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Stanford CS224W: Graph Neural Networks

CS224W: Machine Learning with Graphs

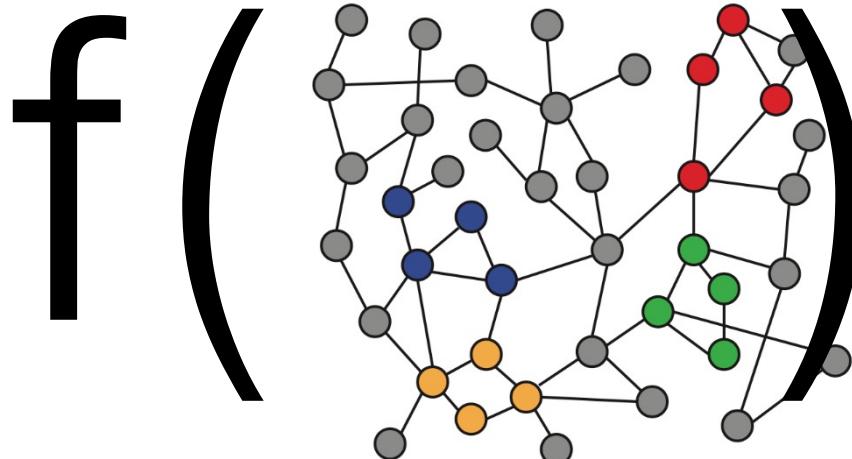
Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>

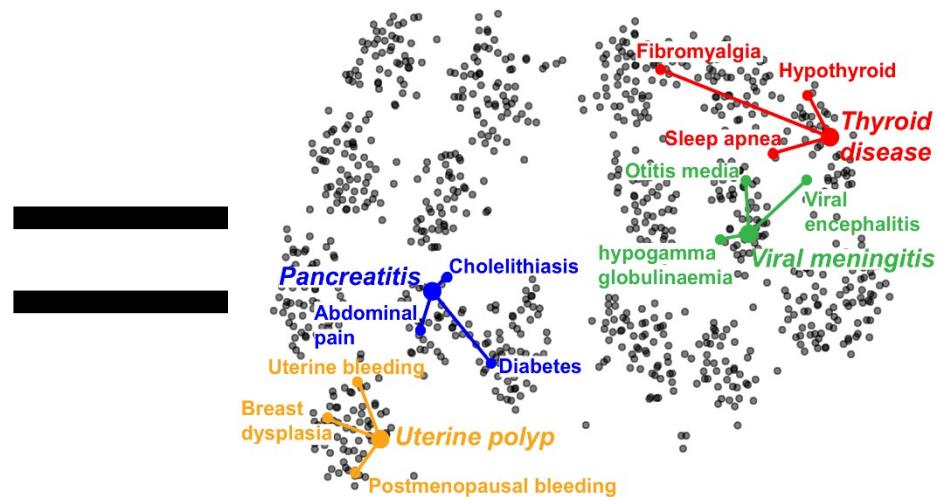


Recap: Node Embeddings

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



Input graph



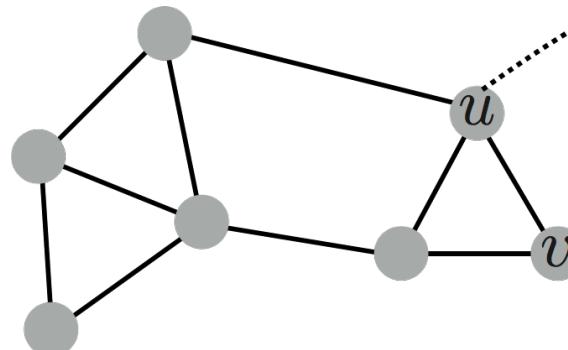
2D node embeddings

How to learn mapping function f ?

Recap: Node Embeddings

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

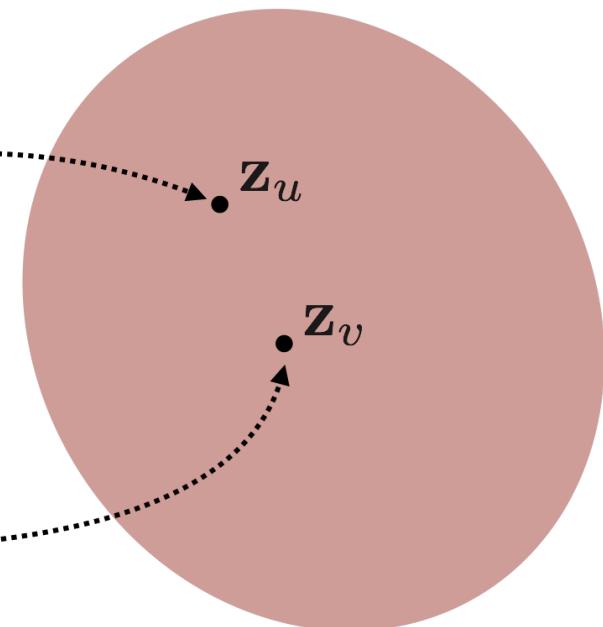
Need to define!



encode nodes

$\text{ENC}(u)$

$\text{ENC}(v)$

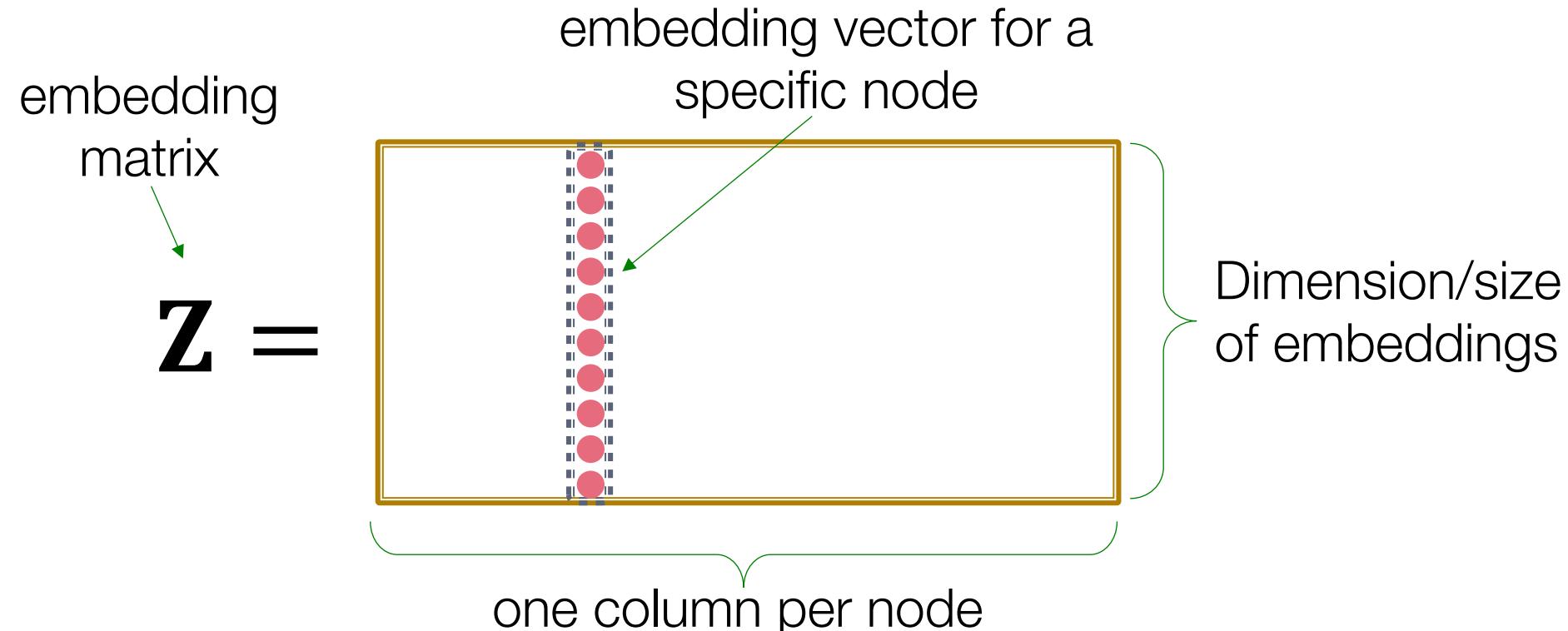


Input network

d -dimensional
embedding space

Recap: “Shallow” Encoding

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



Today: Deep Graph Encoders

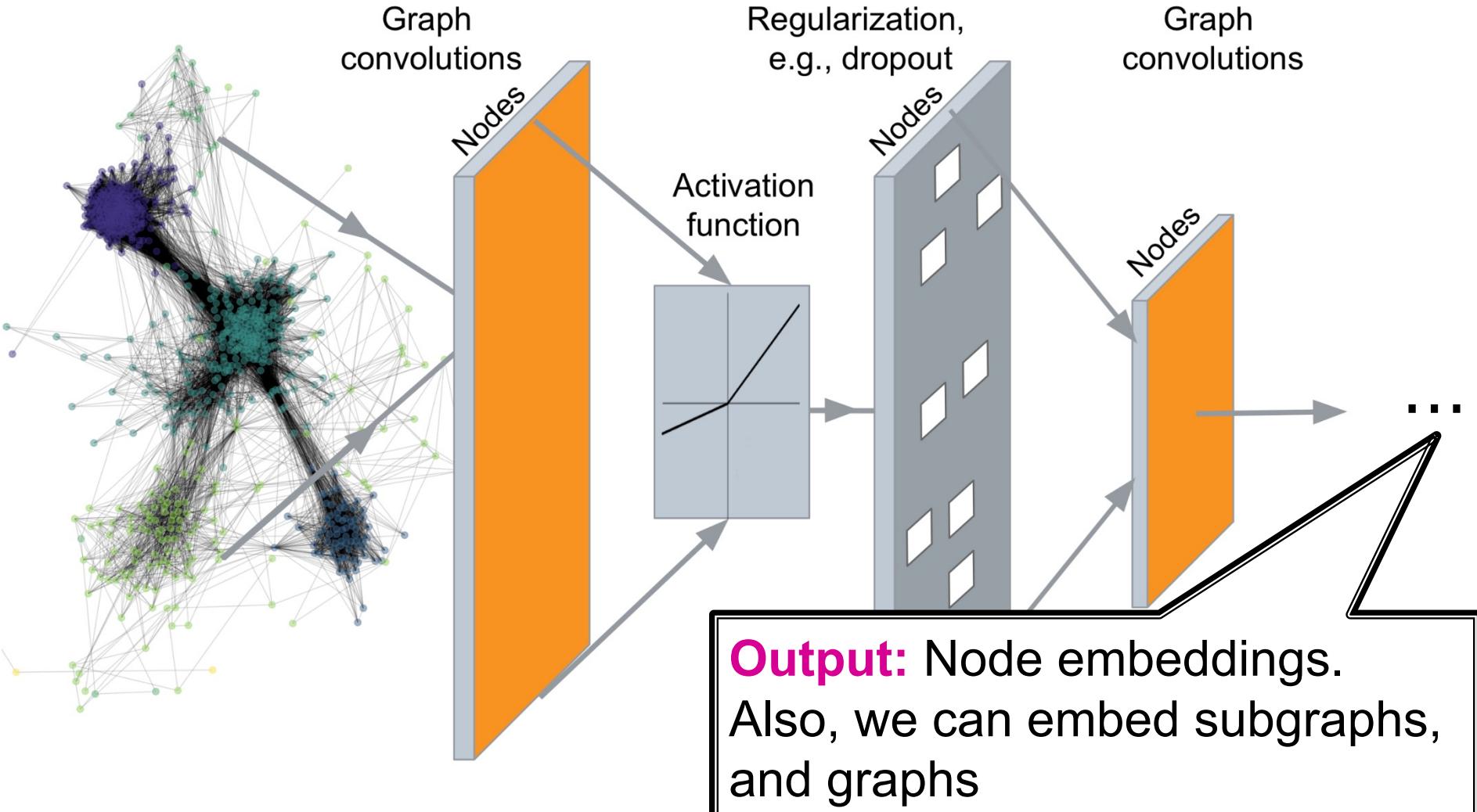
- **Today:** We will now discuss deep learning methods based on **graph neural networks (GNNs)**:

$$\text{ENC}(v) =$$

**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



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
- Community detection
 - Identify densely linked clusters of nodes
- Network similarity
 - How similar are two (sub)networks

Outline of Today's Lecture

1. Deep learning for graphs



2. Graph Convolutional Networks

3. GNNs subsume CNNs

Summary: Basics of Deep Learning

- Loss function \mathcal{L} :

$$\min_{\Theta} \mathcal{L}(y, f_{\Theta}(x))$$

- f can be a simple linear layer, an MLP, or other neural networks (e.g., a GNN later)
- Sample a minibatch of input data x
- Forward propagation: Compute \mathcal{L} given x
- Back-propagation: Obtain gradient $\nabla_{\Theta} \mathcal{L}$ using a chain rule.
- Use stochastic gradient descent (SGD) to optimize \mathcal{L} for weights Θ over many iterations.

Stanford CS224W: Deep Learning for Graphs

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Content

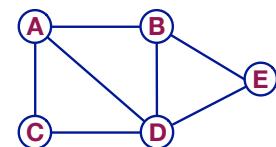
- **Local network neighborhoods:**
 - Describe aggregation strategies
 - Define computation graphs
- **Stacking multiple layers:**
 - Describe the model, parameters, training
 - How to fit the model?
 - Simple example for unsupervised and supervised training

Setup

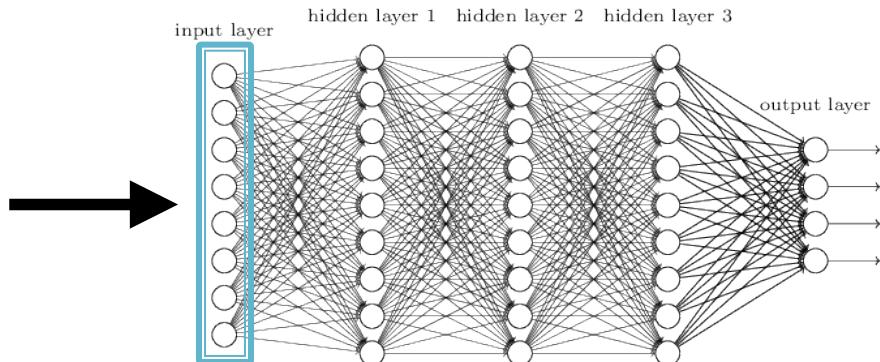
- Assume we have a graph G :
 - V is the **vertex set**
 - A is the **adjacency matrix** (assume binary)
 - $X \in \mathbb{R}^{|V| \times m}$ is a matrix of **node features**
 - v : a node in V ; $N(v)$: the set of neighbors of v .
 - **Node features:**
 - Social networks: User profile, User image
 - Biological networks: Gene expression profiles, gene functional information
 - When there is no node feature in the graph dataset:
 - Indicator vectors (one-hot encoding of a node)
 - Vector of constant 1: [1, 1, ..., 1]

