Graph Neural Networks

COMP9312_23T2

UNSW SYDNEY

Several slides are from Standford CS224W: Machine Learning with Graphs

Recap: Feature Engineering

Given an input graph, extract node, link and graph-level features, learn a model (SVM, neural network, etc.) that maps features to labels.

Raw Data → Graph → Structured Features → Learning Algorithm → Prediction

↑

Feature Engineering

Covered in Topic 6

Recap: Feature Engineering

Node / Edge / Graph

Various metric/methods to design features to represent graph.

Which metric is the best? **Ask machine!**

Raw Data → Graph → Structured Features → Learning Algorithm → Prediction

↑

Representation Learning to Learn the features

Graph Representation Learning alleviates the need to do feature engineering every single time.

Node Embedding

Graph Representation Learning

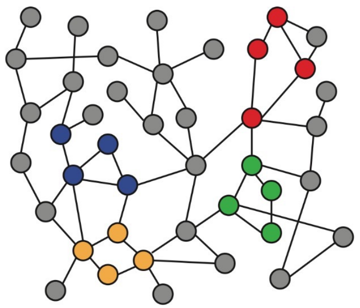
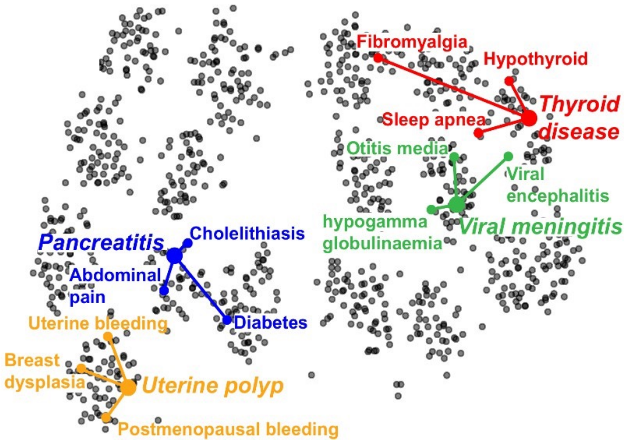
Representation **node/**edge/graph by features (i.e., vectors)

Represent a graph structure using features is also called

Graph Embedding.

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

Why Node Embedding

Map nodes into an embedding space

- Similarity of embeddings between nodes indicates their similarity in the network. For example:
  - Both nodes are close to each other (connected by an edge)
- Encode network information
- Potentially used for many downstream predictions

With embeddings (features), we can use ML/DL techniques to solve may real problems.

Node Embedding: A Case Study

2D embedding of nodes of the Zachary's Karate Club network:

