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Stanford CS224W: Graph Neural Networks

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

<http://cs224w.stanford.edu>



ANNOUNCEMENTS

- **Next Thursday (10/12): Colab 1 due**

CS224W: Machine Learning with Graphs

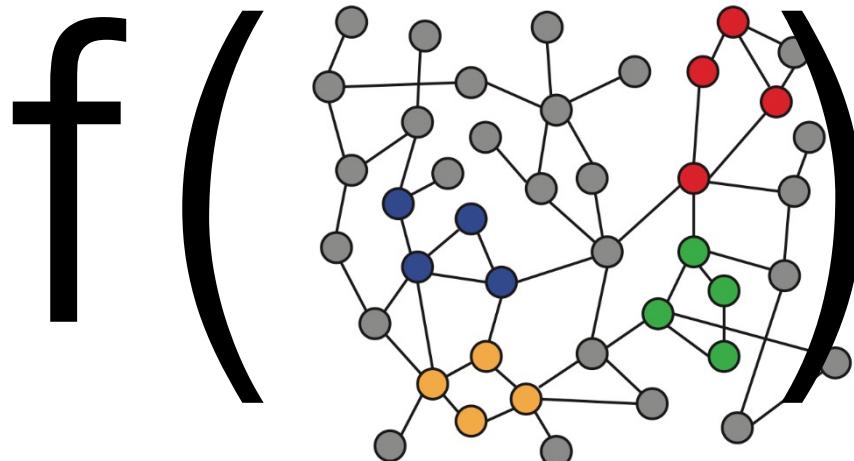
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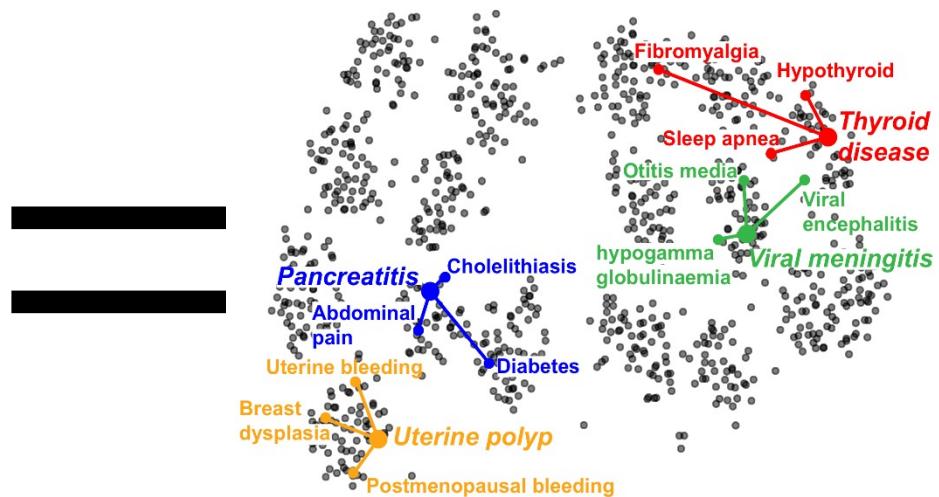


Recap: Node Embeddings

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



Input graph



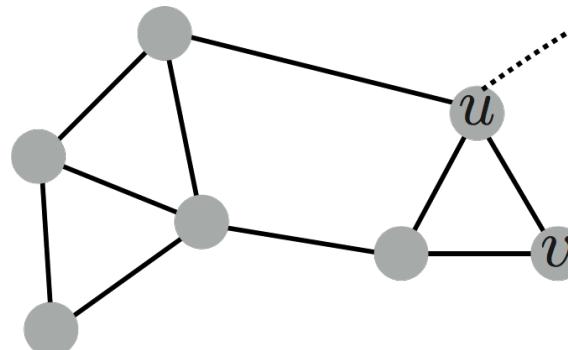
2D node embeddings

How to learn mapping function f ?

Recap: Node Embeddings

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

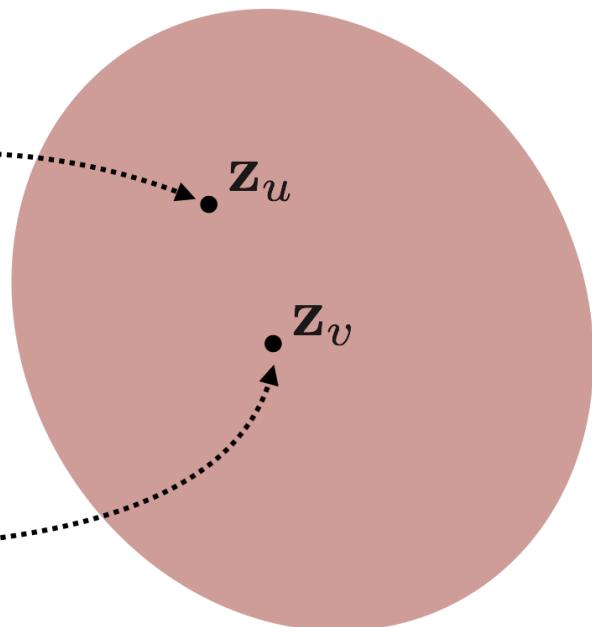
Need to define!



encode nodes

$\text{ENC}(u)$

$\text{ENC}(v)$



Input network

d -dimensional
embedding space

Recap: Two Key Components

- **Encoder:** Maps each node to a low-dimensional vector

$\text{ENC}(v) = \mathbf{z}_v$

d-dimensional embedding

node in the input graph

- **Similarity function:** Specifies how the relationships in vector space map to the relationships in the original network

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

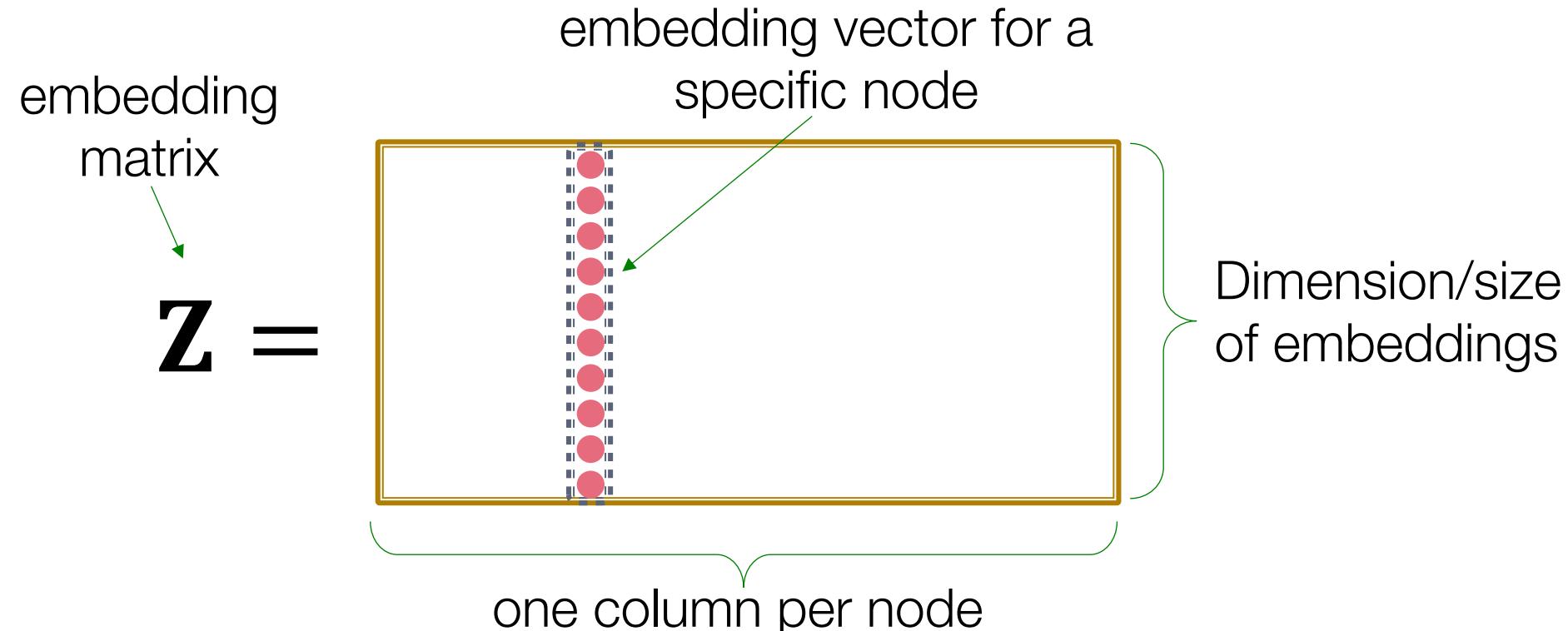
Similarity of u and v in
the original network

Decoder

dot product between node
embeddings

Recap: “Shallow” Encoding

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



Recap: Shallow Encoders

- Limitations of shallow embedding methods:
 - **$O(|V|d)$ 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

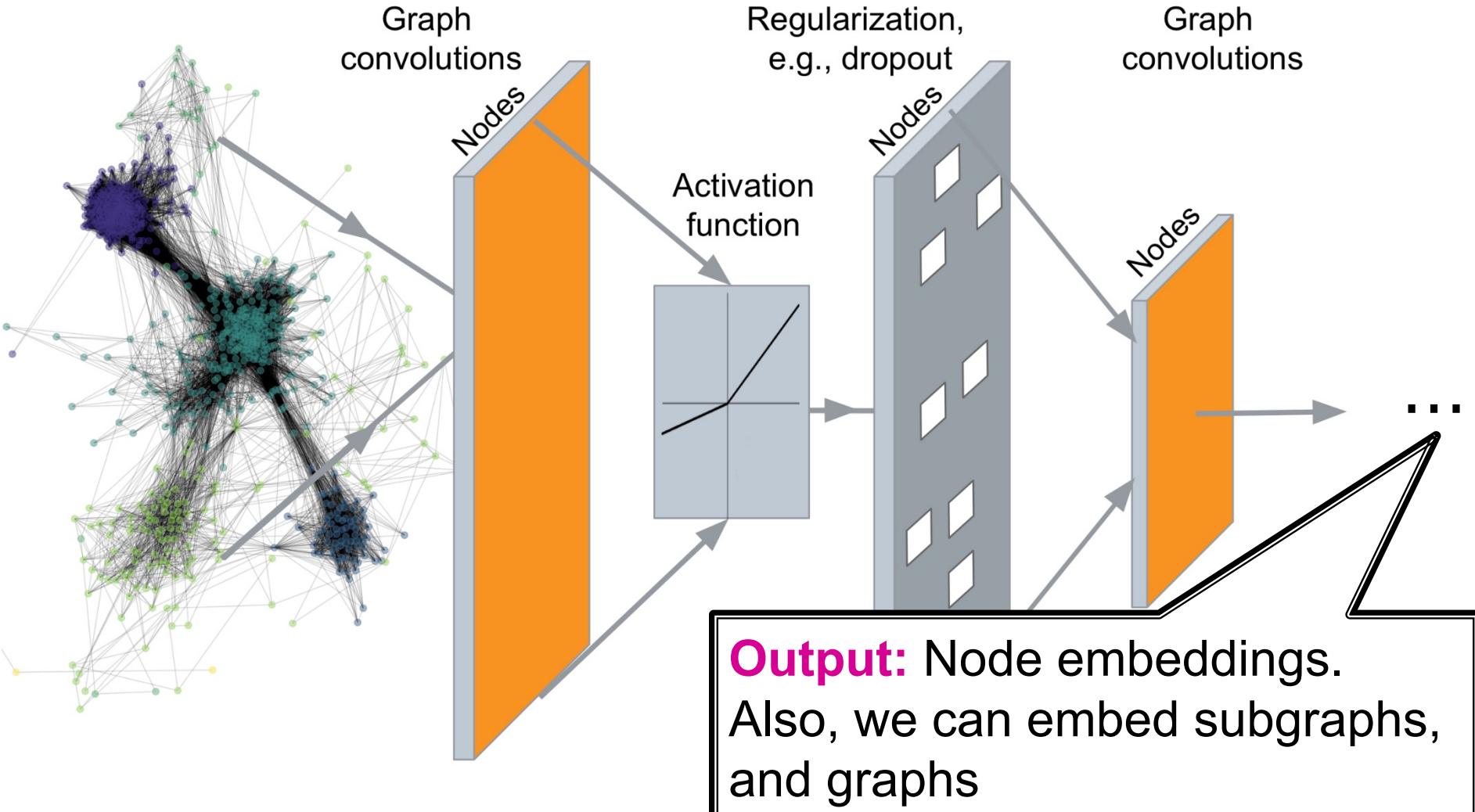
- **Today:** We will now discuss deep learning methods based on **graph neural networks (GNNs)**:

