Stanford CS224W: Graph Neural Networks

CS224W: Machine Learning with Graphs
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http://cs224w.stanford.edu

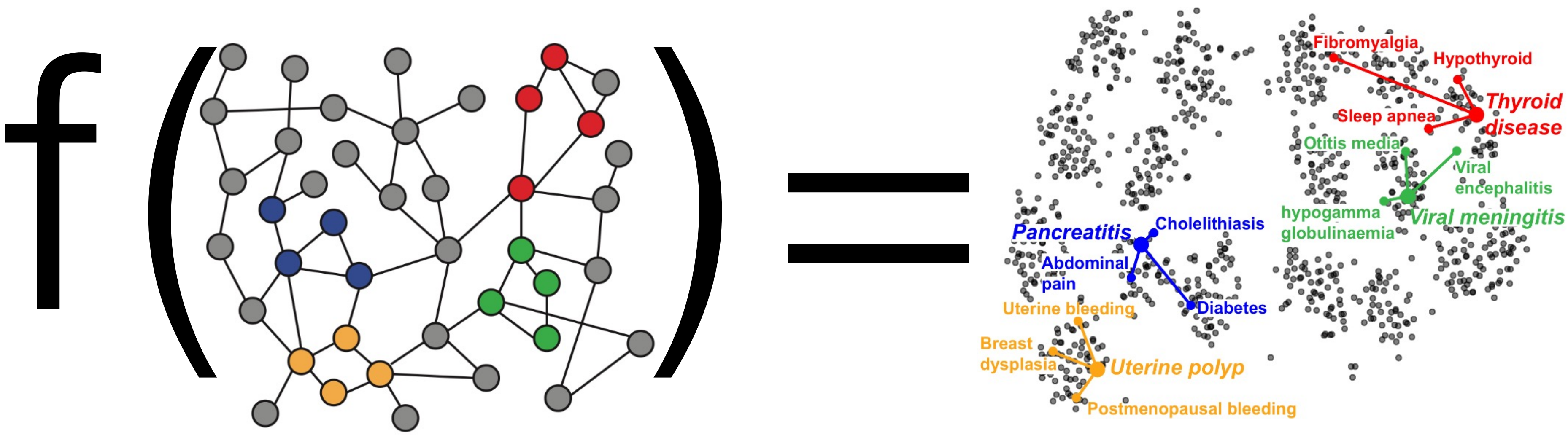
ANNOUNCEMENTS

- **Today (10/07):** Colab 1 due, Colab 2 out
- **Next Thursday (10/14):** HW 1 due, HW 2 out
- Project proposals **due on Tuesday 10/19**
  - If you are looking for **project** partners, check out / add yourself to our pinned Ed post ("Project Partner Thread") -- reach out to each other!
  - We strongly encourage groups of 3, but groups of 1 or 2 are allowed

Recap: Node Embeddings

图嵌入表示学习

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



Input graph

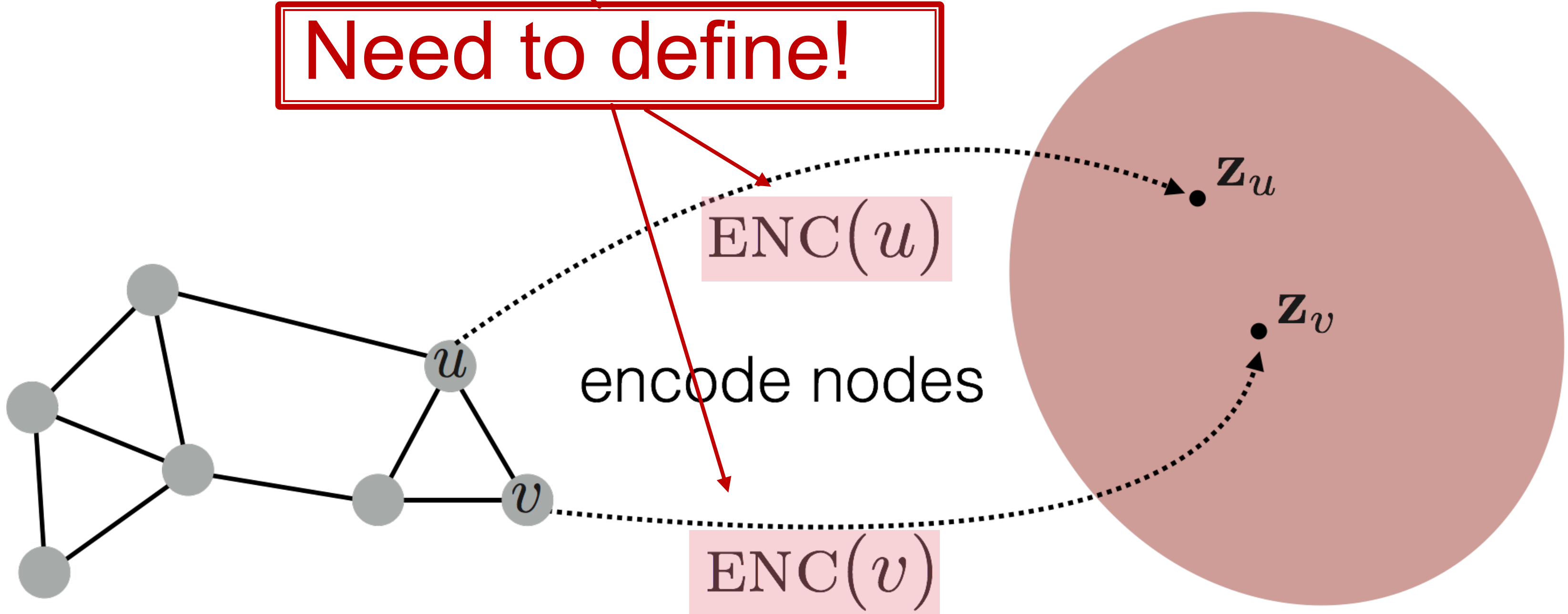
2D node embeddings

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

Recap: Node Embeddings

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

Need to define!



Input network

d-dimensional embedding space

Recap: Two Key Components

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

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

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

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

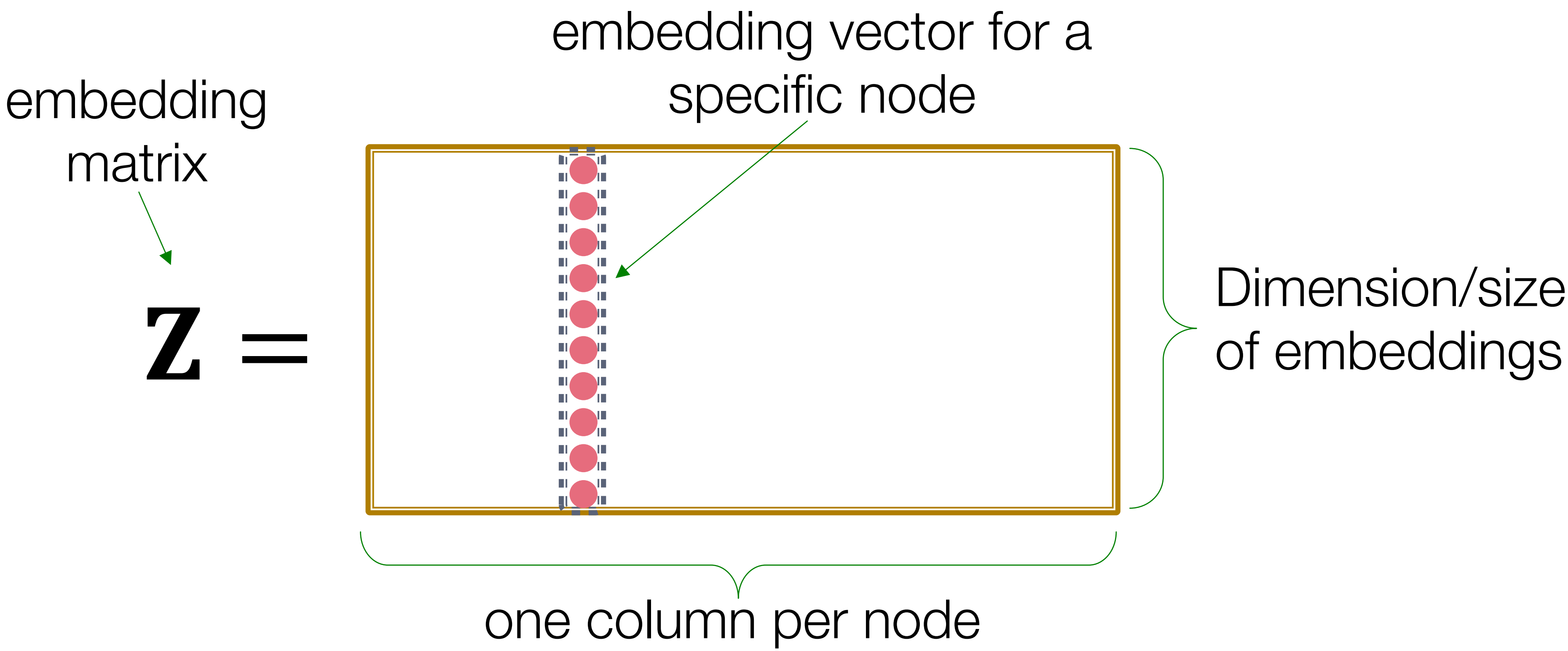
Decoder

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

DeepWalk, Node2vec, LINE

- **Limitations** of shallow embedding methods:
  - **$O(|V|)$ parameters are needed:** 每个节点的嵌入向量都需单独训练
    - No sharing 参数共享 of parameters between nodes
    - Every node has its own unique embedding
  - **Inherently "transductive":** 直推式 无法泛化到新图/新节点
    - Cannot generate embeddings for nodes that are not seen during training
  - **Do not incorporate 纳入 node features:** 没有用到节点属性特征
    - Nodes in many graphs have features 标注 that we can and should leverage 利用

Today: Deep Graph Encoders

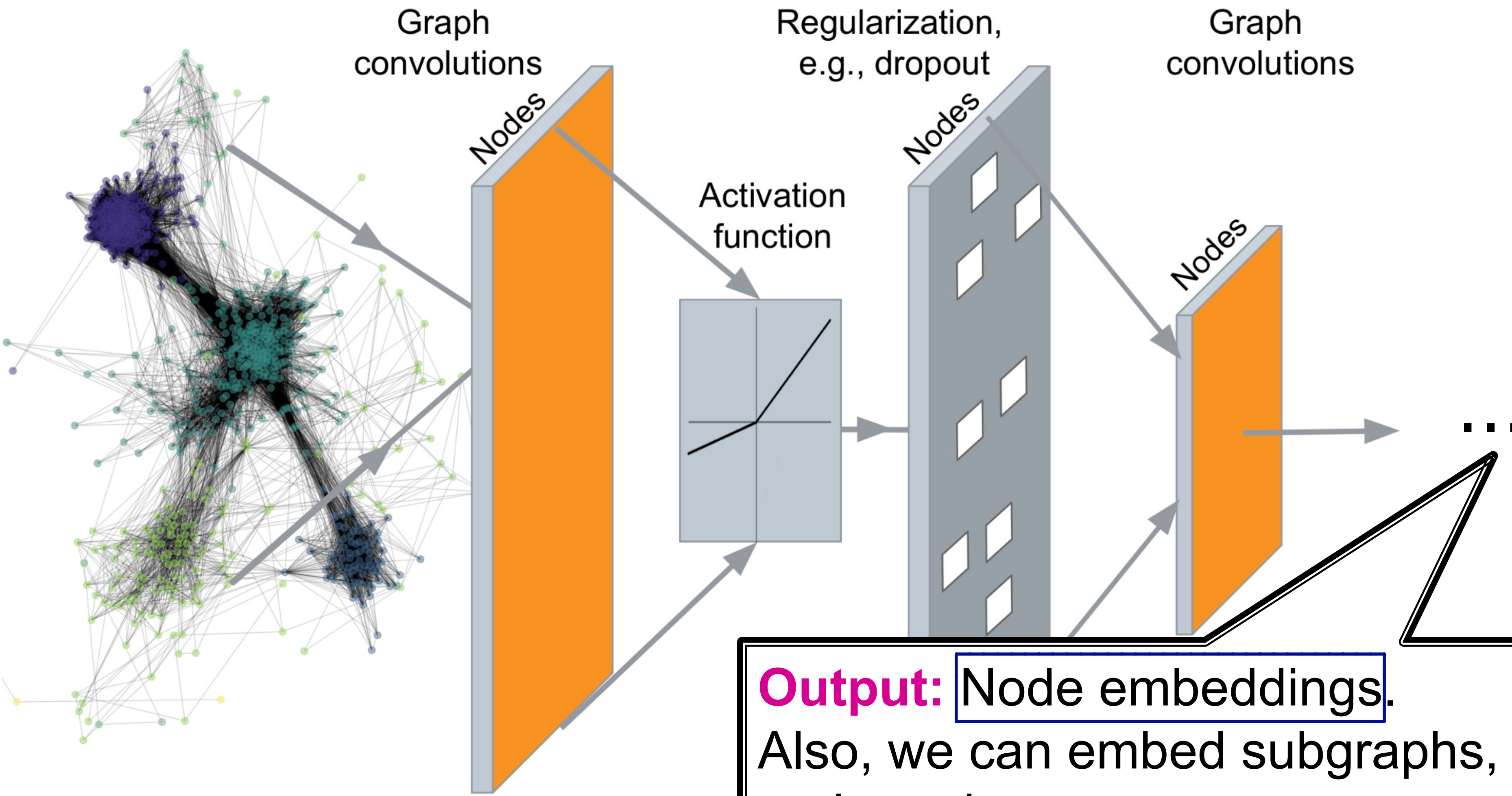
图深度学习 图神经网络

- **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



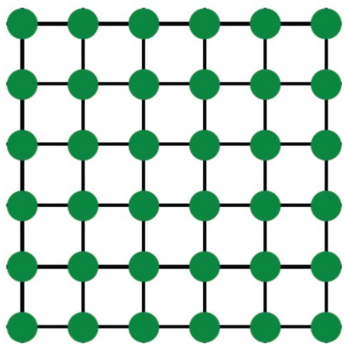
Output: Node embeddings. Also, we can embed subgraphs, and graphs

Tasks on Networks

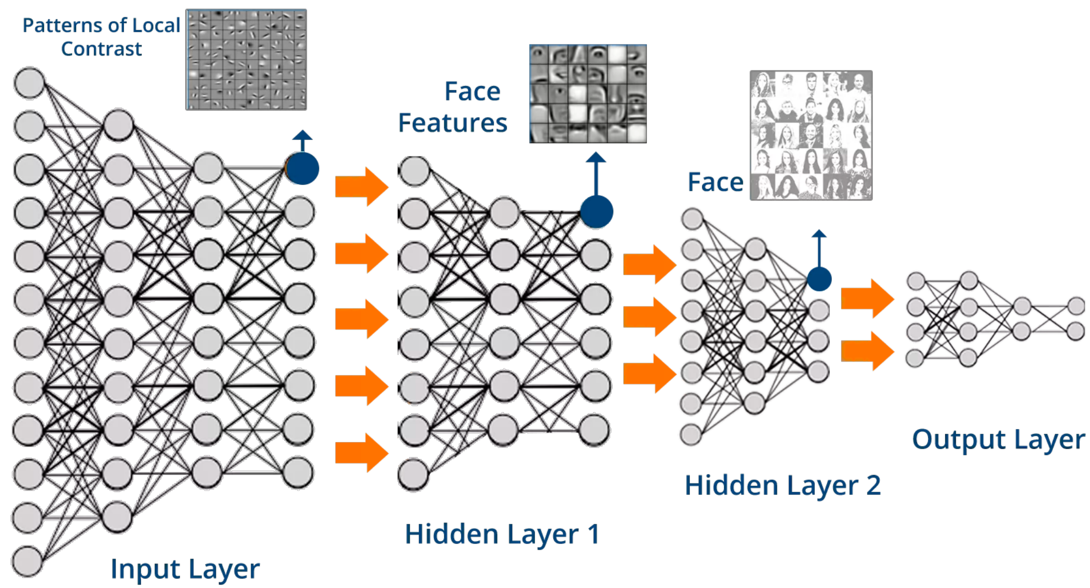
Tasks we will be able to solve:

- Node classification
  - Predict a 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

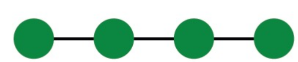
Modern ML Toolbox

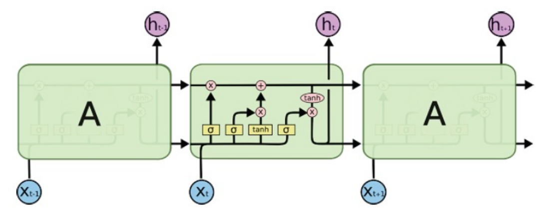


Images



Text/Speech



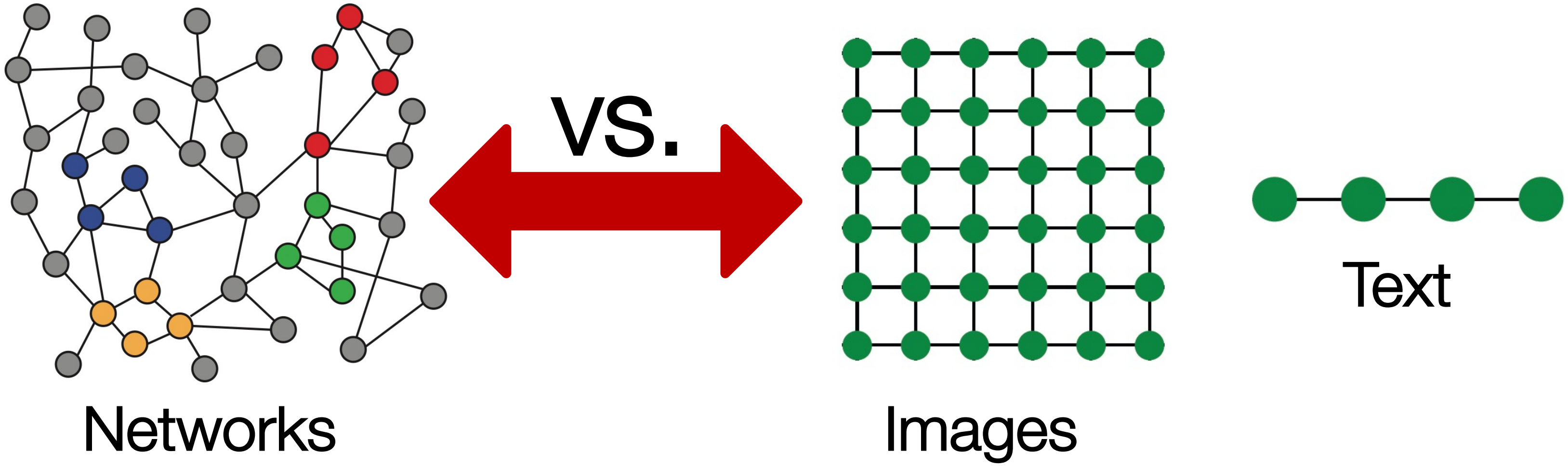


Modern deep learning toolbox is designed for simple sequences & grids

Why is it Hard?