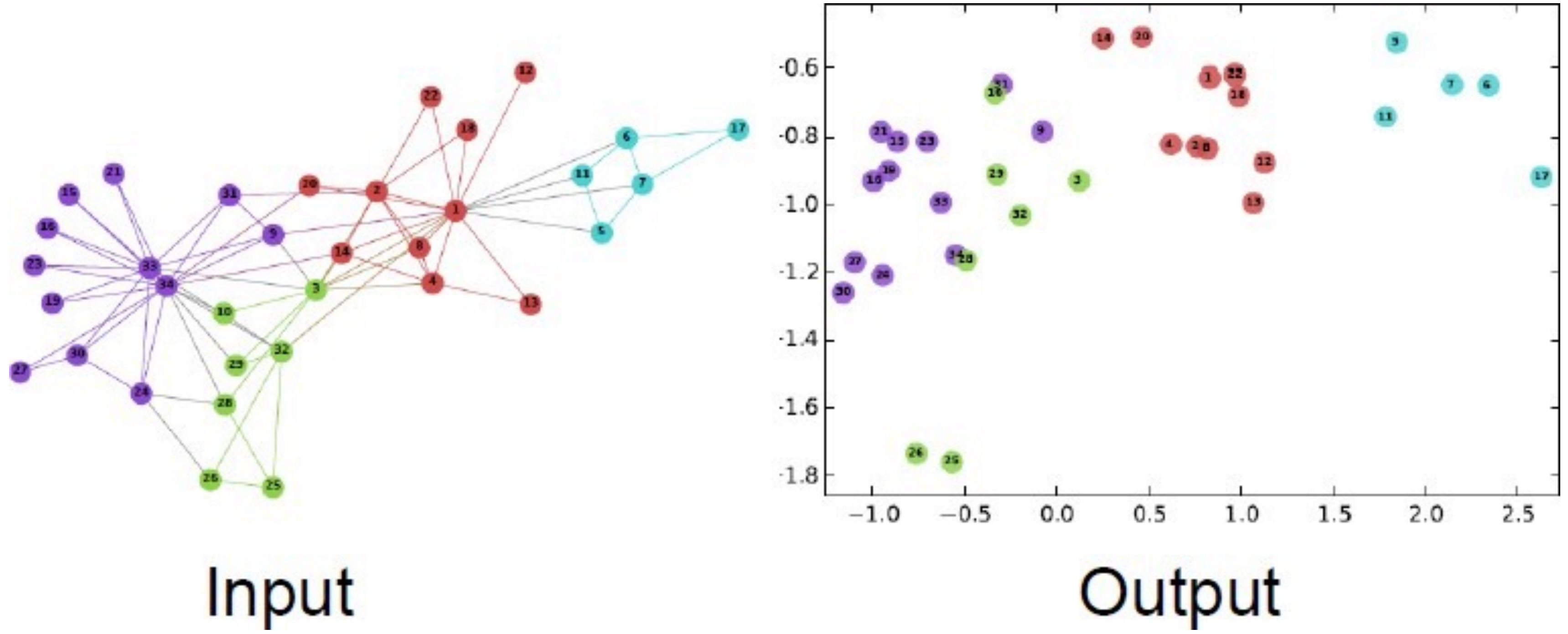
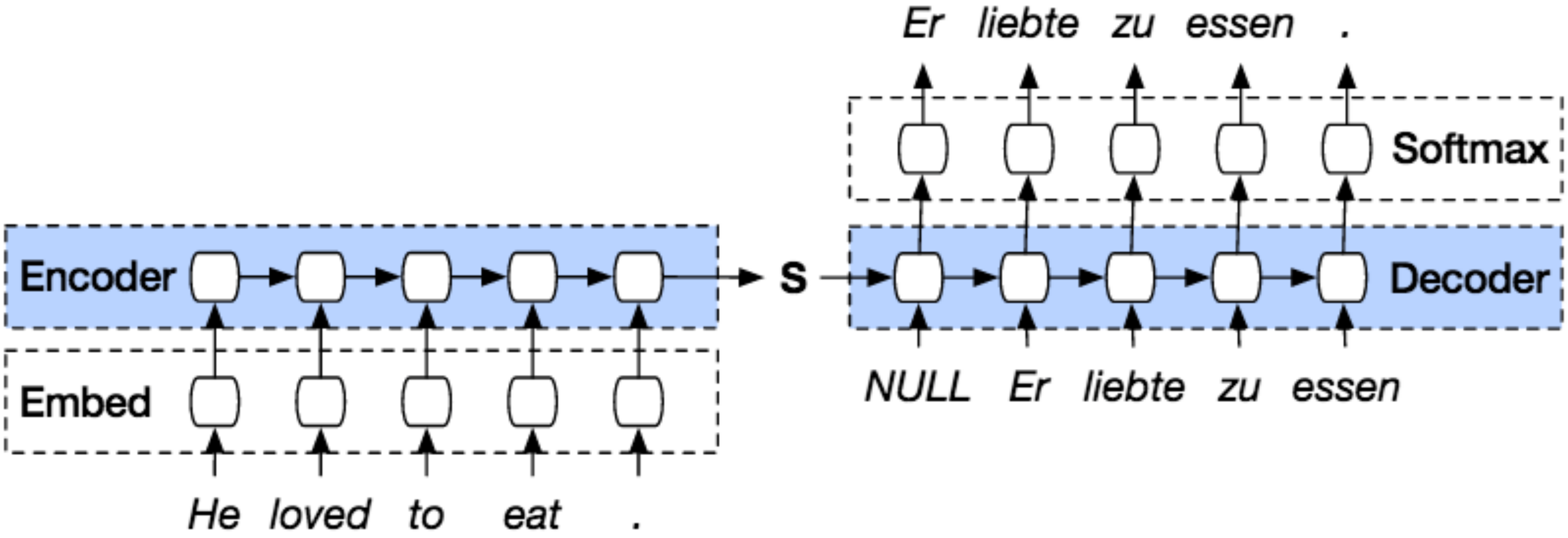


