* of students who would like to ask general questions (and listen to answers to questions from other students) about how to approach or start working through homework questions.

Answering these general questions with batches of students seems likely to increase the efficiency of office hours a lot. From past experience, students can also get answers to questions that will inevitably pop up for them when they reach the corresponding problems on the assignments which will, in turn, alleviate the pressure on future office hours, as well.

Comment Edit Delete Endorse ···

- We will be hosting 1 group OH in person a week. CA Zhuoyi Huang will lead these.

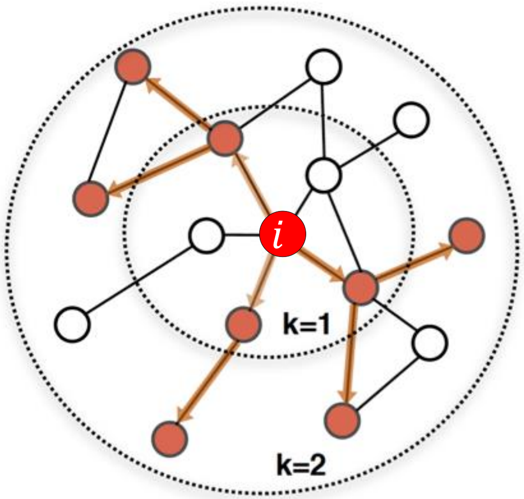
Recap: Deep Graph Encoders

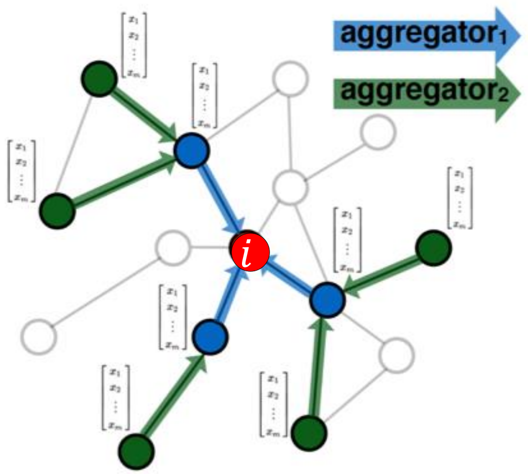


Output: Node embeddings. Also, we can embed subgraphs, graphs

Recap: Graph Neural Networks

Idea: Node's neighborhood defines a computation graph





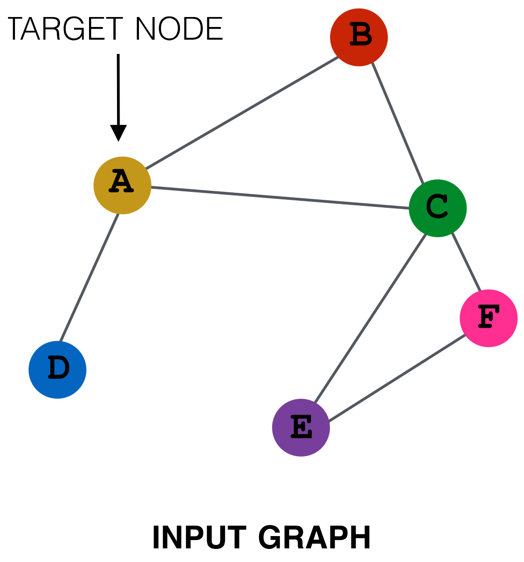
Determine node computation graph

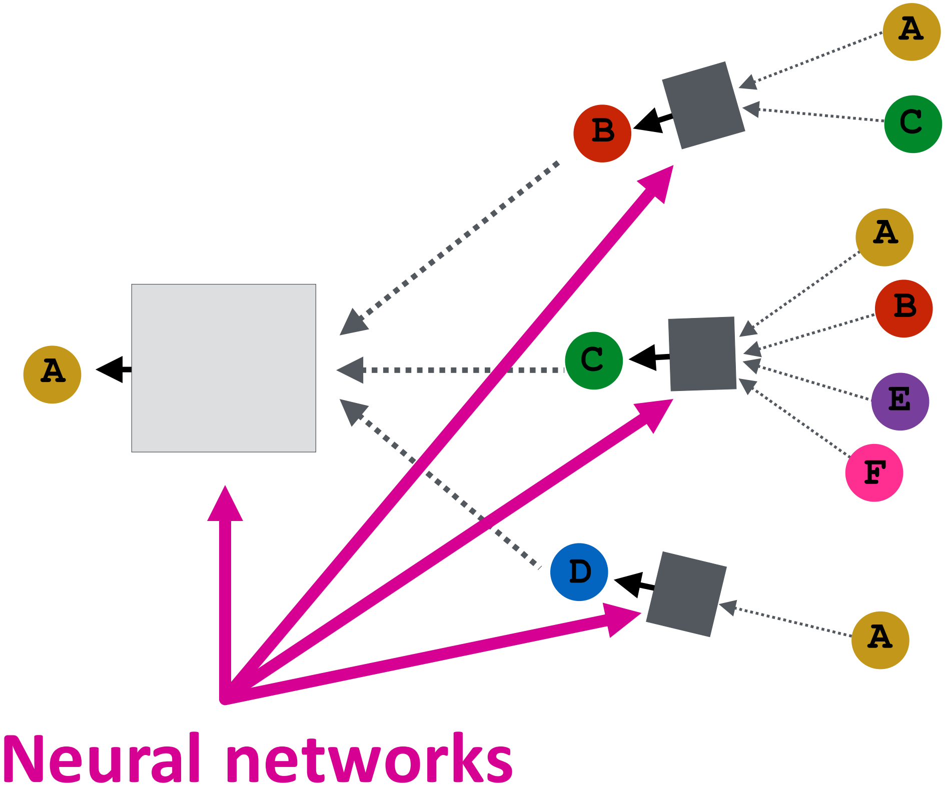
Propagate and transform information

Learn how to propagate information across the graph to compute node features

Recap: Aggregate from Neighbors

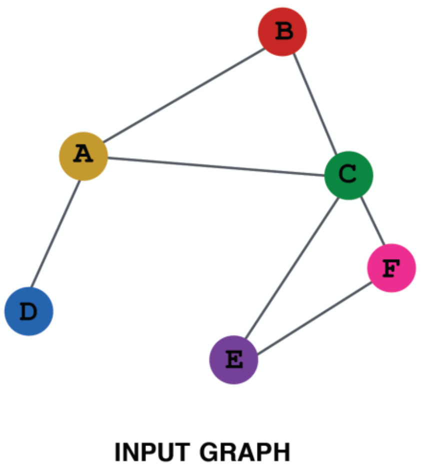
- **Intuition:** Nodes aggregate information from their neighbors using neural networks



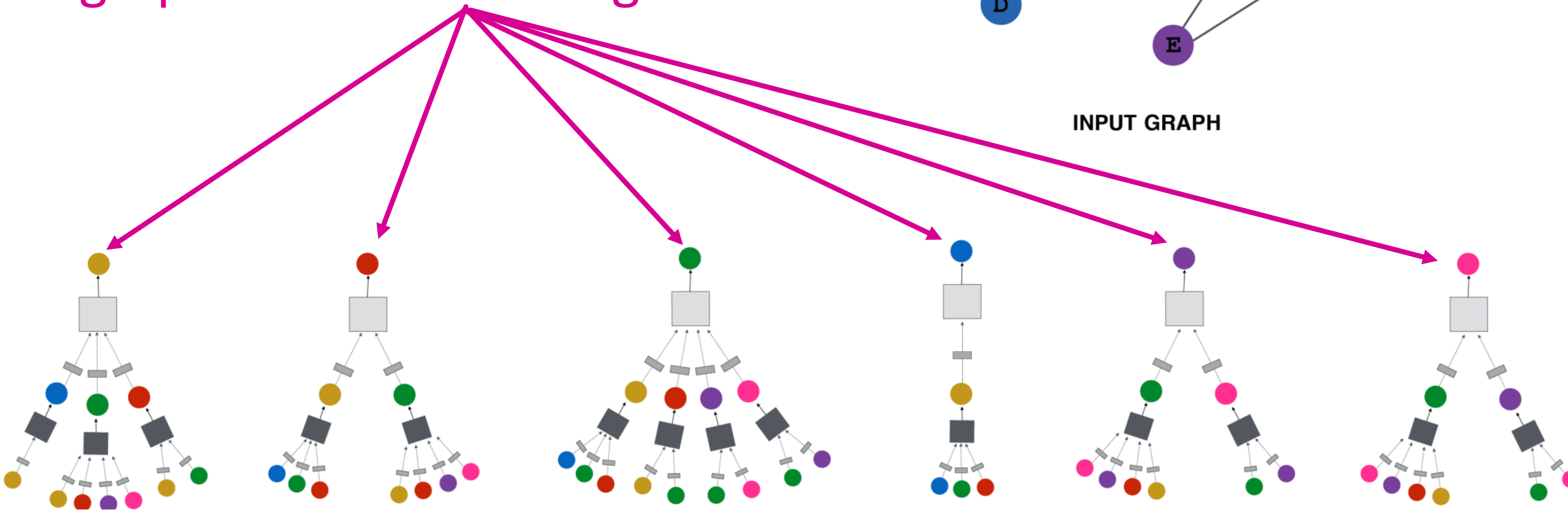


Recap: Aggregate Neighbors

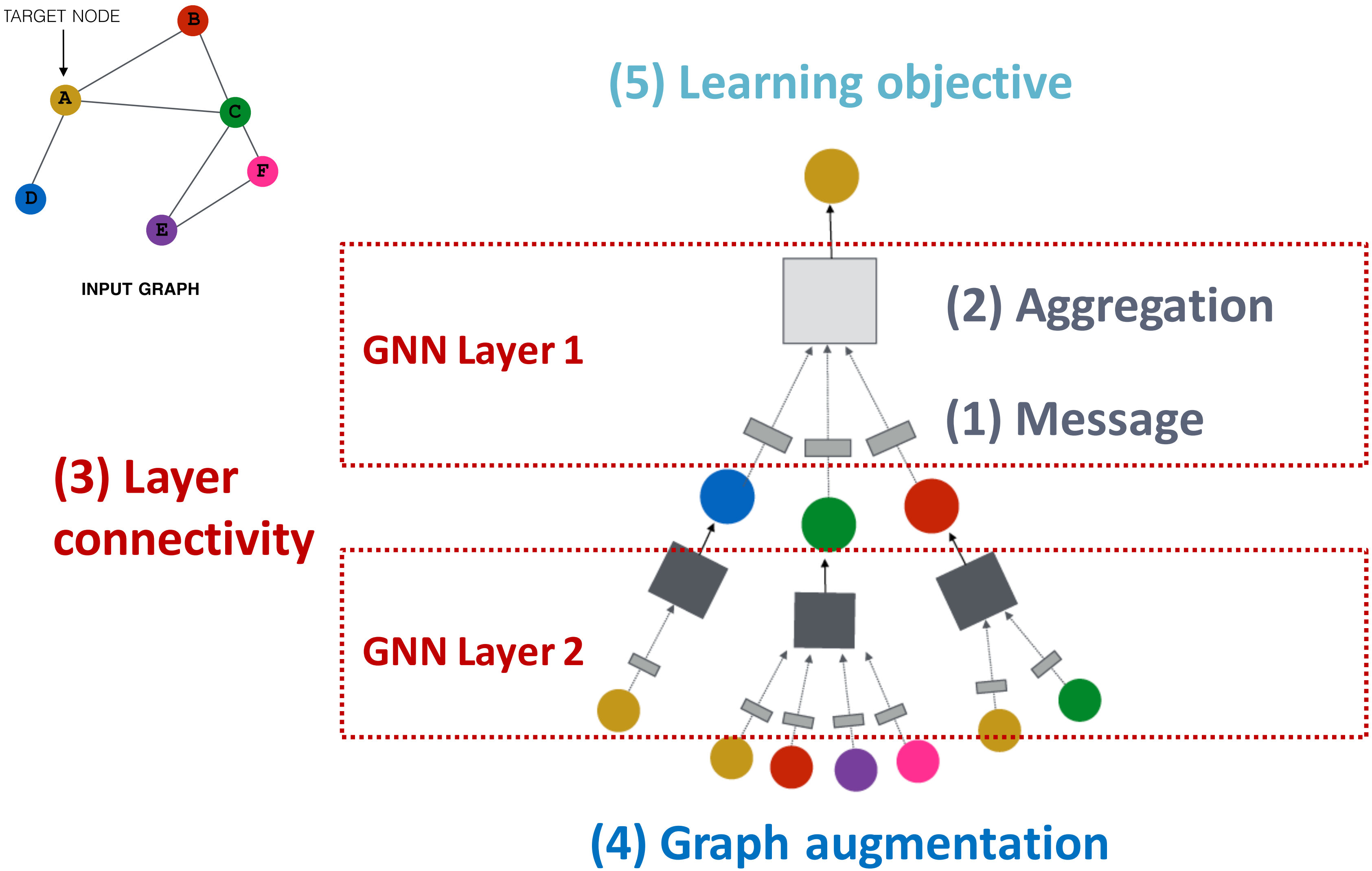
- **Intuition:** Network neighborhood defines a computation graph



Every node defines a computation graph based on its neighborhood!

