A General Perspective on Graph Neural Networks

CS246: Mining Massive Datasets

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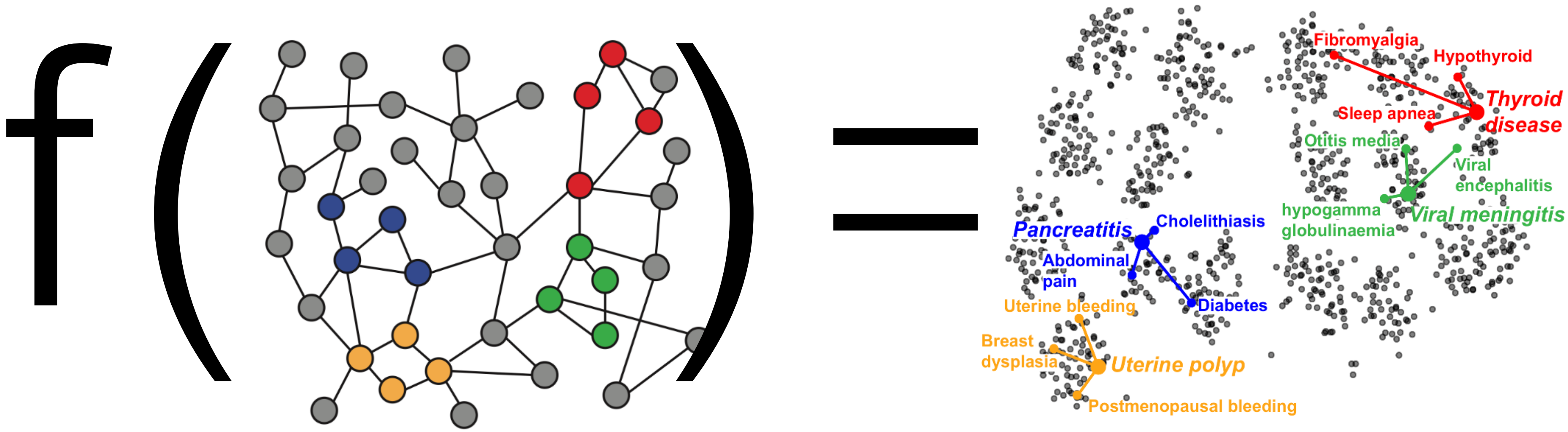
Announcements

- **Assignment 3 and Colab 6 are due Thursday (2/20 at 11:59 pm)**

Recap: Node Embeddings

- **Intuition:** Map nodes to d-dimensional embeddings such that similar nodes in the graph are embedded close together



Input graph

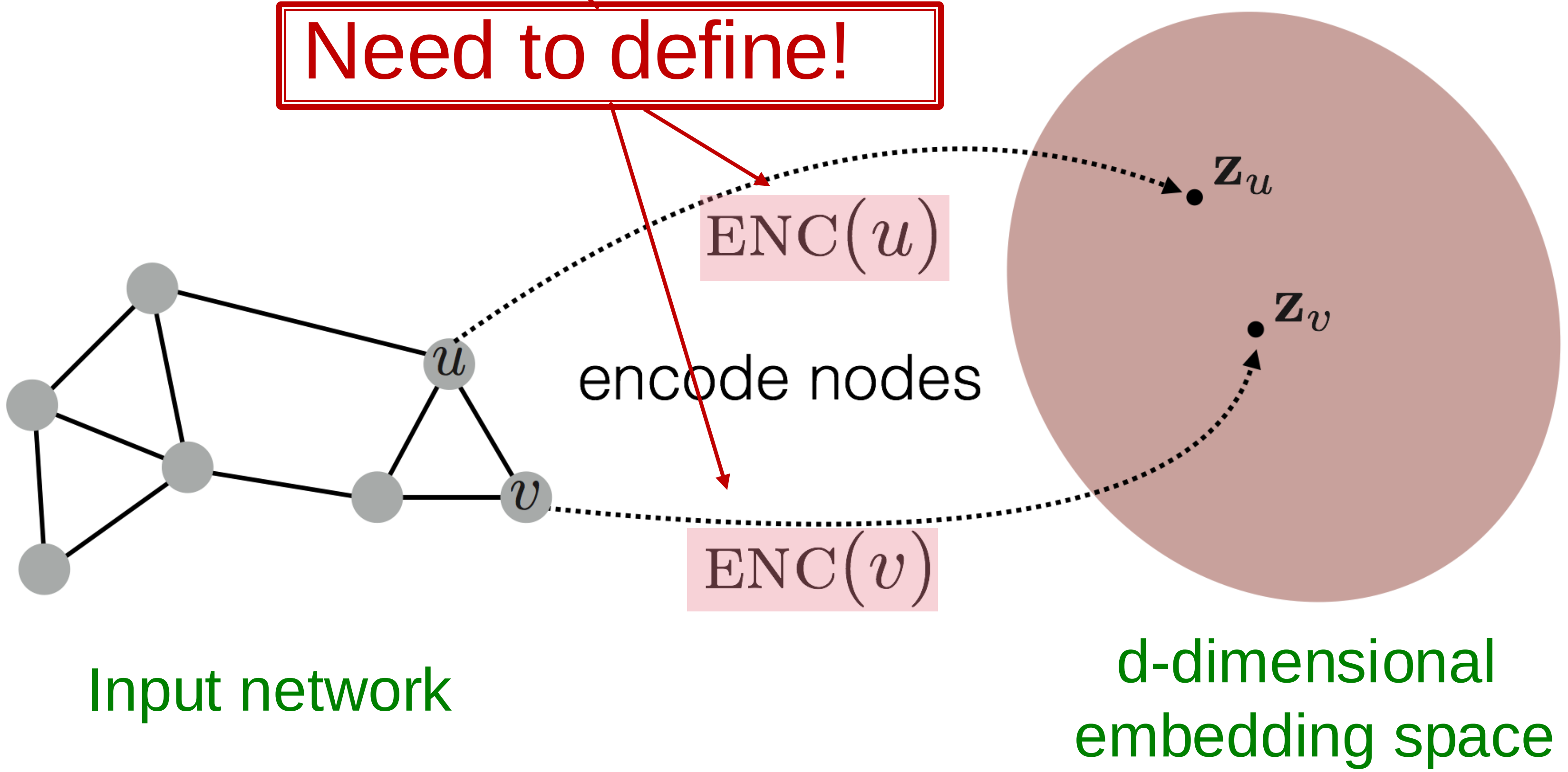
2D node embeddings

How to <u>learn</u> mapping function f?

Recap: Node Embeddings

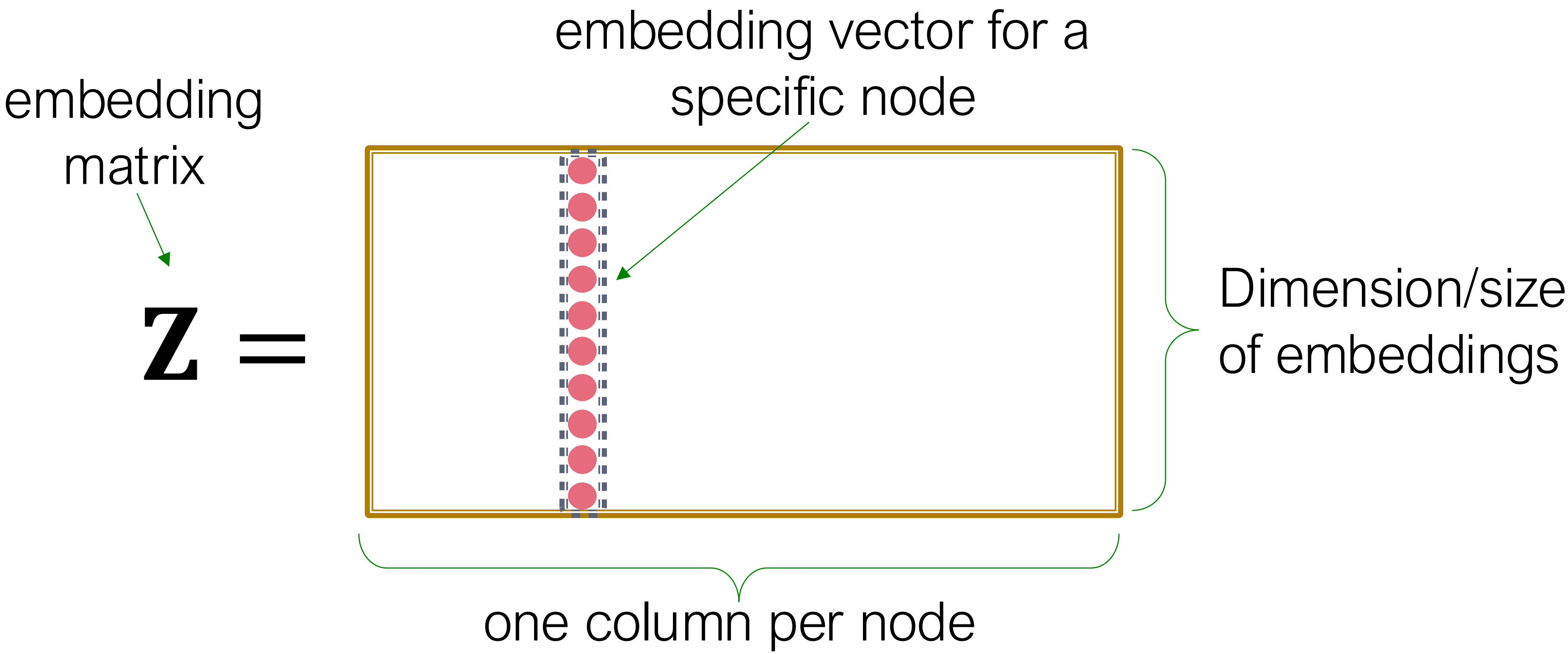
Goal: $\text{similarity}(u, v) \approx \mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$

Need to define!



Recap: “Shallow” Encoding

Simplest encoding approach: **Encoder is just an embedding-lookup**



Recap: Shallow Encoders

- **Limitations** of shallow embedding methods:
  - $\boldsymbol{O}(|\boldsymbol{V}|\boldsymbol{d})$ **parameters are needed**:
    - No sharing of parameters between nodes
    - Every node has its own unique embedding
  - **Inherently "transductive"**:
    - Cannot generate embeddings for nodes that are not seen during training
  - **Do not incorporate node features**:
    - Nodes in many graphs have features that we can and should leverage

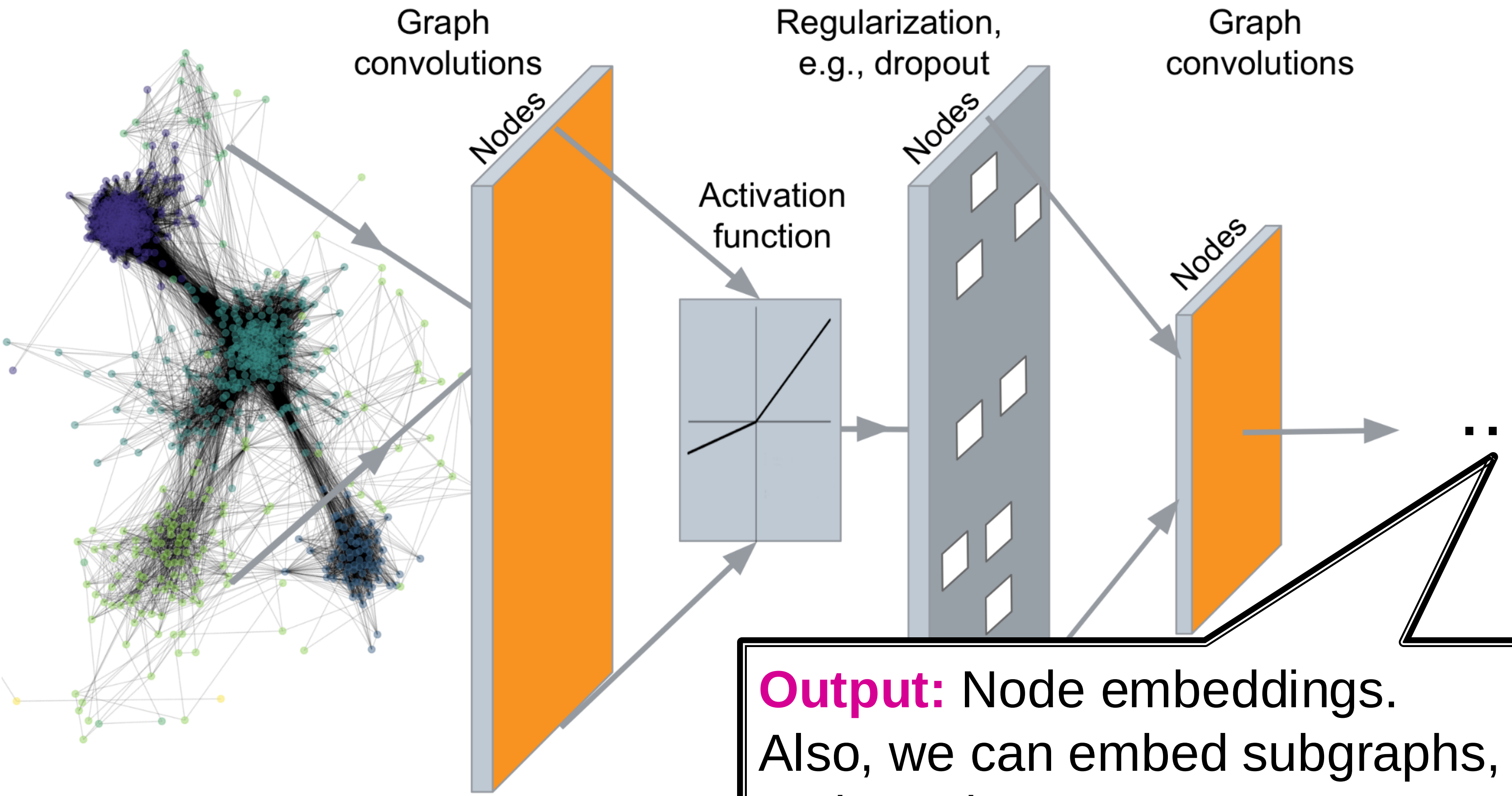
Today: Deep Graph Encoders

- **Today:** We will now discuss deep learnig methods based on **graph neural networks (GNNs):**

$$\mathrm{ENC}(v) = \text{multiple layers of non-linear transformations based on graph structure}$$

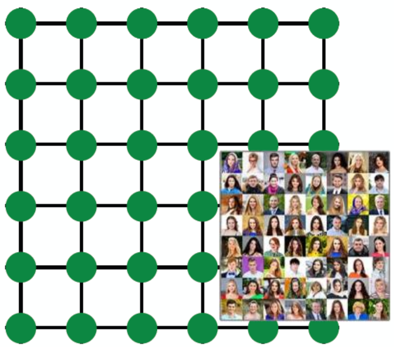
- **Note:** All these deep encoders can be **combined with node similarity functions** defined in the Lecture 2.