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

**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 3.

Deep Graph Encoders

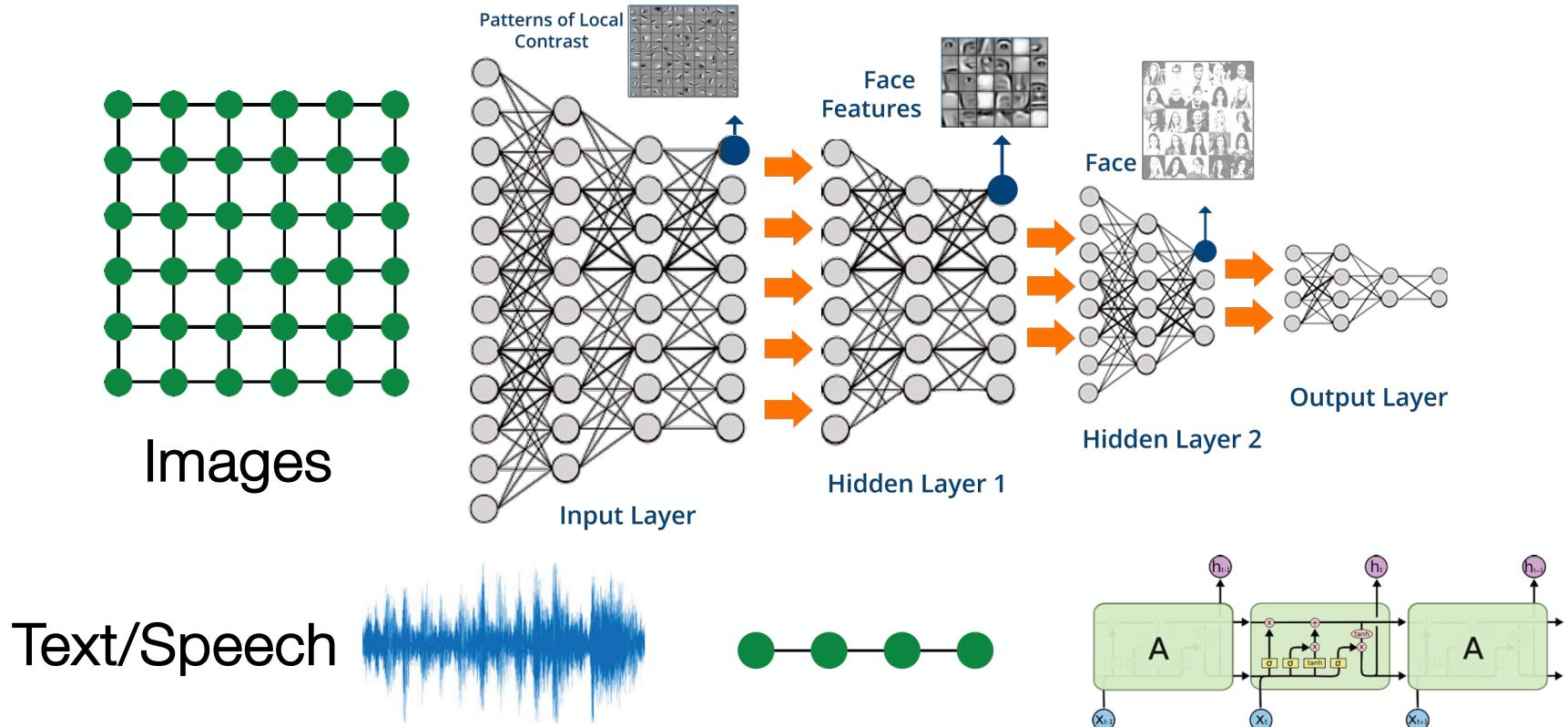


Tasks on Networks

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

Modern ML Toolbox

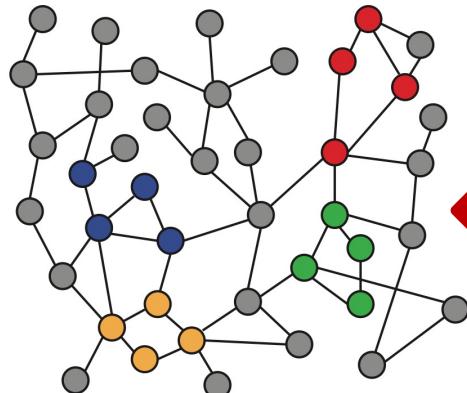


Modern deep learning toolbox is designed
for simple sequences & grids

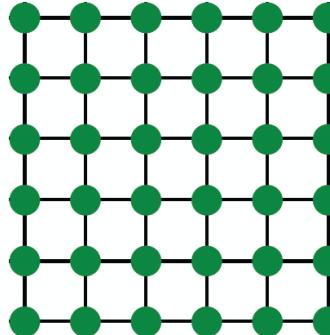
Why is it Hard?

But networks are far more complex!

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



Networks



Images



Text

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

Outline of Today's Lecture

1. Basics of deep learning



2. Deep learning for graphs

3. Graph Convolutional Networks

4. GNNs subsume CNNs

Summary: Basics of Deep Learning

- **Loss function:**

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

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

Stanford CS224W: Deep Learning for Graphs

CS224W: Machine Learning with Graphs

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Content

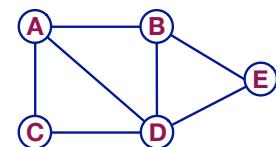
- **Local network neighborhoods:**
 - Describe aggregation strategies
 - Define computation graphs
- **Stacking multiple layers:**
 - Describe the model, parameters, training
 - How to fit the model?
 - Simple example for unsupervised and supervised training

Setup

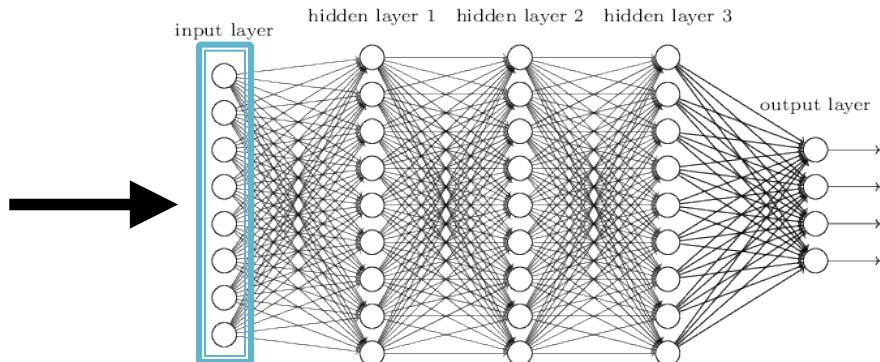
- Assume we have a graph G :
 - V is the **vertex set**
 - A is the **adjacency matrix** (assume binary)
 - $X \in \mathbb{R}^{|V| \times m}$ is a matrix of **node features**
 - v : a node in V ; $N(v)$: the set of neighbors of v .
- **Node features:**
 - Social networks: User profile, User image
 - 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:



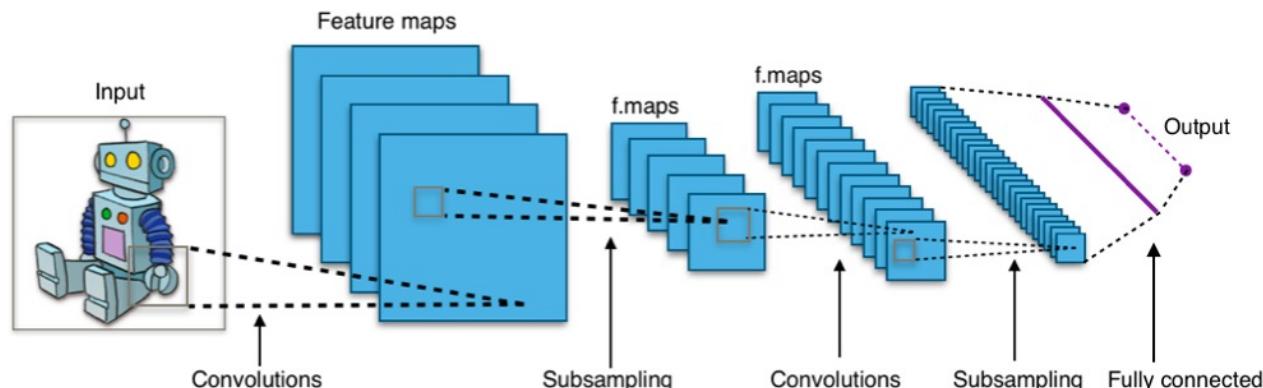
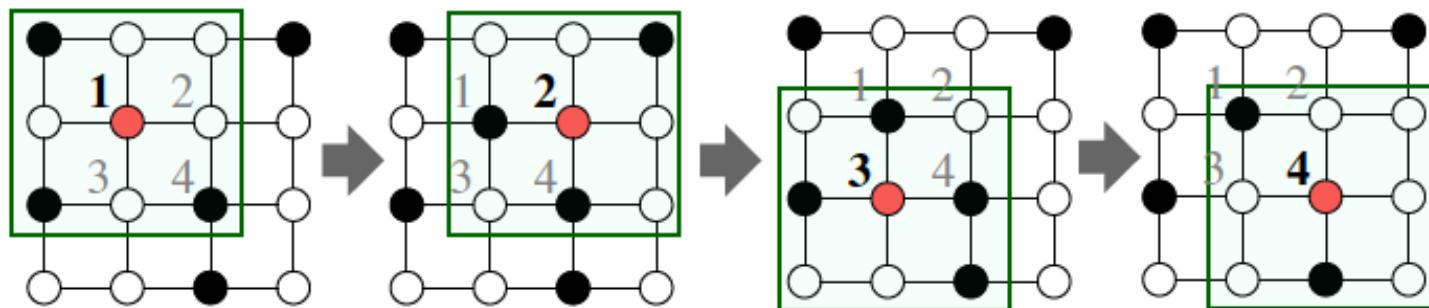
	A	B	C	D	E	Feat
A	0	1	1	1	0	1 0
B	1	0	0	1	1	0 0
C	1	0	0	1	0	0 1
D	1	1	1	0	1	1 1
E	0	1	0	1	0	1 0



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

Idea: Convolutional Networks

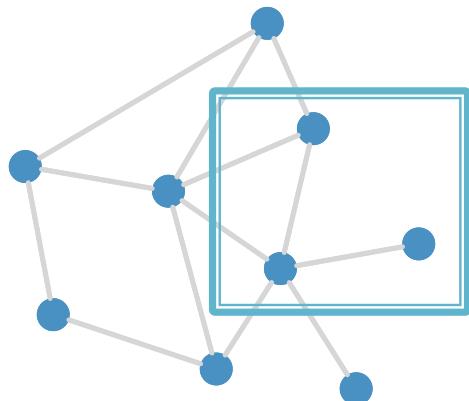
CNN on an image:



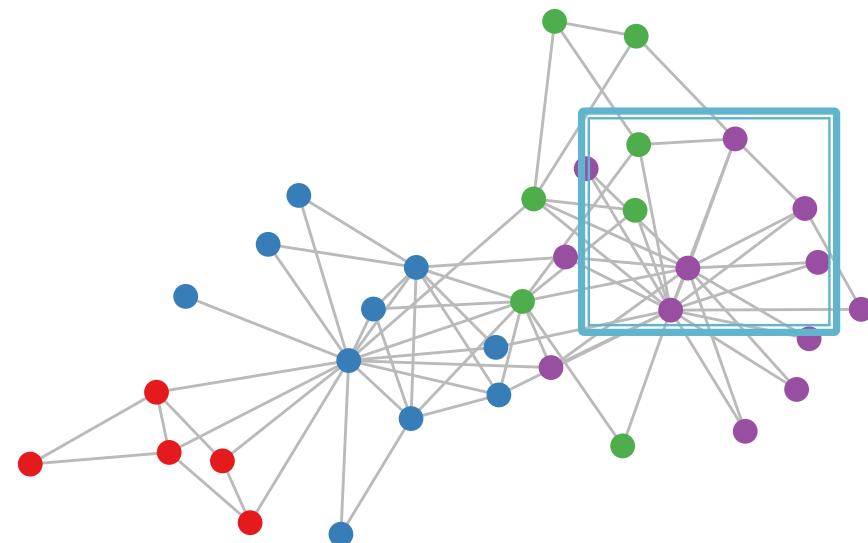
Goal is to generalize convolutions beyond simple lattices
Leverage node features/attributes (e.g., text, images)

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

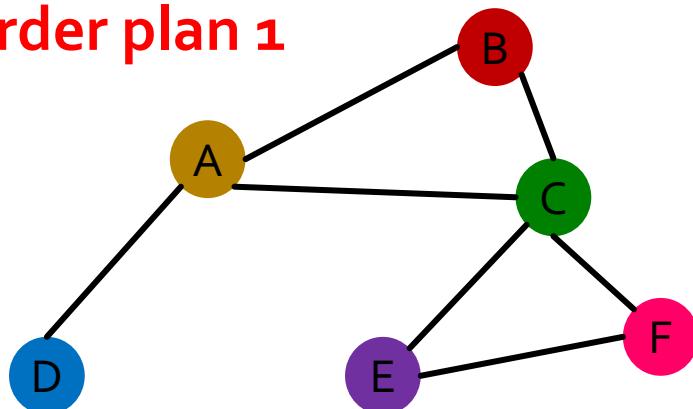
Permutation Invariance

- **Graph does not have a canonical order of the nodes!**
- We can have many different order plans.

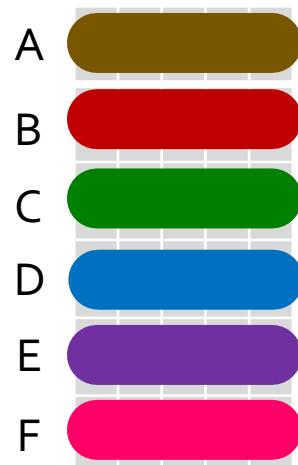
Permutation Invariance

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

Order plan 1



Node features X_1



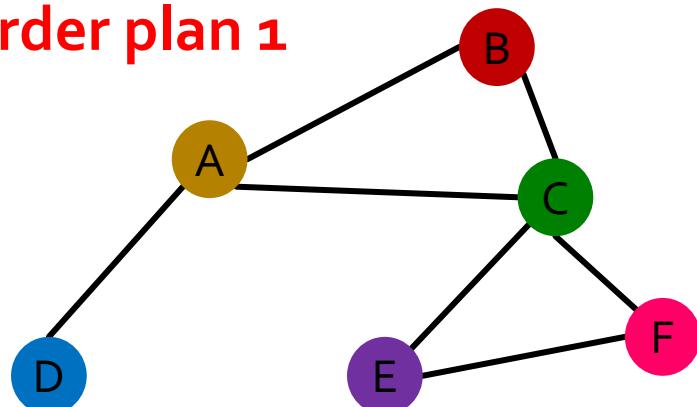
Adjacency matrix A_1

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

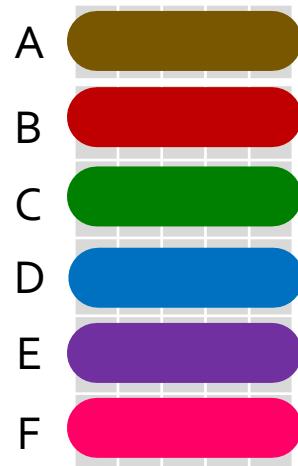
Permutation Invariance

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

Order plan 1



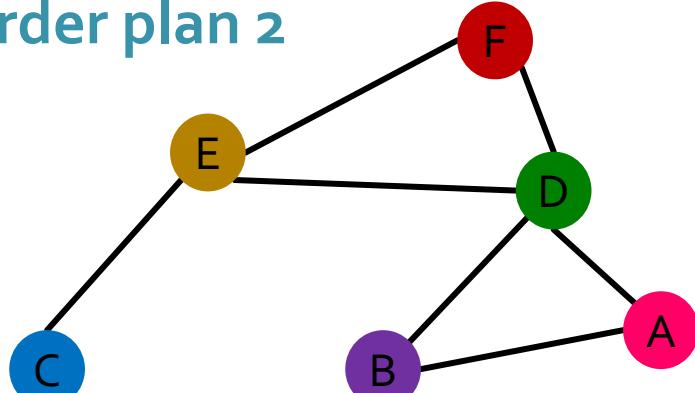
Node features X_1



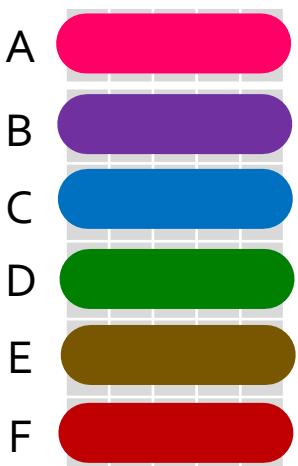
Adjacency matrix A_1

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

Order plan 2



Node features X_2



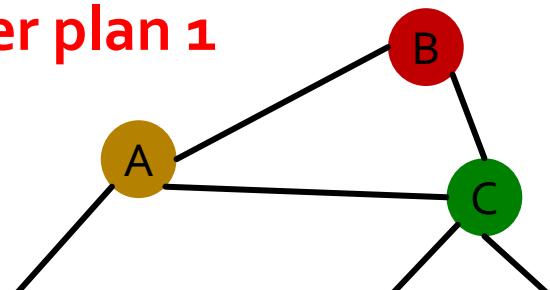
Adjacency matrix A_2

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

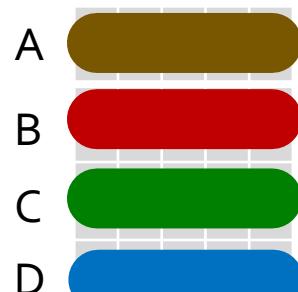
Permutation Invariance

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

Order plan 1



Node features X_1

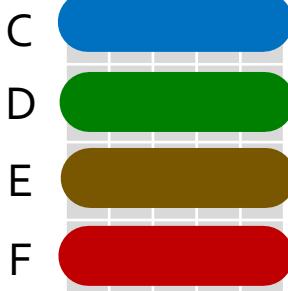
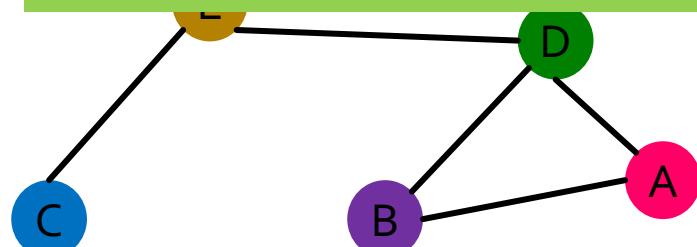