But networks are far more complex!

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



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

Outline of Today's Lecture

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

Stanford CS224W: Basics of Deep Learning

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
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Machine Learning as Optimization

监督学习 特征

- **Supervised learning:** we are given input $\boldsymbol{x}$, and the goal is to predict label $\boldsymbol{y}$.

标签

- **Input x can be:**
  - Vectors of real numbers 向量
  - Sequences (natural language) 文本序列
  - Matrices (images) 栅格图片
  - Graphs (potentially with node and edge features) 图
- **We formulate the task as an optimization problem.**

Machine Learning as Optimization

- **Formulate the task as an optimization problem:**

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

Objective function

- Θ: a set of **parameters** we optimize
  - Could contain one or more scalars, vectors, matrices …
  - E.g. $\Theta = \{Z\}$ in the shallow encoder (the embedding lookup)

- $\mathcal{L}$: **loss function**. Example: L2 loss

$$\mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x})) = \|y - f(x)\|_2$$

  - Other common loss functions:
    - L1 loss, huber loss, max margin (hinge loss), cross entropy …
    - See https://pytorch.org/docs/stable/nn.html#loss-functions

Loss Function Example

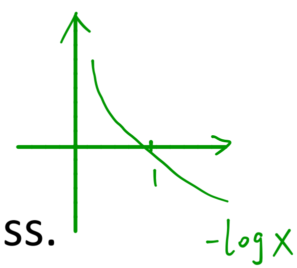
多分类 交叉熵损失函数

- One common loss for classification: **cross entropy (CE)**
- Label $\boldsymbol{y}$ is a categorical vector (one-hot encoding)
  - e.g. $\boldsymbol{y} = \begin{bmatrix} 0 & 0 & \boxed{1} & 0 & 0 \end{bmatrix}$

    y is of class “3”
- $f(\boldsymbol{x}) = \text{Softmax}(g(\boldsymbol{x}))$
  - Recall from lecture 3: $f(\boldsymbol{x})_i = \dfrac{e^{g(x)_i}}{\sum_{j=1}^{C} e^{g(x)_j}}$

    $g(x)_i$ denotes i-th coordinate of the vector output of func. $g(x)$

  where C is the number of classes.
  - e.g. $f(\boldsymbol{x}) = \begin{bmatrix} 0.1 & 0.3 & \boxed{0.4} & 0.1 & 0.1 \end{bmatrix}$
- $\text{CE}(\boldsymbol{y}, f(\boldsymbol{x})) = -\sum_{i=1}^{C}(y_i \log f(x)_i)$ $-\log 0.4$

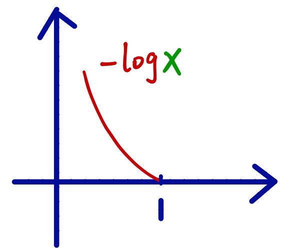


  - y_i and $f(x)_i$ are the **actual** and **predicted** values of the i-th class.
  - **Intuition:** the lower the loss, the closer the prediction is to one-hot
- **Total loss over all training examples:**
  - $\mathcal{L} = \sum_{(\boldsymbol{x},\boldsymbol{y})\in\mathcal{T}} \text{CE}(\boldsymbol{y}, f(\boldsymbol{x}))$
    - $\mathcal{T}$: training set containing all pairs of data and labels $(\boldsymbol{x}, \boldsymbol{y})$

交叉熵损失函数

同济子豪兄 2023-3-1
公众号 人工智能小技巧 回复 交叉熵 下载原图

		猫	狗	马	猪	交叉熵 $-y_i \log P_i$
训练集样本1	标签	0	1	0	0	$-\log 0.6$
	预测	0.2	0.6	0.1	0.1	
训练集样本2	标签	0	0	1	0	$-\log 0.3$
	预测	0.1	0.5	0.3	0.1	
训练集样本3	标签	1	0	0	0	$-\log 0.7$
	预测	0.7	0.1	0.1	0.1	



P_i越接近1
交叉熵越小

样本之间独立同分布

随机事件"所有样本都被正确预测"发生的概率 $\boxed{P = 0.6 \times 0.3 \times 0.7}$

P越大 ⟹ 预测结果越好 ⟹ 算法模型越好

优化目标：更新算法模型参数 使得 P最大化 极大似然估计

最大化 P ⟺ 最大化 P 取对数 $\log P = \log 0.6 + \log 0.3 + \log 0.7$ ⟺ 最小化负对数 $-\log 0.6 - \log 0.3 - \log 0.7$

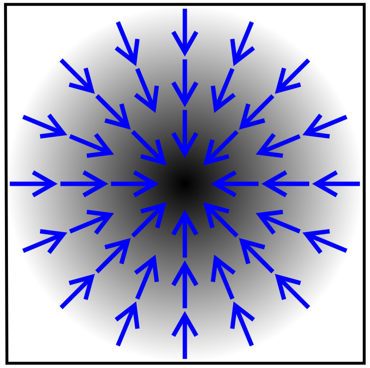
交叉熵损失函数 $\boxed{L = -\sum_i y_i \log P_i}$

Machine Learning as Optimization

目标函数
- **How to optimize the objective function?**
- **Gradient vector:** Direction and rate of fastest increase

Partial derivative
偏导数

$$\nabla_{\Theta}\mathcal{L} = \left(\frac{\partial \mathcal{L}}{\partial \Theta_1}, \frac{\partial \mathcal{L}}{\partial \Theta_2}, \ldots\right)$$



https://en.wikipedia.org/wiki/Gradient

  - $\Theta_1, \Theta_2 \ldots$: components of Θ
- Recall **directional derivative** of a multi-variable function (e.g. $\mathcal{L}$) along a given vector represents the instantaneous rate of change of the function along the vector. （斜率）

  多元函数
- Gradient is the directional derivative in the **direction of largest increase.** 斜率最大的方向

Gradient Descent

梯度下降

- **Iterative algorithm:** repeatedly update weights in the (opposite) direction of gradients until convergence

$$\Theta \leftarrow \Theta - \eta \nabla_{\Theta} \mathcal{L}$$

- **Training:** Optimize Θ iteratively
  - **Iteration**: 1 step of gradient descent
- **Learning rate (LR) η:** 学习率
  - Hyperparameter that controls the size of gradient step
  - Can vary over the course of training (LR scheduling)
- **Ideal termination condition:** gradient = **0** (碗底)
  - In practice, we stop training if it no longer improves performance on **validation set** (part of dataset we hold out from training).

Stochastic Gradient Descent (SGD)

- **Problem with gradient descent:**
  - Exact gradient requires computing $\nabla_{\Theta}\mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x}))$, where $\boldsymbol{x}$ is the **entire** dataset! 每迭代一次，需输入所有样本计算损失函数
    - This means summing gradient contributions over all the points in the dataset
    - Modern datasets often contain billions of data points
    - Extremely expensive for every gradient descent step
- **Solution: Stochastic gradient descent (SGD)**
  - At every step, pick a different **minibatch** $\mathcal{B}$ containing a subset of the dataset, use it as input $\boldsymbol{x}$

每迭代一次，只输入batch size个样本计算损失函数

Minibatch SGD

- **Concepts:**
  - 一次迭代输入的样本数
  - **Batch size**: the number of data points in a minibatch
    - E.g. number of nodes for node classification task
  - **Iteration**: 1 step of SGD on a minibatch
  - **Epoch**: one full pass over the dataset (# iterations is equal to ratio of dataset size and batch size)

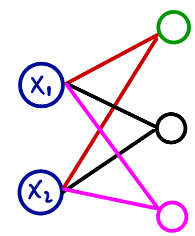
    遍历训练集全部样本

无偏估计

- **SGD is unbiased estimator of full gradient:**
  - But there is no guarantee on the rate of convergence
  - In practice often requires tuning of learning rate
- Common optimizer that improves over SGD:
  - Adam, Adagrad, Adadelta, RMSprop …

Neural Network Function

- **Objective:** $\min_{\Theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x}))$
- In deep learning, function f can be very complex
- **Example:**
  - To start simple, consider linear function



$$\underset{3\times 1}{f(\boldsymbol{x})} = \underset{3\times 2}{W} \cdot \underset{2\times 1}{\boldsymbol{x}}, \qquad \Theta = \{W\}$$

  - Then, if f returns a scalar, then W is a learnable **vector**

$$\nabla_W f = \left(\frac{\partial f}{\partial w_1}, \frac{\partial f}{\partial w_2}, \frac{\partial f}{\partial w_3} \ldots\right)$$

偏导数向量

  - But, if f returns a vector, then W is the **weight matrix**

$$\nabla_W f = \begin{bmatrix} \frac{\partial f_1}{\partial w_{11}} & \frac{\partial f_2}{\partial w_{12}} \\ \frac{\partial f_1}{\partial w_{21}} & \frac{\partial f_2}{\partial w_{22}} \end{bmatrix}$$

雅克比矩阵
Jacobian matrix of f

Intuition: Back Propagation

- **Goal:** $\min_{\Theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x}))$
  - To minimize $\mathcal{L}$, we need to evaluate the gradient: $\nabla_W \mathcal{L} = \left(\frac{\partial \mathcal{L}}{\partial w_1}, \frac{\partial \mathcal{L}}{\partial w_2}, \frac{\partial \mathcal{L}}{\partial w_3} \dots\right)$ which means we need to derive derivative of $\mathcal{L}$.
- **Overview of Back-propagation:** 复合函数求偏导
  - $\mathcal{L}$ is composed from some set of predefined building block functions $g(\cdot)$
  - For each such g we also have its derivative g'
  - Then we can automatically compute$\nabla_{\Theta} \mathcal{L}$ by evaluating appropriate funcs. g' on the minibatch $\boldsymbol{\mathcal{B}}$.

Back-propagation

$f = g \cdot h$

- **How about a more complex function:**

$$f(\boldsymbol{x}) = W_2(W_1\boldsymbol{x}), \Theta = \{W_1, W_2\}$$

$2\times1 \quad 2\times3 \quad 3\times2 \quad 2\times1$

In other words:

$f(\boldsymbol{x}) = W_2(W_1\boldsymbol{x})$

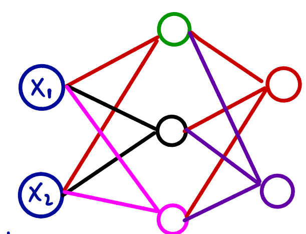
$h(x) = W_1\boldsymbol{x}$

$g(z) = W_2 z$

- Recall **chain rule**:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \frac{\mathrm{d}g}{\mathrm{d}h} \cdot \frac{\mathrm{d}h}{\mathrm{d}x} \text{ or } f'(x) = g'\big(h(x)\big)h'(x)$$

- **Example:** $\nabla_{\boldsymbol{x}} f = \dfrac{\partial f}{\partial(W_1\boldsymbol{x})} \cdot \dfrac{\partial(W_1\boldsymbol{x})}{\partial \boldsymbol{x}}$



链式法则

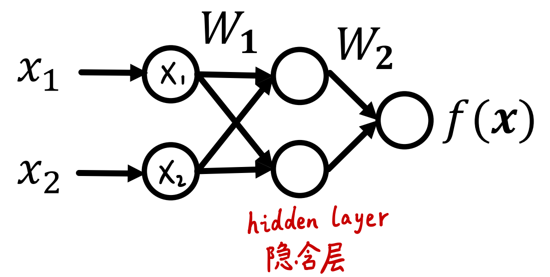
- **Back-propagation**: Use of **chain rule** to propagate gradients of intermediate steps, and finally obtain gradient of $\mathcal{L}$ w.r.t. Θ.

$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$

Back-propagation Example (1)

- **Example:** Simple 2-layer linear network
- $f(\boldsymbol{x}) = g(h(x)) = W_2(W_1\boldsymbol{x})$

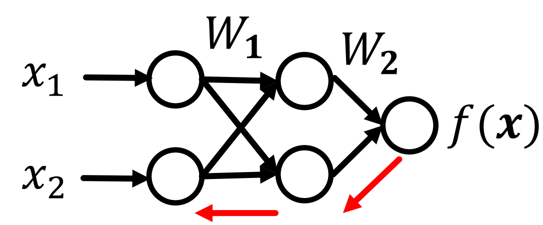
  标量 1×1　　1×2　2×2　2×1



- $\mathcal{L} = \sum_{(\boldsymbol{x},\boldsymbol{y})\in\boldsymbol{\mathcal{B}}} \left\|\left(\boldsymbol{y}, -f(\boldsymbol{x})\right)\right\|_2$
  - The loss $\mathcal{L}$ sums the L2 loss in a minibatch $\boldsymbol{\mathcal{B}}$.
- **Hidden layer:**
  - Intermediate representation of input $\boldsymbol{x}$
  - Here we use $h(x) = W_1\boldsymbol{x}$ to denote the hidden layer
  - $f(\boldsymbol{x}) = W_2 h(x)$

Back-propagation Example (2)

Remember:
$f(\boldsymbol{x}) = W_2(W_1\boldsymbol{x})$
$h(x) = W_1\boldsymbol{x}$
$g(z) = W_2 z$



- **Forward propagation:** 前向预测 求损失函数
  Compute loss starting from input
  - $\boldsymbol{x} \xrightarrow[\text{Multiply } W_1]{} h \xrightarrow[\text{Multiply } W_2]{} g \xrightarrow[\text{Loss}]{} \mathcal{L}$

- **Back-propagation to compute gradient of**
  反向传播 求梯度

$$\Theta = \{W_1, W_2\}$$

Start from loss, compute the gradient

$$\frac{\partial \mathcal{L}}{\partial W_2} = \frac{\partial \mathcal{L}}{\partial f} \cdot \frac{\partial f}{\partial W_2}, \qquad \frac{\partial \mathcal{L}}{\partial W_1} = \frac{\partial \mathcal{L}}{\partial f} \cdot \frac{\partial f}{\partial W_2} \cdot \frac{\partial W_2}{\partial W_1}$$

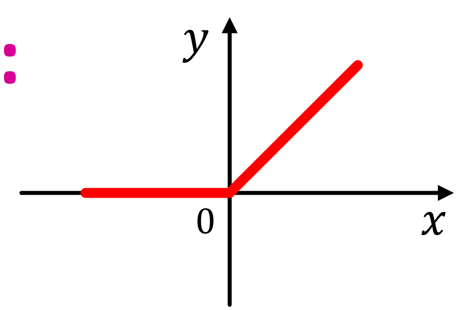
Compute backwards **Compute backwards**

Non-linearity

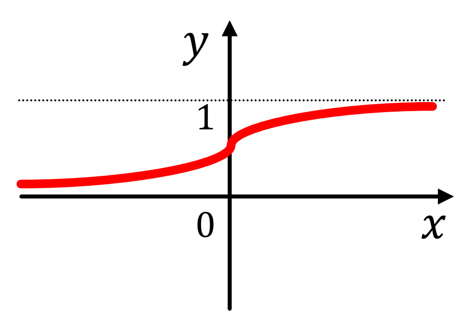
- Note that in $f(\boldsymbol{x}) = W_2(W_1\boldsymbol{x})$, W_2W_1 is another matrix (vector, if we do binary classification)
  - Hence $f(\boldsymbol{x})$ is still linear w.r.t. $\boldsymbol{x}$ no matter how many weight matrices we compose 矩阵代表线性变换

非线性激活函数

- **We introduce non-linearity:**
  - **Rectified linear unit (ReLU)**
    $ReLU(x) = \max(x, 0)$



  - **Sigmoid**
    $$\sigma(x) = \frac{1}{1 + e^{-x}}$$

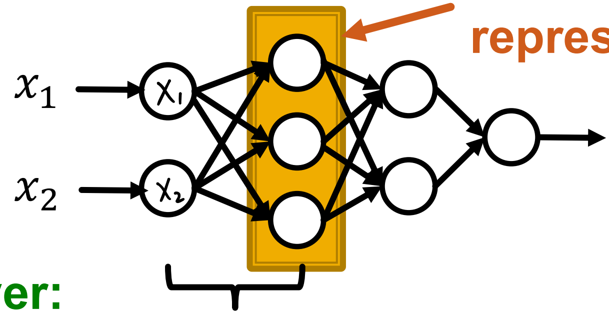


Multi-layer Perceptron (MLP)

- **Each layer of MLP combines linear transformation and non-linearity:**

$$\boldsymbol{x}^{(l+1)} = \sigma(W_l \boldsymbol{x}^{(l)} + b^l)$$

  - where W_l is weight matrix that transforms hidden representation at layer l to layer $l + 1$
  - b^l is bias at layer l, and is added to the linear transformation of $\boldsymbol{x}$ 偏置项
  - σ is non-linearity function (e.g., sigmod) 非线性激活函数
- Suppose $\boldsymbol{x}$ is 2-dimensional, with entries x_1 and x_2



Summary

- **Objective function:**
$$\min_{\Theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{x}))$$
- 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 $\nabla_{\mathrm{W}}\mathcal{L}$ using a chain rule.
- Use **stochastic gradient descent (SGD)** to optimize for Θ over many iterations.