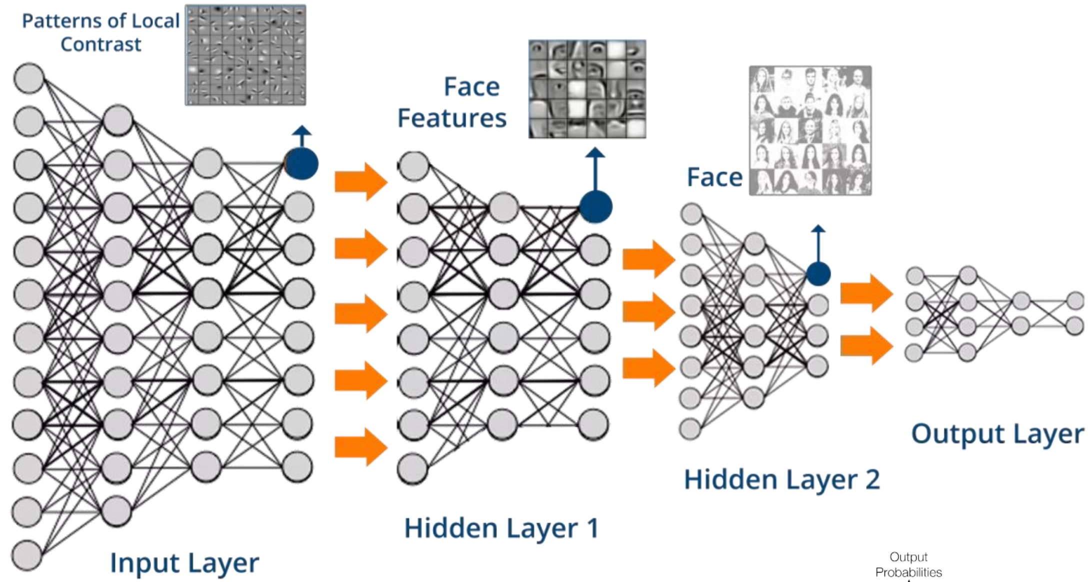
Deep Graph Encoders



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

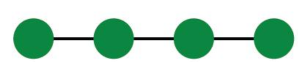
Modern ML Toolbox

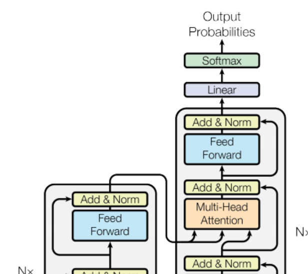




Images

Text/Speech



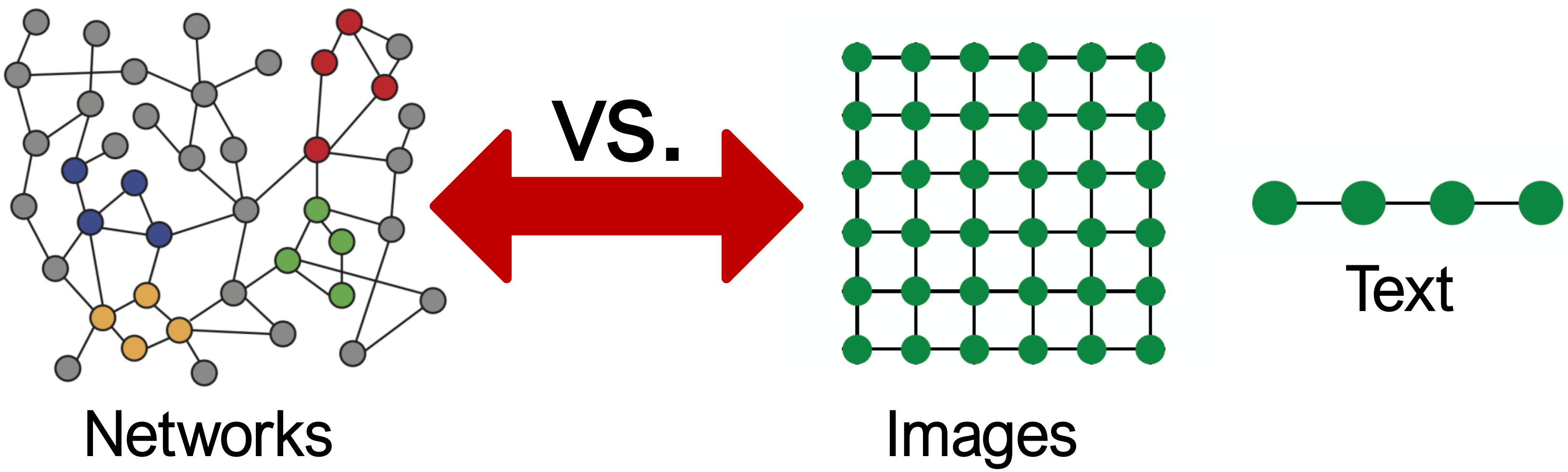


Modern deep learning toolbox is designed for simple sequences & grids

Why is it Hard?

But networks are far more complex!

- Arbitrary size and complex topological structure (i.e., no spatial locality like grids)

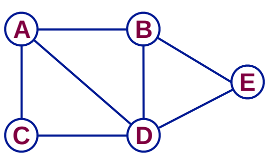


- No fixed node ordering or reference point
- Often dynamic and have multimodal features

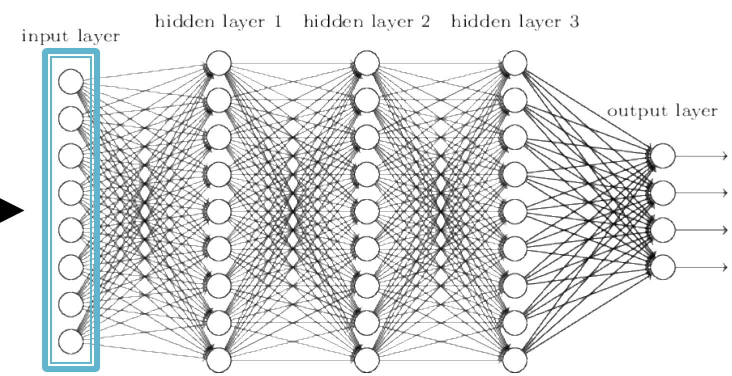
Graph Neural Networks

A Naïve Approach

- Join adjacency matrix and features
- Feed them into a deep neural net:



	A	B	C	D	E	Feat	
A	0	1	1	1	0	1	0
B	1	0	0	1	1	0	0
C	1	0	0	1	0	0	1
D	1	1	1	0	1	1	1
E	0	1	0	1	0	1	0

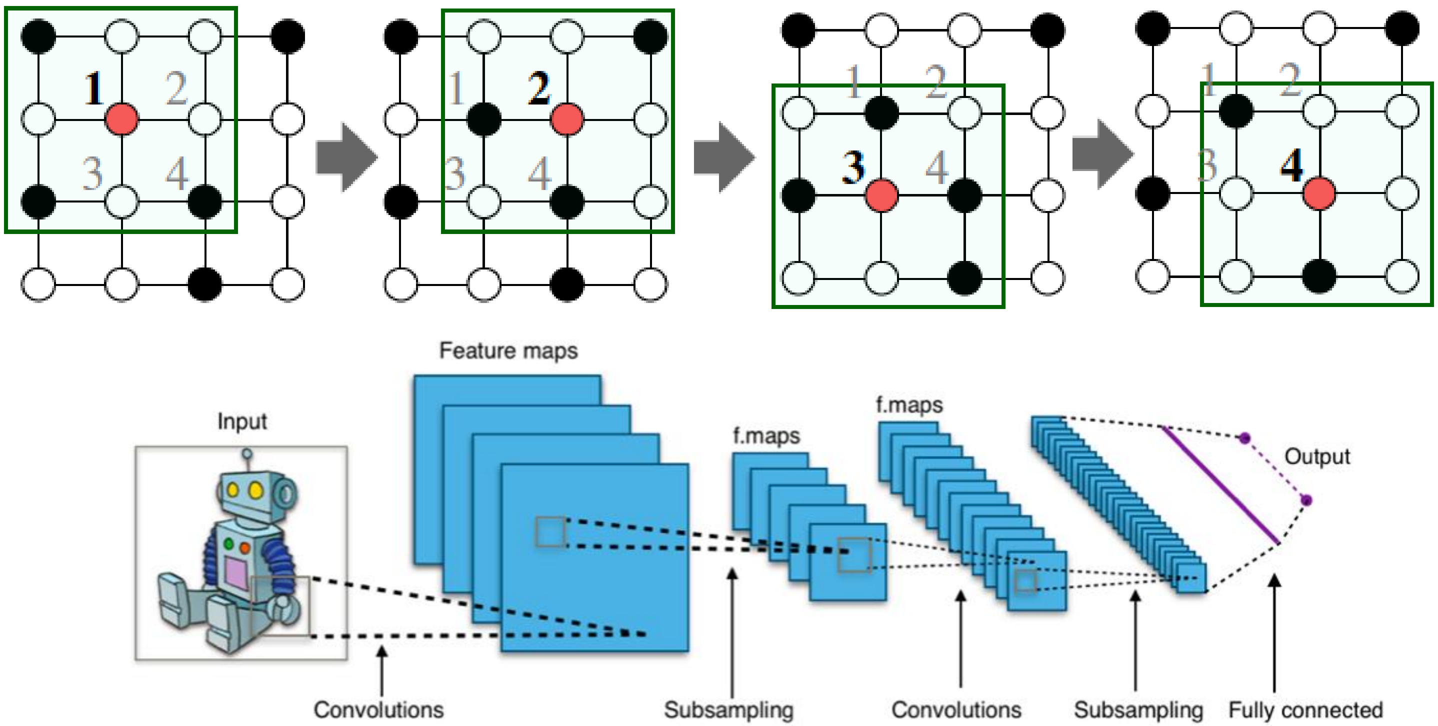


?

- Issues with this idea:
  - $O(|V|)$ parameters
  - Not applicable to graphs of different sizes
  - Sensitive to node ordering

Idea: Convolutional Networks

CNN on an image:

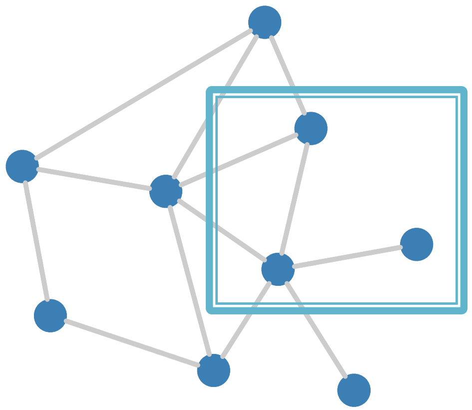


Goal is to generalize convolutions to graphs

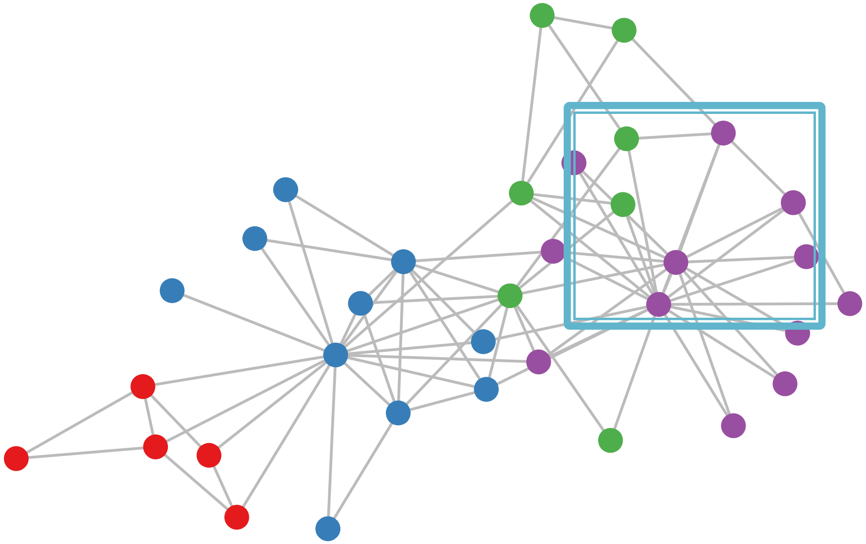
Credit: [Stanford CS224W]