Adjacency matrix A_1

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

Graph and node representations
should be the same for Order plan 1
and Order plan 2

Order plan 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	Gray	Blue
F	Gray	Gray	Gray	Blue	Gray

Permutation Invariance

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

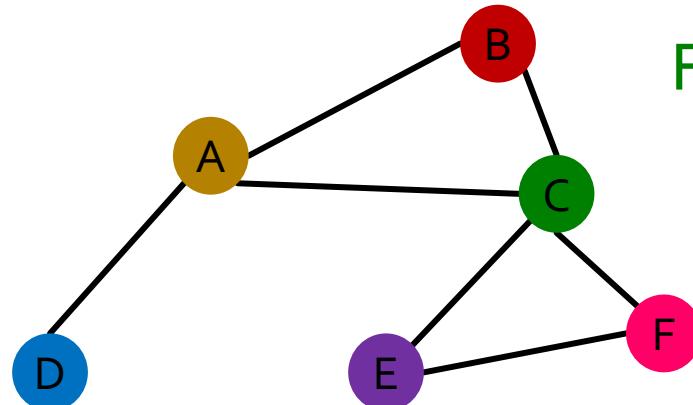
In other words, f maps a graph to a d -dim embedding

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

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

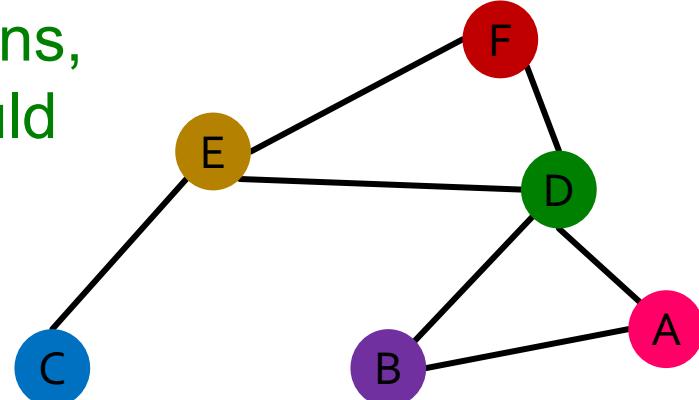
A is the adjacency matrix
 X is the node feature matrix

Order plan 1: A_1, X_1



For two order plans,
output of f should
be the same!

Order plan 2: A_2, X_2



Permutation Invariance

What does it mean by “graph representation is 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 order plan i and j , we formally say f is a **permutation invariant function**.
For a graph with $|V|$ nodes, there are $|V|!$ different order plans.
 m ... each node has a m -dim feature vector associated with it.
- Definition:** For any **graph** function $f: \mathbb{R}^{|V| \times m} \times \mathbb{R}^{|V| \times |V|} \rightarrow \mathbb{R}^d$, f is **permutation-invariant** if $f(A, X) = f(PAP^T, PX)$ for any permutation P .

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

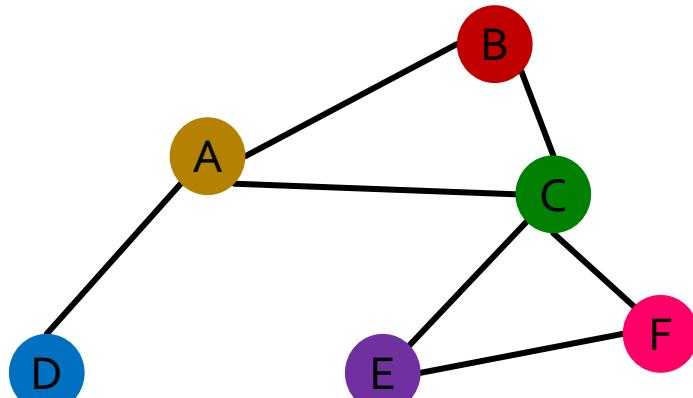
Permutation P : a shuffle of the node order
Example: (A,B,C)->(B,C,A)

Permutation Equivariance

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

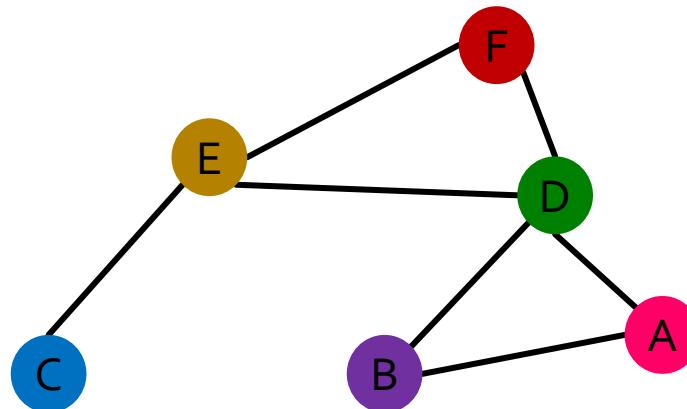
In other words, each node in V is mapped to a d -dim embedding.

Order plan 1: A_1, X_1



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

Order plan 2: A_2, X_2

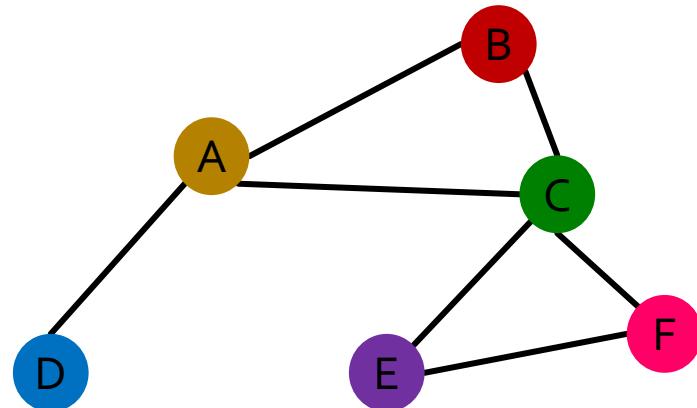


$$f(A_2, X_2) = \begin{array}{c|c|c} & \text{A} & \text{B} \\ \text{A} & \text{A} & \text{A} \\ \text{B} & \text{B} & \text{B} \\ \text{C} & \text{C} & \text{C} \\ \text{D} & \text{D} & \text{D} \\ \text{E} & \text{E} & \text{E} \\ \text{F} & \text{F} & \text{F} \end{array}$$

Permutation Equivariance

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

Order plan 1: A_1, X_1

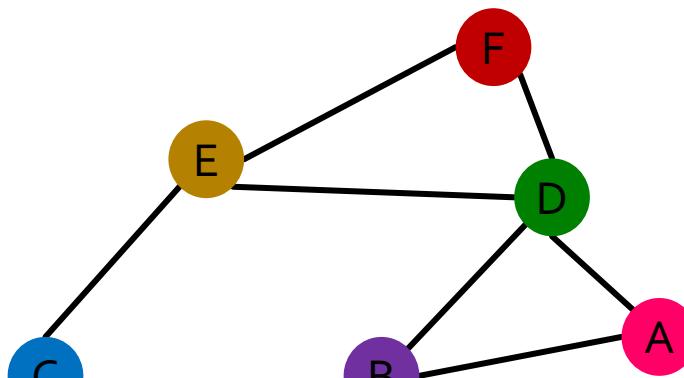


Representation vector
of the brown node A

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

$$f(A_1, X_1) =$$

Order plan 2: A_2, X_2



$$f(A_2, X_2) =$$

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

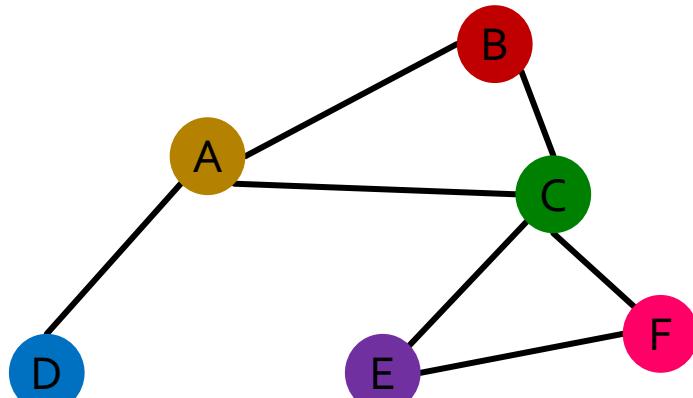
E	[brown]	[brown]
F	[red]	[red]
C	[blue]	[blue]
D	[green]	[green]
B	[purple]	[purple]
A	[pink]	[pink]

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 plan 1: A_1, X_1

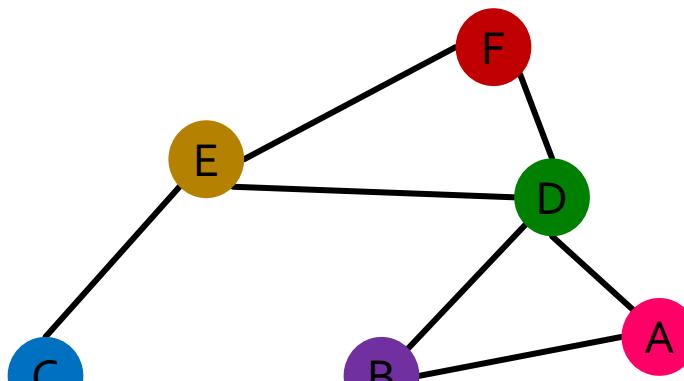


$$f(A_1, X_1) = \begin{matrix} & \text{A} & \text{B} & \text{C} & \text{D} & \text{E} & \text{F} \\ \text{A} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{B} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \text{C} & \text{---}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

Representation vector of the green node C

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

Order plan 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 order plan, we say f is **permutation equivariant**.
- Definition:** For any **node** function $f: \mathbb{R}^{|V| \times m} \times \mathbb{R}^{|V| \times |V|} \rightarrow \mathbb{R}^{|V| \times d}$, 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.

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

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

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

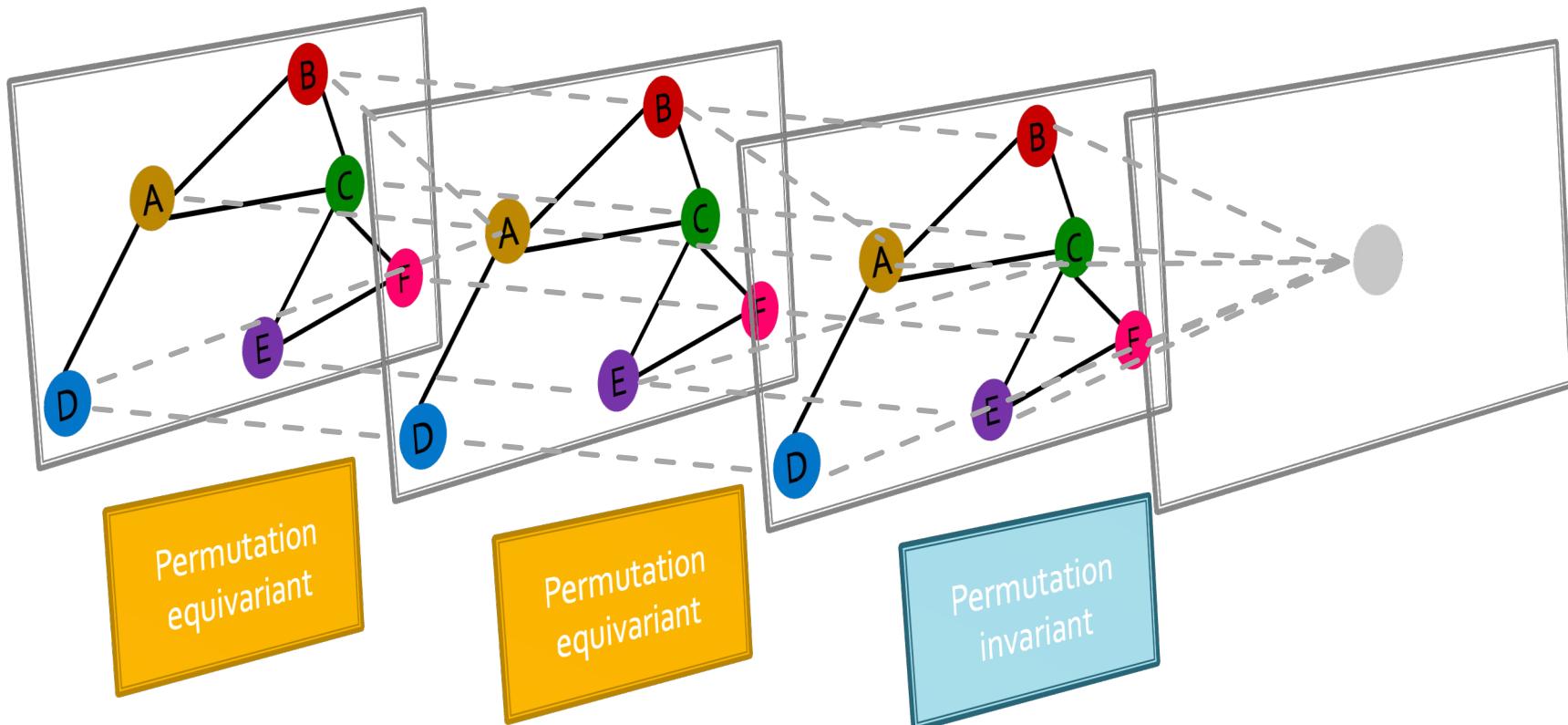
Permute the input, output also permutes accordingly.
(map a graph to a matrix)

■ 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.