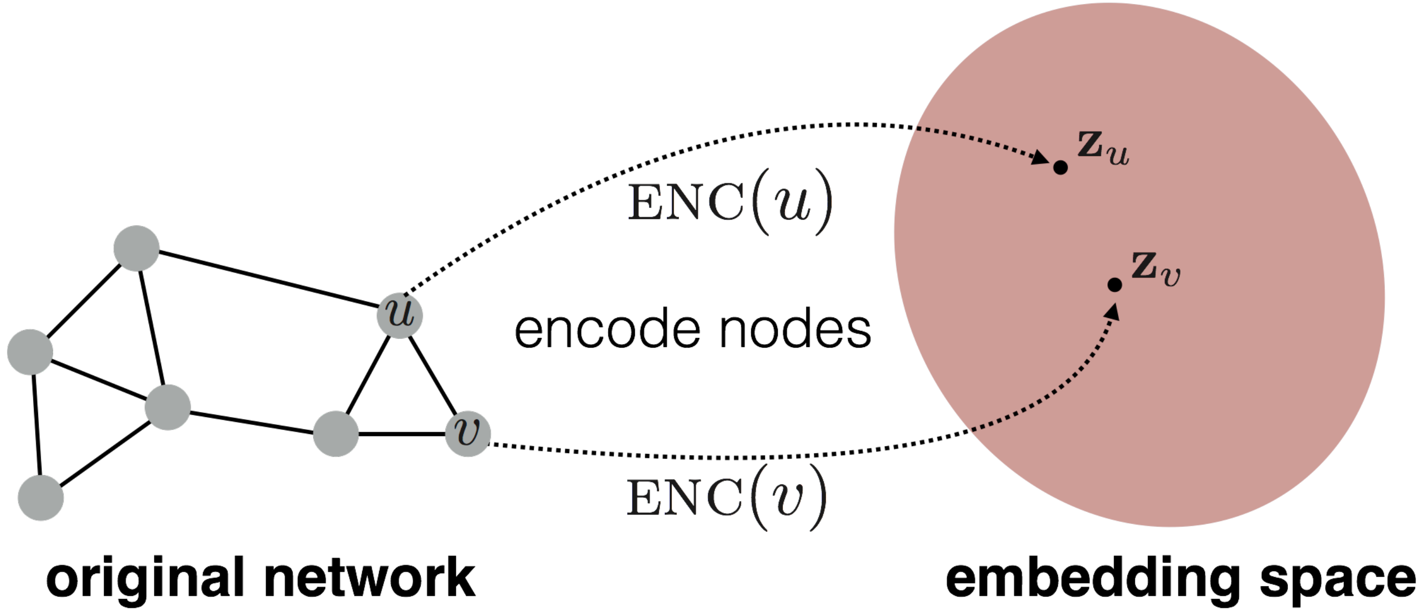
Image from: [Perozzi et al](). DeepWalk: Online Learning of Social Representations. *KDD 2014.*

Encoder & Decoder in NLP



Embedding Nodes

Encode nodes so that similarity in the embedding space (e.g., dot product) approximates similarity in the graph.