A Naïve Approach

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



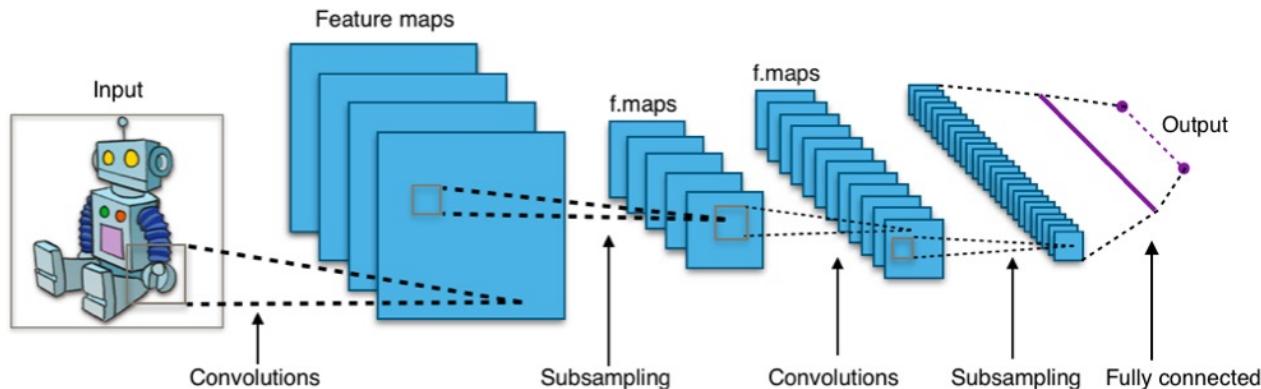
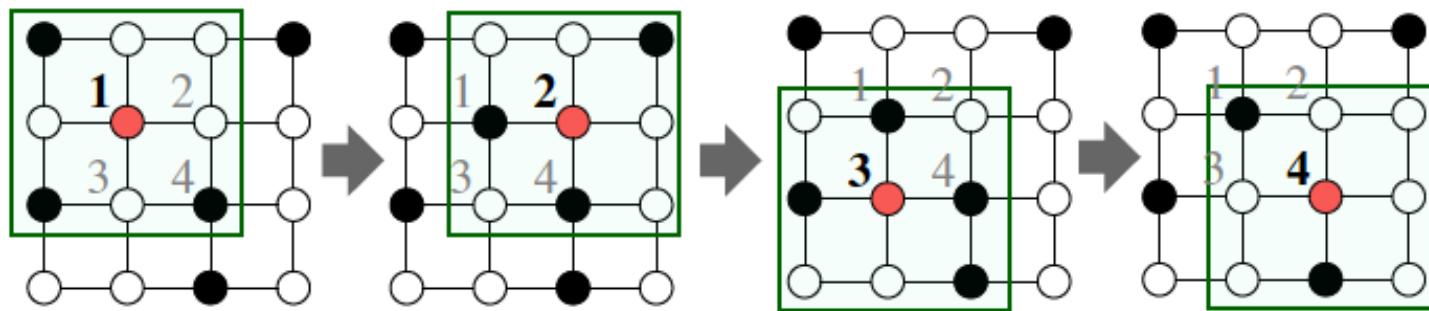
	A	B	C	D	E	Feat
A	0	1	1	1	0	1 0
B	1	0	0	1	1	0 0
C	1	0	0	1	0	0 1
D	1	1	1	0	1	1 1
E	0	1	0	1	0	1 0



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

Idea: Convolutional Networks

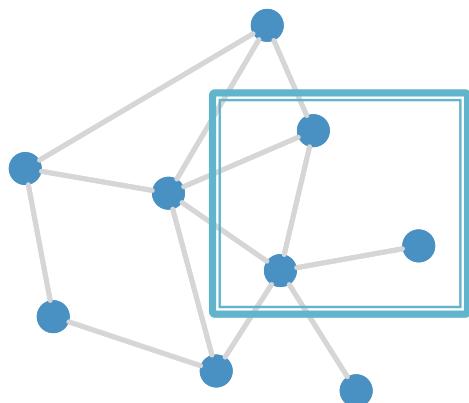
CNN on an image:



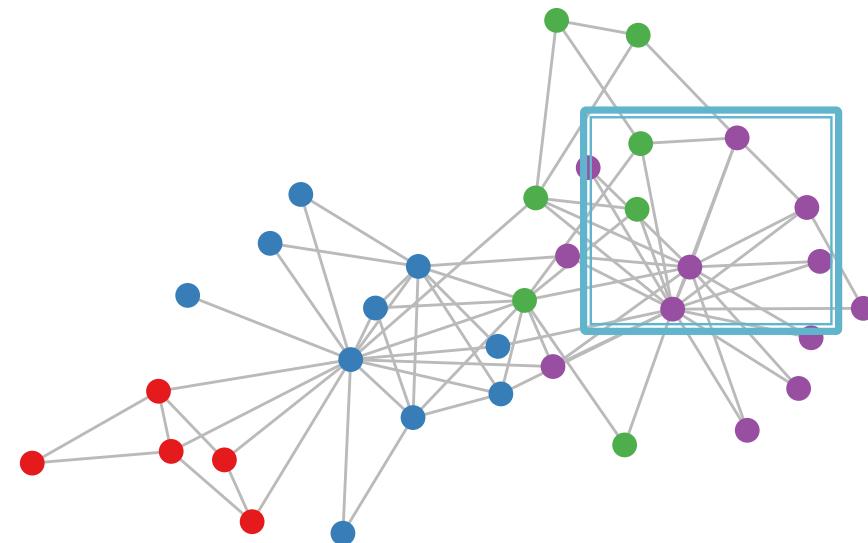
Goal is to generalize convolutions beyond simple lattices
Leverage node features/attributes (e.g., text, images)

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**

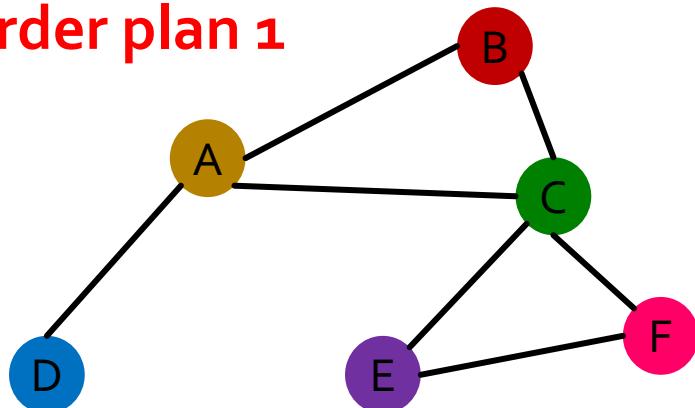
Permutation Invariance

- Consider we want to embed an entire graph
- Observation: A graph does not have a canonical ordering of its nodes
 - We can have many different node orderings of the same graph.
- What do we want: If we learn an embedding function over a graph, we should get the same result (the same embedding) regardless of how the nodes are numbered.

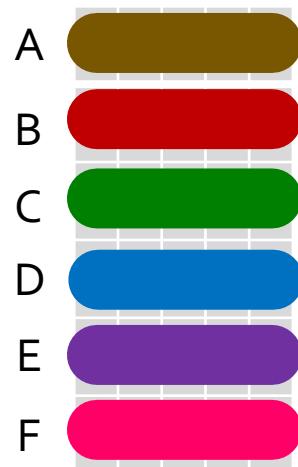
Permutation Invariance

- Graph does not have a canonical ordering of the nodes!

Order plan 1



Node features X_1



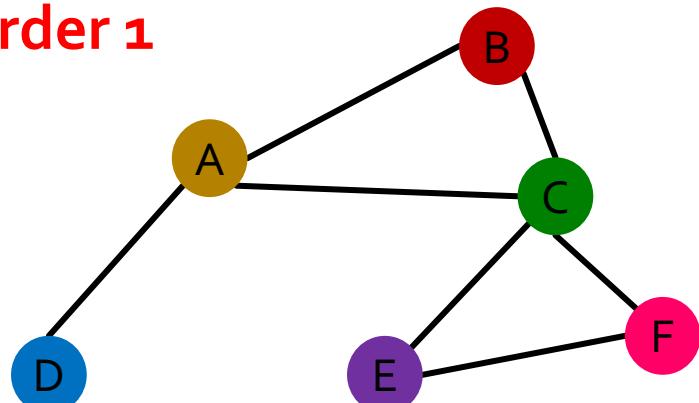
Adjacency matrix A_1

	A	B	C	D	E	F
A	Gray	Blue	Blue	Blue	Gray	Gray
B	Blue	Gray	Blue	Blue	Gray	Gray
C	Blue	Blue	Gray	Gray	Blue	Blue
D	Blue	Gray	Gray	Gray	Gray	Gray
E	Gray	Gray	Blue	Blue	Gray	Blue
F	Gray	Gray	Gray	Blue	Gray	Gray

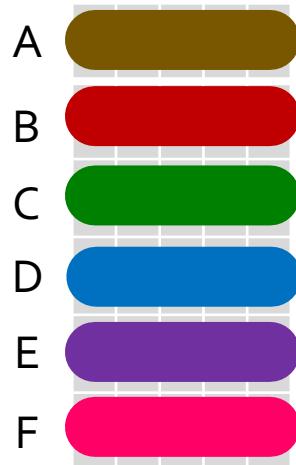
Permutation Invariance

- Graph does not have a canonical ordering of the nodes!

Order 1



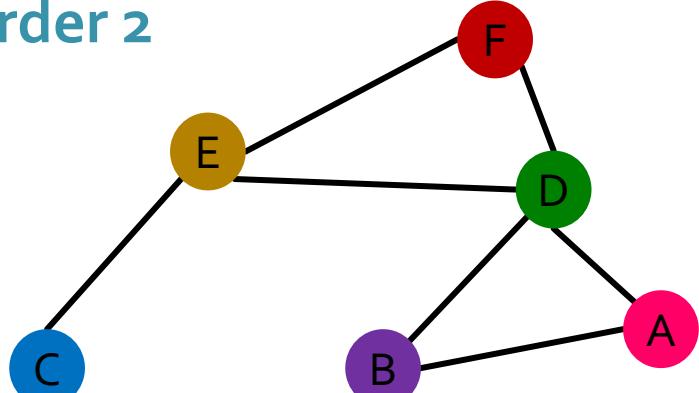
Node features X_1



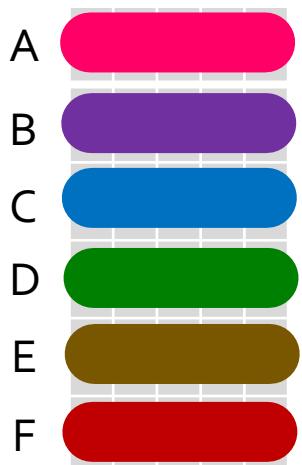
Adjacency matrix A_1

	A	B	C	D	E	F
A	Gray	Blue	Gray	Blue	Gray	Gray
B	Blue	Gray	Blue	Gray	Gray	Gray
C	Blue	Blue	Gray	Gray	Blue	Blue
D	Blue	Gray	Gray	Gray	Gray	Gray
E	Gray	Gray	Blue	Blue	Gray	Blue
F	Gray	Gray	Gray	Blue	Blue	Gray

Order 2



Node features X_2



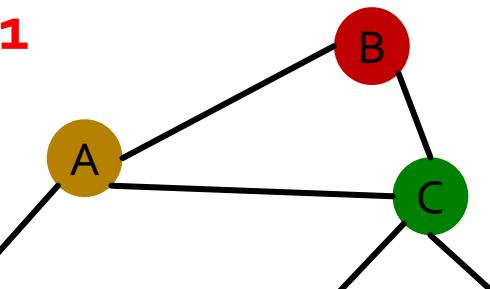
Adjacency matrix A_2

	A	B	C	D	E	F
A	Gray	Blue	Gray	Blue	Gray	Gray
B	Blue	Gray	Gray	Gray	Blue	Blue
C	Gray	Gray	Gray	Gray	Blue	Gray
D	Blue	Blue	Gray	Gray	Blue	Blue
E	Gray	Gray	Blue	Blue	Gray	Blue
F	Gray	Gray	Gray	Blue	Blue	Gray

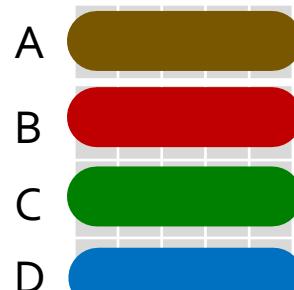
Permutation Invariance

- Graph does not have a canonical ordering of the nodes!

Order 1



Node features X_1

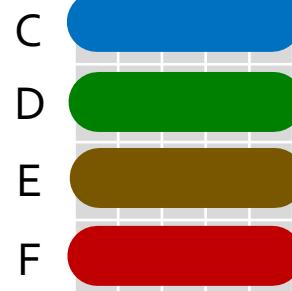
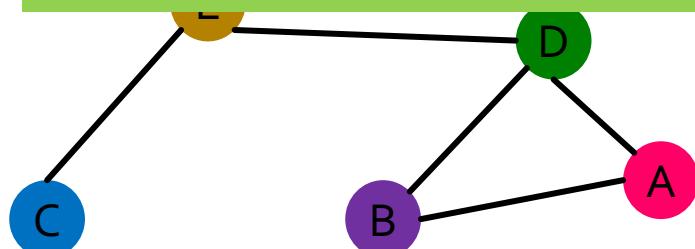


Adjacency matrix A_1

	A	B	C	D	E	F
A	Gray	Blue	Gray	Gray	Gray	Gray
B	Blue	Gray	Blue	Gray	Gray	Gray
C	Gray	Gray	Gray	Blue	Blue	Gray
D	Blue	Gray	Gray	Gray	Blue	Gray

Learned graph representation
should be the same for Order 1
and Order 2

Order 2



	B	C	D	E	F
B	Blue	Gray	Gray	Blue	Gray
C	Gray	Gray	Gray	Blue	Gray
D	Blue	Blue	Gray	Gray	Blue
E	Gray	Gray	Blue	Blue	Gray
F	Gray	Gray	Gray	Blue	Gray

Permutation Invariance

What do we mean by “graph representation is the same for two orderings”?

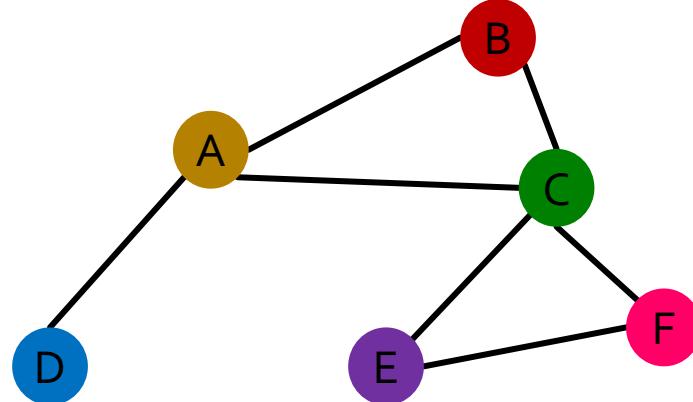
In other words, f maps a graph to a d -dim embedding

- Consider we learn a function f that maps a graph $G = (A, X)$ to a vector \mathbb{R}^d then

$$f(A_1, X_1) = f(A_2, X_2)$$

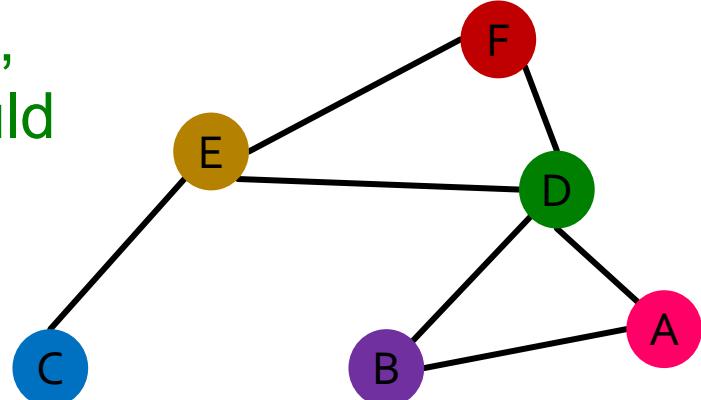
A is the adjacency matrix
 X is the node feature matrix

Order 1: A_1, X_1



For two orders,
output of f should
be the same!

