# Stanford CS224W: Graph Neural Networks

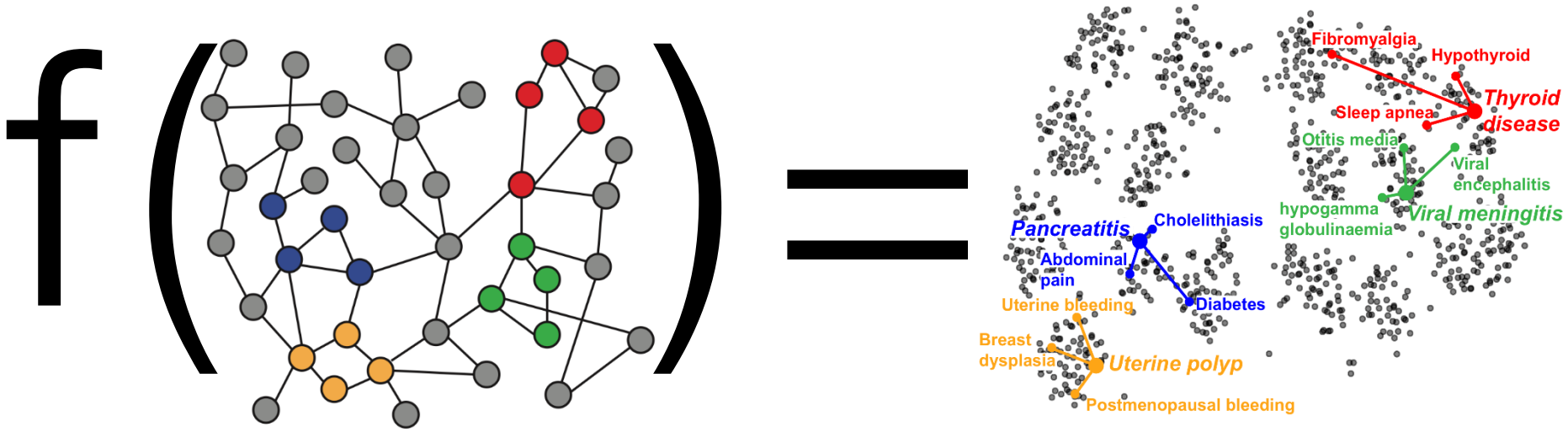
CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

# Recap: Node Embeddings

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




Input graph

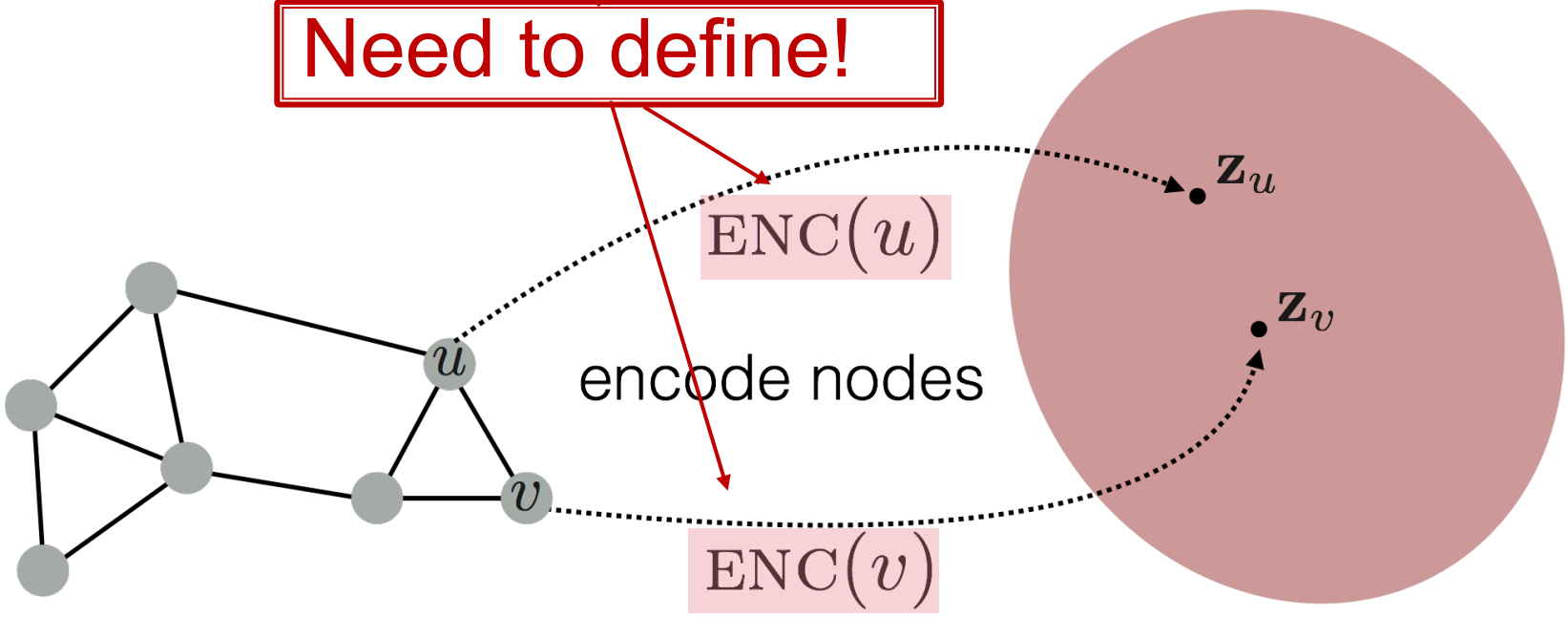
2D node embeddings

**How to learn mapping function $f$?**

# Recap: Node Embeddings

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

Need to define!




Input network

d-dimensional embedding space

# Recap: Two Key Components

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

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

$d$-dimensional embedding

node in the input graph

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

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

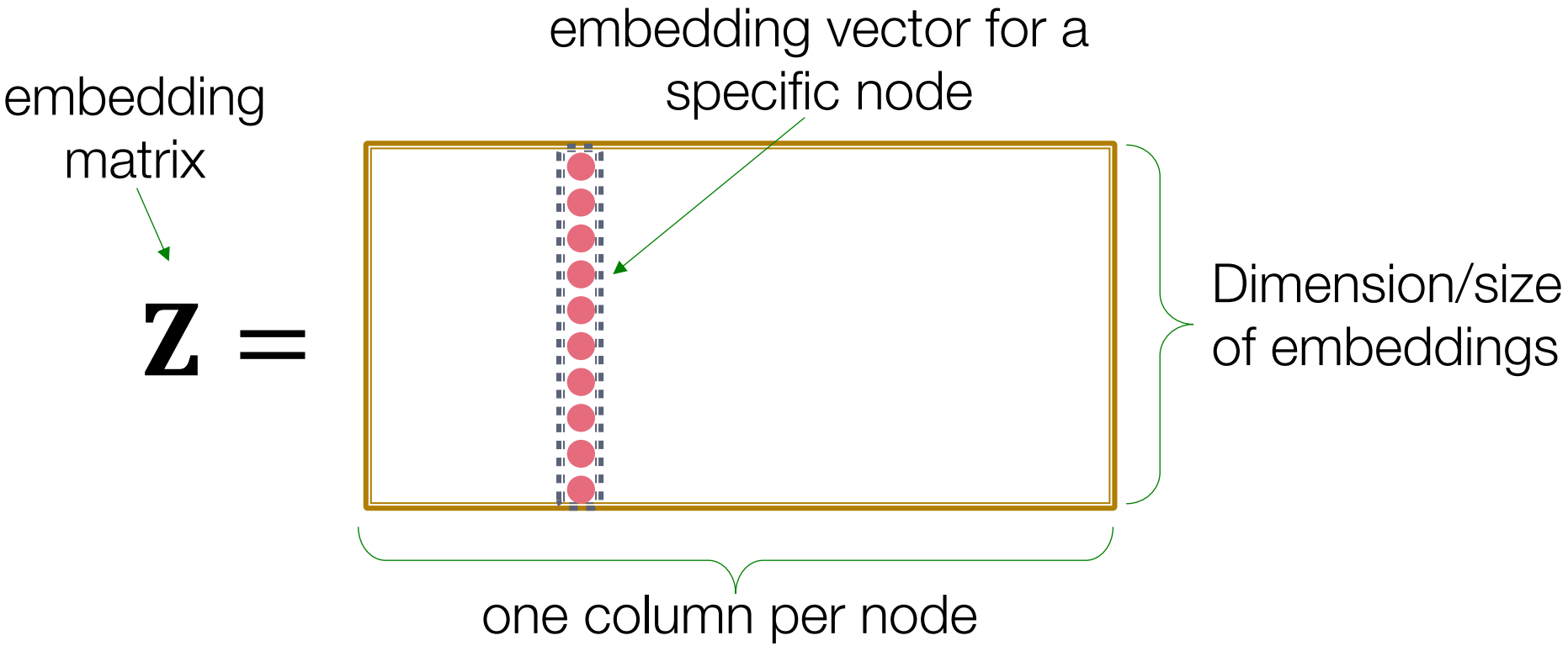
**Decoder**

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

- **Limitations** of shallow embedding methods:
  - $O(|V|)$ **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**:
    - Many graphs have features that we can and should leverage

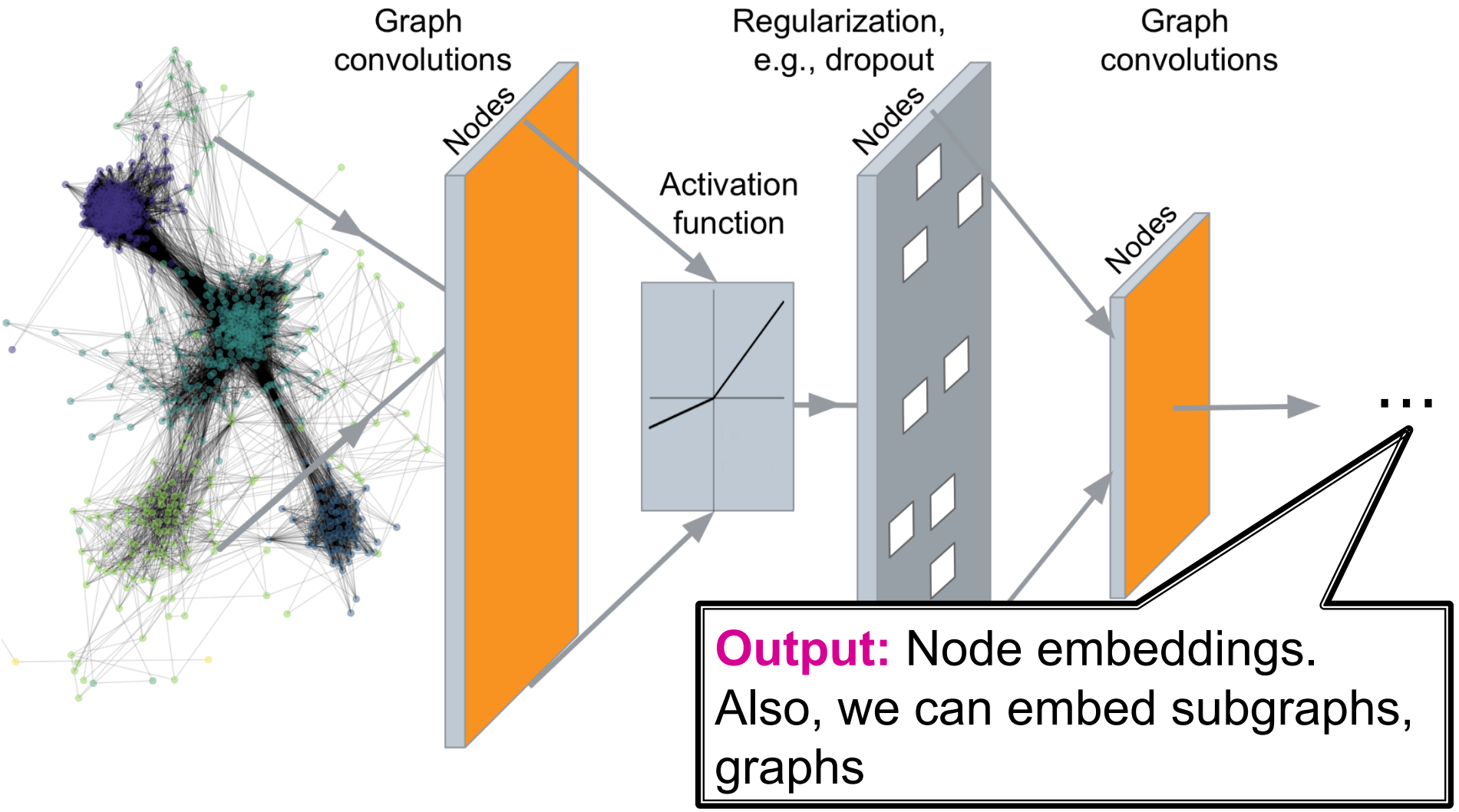
# Today: Deep Graph Encoders

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

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

- **Note:** All these deep encoders can be **combined with node similarity functions** defined in the lecture 3