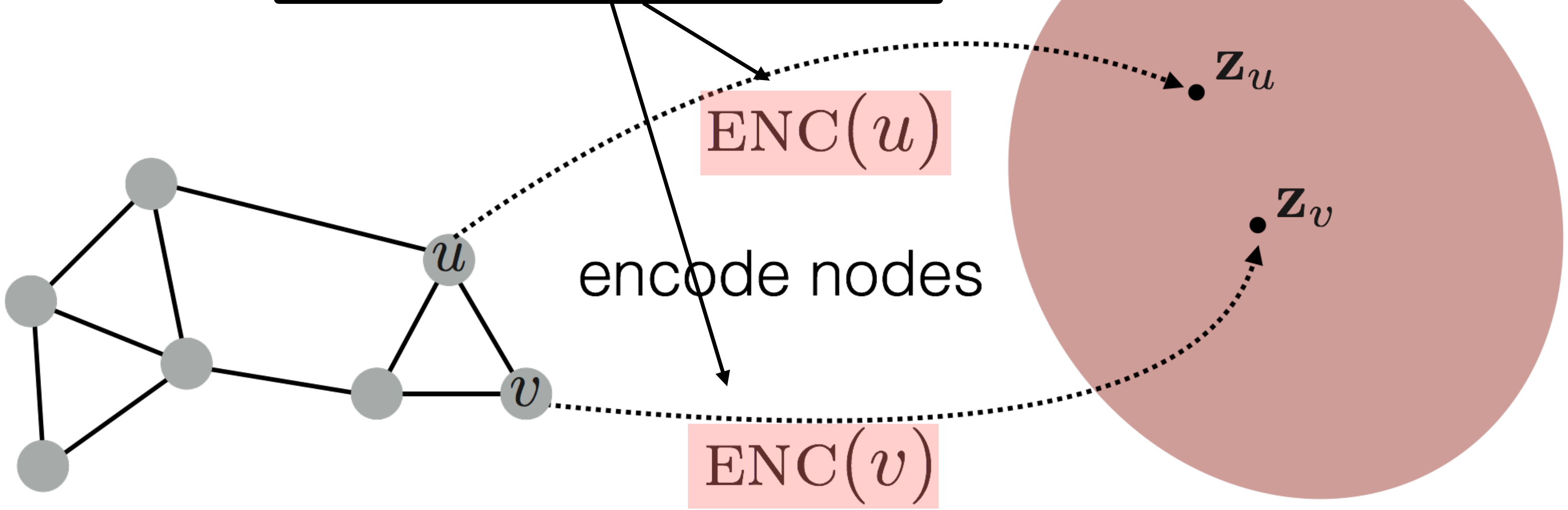


Embedding Nodes

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

in the original network — Similarity of the embedding

Need to define!



original network **embedding space**

Embedding Nodes

1. Encoder maps from nodes to embeddings
2. Define a node similarity function (i.e., a measure of similarity in the original network)
3. Decoder **DEC** maps from embeddings to the similarity score
4. Optimize the parameters of the encoder so that

$$\mathrm{DEC}(\boldsymbol{z}_v, \boldsymbol{z}_u) = \mathbf{z}_v^{\mathrm{T}} \mathbf{z}_u$$

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

in the original network   Similarity of the embedding

Two Key Components

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

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

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

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

Decoder

Similarity of u and v in the original network

dot product between node embeddings

"Shallow" Encoding

Simplest encoding approach: encoder is just an embedding-lookup.

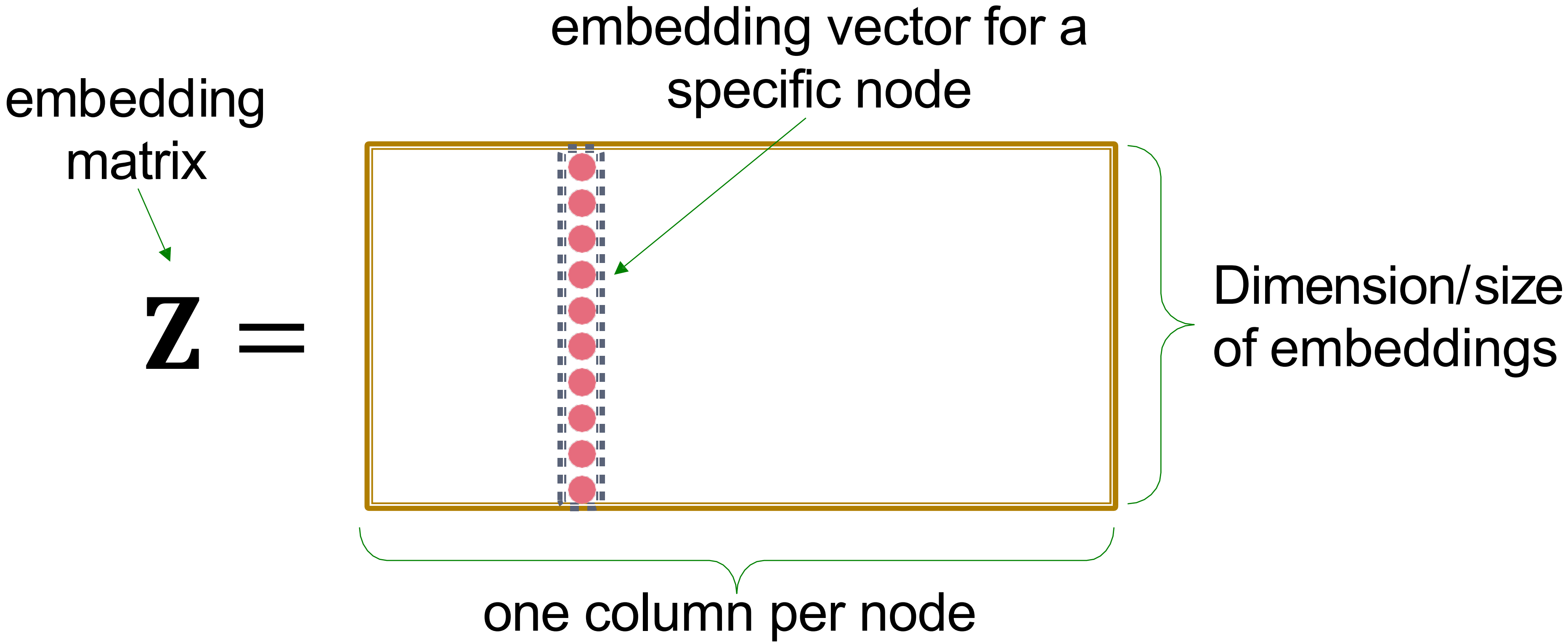
$$\mathrm{ENC}(v) = \mathbf{z}_v = \mathbf{Z} \cdot v$$