Order 2: A_2, X_2



Permutation Invariance

What does it mean by “graph representation is the same for two order plans”?

- Consider we learn a function f that maps a graph $G = (A, X)$ to a vector \mathbb{R}^d .
 A is the adjacency matrix
 X is the node feature matrix
- Then, if $f(A_i, X_i) = f(A_j, X_j)$ for any ordering i and j , we formally say f is a **permutation invariant function**.
For a graph with $|V|$ nodes, there are $|V|!$ different orderings.
 m ... each node has a m -dim feature vector associated with it.
- Definition:** For any **graph** function $f: \mathbb{R}^{|V| \times |V|} \times \mathbb{R}^{|V| \times m} \rightarrow \mathbb{R}^d$, f is **permutation invariant** if $f(A, X) = f(PAP^T, PX)$ for any permutation P .

d ... output embedding dimensionality of embedding the graph $G = (A, X)$

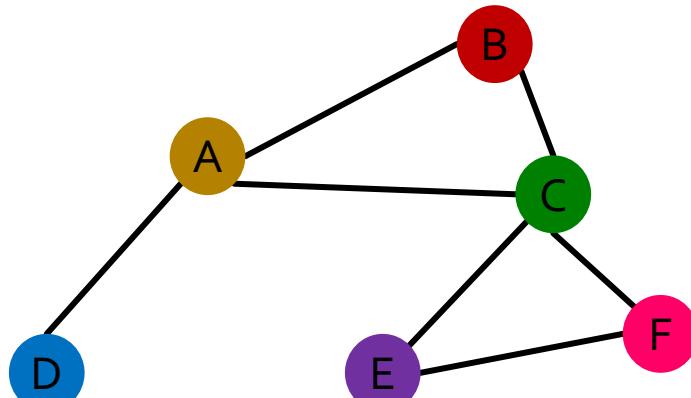
Permutation P : a shuffle of the node order
Example: (A,B,C)->(B,C,A)

Permutation Equivariance

For node representation: We learn a function f that maps nodes of G to a matrix $\mathbb{R}^{|V| \times d}$.

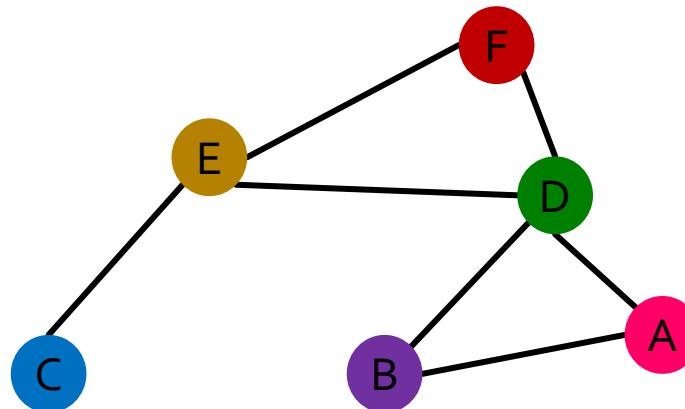
In other words, each node in V is mapped to a d -dim embedding.

Order 1: A_1, X_1



$$f(A_1, X_1) = \begin{array}{c|cc|cc|cc} & \text{A} & \text{B} & \text{C} & \text{D} & \text{E} & \text{F} \\ \text{A} & \text{Yellow} & & & & & \\ \text{B} & & \text{Red} & \text{Red} & & & \\ \text{C} & & & \text{Green} & \text{Green} & & \\ \text{D} & & & & \text{Blue} & \text{Blue} & \\ \text{E} & & & & & \text{Purple} & \text{Purple} \\ \text{F} & & & & & & \text{Red} \end{array}$$

Order 2: A_2, X_2

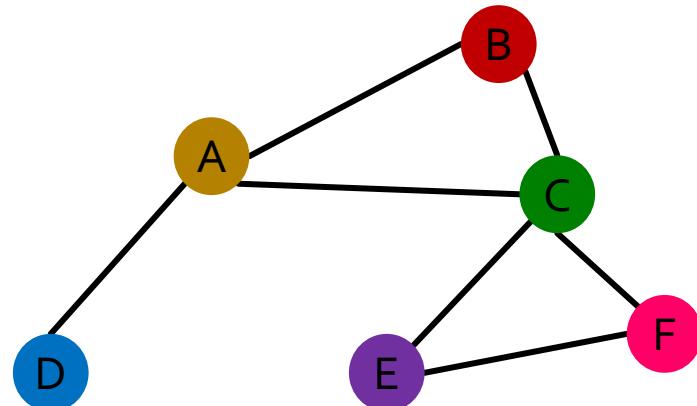


$$f(A_2, X_2) = \begin{array}{c|cc|cc|cc} & \text{A} & \text{B} & \text{C} & \text{D} & \text{E} & \text{F} \\ \text{A} & \text{Red} & \text{Red} & & & & \\ \text{B} & \text{Purple} & \text{Purple} & & & & \\ \text{C} & & \text{Blue} & \text{Blue} & & & \\ \text{D} & & & \text{Green} & \text{Green} & & \\ \text{E} & & & & \text{Yellow} & \text{Yellow} & \\ \text{F} & & & & & \text{Red} & \text{Red} \end{array}$$

Permutation Equivariance

For node representation: We learn a function f that maps nodes of G to a matrix $\mathbb{R}^{|V| \times d}$.

Order 1: A_1, X_1

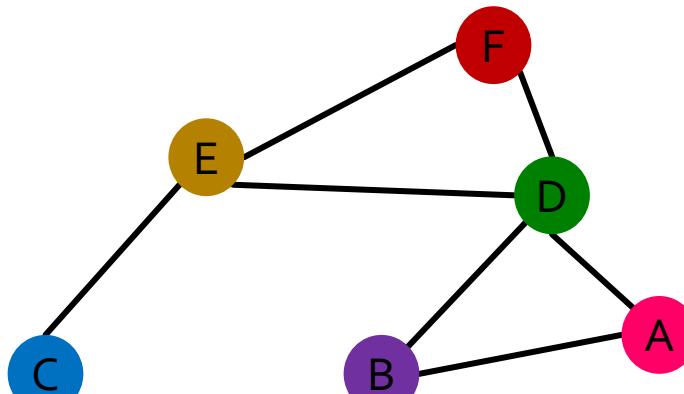


Representation vector
of the brown node A

A	[brown]	[brown]
B	[red]	[red]
C	[green]	[green]
D	[blue]	[blue]
E	[purple]	[purple]
F	[pink]	[pink]

$$f(A_1, X_1) =$$

Order 2: A_2, X_2



$$f(A_2, X_2) =$$

For two orderings, the vector of node at the same position in the graph is the same!

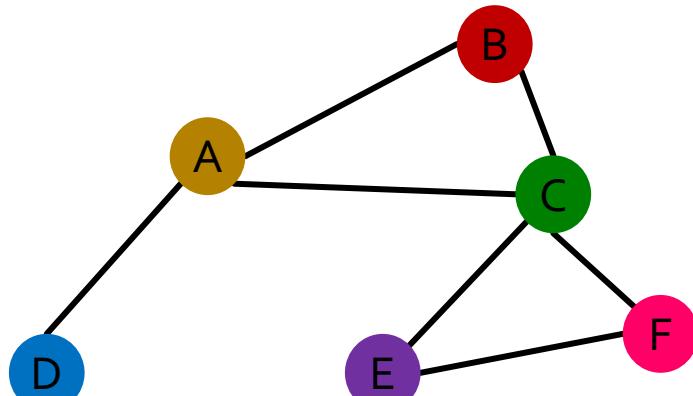
A	[red]	[red]
B	[purple]	[purple]
C	[blue]	[blue]
D	[green]	[green]
E	[brown]	[brown]
F	[pink]	[pink]

Representation vector
of the brown node E

Permutation Equivariance

For node representation: We learn a function f that maps nodes of G to a matrix $\mathbb{R}^{|V| \times d}$.

Order 1: A_1, X_1

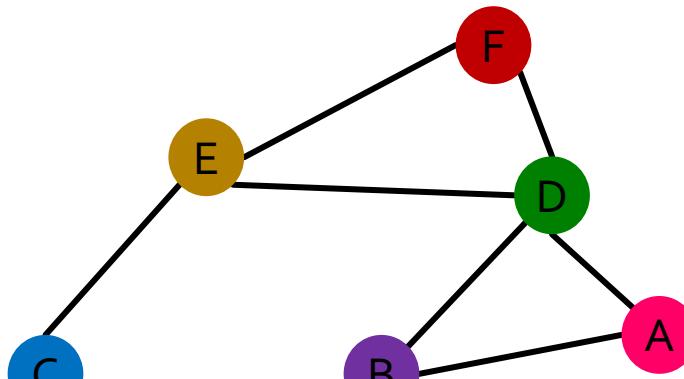


$$f(A_1, X_1) = \begin{matrix} & \text{A} & \text{B} & \text{C} & \text{D} & \text{E} & \text{F} \\ \text{A} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{B} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{C} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{D} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{E} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{F} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \end{matrix}$$

Representation vector of the green node C

For two orderings, the vector of node at the same position in the graph is the same!

Order 2: A_2, X_2



$$f(A_2, X_2) = \begin{matrix} & \text{A} & \text{B} & \text{C} & \text{D} & \text{E} & \text{F} \\ \text{A} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{B} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{C} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{D} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{E} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{F} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \end{matrix}$$

Representation vector of the green node D

Permutation Equivariance

For node representation:

- Consider we learn a function f that maps a graph $G = (A, X)$ to a matrix $\mathbb{R}^{|V| \times d}$
- If the output vector of a node at the same position in the graph remains unchanged for any ordering, we say f is **permutation equivariant**.

m... each node has a m -dim feature vector associated with it.

- Definition:** For any **node** function $f: \mathbb{R}^{|V| \times |V|} \times \mathbb{R}^{|V| \times m} \rightarrow \mathbb{R}^{|V| \times d}$, f is **permutation-equivariant** if $Pf(A, X) = f(PAP^T, PX)$ for any permutation P .

f maps each node in V to a d -dim embedding.

Summary: Invariance and Equivariance

■ Permutation-invariant

$$f(A, X) = f(PAP^T, PX)$$

Permute the input, the output stays the same.
(map a graph to a vector)

■ Permutation-equivariant

$$Pf(A, X) = f(PAP^T, PX)$$

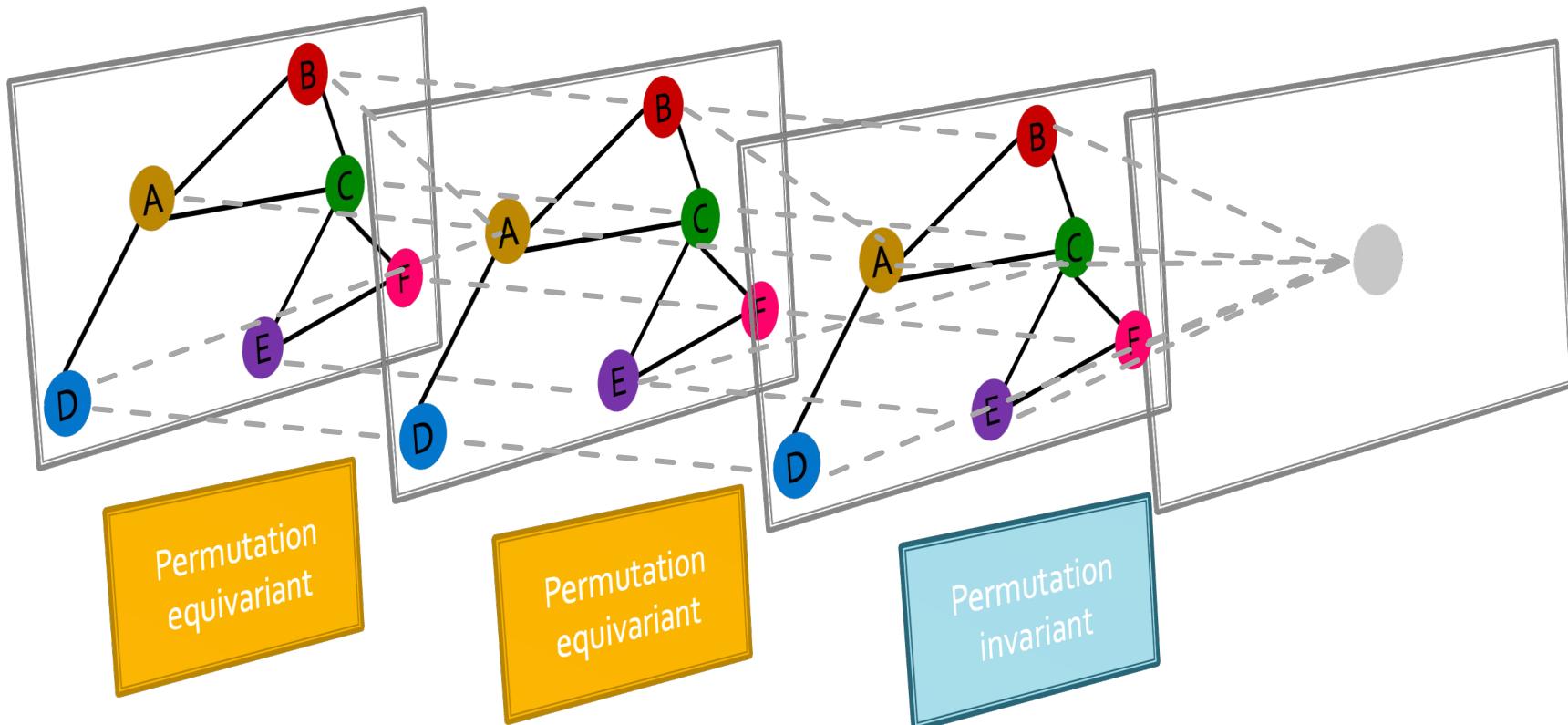
Permute the input, output also permutes accordingly.
(map a graph to a matrix)

■ Examples:

- $f(A, X) = \mathbf{1}^T X$: Permutation-**invariant**
 - Reason: $f(PAP^T, PX) = \mathbf{1}^T \mathbf{P}X = \mathbf{1}^T X = f(A, X)$
- $f(A, X) = X$: Permutation-**equivariant**
 - Reason: $f(PAP^T, PX) = \mathbf{P}X = Pf(A, X)$
- $f(A, X) = AX$: Permutation-**equivariant**
 - Reason: $f(PAP^T, PX) = PAP^T PX = \mathbf{P}AX = Pf(A, X)$

Graph Neural Network Overview

- Graph neural networks consist of multiple permutation equivariant / invariant functions.