Real-World Graphs

But our graphs look like this:



or this:

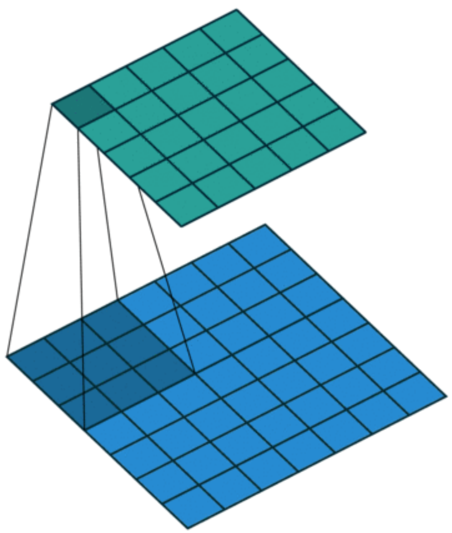


- There is no fixed notion of locality or sliding window on the graph
- Graph is permutation invariant

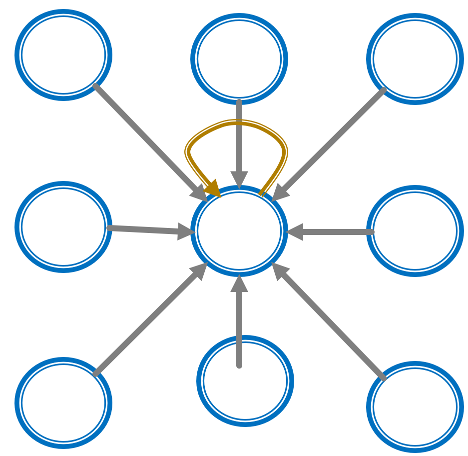
Credit: [Stanford CS224W]

From Images to Graphs

Single Convolutional neural network (CNN) layer with 3x3 filter:



Image



Graph

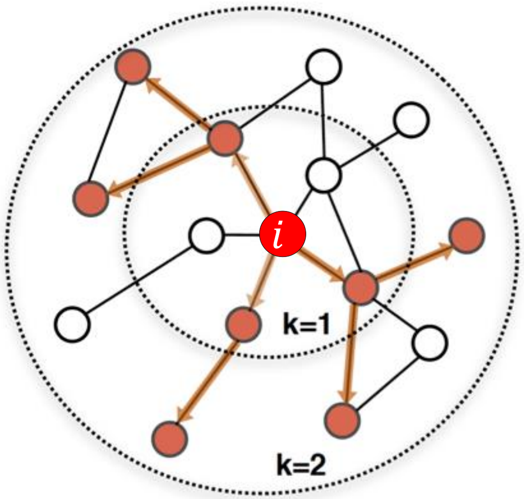
Idea: transform information at the neighbors and combine it:

- Transform “messages” h_i from neighbors: $W_i\ h_i$
- Add them up: $\sum_i W_i\ h_i$

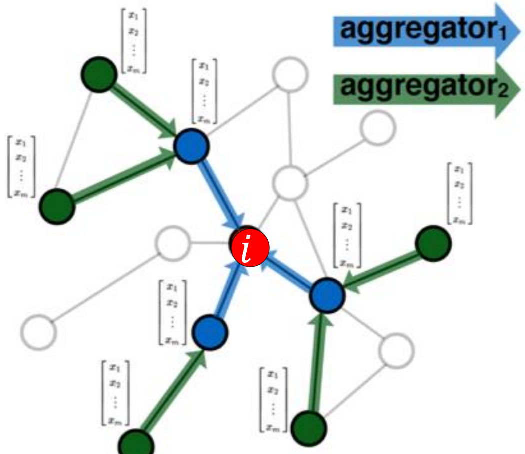
Credit: [Stanford CS224W]

Graph Convolutional Networks

Idea: Node's neighborhood defines a computation graph



Determine node computation graph



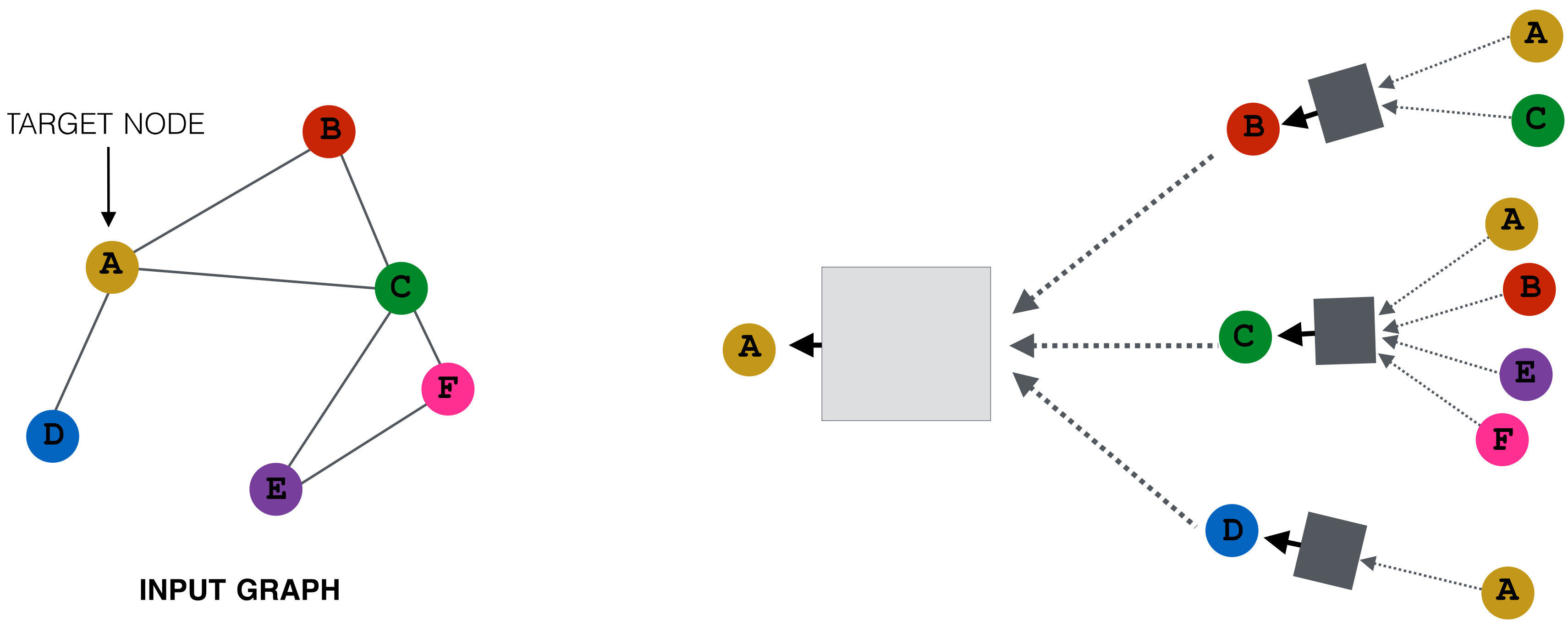
Propagate and transform information

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

Credit: Stanford CS224W

Idea: Aggregate Neighbors

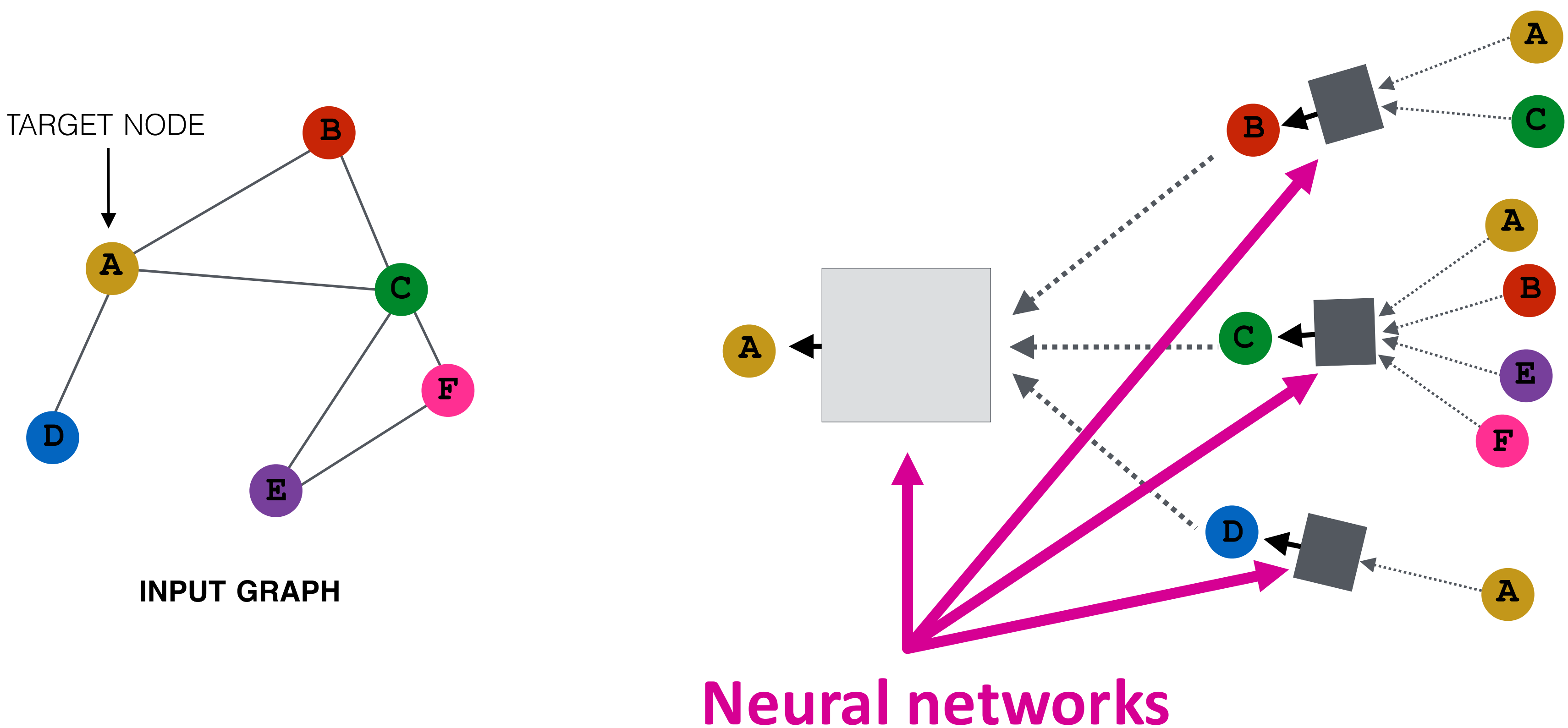
- **Key idea:** Generate node embeddings based on **local network neighborhoods**



Credit: Stanford CS224W

Idea: Aggregate Neighbors

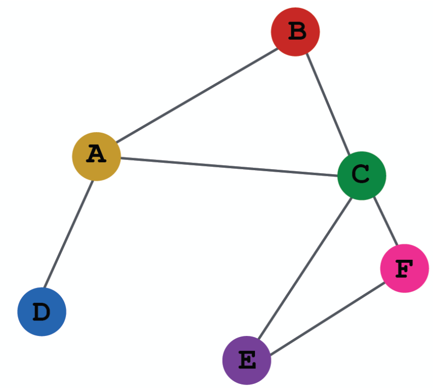
- **Intuition:** Nodes aggregate information from their neighbors using neural networks



Credit: [Stanford CS224W]

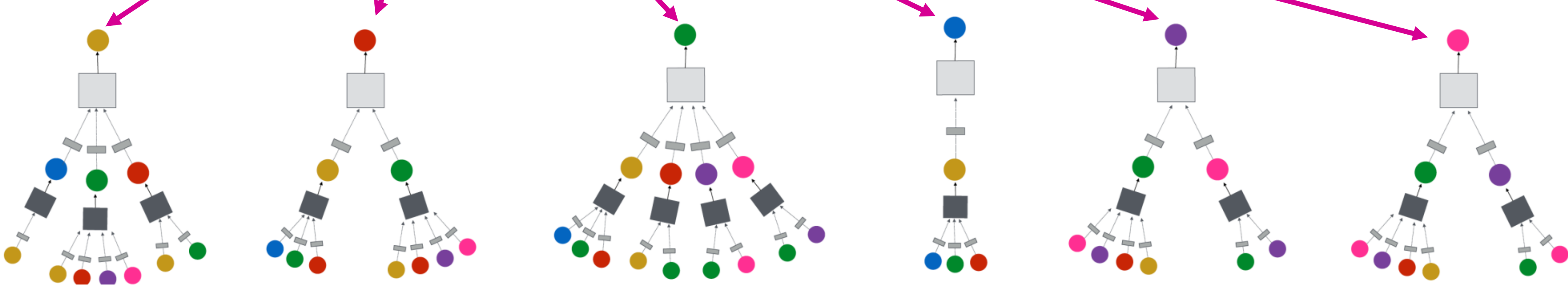
Idea: Aggregate Neighbors

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



INPUT GRAPH

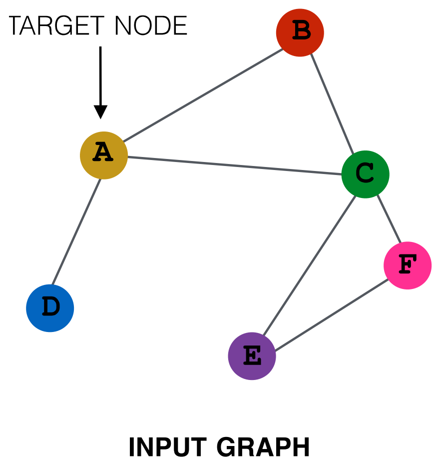
Every node defines a computation graph based on its neighborhood!