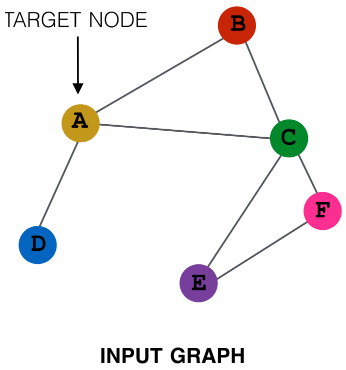


Today: A General GNN Framework



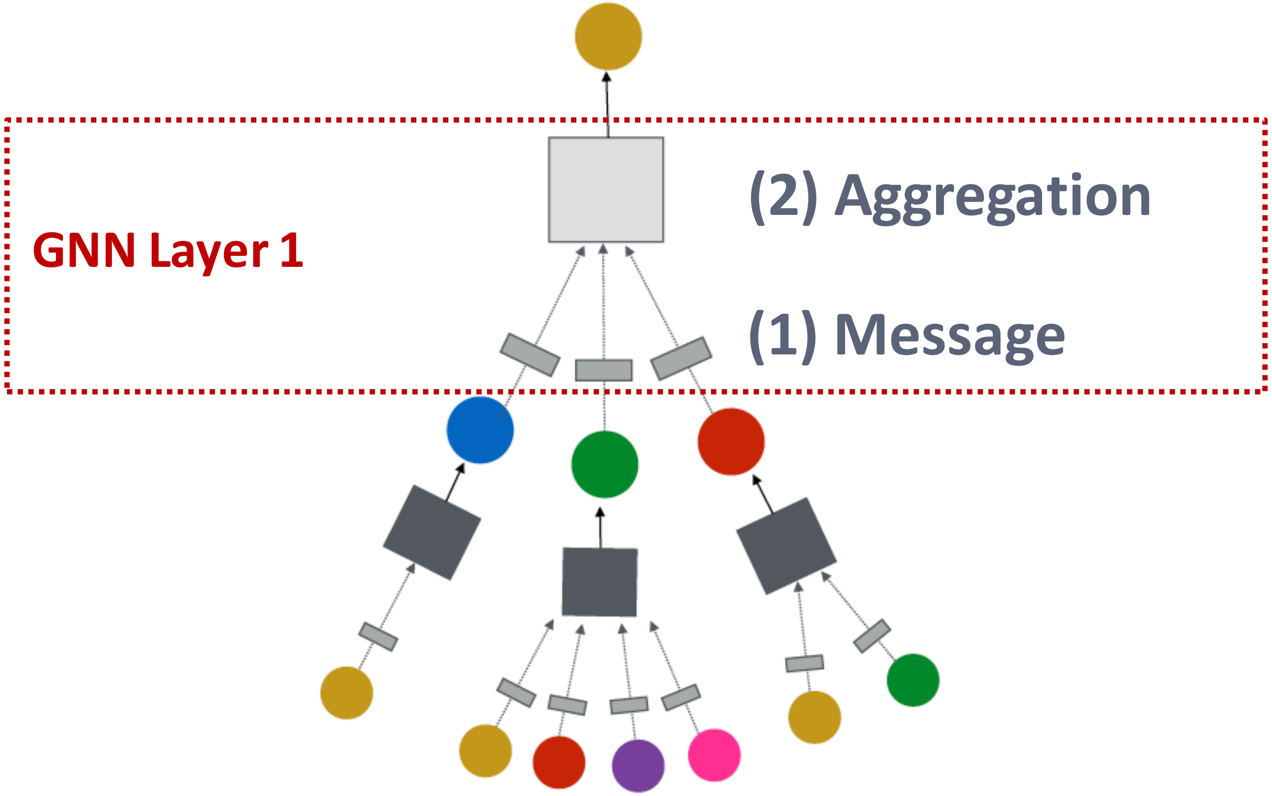
J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020

A General GNN Framework (1)

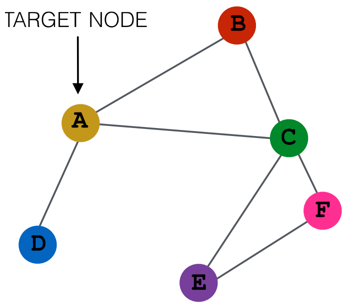


GNN Layer = Message + Aggregation

- Different instantiations under this perspective
- GCN, GraphSAGE, GAT, …



A General GNN Framework (2)

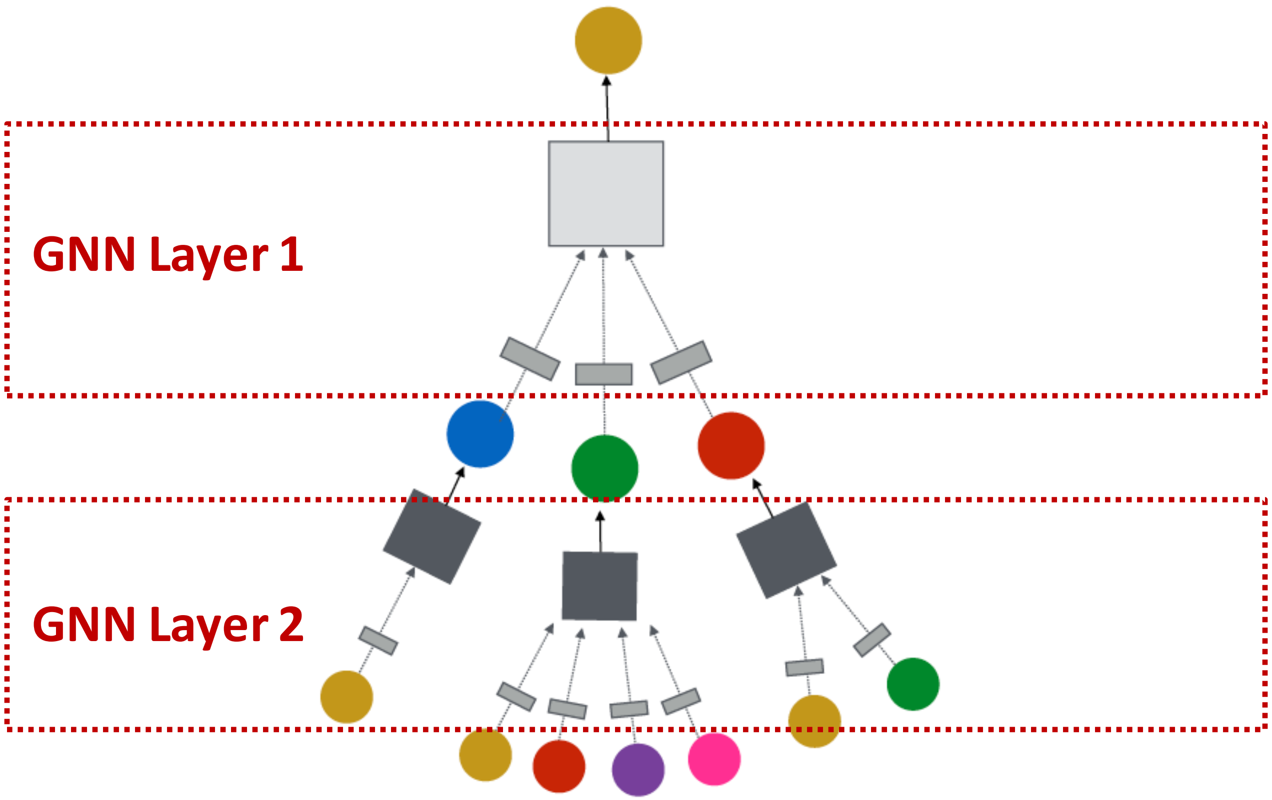


INPUT GRAPH

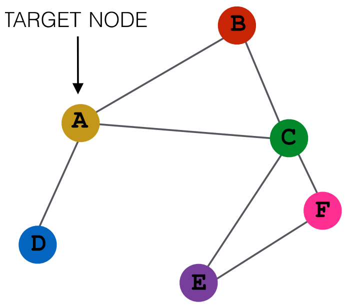
Connect GNN layers into a GNN

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

(3) Layer connectivity



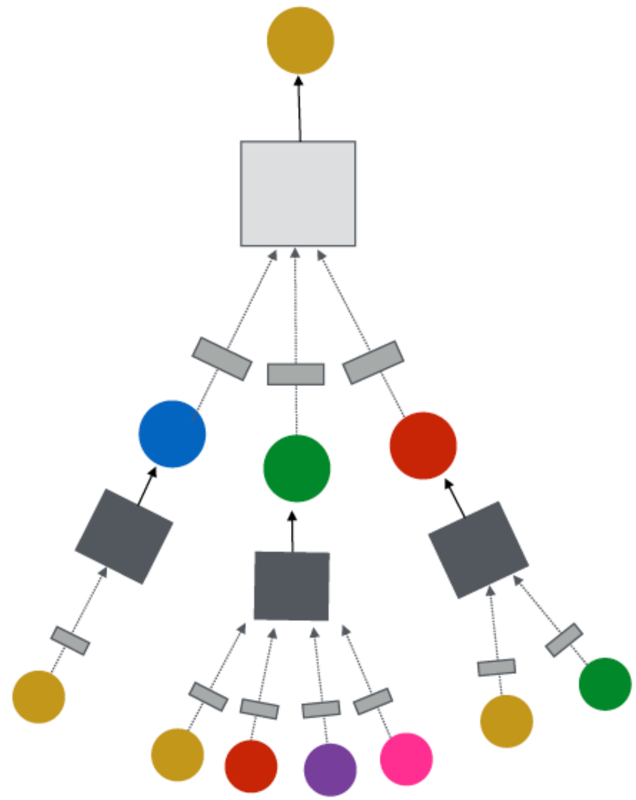
A General GNN Framework (3)



INPUT GRAPH

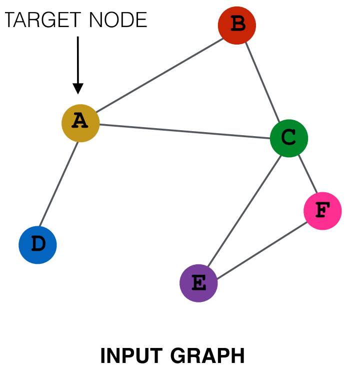
Idea: Raw input graph ≠ computational graph

- **Graph feature augmentation**
- **Graph structure augmentation**

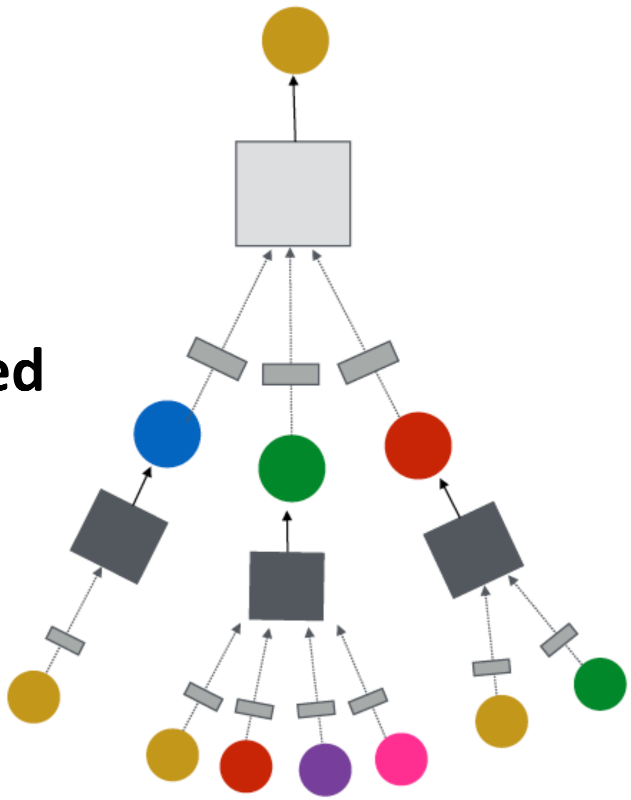


(4) Graph augmentation

A General GNN Framework (4)