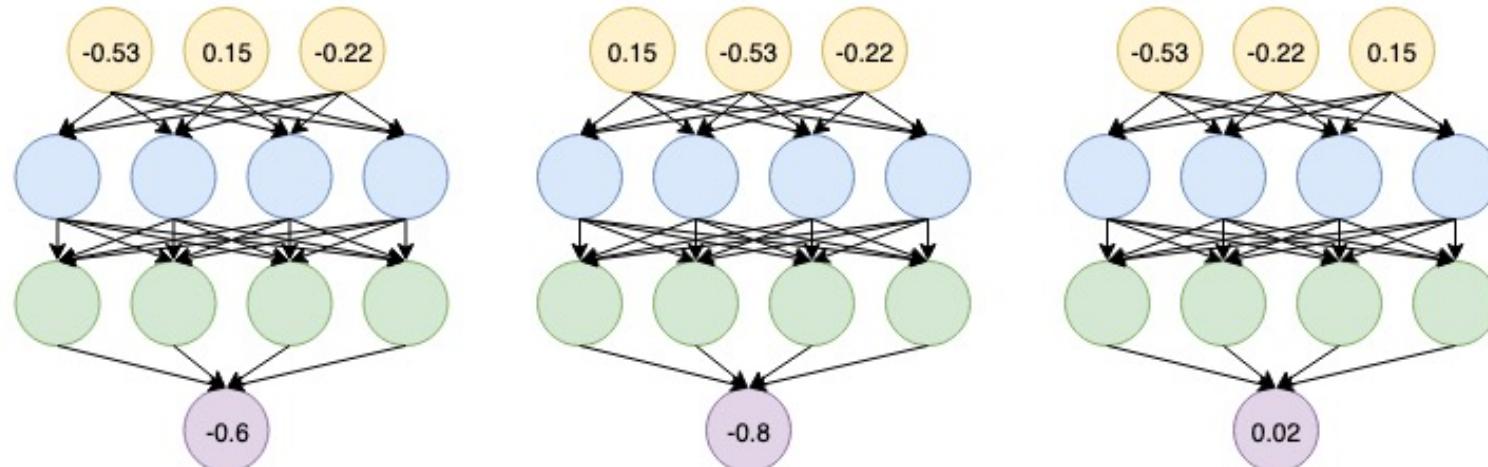


Graph Neural Network Overview

Are other neural network architectures, e.g.,
MLPs, permutation invariant / equivariant?

- No.

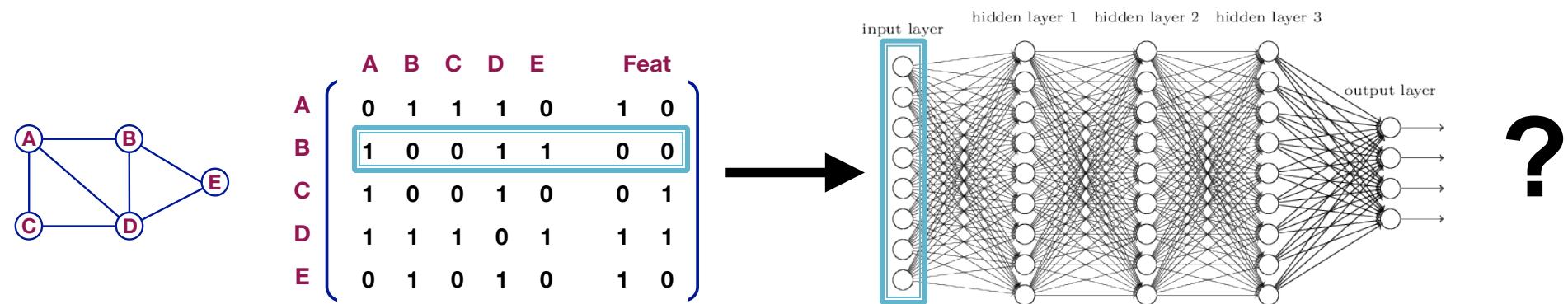
Switching the order of the
input leads to different
outputs!



Graph Neural Network Overview

Are other neural network architectures, e.g.,
MLPs, permutation invariant / equivariant?

- No.

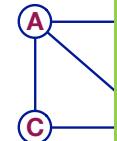


This explains why **the naïve MLP approach fails for graphs!**

Graph Neural Network Overview

- Are any neural network architectures, e.g.,

Next: Design graph neural networks that are permutation invariant / equivariant by **passing and aggregating information from neighbors!**



Outline of Today's Lecture

1. Basics of deep learning



2. Deep learning for graphs



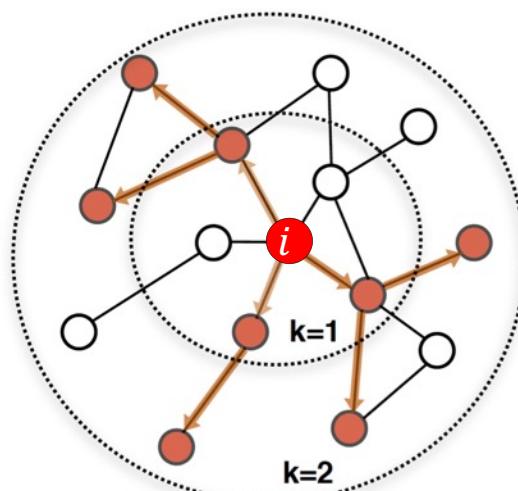
3. Graph Convolutional Networks



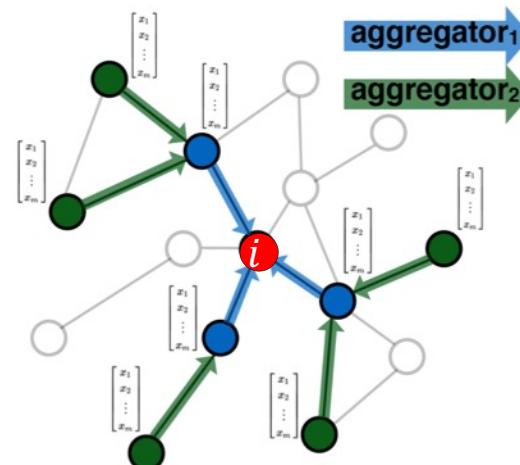
4. GNNs subsume CNNs

Graph Convolutional Networks

Idea: Node's neighborhood defines a computation graph



Determine node computation graph

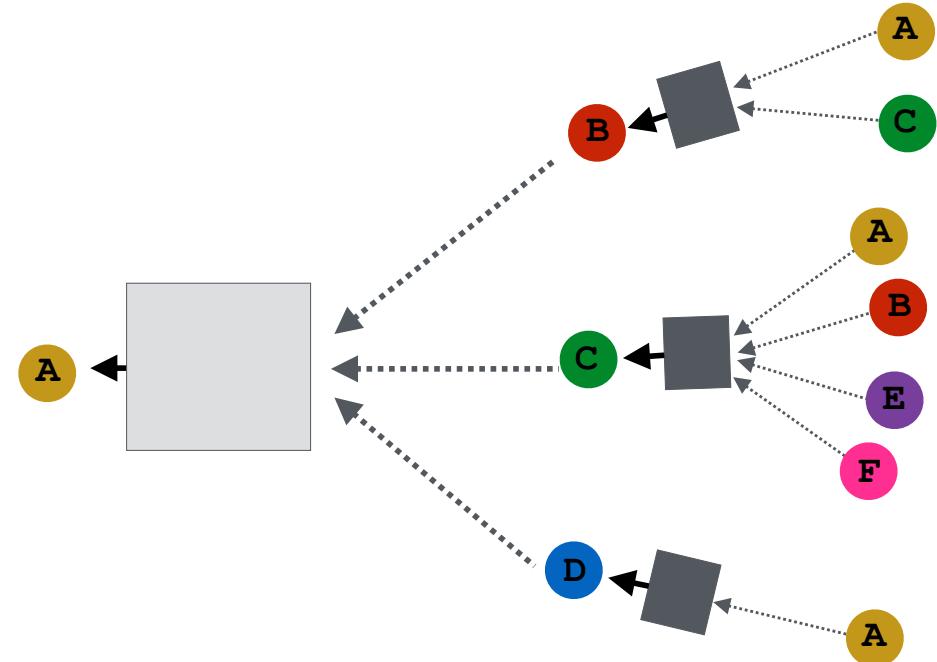
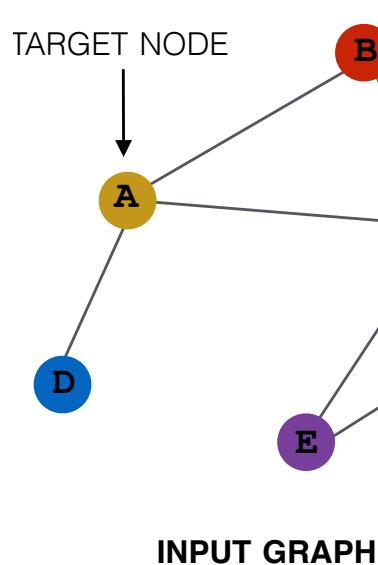


Propagate and transform information

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

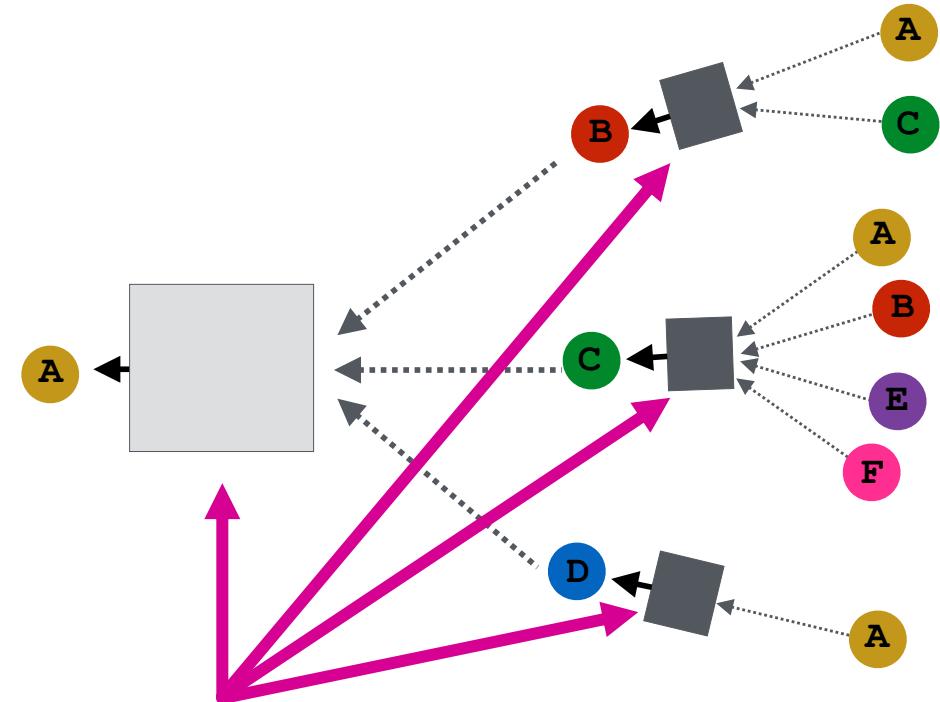
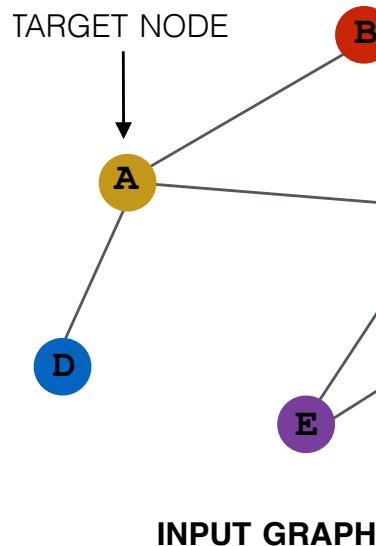
Idea: Aggregate Neighbors

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



Idea: Aggregate Neighbors

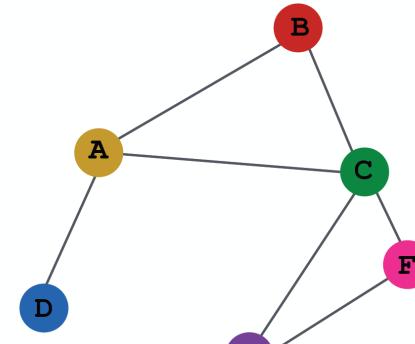
- **Intuition:** Nodes aggregate information from their neighbors using neural networks



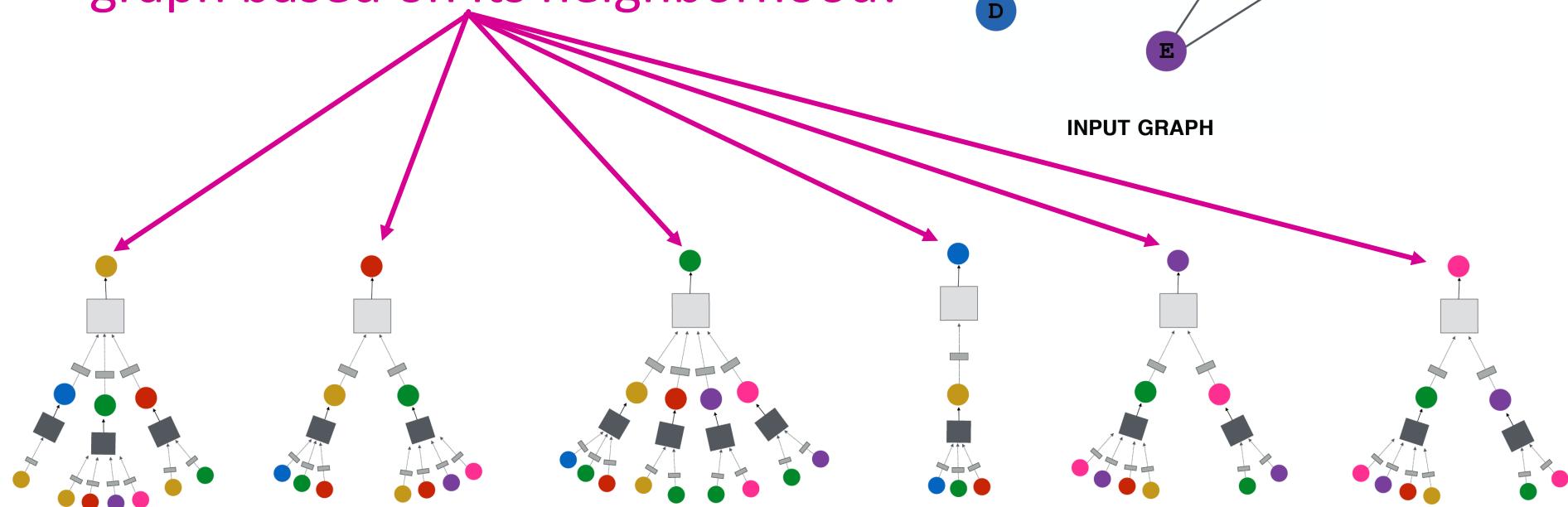
Idea: Aggregate Neighbors

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

Every node defines a computation graph based on its neighborhood!

