Stanford CS224W: Graph Neural Networks

CS224W: Machine Learning with Graphs

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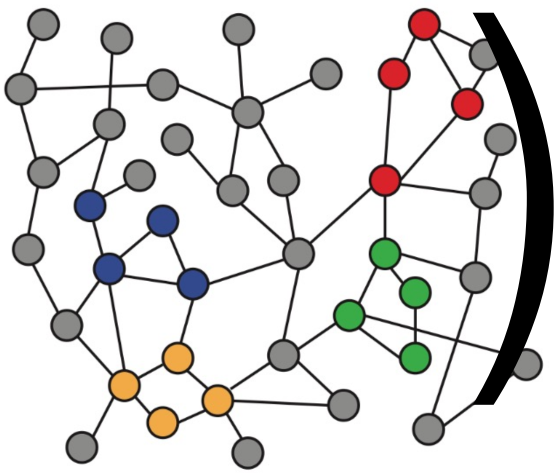
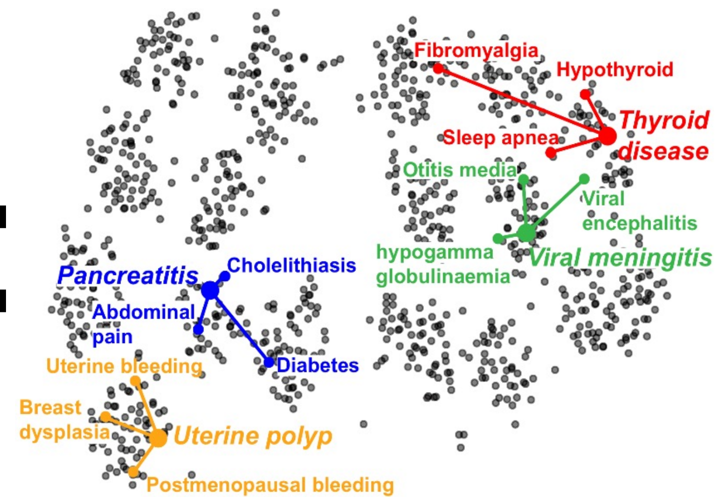
http://cs224w.stanford.edu

ANNOUNCEMENTS

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

Recap: Node Embeddings

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

f() = 

Input graph

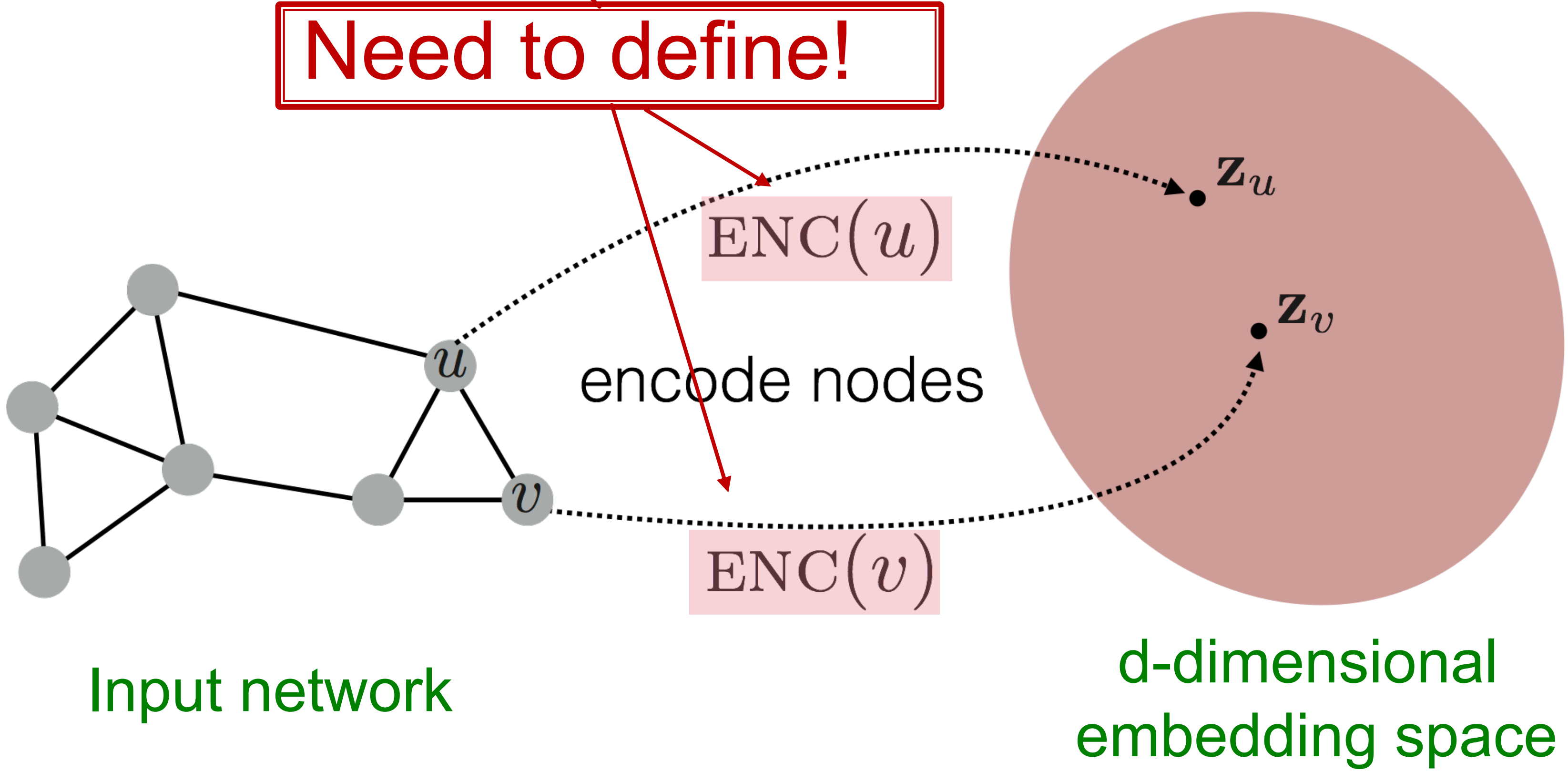
2D node embeddings

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: Two Key Components

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

d-dimensional embedding

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

node in the input graph

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

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

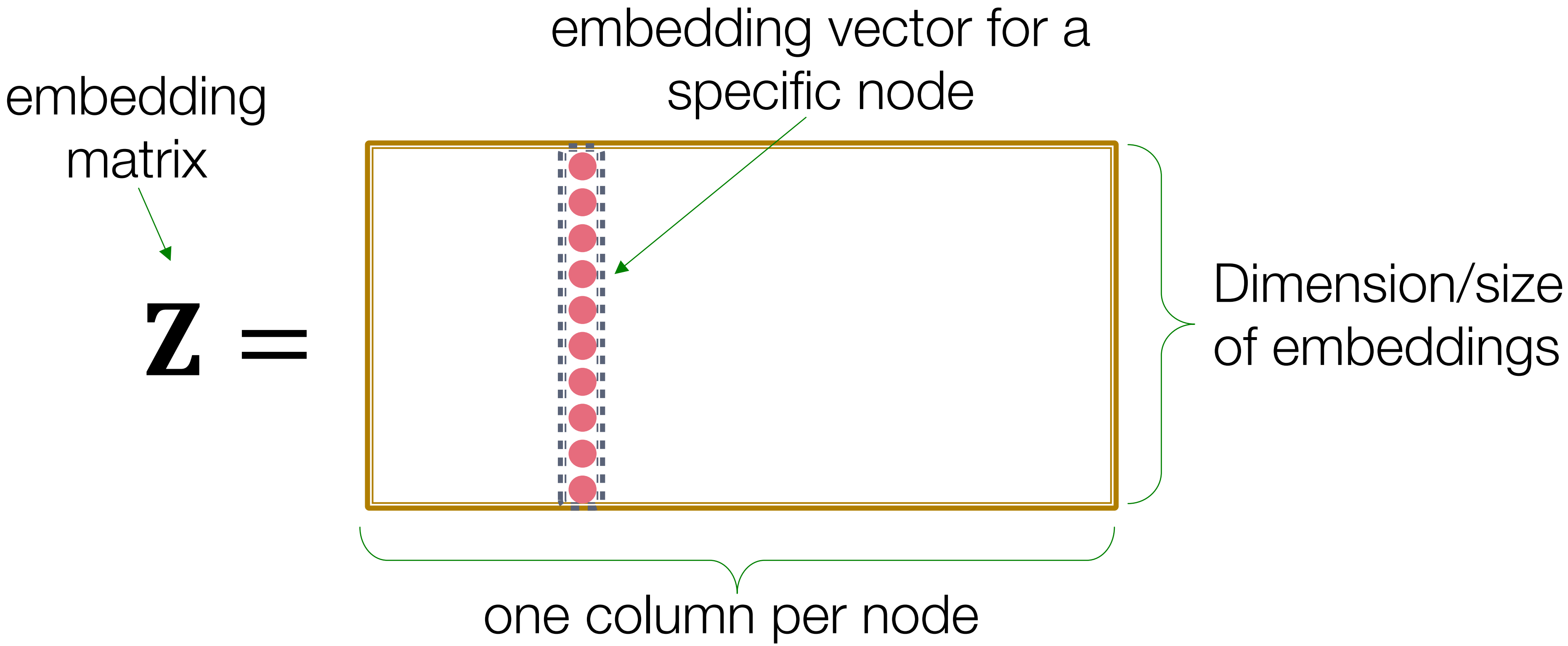
Decoder

Similarity of u and v in the original network

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

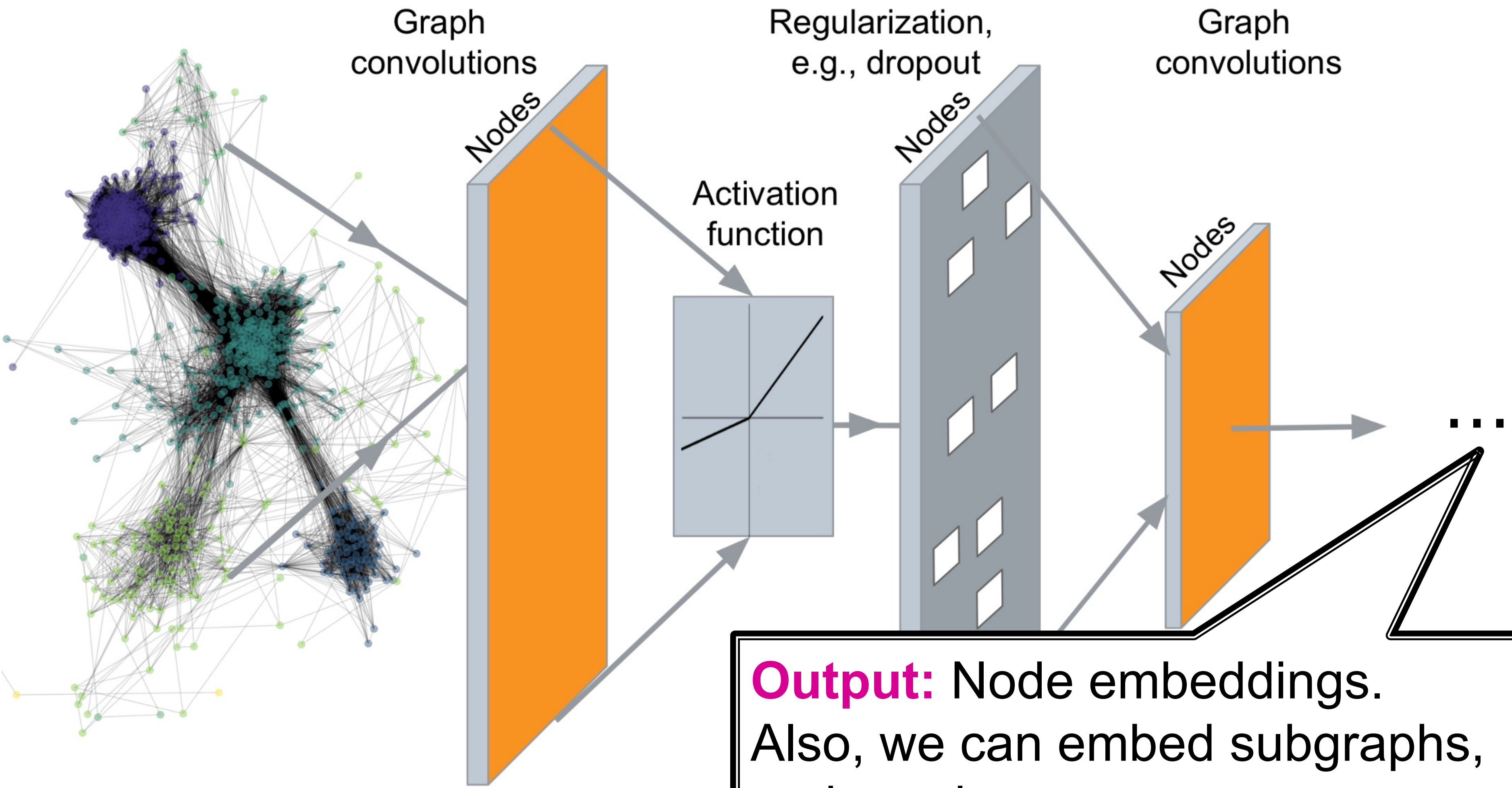
Today: Deep Graph Encoders

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

$$\mathrm{ENC}(v) = $$ **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 3.

Deep Graph Encoders



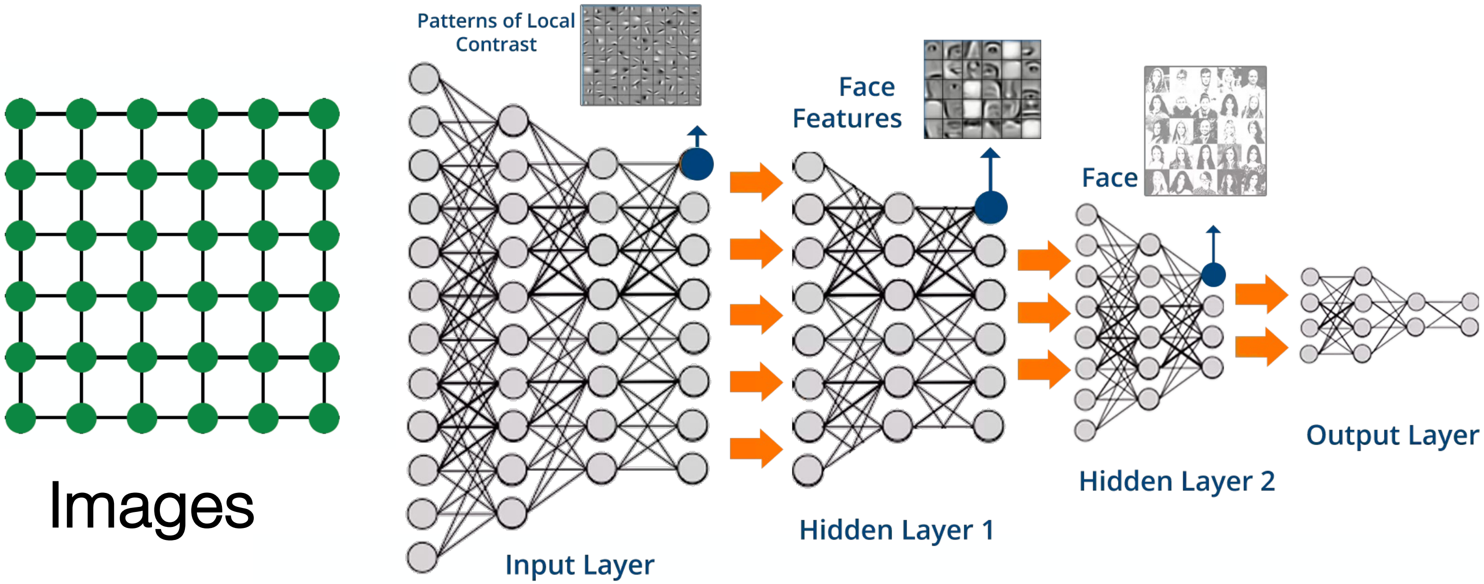
Output: Node embeddings. Also, we can embed subgraphs, and graphs