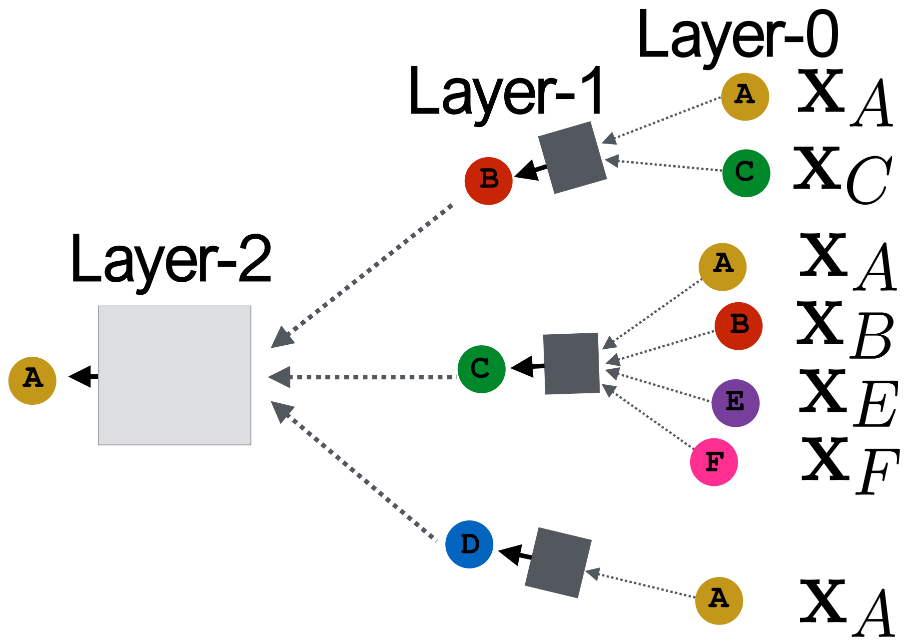


Credit: [Stanford CS224W]

Deep Model: Many Layers

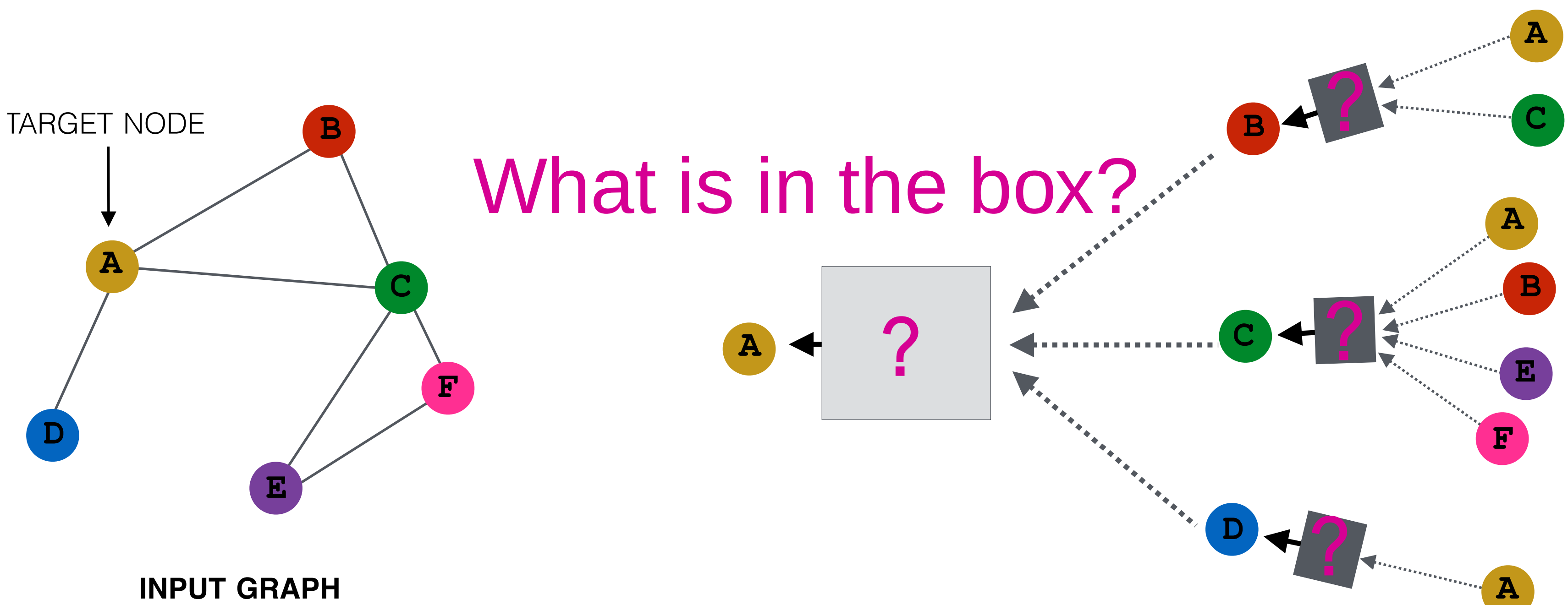
- Model can be of arbitrary depth:
  - Nodes have embeddings at each layer
  - Layer-0 embedding of node u is its input feature, x_u
  - Layer-k embedding gets information from nodes that are K hops away





Neighborhood Aggregation

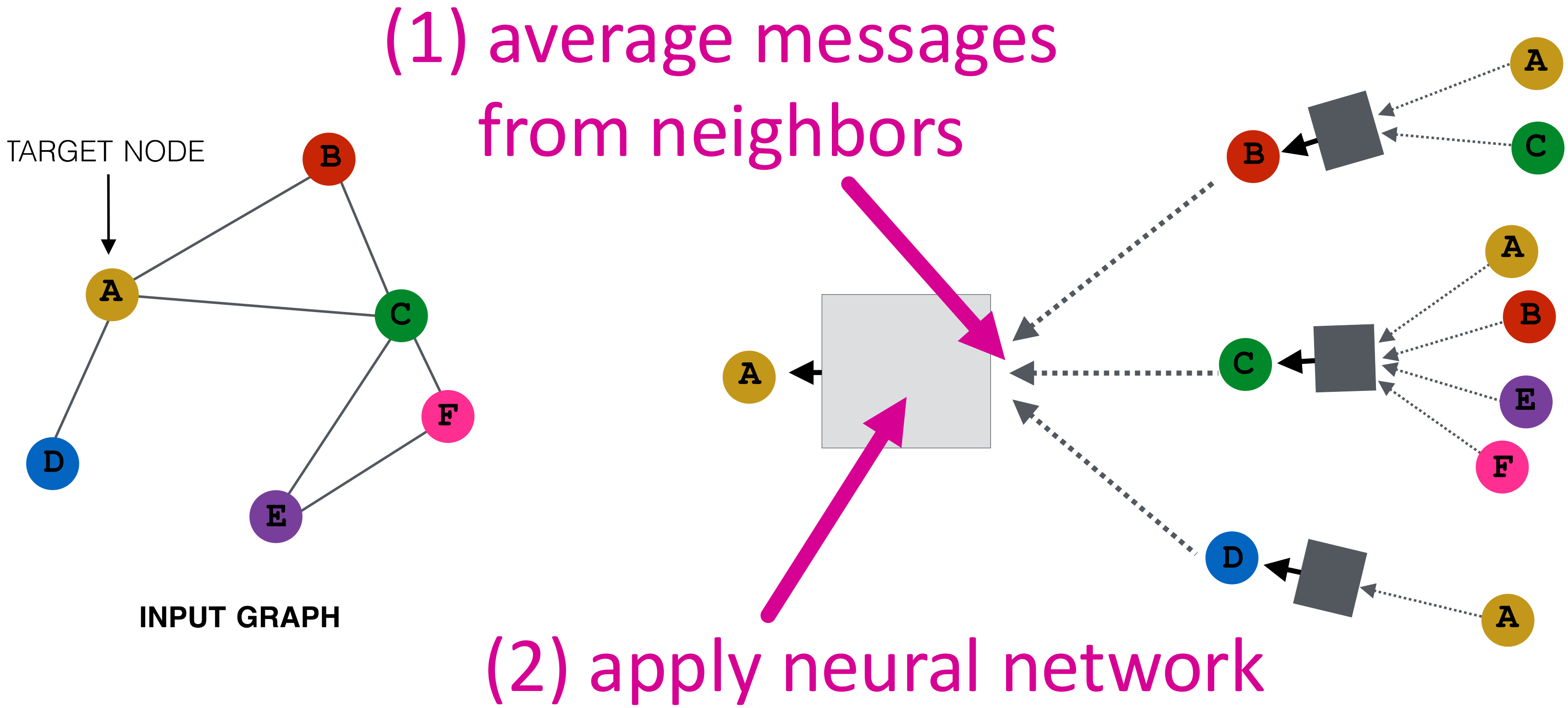
- **Neighborhood aggregation:** Key distinctions are in how different approaches aggregate information across the layers



Credit: [Stanford CS224W]()

Neighborhood Aggregation

- **Basic approach:** Average information from neighbors and apply a neural network



Credit: [Stanford CS224W]

Setup: Learning from Graphs

- **Assume we have a graph G:**
  - V is the **vertex set**
  - $\boldsymbol{A}$ is the **adjacency matrix** (assume binary)
  - $\boldsymbol{X} \in \mathbb{R}^{m \times |V|}$ is a matrix of **node features**
  - v: a node in V; $N(v)$: the set of neighbors of v.
  - **Node features:**
    - Relational data: User/item descriptions, categories
    - Social networks: User profile, User image
    - Biological networks: Gene expression profiles, gene functional information
    - What if there is no node feature in the graph dataset?

Tasks on Networks

Tasks we will be able to solve:

- Node classification
  - Predict the type of a given node
- Link prediction
  - Predict whether two nodes are linked
- Graph/subgraph classification
  - What is the label of a (sub)network

The Math: Deep Encoder

- **Basic approach:** Average neighbor messages and apply a neural network

Initial 0-th layer embeddings are equal to node features

$$\boxed{h_v^0 = x_v}$$

embedding of v at layer l

$$h_v^{(l+1)} = \boxed{\sigma}\left(W_l \boxed{\sum_{u \in N(v)} \frac{h_u^{(l)}}{|N(v)|}} + B_l \boxed{h_v^{(l)}}\right), \forall l \in \{0, \dots, \boxed{L} - 1\}$$

$$\boxed{z_v} = h_v^{(L)}$$

Embedding after L layers of neighborhood aggregation

Non-linearity (e.g., ReLU)

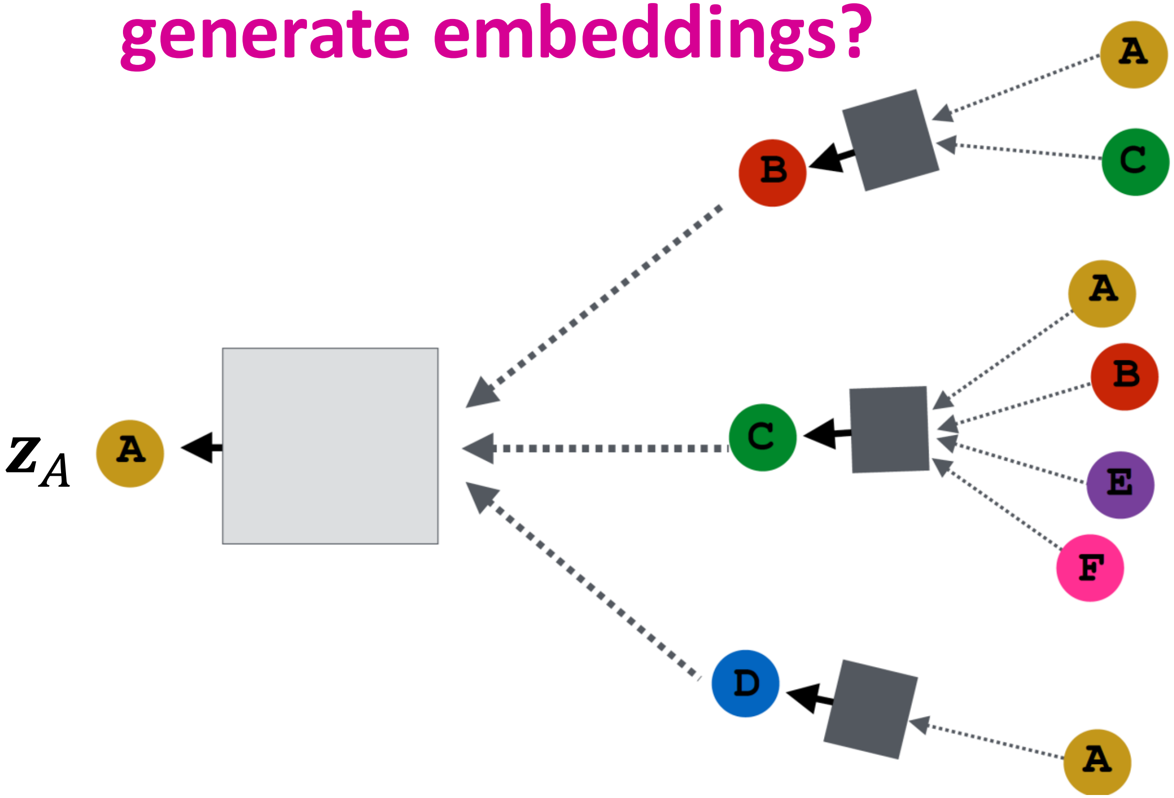
Average of neighbor's previous layer embeddings

Total number of layers

Credit: [Stanford CS224W]

Training the Model

How do we train the model to generate embeddings?