(5) Learning objective

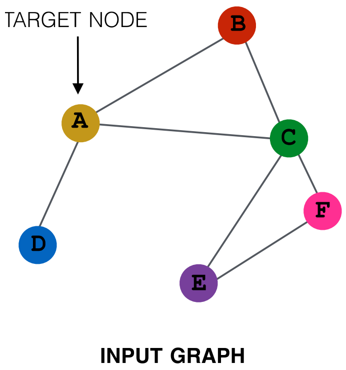


How do we train a GNN

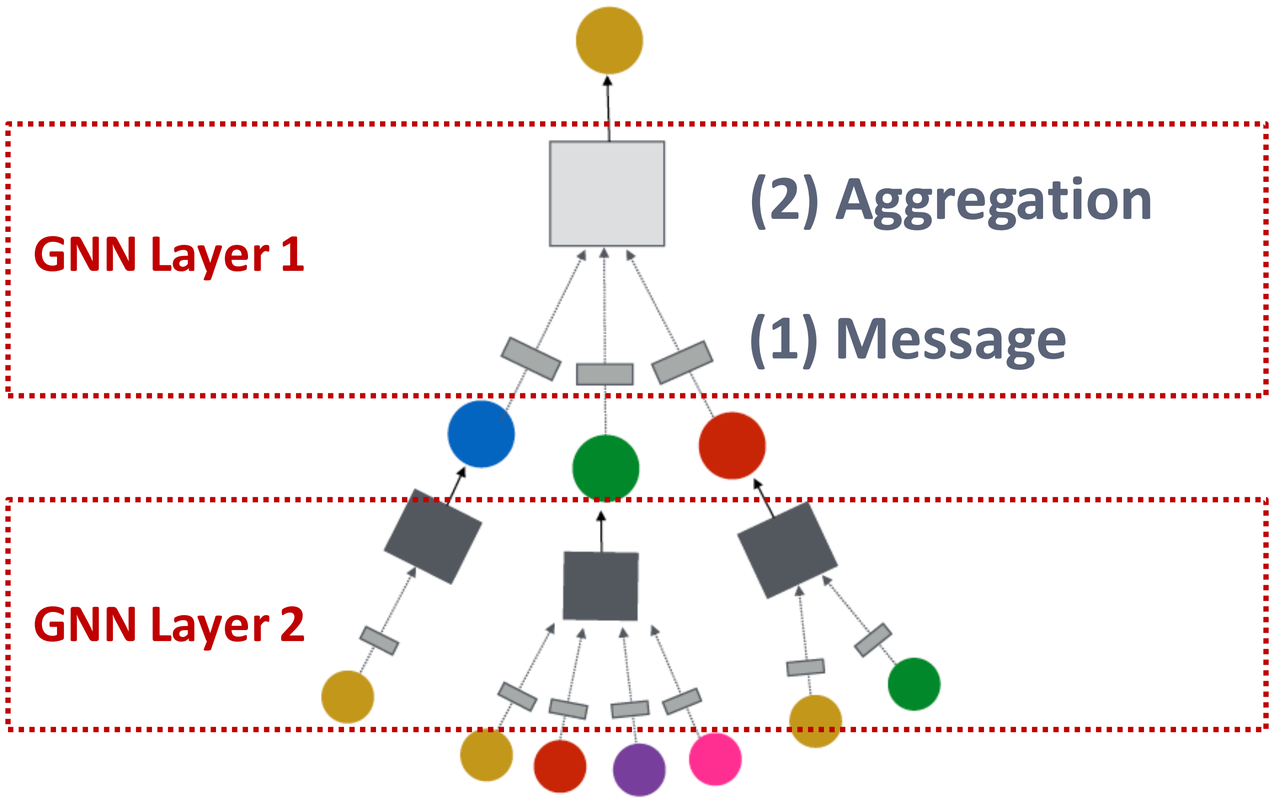
- **Supervised/Unsupervised objectives**
- **Node/Edge/Graph level objectives**

(We will discuss all of these later in class)

GNN Framework: Summary



(5) Learning objective



(3) Layer connectivity

(4) Graph augmentation

Stanford CS224W: A Single Layer of a GNN

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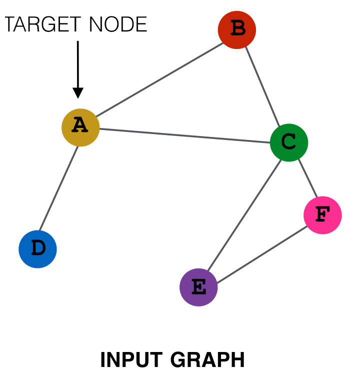
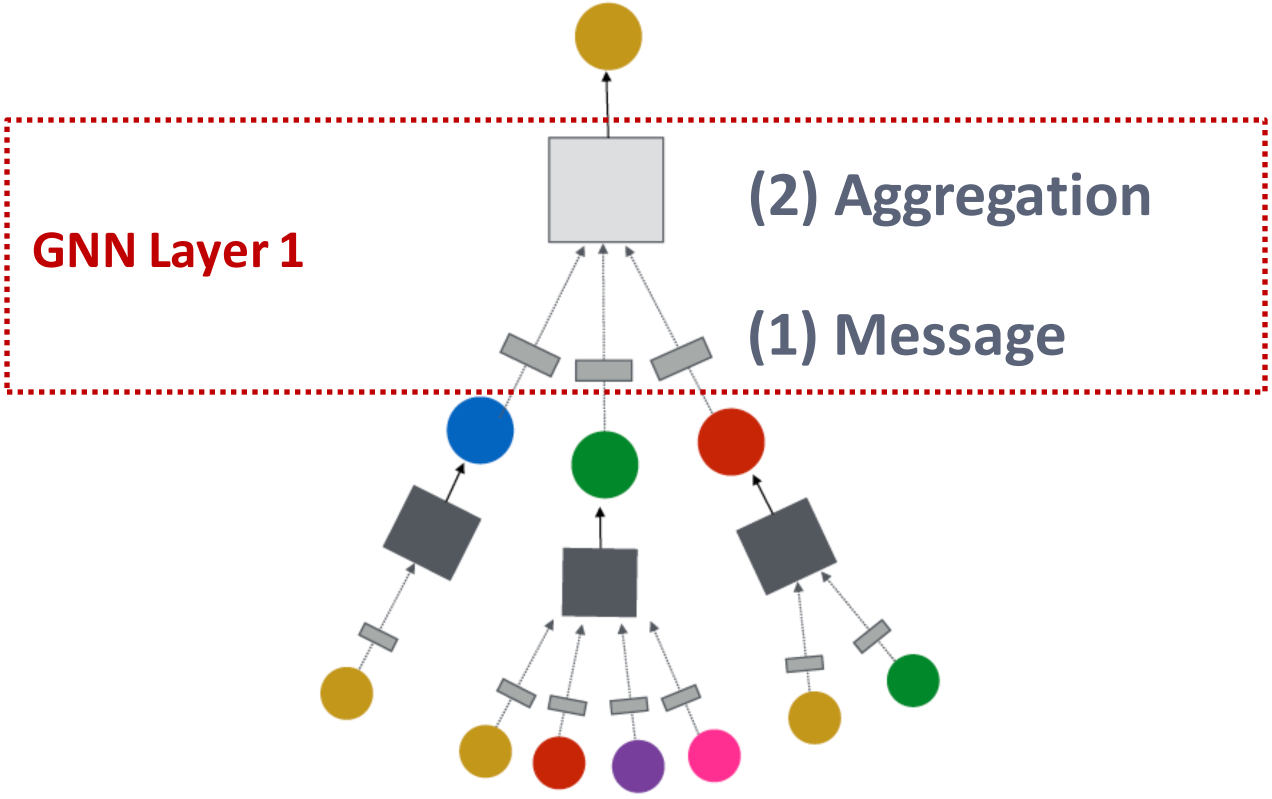
J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020

A GNN Layer

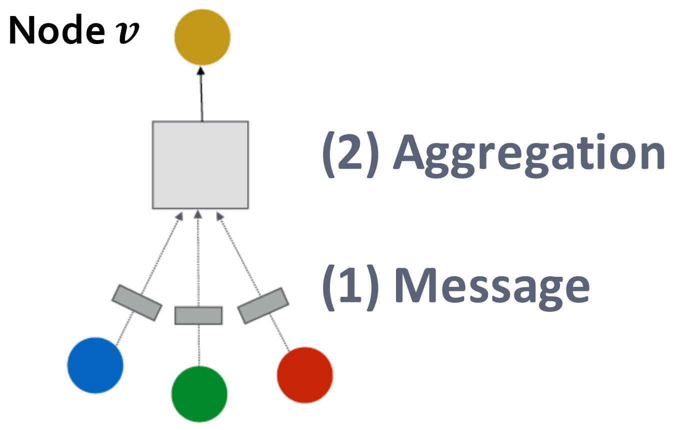


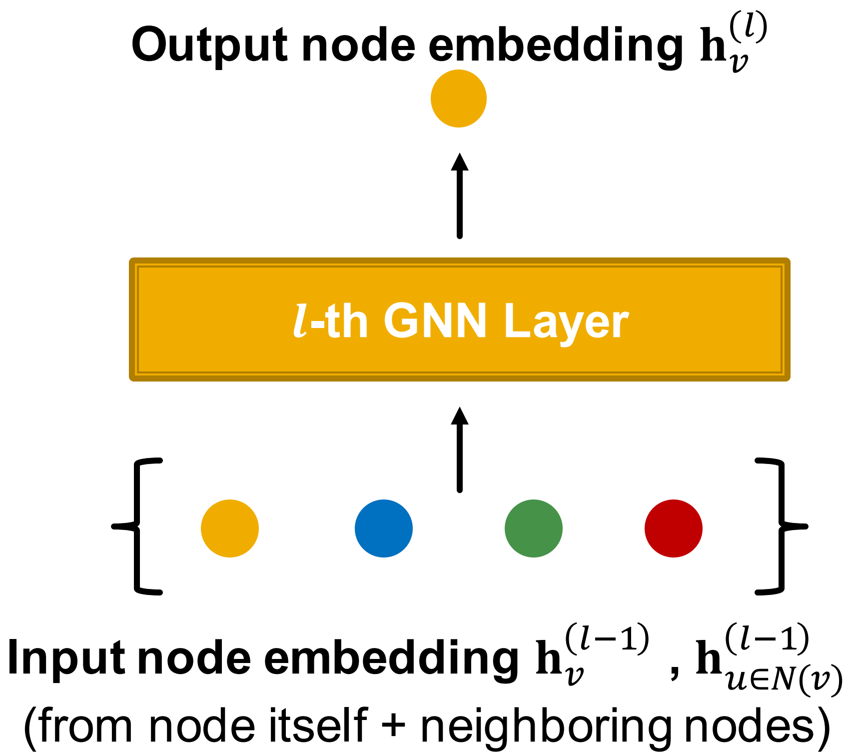
GNN Layer = Message + Aggregation
- **Different instantiations under this perspective**
- **GCN, GraphSAGE, GAT, …**



A Single GNN Layer

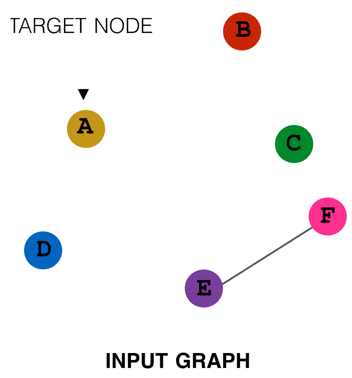
- **Idea of a GNN Layer:**
  - Compress a set of vectors into a single vector
  - **Two-step process:**
    - **(1) Message**
    - **(2) Aggregation**

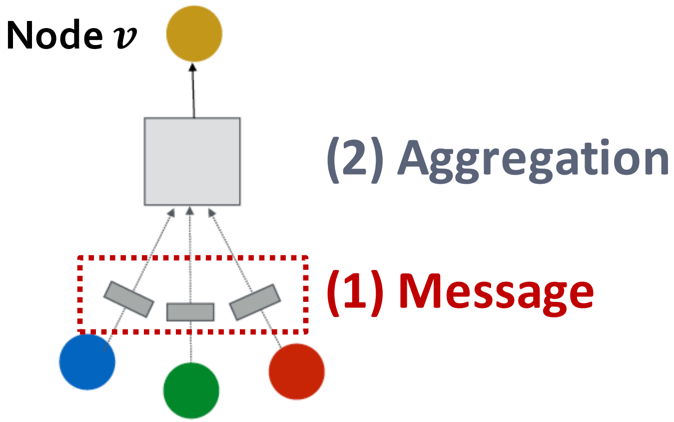




Message Computation

- **(1) Message computation**
  - **Message function:** $\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right)$
    - **Intuition:** Each node will create a message, which will be sent to other nodes later
    - **Example:** A Linear layer $\mathbf{m}_u^{(l)} = \mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}$
      - Multiply node features with weight matrix $\mathbf{W}^{(l)}$