Outline of Today's Lecture

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

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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

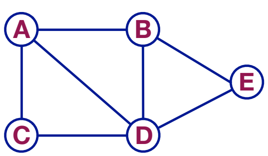
Setup

- **Assume we have a graph G:**
  - V is the **vertex set**
  - $\boldsymbol{A}$ is the **adjacency matrix** (assume binary)
  - $\boldsymbol{X} \in \mathbb{R}^{m \times |V|}$ is a matrix of **node features** 节点属性特征
  - v: a node in V; $\boxed{N(v)}$: the set of neighbors of v.
  - **Node features:** 节点v的邻域(相连节点)
    - 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]

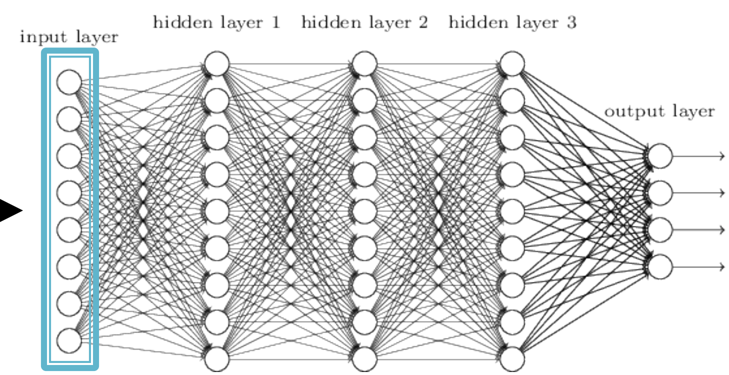
A Naïve Approach

朴素想法：直接输入邻接矩阵A

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



$$
\begin{array}{c}
\\ A \\ B \\ C \\ D \\ E
\end{array}
\begin{array}{c}
\begin{array}{ccccccc} A & B & C & D & E & \multicolumn{2}{c}{\text{Feat}} \end{array} \\
\left(\begin{array}{ccccccc}
0 & 1 & 1 & 1 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 \\
1 & 1 & 1 & 0 & 1 & 1 & 1 \\
0 & 1 & 0 & 1 & 0 & 1 & 0
\end{array}\right)
\end{array}
\longrightarrow
$$

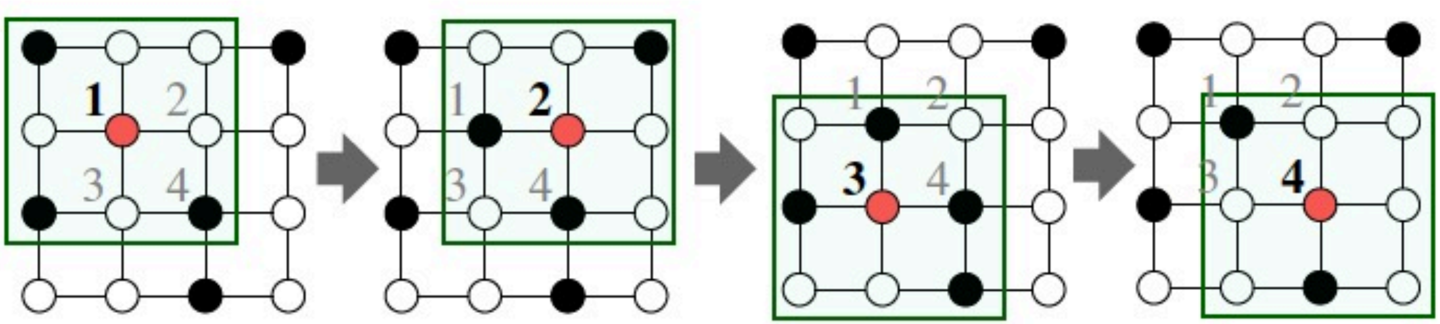


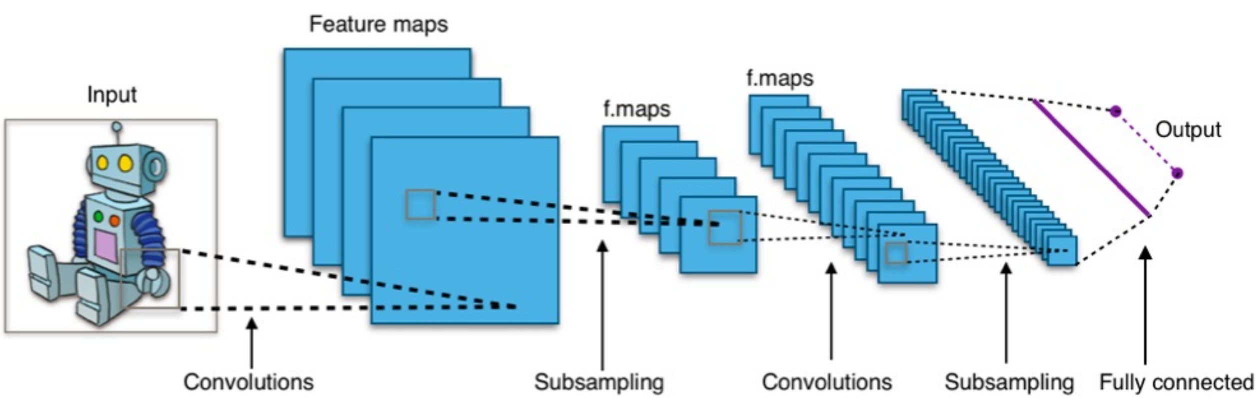
?

- Issues with this idea:
  - $O(|V|)$ parameters 过拟合
  - Not applicable to graphs of different sizes 无法泛化到新节点
  - Sensitive to node ordering 不具备"变换不变性"

Idea: Convolutional Networks

CNN on an image:



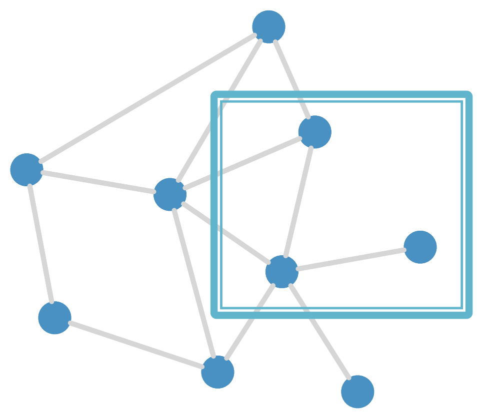


栅格
Goal is to generalize convolutions beyond simple lattices

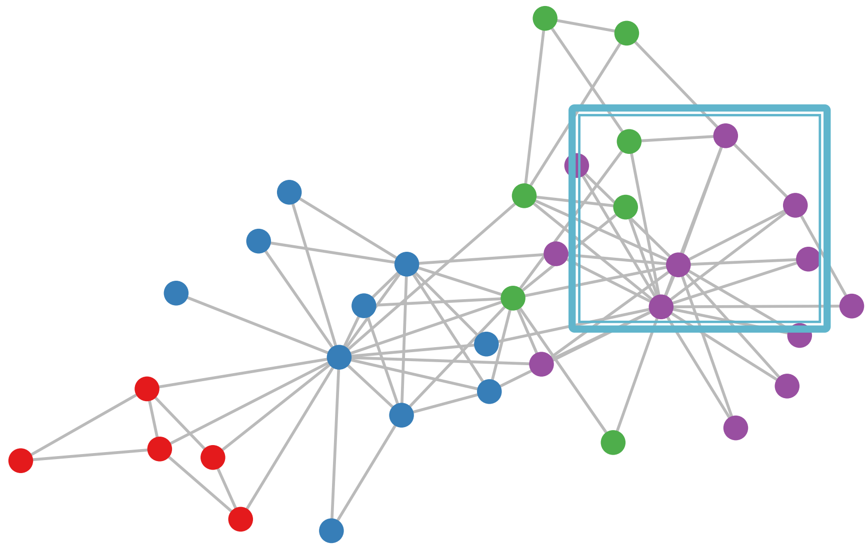
Leverage node features/attributes (e.g., text, images)

Real-World Graphs

But our graphs look like this:



or this:



- There is no fixed 固定的 notion of locality or sliding window on the graph
- Graph is permutation invariant 图具有"变换不变性"

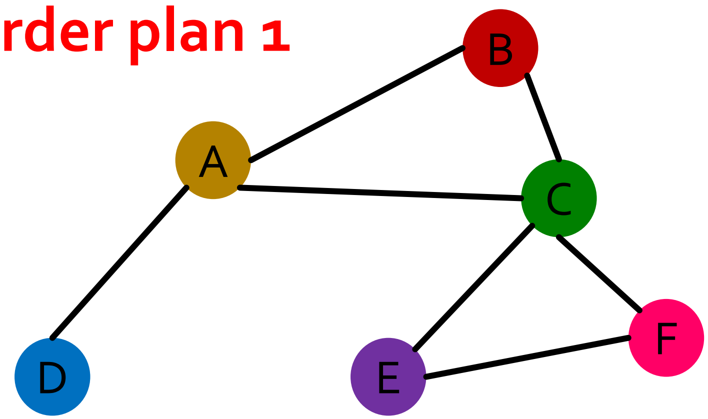
Permutation Invariance

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

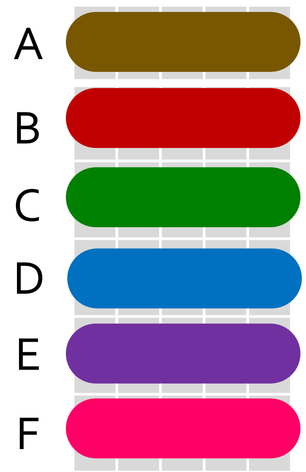
Permutation Invariance

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

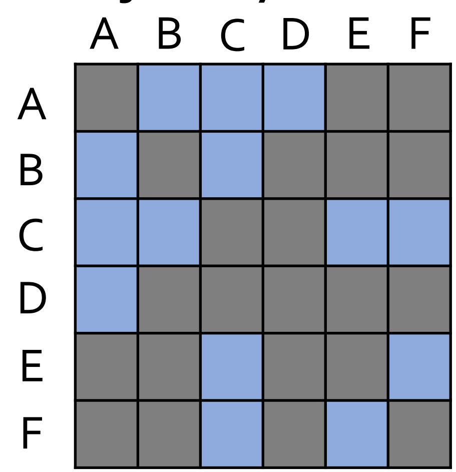
Order plan 1



Node features X_1



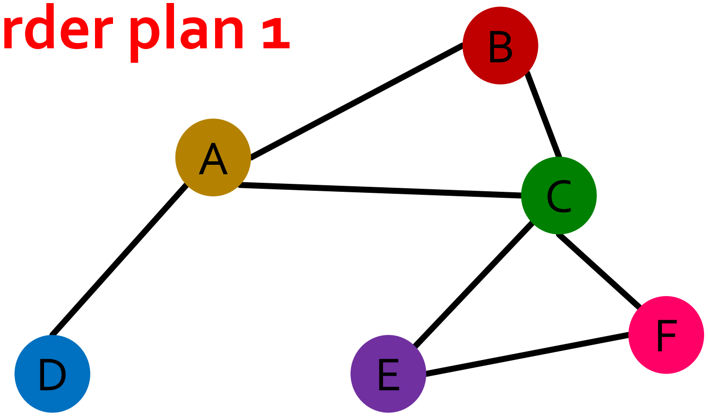
Adjacency matrix A_1



Permutation Invariance

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

Order plan 1



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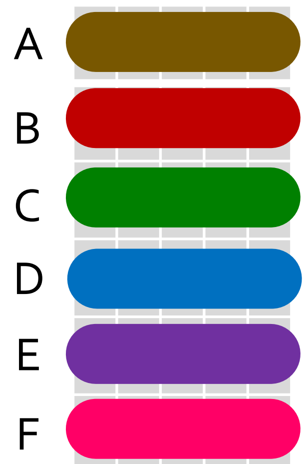
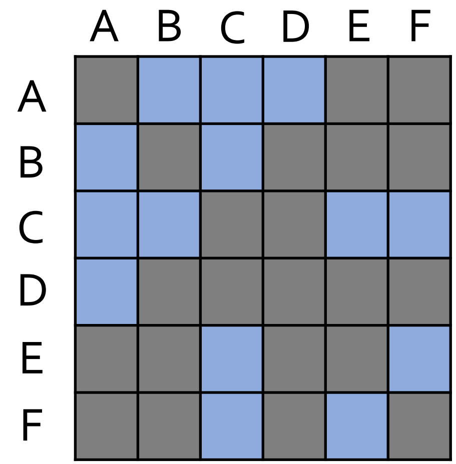
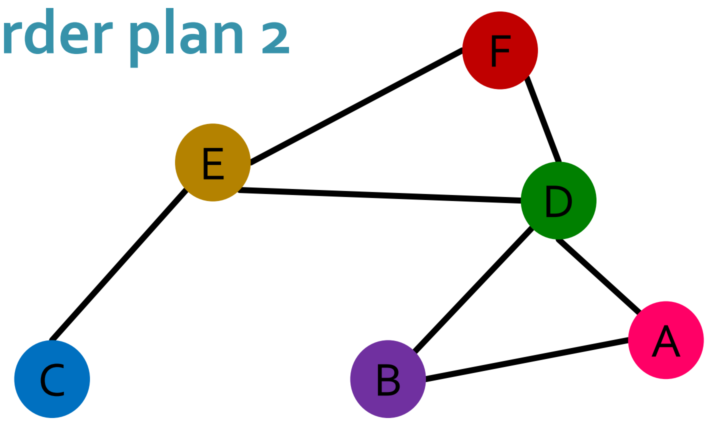


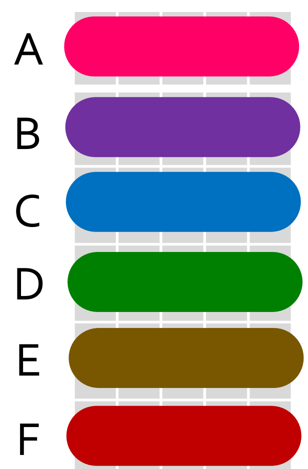
Adjacency matrix A_1



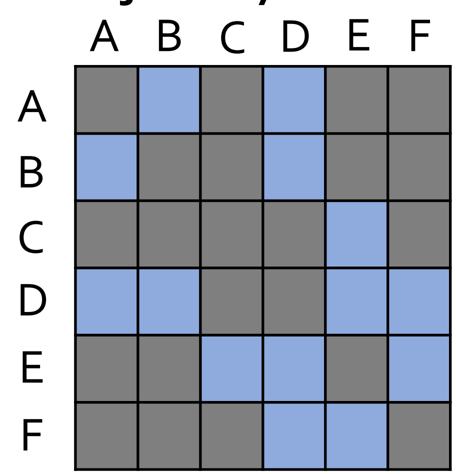
Order plan 2



Node features X_2

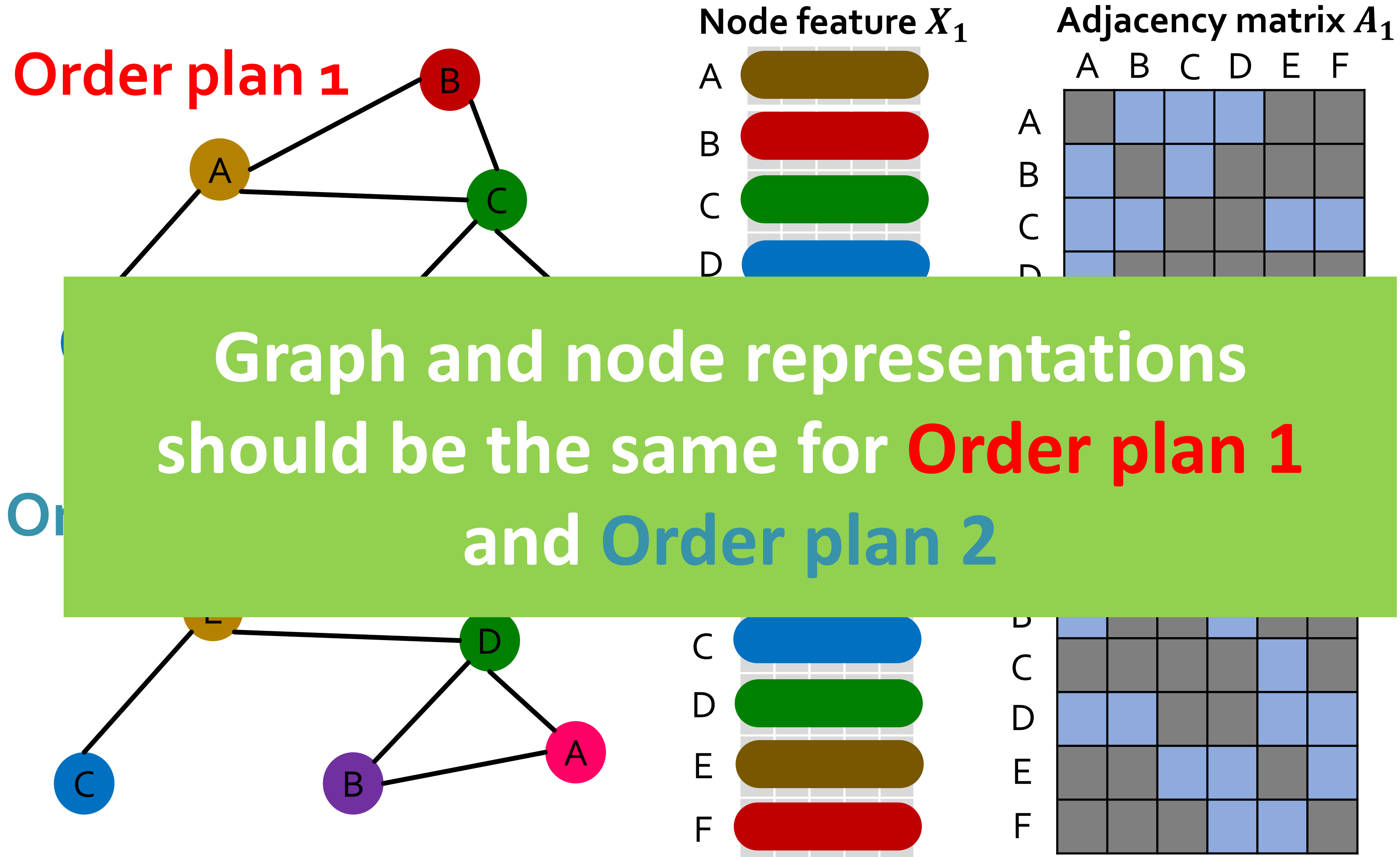


Adjacency matrix A_2



Permutation Invariance

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



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

Permutation Invariance

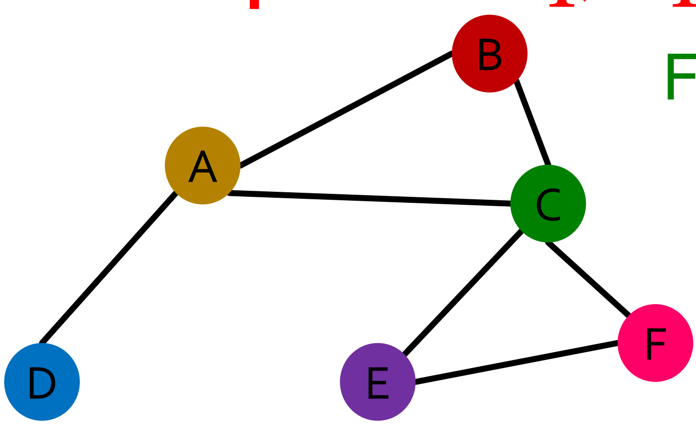
What does it mean by "graph representation is same for two order plans"?