Need to define a loss function on the embeddings

Credit: [Stanford CS224W]

Model Parameters

Trainable weight matrices
(i.e., what we learn)

$$\mathrm{h}_v^{(0)} = \mathrm{x}_v$$

$$\mathrm{h}_v^{(l+1)} = \sigma\left(\boxed{\mathrm{W}_l} \sum_{u \in \mathrm{N}(v)} \frac{\mathrm{h}_u^{(l)}}{|\mathrm{N}(v)|} + \boxed{\mathrm{B}_l}\mathrm{h}_v^{(l)}\right), \forall l \in \{0, \dots, L-1\}$$

$$\mathrm{z}_v = \mathrm{h}_v^{(L)}$$

Final node embedding

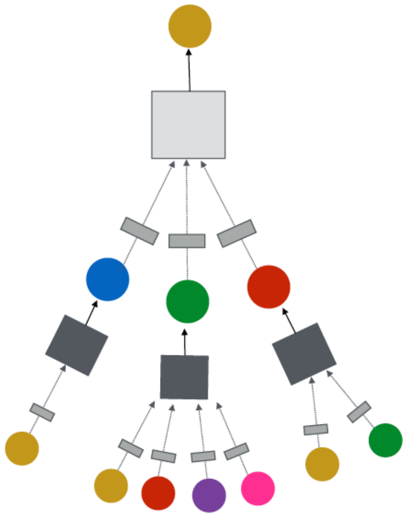
We can feed these **embeddings into any loss function** and run SGD to **train the weight parameters**

h_v^l: the hidden representation of node v at layer l
- W_l: weight matrix for neighborhood aggregation
- B_l: weight matrix for transforming hidden vector of self

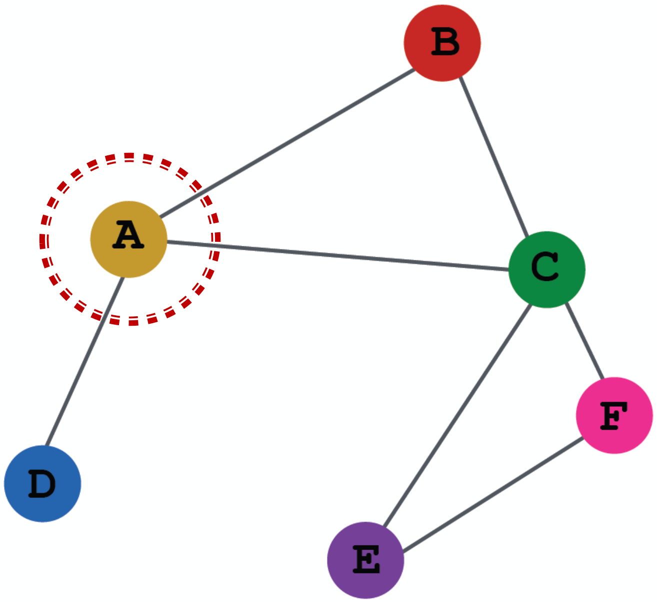
Credit: Stanford CS224W

Supervised Training

Directly train the model for a supervised task (e.g., node classification)



Is user going to churn in the next week?



E.g., a relational graph of users, sales, products

How to train a GNN

- Node embedding $\boldsymbol{z}_v$ is a function of input graph
- **Supervised setting**: we want to minimize the loss $\mathcal{L}$:

$$\min_{\Theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{z}_v))$$

  - $\boldsymbol{y}$: node label
  - $\mathcal{L}$ could be L2 if $\boldsymbol{y}$ is real number, or cross entropy if $\boldsymbol{y}$ is categorical

Credit: [Stanford CS224W]

Supervised Training

Directly train the model for a supervised task (e.g., **node classification**)

- Use cross entropy loss

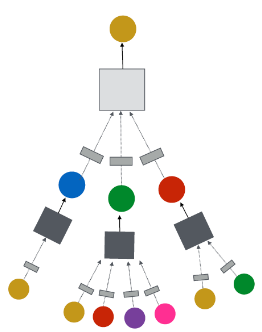
$$\mathcal{L} = \sum_{v\in V} \boxed{y_v}\log(\sigma(\boxed{\mathrm{z}_v^{\mathrm{T}}}\boxed{\theta})) + (1-\boxed{y_v})\log(1-\sigma(\boxed{\mathrm{z}_v^{\mathrm{T}}}\boxed{\theta}))$$

Encoder output:
node embedding

Classification
weights

Node class
label

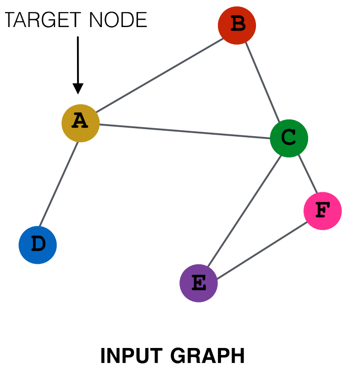
Is user going to churn
in the next week?



Credit: Stanford CS224W

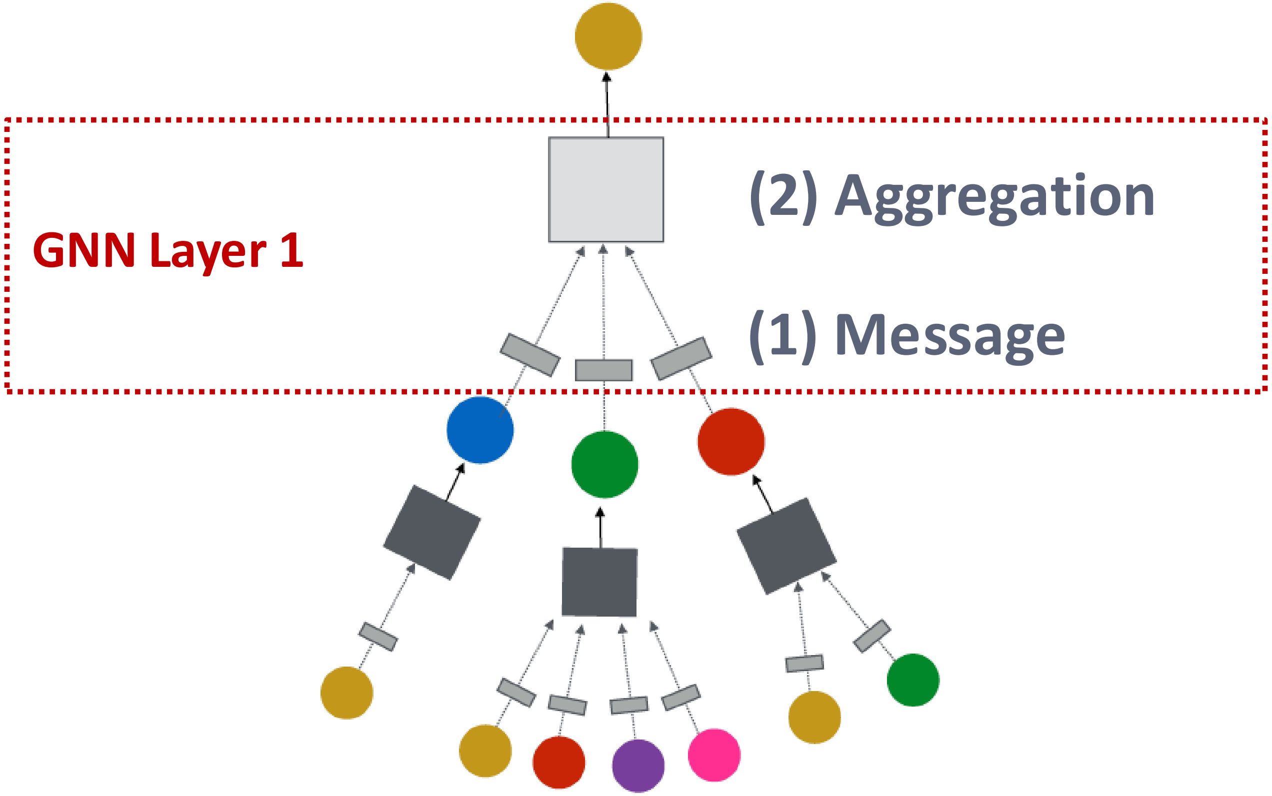
Designing a GNN

A General GNN Framework (1)

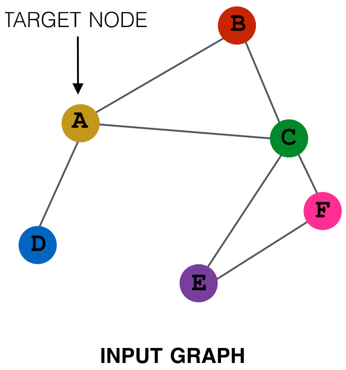


GNN Layer = Message + Aggregation

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



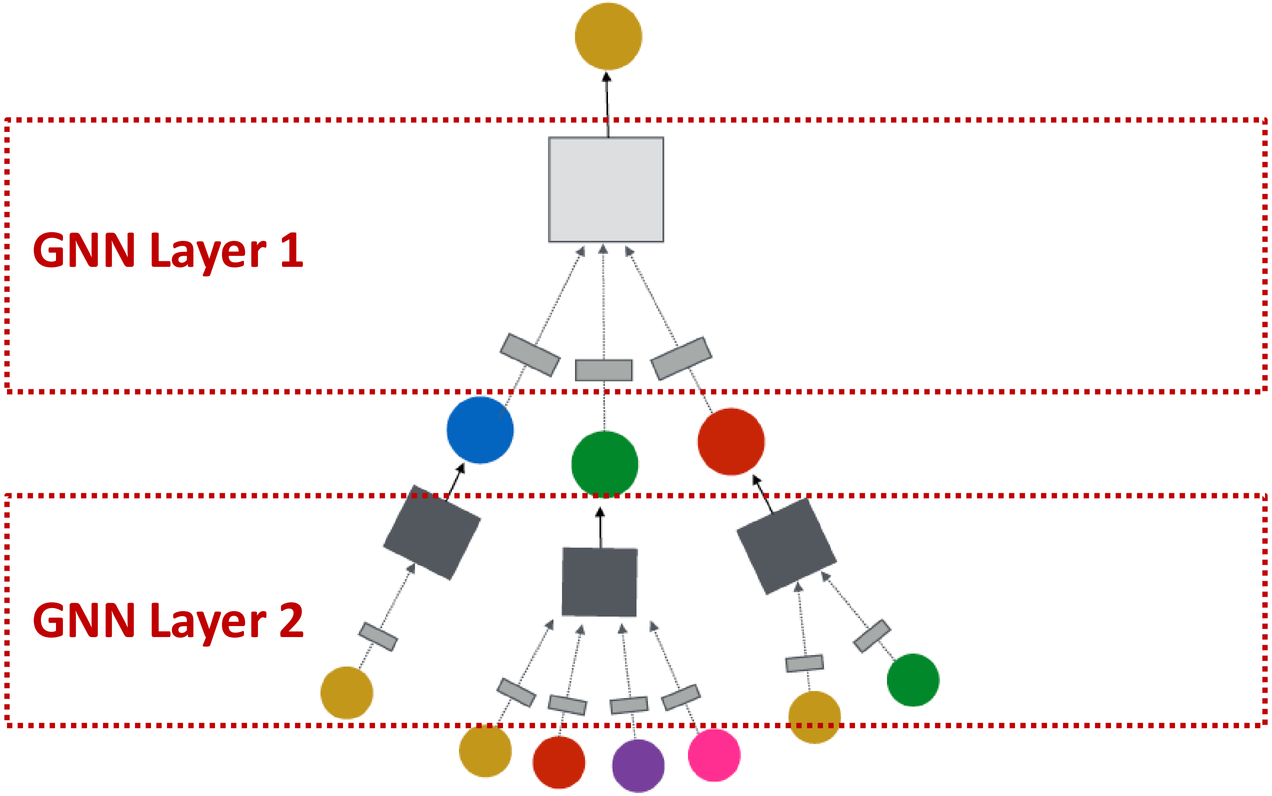
A General GNN Framework (2)