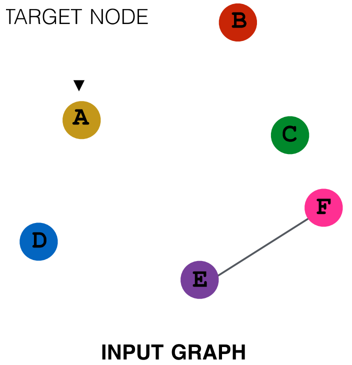


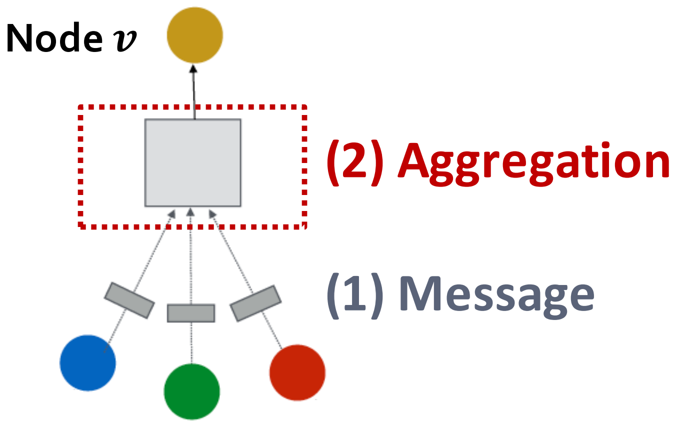
Message Aggregation

- **(2) Aggregation**
  - **Intuition:** Each node will aggregate the messages from node v's neighbors

$$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}\right)$$

  - **Example:** $\mathrm{Sum}(\cdot)$, $\mathrm{Mean}(\cdot)$ or $\mathrm{Max}(\cdot)$ aggregator
    - $\mathbf{h}_v^{(l)} = \mathrm{Sum}(\{\mathbf{m}_u^{(l)}, u \in N(v)\})$





Message Aggregation: Issue

- **Issue:** Information from node v itself **could get lost**
  - Computation of $\mathbf{h}_v^{(l)}$ does not directly depend on $\mathbf{h}_v^{(l-1)}$
- **Solution:** Include $\mathbf{h}_v^{(l-1)}$ when computing $\mathbf{h}_v^{(l)}$
  - **(1) Message: compute message from node v itself**
    - Usually, a **different message computation** will be performed

$$\mathbf{m}_u^{(l)} = \mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)} \qquad \mathbf{m}_v^{(l)} = \mathbf{B}^{(l)}\mathbf{h}_v^{(l-1)}$$

  - **(2) Aggregation:** After aggregating from neighbors, we can **aggregate the message from node v itself**
    - Via **concatenation** or **summation**

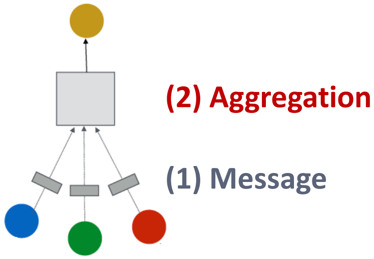
Then aggregate from node itself

$$\mathbf{h}_v^{(l)} = \mathrm{CONCAT}\left(\mathrm{AGG}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}\right), \mathbf{m}_v^{(l)}\right)$$

First aggregate from neighbors

A Single GNN Layer

- **Putting things together:**
  - **(1) Message**: each node computes a message
    $$\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$
  - **(2) Aggregation**: aggregate messages from neighbors
    $$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}, \mathbf{m}_v^{(l)}\right)$$
  - **Nonlinearity (activation):** Adds expressiveness
    - Often written as $\sigma(\cdot)$: $\mathrm{ReLU}(\cdot)$, $\mathrm{Sigmoid}(\cdot)$, …
    - Can be added to **message or aggregation**



Classical GNN Layers: GCN (1)

- **(1) Graph Convolutional Networks (GCN)**

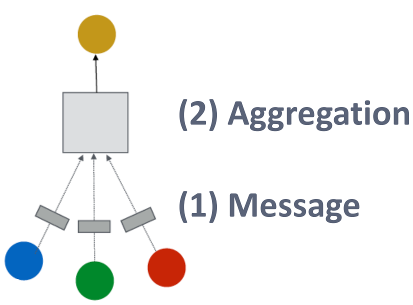
$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}^{(l)} \sum_{u \in N(v)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}\right)$$

- **How to write this as Message + Aggregation?**

Message

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

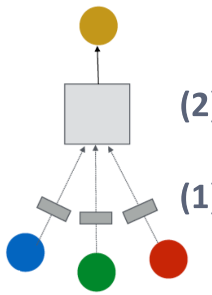
Aggregation



Classical GNN Layers: GCN (2)

- **(1) Graph Convolutional Networks (GCN)**

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



- **Message:**
  - Each Neighbor: $\mathbf{m}_u^{(l)} = \frac{1}{|N(v)|}\mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}$

Normalized by node degree
(In the GCN paper they use a slightly different normalization)

- **Aggregation:**
  - **Sum** over messages from neighbors, then apply activation
  - $\mathbf{h}_v^{(l)} = \sigma\left(\mathrm{Sum}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}\right)\right)$

In GCN graph is assumed to have self-edges that are included in the summation.

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 Aggregation

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

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

Aggregation — Message computation

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

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

Aggregation — Message computation

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

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

Aggregation

GraphSAGE: L2 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**

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

Attention weights

- **In GCN / GraphSAGE**
  - $\alpha_{vu} = \frac{1}{|N(v)|}$ is the **weighting factor (importance)** of node u's message to node v
  - $\Longrightarrow \alpha_{vu}$ 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**

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

Attention weights

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?

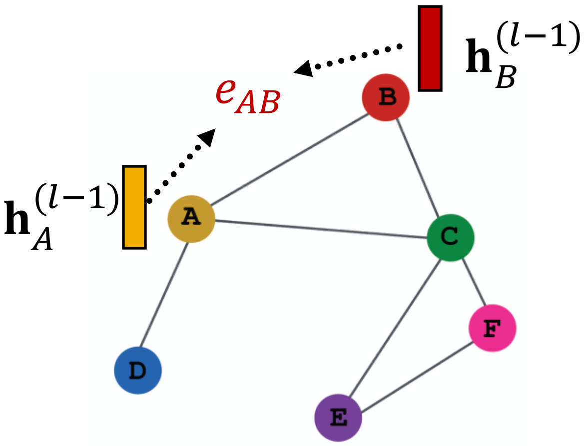
- **Goal:** Specify **arbitrary importance** to different neighbors of each node in the graph
- **Idea:** Compute embedding $\boldsymbol{h}_v^{(l)}$ of each node in the graph following an **attention strategy**:
  - Nodes attend over their neighborhoods' message
  - Implicitly specifying different weights 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 $\sum_{u \in N(v)} \alpha_{vu} = 1$:

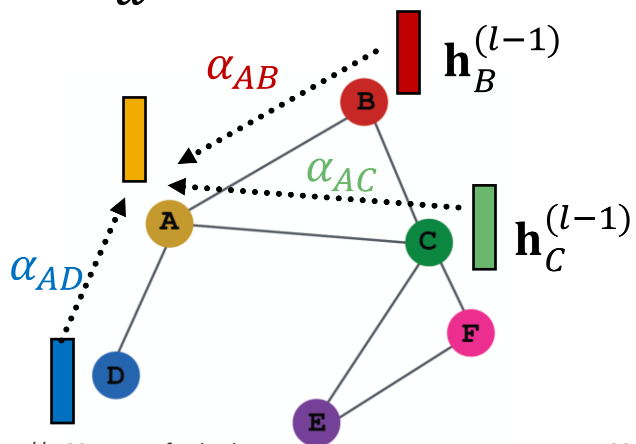
$$\alpha_{vu} = \frac{\exp(e_{vu})}{\sum_{k \in N(v)} \exp(e_{vk})}$$

- **Weighted sum** based on the **final attention weight** α_{vu}

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

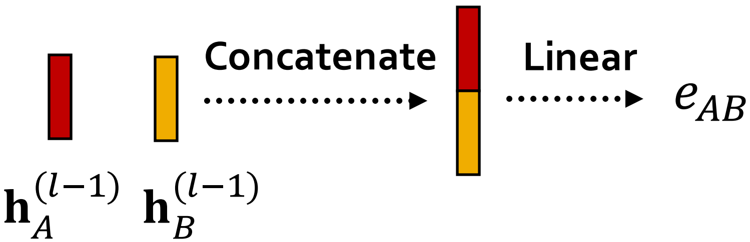
Weighted sum using α_{AB}, α_{AC}, α_{AD}**:**

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



Attention Mechanism (3)

- **What is the form of attention mechanism a?**
  - The approach is agnostic to the choice of a
    - E.g., use a simple single-layer neural network
      - a have trainable parameters (weights in the Linear layer)



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

  - 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):

$$\mathbf{h}_v^{(l)}[1] = \sigma(\sum_{u \in N(v)} \alpha_{vu}^{1} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$
$$\mathbf{h}_v^{(l)}[2] = \sigma(\sum_{u \in N(v)} \alpha_{vu}^{2} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$
$$\mathbf{h}_v^{(l)}[3] = \sigma(\sum_{u \in N(v)} \alpha_{vu}^{3} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)})$$