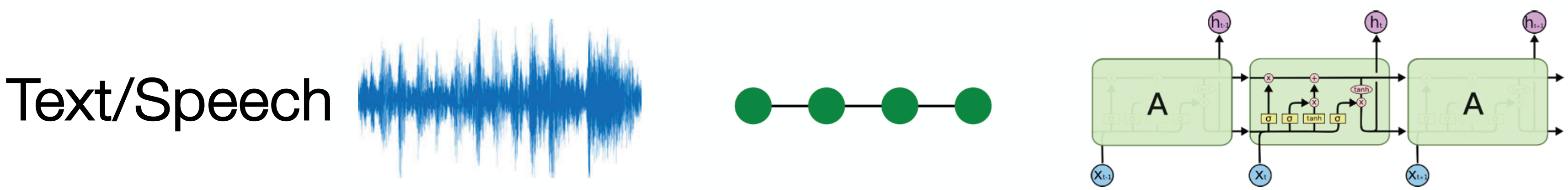
Tasks on Networks

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



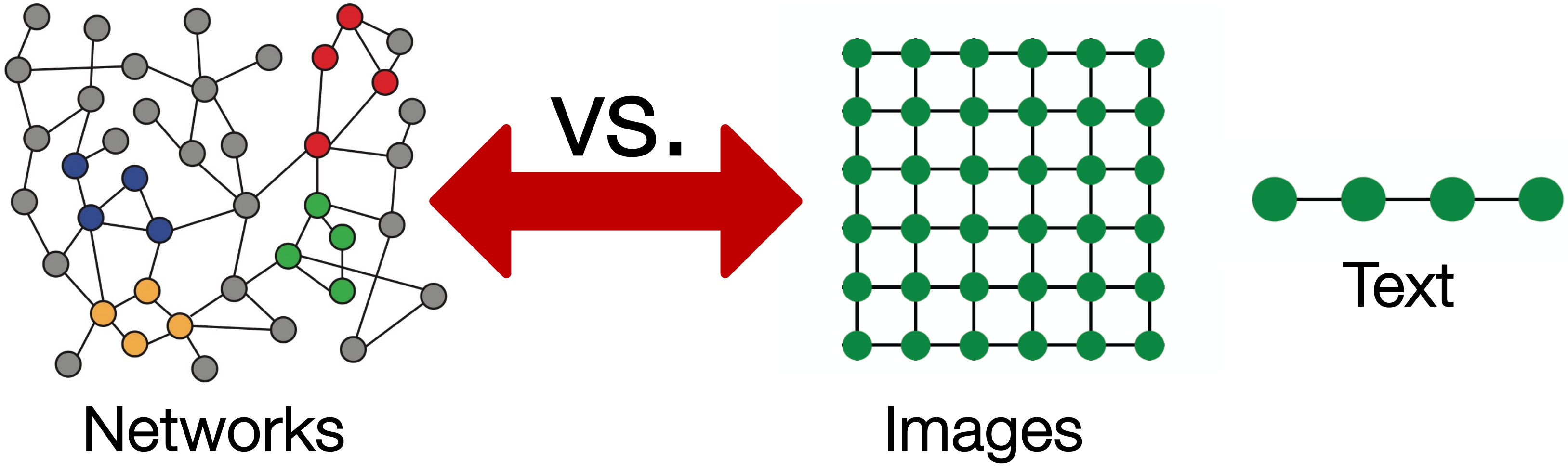


Modern deep learning toolbox is designed for simple sequences & grids

Why is it Hard?

But networks are far more complex!

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



- 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:**

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

- f can be a simple linear layer, an MLP, or other neural networks (e.g., a GNN later)
- Sample a minibatch of input $\boldsymbol{x}$
- **Forward propagation:** Compute $\mathcal{L}$ given $\boldsymbol{x}$
- **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
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Content

- **Local network neighborhoods:**
  - Describe aggregation strategies
  - Define computation graphs

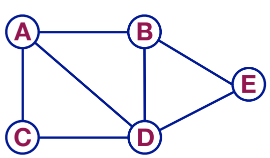
- **Stacking multiple layers:**
  - Describe the model, parameters, training
  - How to fit the model?
  - Simple example for unsupervised and supervised training

Setup

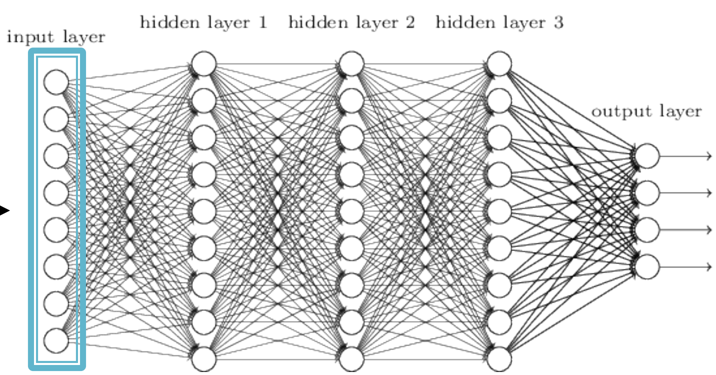
- **Assume we have a graph G:**
  - V is the **vertex set**
  - $\boldsymbol{A}$ is the **adjacency matrix** (assume binary)
  - $\boldsymbol{X} \in \mathbb{R}^{|V| \times m}$ is a matrix of **node features**
  - v: a node in V; $N(v)$: the set of neighbors of v.
  - **Node features:**
    - Social networks: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

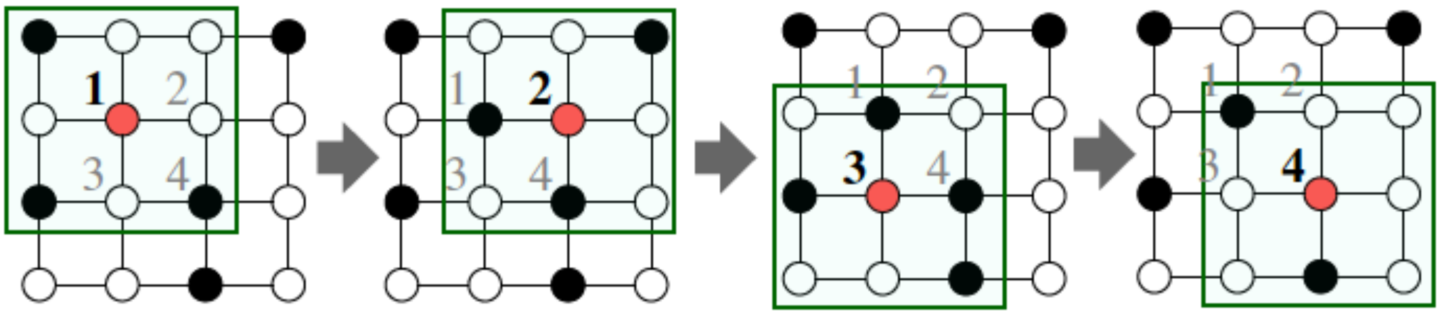


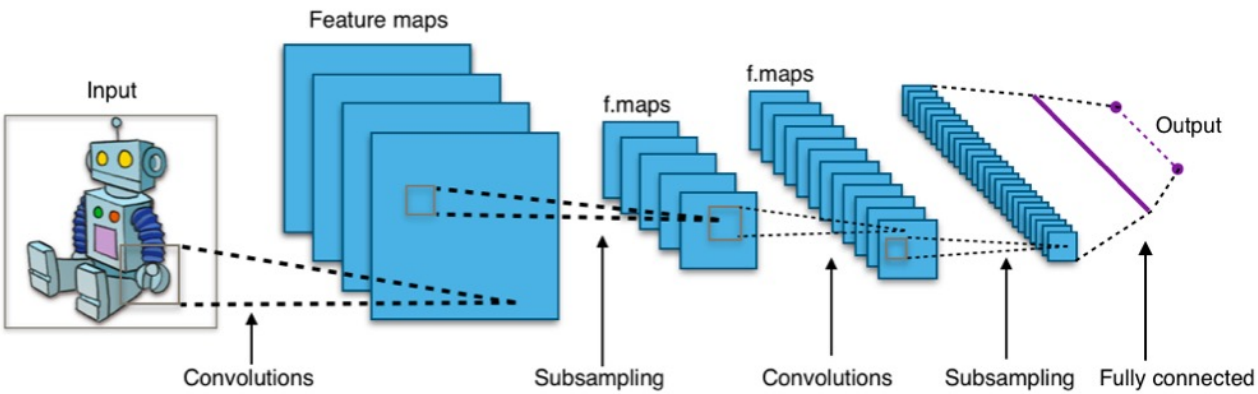
?

- 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:

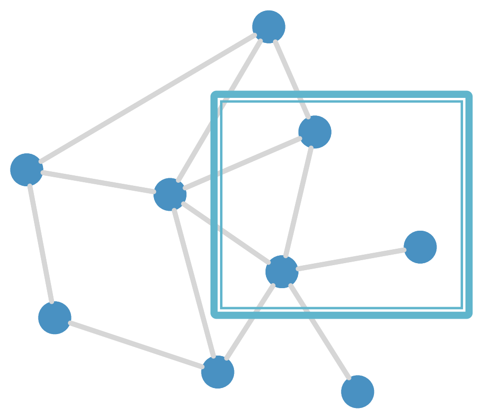




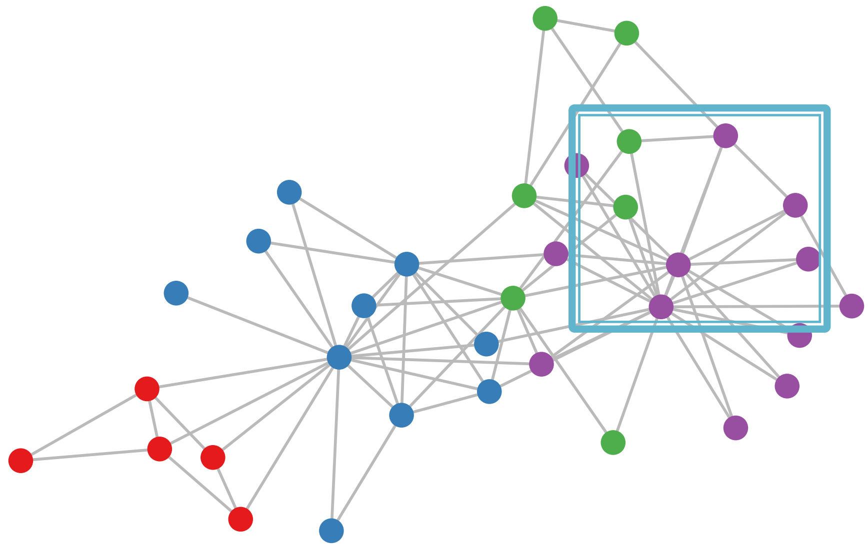
Goal is to generalize convolutions beyond simple lattices
Leverage node features/attributes (e.g., text, images)

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

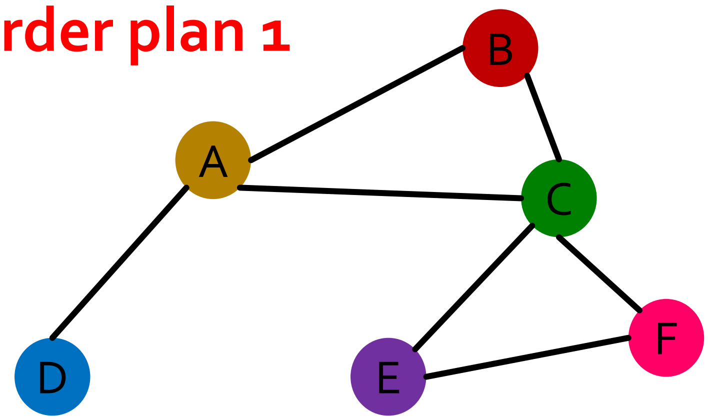
Permutation Invariance

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

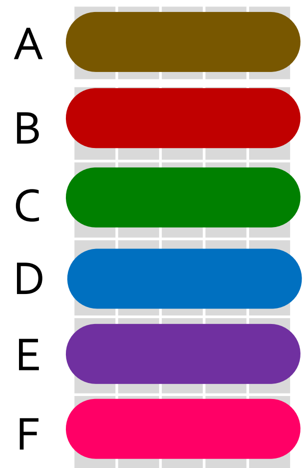
Permutation Invariance

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

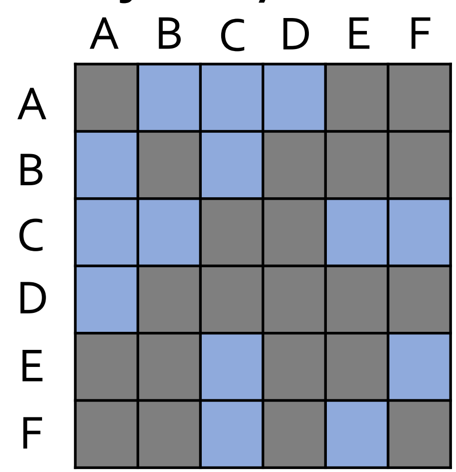
Order plan 1



Node features X_1



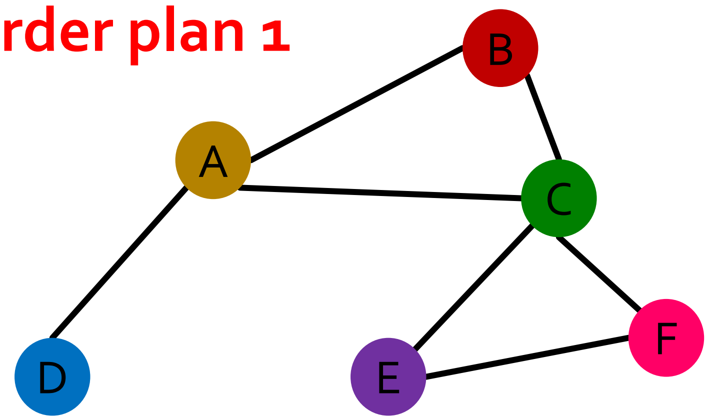
Adjacency matrix A_1



Permutation Invariance

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

Order plan 1



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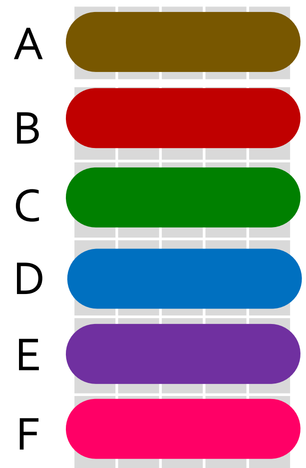

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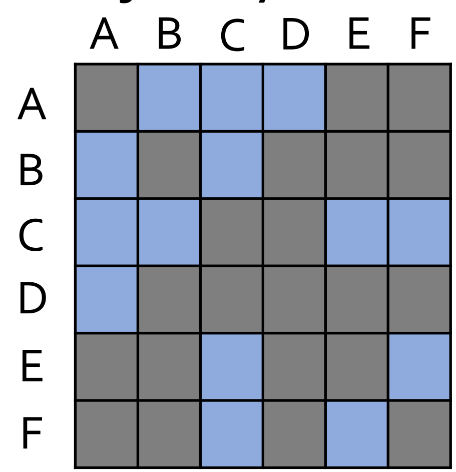
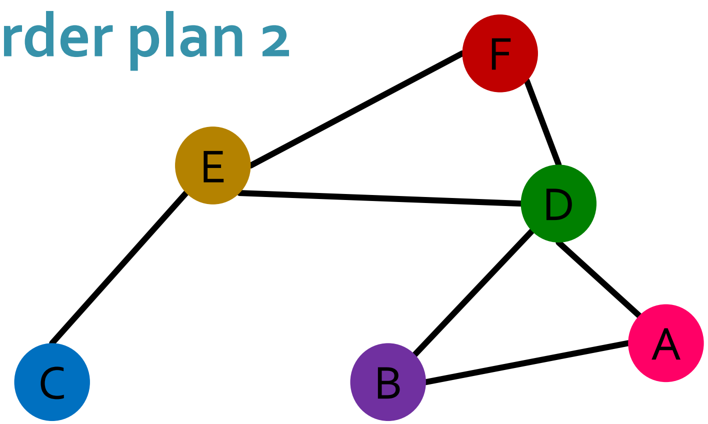
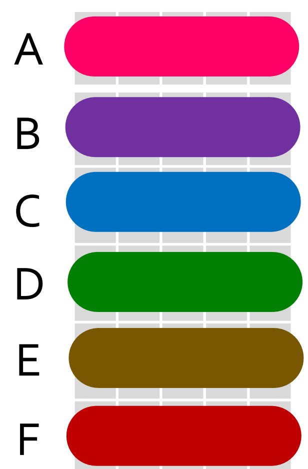