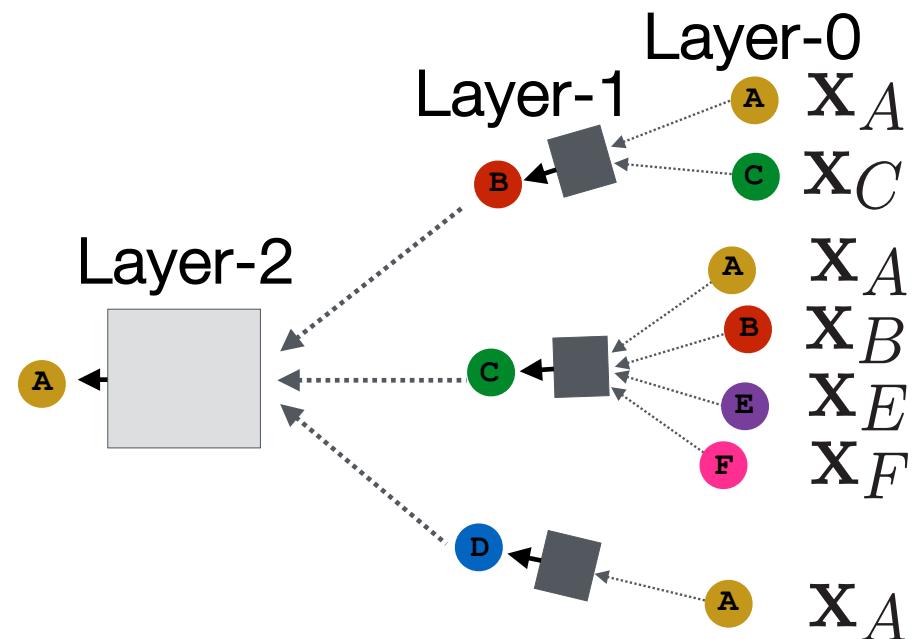
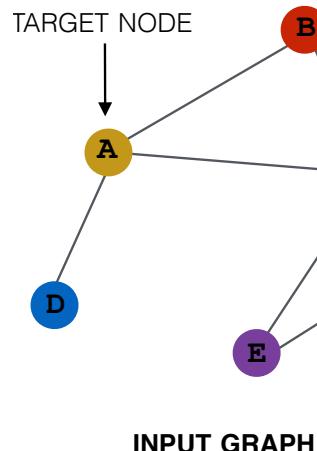


INPUT GRAPH



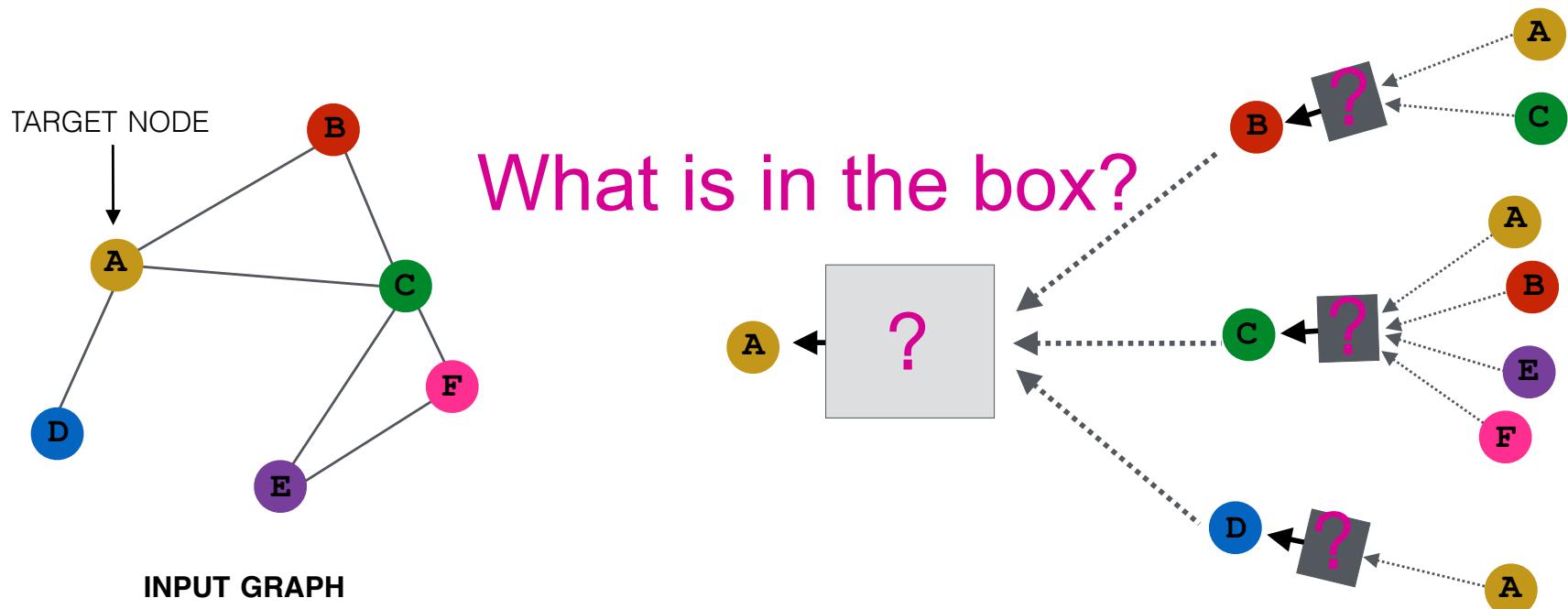
Deep Model: Many Layers

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



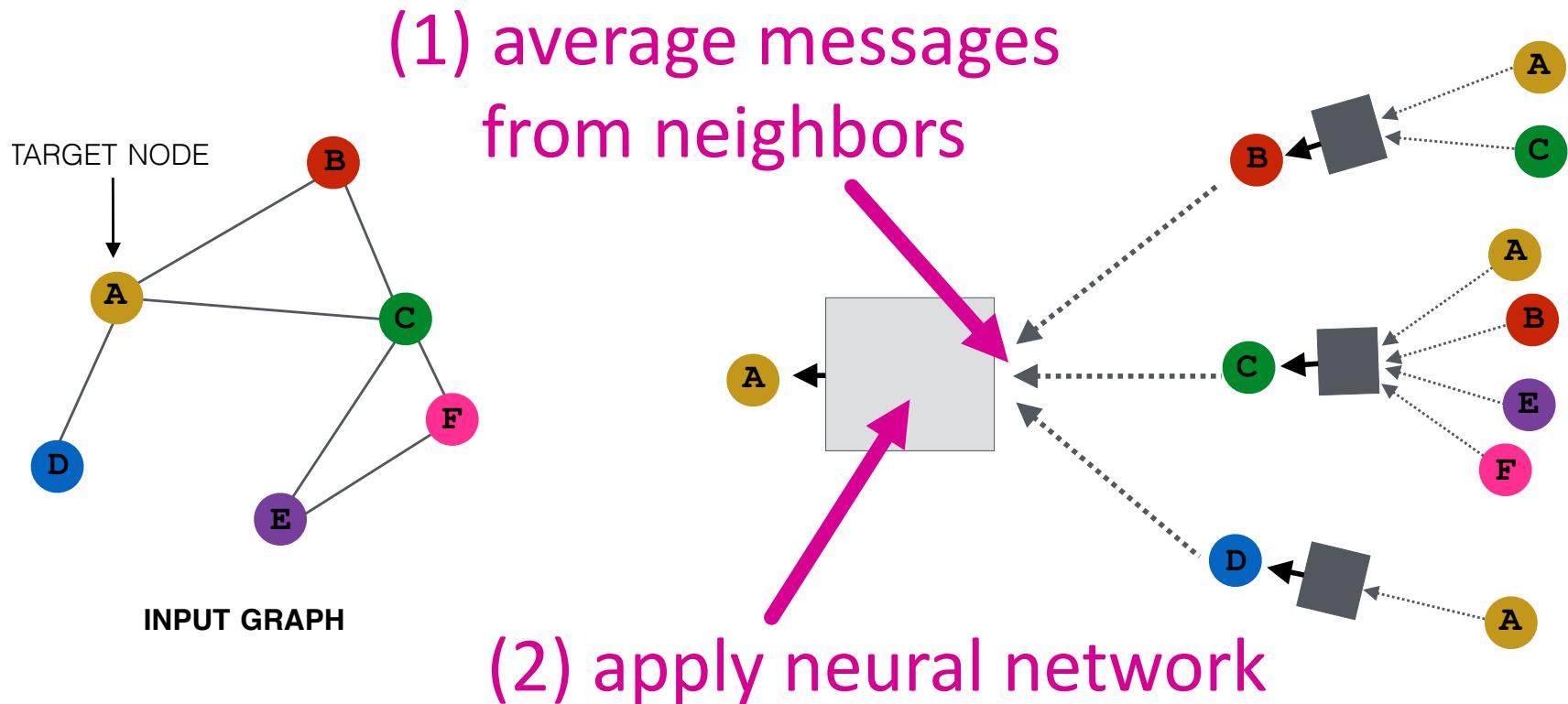
Neighborhood Aggregation

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



Neighborhood Aggregation

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



The Math: Deep Encoder of a GCN

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

Initial 0-th layer embeddings are equal to node features

$$h_v^0 = x_v$$

embedding of v at layer k

$$h_v^{(k+1)} = \sigma(W_k \sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|} + B_k h_v^{(k)}), \forall k \in \{0, \dots, K-1\}$$

Total number of layers

$z_v = h_v^{(K)}$

Embedding after K layers of neighborhood aggregation

Average of neighbor's previous layer embeddings

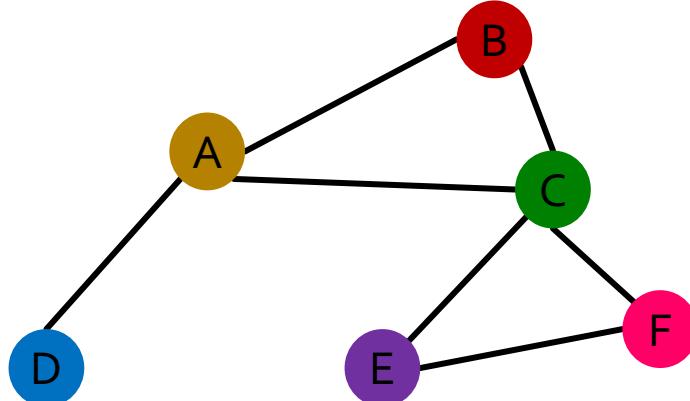
Non-linearity (e.g., ReLU)

Notice summation is a permutation invariant pooling/aggregation.

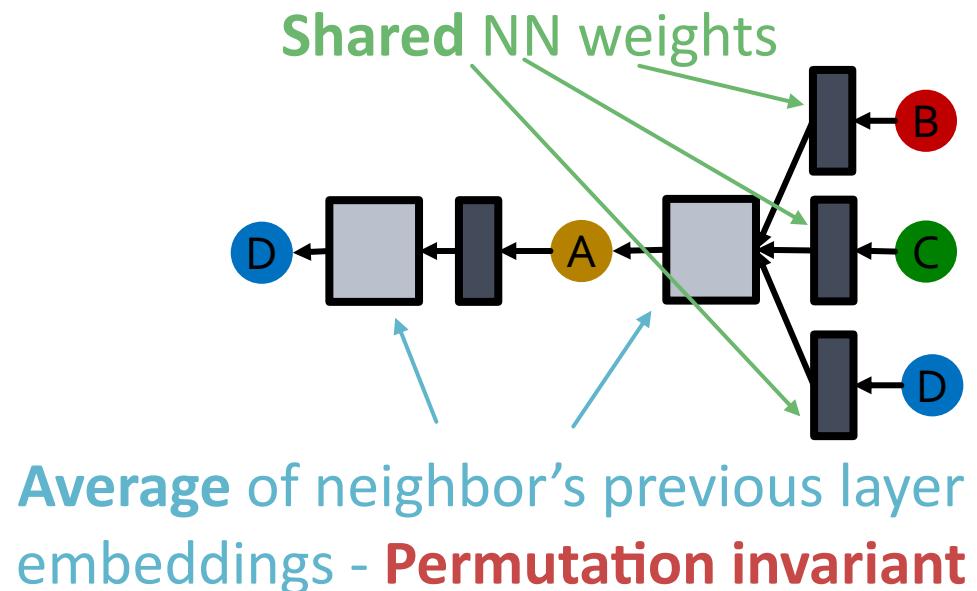
GCN: Invariance and Equivariance

What are the **invariance** and **equivariance** properties for a GCN?

- Given a node, the GCN that computes its embedding is **permutation invariant**



Target Node

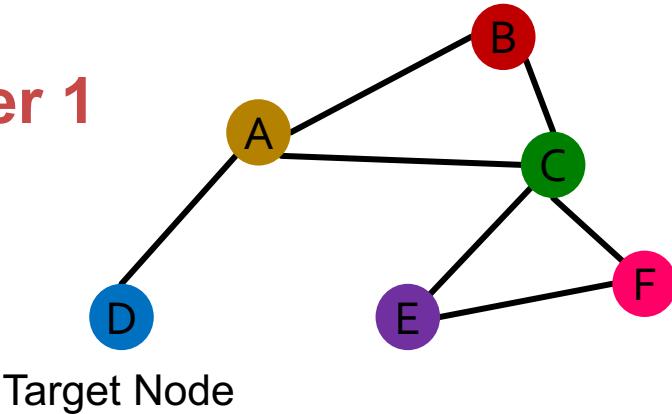


Average of neighbor's previous layer embeddings - **Permutation invariant**

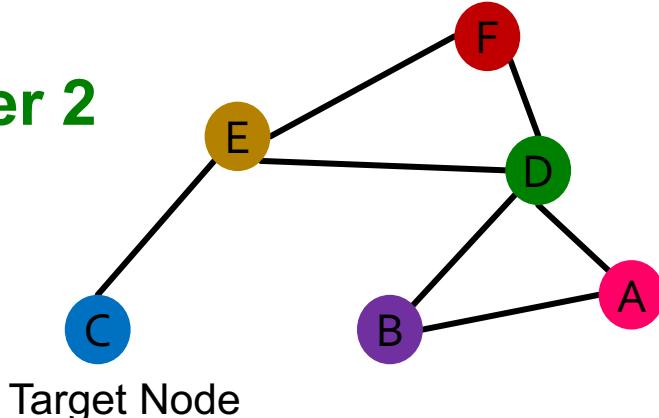
GCN: Invariance and Equivariance

- Considering all nodes in a graph, GCN computation is **permutation equivariant**

Order 1



Order 2



Node feature X_1

A	[Yellow]
B	[Red]
C	[Green]
D	[Blue]
E	[Purple]
F	[Pink]

Adjacency matrix A_1

A	1	0	1	0	0
B	0	1	0	1	0
C	1	0	1	0	1
D	0	1	0	1	0
E	0	0	1	0	1
F	0	0	0	1	1

Embeddings H_1

A	[Yellow]
B	[Red]
C	[Green]
D	[Blue]
E	[Purple]
F	[Pink]

Permute the input, the output also permutes accordingly - permutation equivariant

Node feature X_2

A	[Pink]
B	[Purple]
C	[Blue]
D	[Green]
E	[Brown]
F	[Red]