# Deep Graph Encoders

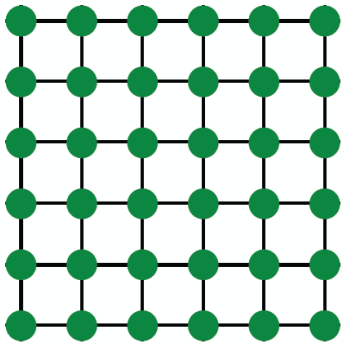


# Tasks on Networks

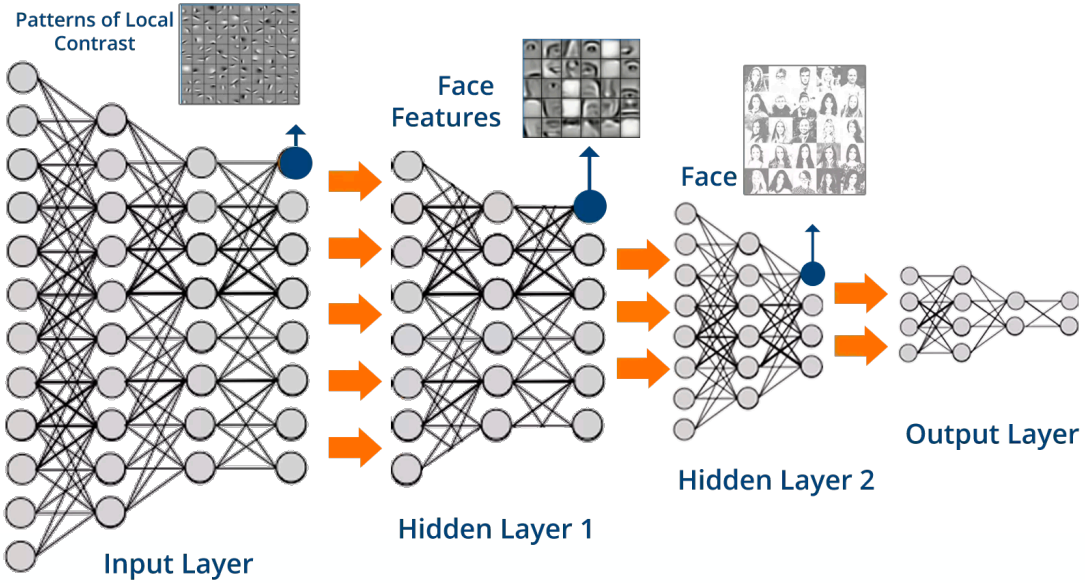
## Tasks we will be able to solve:

- 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

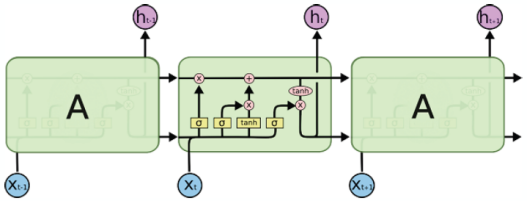


Images




Text/Speech



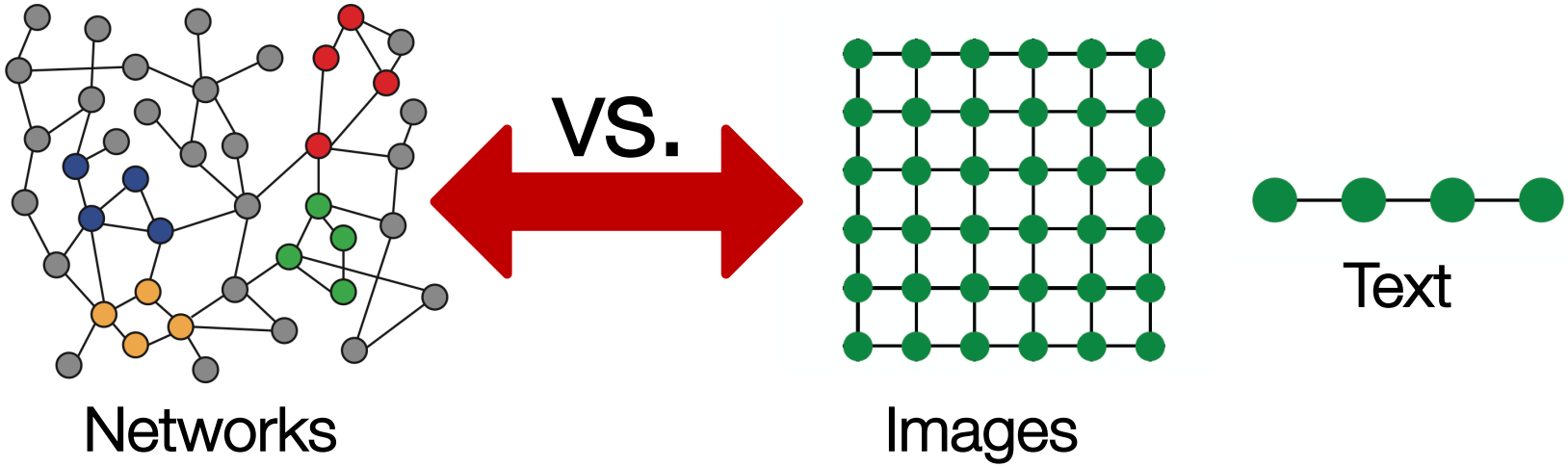



**Modern deep learning toolbox is designed for simple sequences & grids**

# 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 and GraphSAGE**

# Stanford CS224W: Basics of Deep Learning

CS224W: Machine Learning with Graphs

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# Machine Learning as Optimization

- **Supervised learning:** we are given input $x$, and the goal is to predict label $y$
- **Input $x$ can be:**
  - Vectors of real numbers
  - Sequences (natural language)
  - Matrices (images)
  - Graphs (potentially with node and edge features)
- **We formulate the task as an optimization problem**

# Machine Learning as Optimization

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

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

**Objective function**

- $\Theta$: 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

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

  - 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

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

$y$ is of class "3"

- $f(\boldsymbol{x}) = \text{Softmax}(g(\boldsymbol{x}))$
  - Recall from lecture 3: $f(\boldsymbol{x})_i = \frac{e^{g(x)_i}}{\sum_{j=1}^{C} e^{g(x)_j}}$,

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

where $C$ is the number of classes.

  - e.g. $f(\boldsymbol{x}) =$ | 0.1 | 0.3 | 0.4 | 0.1 | 0.1 |

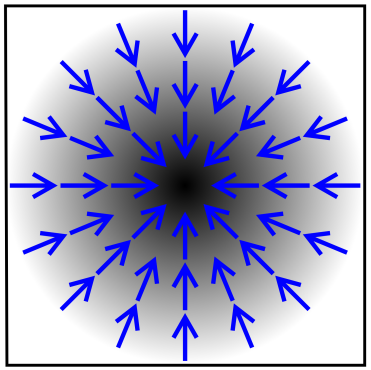
- $\text{CE}(\boldsymbol{y}, f(\boldsymbol{x})) = -\sum_{i=1}^{C}(y_i \log f(x)_i)$
  - $y_i, f(x)_i$ are the **actual** and **predicted** value of the $i$-th class.
  - **Intuition:** the lower the loss, the closer the prediction is to one-hot
- **Total loss over all training examples:**
  - $\mathcal{L} = \sum_{(\boldsymbol{x},\boldsymbol{y})\in\mathcal{T}} \text{CE}(\boldsymbol{y}, f(\boldsymbol{x}))$
  - $\mathcal{T}$: training set containing all pairs of data and labels $(\boldsymbol{x}, \boldsymbol{y})$

# Machine Learning as Optimization

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

Partial derivative

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



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

  - $\Theta_1, \Theta_2$ … : components of $\Theta$
- 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.
- Gradient is the directional derivative in the **direction of largest increase**

# Gradient Descent

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

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

- **Training:** Optimize $\Theta$ iteratively
  - **Iteration**: 1 step of gradient descent

- **Learning rate (LR) $\eta$:**
  - Hyperparameter that controls the size of gradient step
  - Can vary over the course of training (LR scheduling)
- Ideal termination condition: **0** gradient
  - 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!
    - 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** $\boldsymbol{\mathcal{B}}$ containing a subset of the dataset, use it as input $\boldsymbol{x}$

# Minibatch SGD

- **Concepts:**
  - **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)

- 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, the function $f$ can be very complex
- To start simple, consider linear function

$$f(\boldsymbol{x}) = W \cdot \boldsymbol{x}, \qquad \Theta = \{W\}$$

- If $f$ returns a scalar, then $W$ is a learnable **vector**

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

- If $f$ returns a vector, then $W$ is the **weight matrix**

$$\nabla_W f = W^T$$

**Jacobian matrix of $f$**

# Back-propagation

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

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

- Recall **chain rule**:

$$\frac{\mathrm{d}z}{\mathrm{d}x} = \frac{\mathrm{d}z}{\mathrm{d}y} \cdot \frac{\mathrm{d}y}{\mathrm{d}x}$$

In other words:

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

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

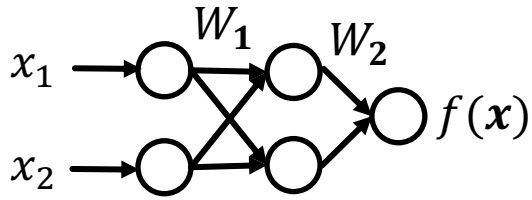
$\mathrm{g}(z) = W_2 z$

- E.g. $\nabla_{\boldsymbol{x}} f = \frac{\partial f}{\partial (W_1\boldsymbol{x})} \cdot \frac{\partial (W_1\boldsymbol{x})}{\partial \boldsymbol{x}}$

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

# Back-propagation Example (1)

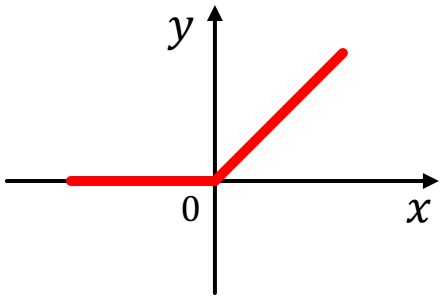
- **Example:** Simple 2-layer linear network
- $f(\boldsymbol{x}) = g\big(h(x)\big) = W_2(W_1\boldsymbol{x})$

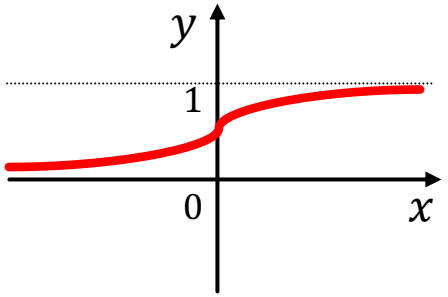



- $\mathcal{L} = \sum_{(\boldsymbol{x},\boldsymbol{y})\in\mathcal{B}} \big|\big|\big(\boldsymbol{y}, -f(\boldsymbol{x})\big)\big|\big|_2$ sums the L2 loss in a minibatch $\mathcal{B}$
- **Hidden layer:** intermediate representation for input $\boldsymbol{x}$
  - Here we use $h(x) = W_1\boldsymbol{x}$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