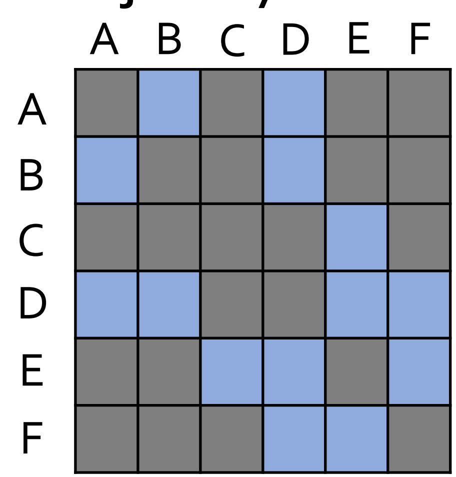
Order plan 2



Node features X_2



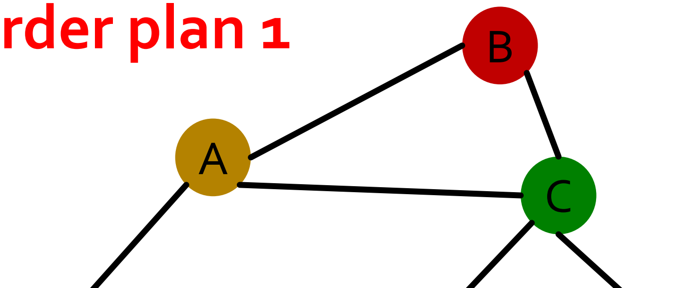
Adjacency matrix A_2

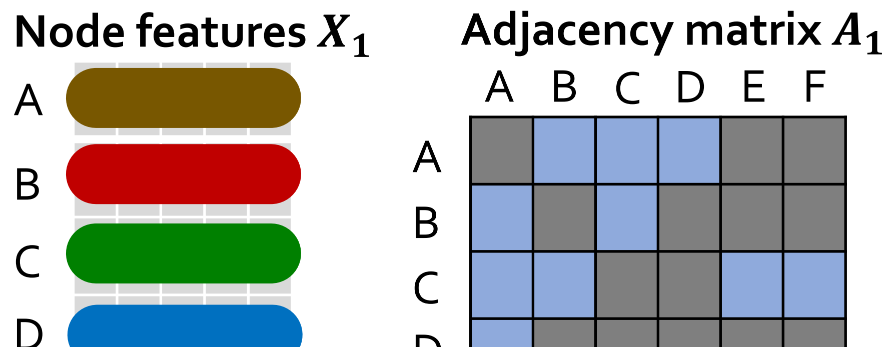


Permutation Invariance

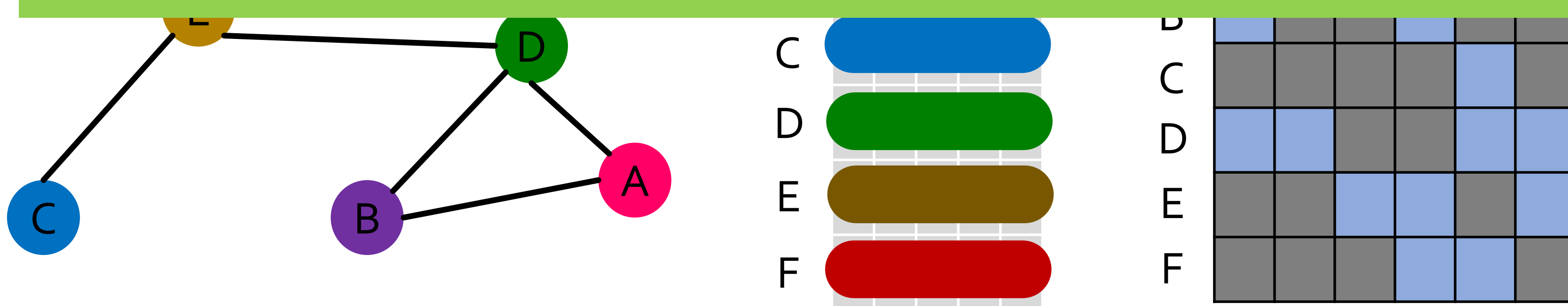
- **Graph does not have a canonical order of the nodes!**

Order plan 1





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



Permutation Invariance

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

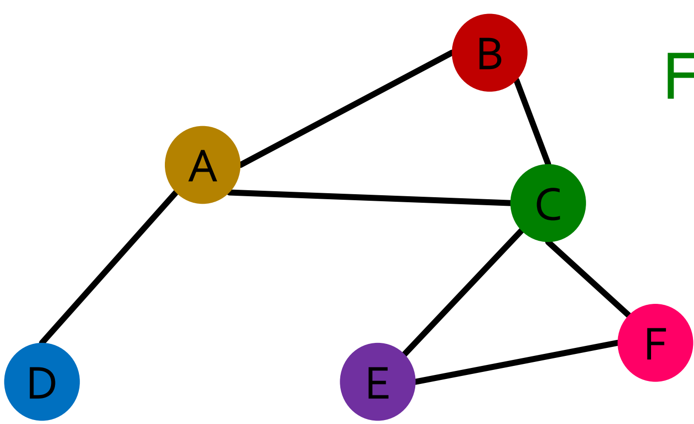
In other words, f maps a graph to a d-dim embedding

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

$$f(\boldsymbol{A}_1, \boldsymbol{X}_1) = f(\boldsymbol{A}_2, \boldsymbol{X}_2)$$

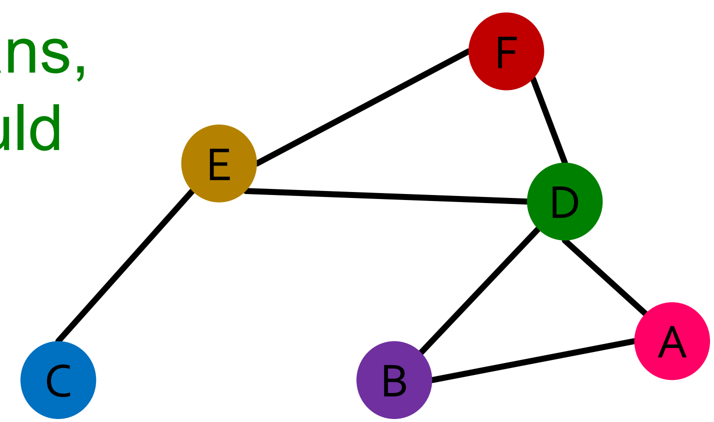
$\boldsymbol{A}$ is the adjacency matrix
$\boldsymbol{X}$ is the node feature matrix

Order plan 1: $\boldsymbol{A}_1, \boldsymbol{X}_1$



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

Order plan 2: $\boldsymbol{A}_2, \boldsymbol{X}_2$



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 $G = (\boldsymbol{A}, \boldsymbol{X})$ to a vector $\mathbb{R}^d$.

$\boldsymbol{A}$ is the adjacency matrix
$\boldsymbol{X}$ is the node feature matrix

- Then, if $f(\boldsymbol{A}_i, \boldsymbol{X}_i) = f(\boldsymbol{A}_j, \boldsymbol{X}_j)$ 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 $G = (A, X)$

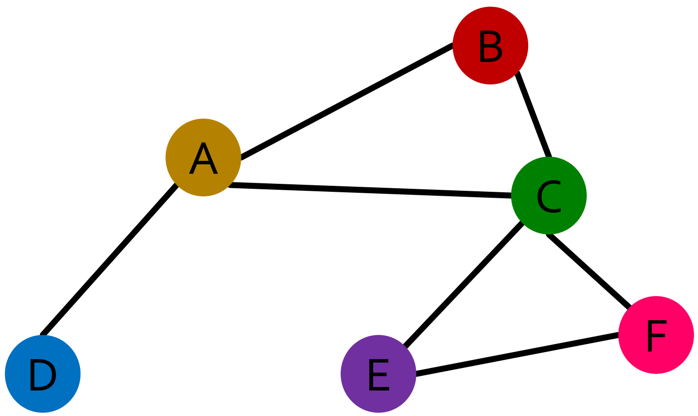
Permutation P: a shuffle of the node order
Example: (A,B,C)->(B,C,A)

Permutation Equivariance

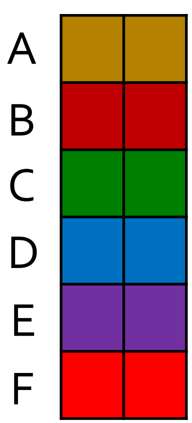
For node representation: We learn a function f that maps nodes of G to a matrix $\mathbb{R}^{|V|\times d}$.

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

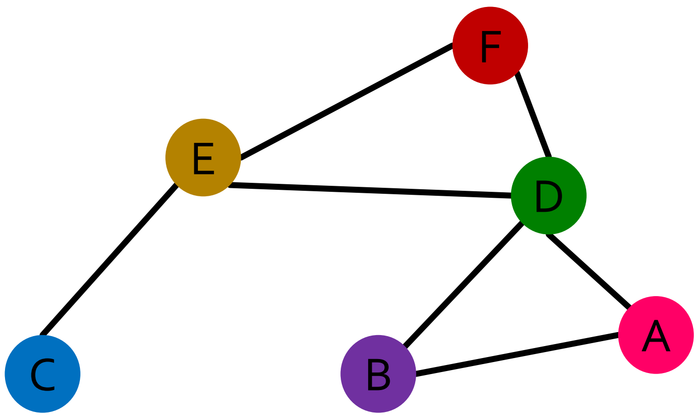
Order plan 1: A_1, X_1



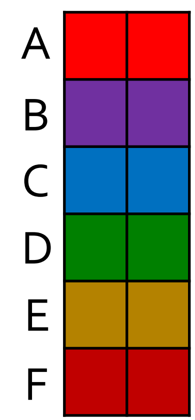
$f(\boldsymbol{A}_1, \boldsymbol{X}_1) =$



Order plan 2: A_2, X_2



$f(\boldsymbol{A}_2, \boldsymbol{X}_2) =$



Permutation Equivariance

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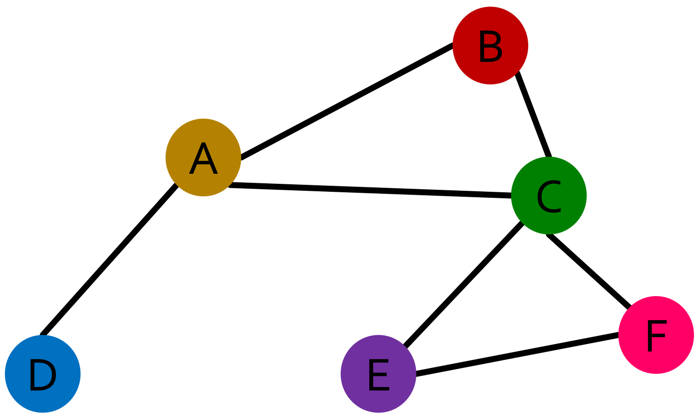
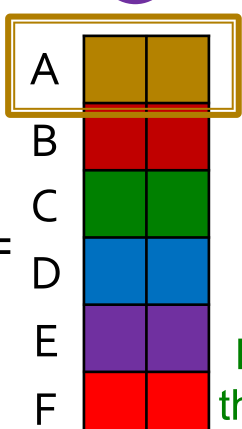
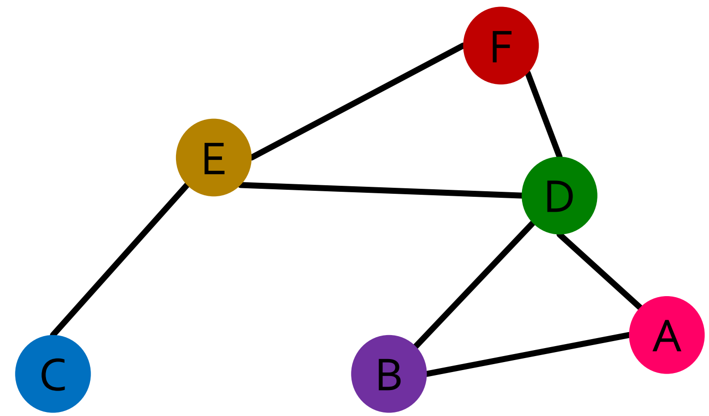


Representation vector of the brown node A

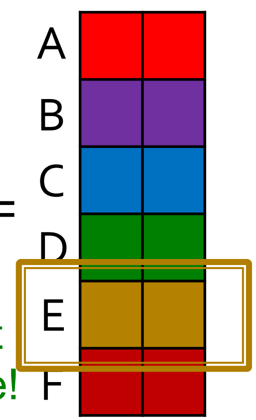
$$f(\boldsymbol{A}_1, \boldsymbol{X}_1) =$$



Order plan 2: A_2, X_2



$$f(\boldsymbol{A}_2, \boldsymbol{X}_2) =$$



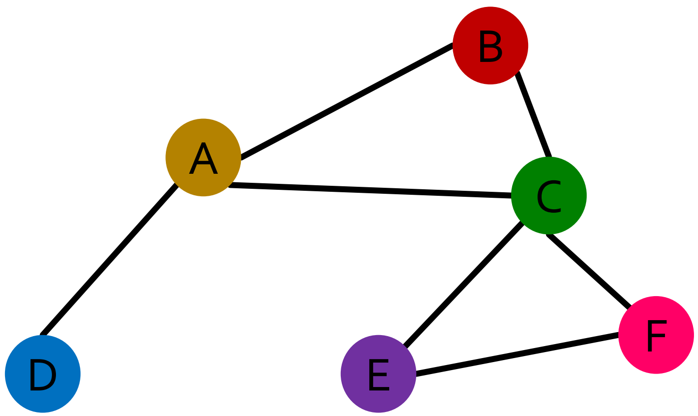
Representation vector of the brown node E

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

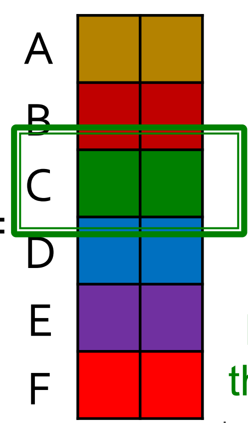
Permutation Equivariance

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

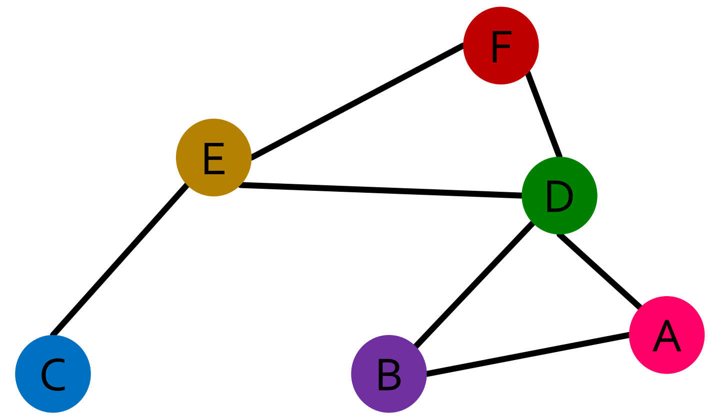


$$f(\boldsymbol{A}_1, \boldsymbol{X}_1) =$$

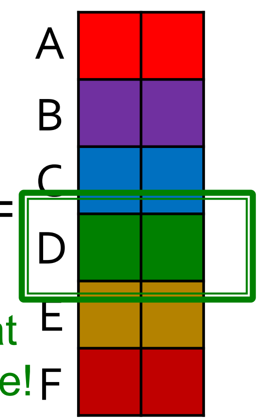


Representation vector of the green node C

Order plan 2: A_2, X_2



$$f(\boldsymbol{A}_2, \boldsymbol{X}_2) =$$



Representation vector of the green node D

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

Permutation Equivariance

For node representation:

- Consider we learn a function f that maps a graph $G = (\boldsymbol{A}, \boldsymbol{X})$ 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**.