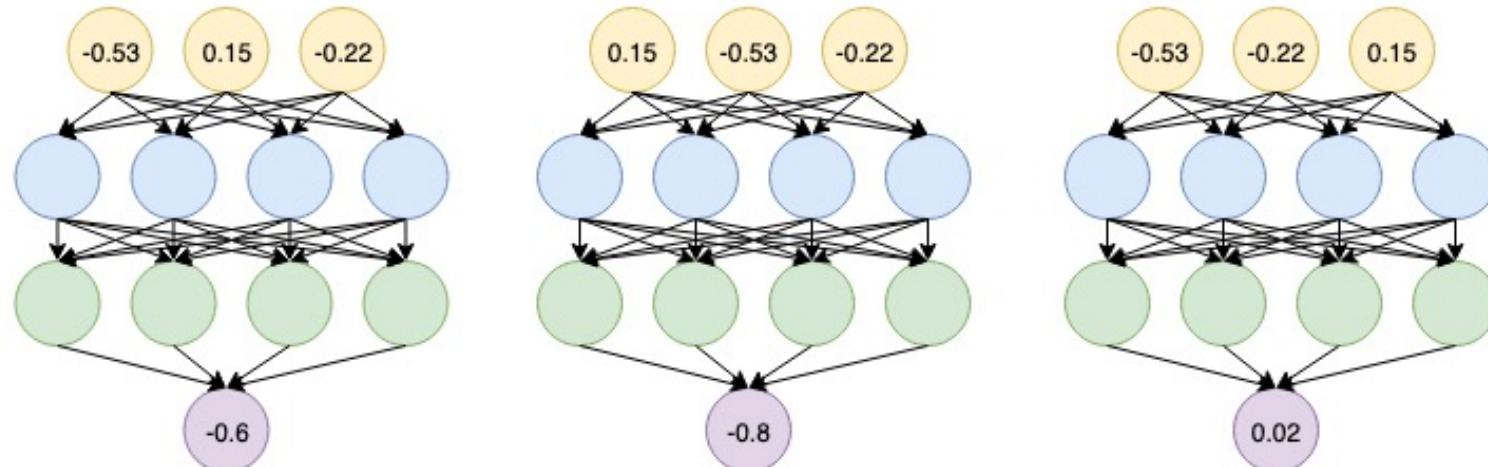


Graph Neural Network Overview

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

- No.

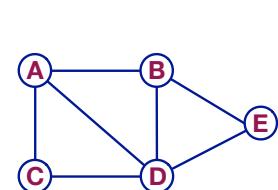
Switching the order of the
input leads to different
outputs!



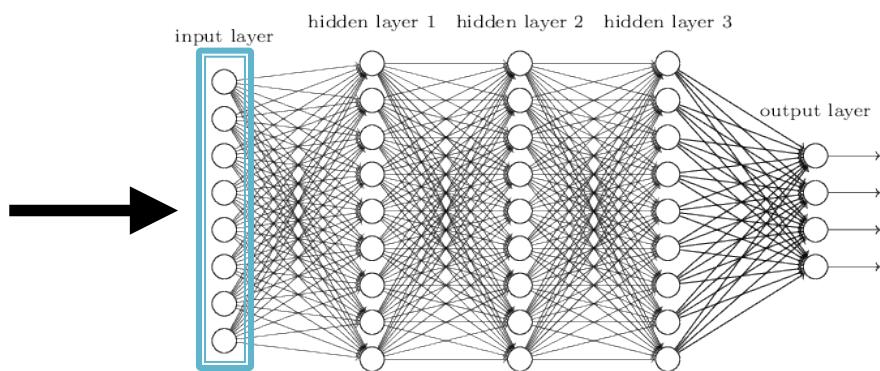
Graph Neural Network Overview

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

- No.



	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

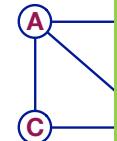


This explains why **the naïve MLP approach fails for graphs!**

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



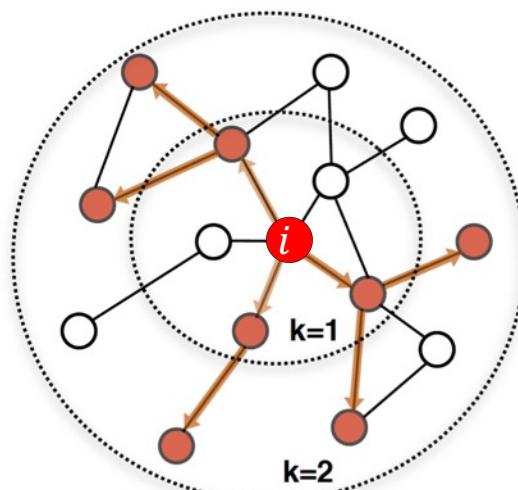
3. Graph Convolutional Networks



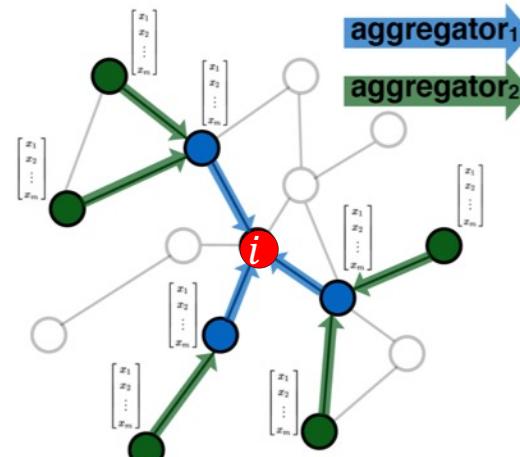
4. GNNs subsume CNNs

Graph Convolutional Networks

Idea: Node's neighborhood defines a computation graph



Determine node computation graph

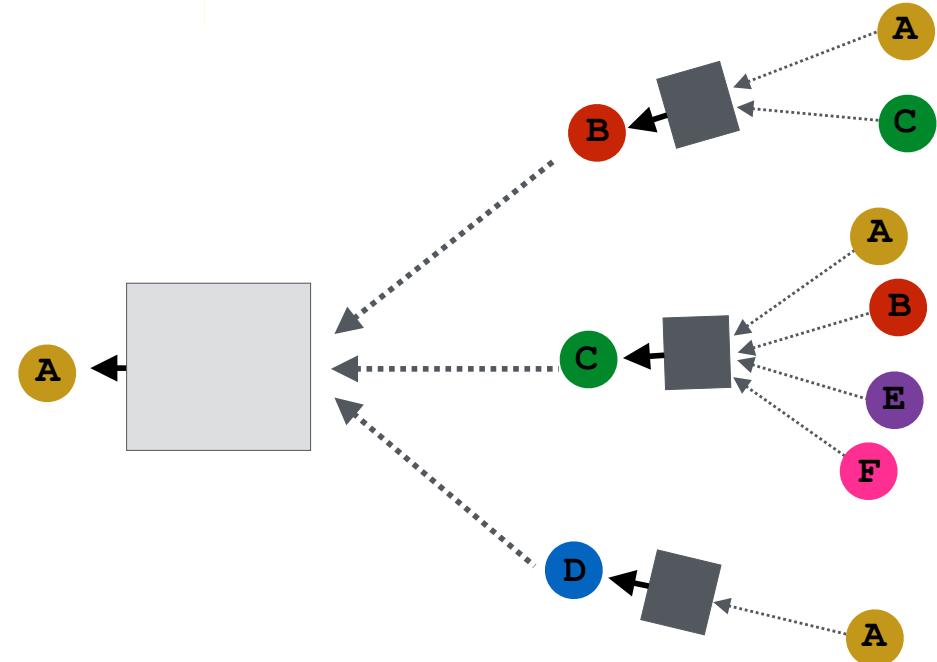
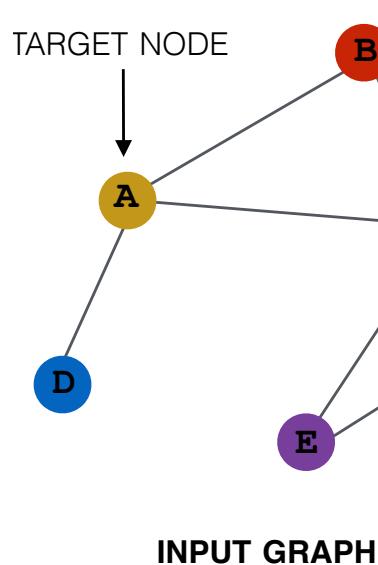


Propagate and transform information

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

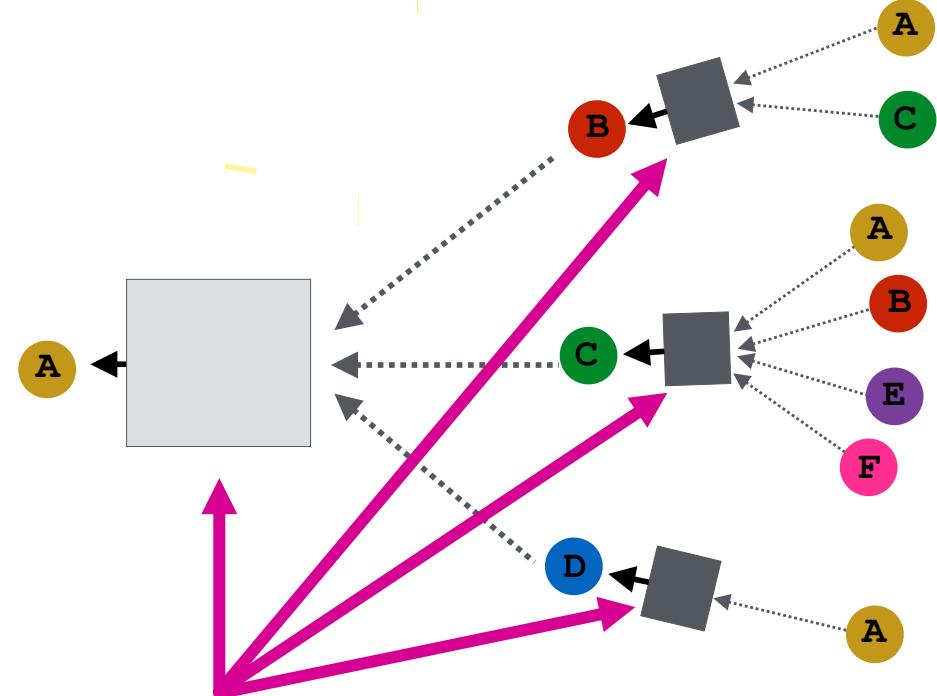
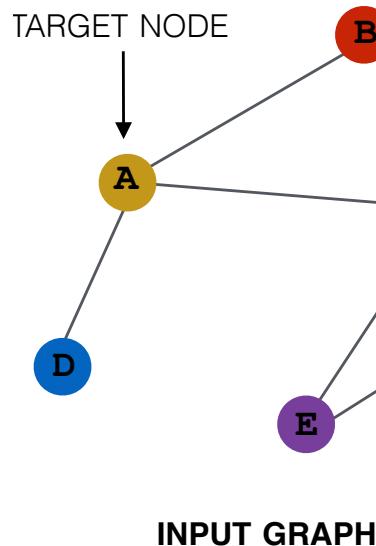
Idea: Aggregate Neighbors

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



Idea: Aggregate Neighbors

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

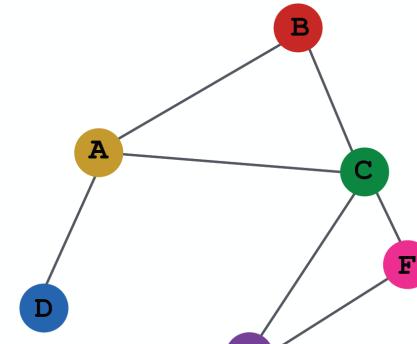


Neural networks

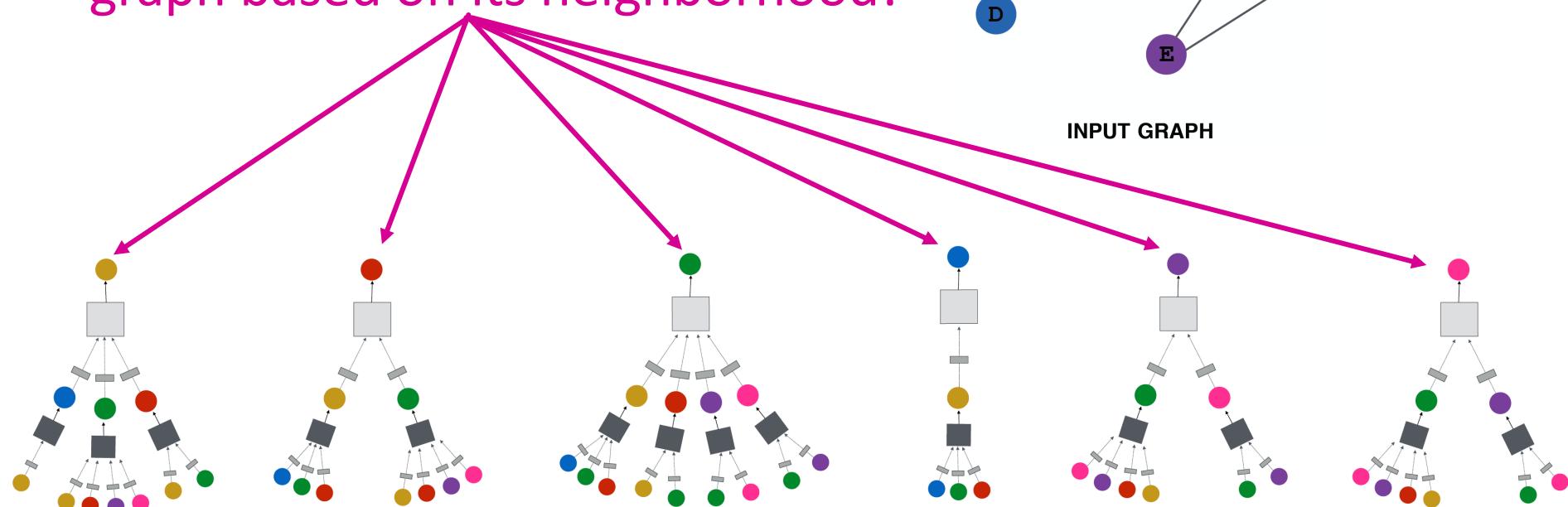
Idea: Aggregate Neighbors

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

Every node defines a computation graph based on its neighborhood!