# 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
- **Introduce non-linearity:**
  - **Rectified linear unit (ReLU)**
    $ReLU(x) = \max(x, 0)$
  - **Sigmoid**
    $$\sigma(x) = \frac{1}{1 + e^{-x}}$$



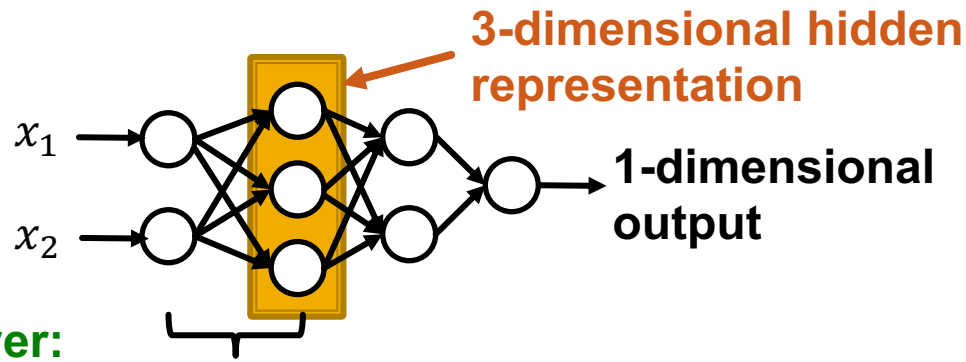



# Multi-layer Perceptron (MLP)

- **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 $\boldsymbol{x}$
  - $\sigma$ is non-linearity function (e.g., sigmod)
- 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 $\nabla_{\Theta}\mathcal{L}$ using a chain rule
- Use **stochastic gradient descent (SGD)** to optimize for $\Theta$ over many iterations

# Outline of Today's Lecture

1. **Basics of deep learning** ✓
2. **Deep learning for graphs** 
3. **Graph Convolutional Networks and GraphSAGE**

# Stanford CS224W: Deep Learning for Graphs

CS224W: Machine Learning with Graphs

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# Content

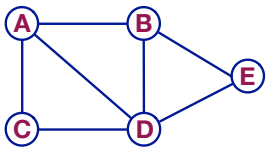
- **Local network neighborhoods:**
  - Describe aggregation strategies
  - Define computation graphs
- **Stacking multiple layers:**
  - Describe the model, parameters, training
  - How to fit the model?
  - Simple example for unsupervised and supervised training

# Setup

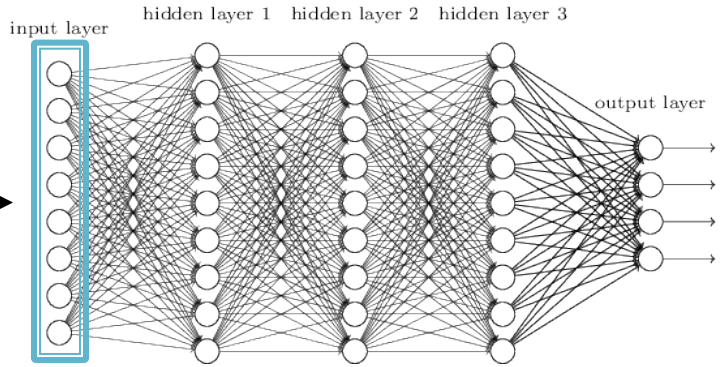
- **Assume we have a graph $G$:**
  - $V$ is the **vertex set**
  - $\boldsymbol{A}$ is the **adjacency matrix** (assume binary)
  - $\boldsymbol{X} \in \mathbb{R}^{m \times |V|}$ is a matrix of **node features**
  - $v$: a node in $V$; $N(v)$: the set of neighbors of $v$.
  - **Node features:**
   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

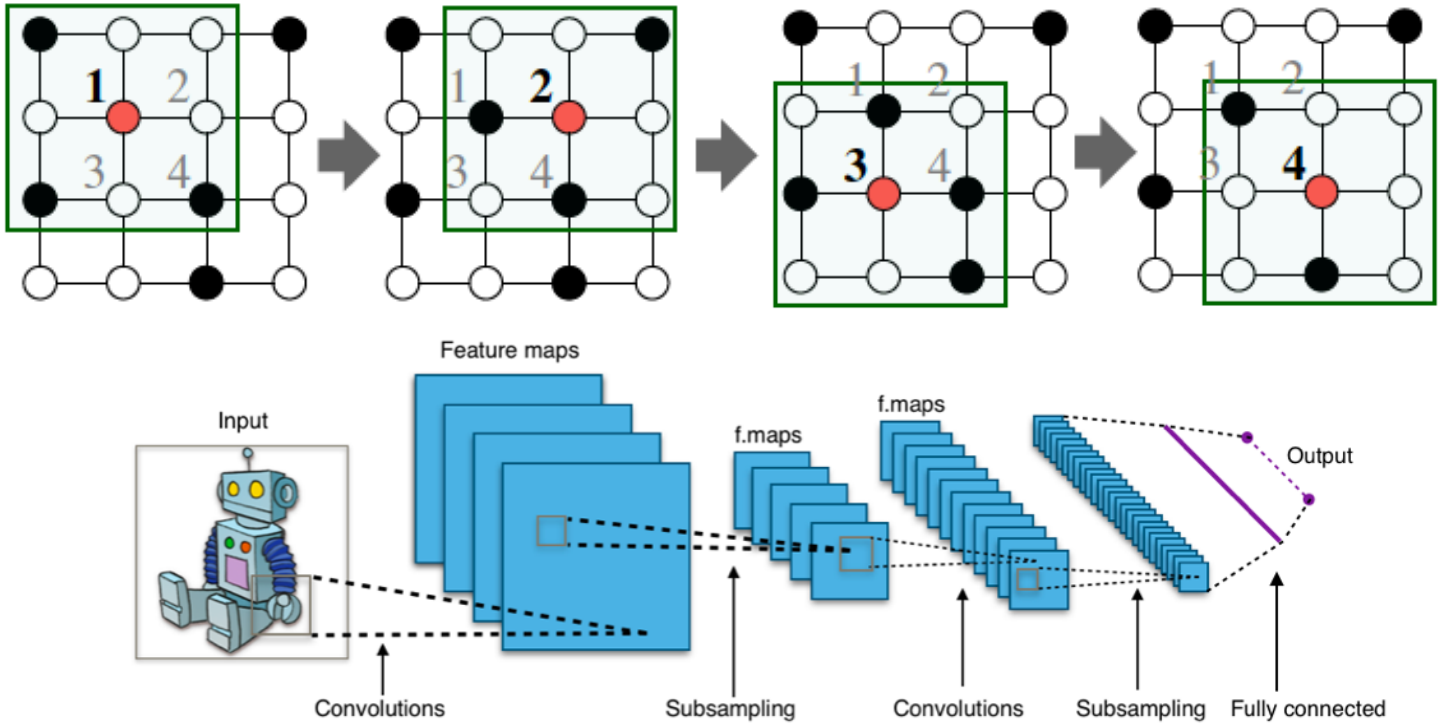



?

- 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:

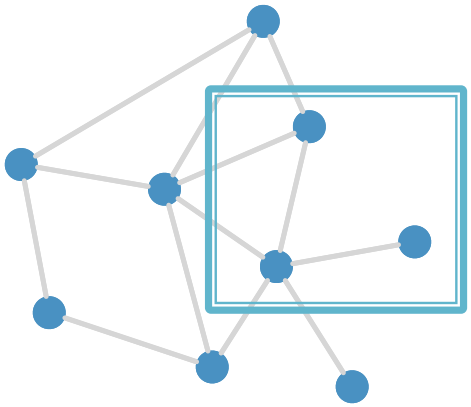



Goal is to generalize convolutions beyond simple lattices

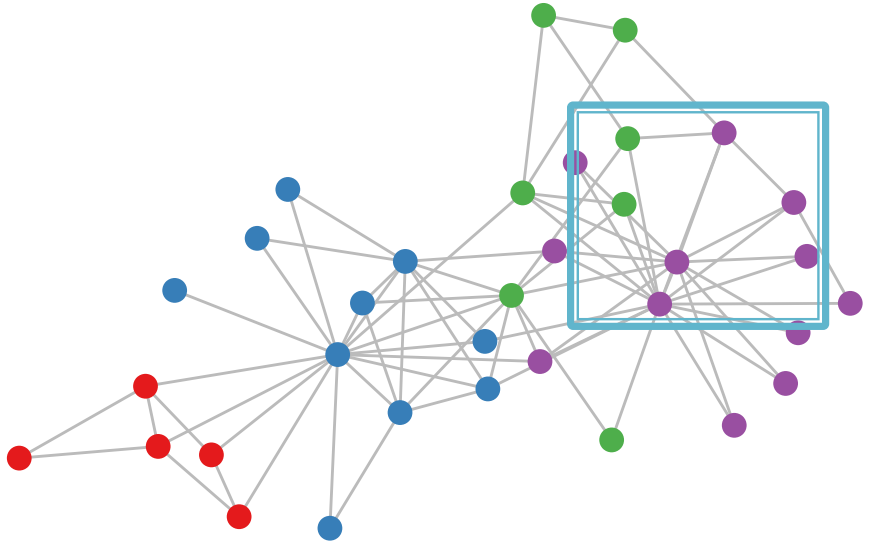
Leverage node features/attributes (e.g., text, images)

# Real-World Graphs

**But our graphs look like this:**



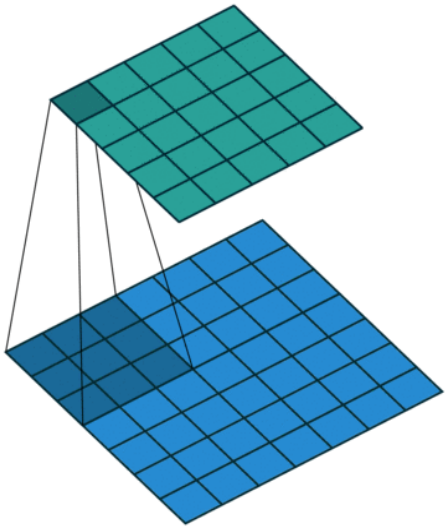
or this:



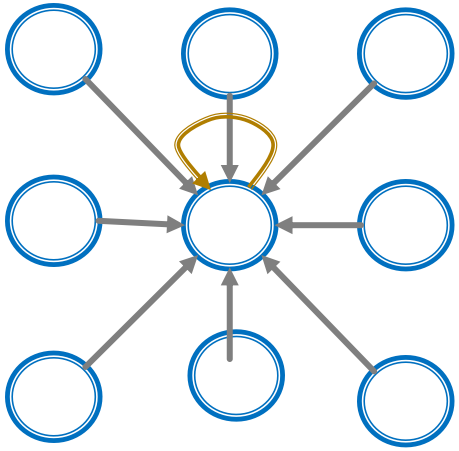
- There is no fixed notion of locality or sliding window on the graph
- Graph is permutation invariant

# From Images to Graphs

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



Image



Graph

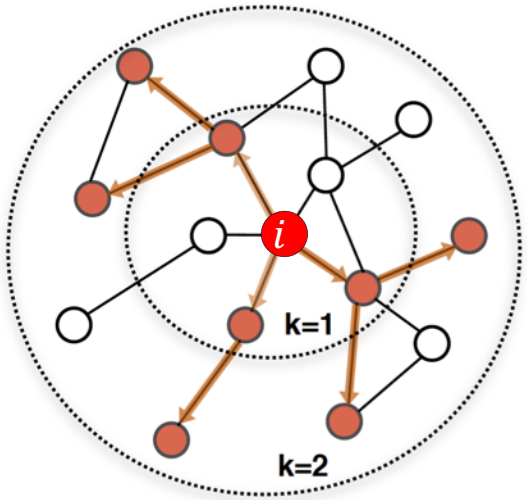
**Idea:** transform information at the neighbors and combine it:

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

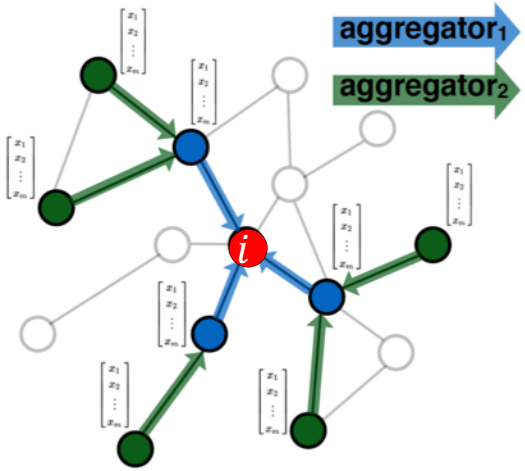
[Kipf and Welling, ICLR 2017]

# Graph Convolutional Networks

Idea: Node's neighborhood defines a computation graph




Determine node computation graph

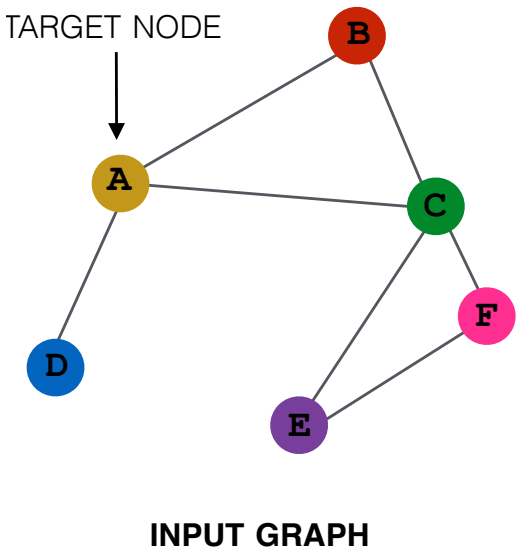



Propagate and transform information

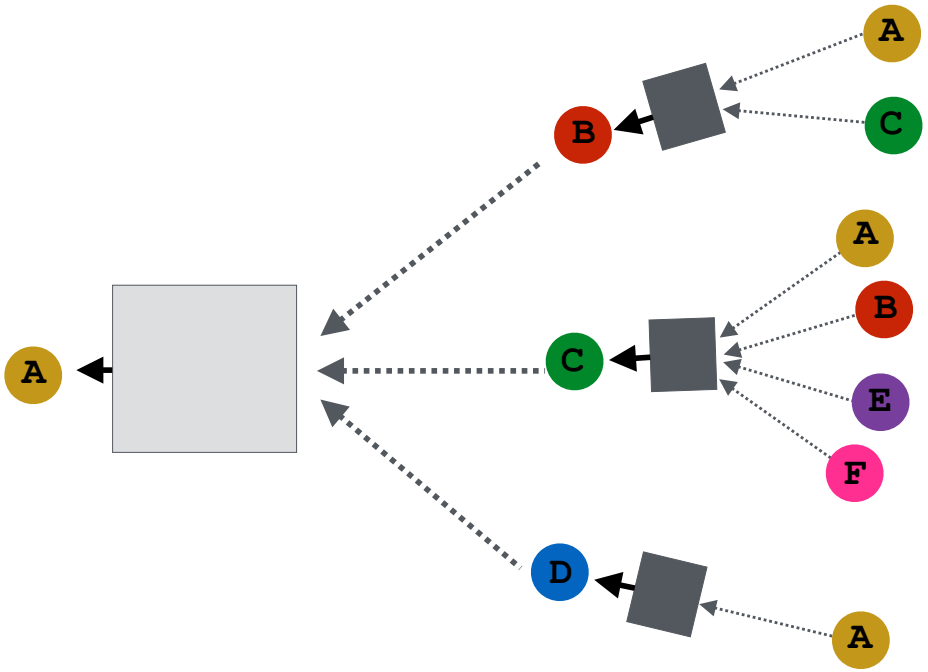
**Learn how to propagate information across the graph to compute node features**

# Idea: Aggregate Neighbors

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

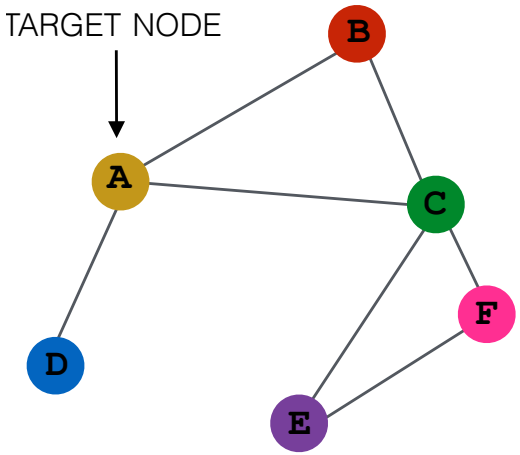



INPUT GRAPH

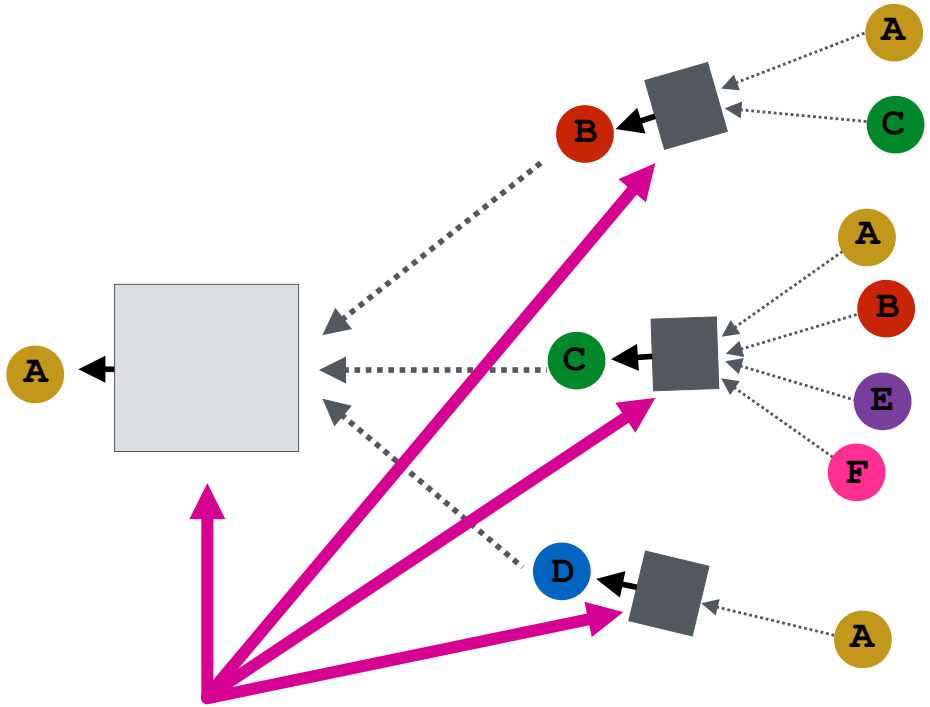


# Idea: Aggregate Neighbors

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




INPUT GRAPH

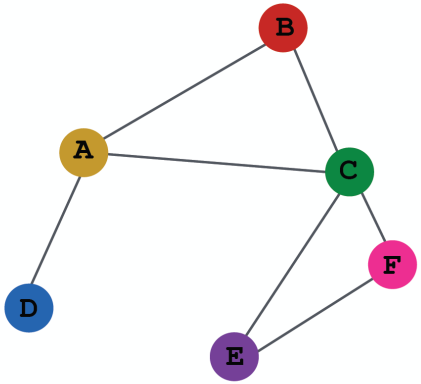



Neural networks

# Idea: Aggregate Neighbors

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

Every node defines a computation graph based on its neighborhood!

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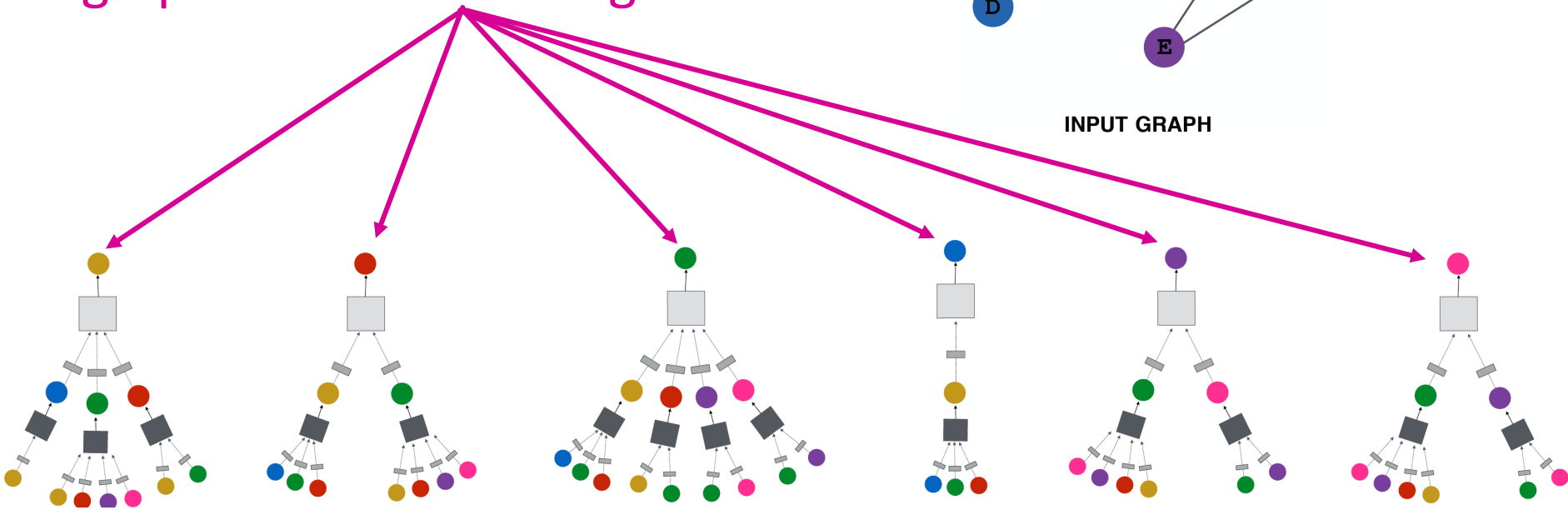
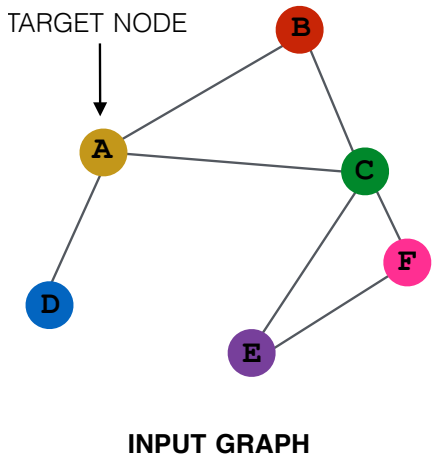
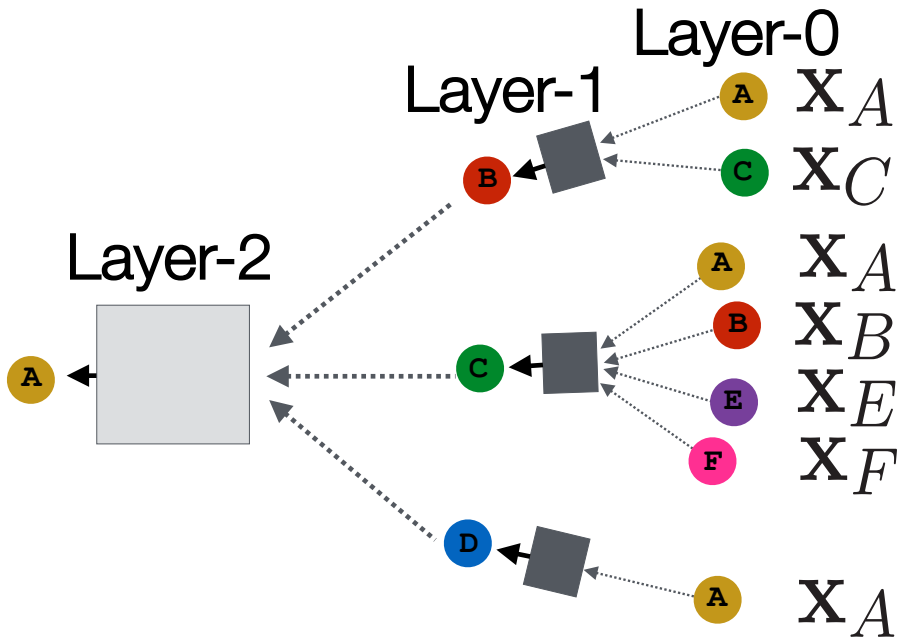