- 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

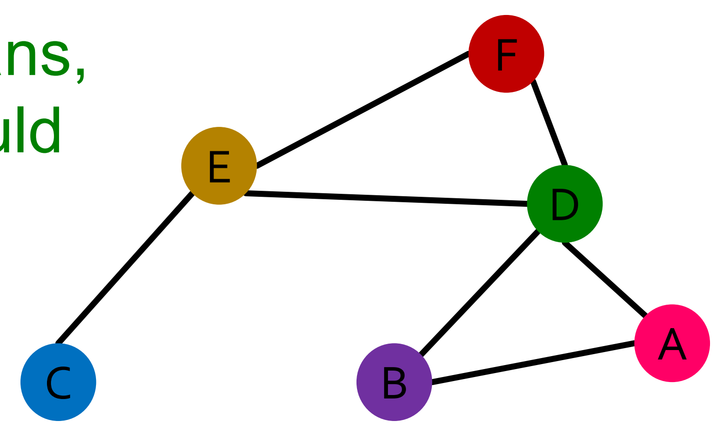
Order plan 1: $\boldsymbol{A}_1, \boldsymbol{X}_1$



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

与节点编号顺序无关
与图的显示方式无关

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**.

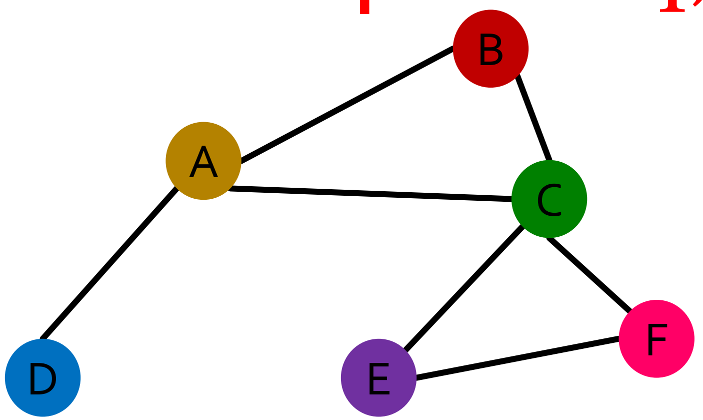
任意顺序

For a graph with m nodes, there are $m!$ different order plans.

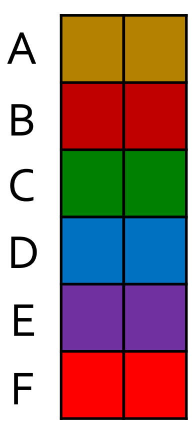
Permutation Equivariance

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

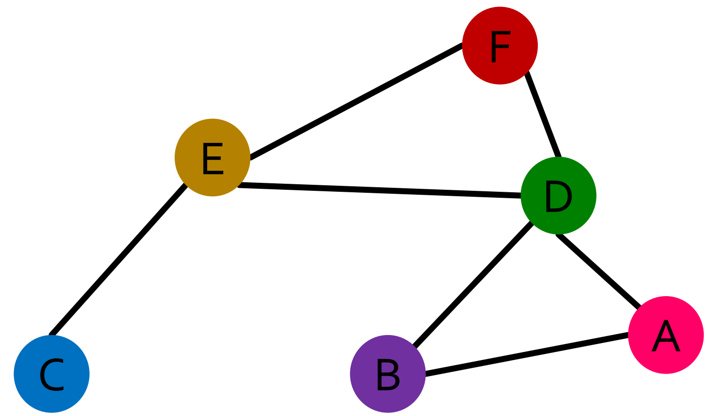
Order plan 1: $\boldsymbol{A}_1, \boldsymbol{X}_1$



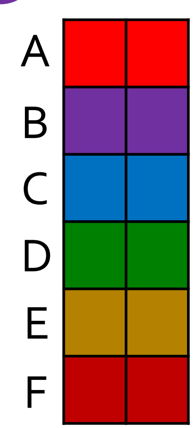
$f(\boldsymbol{A}_1, \boldsymbol{X}_1) =$



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



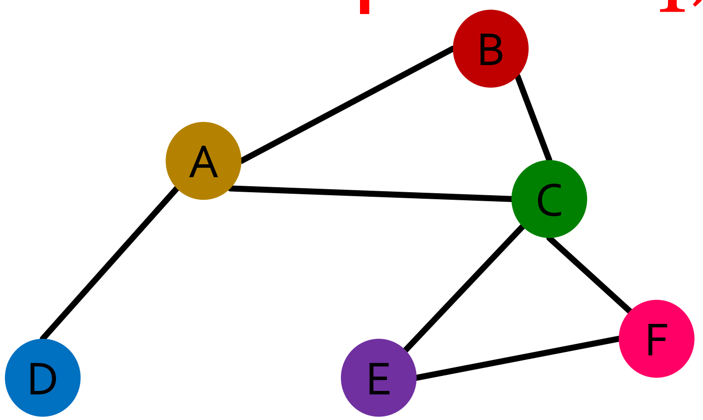
$f(\boldsymbol{A}_2, \boldsymbol{X}_2) =$



Permutation Equivariance

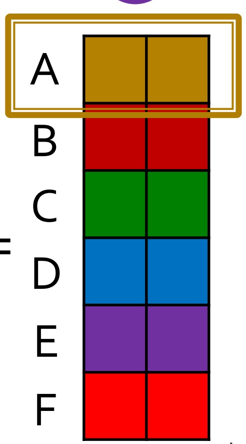
Similarly for node representation: We learn a function f that maps nodes of G to a matrix $\mathbb{R}^{m\times d}$.

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

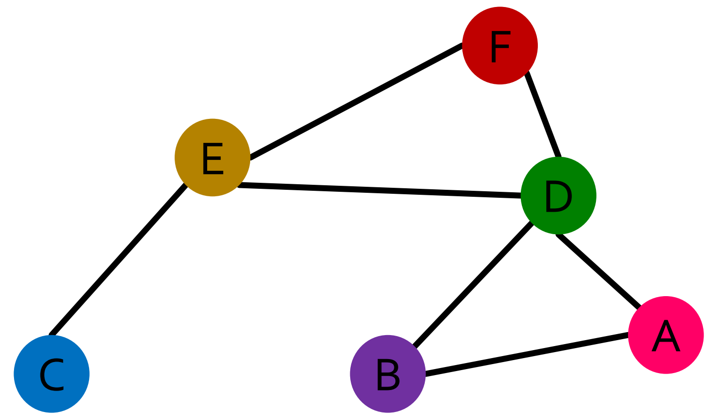


Representation vector of the brown node A

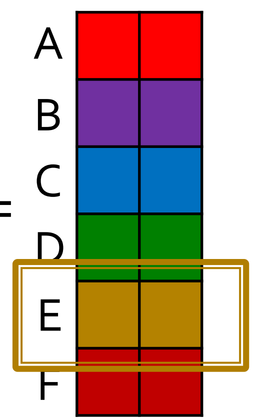
$f(\boldsymbol{A}_1, \boldsymbol{X}_1) =$



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



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



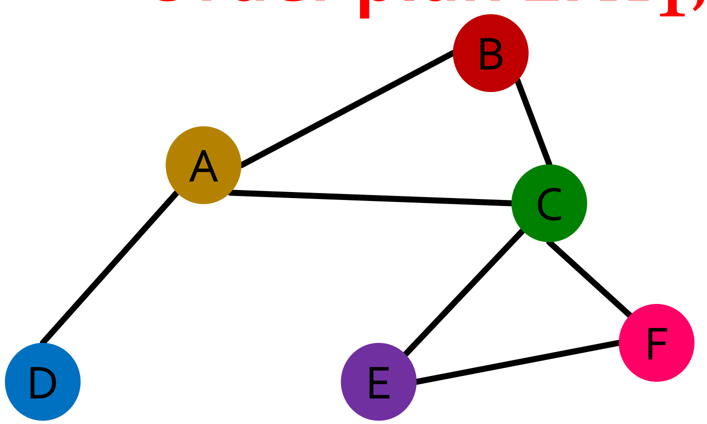
Representation vector of the brown node E

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

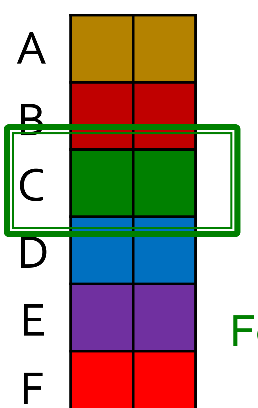
Permutation Equivariance

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

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

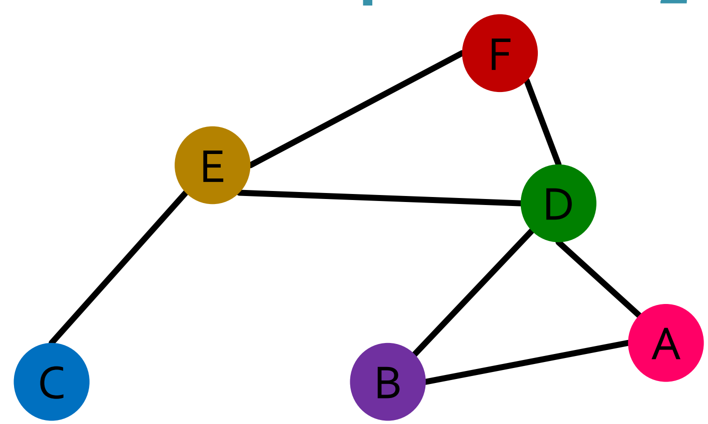


$f(\boldsymbol{A}_1, \boldsymbol{X}_1) =$

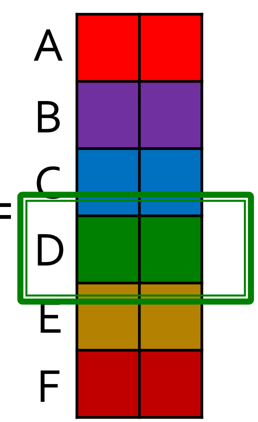


Representation vector of the brown node C

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



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



Representation vector of the brown node D

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

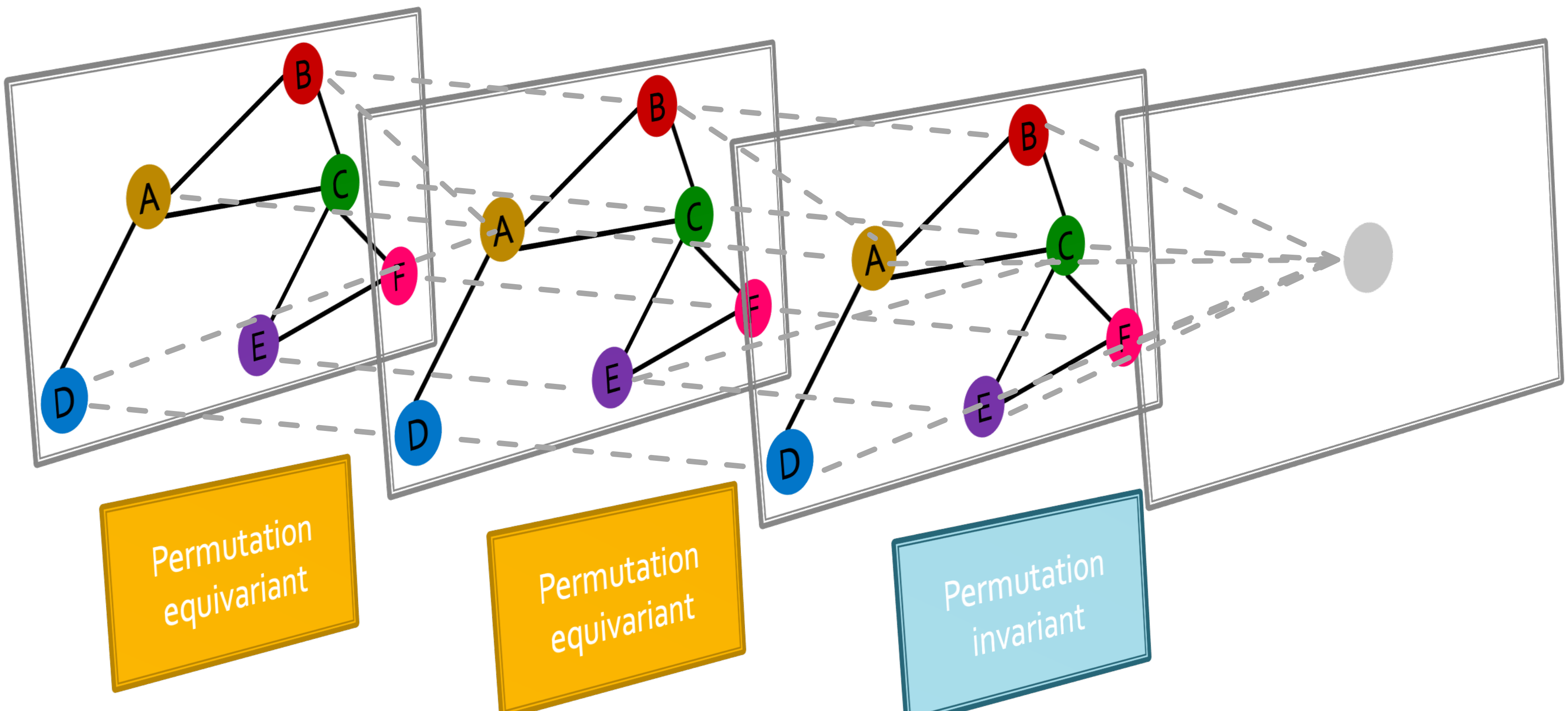
Permutation Equivariance

For node representation

- Consider we learn a function f that maps a graph $G = (\boldsymbol{A}, \boldsymbol{X})$ to a matrix $\mathbb{R}^{m \times d}$
  - graph has m nodes, each row is the embedding of a node.
- Similarly, if this property holds for any pair of order plan i and j, we say f is a **permutation equivariant function**.

Graph Neural Network Overview

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

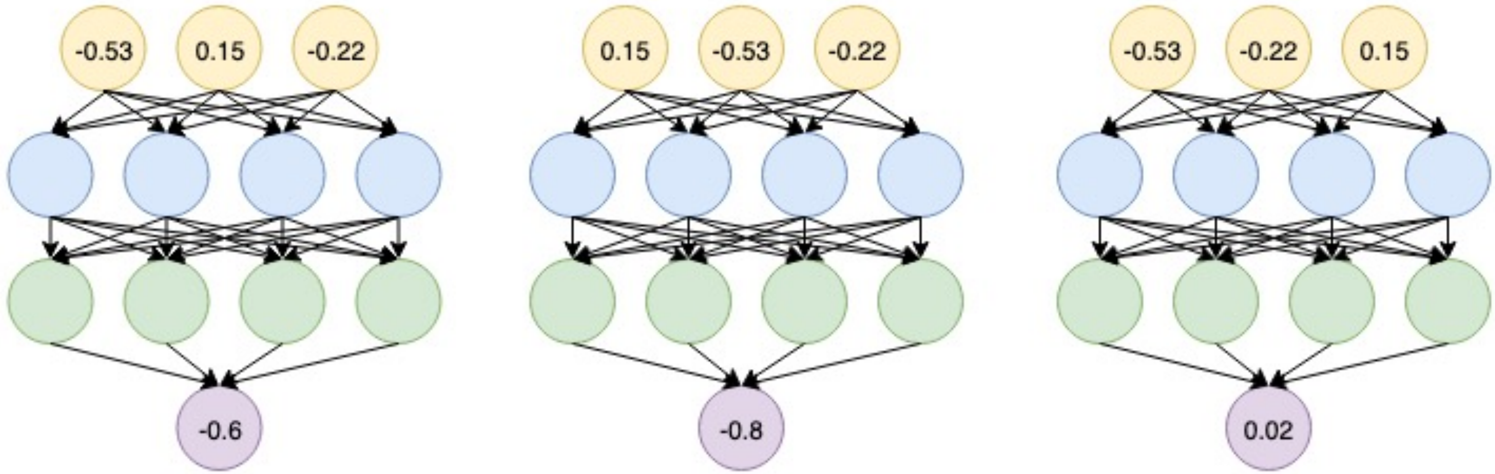


Graph Neural Network Overview

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

- **No.**

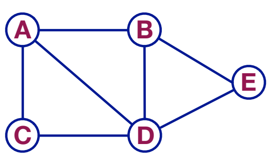
Switching the order of the input leads to different outputs!