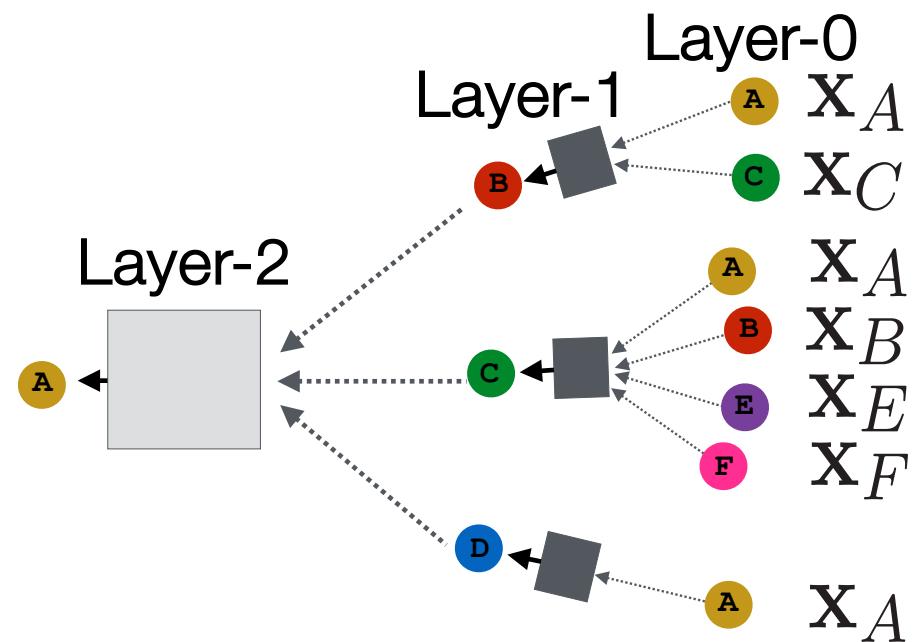
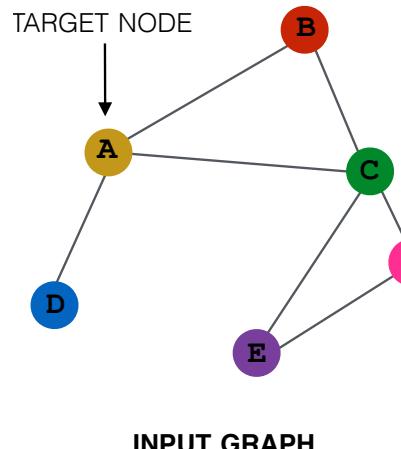


INPUT GRAPH



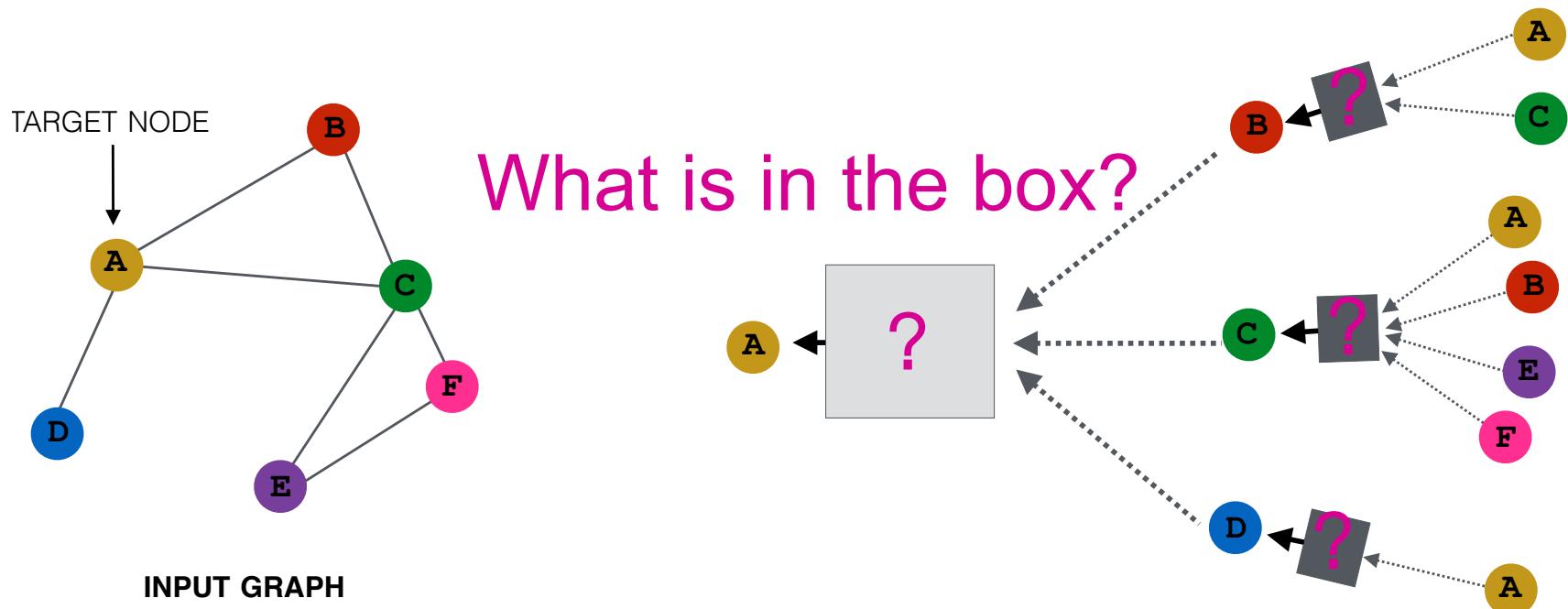
Deep Model: Many Layers

- 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



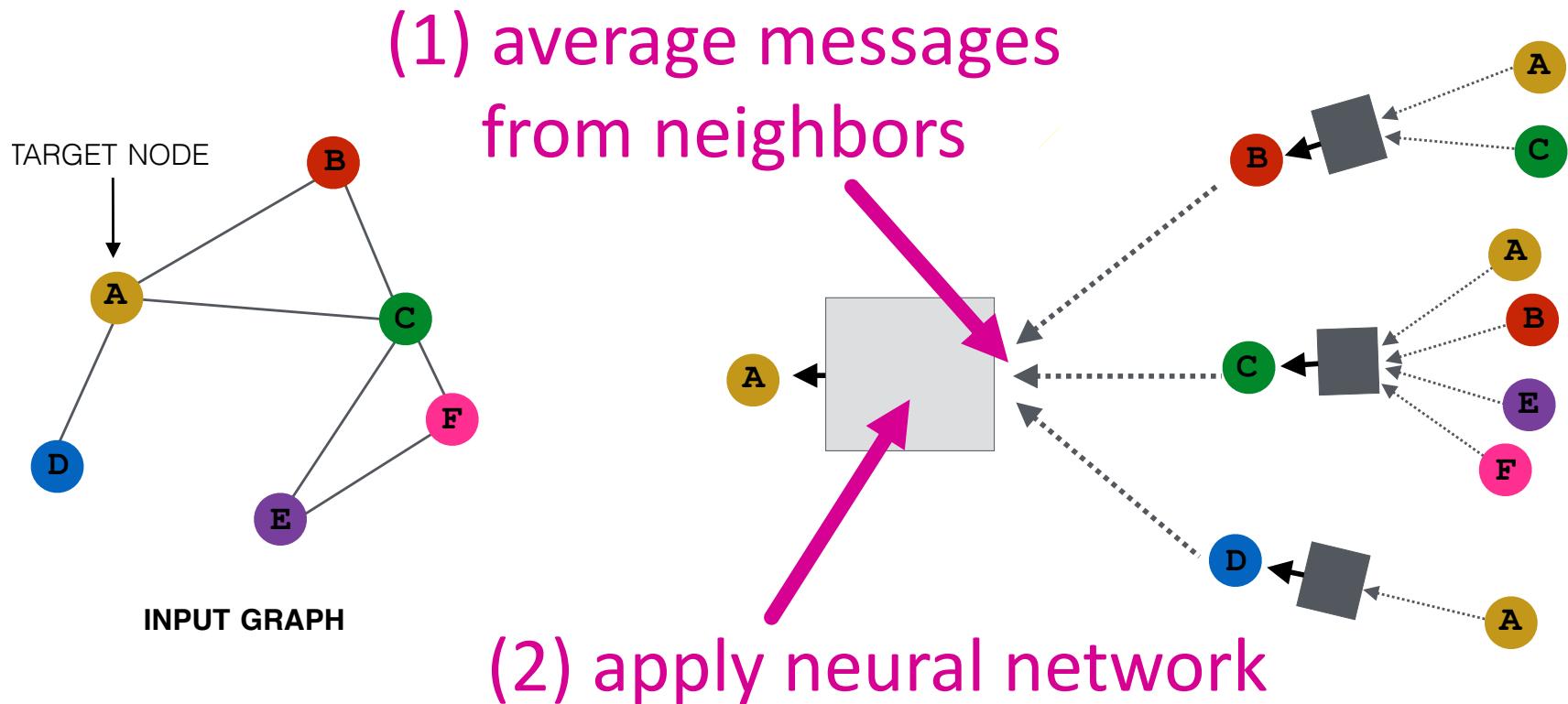
Neighborhood Aggregation

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



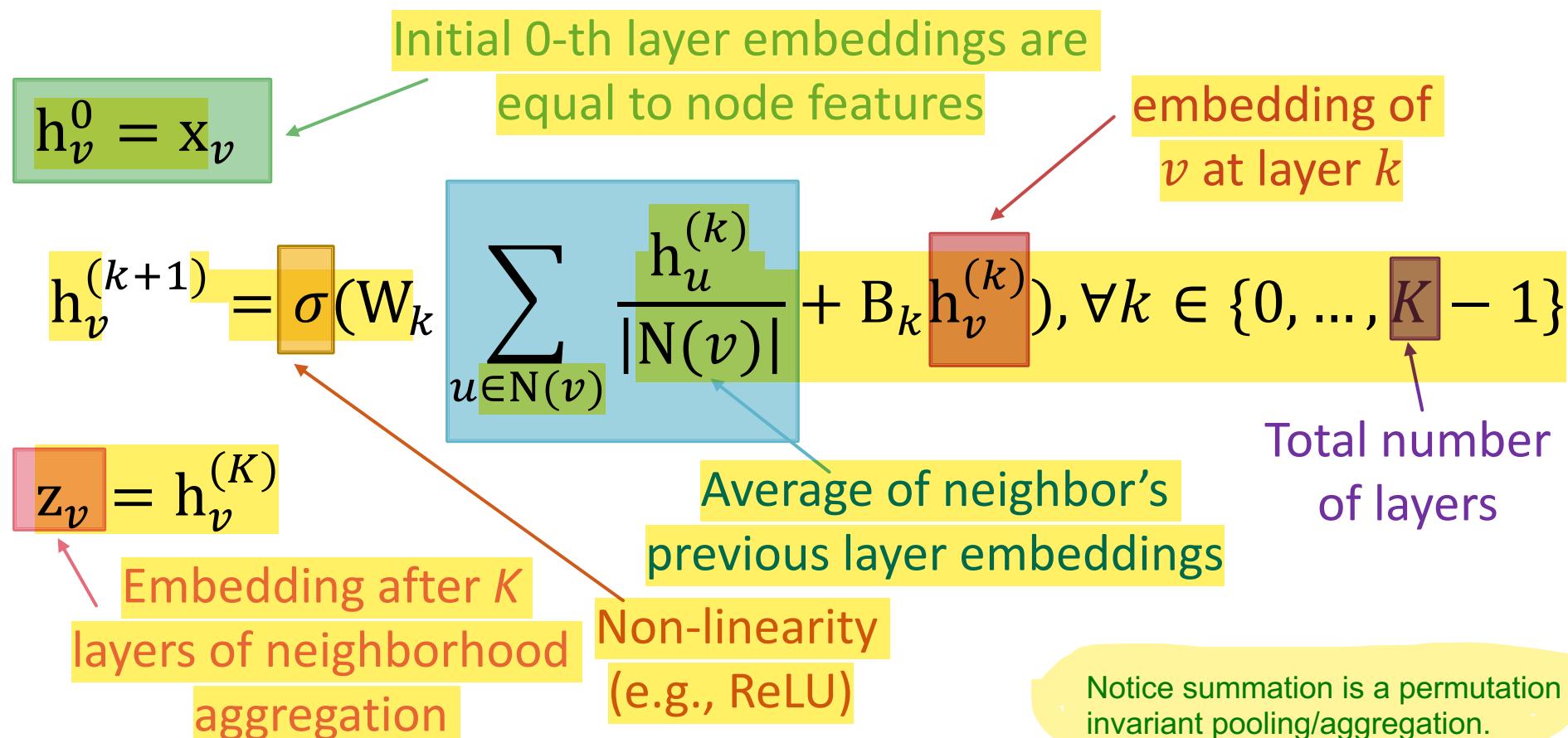
Neighborhood Aggregation

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



The Math: Deep Encoder

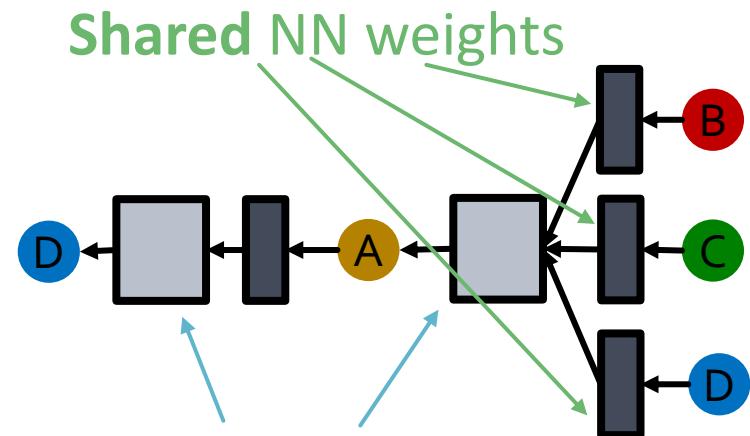
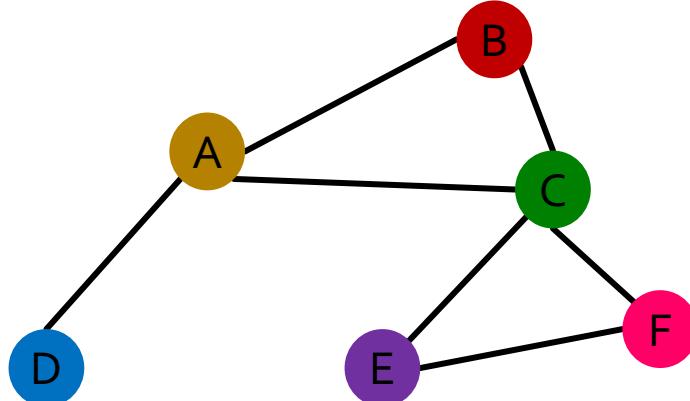
- **Basic approach:** Average neighbor messages and apply a neural network



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**

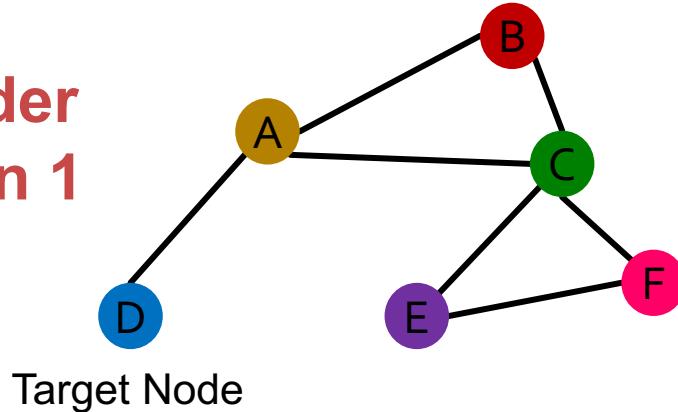


Average of neighbor's previous layer embeddings - **Permutation invariant**

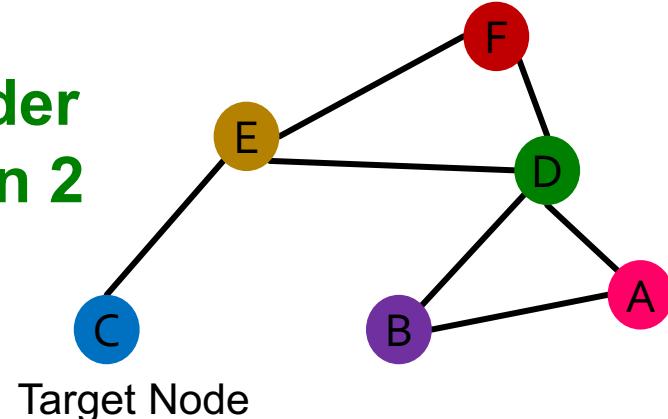
GCN: Invariance and Equivariance

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

Order plan 1



Order plan 2



Node feature X_1

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

Adjacency matrix A_1

	A	B	C	D	E	F
A	■					
B		■				
C			■			
D				■		
E					■	
F						■

Embeddings H_1

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

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	B	C	D	E	F
A	■					
B		■				
C			■			
D				■		
E					■	
F						■