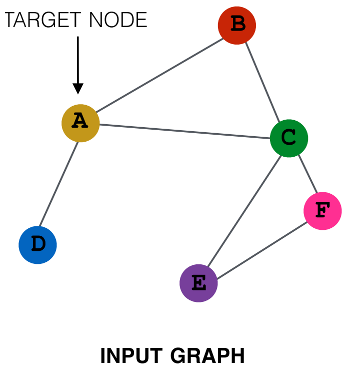
Connect GNN layers into a GNN

- Stack layers sequentially
- Ways of adding skip connections

(3) Layer connectivity

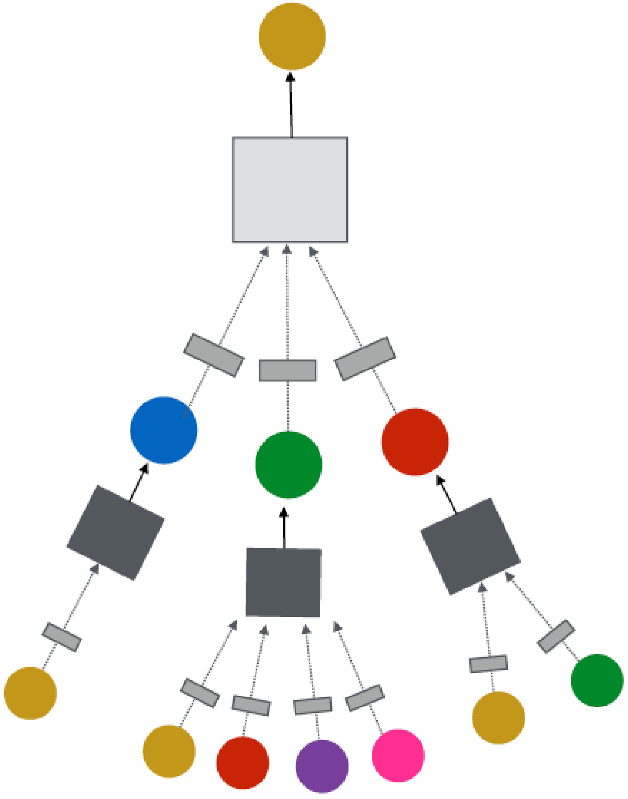


A General GNN Framework (3)



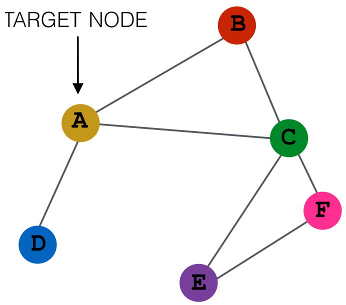
Idea: Raw input graph $\neq$ computational graph

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



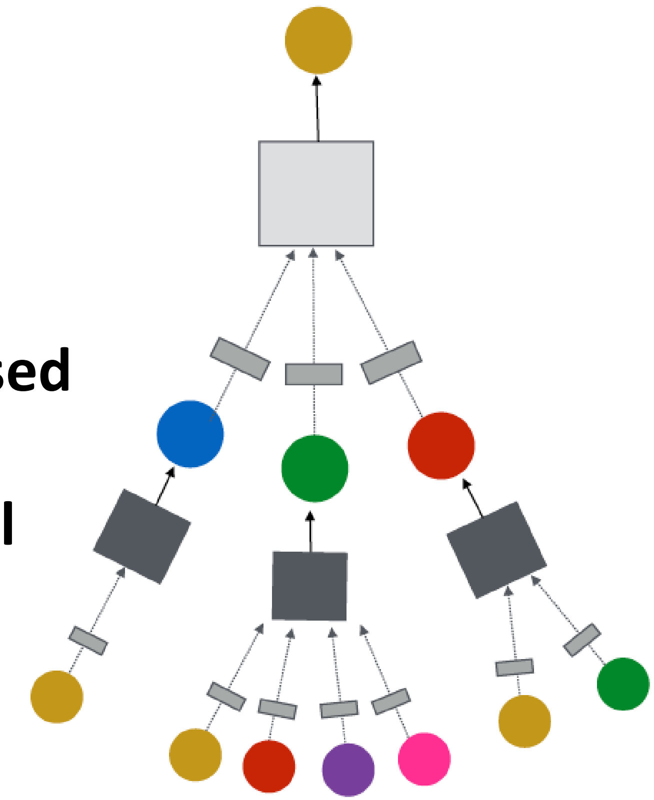
(4) Graph augmentation

A General GNN Framework (4)



INPUT GRAPH

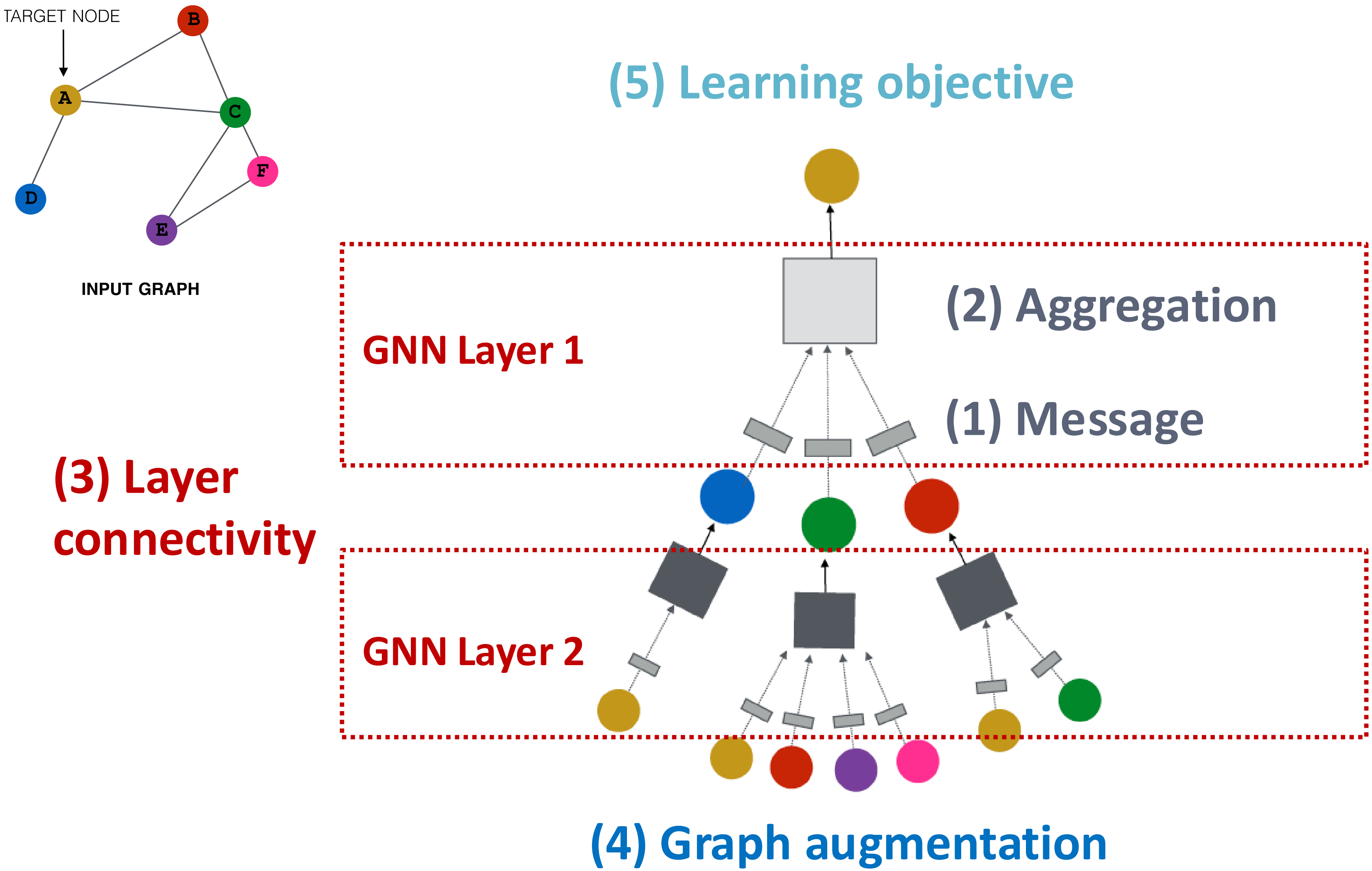
(5) Learning objective



How do we train a GNN

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

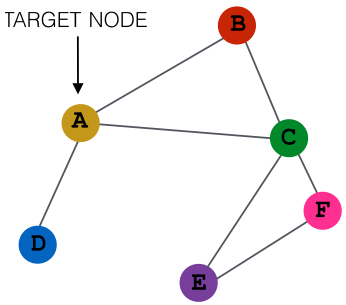
A General GNN Framework (5)



A Single Layer of a GNN

J. You, R. Ying, J. Leskovec. [Design Space of Graph Neural Networks](), NeurIPS 2020

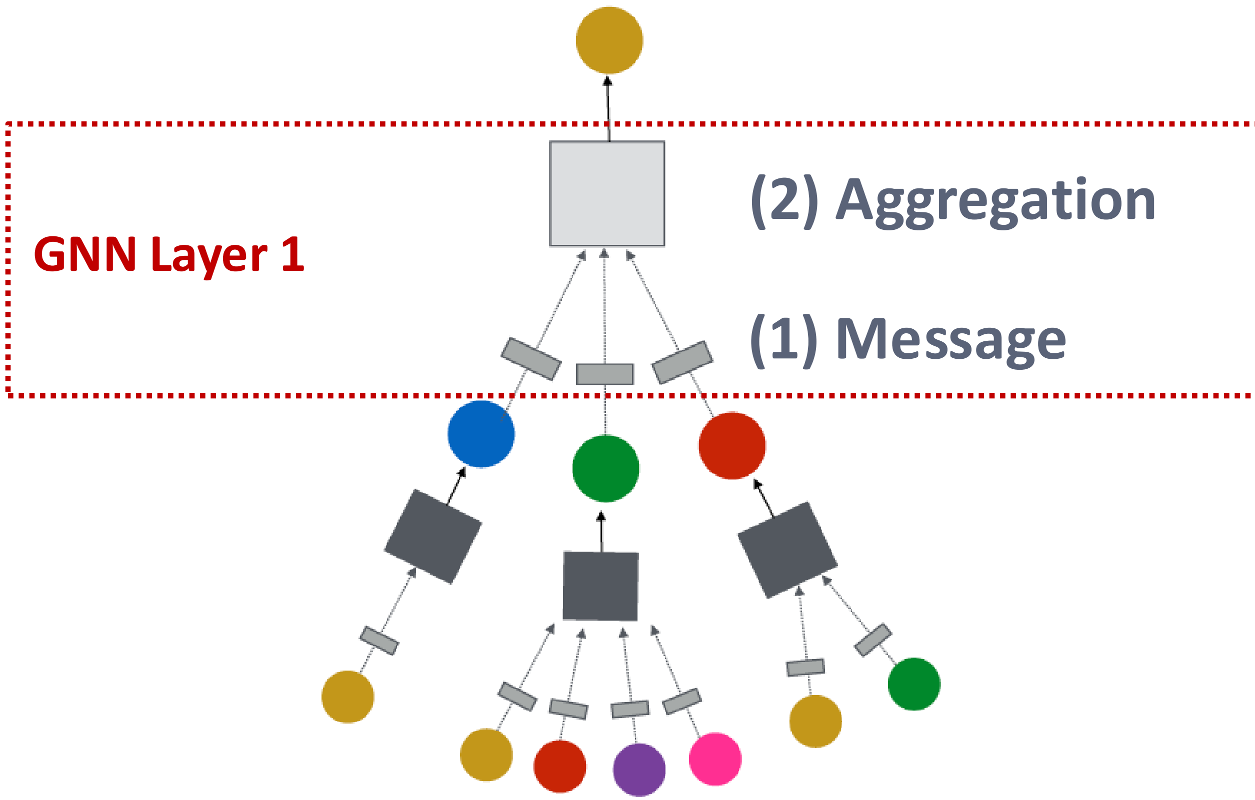
A GNN Layer



INPUT GRAPH

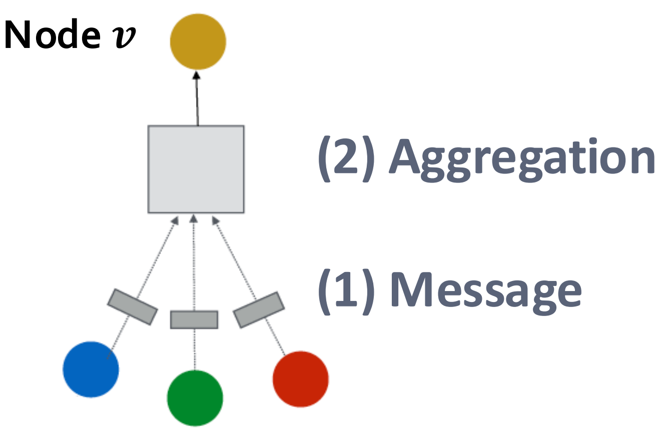
GNN Layer = Message + Aggregation

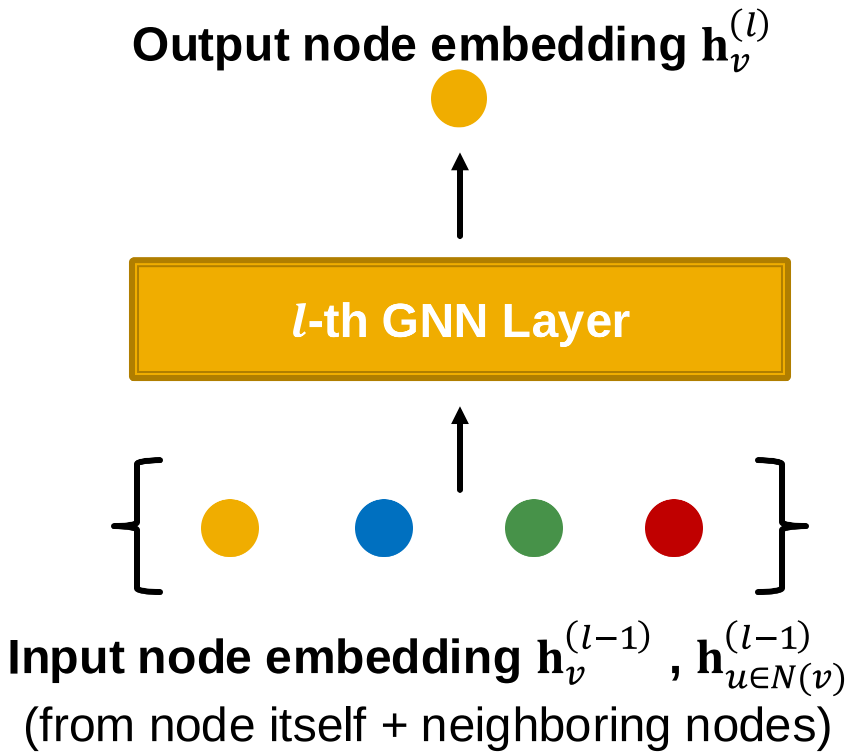
- **Different instantiations under this perspective**
- **GCN, GraphSAGE, GAT, …**