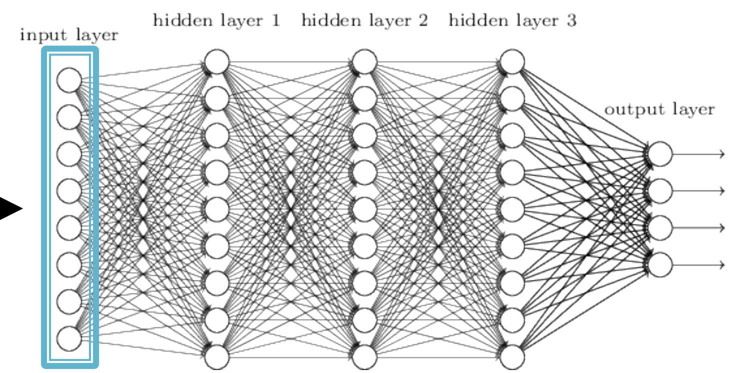
Graph Neural Network Overview

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

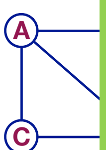


?

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

Graph Neural Network Overview

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



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

消息传递和聚合

?

Outline of Today's Lecture

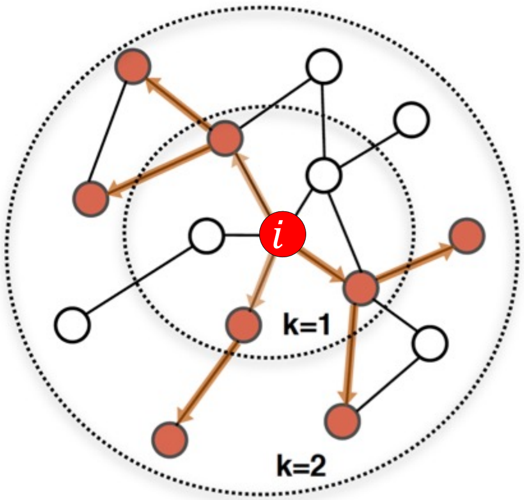
1. Basics of deep learning ✓
2. Deep learning for graphs ✓

   图卷积神经网络
3. Graph Convolutional Networks
4. GNNs subsume CNNs and Transformers

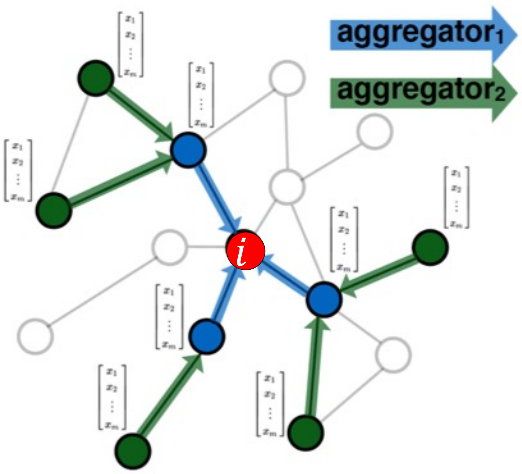
[Kipf and Welling, ICLR 2017]

Graph Convolutional Networks

Idea: Node's neighborhood defines a computation graph 计算图



Determine node computation graph

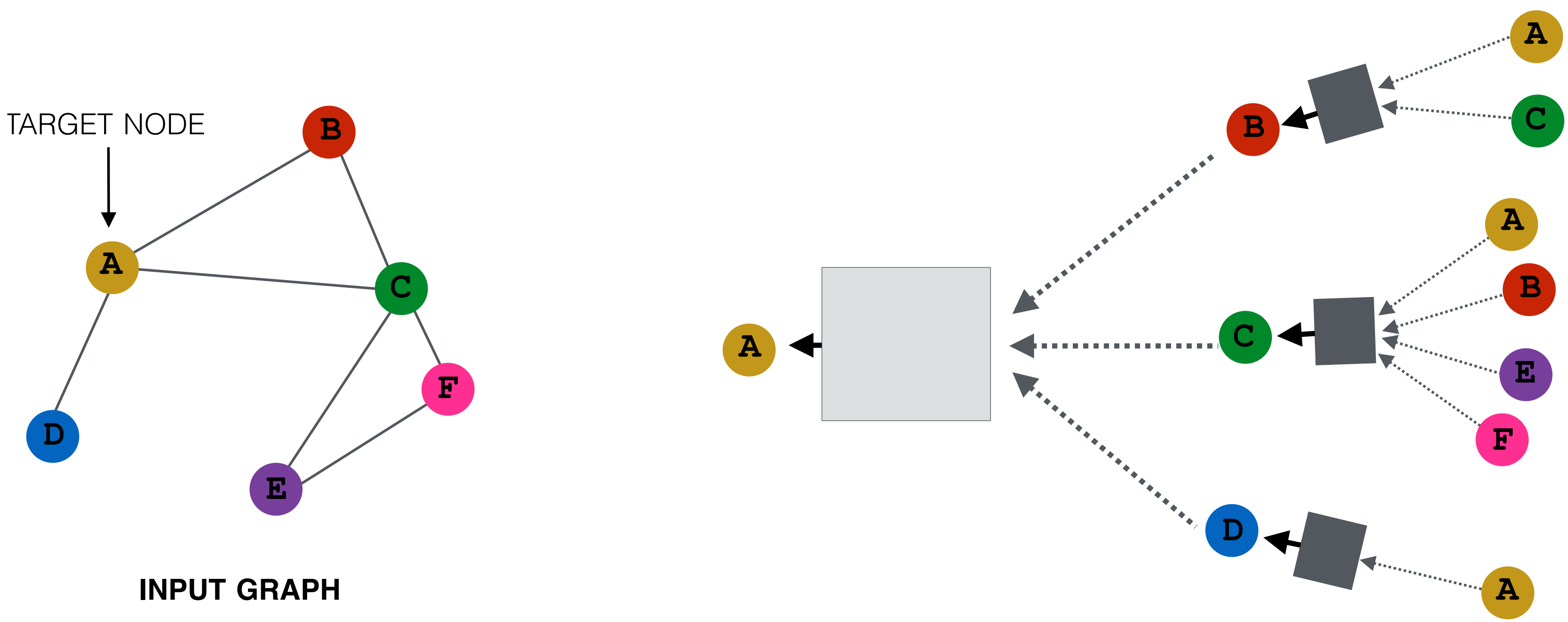


Propagate and transform information

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

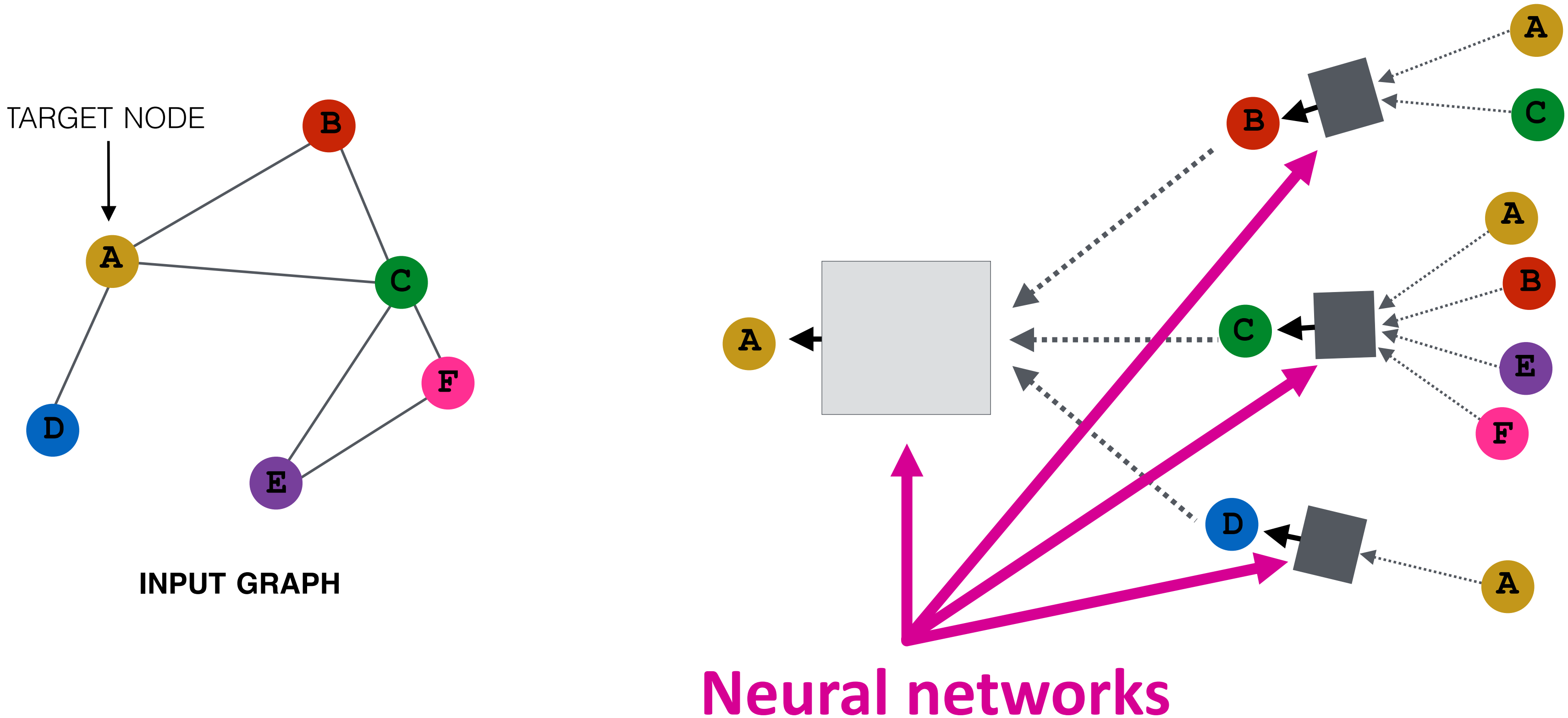
Idea: Aggregate Neighbors

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



Idea: Aggregate Neighbors

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

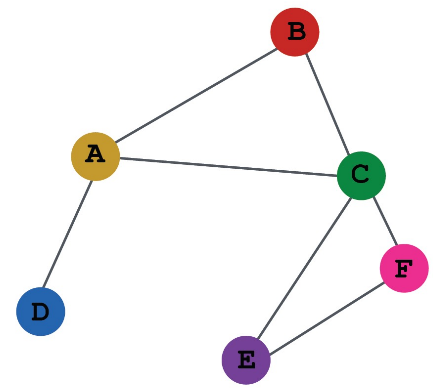


Idea: Aggregate Neighbors

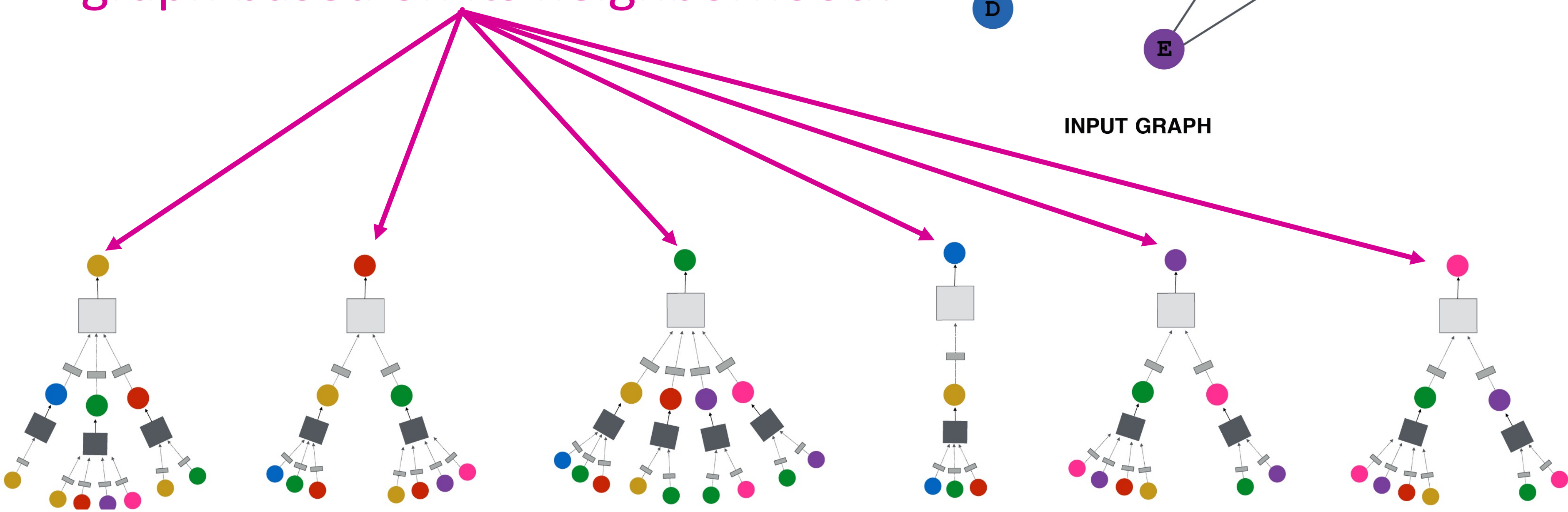
- **Intuition:** Network neighborhood defines a computation graph

每个节点分别构建自己的计算图

Every node defines a computation graph based on its neighborhood!