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

- **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.

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**

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

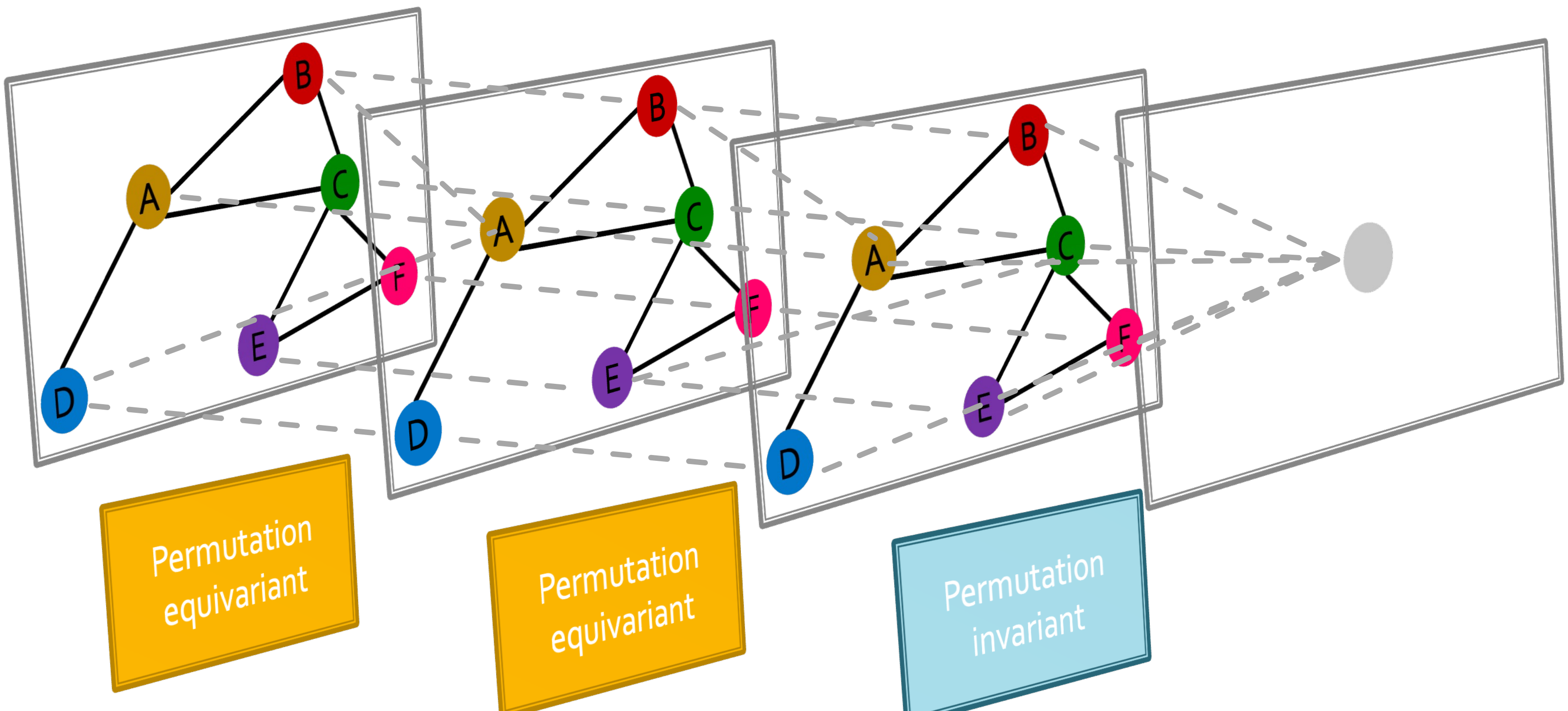
Permute the input, output also permutes accordingly.
(map a graph to a matrix)

- **Examples:**
  - $f(A, X) = 1^T X$: Permutation-**invariant**
    - Reason: $f(PAP^T, PX) = 1^T PX = 1^T X = f(A, X)$
  - $f(A, X) = X$: Permutation-**equivariant**
    - Reason: $f(PAP^T, PX) = PX = Pf(A, X)$
  - $f(A, X) = AX$: Permutation-**equivariant**
    - Reason: $f(PAP^T, PX) = PAP^T PX = PAX = Pf(A, X)$

[Bronstein, ICLR 2021 keynote]

Graph Neural Network Overview

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

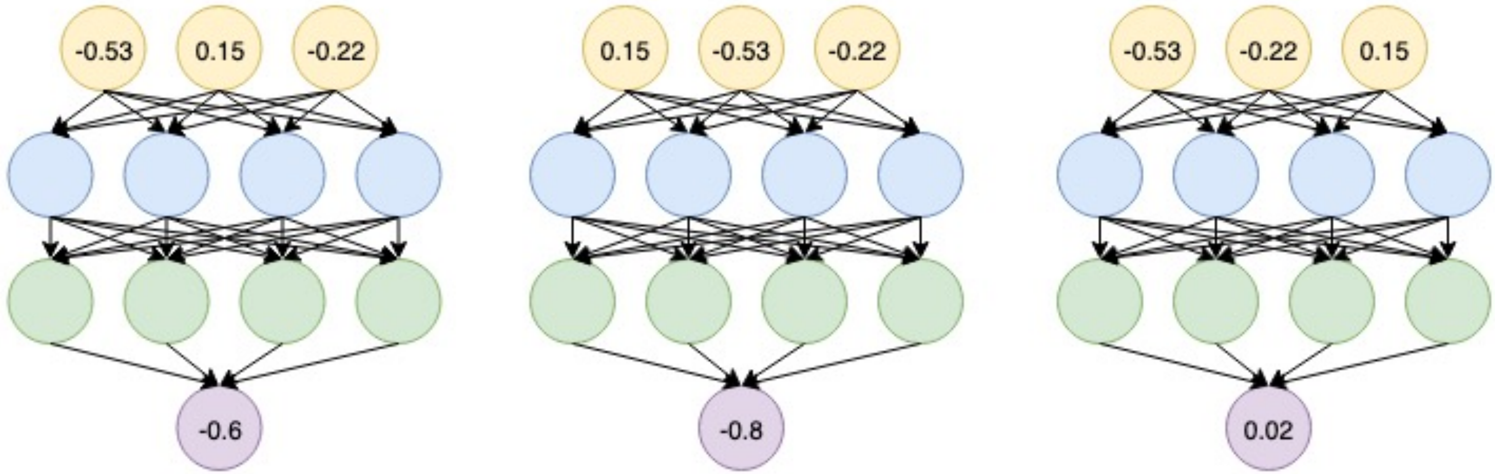


Graph Neural Network Overview

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?

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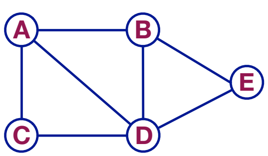

	A	B	C	D	E	Feat	
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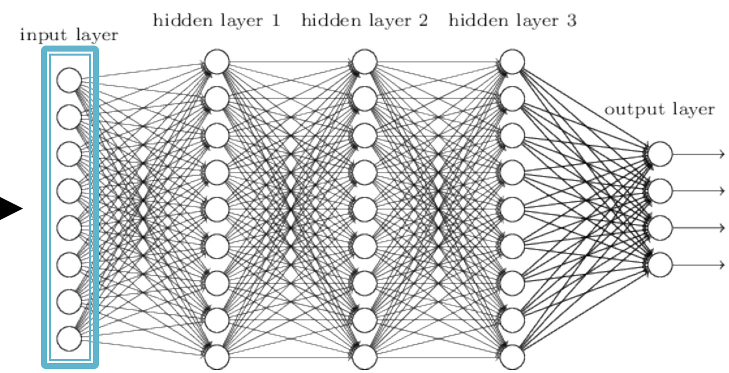

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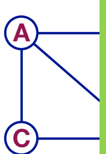
This explains why **the naïve MLP approach fails for graphs**!

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!

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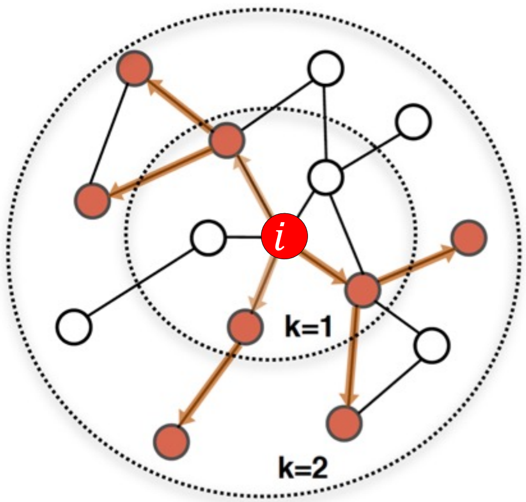
Outline of Today's Lecture

1. Basics of deep learning ✓
2. Deep learning for graphs ✓
3. **Graph Convolutional Networks**
4. GNNs subsume CNNs

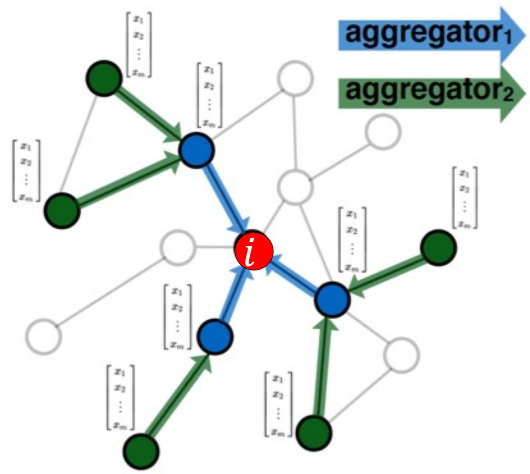
[Kipf and Welling, ICLR 2017]