# Deep Model: Many Layers

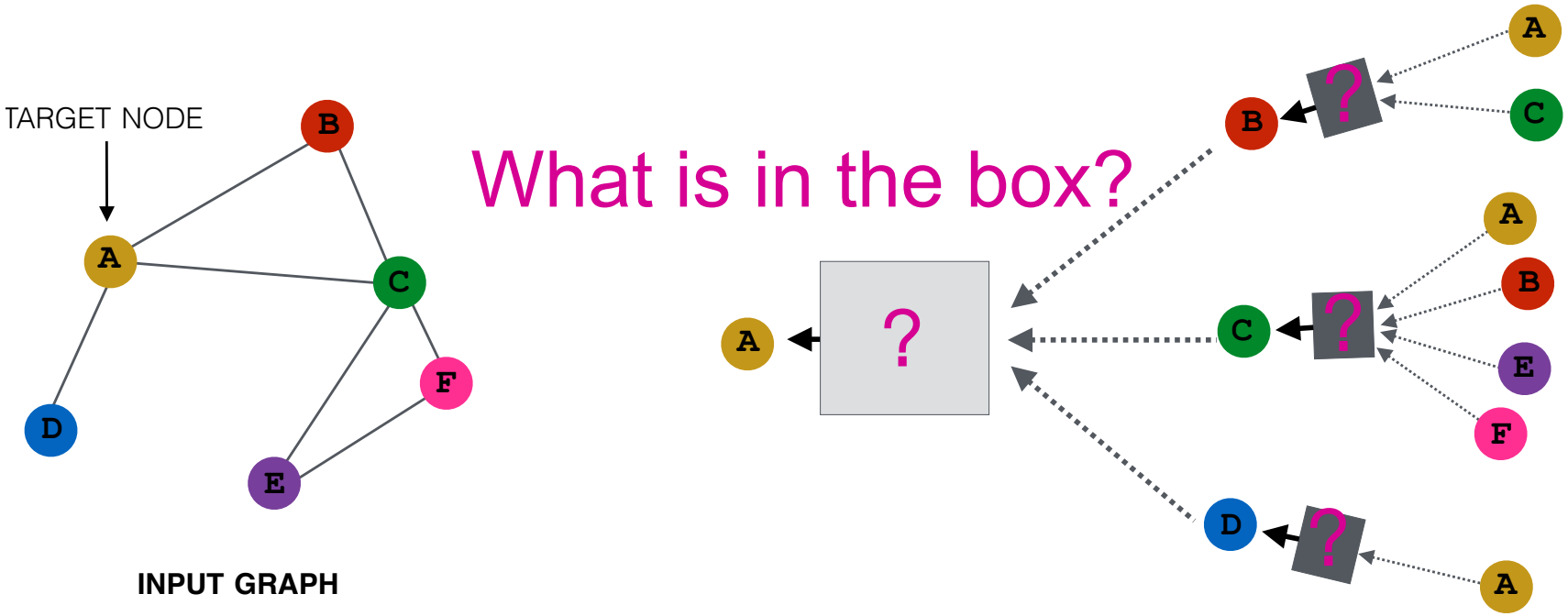
- Model can be of arbitrary depth:
  - Nodes have embeddings at each layer
  - Layer-0 embedding of node $u$ is its input feature, $x_u$
  - Layer-$k$ embedding gets information from nodes that are K hops away



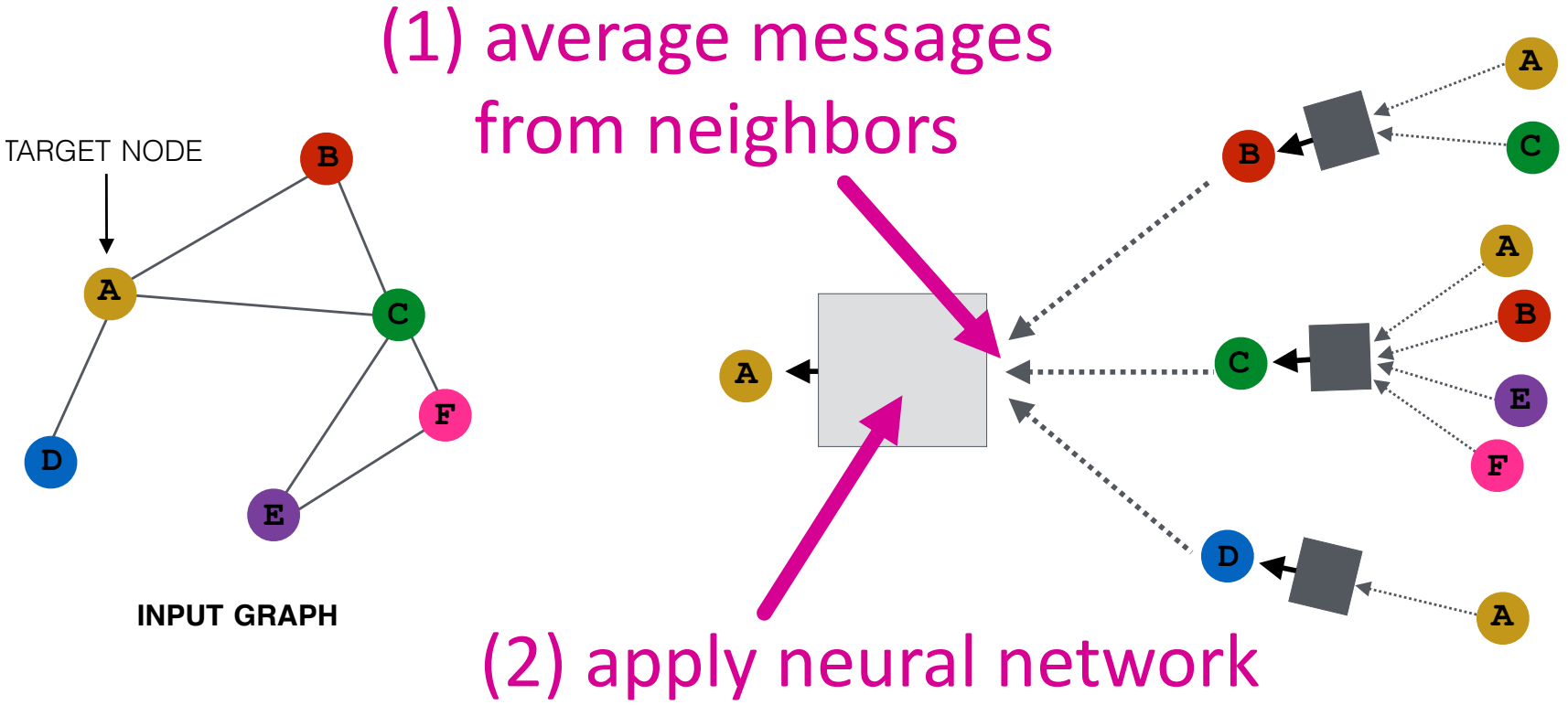
# Neighborhood Aggregation

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



# 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

$$\mathbf{h}_v^0 = \mathbf{x}_v$$

embedding of $v$ at layer $l$

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

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

Embedding after L layers of neighborhood aggregation

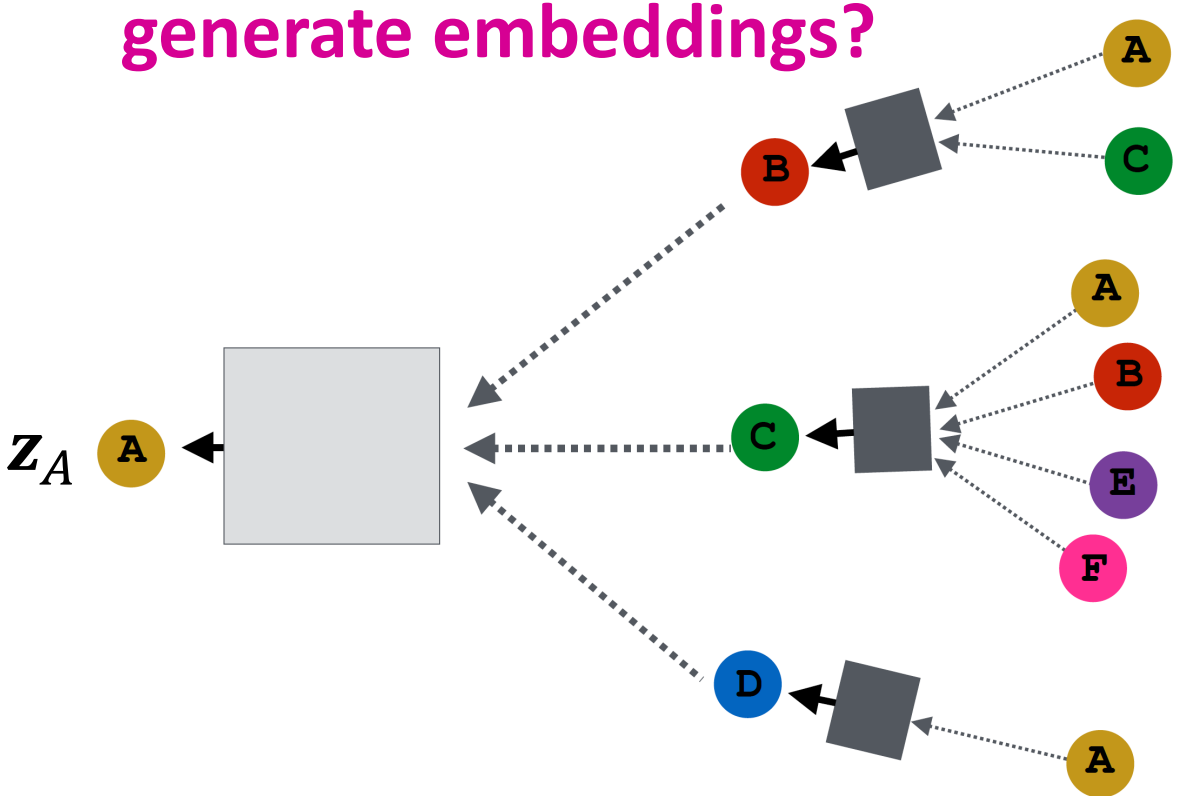
Non-linearity (e.g., ReLU)

Average of neighbor's previous layer embeddings

Total number of layers

# Training the Model

**How do we train the model to generate embeddings?**




**Need to define a loss function on the embeddings**

# Model Parameters

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

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

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

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

Final node embedding

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

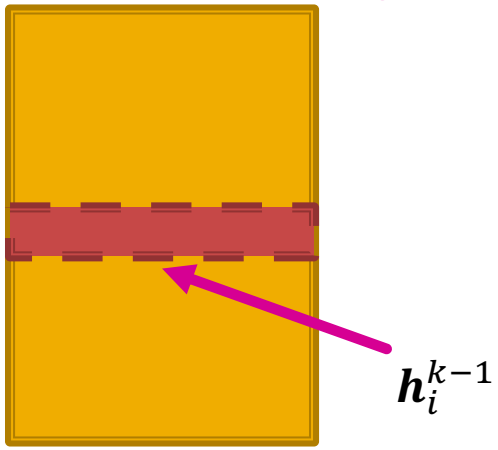
$h_v^l$: the hidden representation of node $v$ at layer $l$