A Single GNN Layer

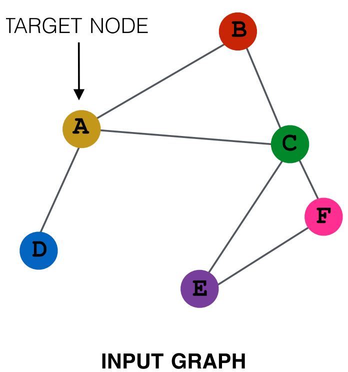
- **Idea of a GNN Layer:**
  - Compress a set of vectors into a single vector
  - **Two step process:**
    - **(1) Message**
    - **(2) Aggregation**

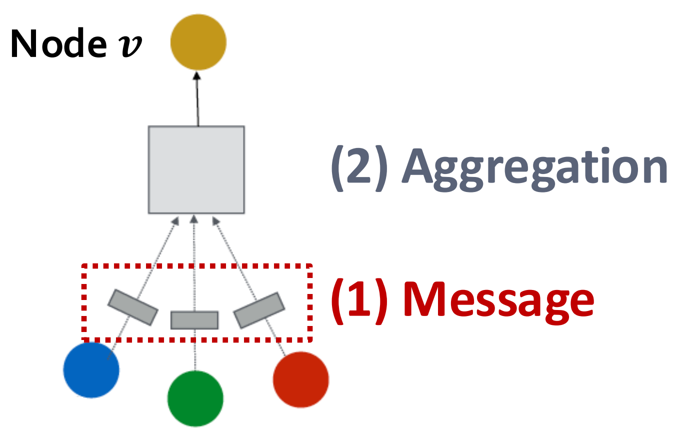




Message Computation

- **(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 $\mathbf{W}^{(l)}$



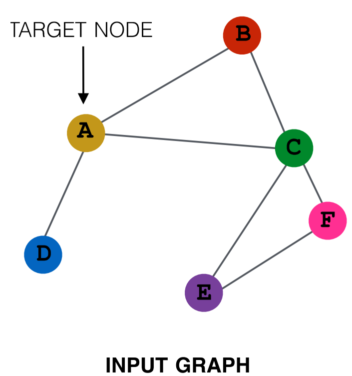


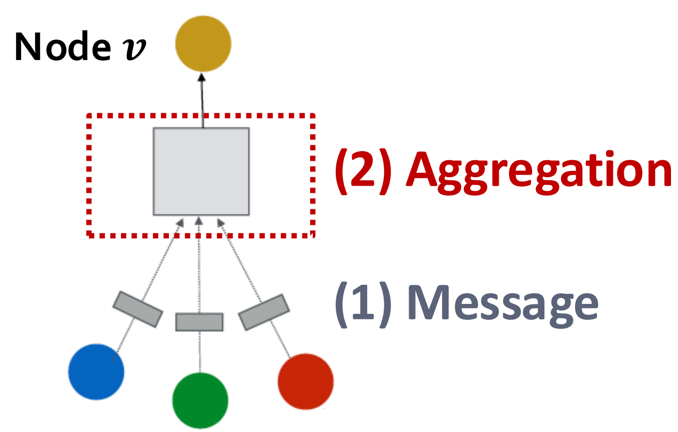
Message Aggregation

- **(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

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

  - **(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

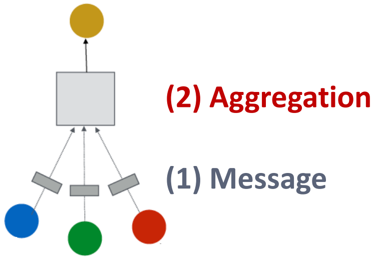
- **Putting things together:**
  - **(1) Message**: each node computes a message

$$\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$

  - **(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**



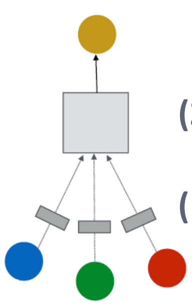
Classical GNN Layers: GCN (1)

- **(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?**

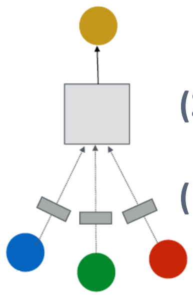
$$\mathbf{h}_v^{(l)} = \sigma\left(\underbrace{\sum_{u \in N(v)}}_{\text{Aggregation}} \overbrace{\mathbf{W}^{(l)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}}^{\text{Message}}\right)$$



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

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

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

Classical GNN Layers: GAT (1)

- **(3) Graph Attention Networks**

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

Attention weights

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

[Velickovic et al., ICLR 2018; Vaswani et al., NIPS 2017]

Classical GNN Layers: GAT (2)

Can we do better than simple neighborhood aggregation?

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

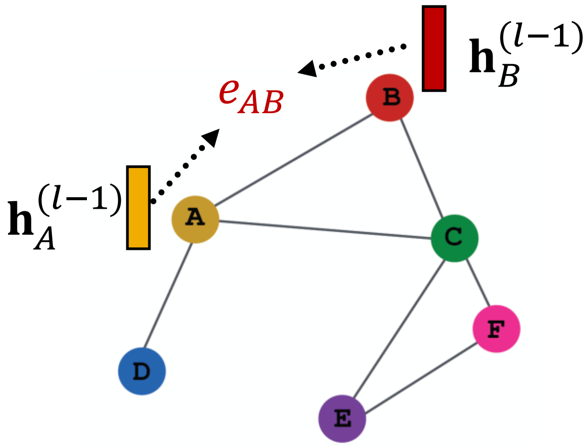
- **Goal:** Specify **arbitrary importance** to different neighbors of each node in the graph
- **Idea:** Compute embedding $\boldsymbol{h}_v^{(l)}$ of each node in the graph following an **attention strategy**:
  - Implicitly specify different weights to different nodes in a neighborhood

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 $\boldsymbol{v}$**



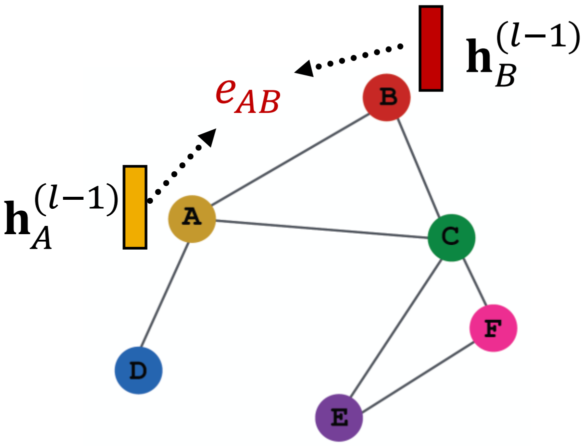
$$e_{AB} = a(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)})$$

Attention Mechanism (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:

$$e_{vu} = a(\boldsymbol{m}_u^{(l)}, \boldsymbol{m}_v^{(l)})$$

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



$$e_{AB} = a(\boldsymbol{m}_A^{(l)}, \boldsymbol{m}_B^{(l)})$$

Attention Mechanism (2)

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

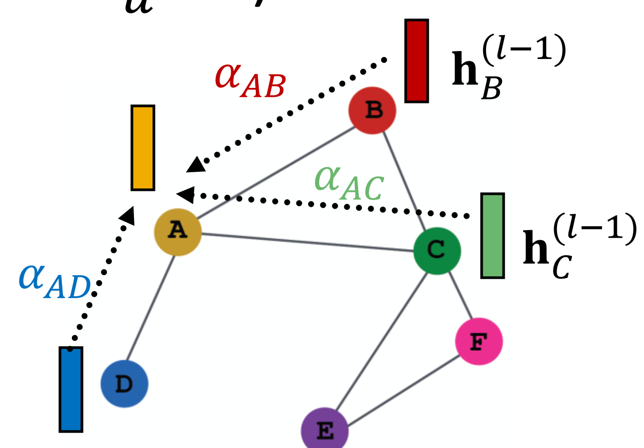
$$\alpha_{vu} = \frac{\exp(e_{vu})}{\sum_{k \in N(v)} \exp(e_{vk})}$$

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

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

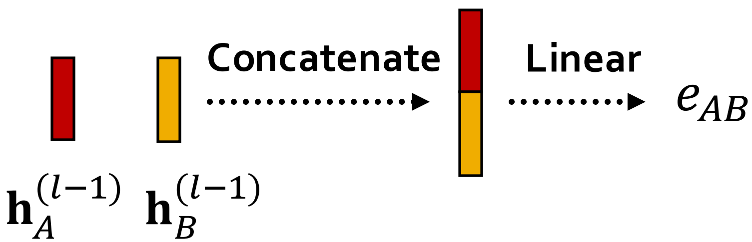
Weighted sum using α_{AB}, α_{AC}, α_{AD}:

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



Attention Mechanism (3)

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



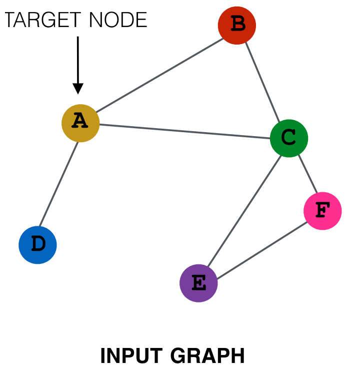
$$e_{AB} = a\left(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)}\right)$$
$$= \text{Linear}\left(\text{Concat}\left(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)}\right)\right)$$

  - 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

Graph Manipulation in GNNs

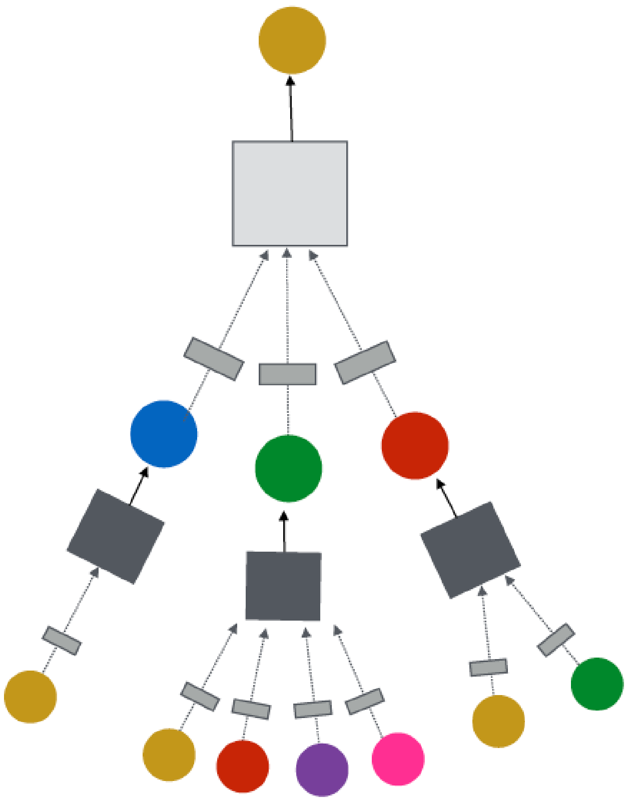
J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020

General GNN Framework



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

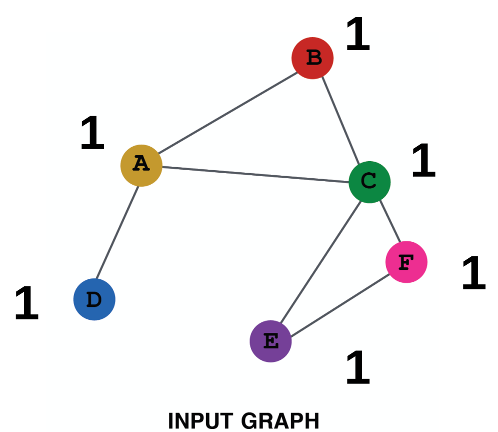
Graph Manipulation Approaches

- **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**

Feature Augmentation on Graphs

Why do we need feature augmentation?