Graph Convolutional Networks

Idea: Node's neighborhood defines a computation graph



Determine node computation graph

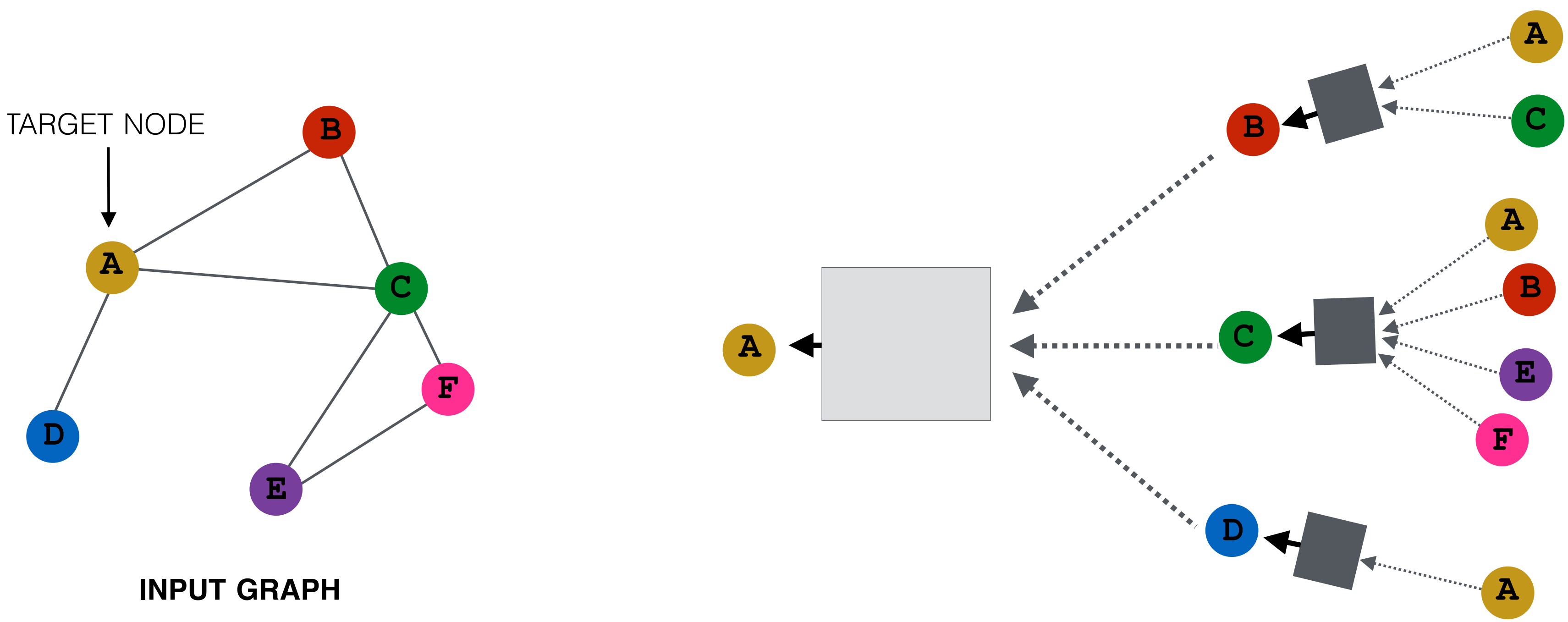


Propagate and transform information

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

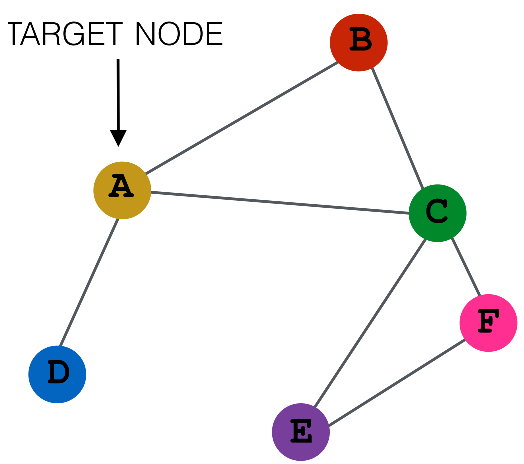
Idea: Aggregate Neighbors

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

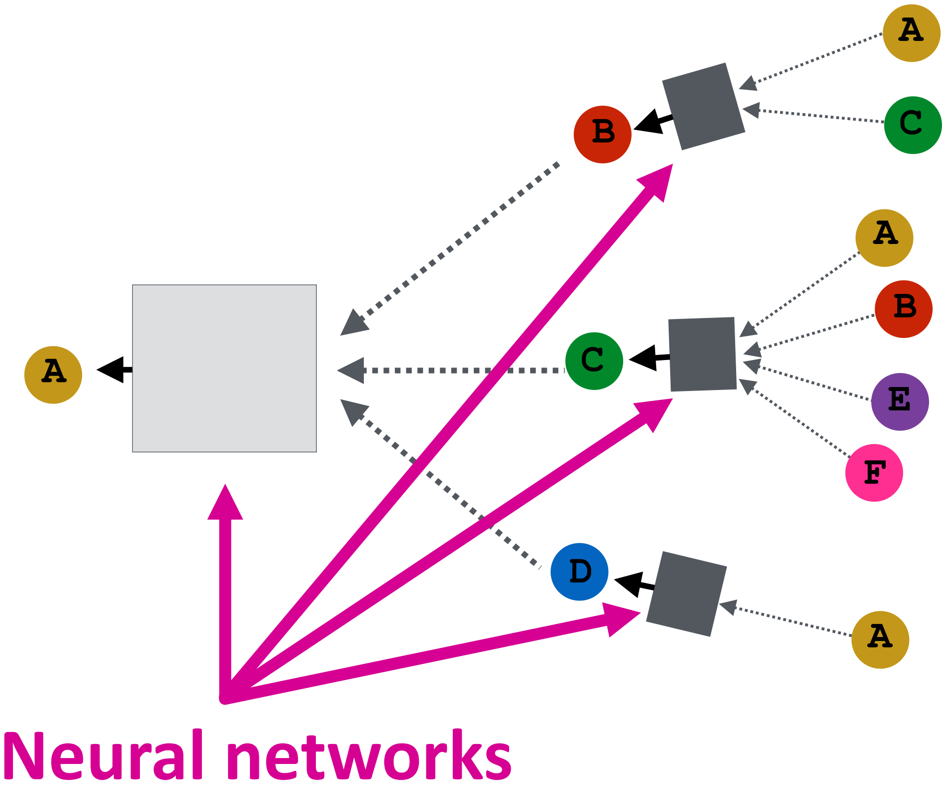


Idea: Aggregate Neighbors

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

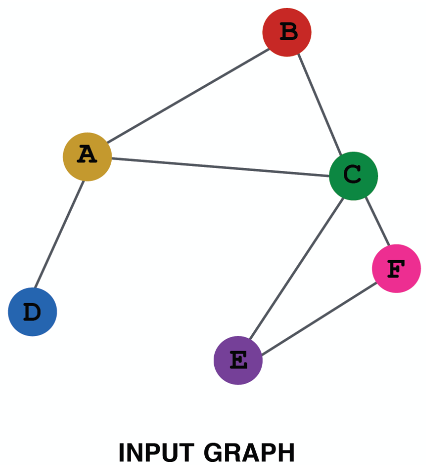


INPUT GRAPH

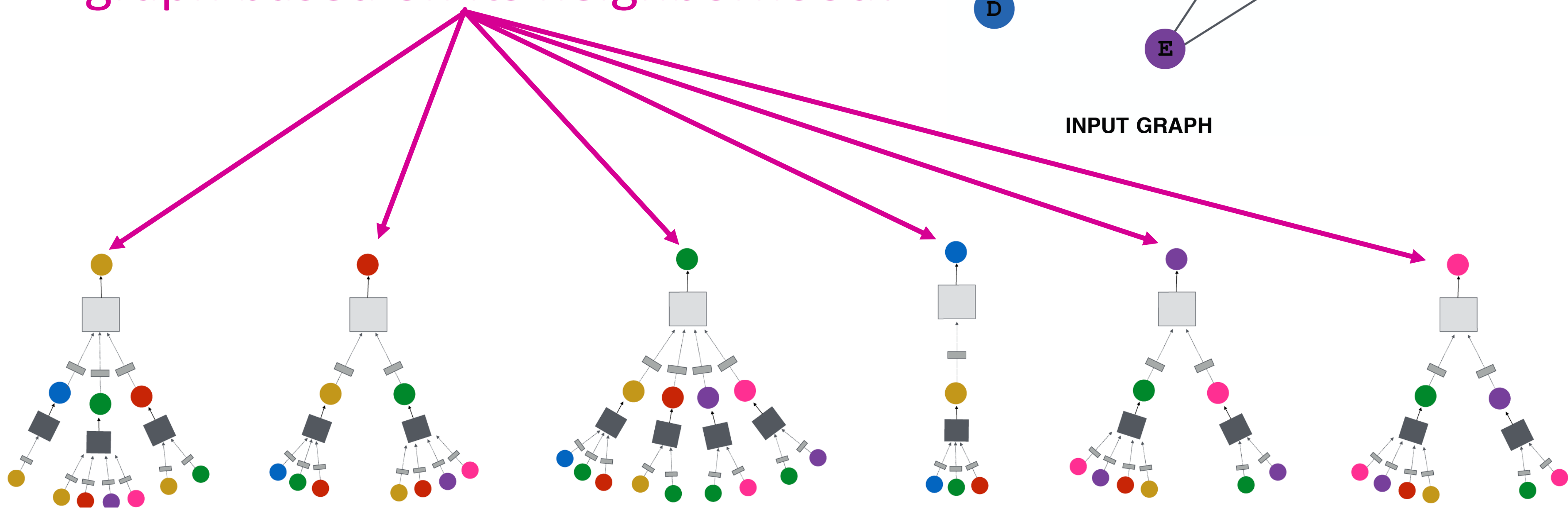


Idea: Aggregate Neighbors

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

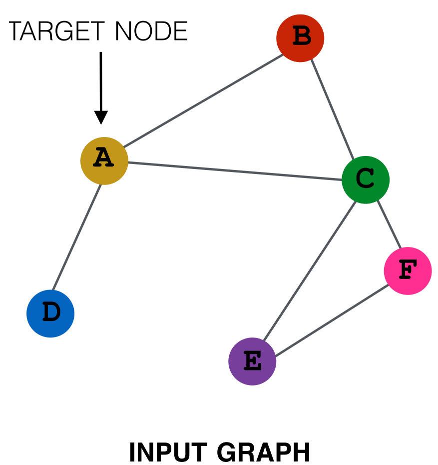


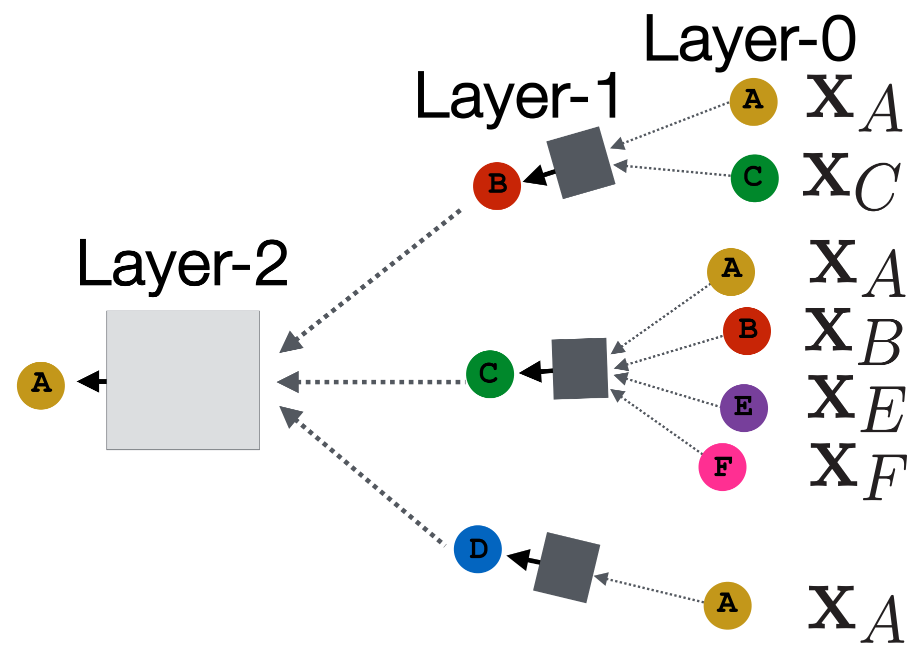
Every node defines a computation graph based on its neighborhood!



Deep Model: Many Layers

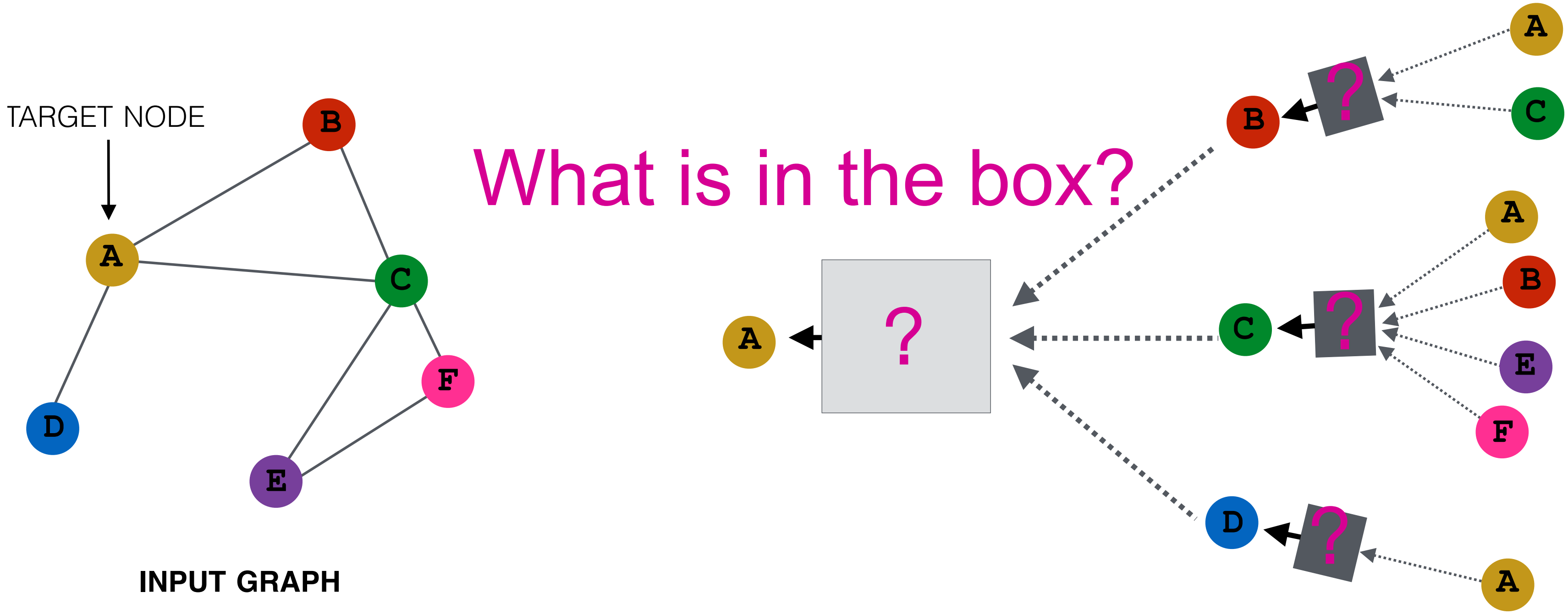
- Model can be of arbitrary depth:
  - Nodes have embeddings at each layer
  - Layer-0 embedding of node v is its input feature, x_v
  - Layer-k embedding gets information from nodes that are k hops away





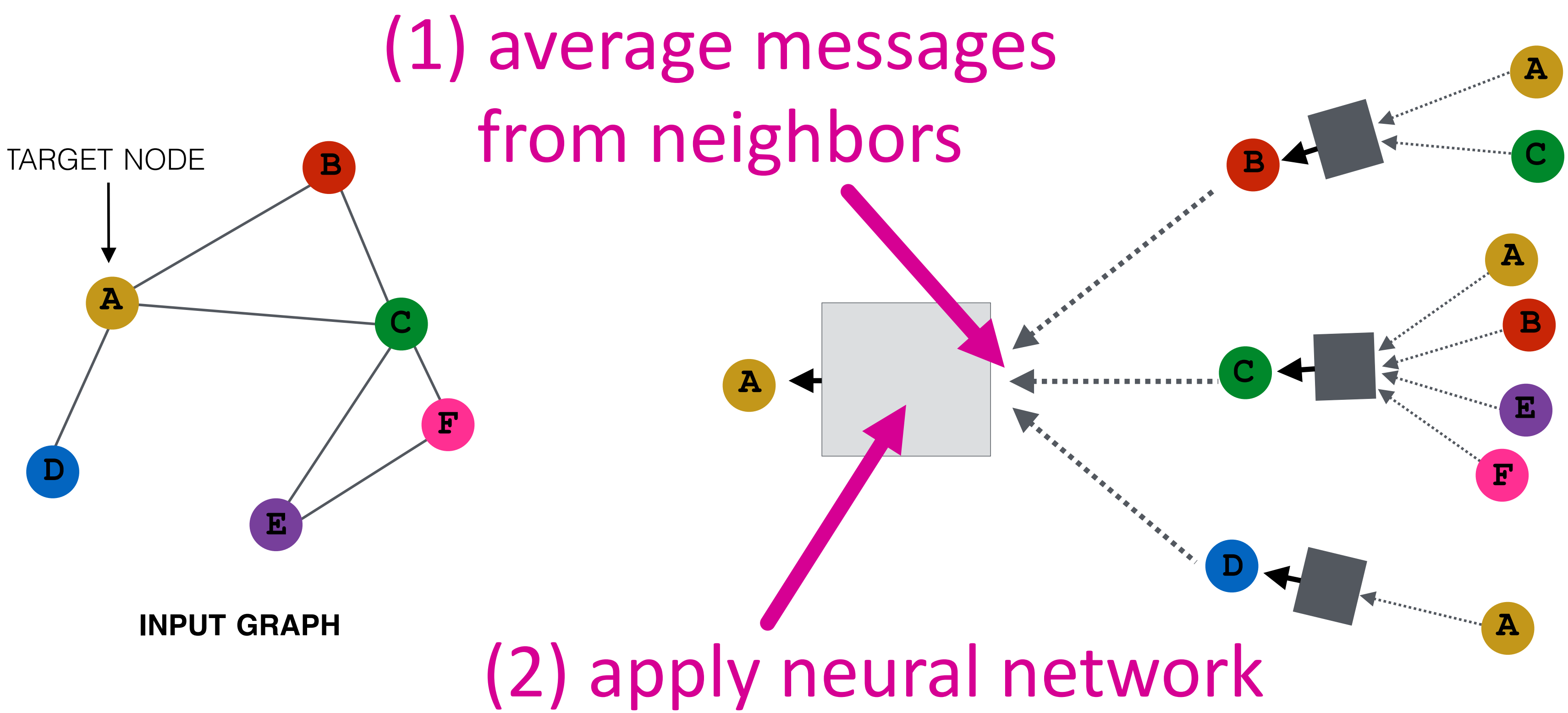
Neighborhood Aggregation

- **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

Initial 0-th layer embeddings are equal to node features

$$\boxed{\mathrm{h}_v^0 = \mathrm{x}_v}$$

embedding of v at layer k

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

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

Total number of layers

Average of neighbor's previous layer embeddings

Embedding after K layers of neighborhood aggregation

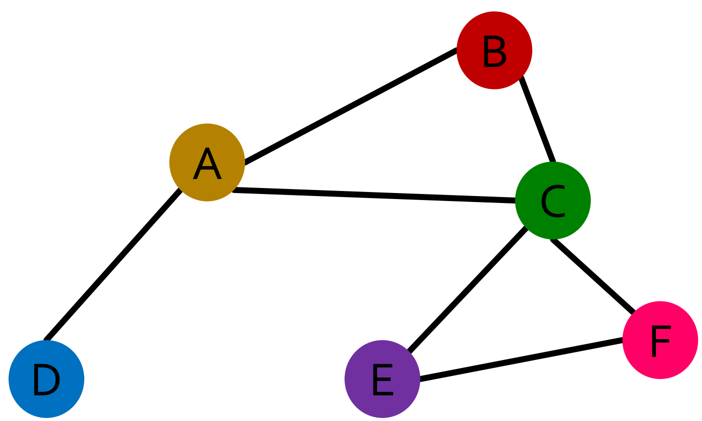
Non-linearity (e.g., ReLU)

Notice summation is a permutation invariant pooling/aggregation.

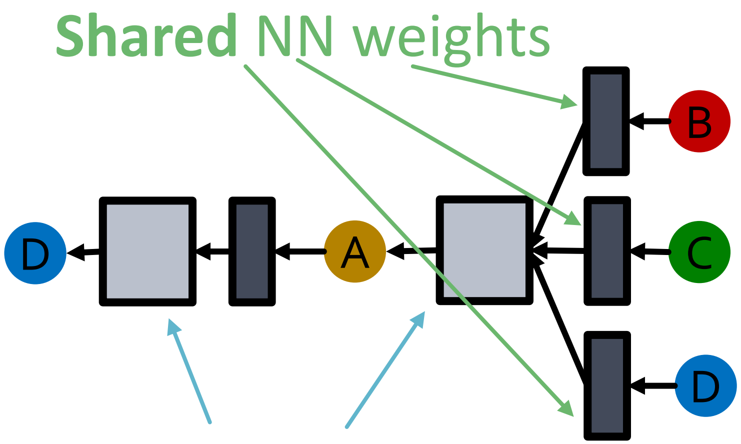
GCN: Invariance and Equivariance

What are the invariance and equivariance properties for a GCN?