INPUT GRAPH



计算图结构相同（结构功能角色）

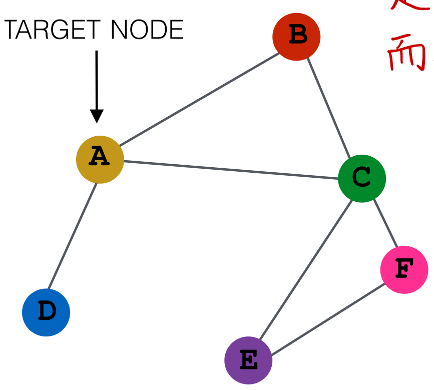
Deep Model: Many Layers

"六度空间"理论

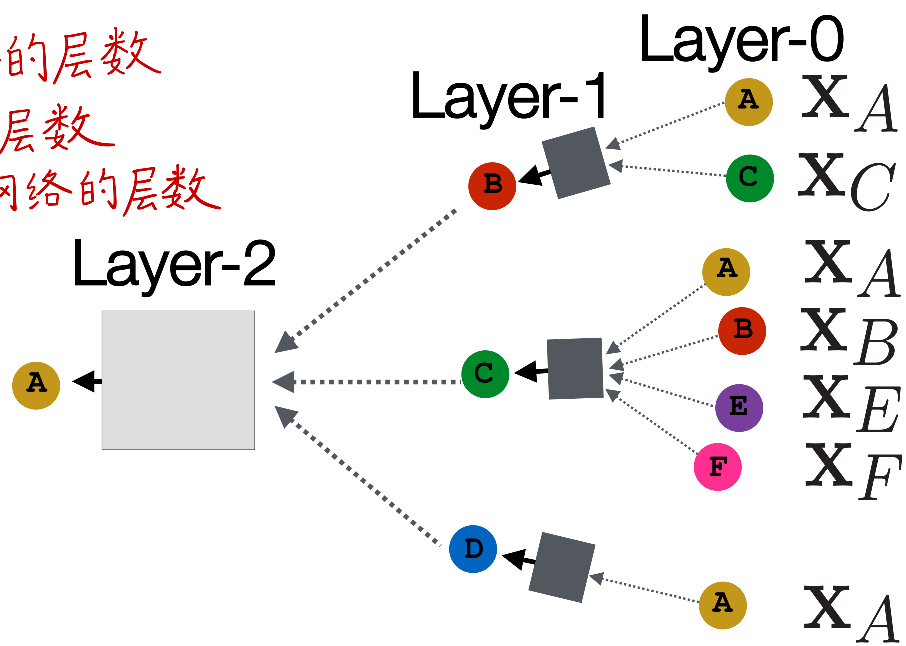
理论上任意深度

- 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

图神经网络的层数
是计算图的层数
而不是神经网络的层数

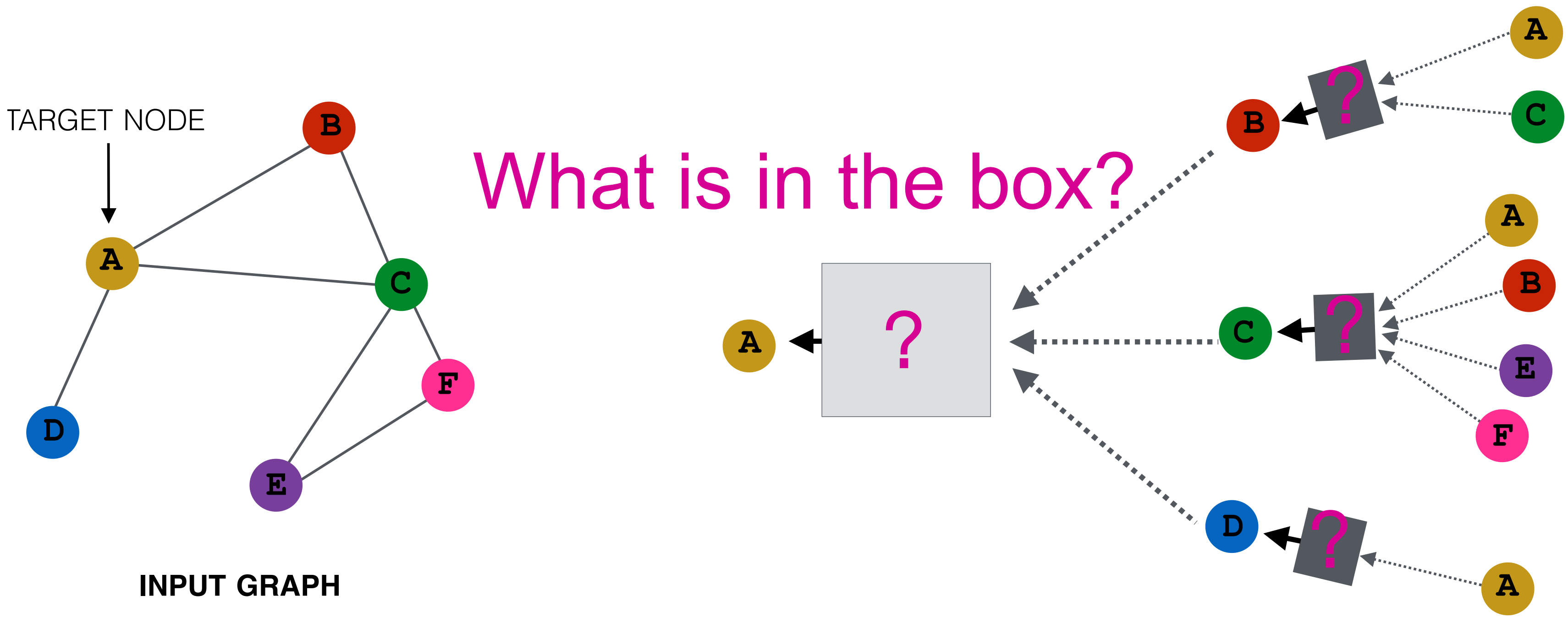


INPUT GRAPH



Neighborhood Aggregation

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

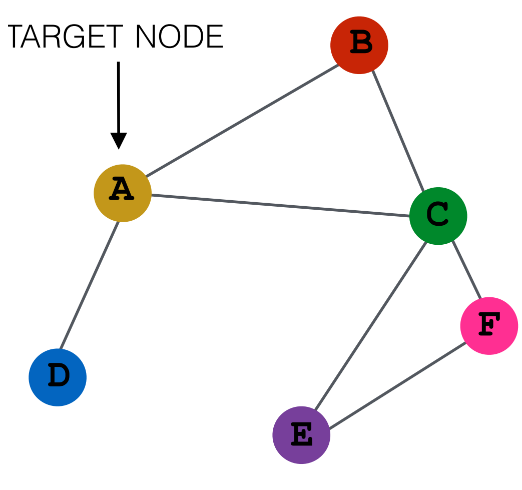


Neighborhood Aggregation

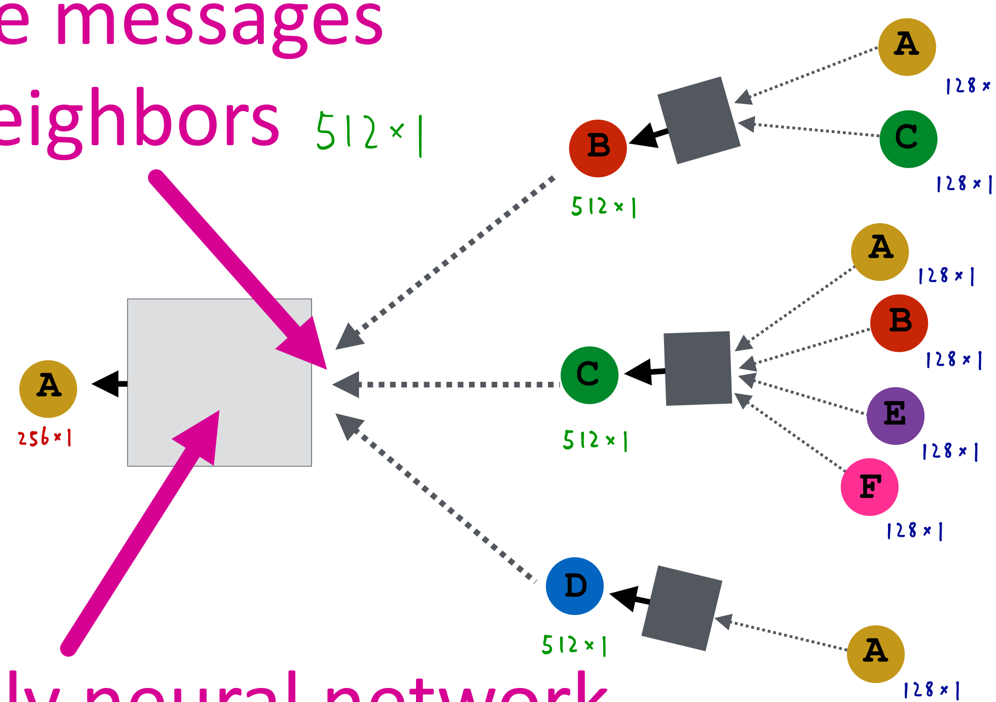
- **Basic approach:** Average information from neighbors and apply a neural network

Order Invariant
Permutation Invariant

(1) average messages from neighbors 512×1



INPUT GRAPH



(2) apply neural network

The Math: Deep Encoder

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

节点属性特征
Initial 0-th layer embeddings are equal to node features

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

本层节点v的嵌入向量

上一层节点v的嵌入向量
embedding of v at layer k

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

总层数
Total number of layers

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

最后一层节点v的嵌入向量作为"表示"
Embedding after L layers of neighborhood aggregation

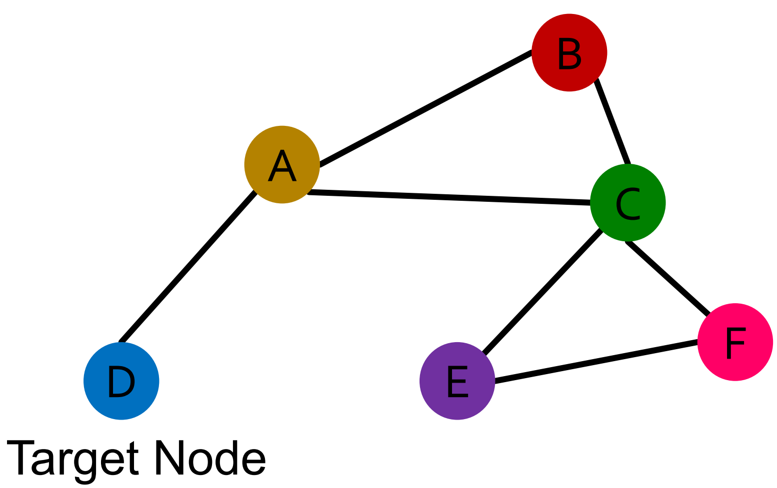
Non-linearity (e.g., ReLU)
非线性激活函数

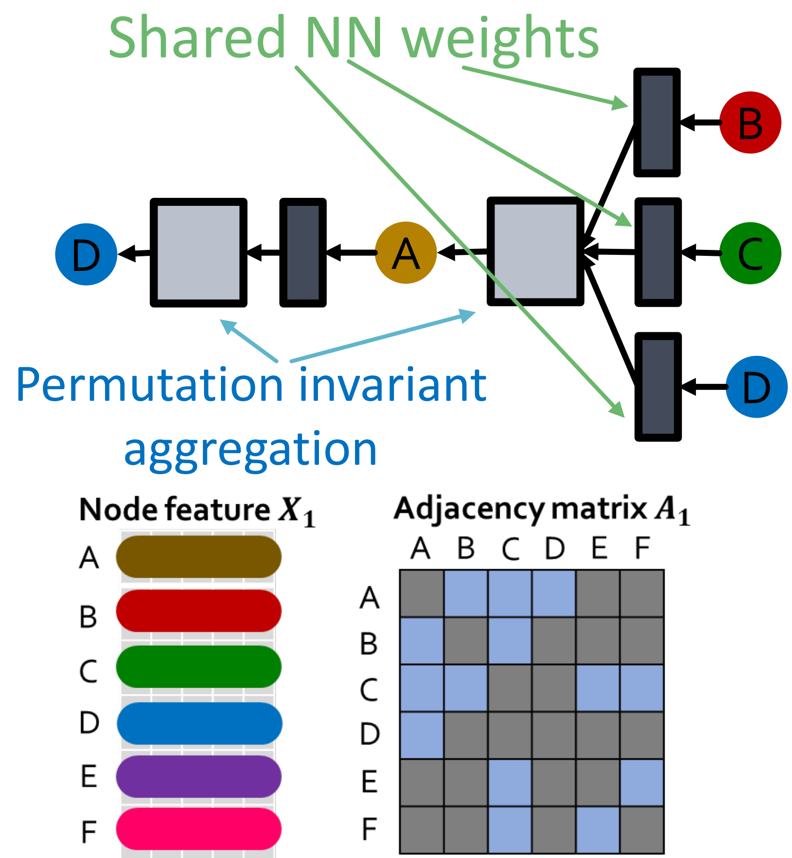
邻域节点上一层平均嵌入向量
Average of neighbor's previous layer embeddings

多个嵌入向量求和(平均)结果，与节点顺序无关
Notice summation is a permutation invariant pooling/aggregation.

Equivariant Property

Message passing and neighbor aggregation in graph convolution networks is permutation equivariant.





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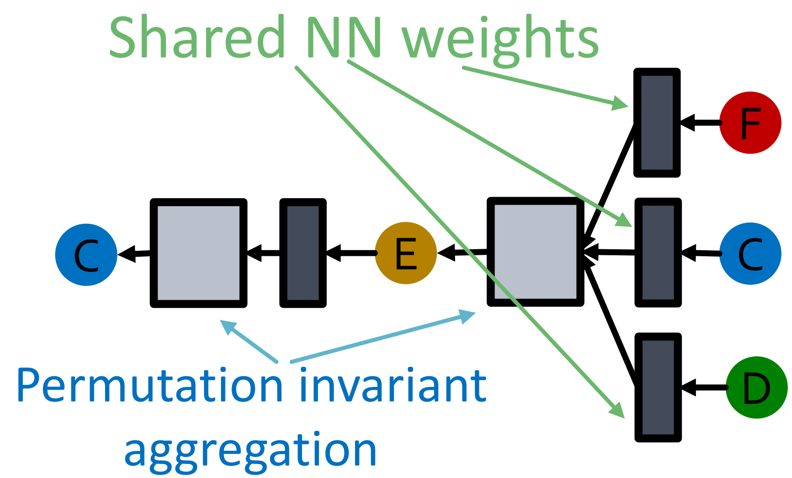
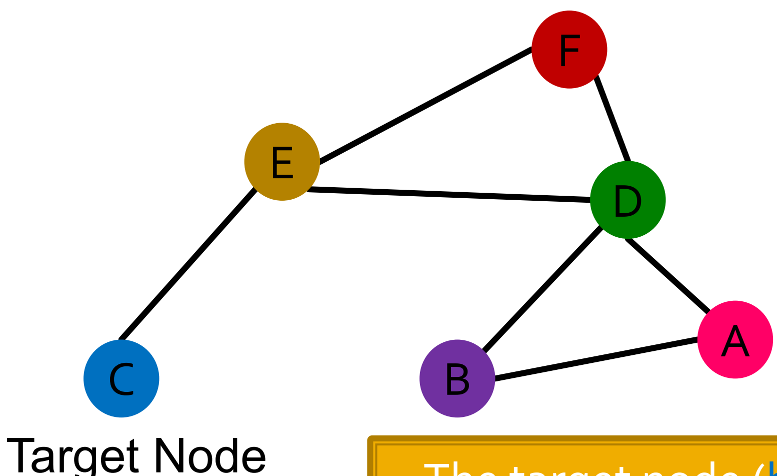
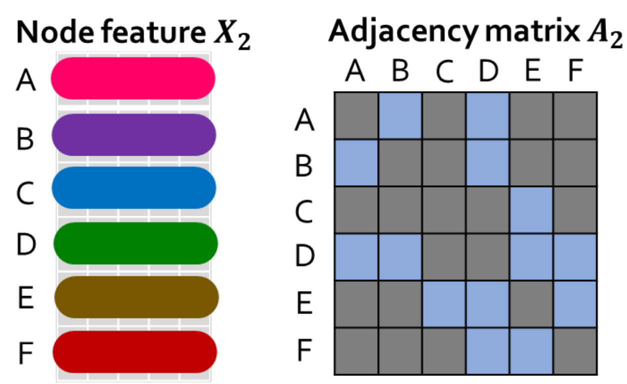


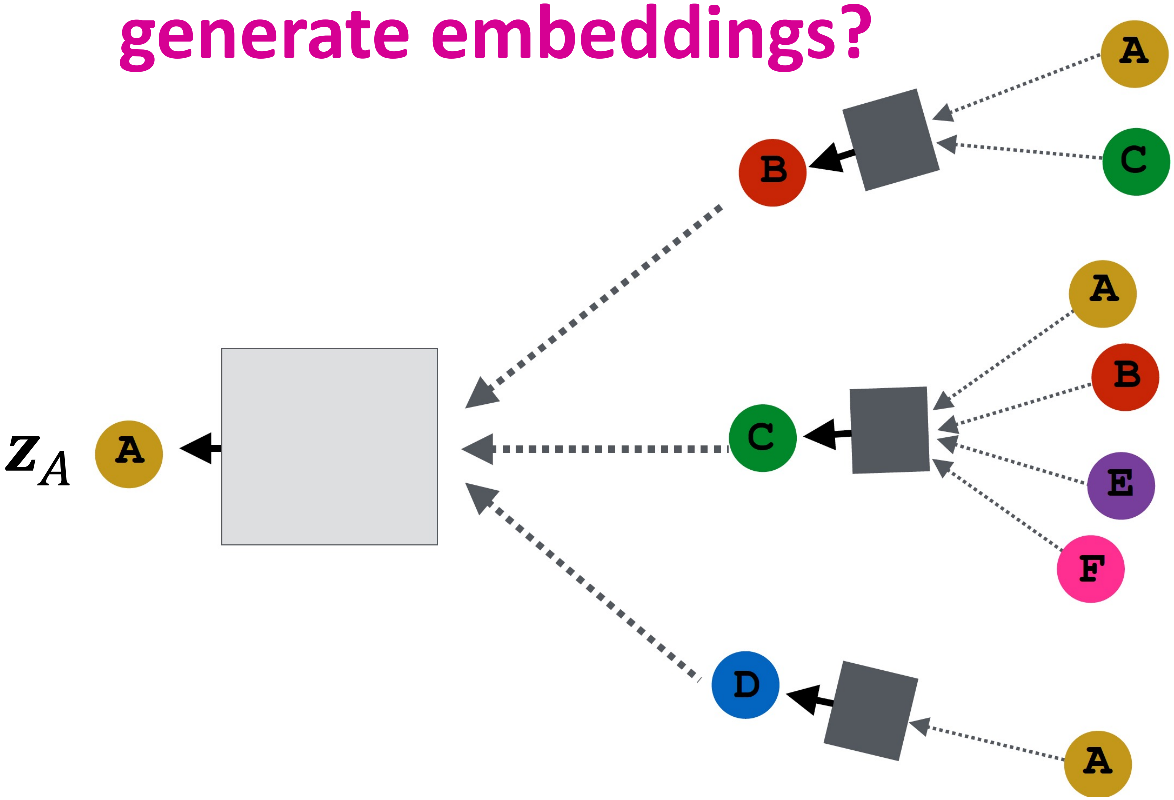


The target node (blue) has the same computation graph for different order plans



Training the Model

How do we train the GCN to generate embeddings?



Need to define a loss function on the embeddings.