Adjacency matrix A_2

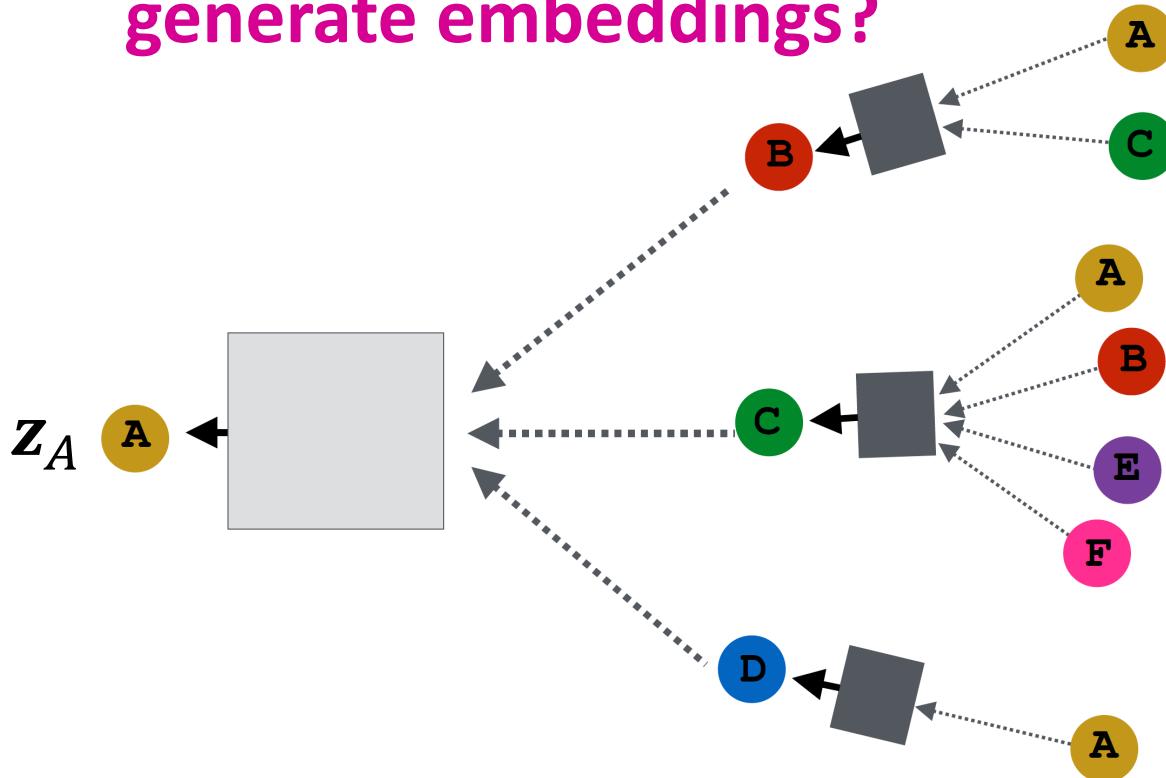
A	1	0	1	0	0
B	0	1	0	1	0
C	1	0	1	0	1
D	0	1	0	1	0
E	0	0	1	0	1
F	0	0	0	1	1

Embeddings H_2

A	[Red]
B	[Purple]
C	[Blue]
D	[Green]
E	[Yellow]
F	[Red]

Training the Model

How do we train the GCN to generate embeddings?



Need to define a loss function on the embeddings.

Model Parameters

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

$$\begin{aligned} h_v^{(0)} &= x_v \\ h_v^{(k+1)} &= \sigma(W_k \sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|} + B_k h_v^{(k)}), \forall k \in \{0..K-1\} \\ z_v &= h_v^{(K)} \end{aligned}$$

Final node embedding

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

h_v^k : the hidden representation of node v at layer k

- W_k : weight matrix for neighborhood aggregation
- B_k : weight matrix for transforming hidden vector of self

Matrix Formulation (1)

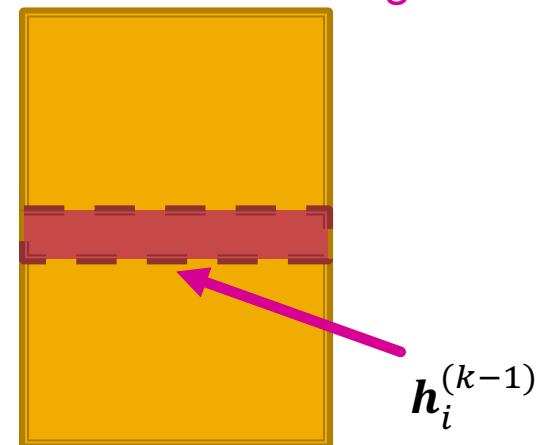
- Many aggregations can be performed efficiently by (sparse) matrix operations
- Let $H^{(k)} = [h_1^{(k)} \dots h_{|V|}^{(k)}]^T$
- Then: $\sum_{u \in N_v} h_u^{(k)} = A_{v,:} H^{(k)}$
- Let D be diagonal matrix where $D_{v,v} = \text{Deg}(v) = |N(v)|$
 - The inverse of D : D^{-1} is also diagonal:
$$D_{v,v}^{-1} = 1/|N(v)|$$
- Therefore,

$$\sum_{u \in N(v)} \frac{h_u^{(k-1)}}{|N(v)|}$$



$$H^{(k+1)} = D^{-1} A H^{(k)}$$

Matrix of hidden embeddings $H^{(k-1)}$

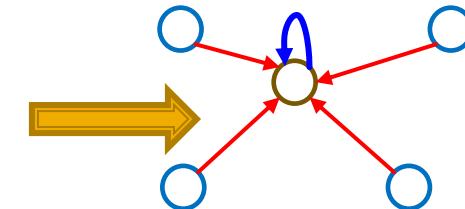


Matrix Formulation (2)

- Re-writing update function in matrix form:

$$H^{(k+1)} = \sigma(\tilde{A}H^{(k)}W_k^T + H^{(k)}B_k^T)$$

where $\tilde{A} = D^{-1}A$



$$H^{(k)} = [h_1^{(k)} \dots h_{|V|}^{(k)}]^T$$

- Red: neighborhood aggregation
- Blue: self transformation
- In practice, this implies that efficient sparse matrix multiplication can be used (\tilde{A} is sparse)
- **Note:** not all GNNs can be expressed in a simple matrix form, when aggregation function is complex

How to Train A GNN

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

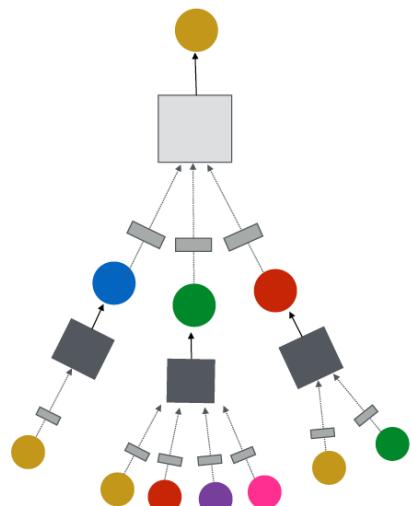
$$\min_{\Theta} \mathcal{L}(\mathbf{y}, f_{\Theta}(\mathbf{z}_v))$$

- \mathbf{y} : node label
- \mathcal{L} could be L2 if \mathbf{y} is real number, or cross entropy if \mathbf{y} is categorical
- **Unsupervised setting:**
 - No node label available
 - **Use the graph structure as the supervision!**

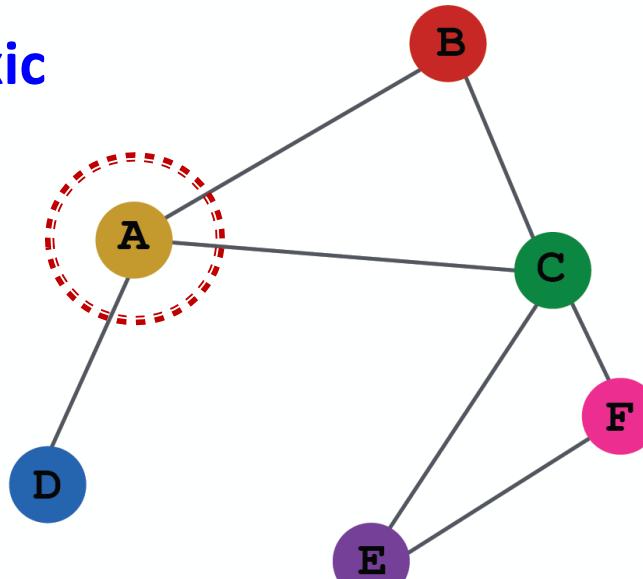
Supervised Training

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

Safe or toxic
drug?



Safe or toxic
drug?