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



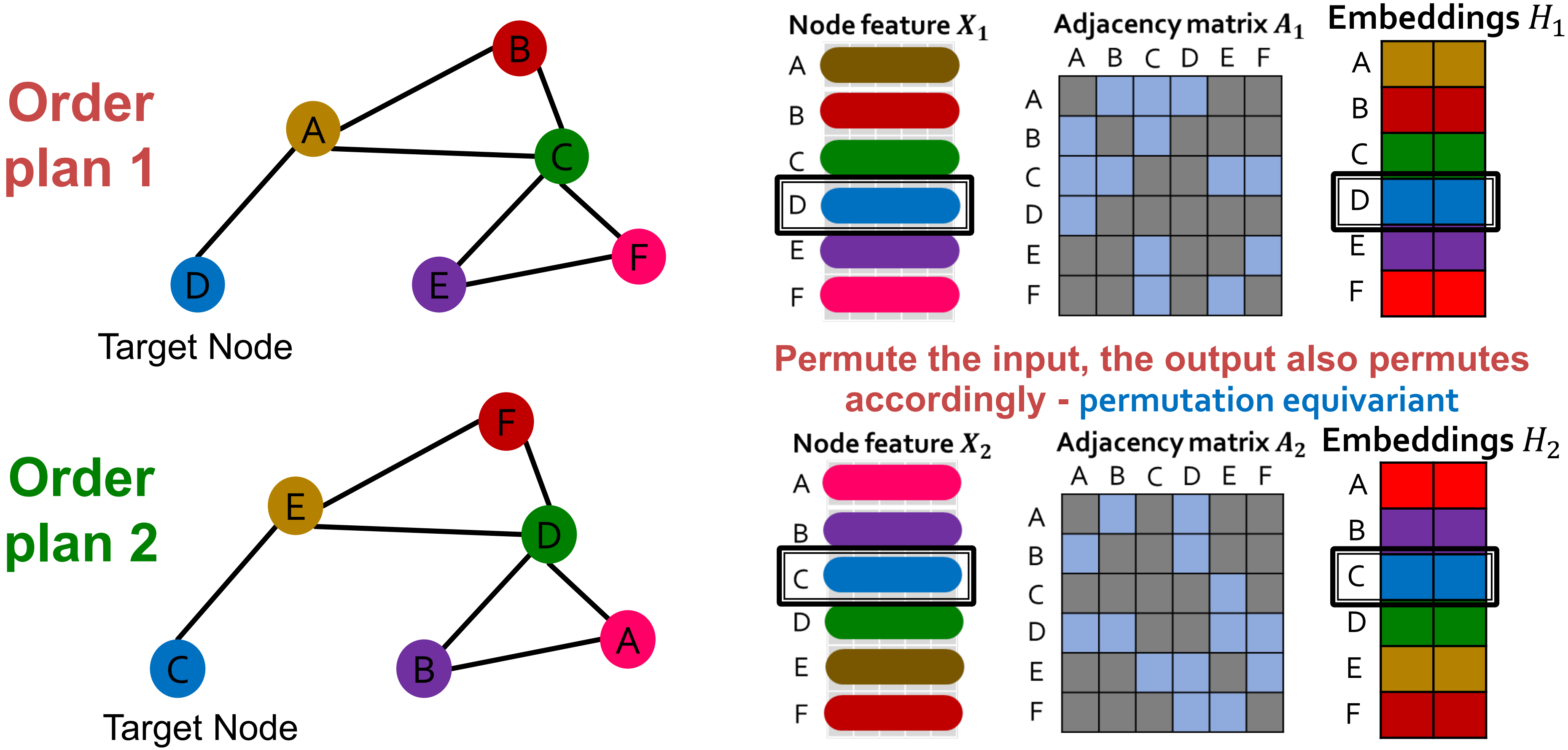
Target Node



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

GCN: Invariance and Equivariance

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



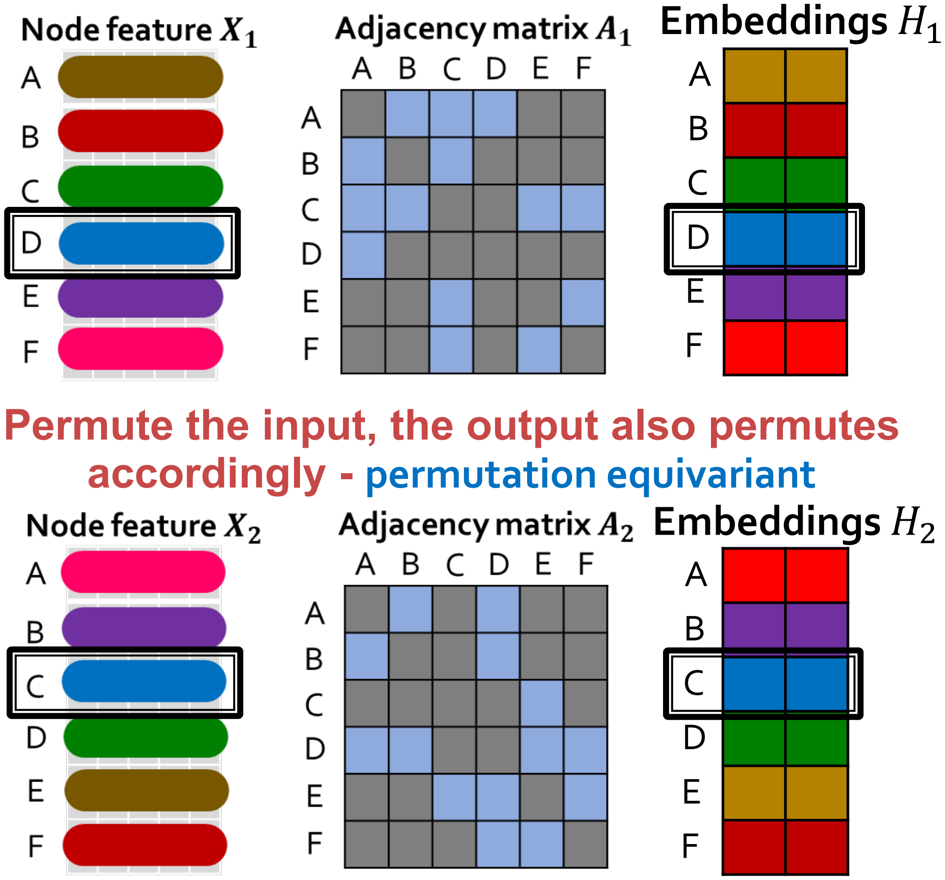
GCN: Invariance and Equivariance

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

Detailed reasoning:

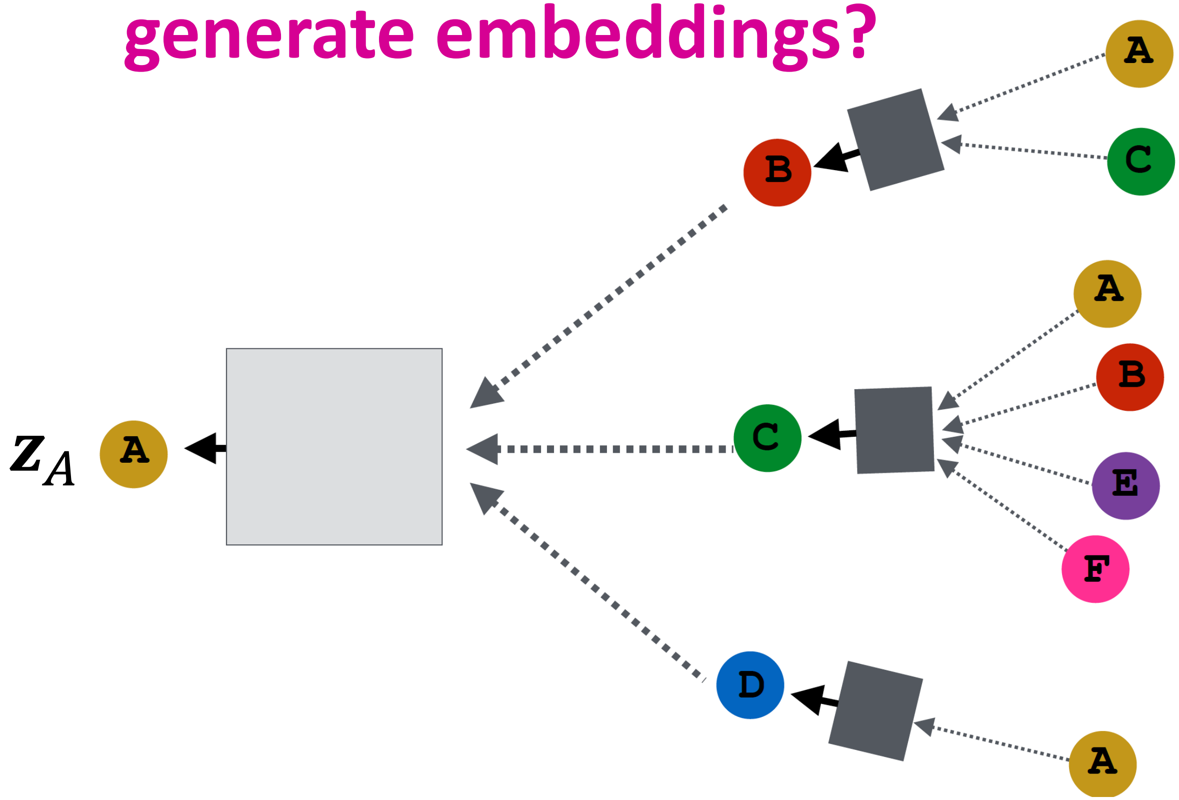
1. The rows of **input node features** and **output embeddings** are **aligned**
2. We know computing the embedding of **a given node** with GCN is **invariant.**
3. So, after permutation, the **location** of **a given node** in the **input node feature** matrix is changed, and the **the output embedding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

This is permutation equivariant



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)

$$h_v^{(0)} = x_v$$

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

$$z_v = h_v^{(K)}$$

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

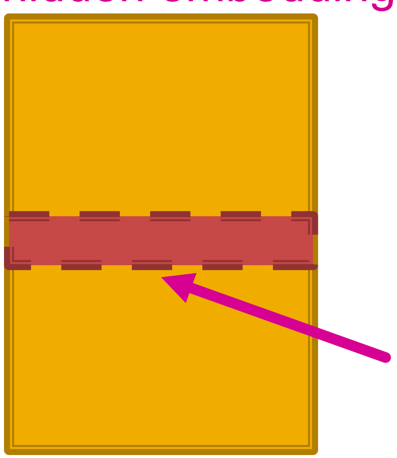
- W_k: weight matrix for neighborhood aggregation
- B_k: weight matrix for transforming hidden vector of self

Matrix Formulation (1)

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

$$\boxed{\sum_{u \in N(v)} \frac{h_u^{(k-1)}}{|N(v)|}} \Rightarrow H^{(k+1)} = D^{-1}AH^{(k)}$$

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



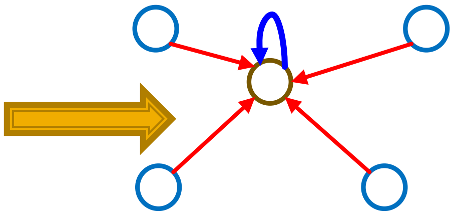
$\boldsymbol{h}_i^{(k-1)}$

Matrix Formulation (2)

- Re-writing update function in matrix form:

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

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

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

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

Unsupervised Training

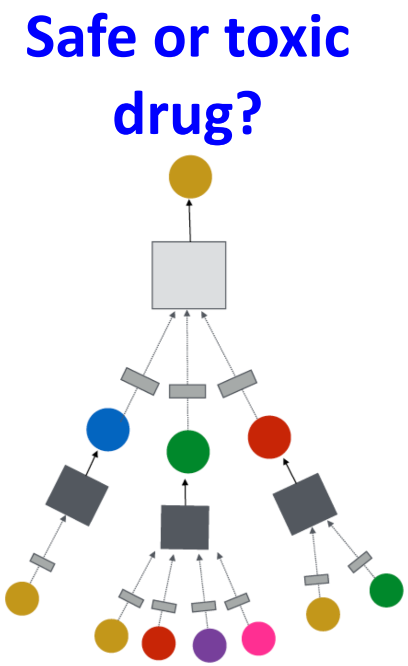
- **One possible idea: "Similar" nodes have similar embeddings:**

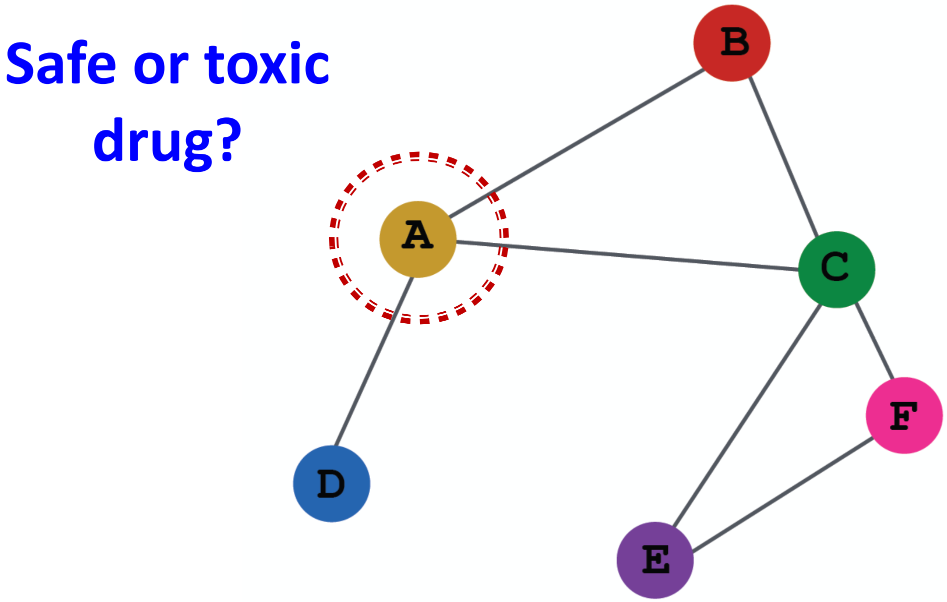
$$\min_{\Theta} \mathcal{L} = \sum_{z_u, z_v} \mathrm{CE}(y_{u,v}, \mathrm{DEC}(z_u, z_v))$$

  - where $y_{u,v} = 1$ when node u and v are **similar**
  - $z_u = f_\Theta(u)$ and $\mathrm{DEC}(\cdot,\cdot)$ is the dot product
- CE is the cross entropy loss:
  - $\mathrm{CE}\big(\boldsymbol{y}, f(\boldsymbol{x})\big) = -\sum_{i=1}^{C}(y_i \log f_\Theta(x)_i)$
    - 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**)





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)

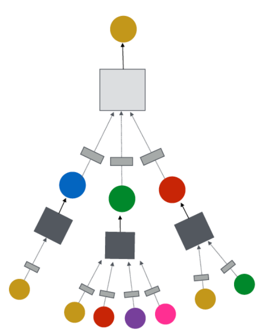
$$\mathcal{L} = -\sum_{v \in V} y_v \log(\sigma(\mathrm{z}_v^{\mathrm{T}}\theta)) + (1 - y_v)\log(1 - \sigma(\mathrm{z}_v^{\mathrm{T}}\theta))$$