- $W_k$: 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 $H^{(l)} = [h_1^{(l)} \dots h_{|V|}^{(l)}]^{\mathrm{T}}$
- Then: $\sum_{u \in N_v} h_u^{(l)} = \mathrm{A}_{v,:}\mathrm{H}^{(l)}$
- 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,**

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



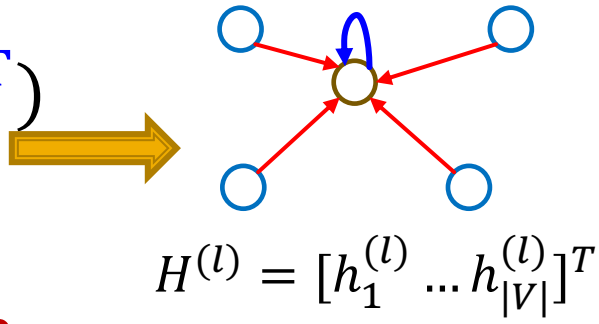

$$\sum_{u \in N(v)} \frac{h_u^{(l-1)}}{|N(v)|} \Longrightarrow H^{(l+1)} = D^{-1}AH^{(l)}$$

# Matrix Formulation (2)

- Re-writing update function in matrix form:

$$H^{(l+1)} = \sigma(\tilde{A}H^{(l)}W_l^{\mathrm{T}} + H^{(l)}B_l^{\mathrm{T}})$$

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




  - 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):

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

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

# Unsupervised Training

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

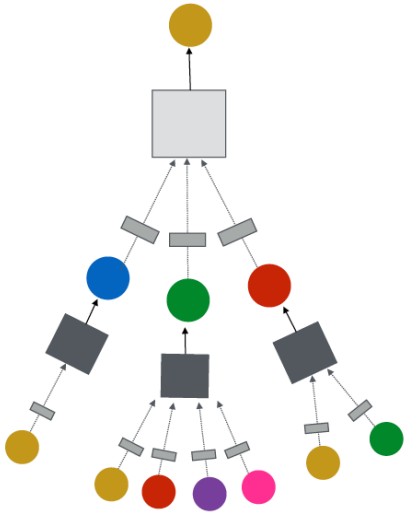
$$\mathcal{L} = \sum_{z_u, z_v} \mathrm{CE}(y_{u,v}, \mathrm{DEC}(z_u, z_v))$$

  - Where $y_{u,v} = 1$ when node $u$ and $v$ are **similar**
  - $\mathrm{CE}$ is the cross entropy (slide 16)
  - $\mathrm{DEC}$ 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**

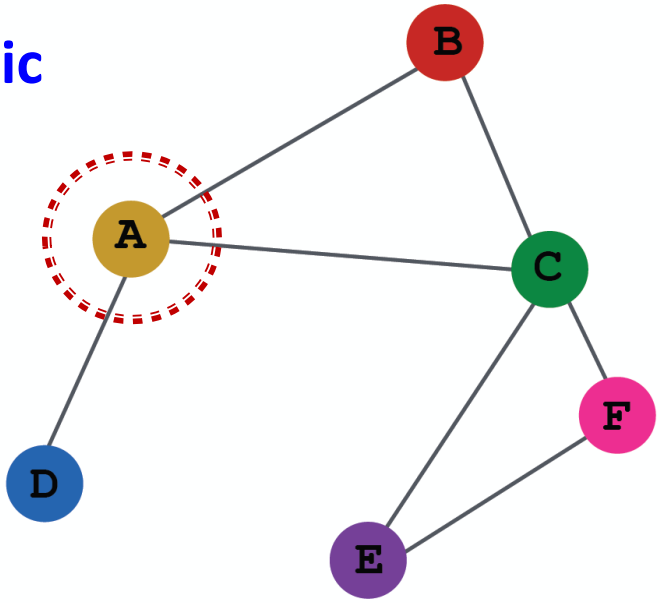
# Supervised Training

**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

# Supervised Training

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

- Use cross entropy loss (slide 16)

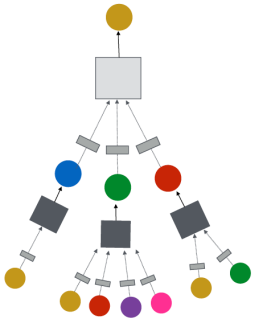
$$\mathcal{L} = \sum_{v \in V} y_v \log(\sigma(z_v^T \theta)) + (1 - y_v) \log(1 - \sigma(z_v^T \theta))$$

**Encoder output:** node embedding

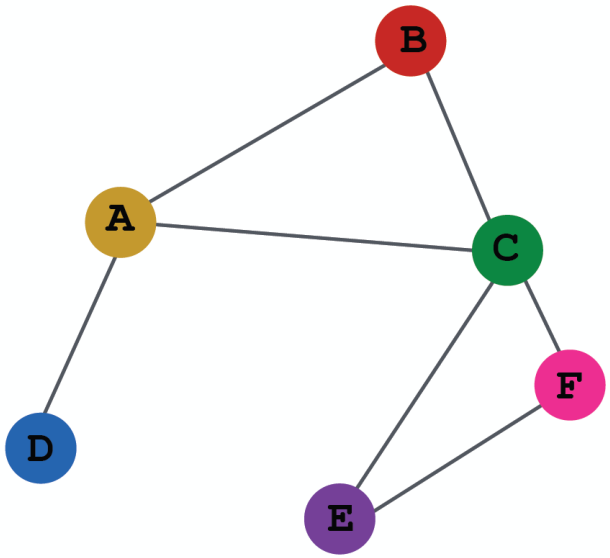
Classification weights

Node class label

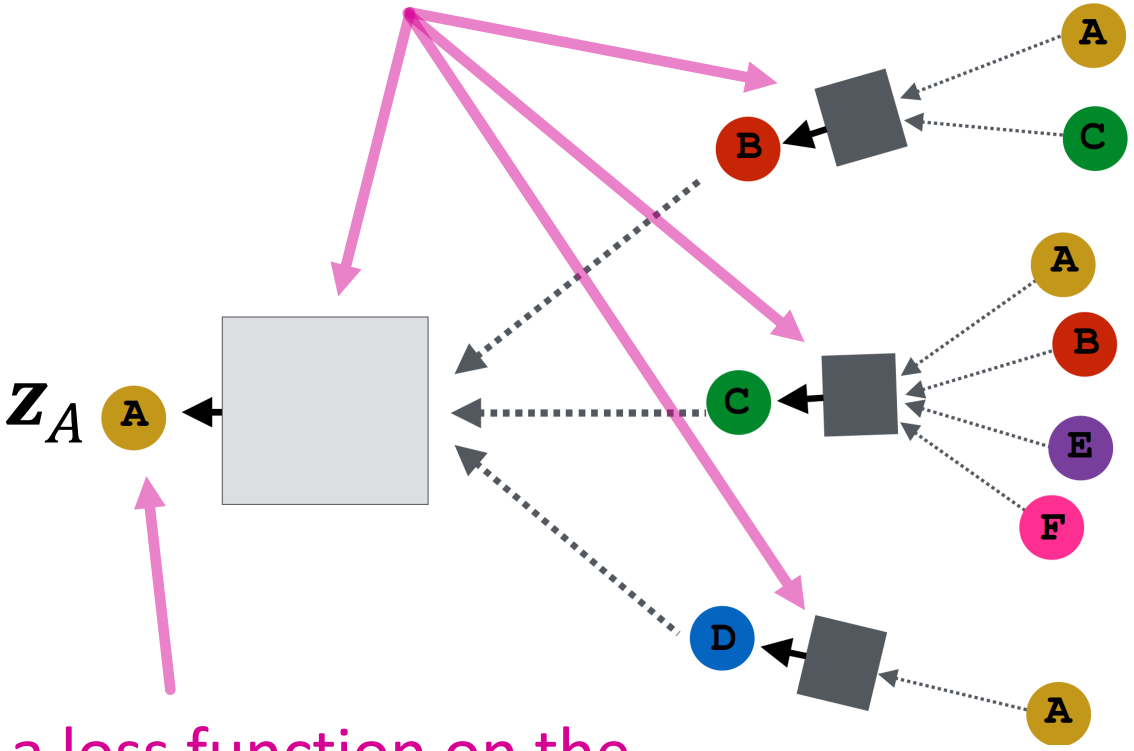
Safe or toxic drug?