Model Parameters

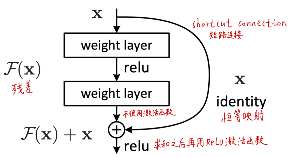
Trainable weight matrices
(i.e., what we learn) 第k层图神经网络
需训练学习得到的权重参数

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

$$h_v^{(k+1)} = \sigma\left(\boxed{W_k} \sum_{u \in N(v)} \frac{h_u^{(k)}}{|N(v)|} + \underbrace{\boxed{B_k} h_v^{(k)}}_{\text{非恒等映射 不是残差连接}}\right), \forall k \in \{0..K-1\}$$

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

Final node embedding



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

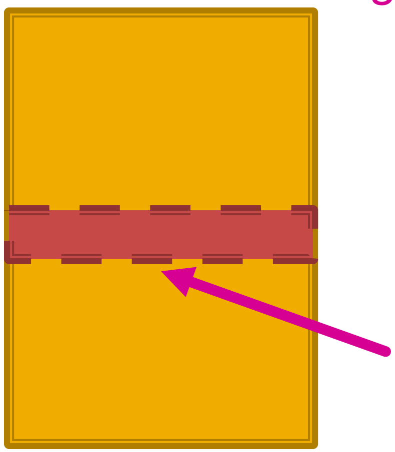
h_v^k: the hidden representation of node v at layer k

- 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,**

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

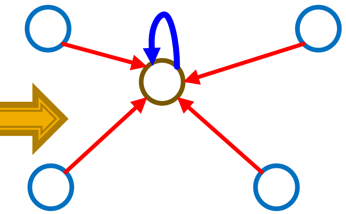


Matrix Formulation (2)

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



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

  - 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 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 the loss $\mathcal{L}$ (see also Slide 15): f:分类或回归预测头

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

  - $\boldsymbol{y}$: node label 节点类别标注
  - $\mathcal{L}$ 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!** 自监督

Unsupervised Training

- **"Similar" nodes have similar embeddings**

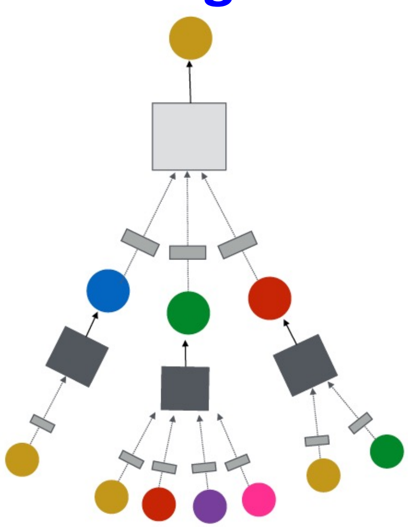
$$\mathcal{L} = \sum_{z_u, z_v} \mathrm{CE}(y_{u,v}, \mathrm{DEC}(z_u, z_v))$$

  - Where $y_{u,v} = 1$ when node u and v are **similar**
  - CE is the cross entropy (Slide 16)
  - DEC is the decoder such as inner product (Lecture 4)
- **Node similarity** can be anything from Lecture 3, e.g., a loss based on:
  - **Random walks** (node2vec, DeepWalk, struc2vec)
  - **Matrix factorization**
  - **Node proximity in the graph**

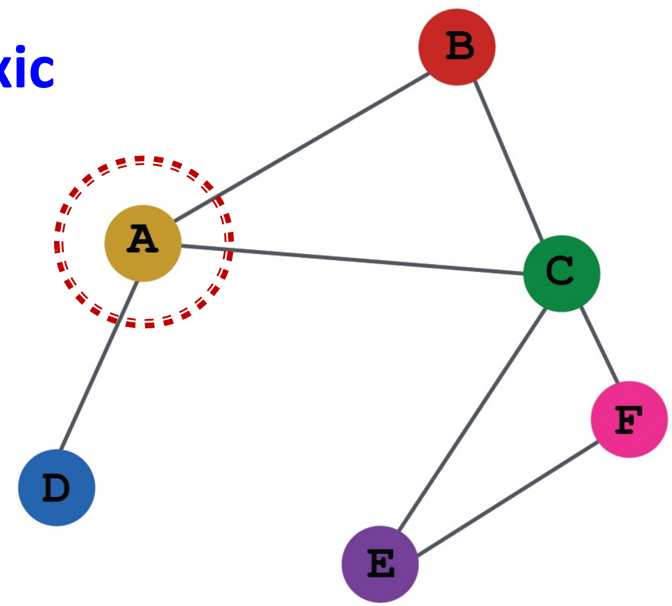
Supervised Training

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

药物-药物相互作用
节点是药物

Supervised Training

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

- Use cross entropy loss (Slide 16)

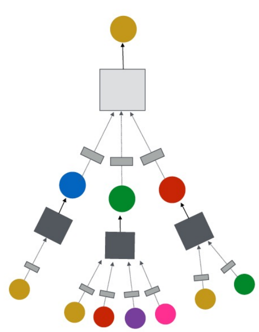
$$\mathcal{L} = \sum_{v \in V} \boxed{y_v} \log(\sigma(\boxed{\mathrm{z}_v^{\mathrm{T}}}\boxed{\theta})) + (1 - \boxed{y_v}) \log(1 - \sigma(\boxed{\mathrm{z}_v^{\mathrm{T}}}\boxed{\theta}))$$

Encoder output:
node embedding

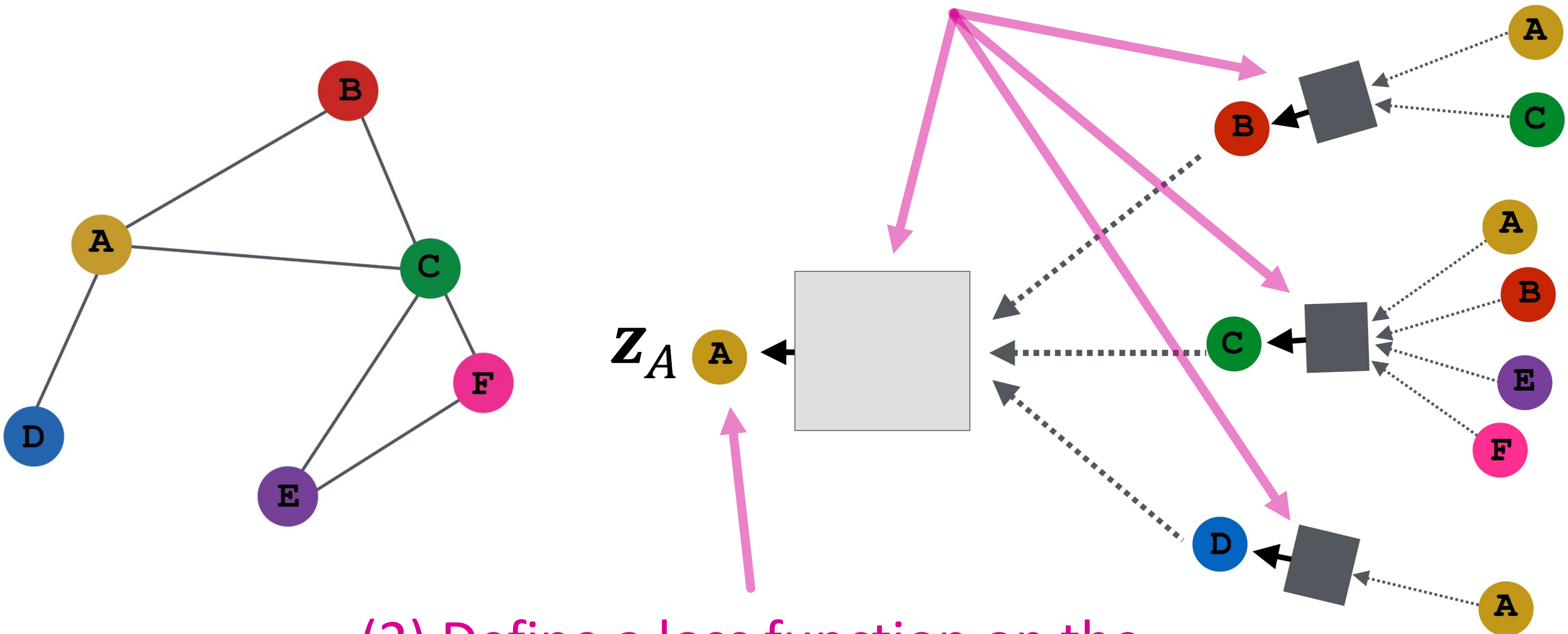
Classification weights
分类预测头权重参数

Node class label

Safe or toxic drug?



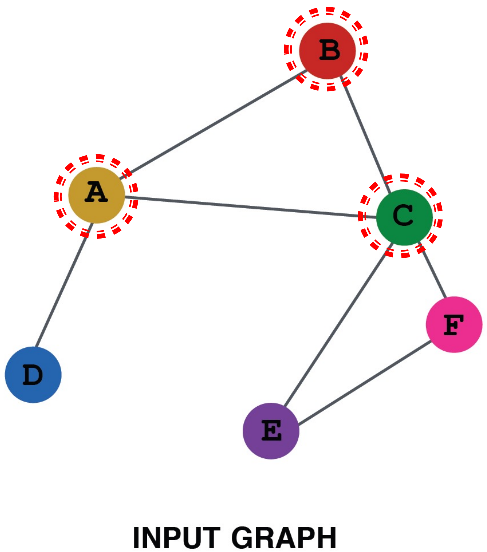
Model Design: Overview



(1) Define a neighborhood aggregation function 聚合邻域信息的方式

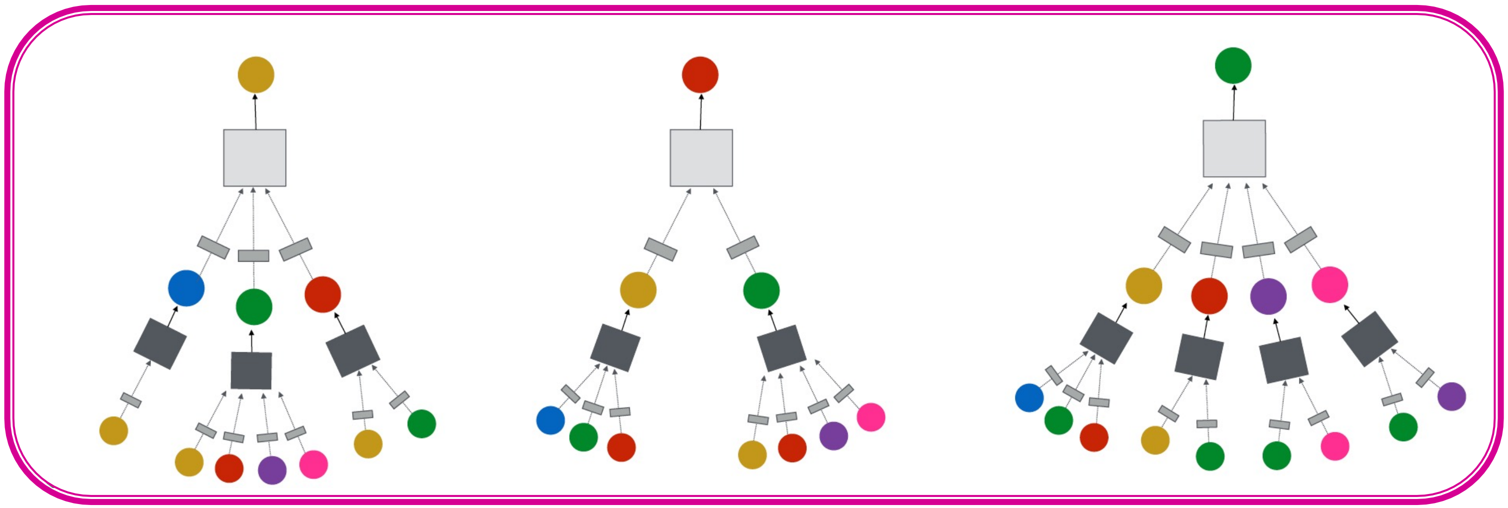
(2) Define a loss function on the embeddings 损失函数

Model Design: Overview

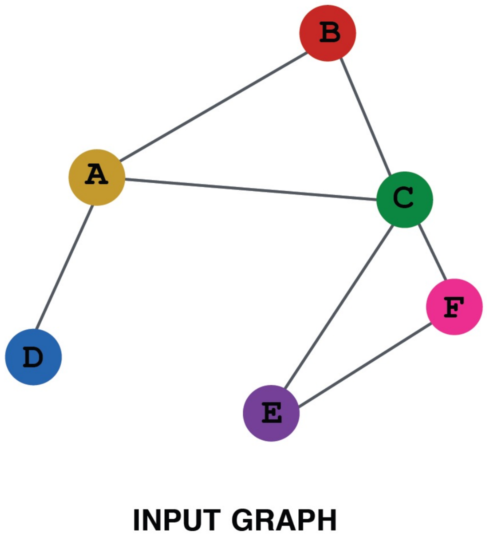


(3) Train on a set of nodes, i.e., a batch of compute graphs

Mini batch 训练



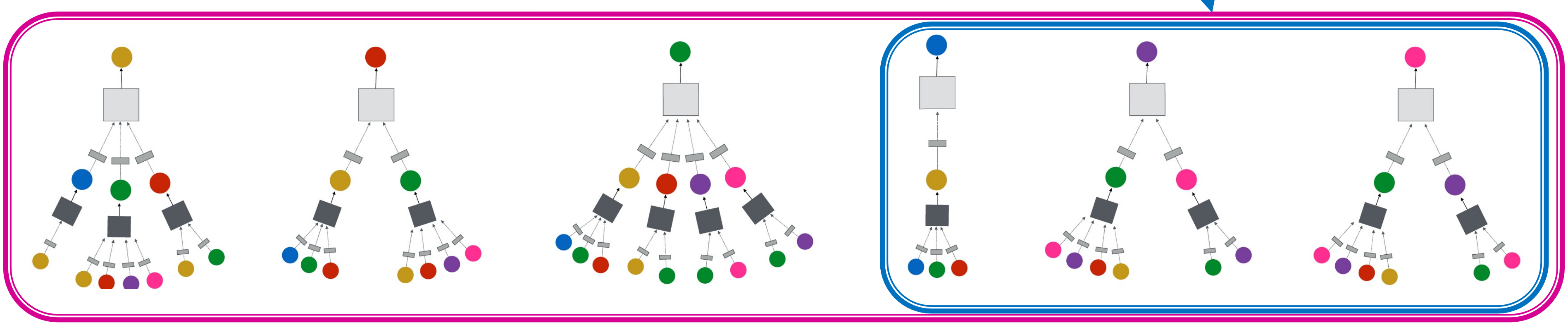
Model Design: Overview



(4) Generate embeddings for nodes as needed

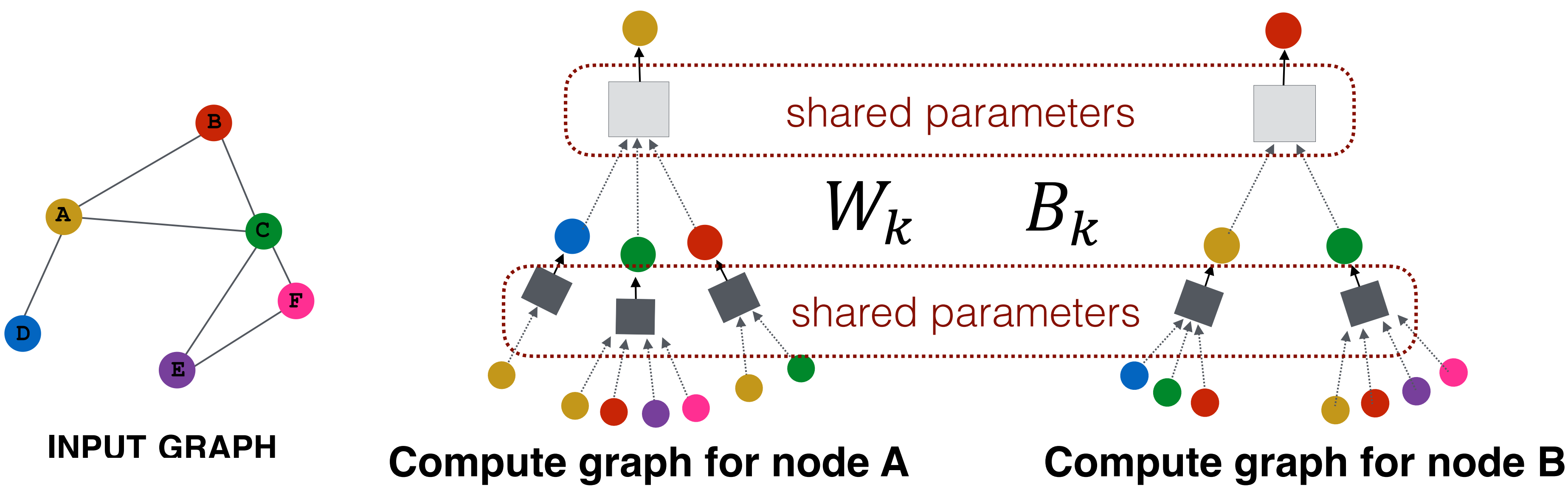
Even for nodes we never trained on!

泛化到新节点、新图
Inductive Learning
归纳式学习



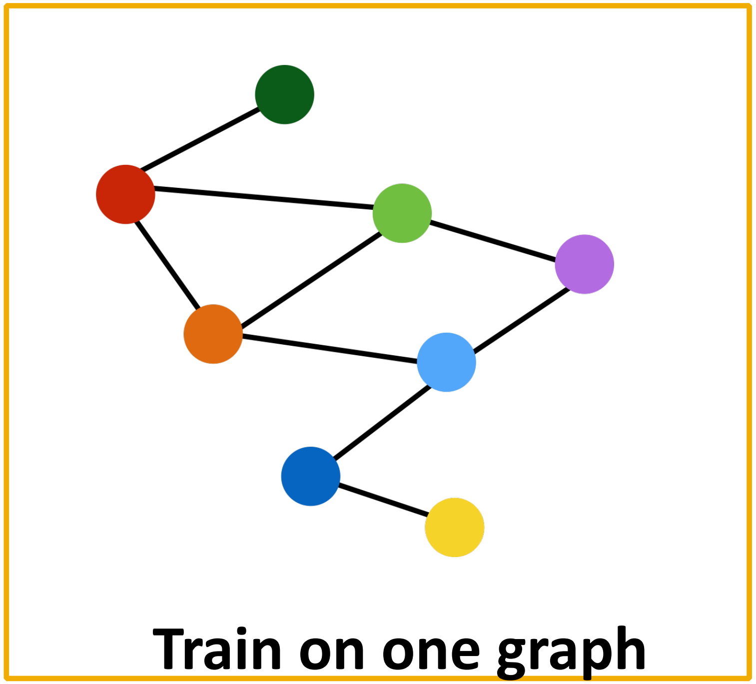
Inductive Capability

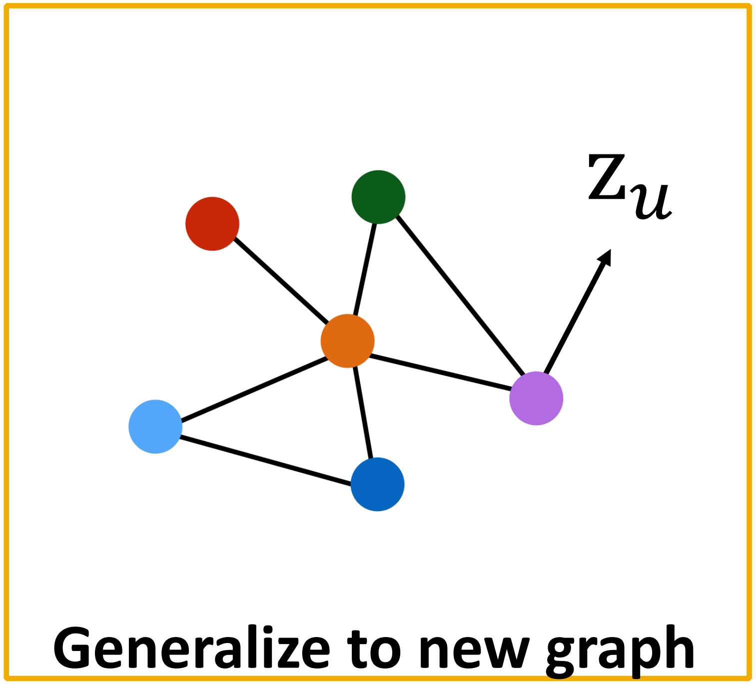
- **The same aggregation parameters are shared for all nodes:**
  - The number of model parameters is sublinear in $|V|$ and we can **generalize to unseen nodes**!