  - **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

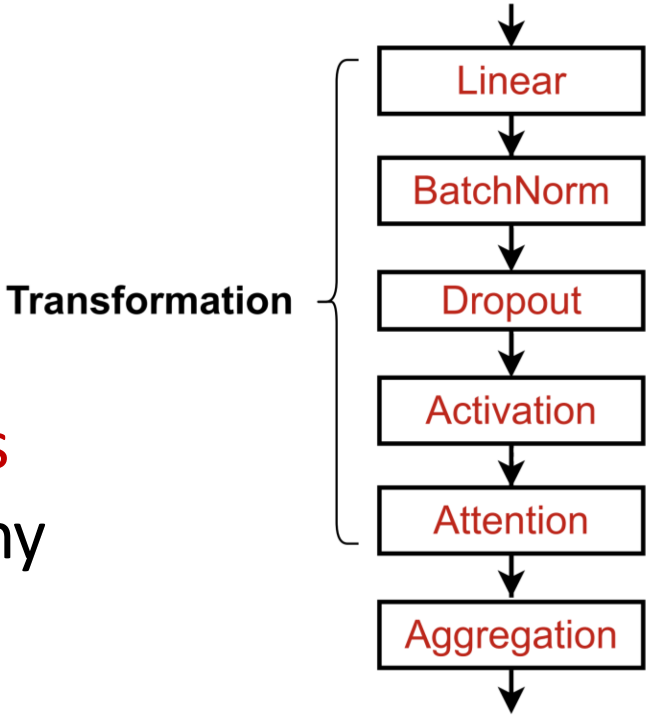
Stanford CS224W: GNN Layers in Practice

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

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

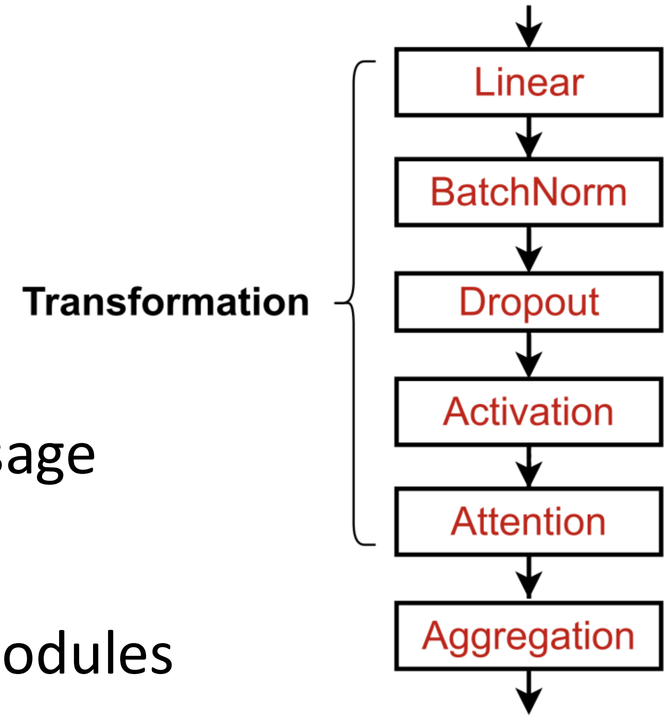
A suggested GNN Layer



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

- **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

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

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

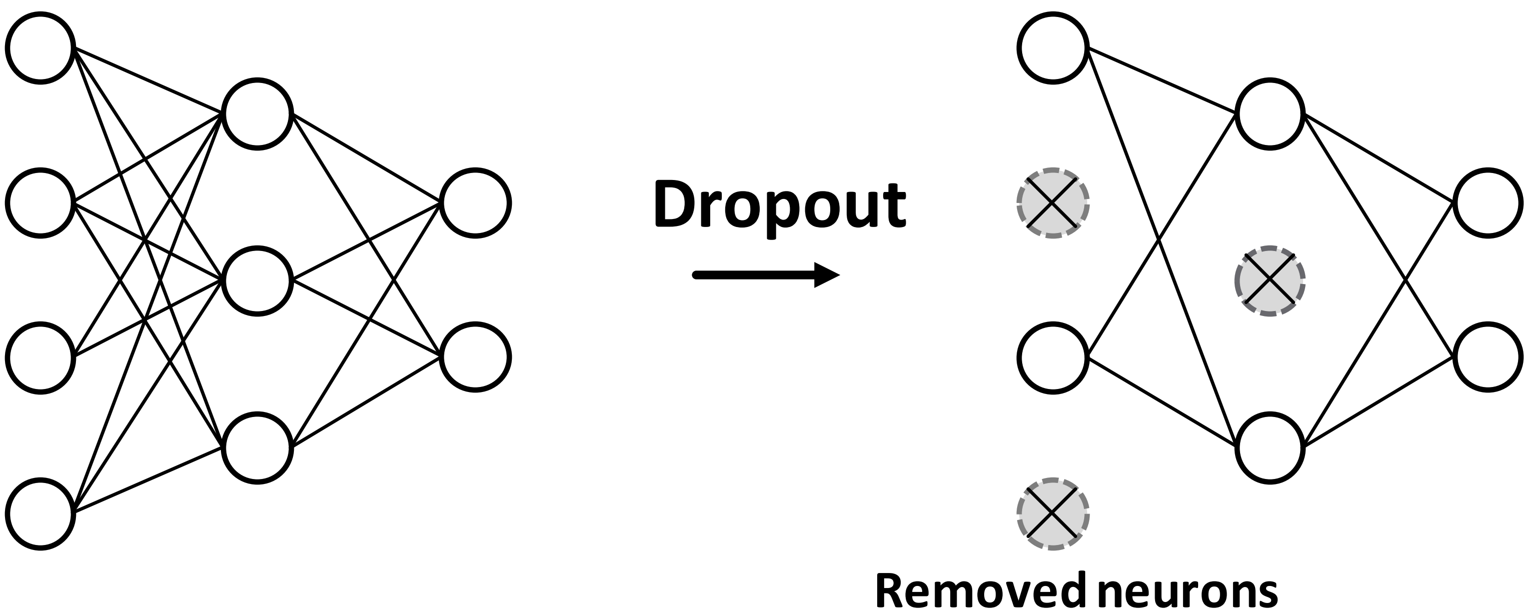
Step 2:
Normalize the feature using computed mean and variance

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

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

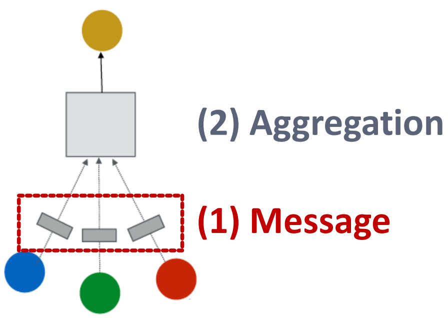
Dropout

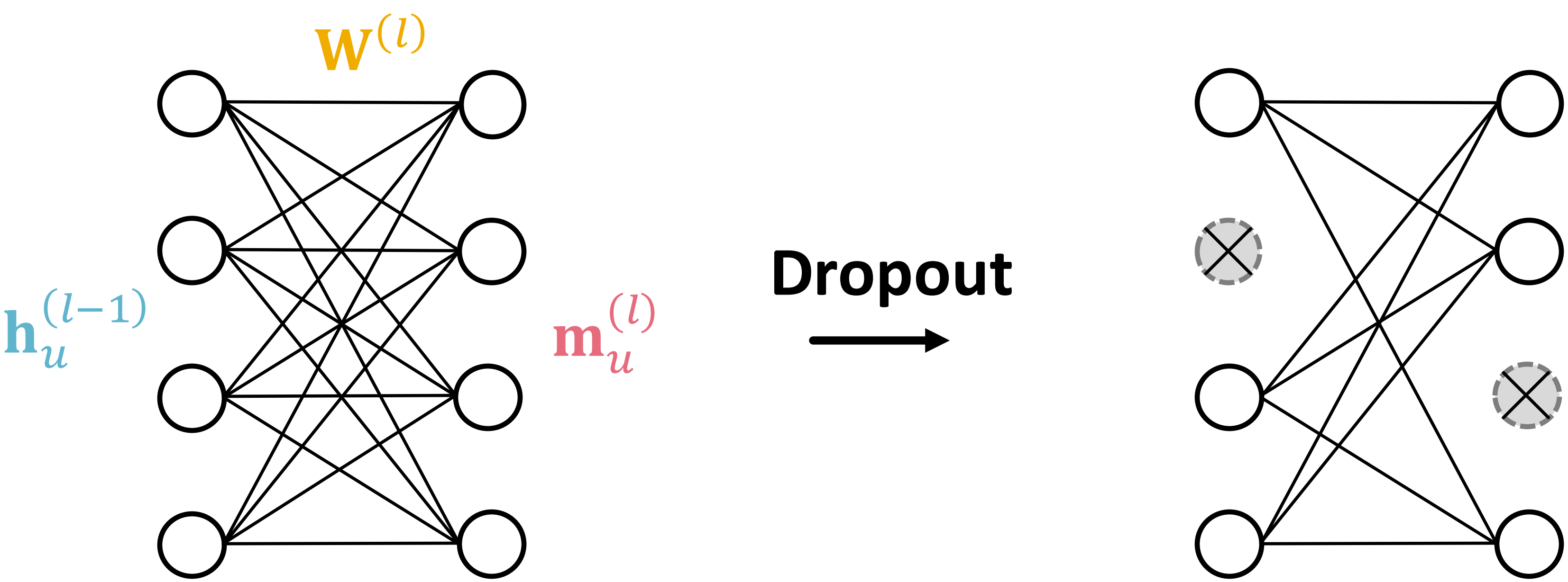
- **Goal**: Regularize a neural net to prevent overfitting.
- **Idea**:
  - **During training**: with some probability p, randomly set neurons to zero (turn off)
  - **During testing:** Use all the neurons for computation



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

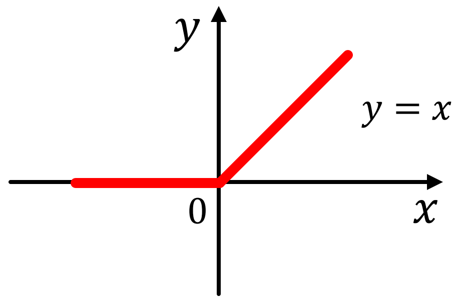
Activation (Non-linearity)

Apply activation to i-th dimension of embedding $\mathbf{x}$

- **Rectified linear unit (ReLU)**

$$\mathrm{ReLU}(\mathbf{x}_i) = \max(\mathbf{x}_i, 0)$$

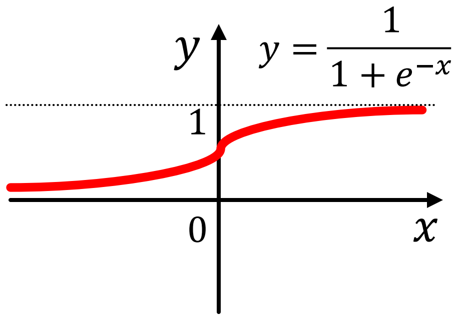
  - Most commonly used



- **Sigmoid**

$$\sigma(\mathbf{x}_i) = \frac{1}{1 + e^{-\mathbf{x}_i}}$$

  - Used only when you want to restrict the range of your embeddings

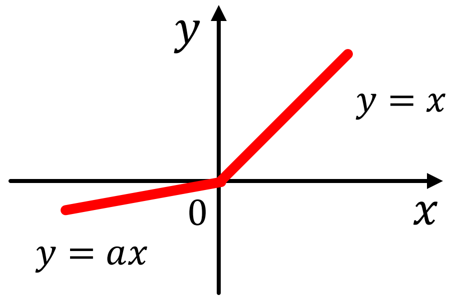


- **Parametric ReLU**

$$\mathrm{PReLU}(\mathbf{x}_i) = \max(\mathbf{x}_i, 0) + a_i \min(\mathbf{x}_i, 0)$$

a_i is a trainable parameter

  - Empirically performs better than ReLU

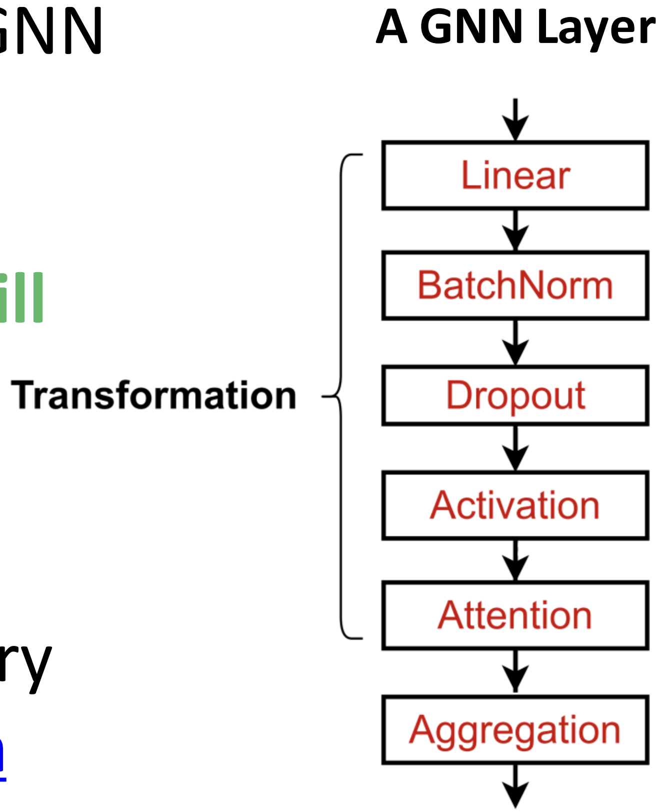


GNN Layer in Practice

- **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



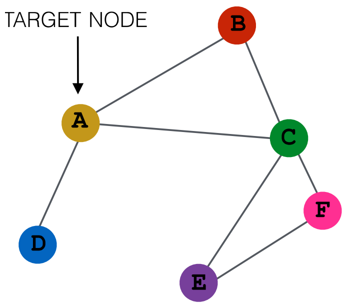
Stanford CS224W: Stacking Layers of a GNN