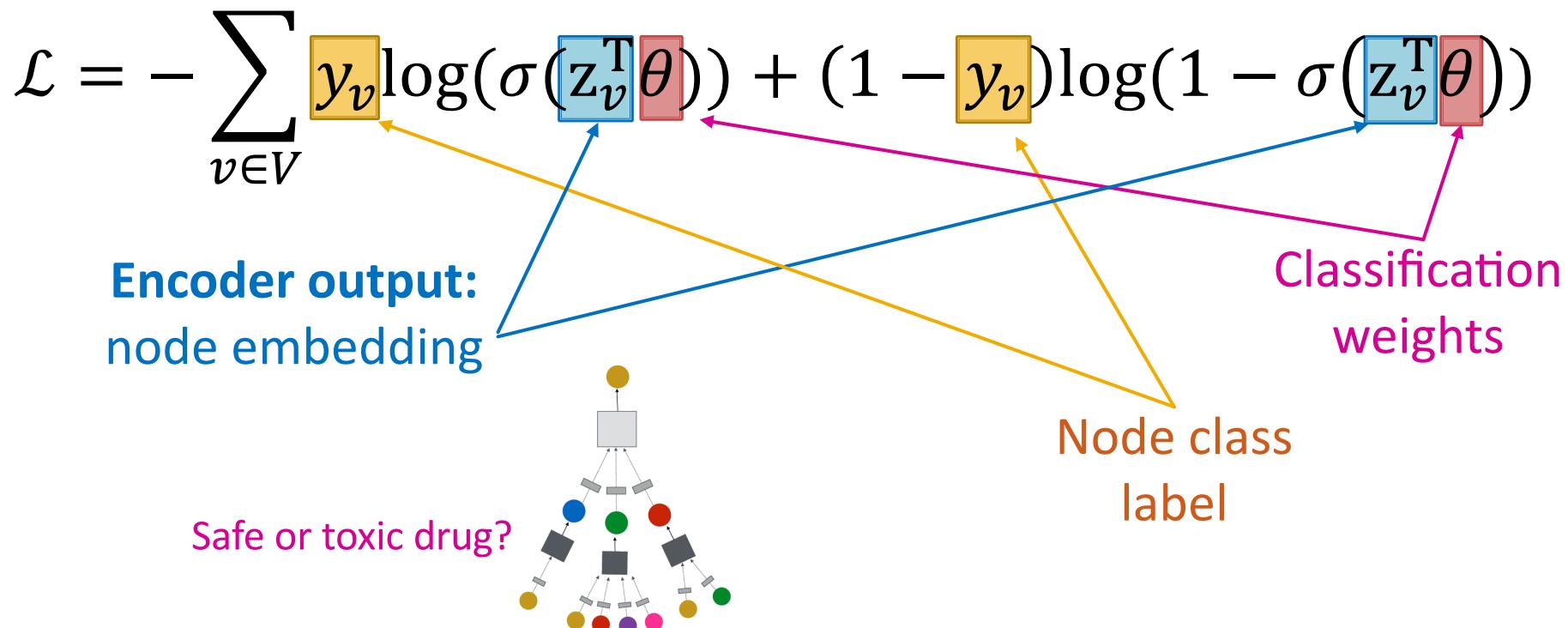


E.g., a drug-drug
interaction network

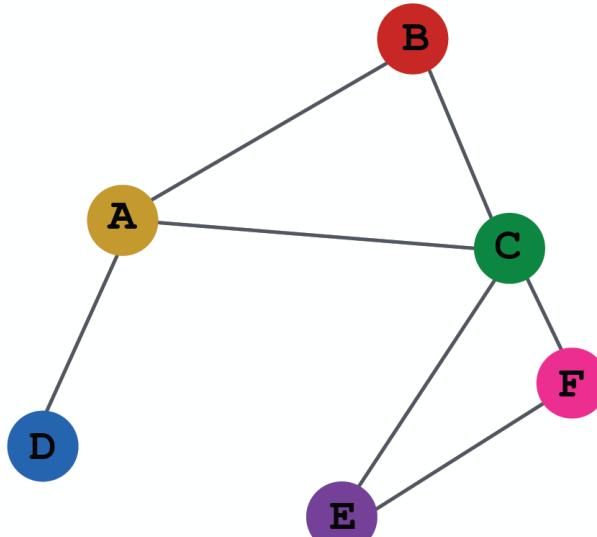
Supervised Training

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

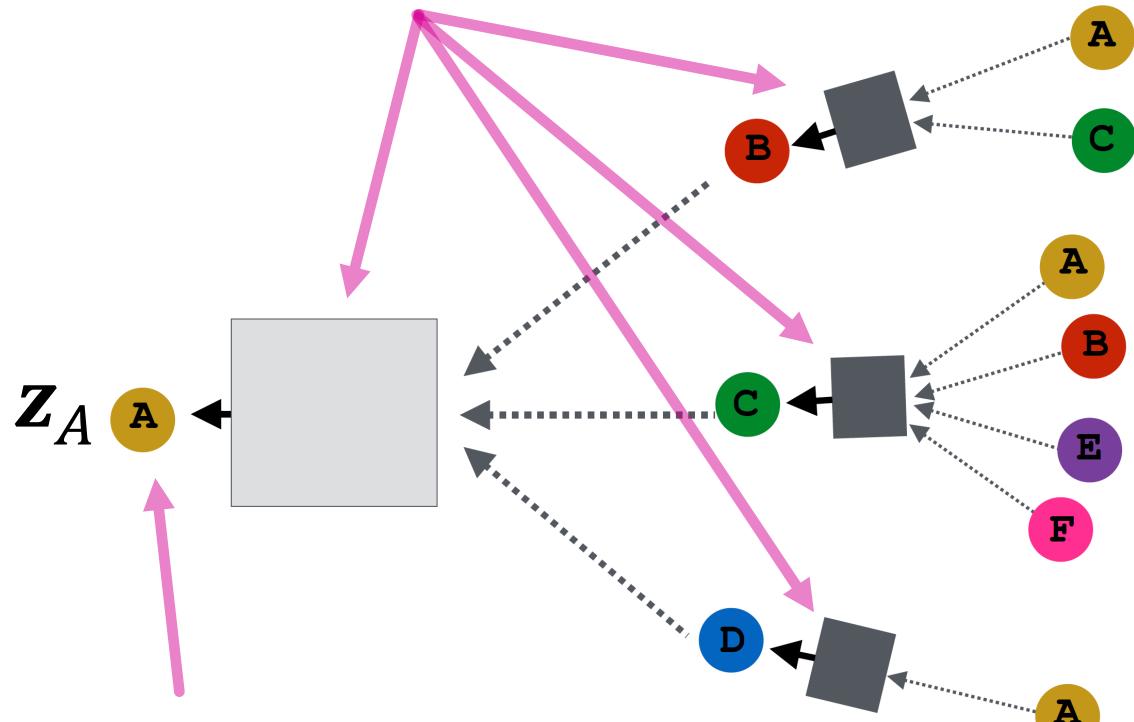
- Use cross entropy loss



Model Design: Overview

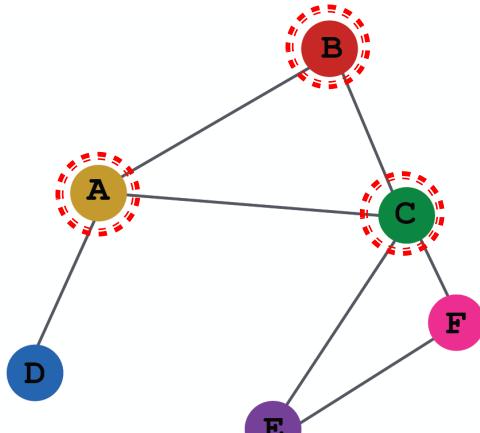


(1) Define a neighborhood aggregation function



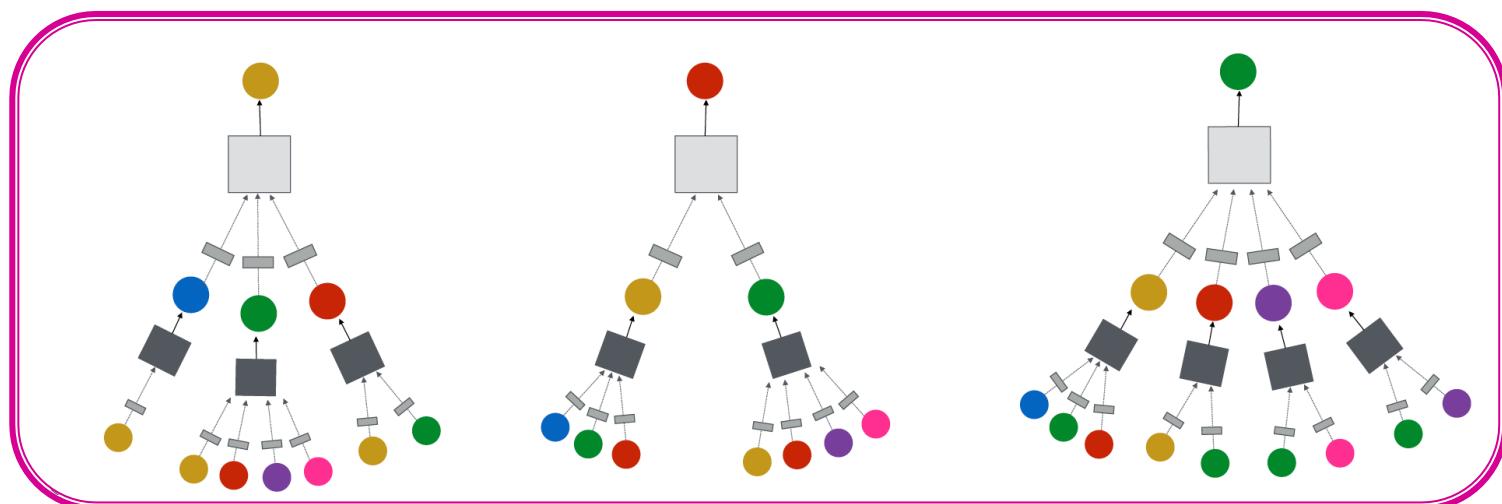
(2) Define a loss function on the embeddings

Model Design: Overview

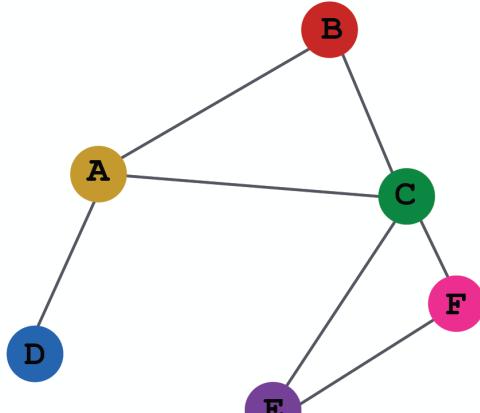


INPUT GRAPH

(3) Train on a set of nodes, i.e.,
a batch of compute graphs



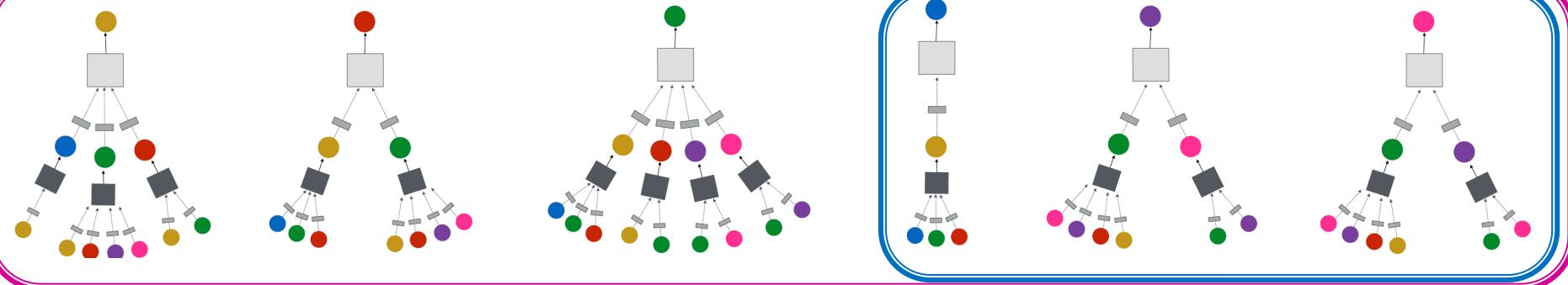
Model Design: Overview



INPUT GRAPH

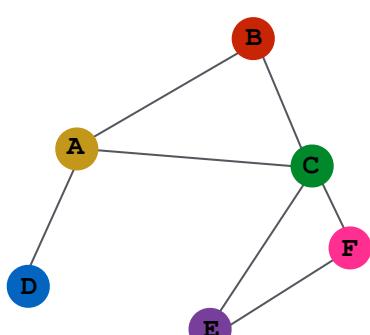
(4) Generate embeddings
for nodes as needed

Even for nodes we never
trained on!

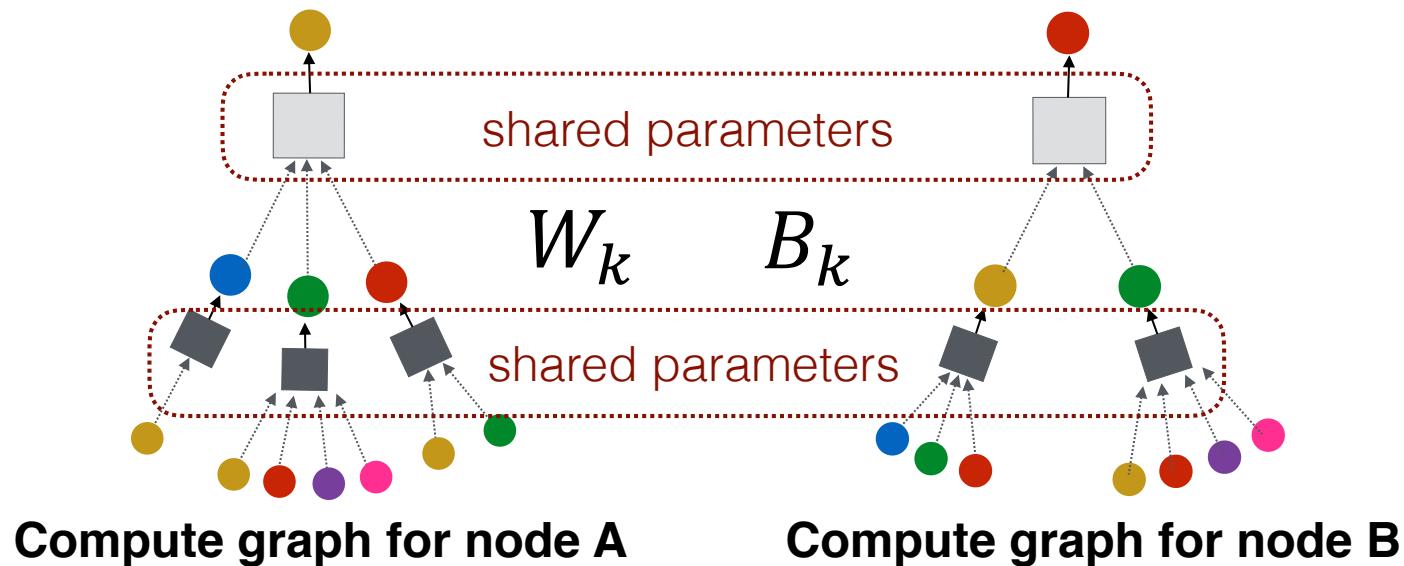


Inductive Capability

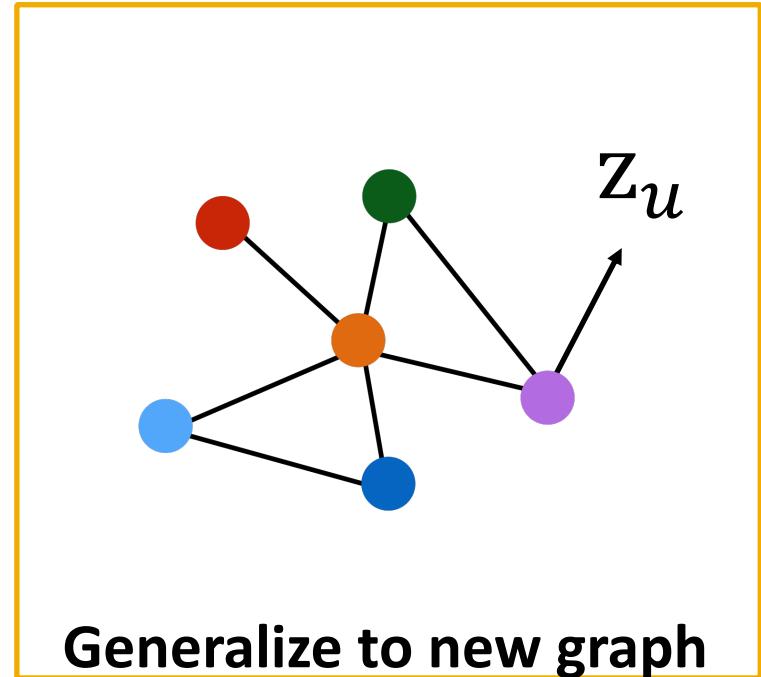
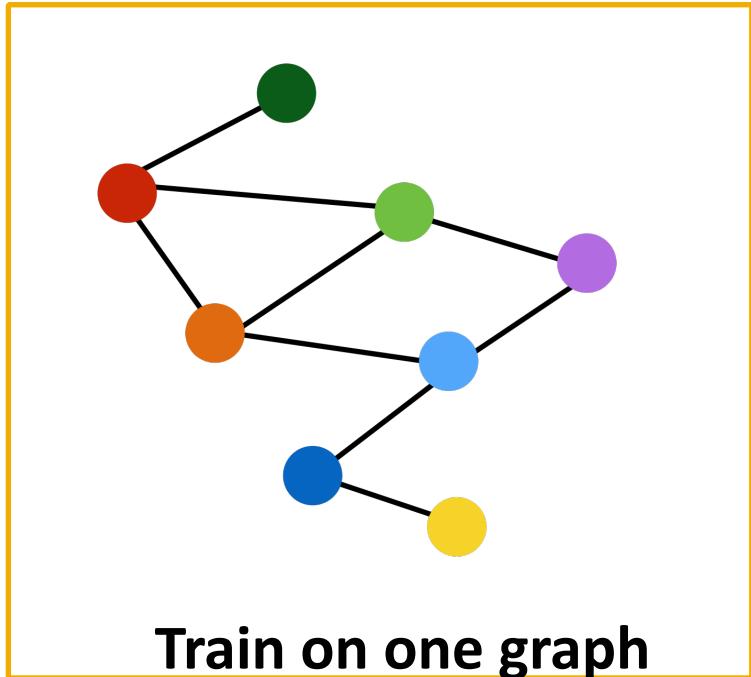
- The same aggregation parameters are shared for all nodes:
 - The number of model parameters is sublinear in $|V|$ and we can **generalize to unseen nodes!**



INPUT GRAPH



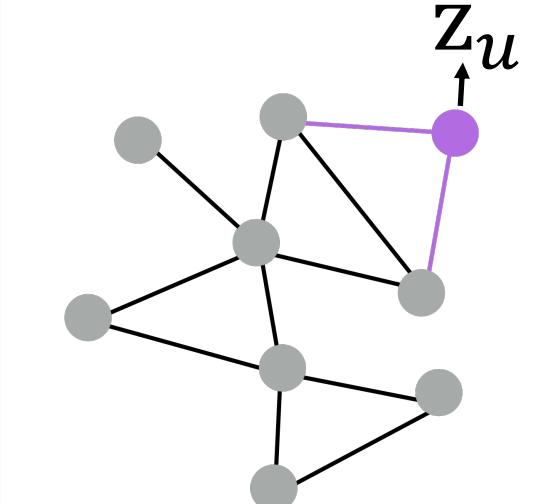
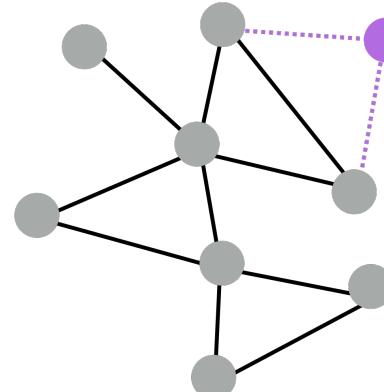
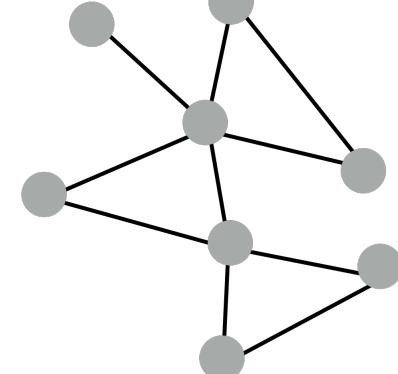
Inductive Capability: New Graphs



Inductive node embedding → Generalize to entirely unseen graphs

E.g., train on protein interaction graph from model organism A and generate embeddings on newly collected data about organism B

Inductive Capability: New Nodes



- Many application settings constantly encounter previously unseen nodes:
 - E.g., Reddit, YouTube, Google Scholar
- Need to generate new embeddings “on the fly”

Outline of Today's Lecture

1. Basics of deep learning



2. Deep learning for graphs



3. Graph Convolutional Networks



4. GNNs subsume CNNs

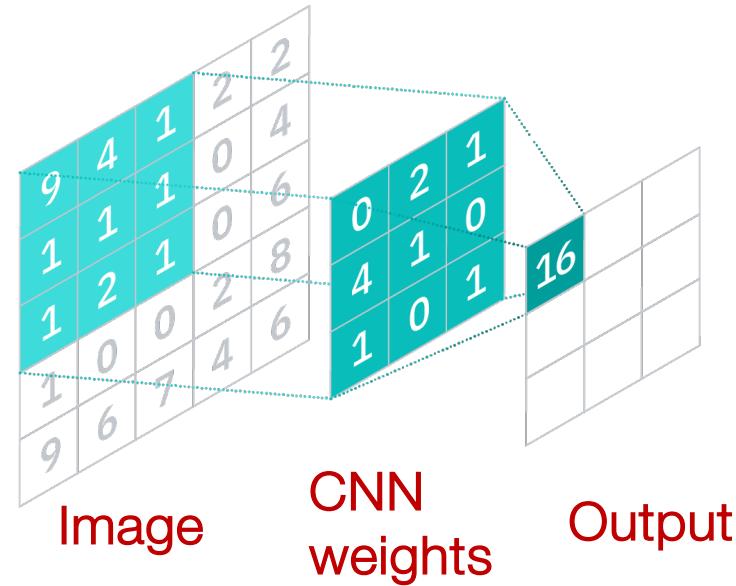
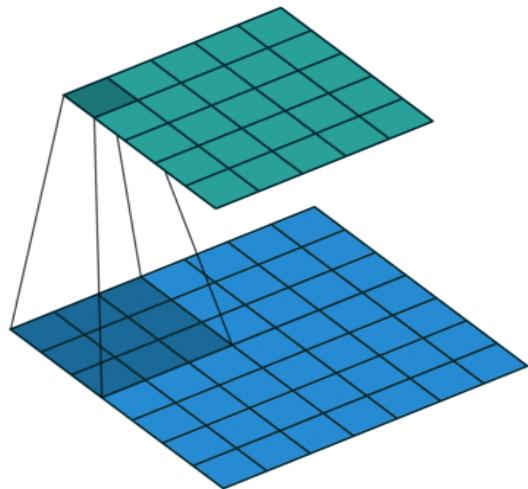


Architecture Comparison

- How do GNNs compare to prominent architectures such as Convolutional Neural Nets?