# Model Design: Overview

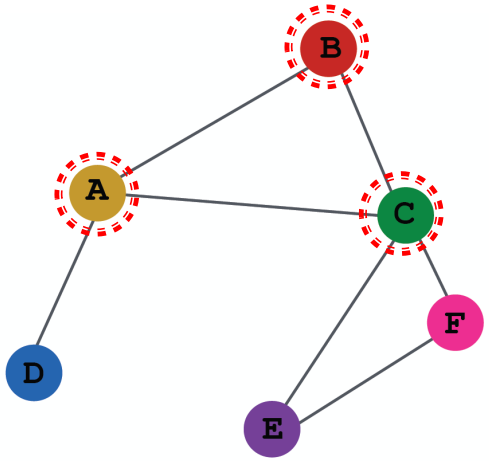



(1) Define a neighborhood aggregation function



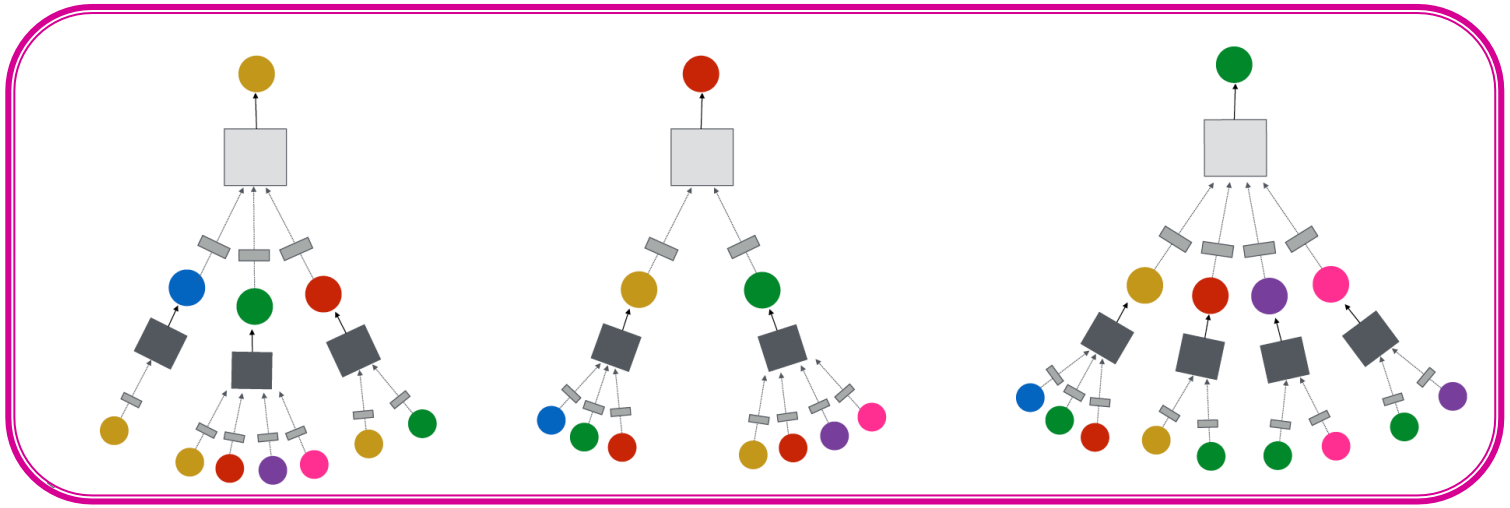

(2) Define a loss function on the embeddings

# Model Design: Overview

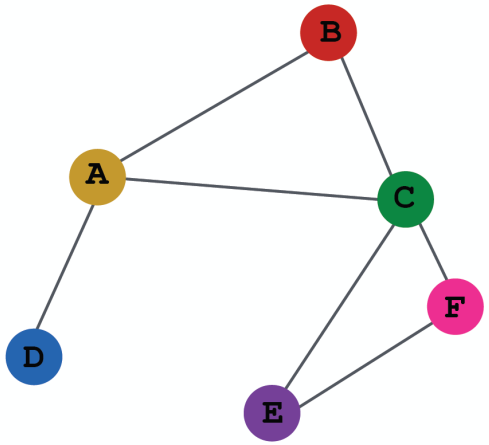



INPUT GRAPH

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



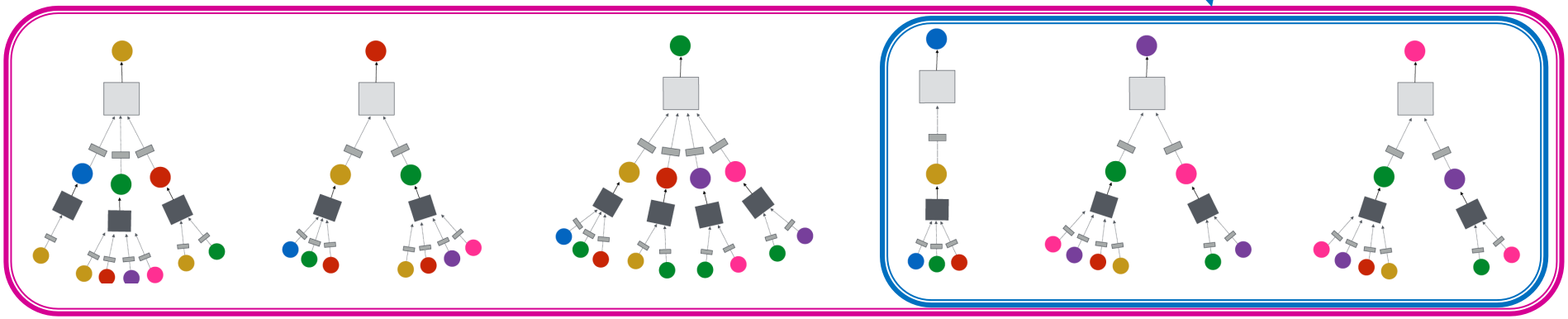
# Model Design: Overview




INPUT GRAPH

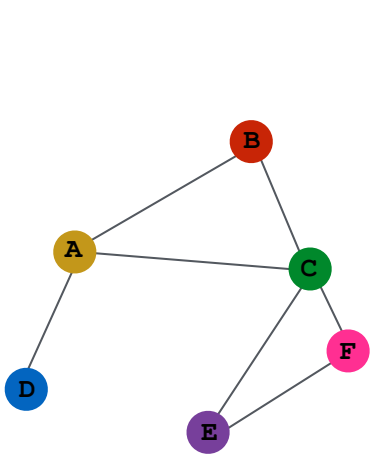
**(4) Generate embeddings for nodes as needed**

**Even for nodes we never trained on!**

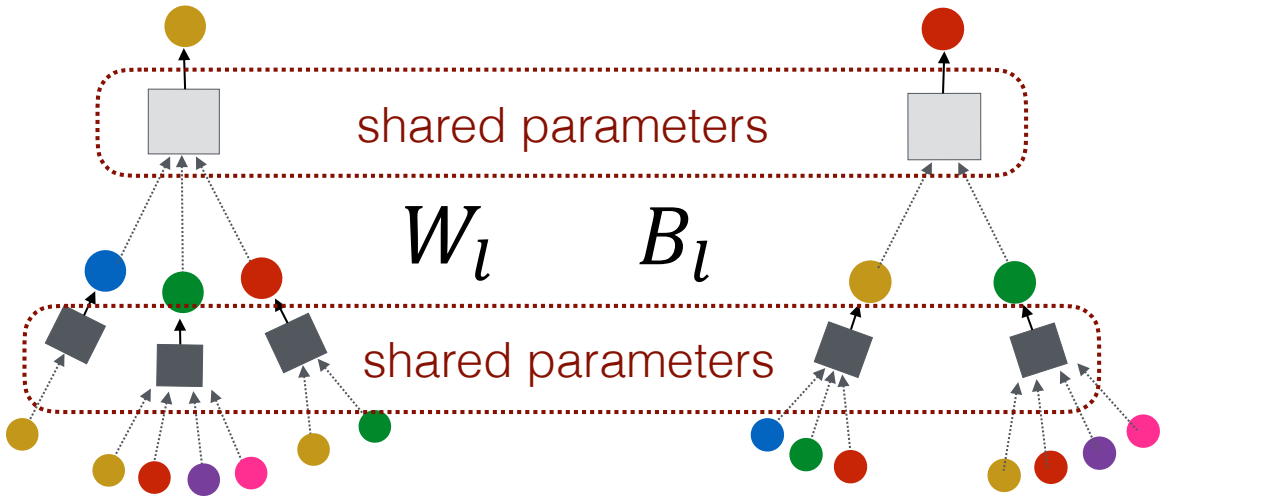


# Inductive Capability

- **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**!



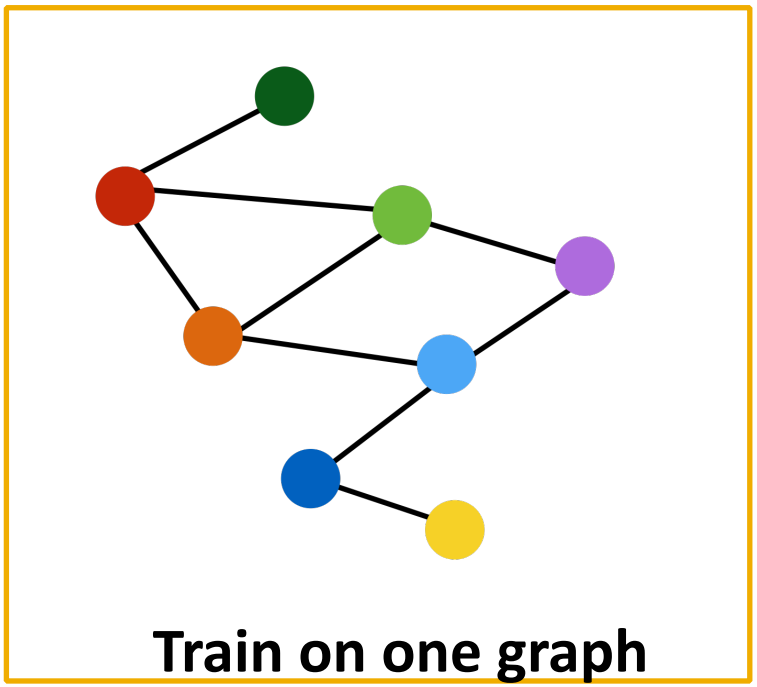

INPUT GRAPH

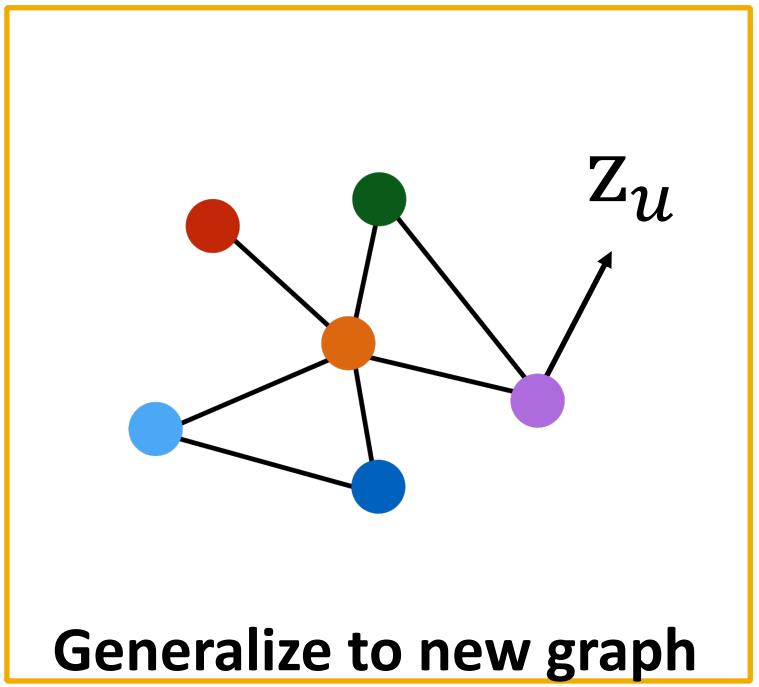



Compute graph for node A

Compute graph for node B

# Inductive Capability: New Graphs

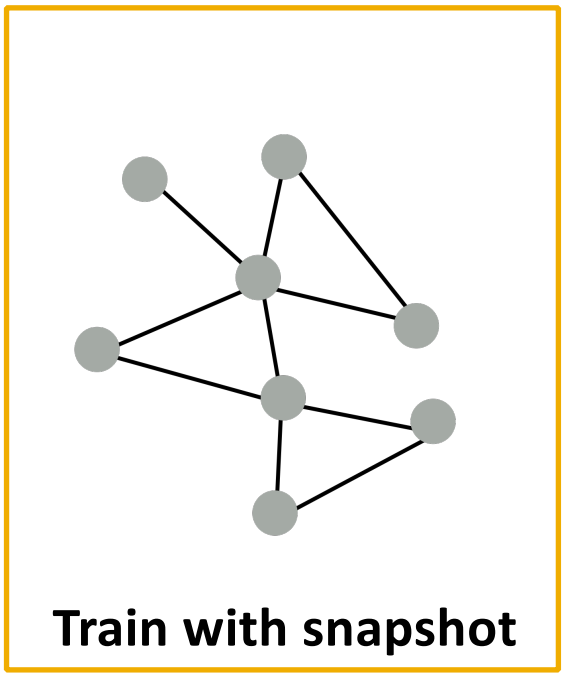


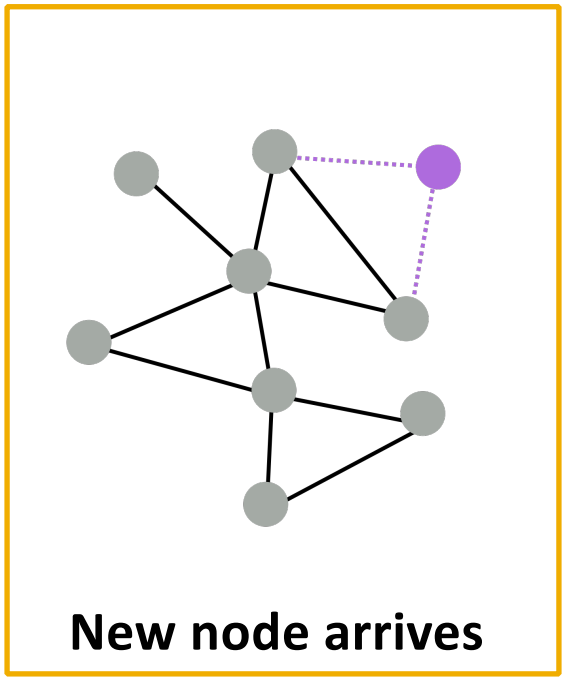



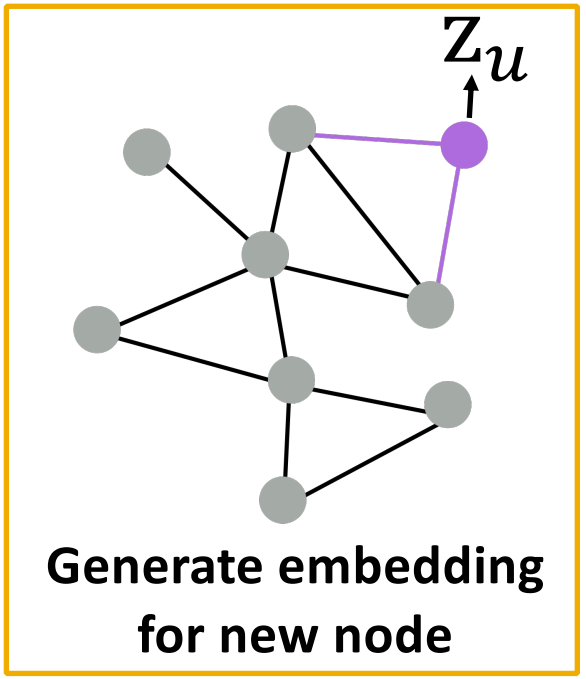

Inductive node embedding → Generalize to entirely unseen graphs

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

# Inductive Capability: New Nodes




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

# Summary

- **Recap:** Generate node embeddings by aggregating neighborhood information
  - We saw a **basic variant of this idea**
  - Key distinctions are in how different approaches aggregate information across the layers