Encoder output: node embedding

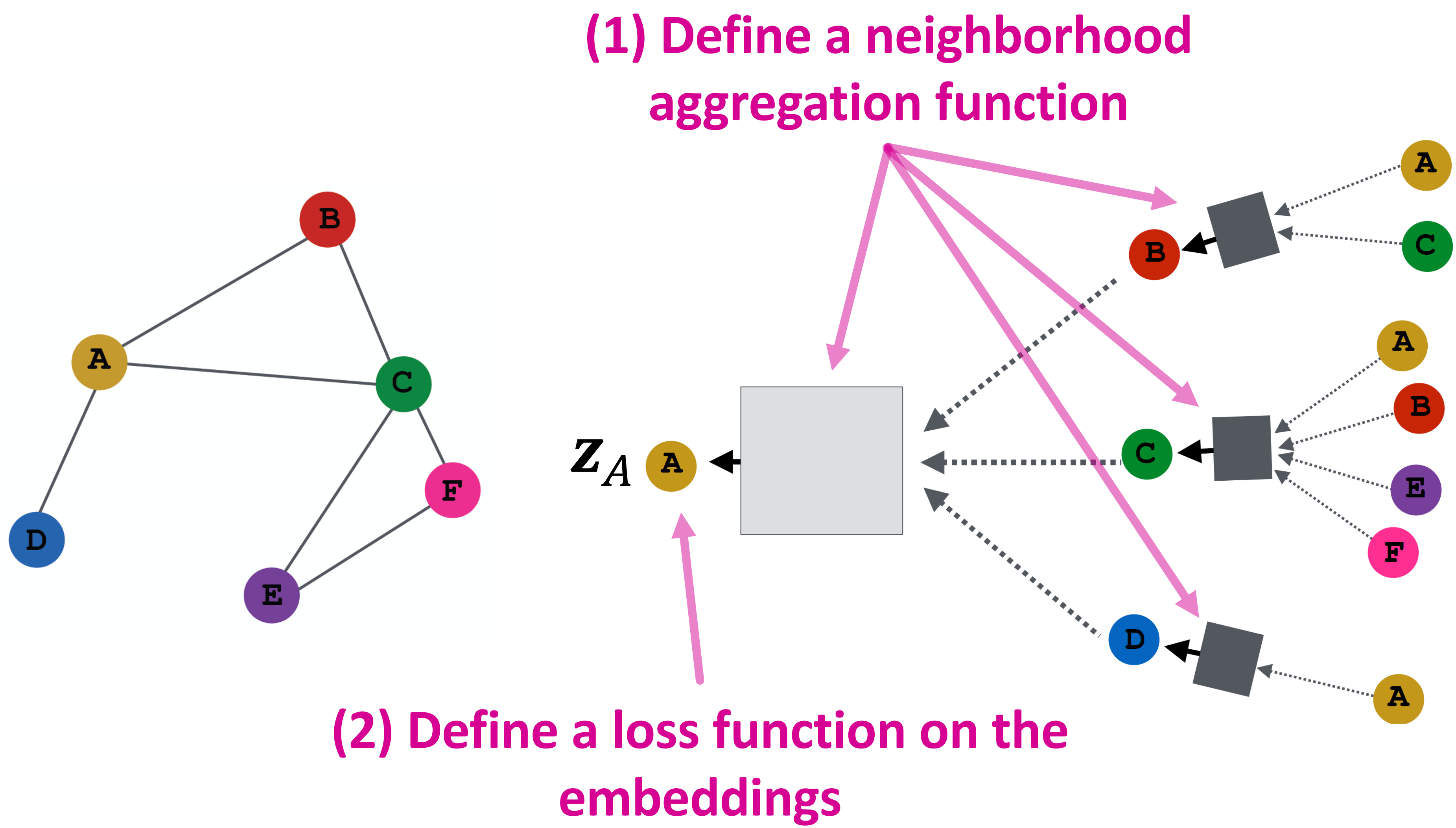
Classification weights

Node class label

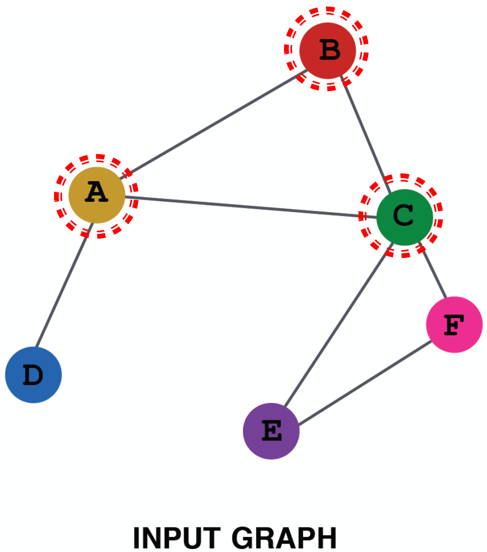
Safe or toxic drug?



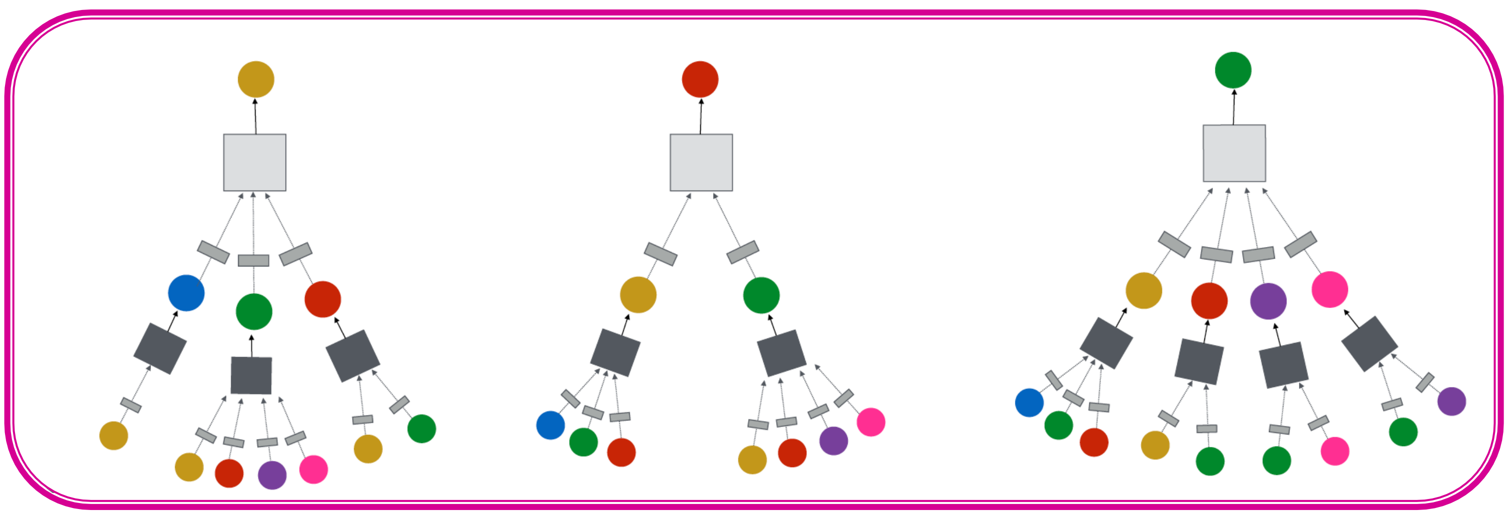
Model Design: Overview



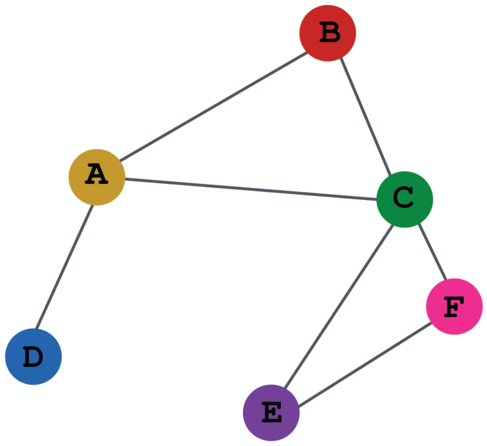
Model Design: Overview



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



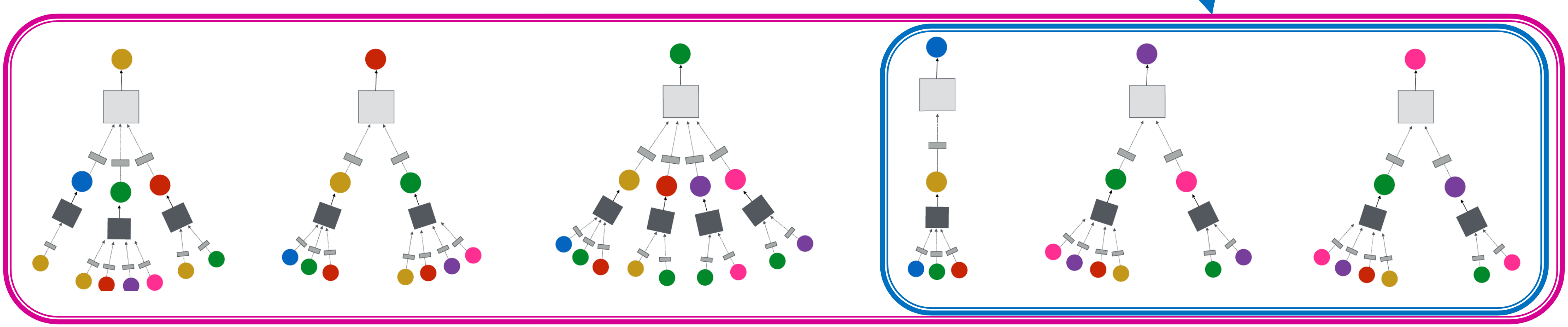
Model Design: Overview



INPUT GRAPH

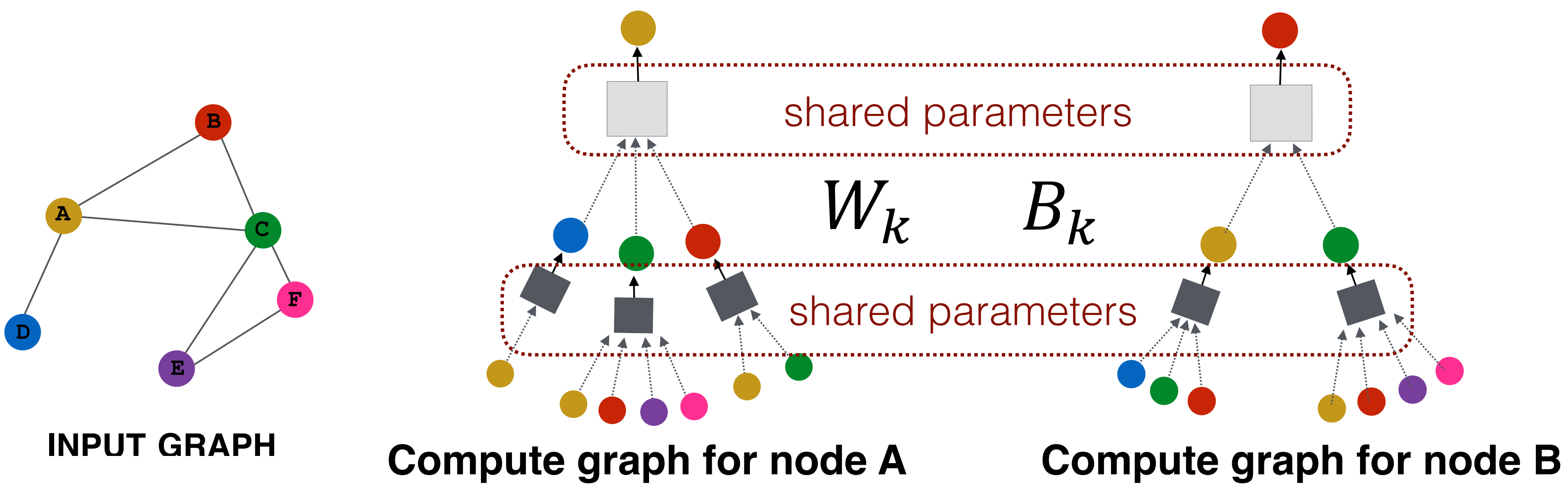
(4) Generate embeddings for nodes as needed

Even for nodes we never trained on!

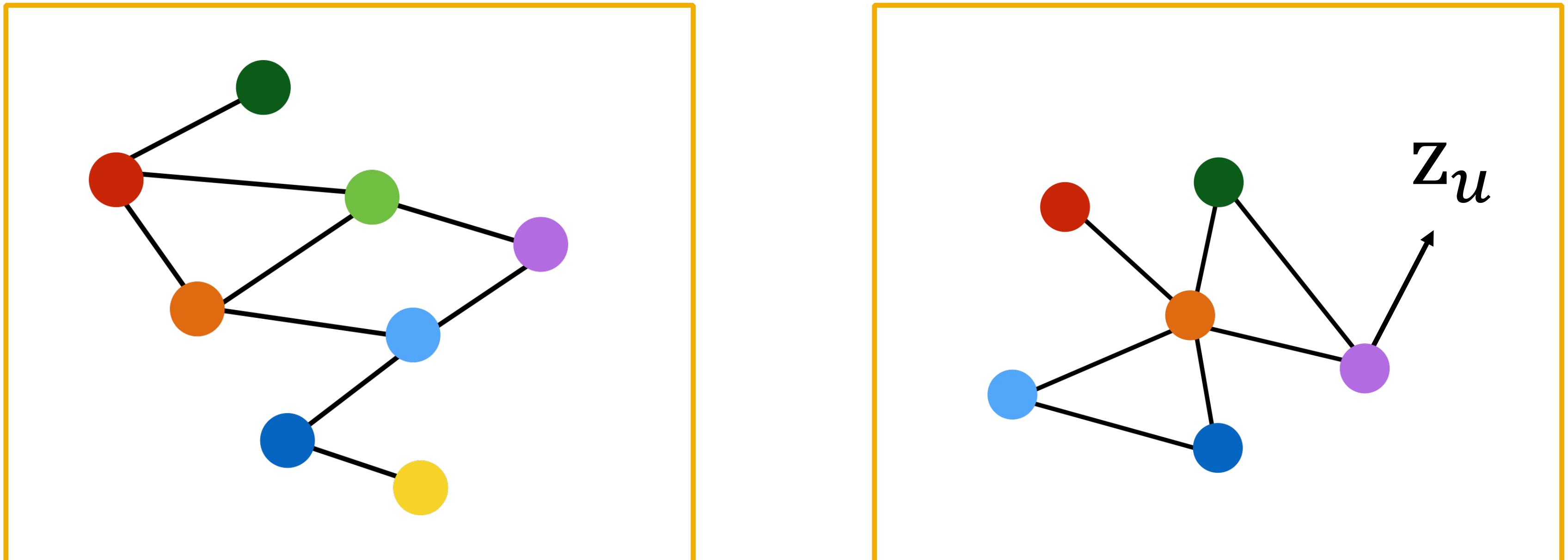


Inductive Capability

- **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**!