Convolutional Neural Network

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

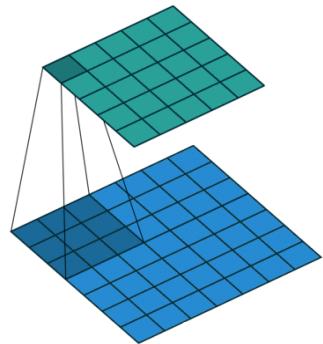


$$\text{CNN formulation: } h_v^{(l+1)} = \sigma(\sum_{u \in N(v) \cup \{v\}} W_l^u h_u^{(l)}), \quad \forall l \in \{0, \dots, L-1\}$$

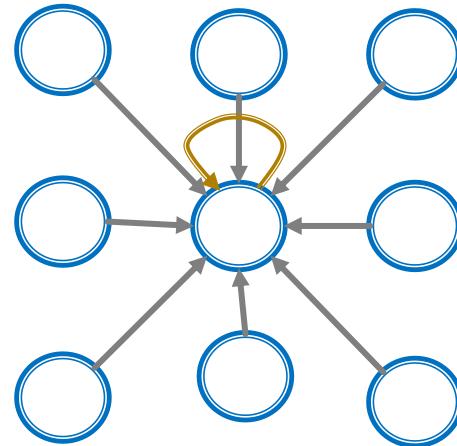
$N(v)$ represents the 8 neighbor pixels of v .

GNN vs. CNN

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



Image

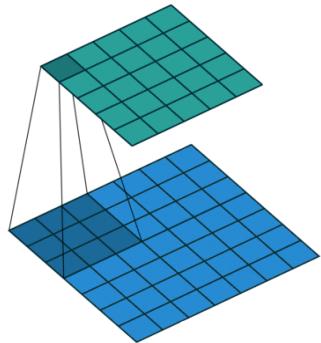


Graph

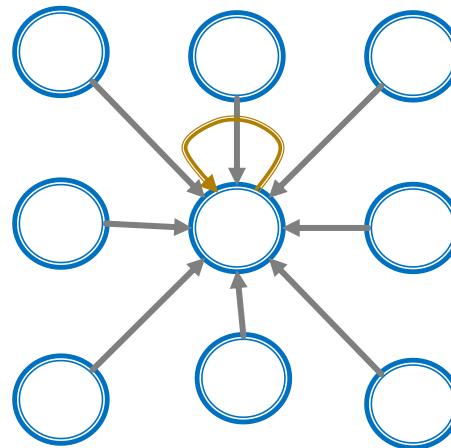
- GNN formulation: $h_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in N(v)} \frac{h_u^{(l)}}{|N(v)|} + B_l h_v^{(l)}), \forall l \in \{0, \dots, L-1\}$
- CNN formulation: (previous slide) $h_v^{(l+1)} = \sigma(\sum_{u \in N(v) \cup \{v\}} W_l^u h_u^{(l)}), \forall l \in \{0, \dots, L-1\}$
if we rewrite: $h_v^{(l+1)} = \sigma(\sum_{u \in N(v)} \mathbf{W}_l^u h_u^{(l)} + B_l h_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

GNN vs. CNN

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



Image



Graph

$$\text{GNN formulation: } h_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in N(v)} \frac{h_u^{(l)}}{|N(v)|} + B_l h_v^{(l)}), \forall l \in \{0, \dots, L-1\}$$

$$\text{CNN formulation: } h_v^{(l+1)} = \sigma(\sum_{u \in N(v)} \mathbf{W}_l^u h_u^{(l)} + B_l h_v^{(l)}), \forall l \in \{0, \dots, L-1\}$$

Key difference: We can learn different W_l^u for different “neighbor” u for pixel v on the image. The reason is we can pick an order for the 9 neighbors using **relative position** to the center pixel: $\{(-1, -1), (-1, 0), (-1, 1), \dots, (1, 1)\}$

GNN vs. CNN

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

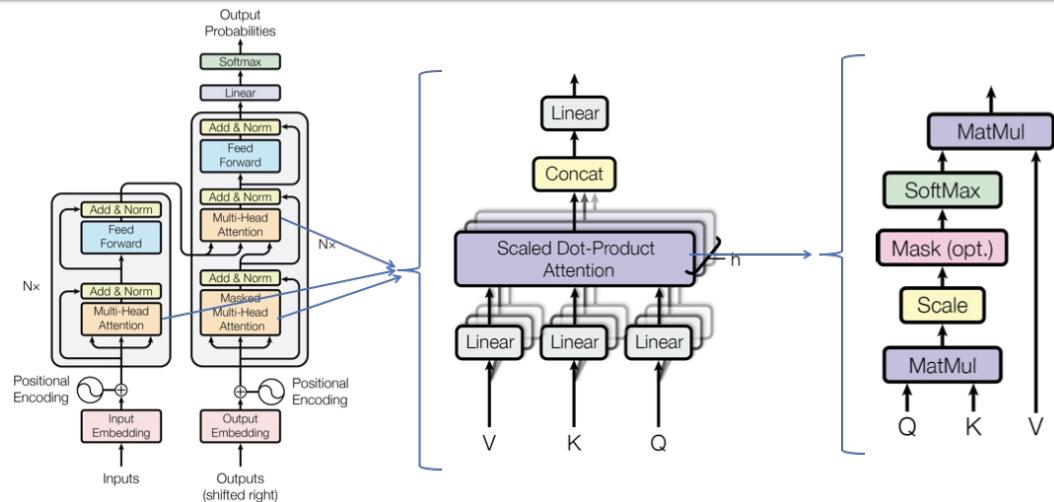


- CNN can be seen as a special GNN with fixed neighbor size and ordering:
 - The size of the filter is pre-defined for a CNN.
 - The advantage of GNN is it processes arbitrary graphs with different degrees for each node.
- CNN is not permutation invariant/equivariant.
 - Switching the order of pixels leads to different outputs.

Key difference: We can learn different W_l^u for different “neighbor” u for pixel v on the image. The reason is we can pick an order for the 9 neighbors using **relative position** to the center pixel: $\{(-1, -1), (-1, 0), (-1, 1), \dots, (1, 1)\}$

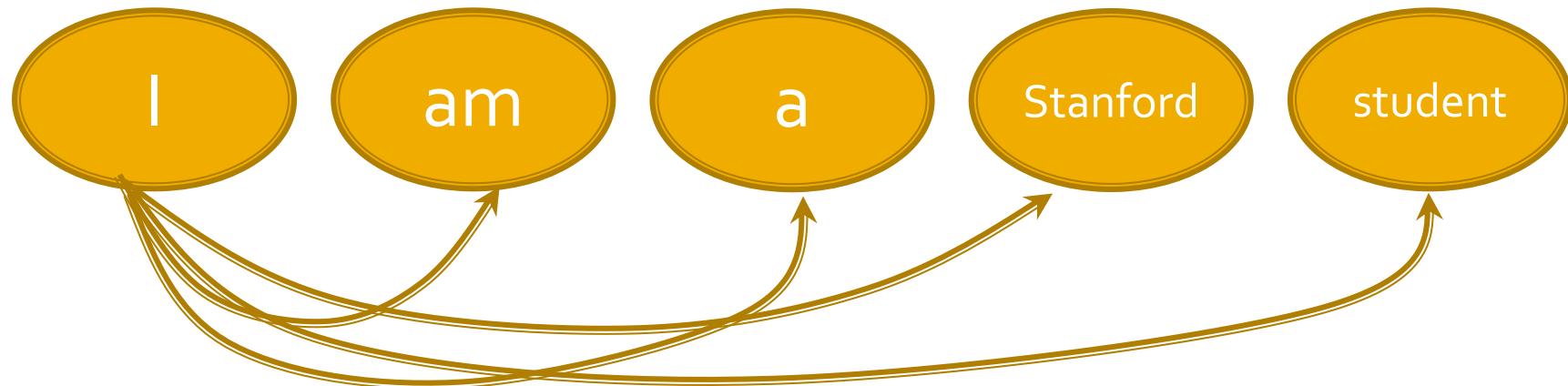
Transformer

Transformer is one of the most popular architectures that achieves great performance in many sequence modeling tasks.



Key component: self-attention

- Every token/word attends to all the other tokens/words via matrix calculation.

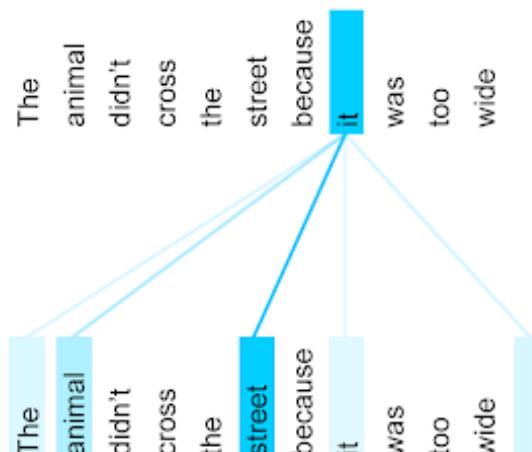
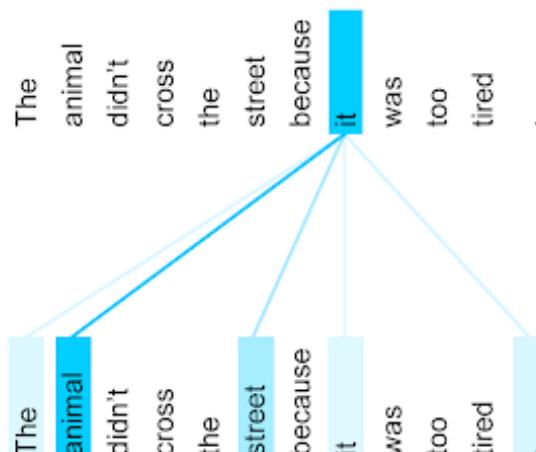


Transformer

A general definition of attention:

Given a set of vector values, and a vector query, **attention** is a technique to compute a weighted sum of the values, dependent on the query.

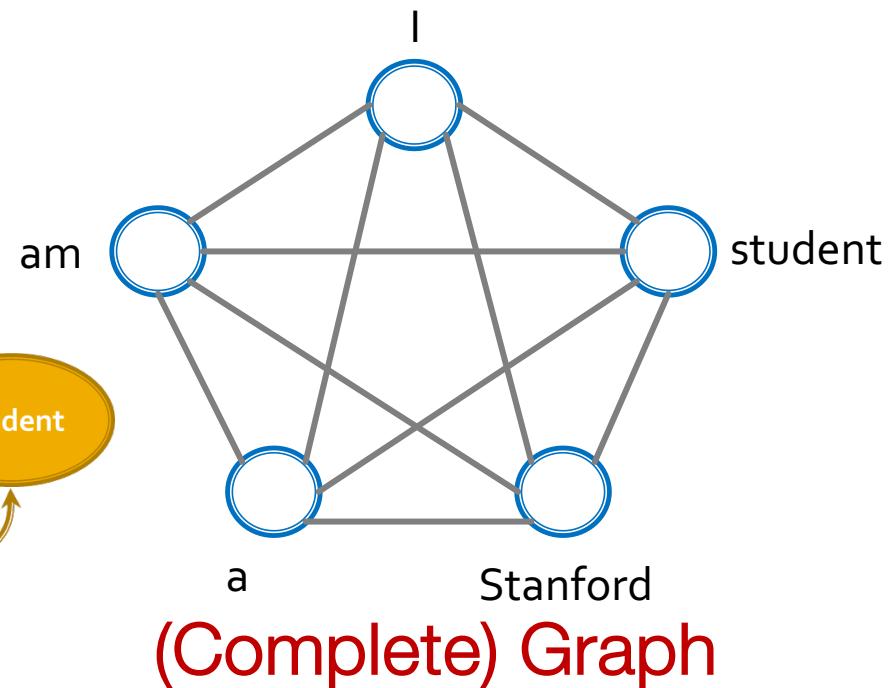
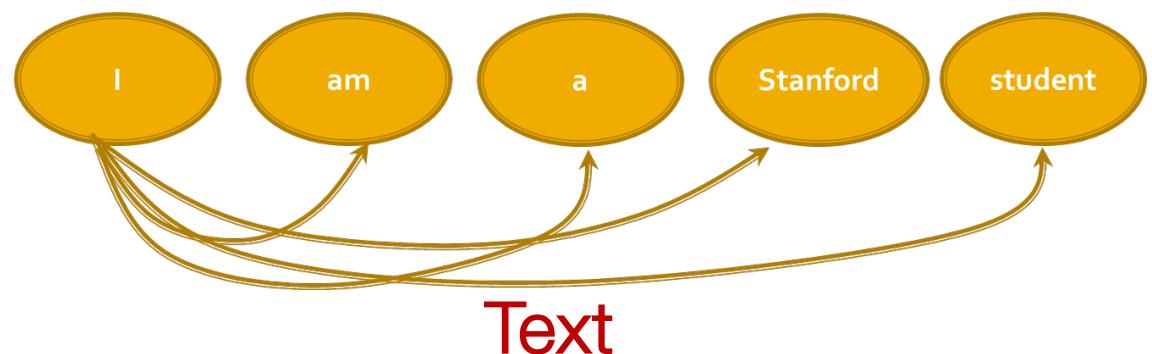
Each token/word has a **value vector** and a **query vector**. The value vector can be seen as the representation of the token/word. We use the query vector to calculate the attention score (weights in the weighted sum).



GNN vs. Transformer

Transformer layer can be seen as a special GNN that runs on a fully-connected “word” graph!

Since each word attends to **all the other words**, **the computation graph** of a transformer layer is identical to that of a GNN on the **fully-connected “word” graph**.



Summary

- In this lecture, we introduced
 - Idea for Deep Learning for Graphs
 - Multiple layers of embedding transformation
 - At every layer, use the embedding at previous layer as the input
 - Aggregation of neighbors and self-embeddings
 - Graph Convolutional Network
 - Mean aggregation; can be expressed in matrix form
 - GNN is a general architecture
 - CNN can be viewed as a special GNN