- **Next:** Describe GraphSAGE graph neural network architecture

# Outline of Today's Lecture

1. **Basics of deep learning** ✓
2. **Deep learning for graphs** ✓
3. **Graph Convolutional Networks and GraphSAGE**

# Stanford CS224W: Graph Convolutional Networks and GraphSAGE

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

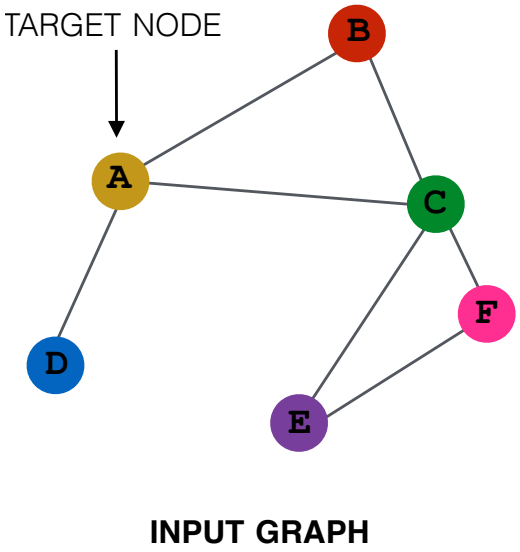
http://cs224w.stanford.edu

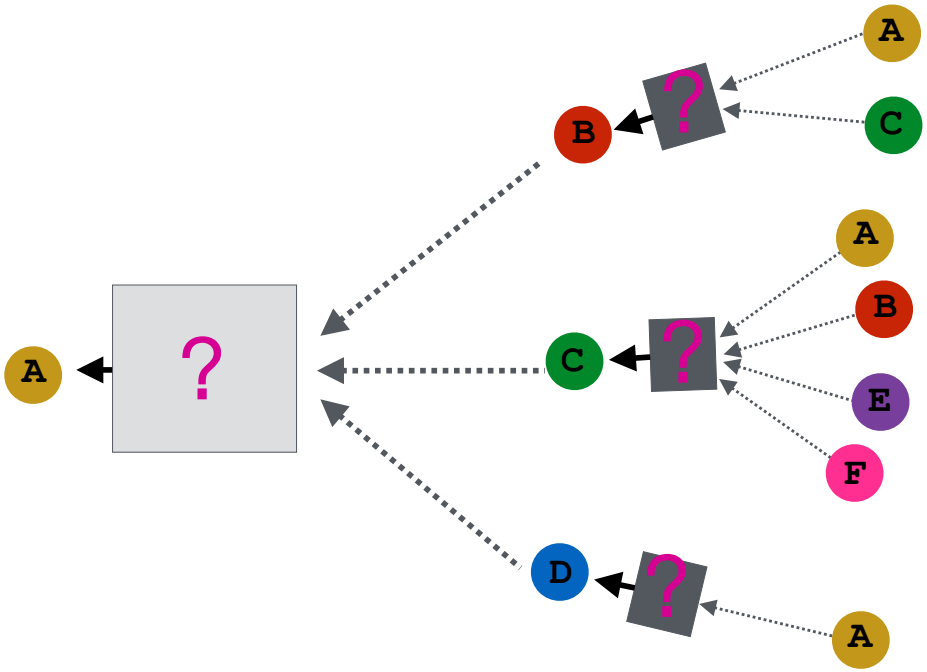
# GraphSAGE Idea

[Hamilton et al., NIPS 2017]

So far we have aggregated the neighbor messages by taking their (weighted) average

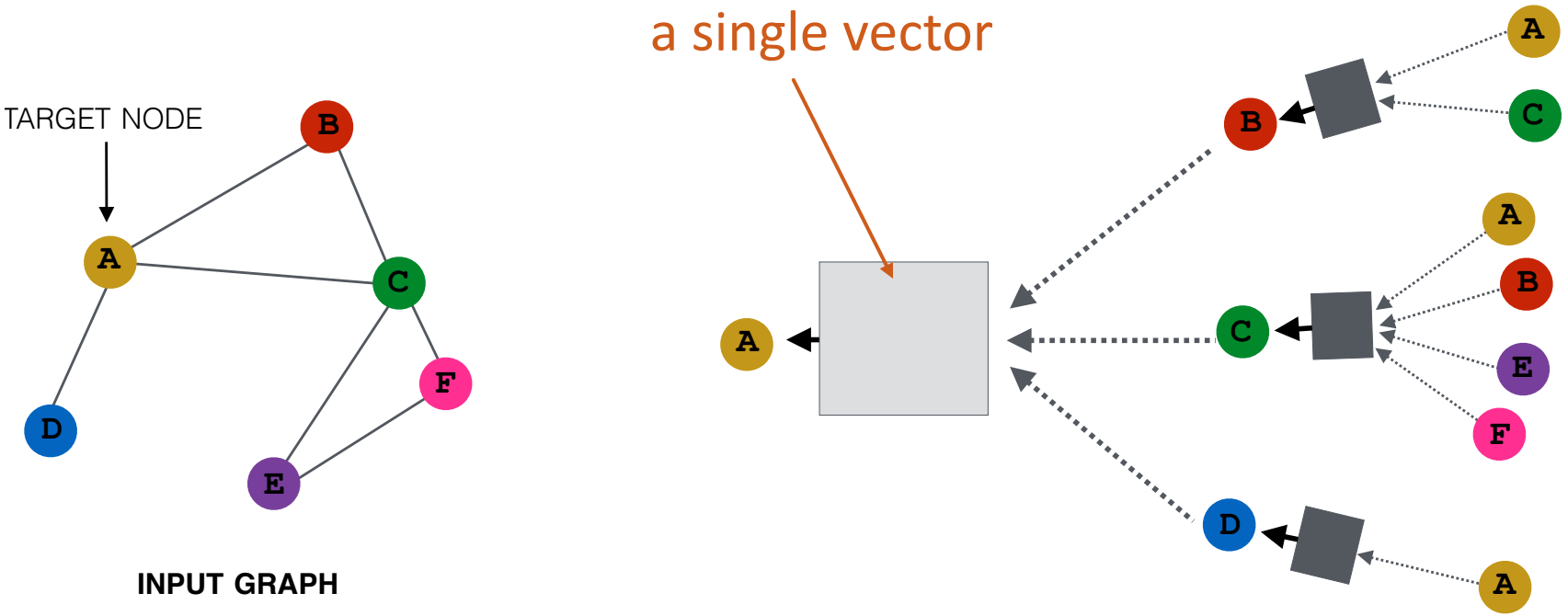
**Can we do better?**



# GraphSAGE Idea (1)

Any differentiable function that maps set of vectors in $N(u)$ to a single vector




$$\mathrm{h}_v^{(l+1)} = \sigma([\mathrm{W}_l \cdot \mathrm{AGG}\left(\left\{\mathrm{h}_u^{(l)}, \forall u \in N(v)\right\}\right), \mathrm{B}_l \mathrm{h}_v^{(l)}])$$

How does this message passing architecture differ?

# GraphSAGE Idea (2)

$$\mathrm{h}_v^{(l+1)} = \sigma([\mathrm{W}_l \cdot \mathrm{AGG}\left(\left\{\mathrm{h}_u^{(l)}, \forall u \in N(v)\right\}\right), \mathrm{B}_l \mathrm{h}_v^{(l)}])$$

Optional: Apply L2 normalization to $\mathrm{h}_v^{(l+1)}$ embedding at every layer

- $\ell_2$ **Normalization:**
  - $h_v^k \leftarrow \frac{h_v^k}{\|h_v^k\|_2}$ $\forall v \in V$ where $\|u\|_2 = \sqrt{\sum_i u_i^2}$ ($\ell_2$-norm)
  - Without $\ell_2$ normalization, the embedding vectors have different scales ($\ell_2$-norm) for vectors
  - In some cases (not always), normalization of embedding results in performance improvement
  - After $\ell_2$ normalization, all vectors will have the same $\ell_2$-norm

# Neighborhood Aggregation

- **Simple neighborhood aggregation:**

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

- **GraphSAGE:**

Concatenate neighbor embedding and self embedding

$$\mathrm{h}_v^{(l+1)} = \sigma\left(\left[\mathrm{W}_l \cdot \mathrm{AGG}\left(\left\{\mathrm{h}_u^{(l)}, \forall u \in N(v)\right\}\right), \mathrm{B}_l \mathrm{h}_v^{(l)}\right]\right)$$

Flexible aggregation function instead of mean

# Neighbor Aggregation: Variants

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

$$\text{AGG} = \sum_{u \in N(v)} \frac{\text{h}_u^{(l)}}{|N(v)|}$$

- **Pool:** Transform neighbor vectors and apply symmetric vector function

Element-wise mean/max

$$\text{AGG} = \gamma(\{\text{MLP}(\text{h}_u^{(l)}), \forall u \in N(v)\})$$

- **LSTM:** Apply LSTM to reshuffled of neighbors

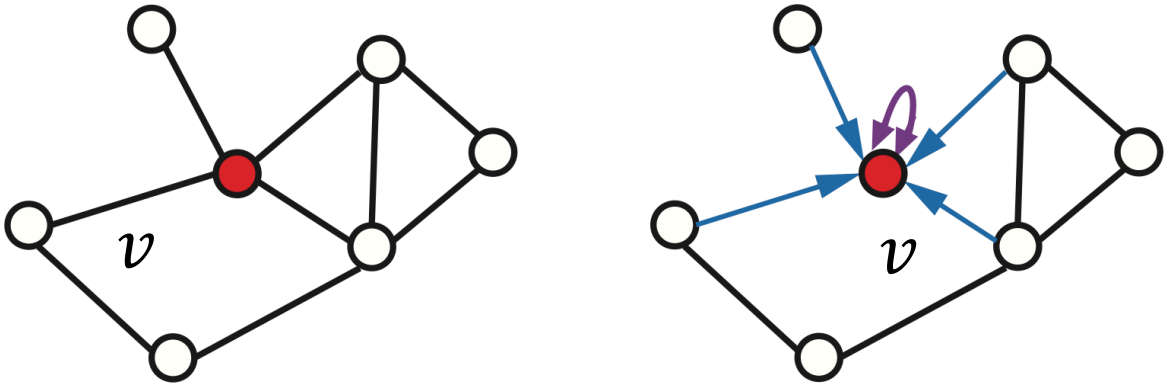
$$\text{AGG} = \text{LSTM}([\text{h}_u^{(l)}, \forall u \in \pi(N(v))])$$

# Recap: GCN, GraphSAGE

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

- Nodes aggregate "messages" from their neighbors using neural networks

- **Graph convolutional networks:**
  - **Basic variant:** Average neighborhood information and stack neural networks
- **GraphSAGE:**
  - Generalized neighborhood aggregation



# Summary

- **In this lecture, we introduced**
  - Basics of neural networks
    - Loss, Optimization, Gradient, SGD, non-linearity, MLP
  - 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
  - GraphSAGE: more flexible aggregation