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Stacking GNN Layers

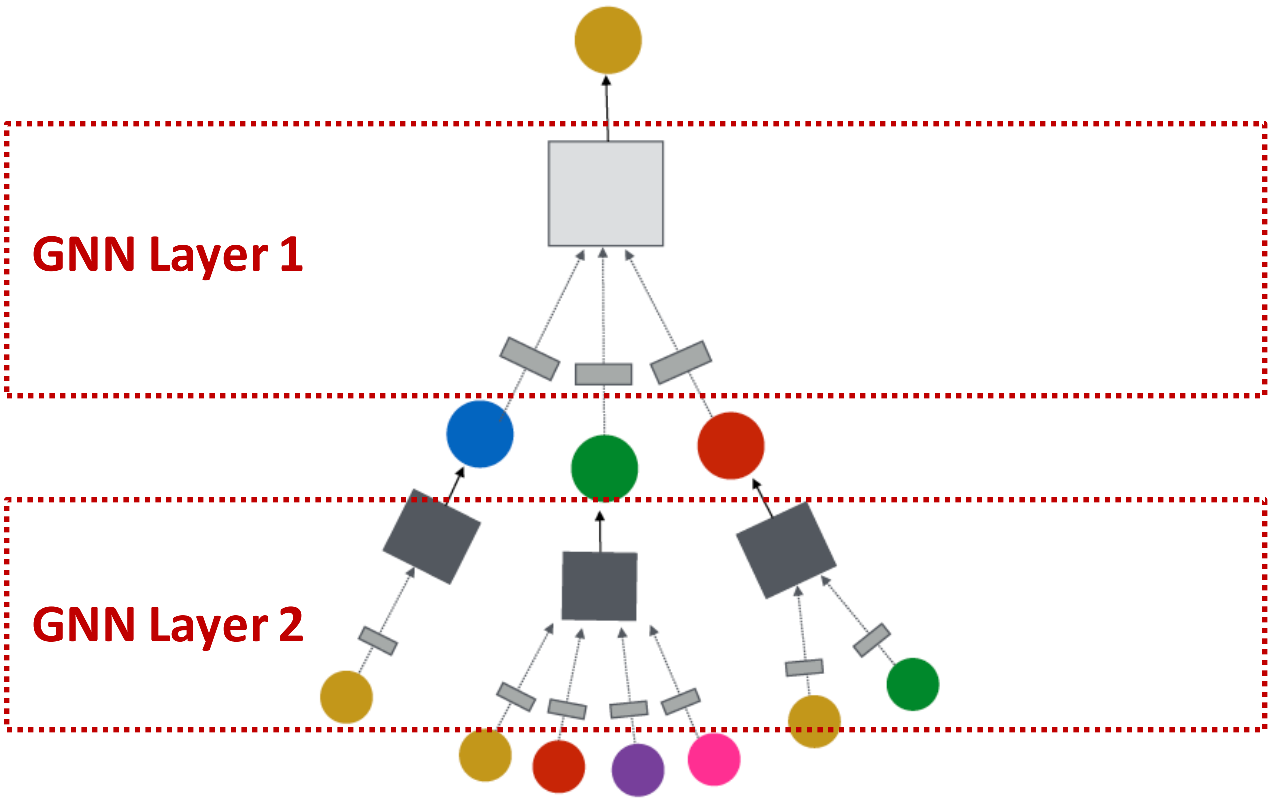


INPUT GRAPH

(3) Layer connectivity

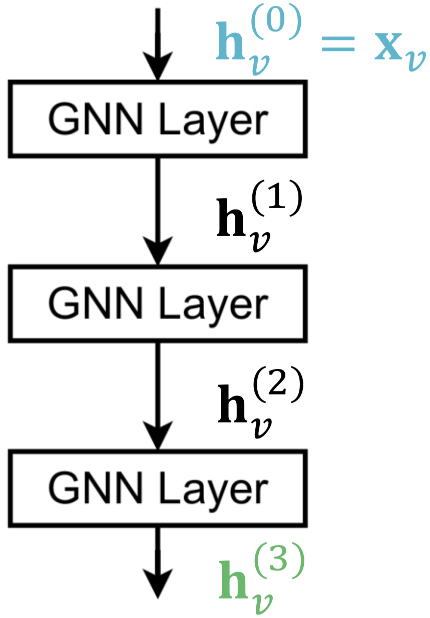
How to connect GNN layers into a GNN?

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



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



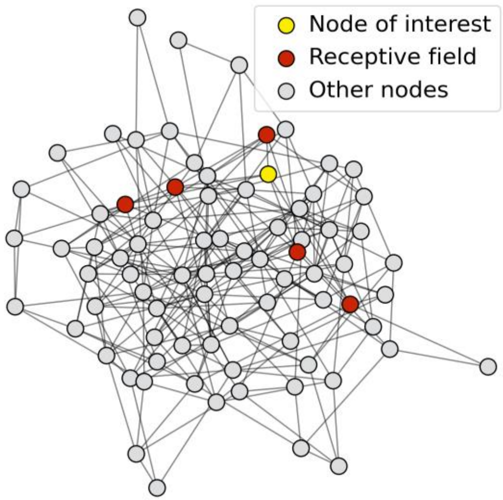
The Over-smoothing Problem

- 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?**

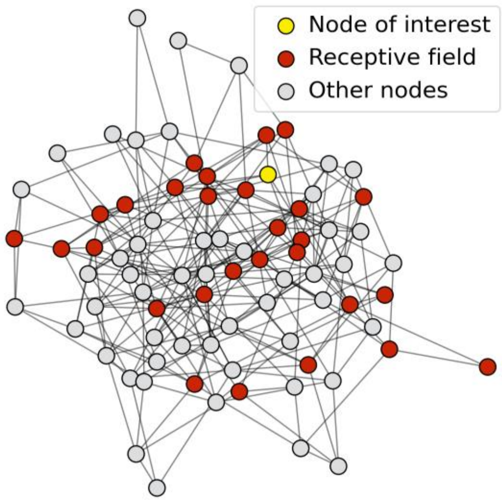
Receptive Field of a GNN

- **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**

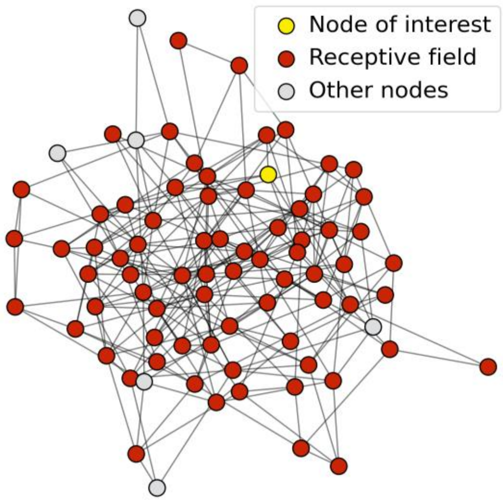
Receptive field for 1-layer GNN



Receptive field for 2-layer GNN



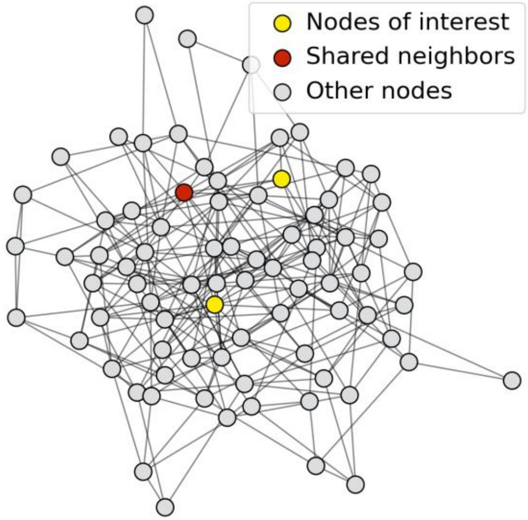
Receptive field for 3-layer GNN



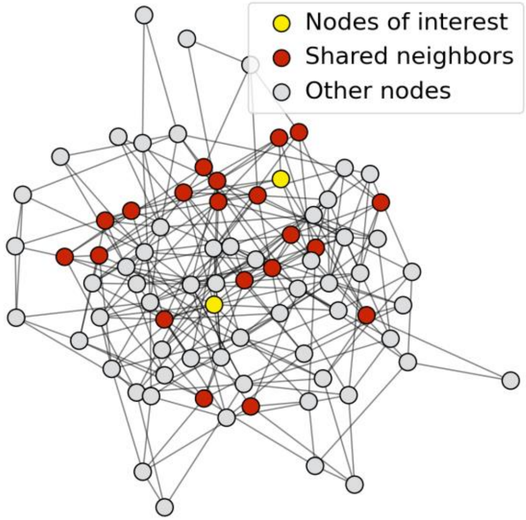
Receptive Field of a GNN

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

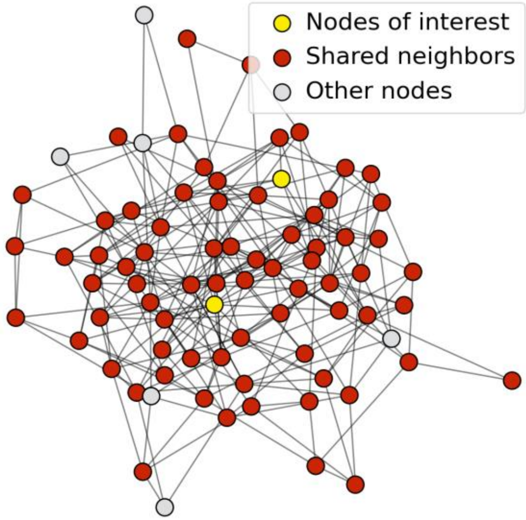
1-hop neighbor overlap
Only 1 node



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

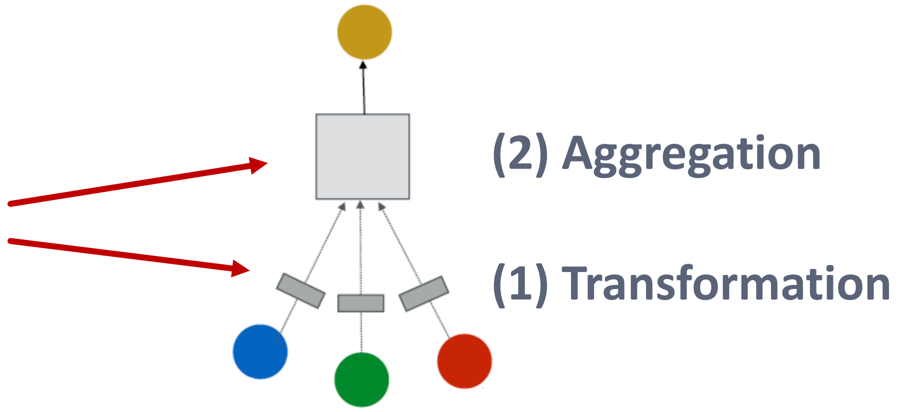
- **What do we learn from the over-smoothing problem?**
- **Lesson 1: Be cautious when adding GNN layers**
  - Unlike neural networks in other domains (CNN for image classification), **adding more GNN layers do not always help**
  - **Step 1: Analyze the necessary receptive field** to solve your problem. 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

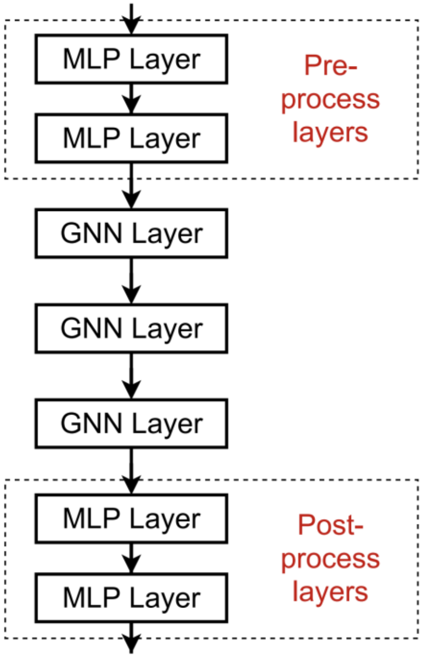
- **How to make a shallow GNN more expressive?**
- **Solution 1**: Increase the expressive power **within each GNN layer**
  - In our previous examples, each transformation or aggregation function only include one linear layer
  - We can **make aggregation / transformation become a deep neural network**!

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

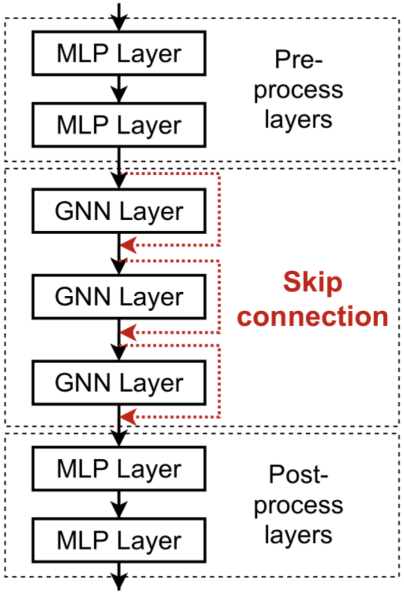
Post-processing layers: Important when reasoning / transformation over node embeddings are needed
E.g., graph classification, knowledge graphs

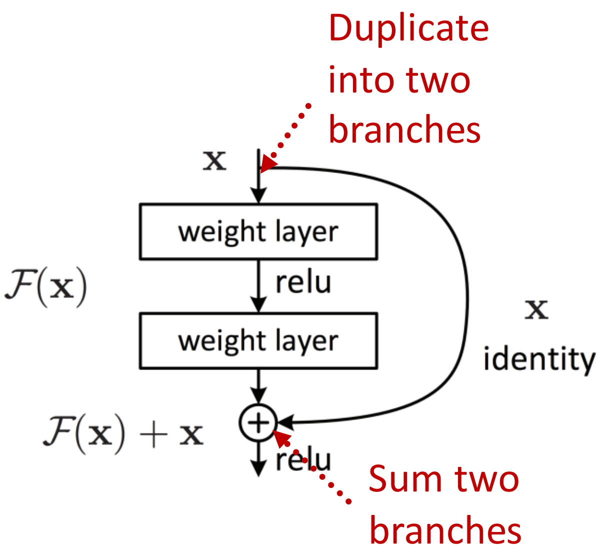
In practice, adding these layers works great!