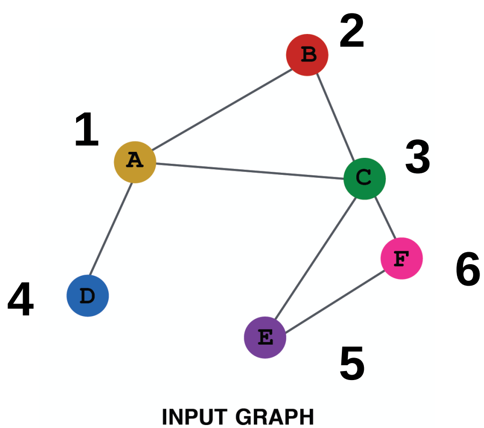
- **(1) Input graph does not have node features**
  - This is common when we only have the adj. matrix
- **Standard approaches:**
- **a) Assign constant values to nodes**



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**



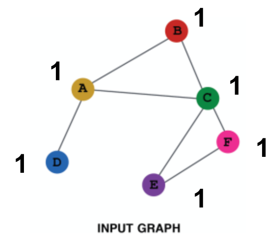
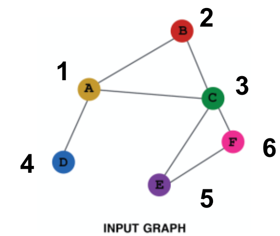
One-hot vector for node with ID=5

ID = 5

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

Feature Augmentation on Graphs

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

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

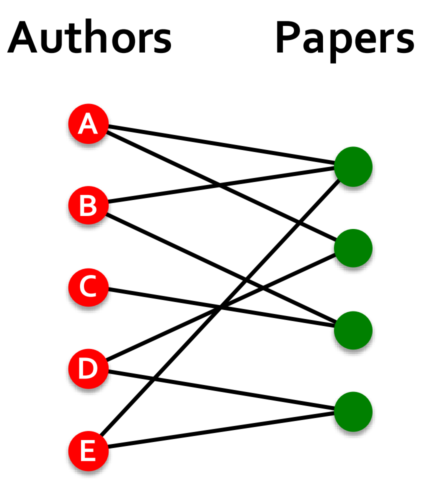
Feature Augmentation on Graphs

Why do we need feature augmentation?

- **(2) Certain features can help GNN learning**
- Other commonly used augmented features:
  - **Node degree**
  - **PageRank**
  - **Clustering coefficient**
  - **…**
- Any **useful graph statistics can be used!**

Add Virtual Nodes / Edges

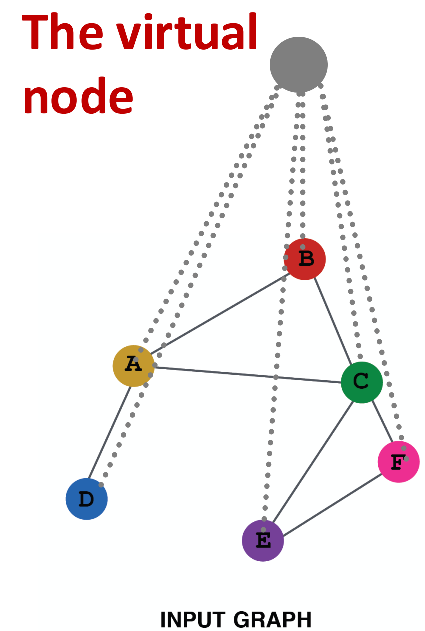
- **Motivation:** Augment sparse graphs
- **(1) Add virtual edges**
  - **Common approach:** Connect 2-hop neighbors via virtual edges
  - **Intuition:** Instead of using adj. matrix A for GNN computation, use $A + A^2$



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

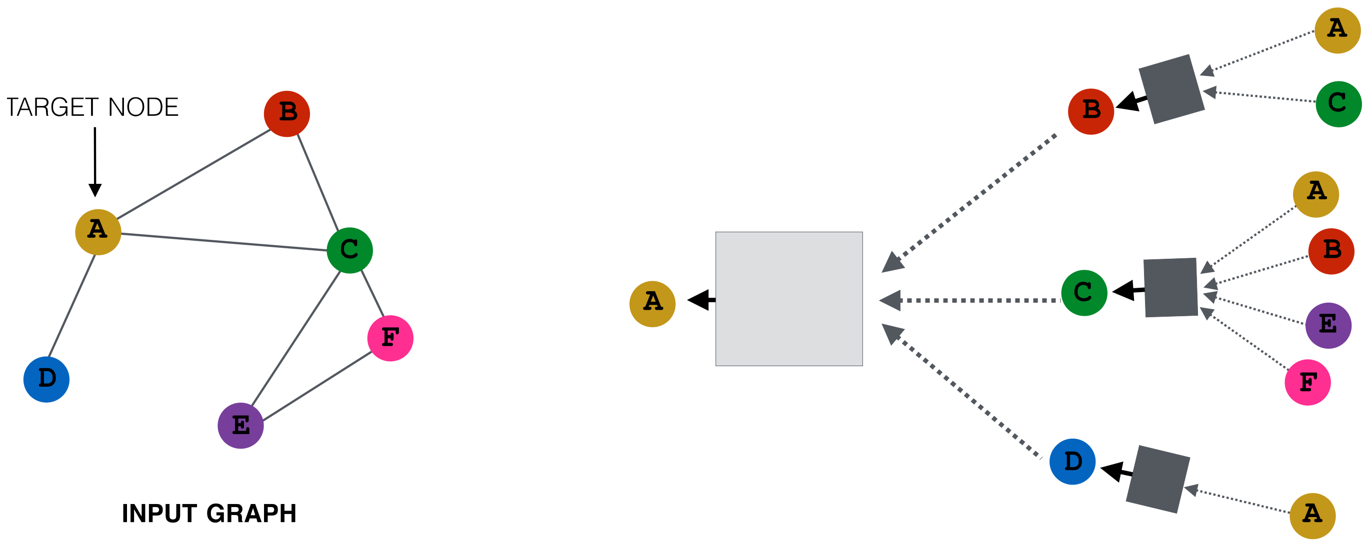
Add Virtual Nodes / Edges

- **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

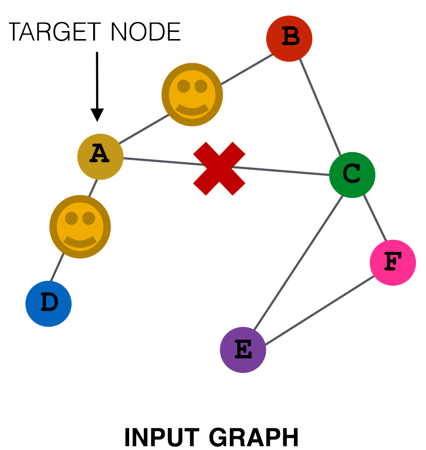
- **Previously:**
  - All the nodes are used for message passing

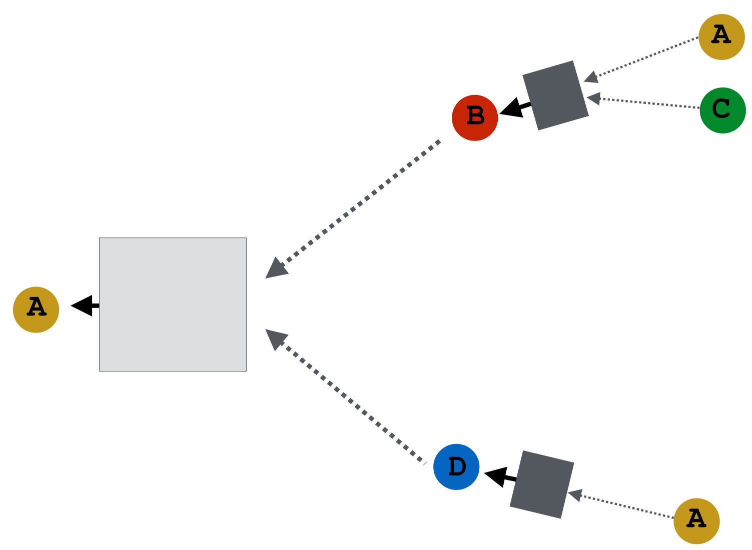


- **New idea:** (Randomly) sample a node's neighborhood for message passing

Neighborhood Sampling Example

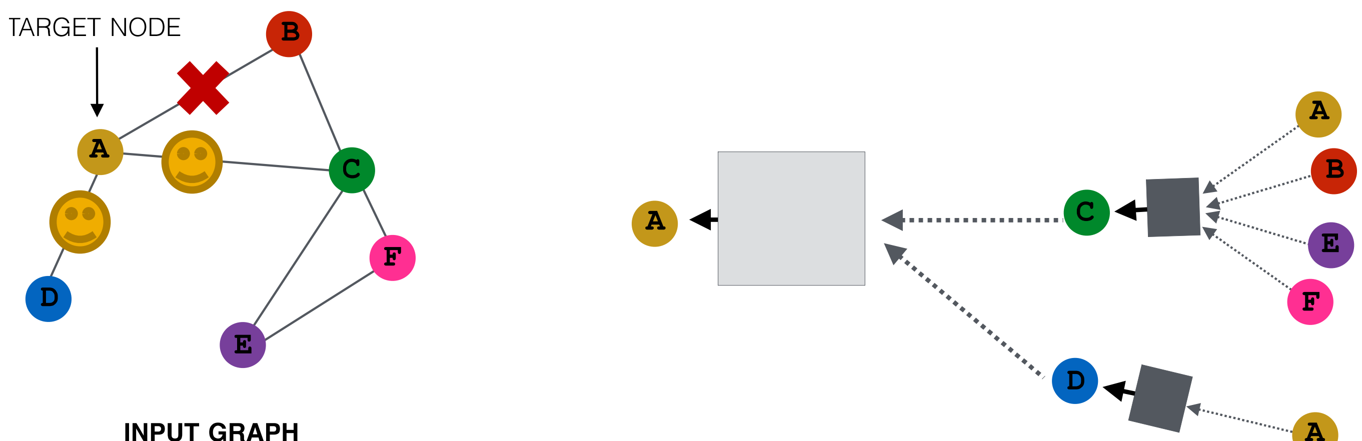
- **For example, we can randomly choose 2 neighbors to pass messages**
  - Only nodes B and D will pass message to A





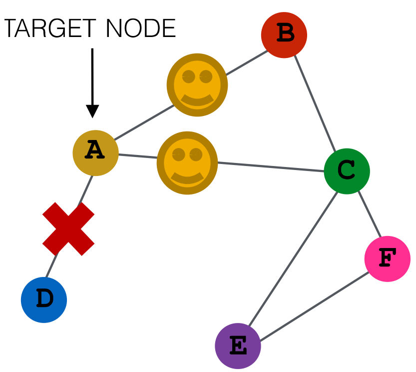
Neighborhood Sampling Example

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

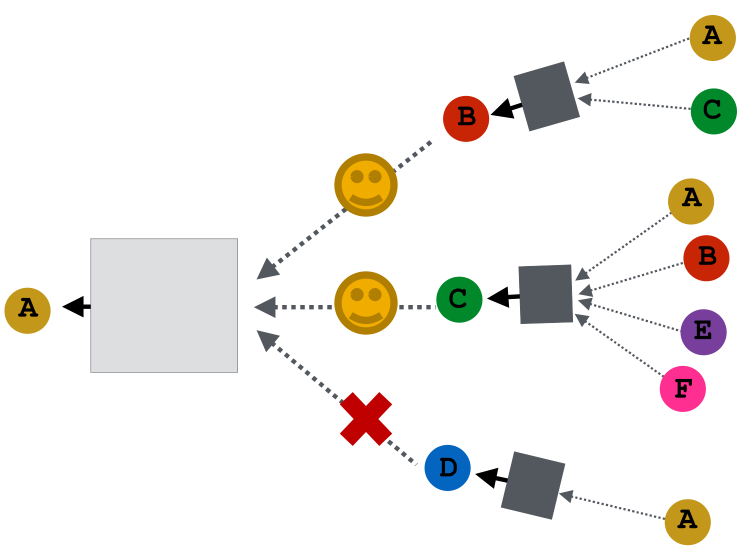


Neighborhood Sampling Example

- 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!



INPUT GRAPH



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

Extras

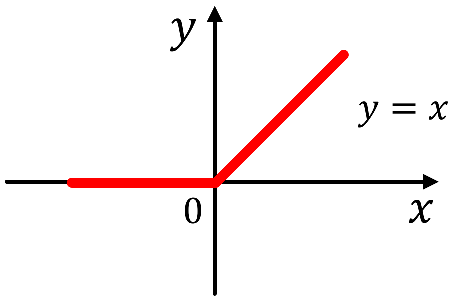
Activation (Non-linearity)

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

- **Rectified linear unit (ReLU)**

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

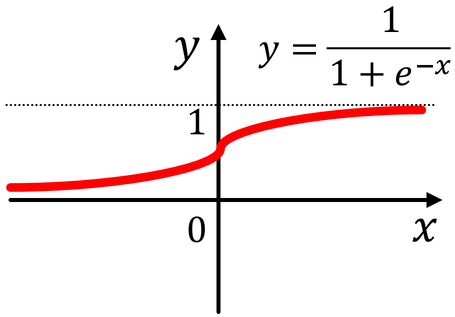
  - Most commonly used



- **Sigmoid**

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

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

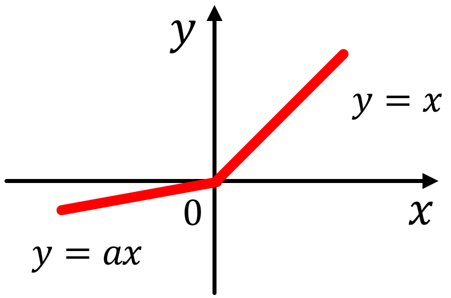


- **Parametric ReLU**

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

  a_i is a trainable parameter

  - Empirically performs better than ReLU



GraphSAGE Neighbor Aggregation

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

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

Aggregation **Message computation**

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

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

Aggregation **Message computation**

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

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