Embeddings H_2

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

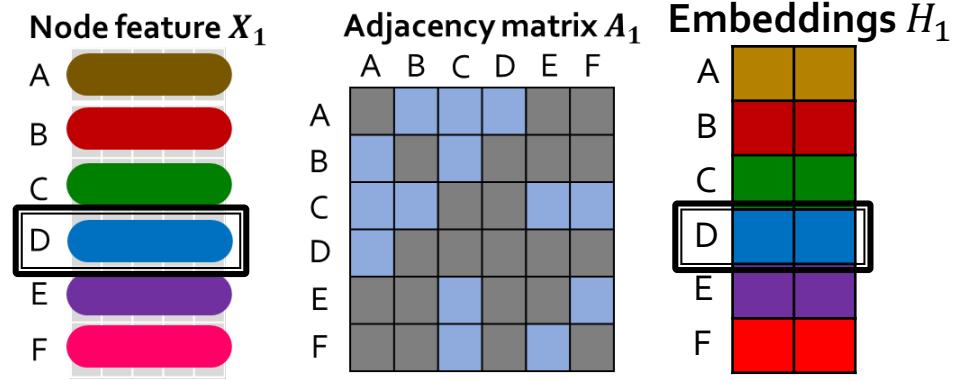
GCN: Invariance and Equivariance

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

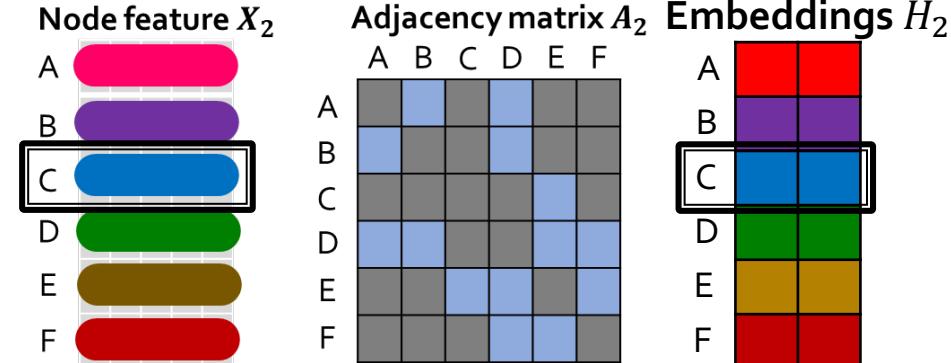
Detailed reasoning:

1. The rows of **input node features** and **output embeddings** are aligned
2. We know computing the embedding of a **given node** with GCN is **invariant**.
3. So, after permutation, the **location of a given node in the input node feature matrix** is changed, and the **the output embedding of a given node stays the same** (the colors of node feature and embedding are **matched**)

This is **permutation equivariant**

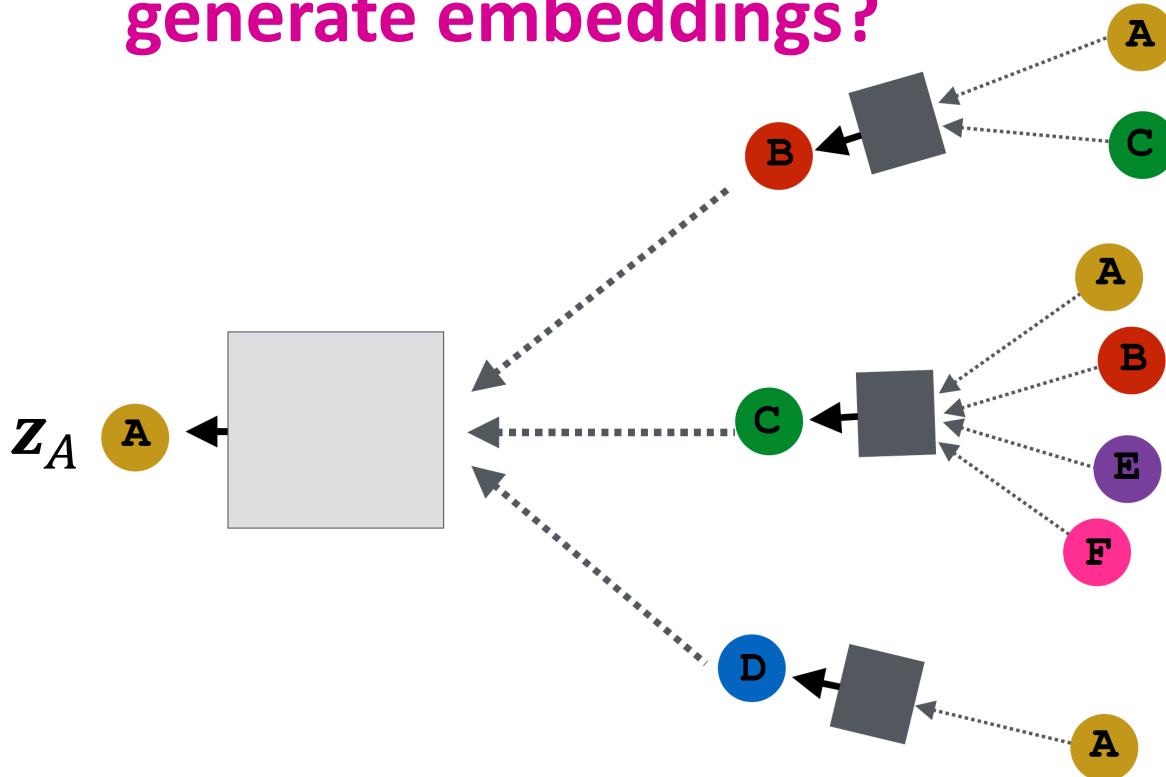


Permute the input, the output also permutes accordingly - **permutation equivariant**



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

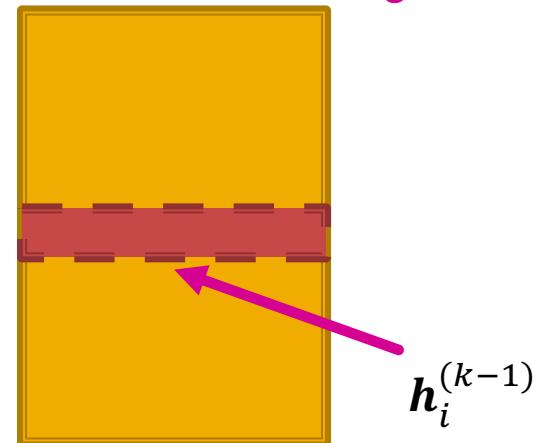
We can feed these **embeddings into any loss function** and run SGD to **train the weight parameters**

- 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,

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



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



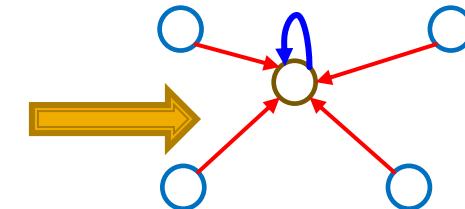
$$H^{(k+1)} = D^{-1} A H^{(k)}$$

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!**

Unsupervised Training

- One possible idea: “Similar” nodes have similar embeddings:

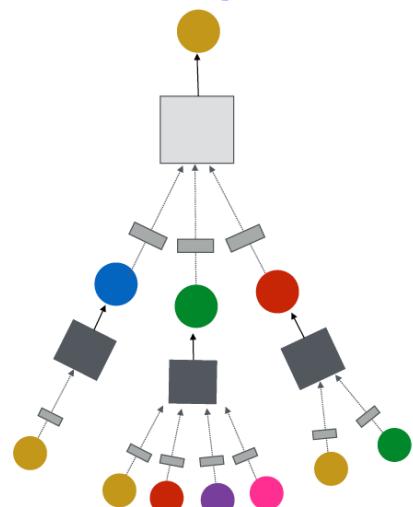
$$\min_{\Theta} \mathcal{L} = \sum_{z_u, z_v} \text{CE}(y_{u,v}, \text{DEC}(z_u, z_v))$$

- where $y_{u,v} = 1$ when node u and v are similar
 - $z_u = f_{\Theta}(u)$ and $\text{DEC}(\cdot, \cdot)$ is the dot product
- CE is the cross entropy loss:
 - $\text{CE}(y, f(x)) = - \sum_{i=1}^C (y_i \log f_{\Theta}(x)_i)$
 - y_i and $f_{\Theta}(x)_i$ are the actual and predicted values of the i -th class.
 - Intuition: the lower the loss, the closer the prediction is to one-hot
- Node similarity can be anything from Lecture 2, e.g., a loss based on:
 - Random walks (node2vec, DeepWalk, struc2vec)
 - Matrix factorization

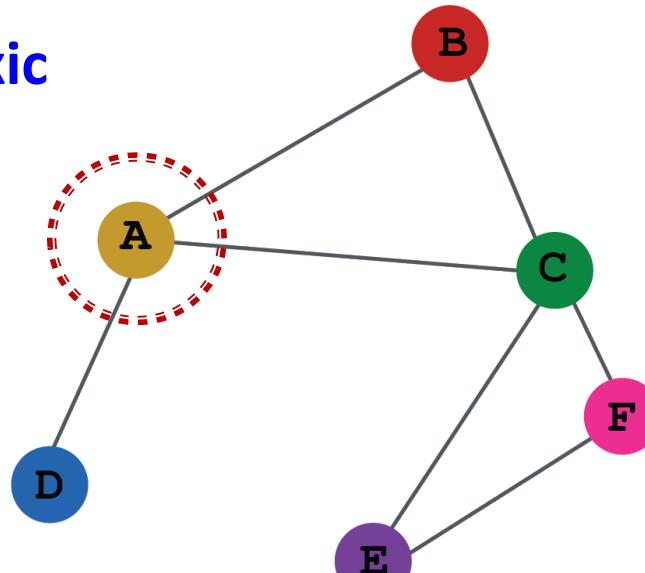
Supervised Training

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

Safe or toxic
drug?



Safe or toxic
drug?