Inductive Capability: New Graphs

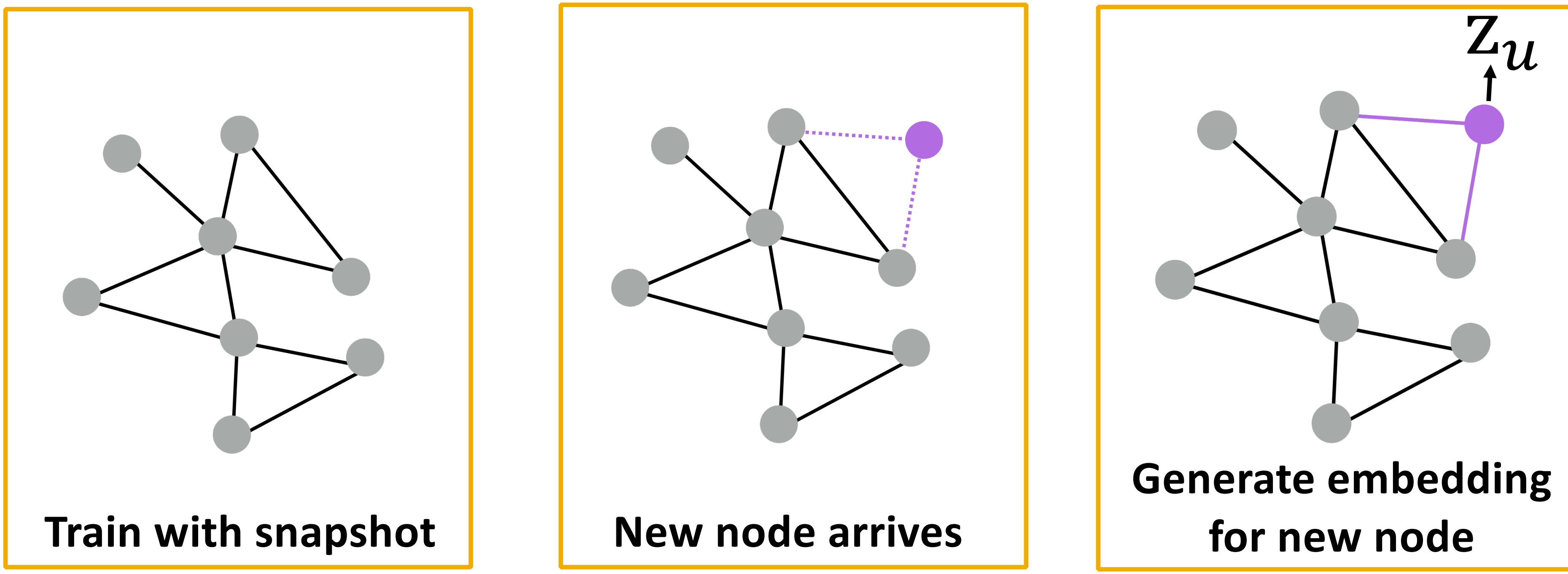


Train on one graph **Generalize to new graph**

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

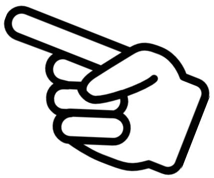
Inductive Capability: New Nodes



- 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**

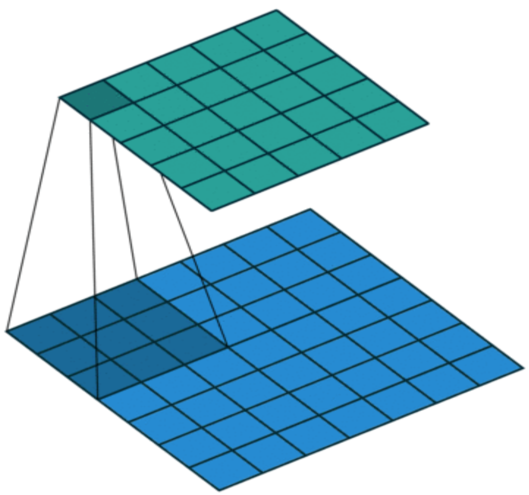


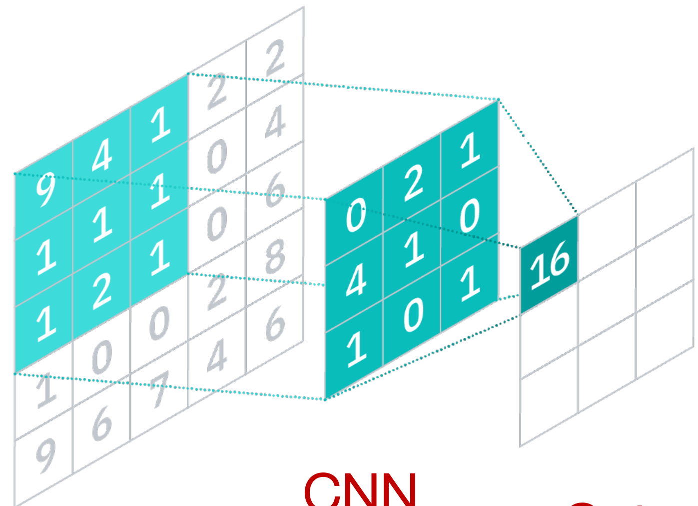
Architecture Comparison

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

Convolutional Neural Network

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



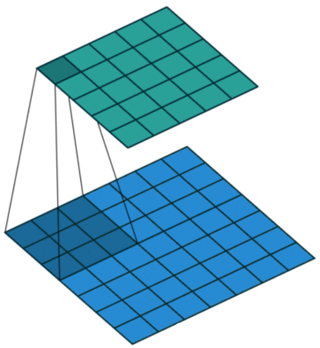


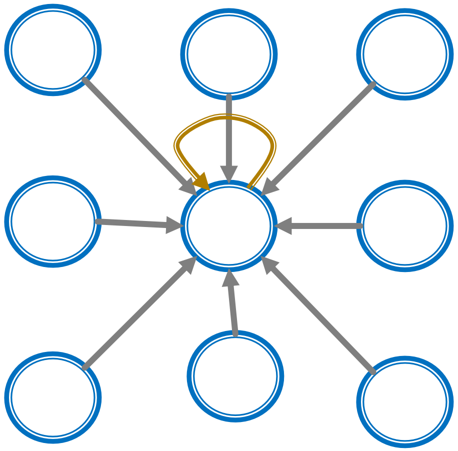
CNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma\left(\sum_{u \in \mathrm{N}(v) \cup \{v\}} \mathrm{W}_l^u \mathrm{h}_u^{(l)}\right), \quad \forall l \in \{0, \dots, L-1\}$

$\boxed{N(v) \text{ represents the 8 neighbor pixels of } v.}$

GNN vs. CNN

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



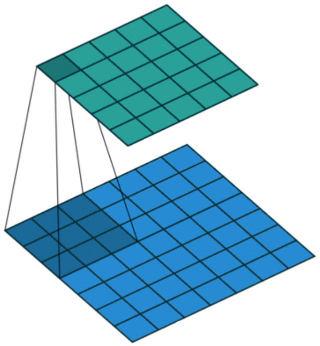


- GNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in \mathrm{N}(v)} \frac{\mathrm{h}_u^{(l)}}{|\mathrm{N}(v)|} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$
- CNN formulation: (previous slide) $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v) \cup \{v\}} \mathrm{W}_l^u \mathrm{h}_u^{(l)}), \forall l \in \{0, \dots, L-1\}$

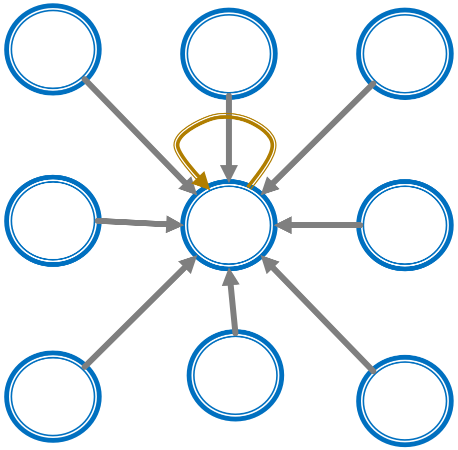
  if we rewrite: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v)} \mathbf{W}_l^u \mathrm{h}_u^{(l)} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

GNN vs. CNN

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



Image



Graph

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

CNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v)} \mathbf{W}_l^u \mathrm{h}_u^{(l)} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

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), …, (1, 1)}

GNN vs. CNN

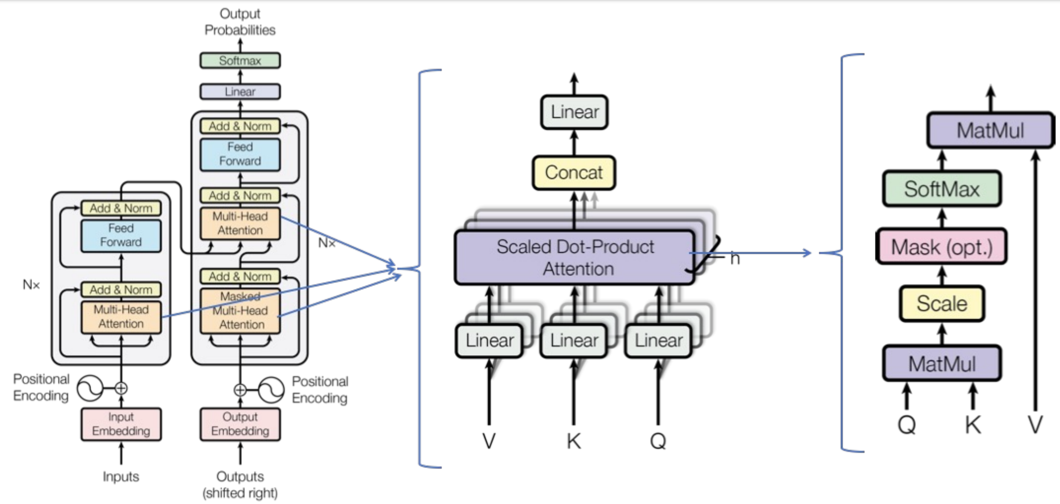
Convolutional neural network (CNN) layer with 3x3 filter:

- **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), …, (1, 1)}

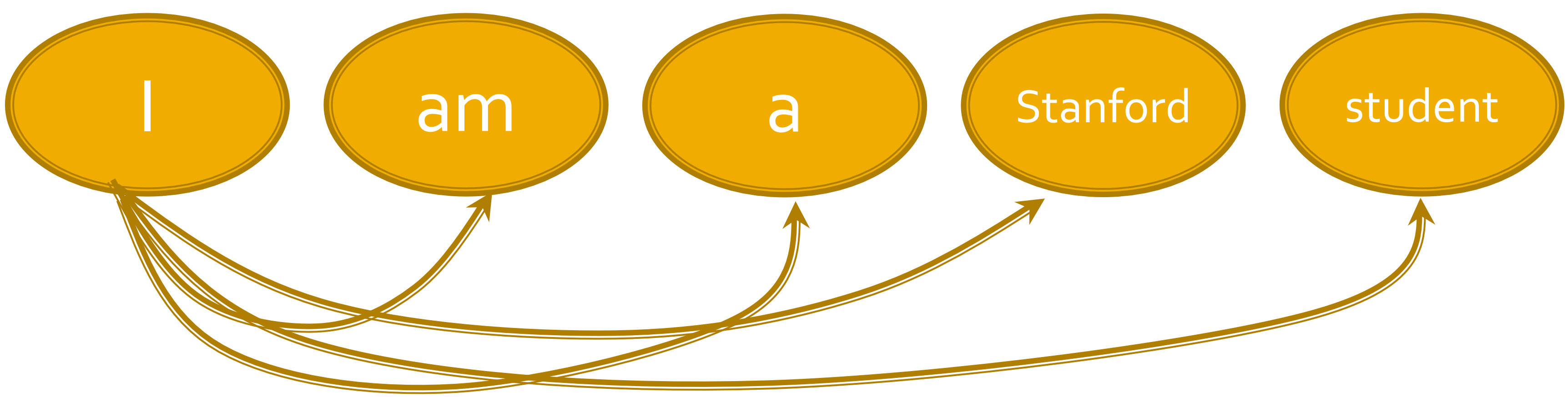
Transformer

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.

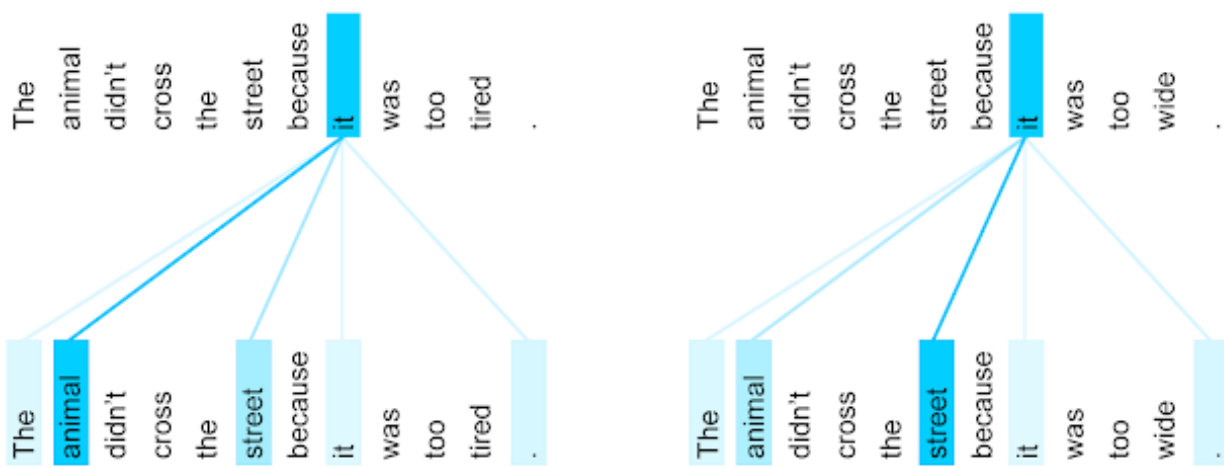


Transformer

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).

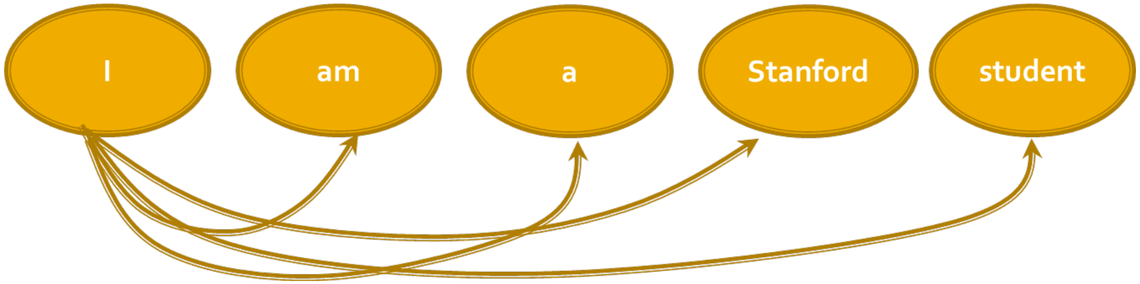


A nice blog plot for this: https://towardsdatascience.com/transformers-are-graph-neural-networks-bca9f75412aa

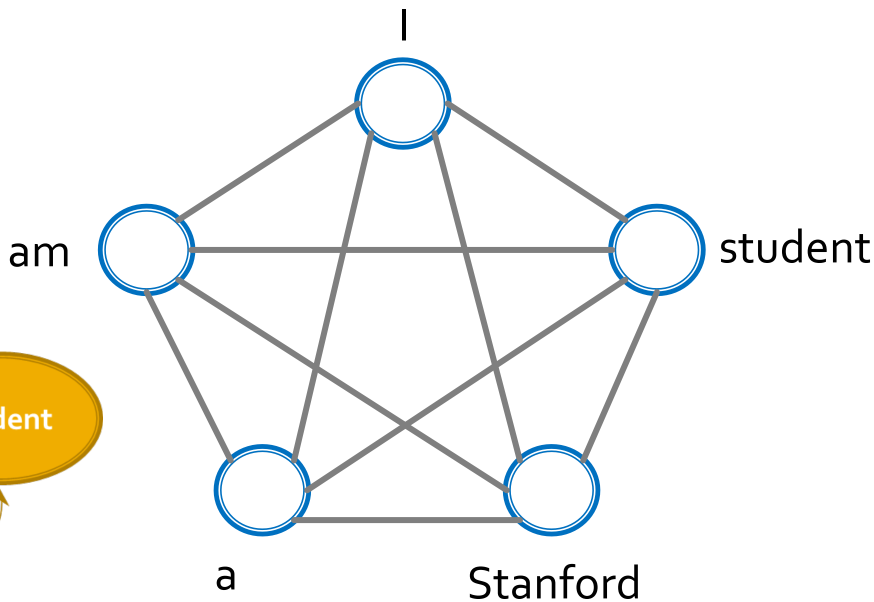
GNN vs. Transformer

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**.



Text



(Complete) 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