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:

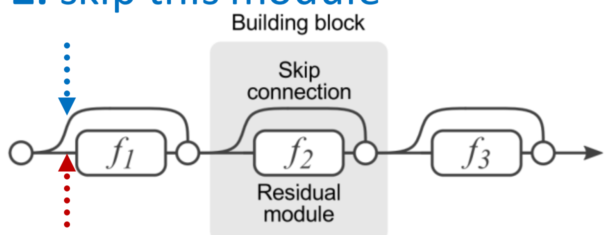
$$\boldsymbol{F}(\mathbf{x}) + \mathbf{x}$$

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

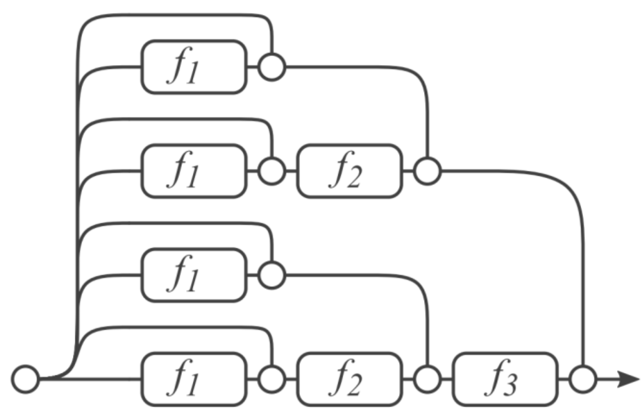
Path 2: skip this module



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

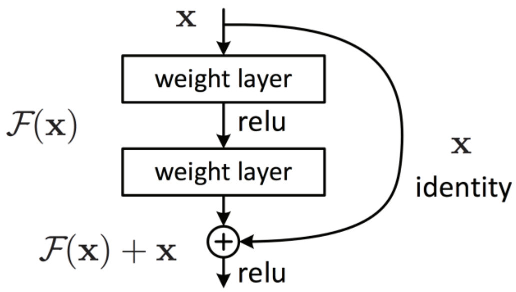
Example: GCN with Skip Connections

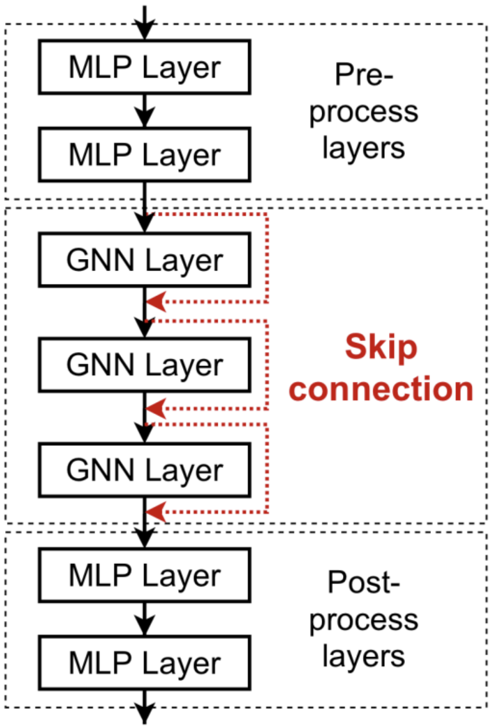
- **A standard GCN layer**
- $$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}\right)$$

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

- **A GCN layer with skip connection**
- $$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|} + \mathbf{h}_v^{(l-1)}\right)$$

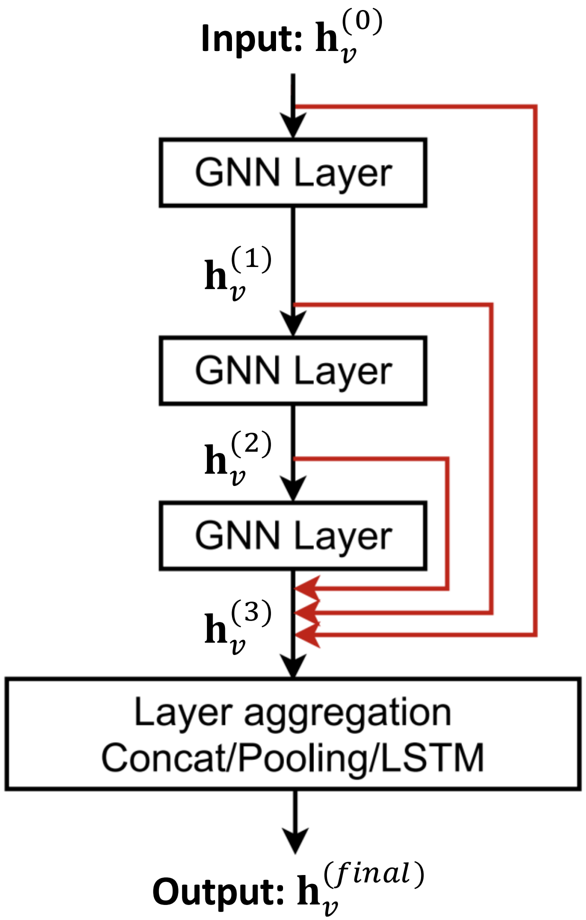
  $F(\mathbf{x}) \quad + \quad \mathbf{x}$





Other Options of Skip Connections

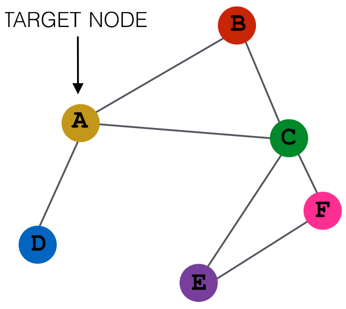
- **Other options:** Directly skip to the last layer
  - The final layer directly **aggregates from the all the node embeddings** in the previous layers



Stanford CS224W: Graph Manipulation in GNNs

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

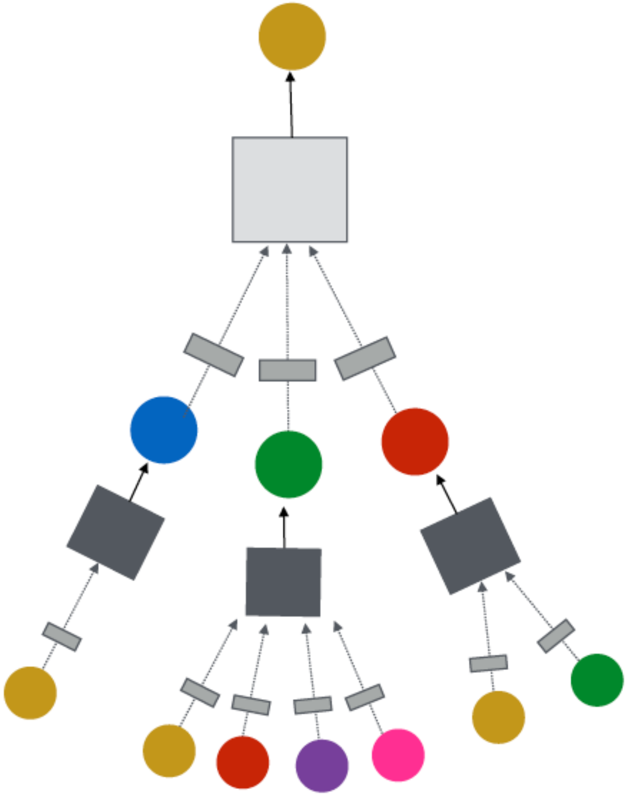
General GNN Framework



INPUT GRAPH

Idea: Raw input graph ≠ computational graph

- **Graph feature augmentation**
- **Graph structure manipulation**



(4) Graph manipulation

Why Manipulate Graphs

Our assumption so far has been

- **Raw input graph = computational graph**

Reasons for breaking this assumption

- **Feature level:**
  - The input graph **lacks features** → feature augmentation
- **Structure level:**
  - 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 just **unlikely that the input graph happens to be the optimal computation graph** for embeddings

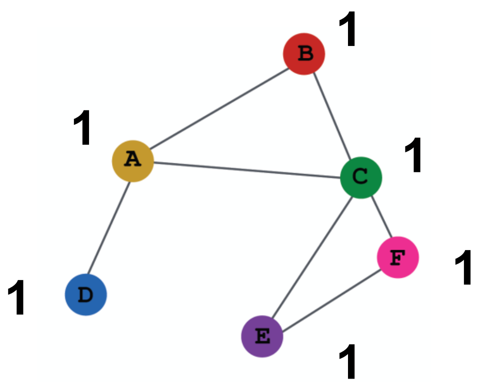
Graph Manipulation Approaches

- **Graph Feature manipulation**
  - The input graph **lacks features** → **feature augmentation**
- **Graph Structure manipulation**
  - 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**

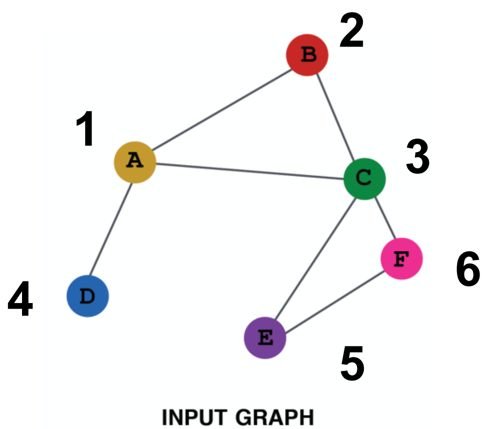


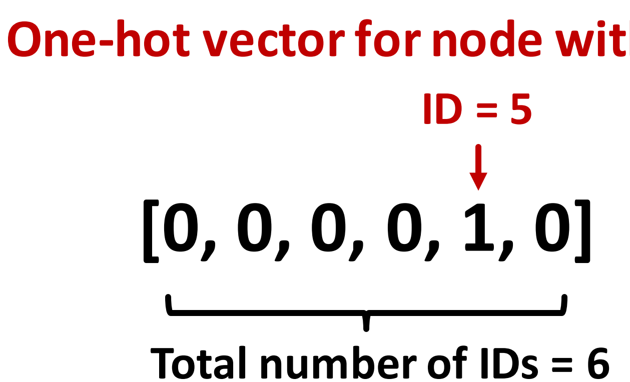
INPUT GRAPH

Feature Augmentation on Graphs

Why do we need feature augmentation?

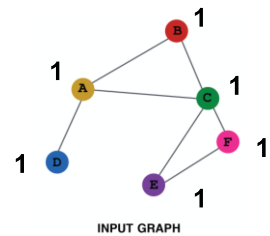
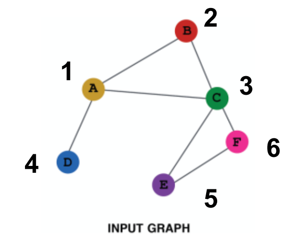
- **(1) Input graph does not have node features**
  - This is common when we only have the adj. matrix
- **Standard approaches:**
- **b) Assign unique IDs to nodes**
  - These IDs are converted into **one-hot vectors**





Feature Augmentation on Graphs

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

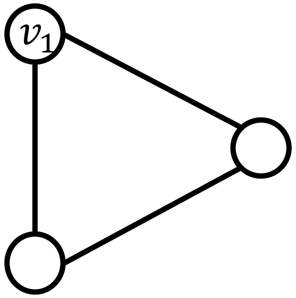
	Constant node feature 	**One-hot node feature** 
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a unique ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple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

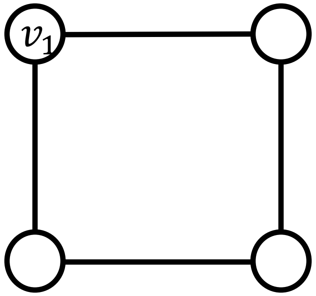
Why do we need feature augmentation?

- **(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



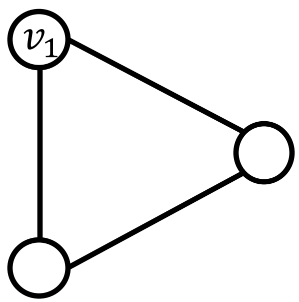
v_1 resides in a cycle with length 4



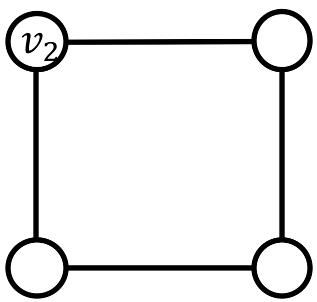
Feature Augmentation on Graphs

- **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

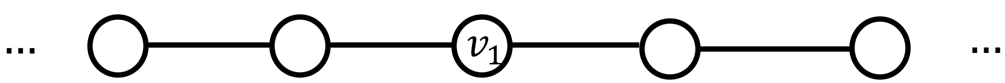
v_1 resides in a cycle with length 3



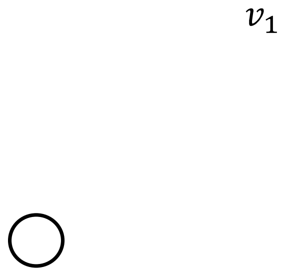
v_1 resides in a cycle with length 4



v_1 resides in a cycle with infinite length



The computational graphs for node v_1 are always the same



Feature Augmentation on Graphs

Why do we need feature augmentation?