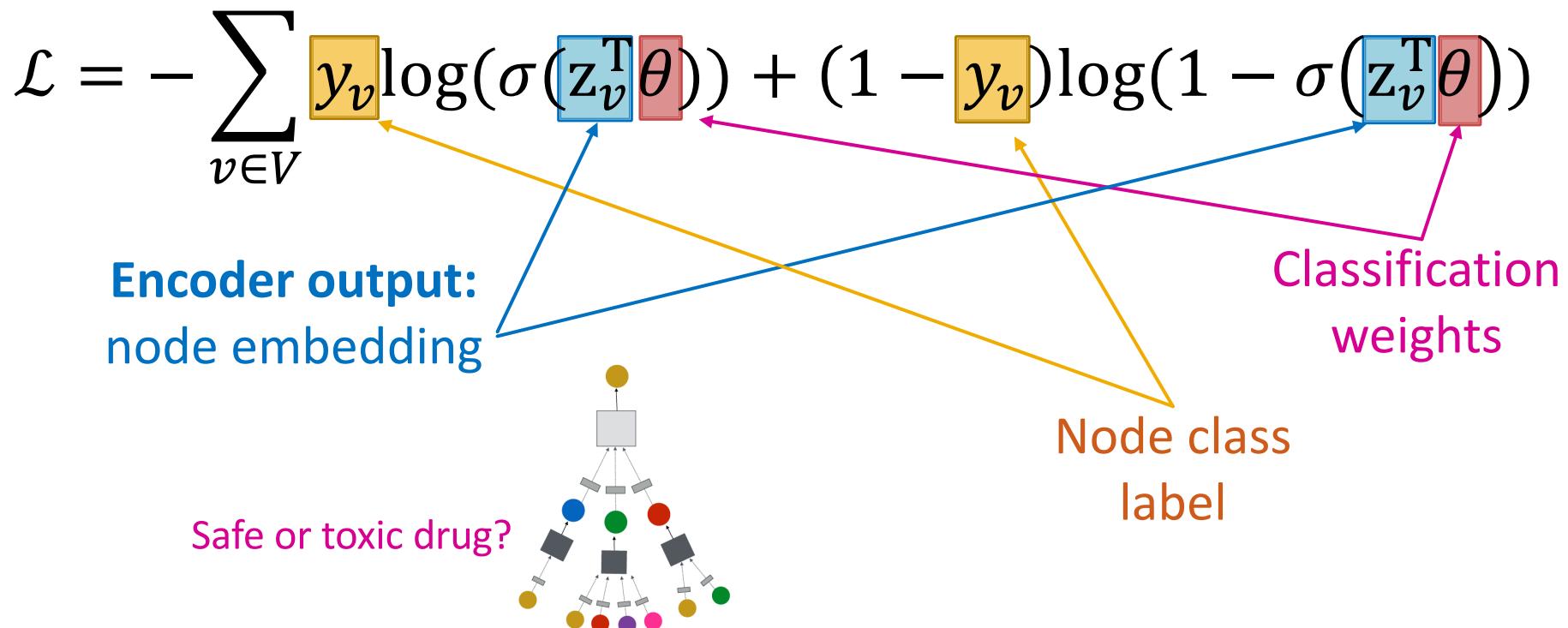


E.g., a drug-drug
interaction network

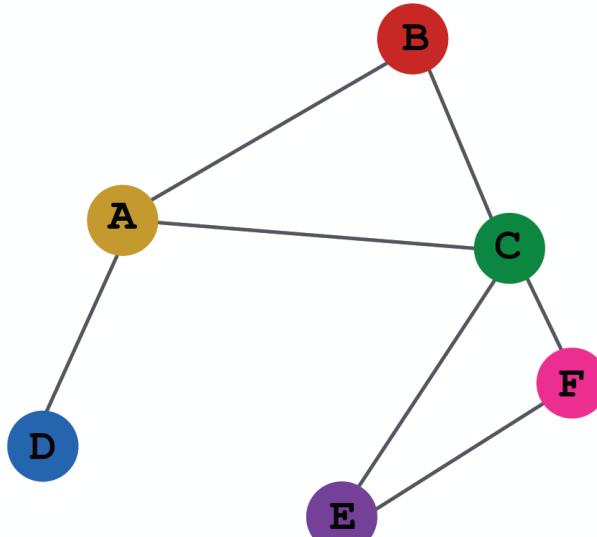
Supervised Training

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

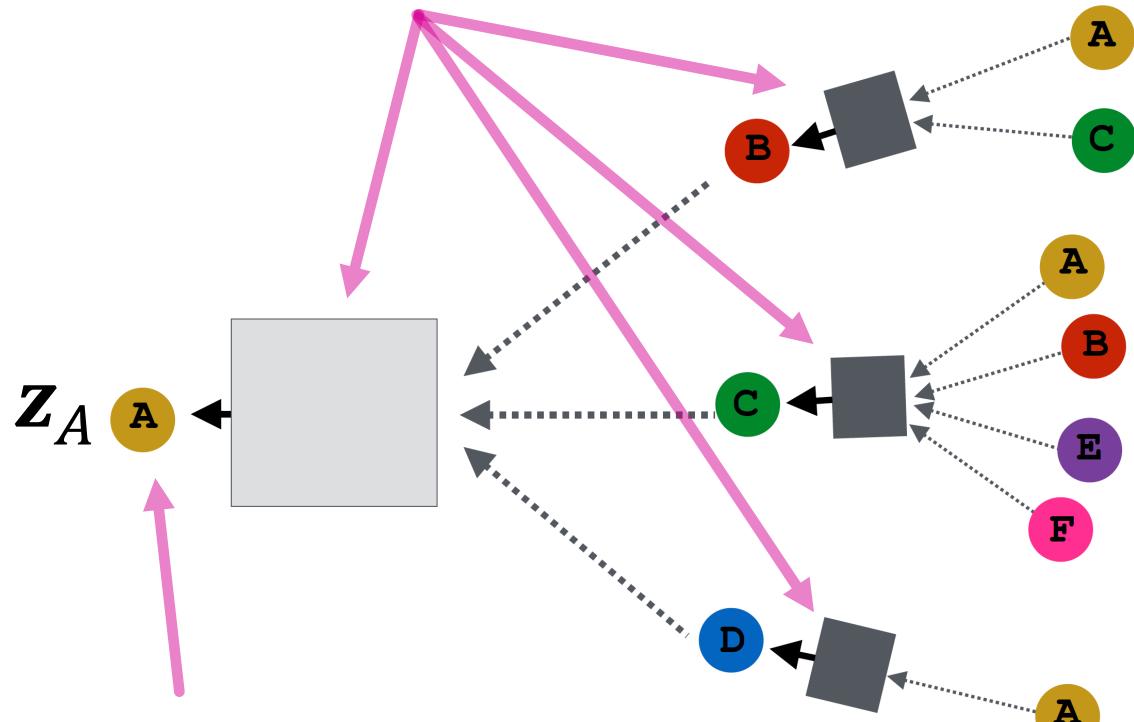
- Use cross entropy loss (Slide 53)



Model Design: Overview

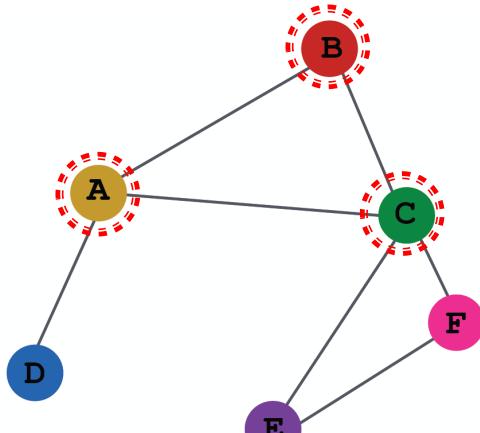


(1) Define a neighborhood aggregation function



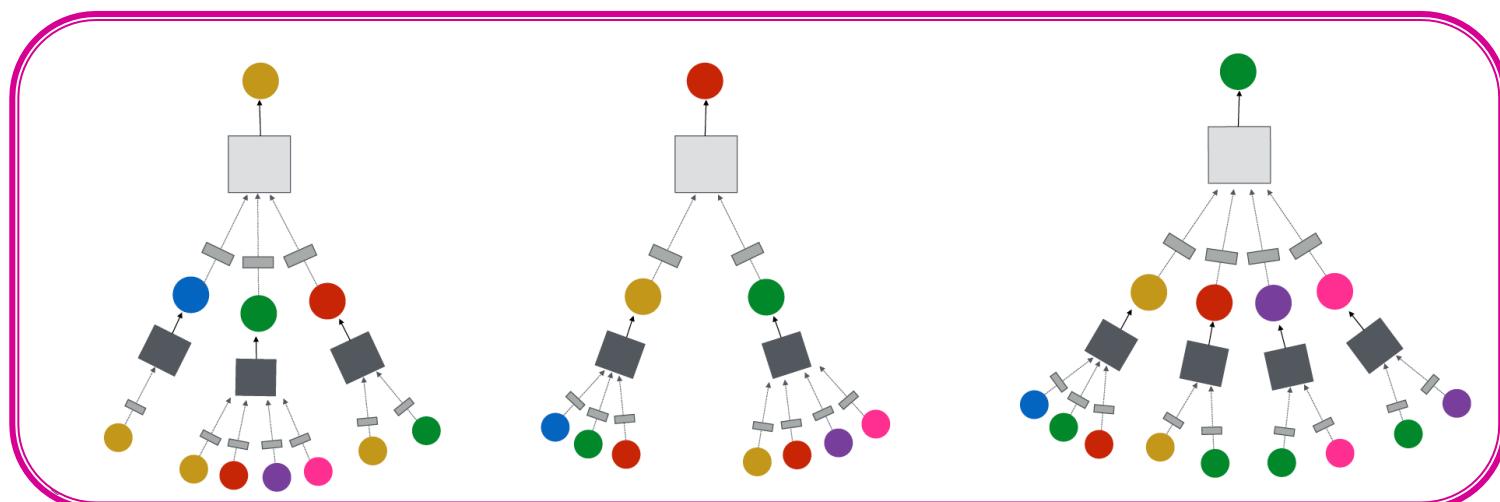
(2) Define a loss function on the embeddings

Model Design: Overview

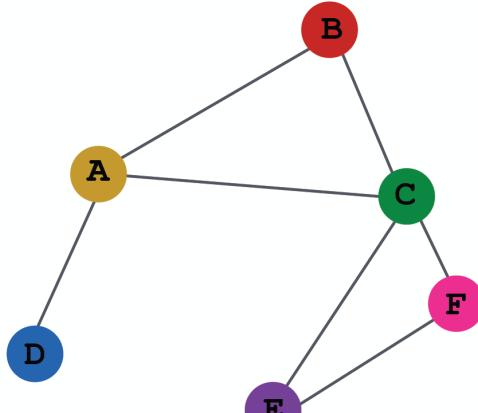


INPUT GRAPH

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



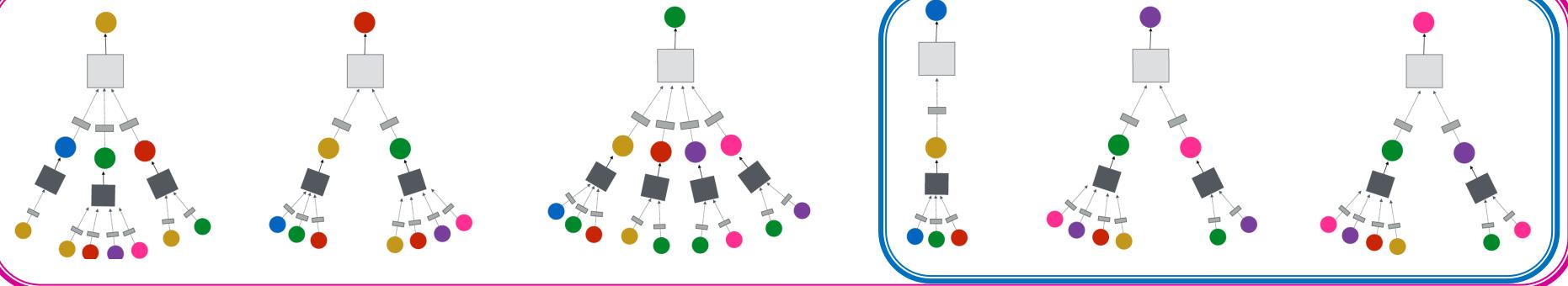
Model Design: Overview



INPUT GRAPH

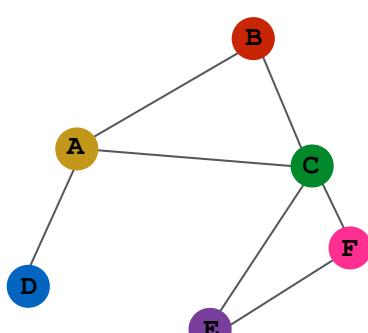
(4) Generate embeddings
for nodes as needed

Even for nodes we never
trained on!

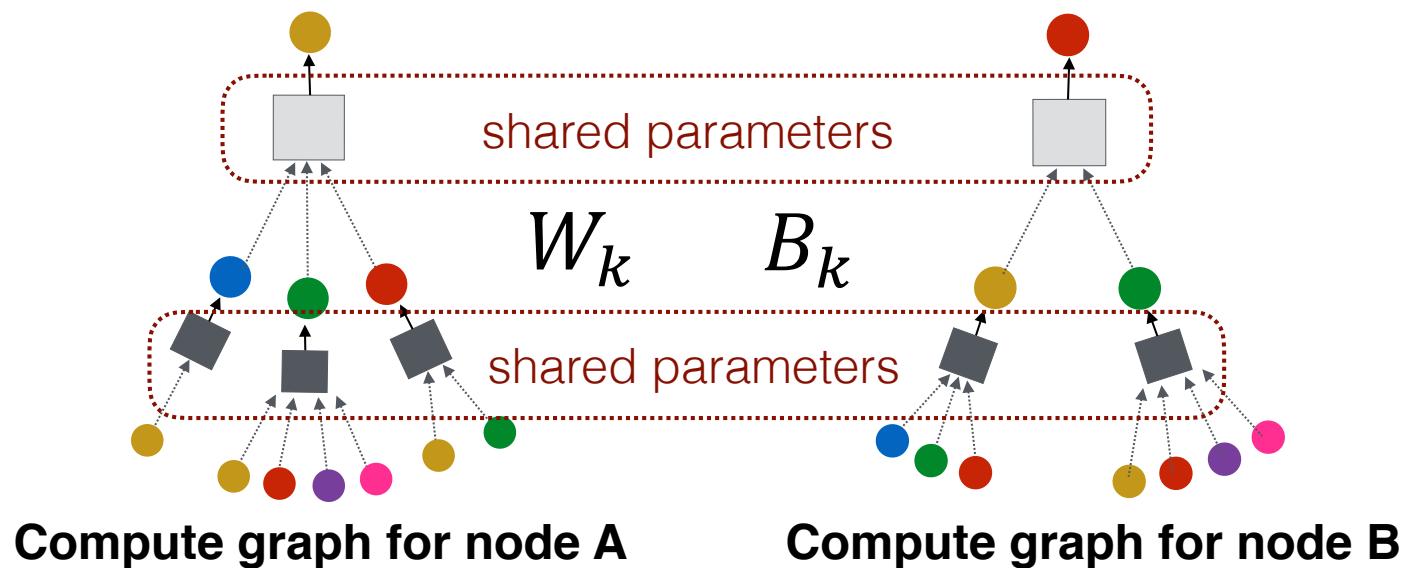


Inductive Capability

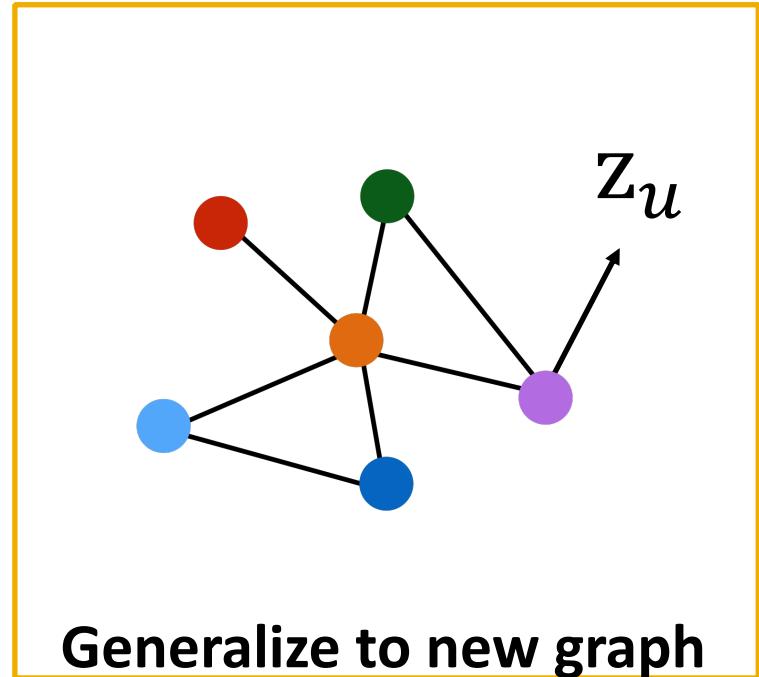
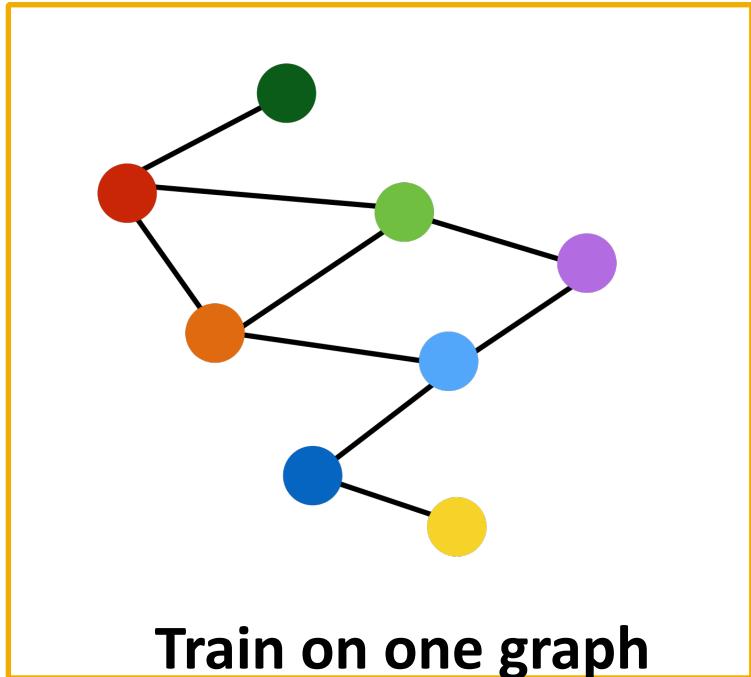
- The same aggregation parameters are shared for all nodes:
 - The number of model parameters is sublinear in $|V|$ and we can **generalize to unseen nodes!**