Inductive Capability: New Graphs

Inductive learning 归纳式学习：泛化到新节点、甚至新图

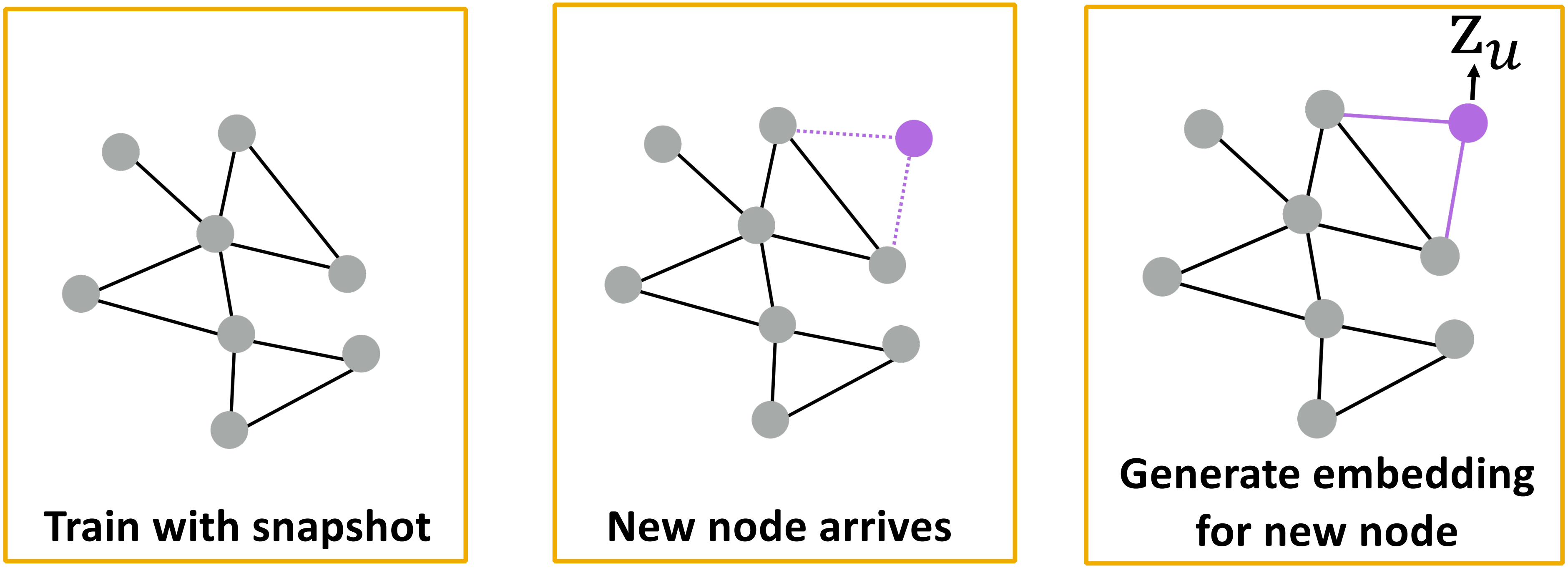




Inductive node embedding → Generalize to entirely unseen graphs

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

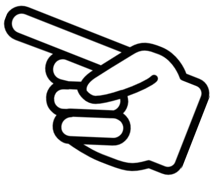
Inductive Capability: New Nodes



- Many application settings constantly encounter previously unseen nodes:
  - E.g., Reddit, YouTube, Google Scholar
- Need to generate new embeddings "on the fly" 随来随用 冷启动

Outline of Today's Lecture

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

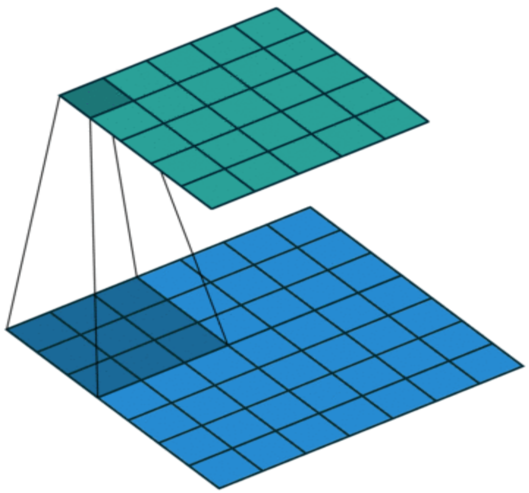


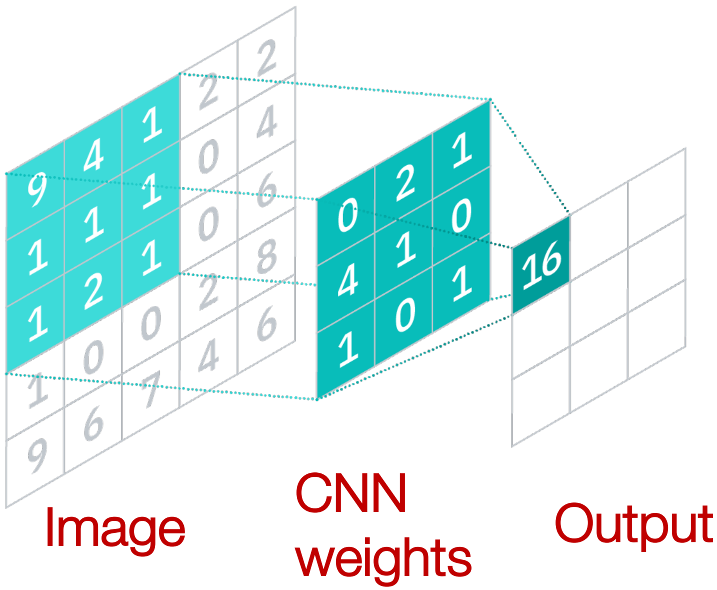
Architecture Comparison

- **How does GNNs compare to 主要的 prominent architectures such as Convolutional Neural Nets, and Transformers?**

Convolutional Neural Network

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



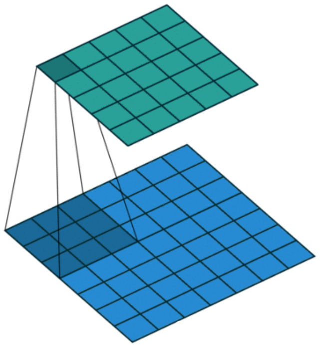


CNN formulation: $h_v^{(l+1)} = \sigma(\sum_{u \in N(v) \cup \{v\}} W_l^u h_u^{(l)}), \quad \forall l \in \{0, \dots, L-1\}$

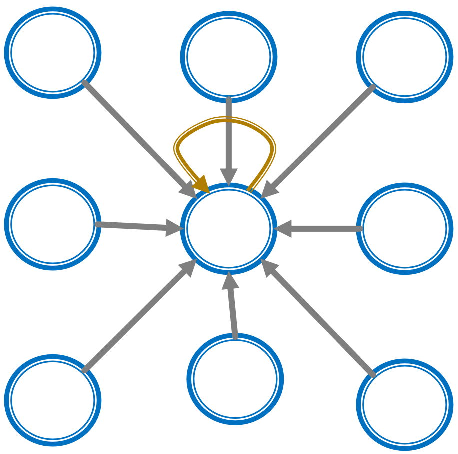
$\boxed{\textbf{\textit{N}}(\boldsymbol{v}) \textbf{ represents the 8 neighbor pixels of } \boldsymbol{v}.}$

GNN vs. CNN

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



Image



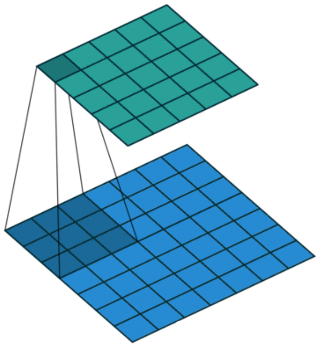
Graph

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

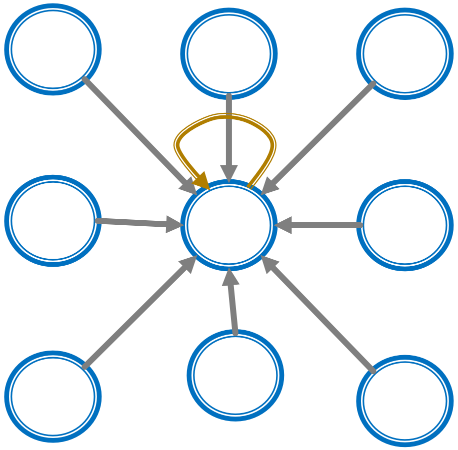
  if we rewrite: $\mathrm{h}_v^{(l+1)} = \sigma(\sum_{u \in \mathrm{N}(v)} \mathbf{W}_l^u \mathrm{h}_u^{(l)} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \ldots, L-1\}$

GNN vs. CNN

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



Image



Graph

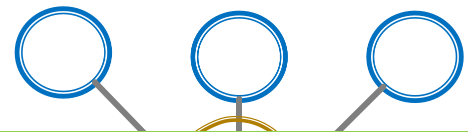
GNN formulation: $\mathrm{h}_v^{(l+1)} = \sigma(\mathbf{W}_l \sum_{u \in \mathrm{N}(v)} \frac{\mathrm{h}_u^{(l)}}{|\mathrm{N}(v)|} + \mathrm{B}_l \mathrm{h}_v^{(l)}), \forall l \in \{0, \dots, L-1\}$

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:



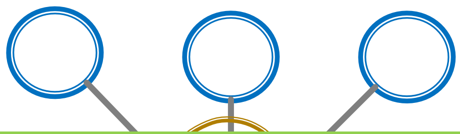
固定的邻域和固定的顺序

- **CNN can be seen as a special GNN with fixed neighbor size and ordering:**
  卷积核
  - **The size of the filter is pre-defined for a CNN.**
  任意的
  - **The advantage of GNN is it processes arbitrary graphs with different degrees for each node.**

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:



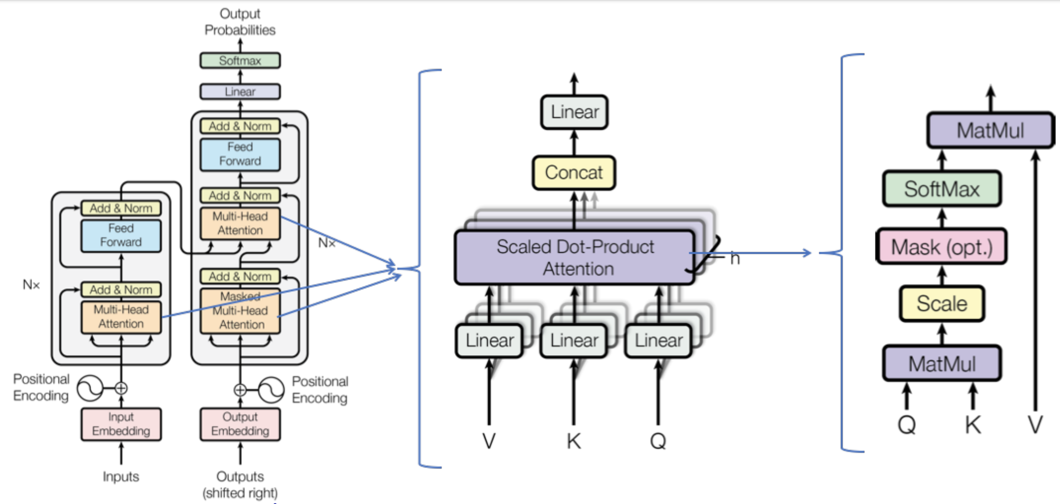
- CNN can be seen as a special GNN with fixed neighbor size and ordering.
- CNN is not permutation equivariant.
  - Switching the order of pixels will leads to different outputs.

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)}

[Attention is all you need. Vaswani et al., NeurIPS 2017]

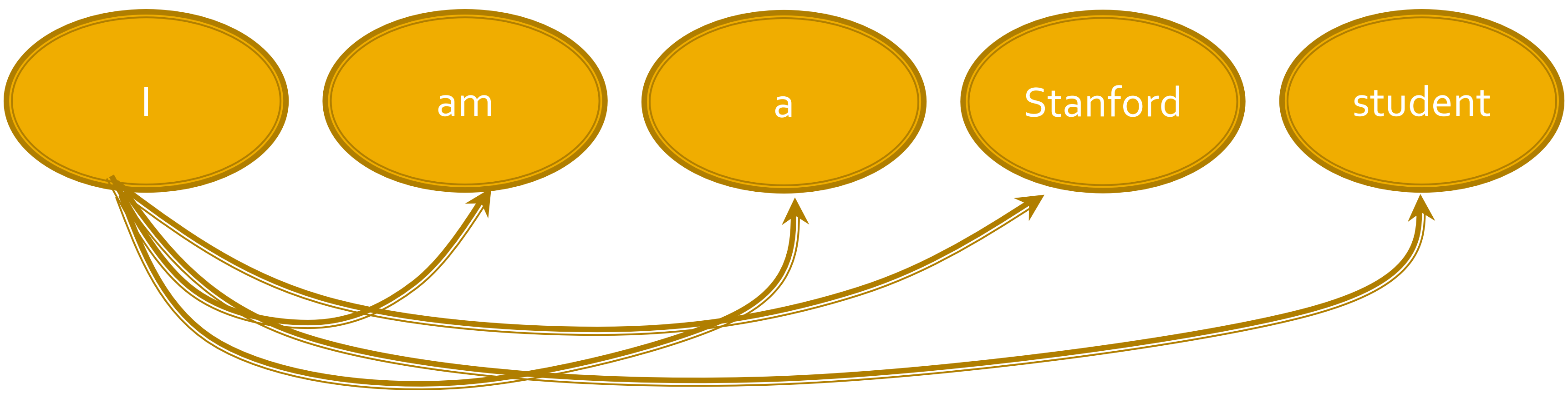
Transformer

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



Key component: self-attention 自注意力

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



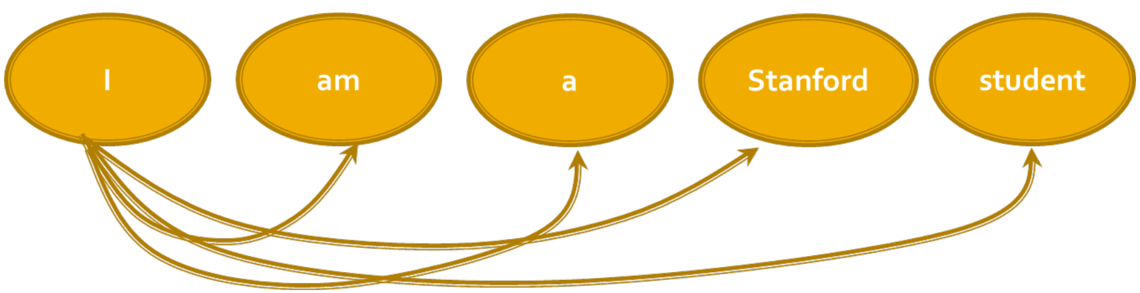
A nice blog plot for this: https://towardsdatascience.com/transformers-are-graph-neural-networks-bca9f75412aa

GNN vs. Transformer

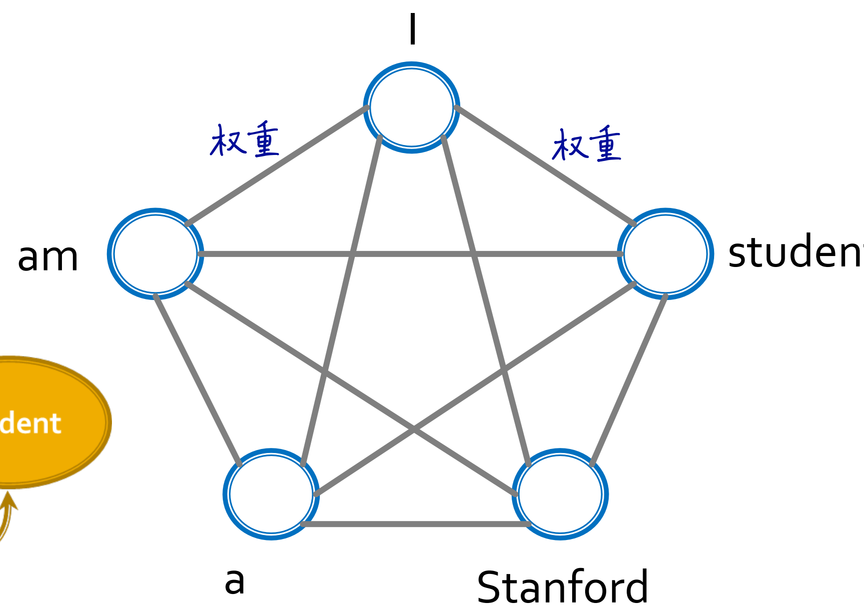
Transformer layer can be seen as a special GNN that runs on a fully-connected “word” graph!

Graph Attention Network (GAT)

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**
  - Basics of neural networks
    - Loss, Optimization, Gradient, SGD, non-linearity, MLP
  - Idea for Deep Learning for Graphs
    计算图
    - 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 图卷积神经网络
    - Mean aggregation; can be expressed in matrix form
  - GNN is a general architecture
    - CNN and Transformer can be viewed as a special GNN