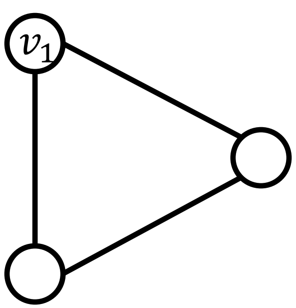
- **(2) Certain structures are hard to learn by GNN**
- **Solution:**
  - We can use cycle count as augmented node features

We start from cycle with length 0

Augmented node feature for v_1

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

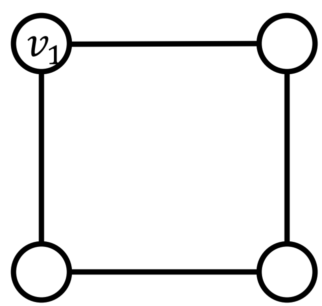
v_1 resides in a cycle with length 3



Augmented node feature for v_1

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

v_1 resides in a cycle with length 4



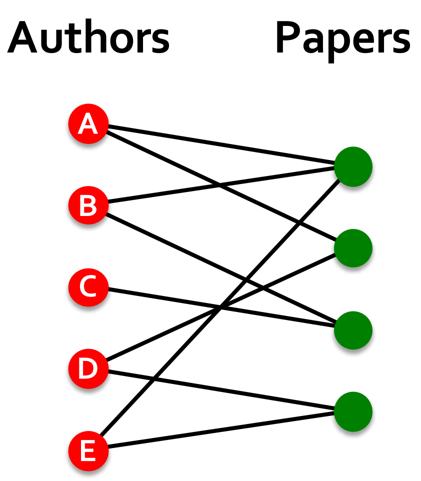
Feature Augmentation on Graphs

Why do we need feature augmentation?

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

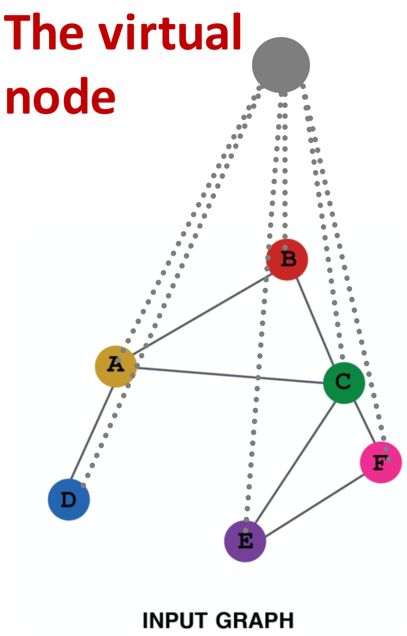
Add Virtual Nodes / Edges

- **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



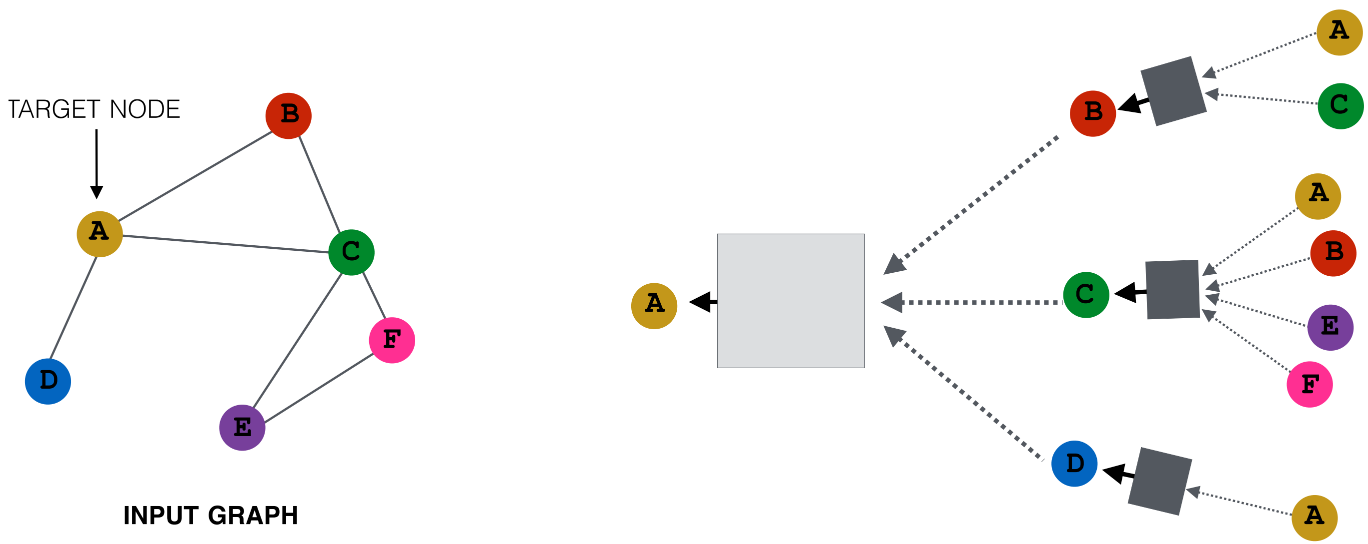
Add Virtual Nodes / Edges

- **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 2**
      - **Node A – Virtual node – Node B**
  - **Benefits:** Greatly **improves message passing in sparse graphs**



Node Neighborhood Sampling

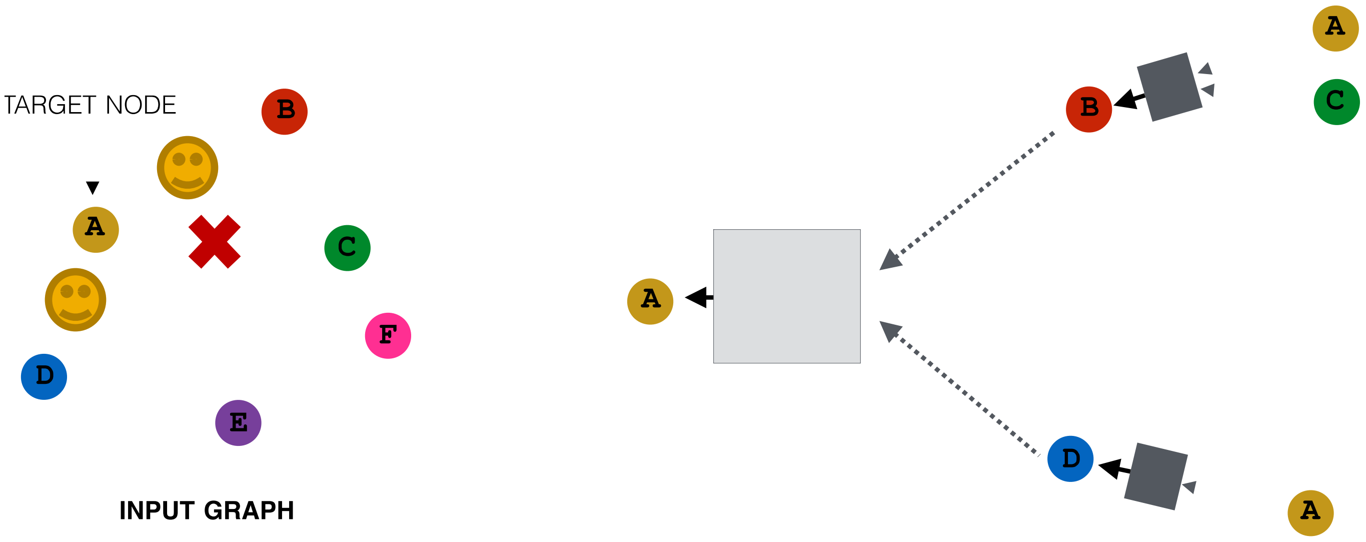
- **Previously:**
  - All the nodes are used for message passing



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

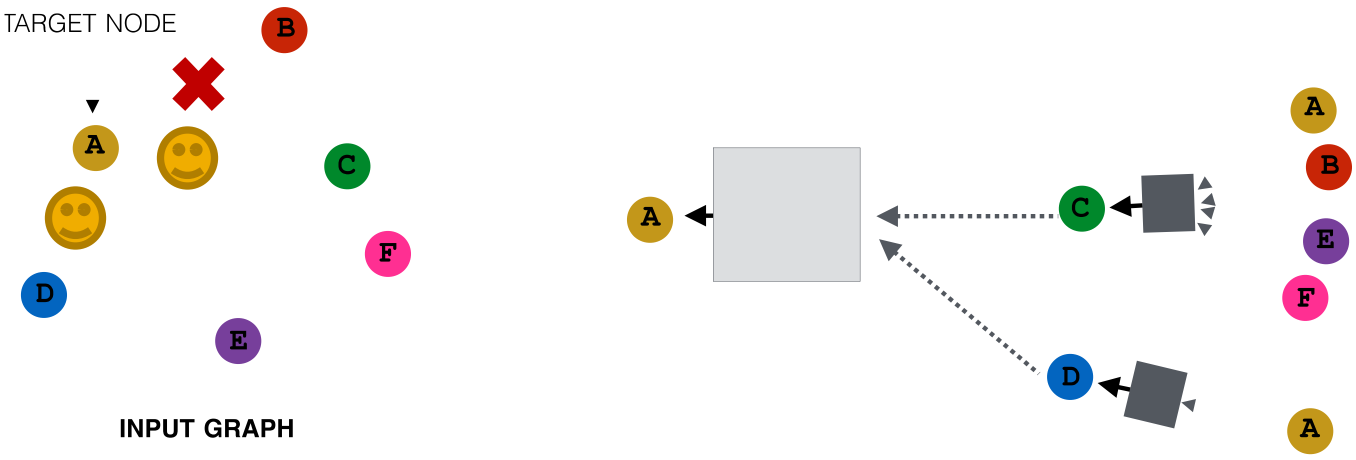
Neighborhood Sampling Example

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



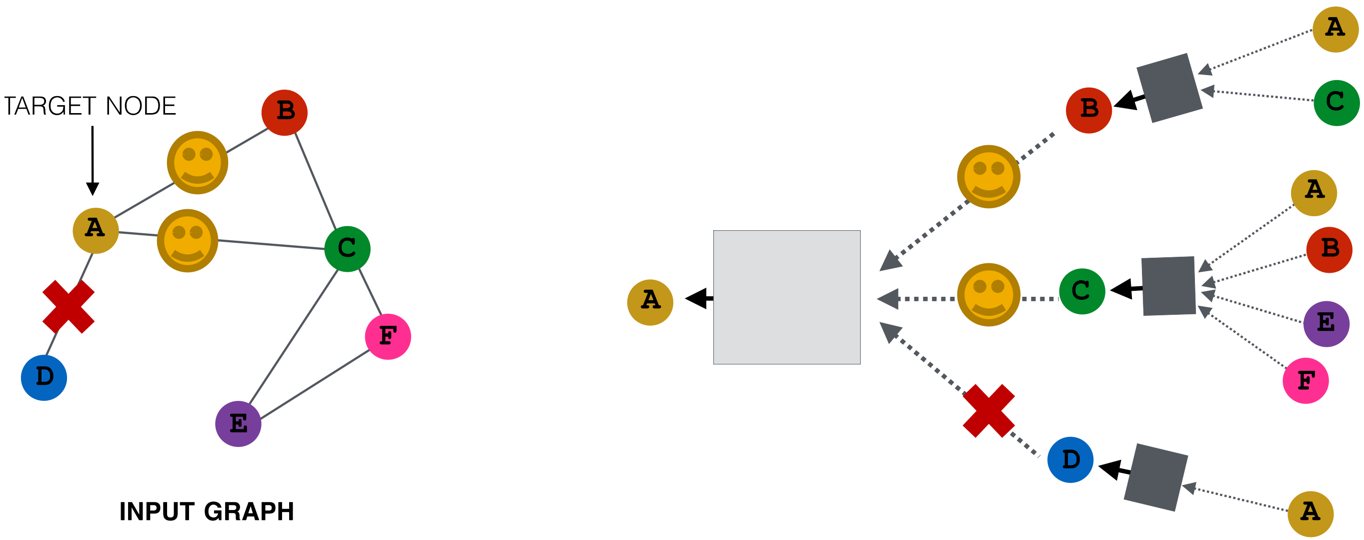
Neighborhood Sampling Example

- **Next time when we compute the embeddings, we can sample different neighbors**
  - Only nodes C and D will pass message to A



Neighborhood Sampling Example

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



Summary of the lecture

- **Recap: A general perspective for GNNs**
  - **GNN Layer**:
    - Transformation + Aggregation
    - Classic GNN layers: GCN, GraphSAGE, GAT
  - **Layer connectivity**:
    - Deciding number of layers
    - Skip connections
  - **Graph Manipulation:**
    - Feature augmentation
    - Structure manipulation
- **Next:** GNN objectives, GNN in practice