INPUT GRAPH



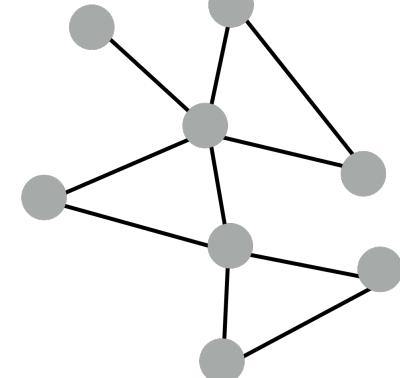
Inductive Capability: New Graphs



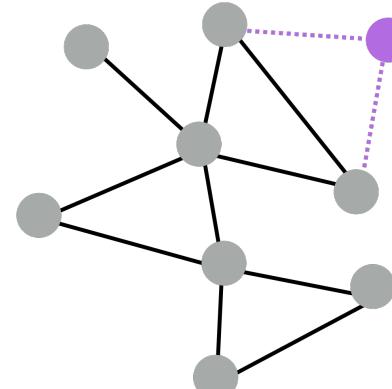
Inductive node embedding → Generalize to entirely unseen graphs

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

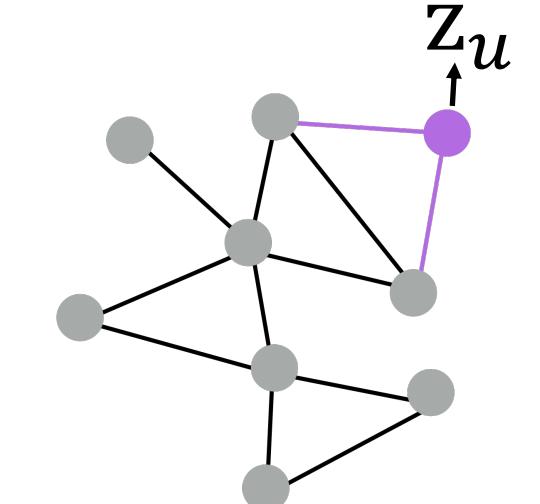
Inductive Capability: New Nodes



Train with snapshot



New node arrives



Generate embedding
for new node

- 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

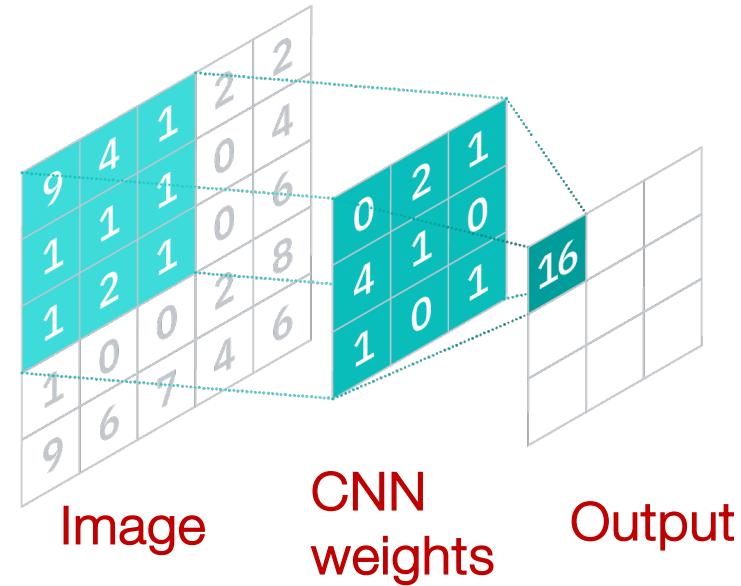
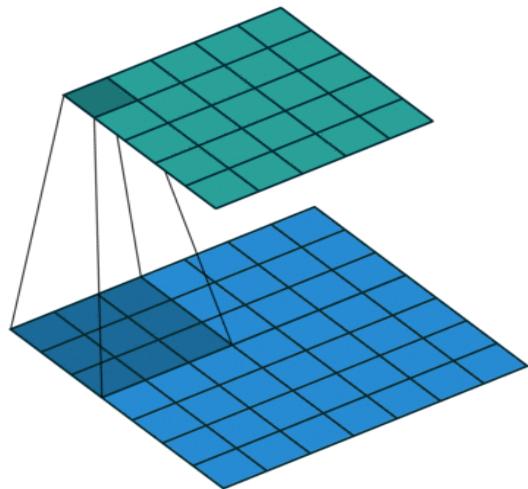


Architecture Comparison

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

Convolutional Neural Network

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

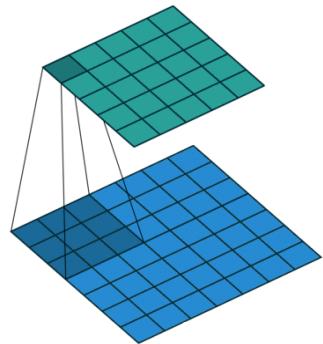


$$\text{CNN formulation: } h_v^{(l+1)} = \sigma(\sum_{u \in N(v) \cup \{v\}} W_l^u h_u^{(l)}), \quad \forall l \in \{0, \dots, L-1\}$$

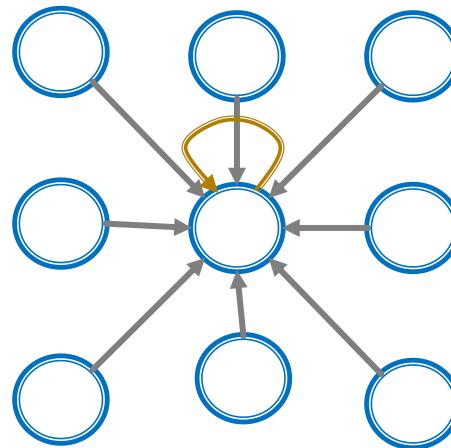
$N(v)$ represents the 8 neighbor pixels of v .

GNN vs. CNN

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



Image

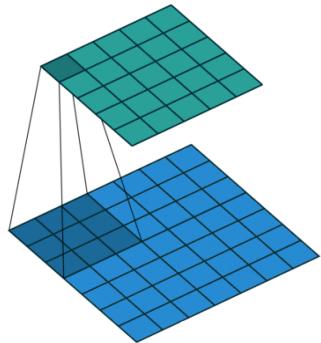


Graph

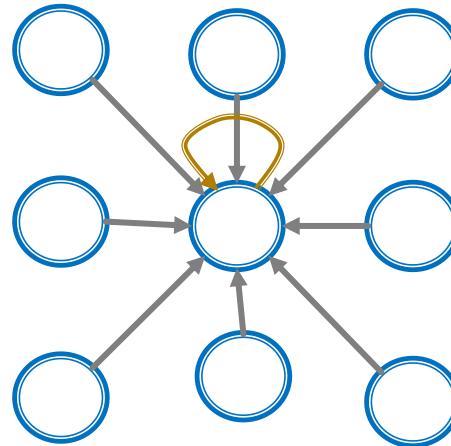
- GNN formulation: $h_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in N(v)} \frac{h_u^{(l)}}{|N(v)|} + B_l h_v^{(l)}), \forall l \in \{0, \dots, L-1\}$
- CNN formulation: (previous slide) $h_v^{(l+1)} = \sigma(\sum_{u \in N(v) \cup \{v\}} W_l^u h_u^{(l)}), \forall l \in \{0, \dots, L-1\}$
if we rewrite: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

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:

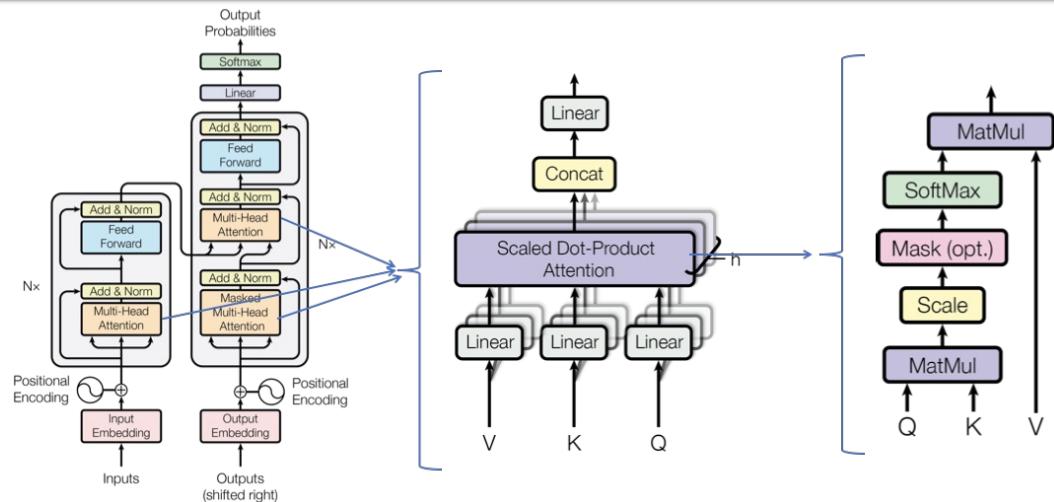


- CNN can be seen as a special GNN with fixed neighbor size and ordering:
 - The size of the filter is pre-defined for a CNN.
 - The advantage of GNN is it processes arbitrary graphs with different degrees for each node.
- CNN is not permutation invariant/equivariant.
 - Switching the order of pixels 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: $\{(-1, -1), (-1, 0), (-1, 1), \dots, (1, 1)\}$

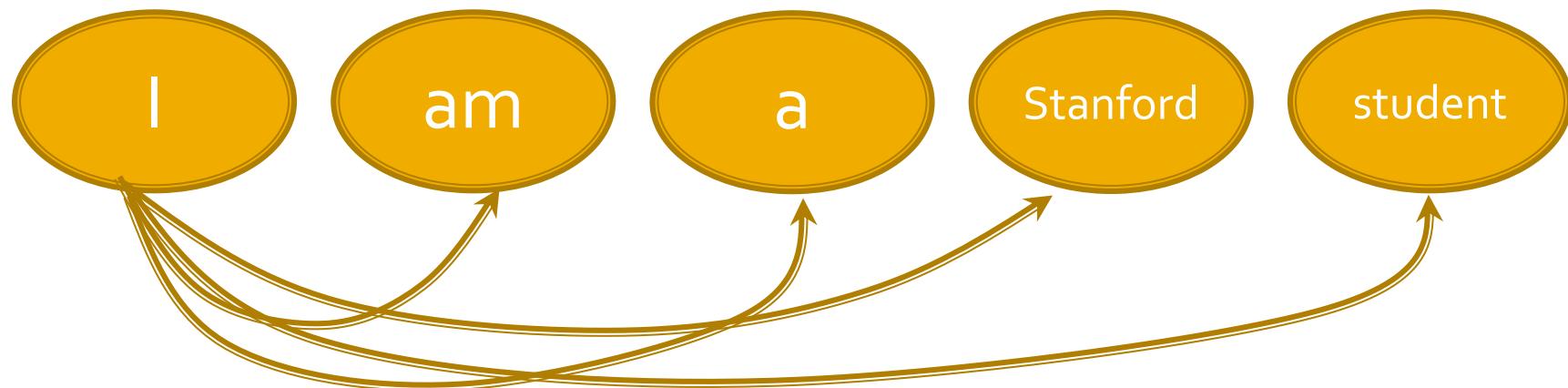
Transformer

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.

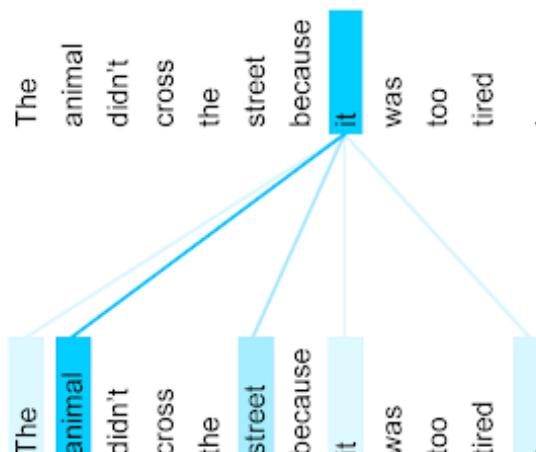


Transformer

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.

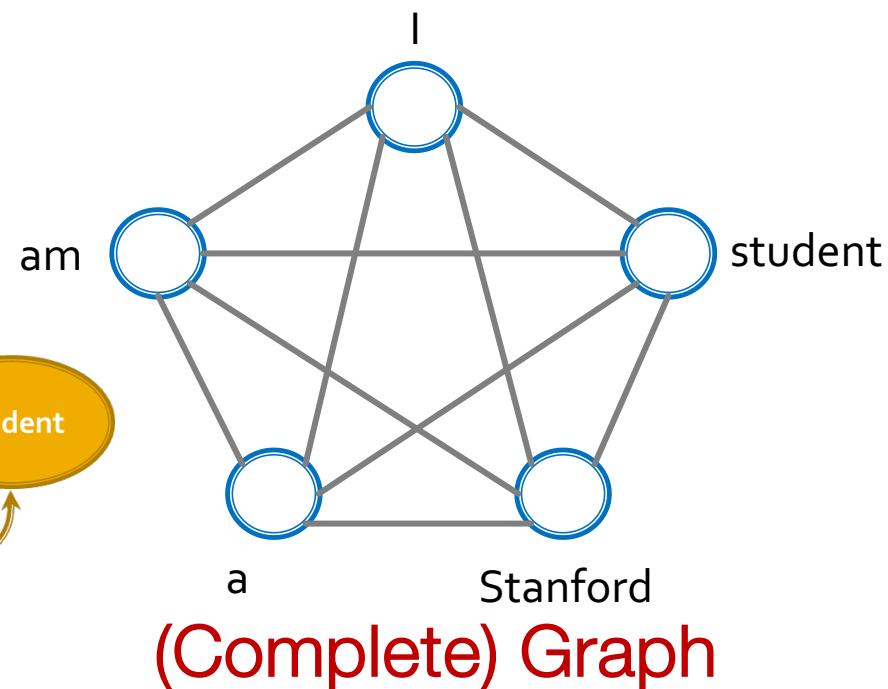
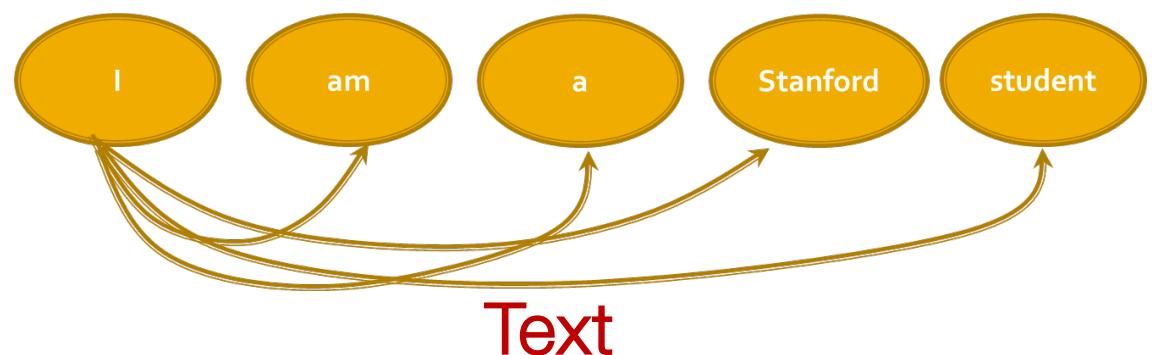
Each token/word has a **value vector** and a **query vector**. The value vector can be seen as the representation of the token/word. We use the query vector to calculate the attention score (weights in the weighted sum).



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