$\mathbf{Z} \in \mathbb{R}^{d \times |\mathcal{V}|}$ matrix, each column is a node embedding [what we learn /optimize]

$v \in \mathbb{I}^{|\mathcal{V}|}$ indicator vector, all zeroes except a one in column indicating node *v*

"Shallow" Encoding

Simplest encoding approach: encoder is just an embedding-lookup



Framework Summary

- Encoder + Decoder Framework
  - Shallow encoder: embedding lookup
  - Parameters to optimize: $\mathbf{Z}$ which contains node embeddings $\mathbf{z}_u$ for all nodes $u \in V$
  - We will cover deep encoders (GNNs) in the future
  - **Decoder:** based on node similarity.
  - **Objective:** maximize $\mathbf{z}_v^{\mathrm{T}}\mathbf{z}_u$ for node pairs (u, v) that are **similar**

Decoder: Node Similarity

- Key choice of methods is **how they define node similarity.**
- Should two nodes have a similar embedding if they…
  - are linked?
  - share neighbors?
  - have similar “structural roles”?
- We will now learn node similarity definition that uses **random walks**, and how to optimize embeddings for such a similarity measure.

  Representative methods: DeepWalk, node2vec

Other important things

- This is **unsupervised/self-supervised** way of learning node embeddings
  - We are **not** utilizing node labels
  - We are **not** utilizing node features
  - The goal is to directly estimate a set of coordinates (i.e., the embedding) of a node so that some aspect of the network structure (captured by DEC) is preserved
- These embeddings are **task independent**
  - They are not trained for a specific task but can be used for any task.

Limitations of shallow embedding

- **$O(|V|)$ parameters are needed**:
  - No sharing of parameters between nodes
  - Every node has its own unique embedding

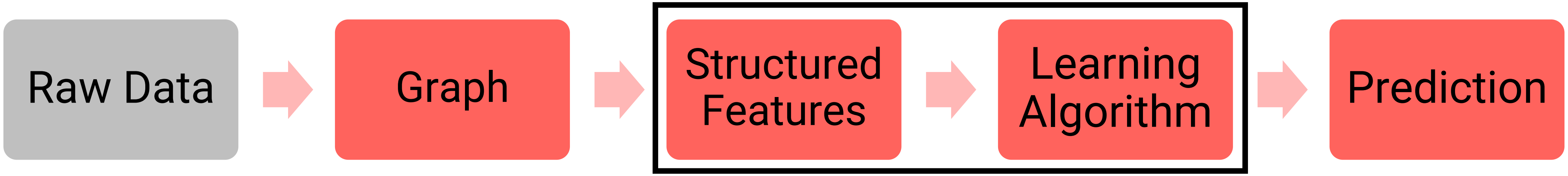
- **Inherently "transductive"**:
  - Cannot generate embeddings for nodes that are not seen during training

- **Do not incorporate node features**:
  - Many graphs have features that we can and should leverage

Deep Encoding

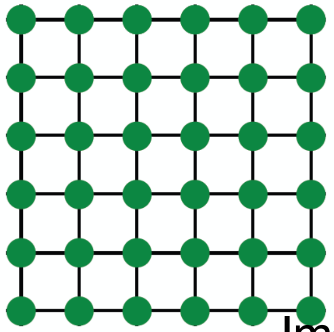
Deep Encoding

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

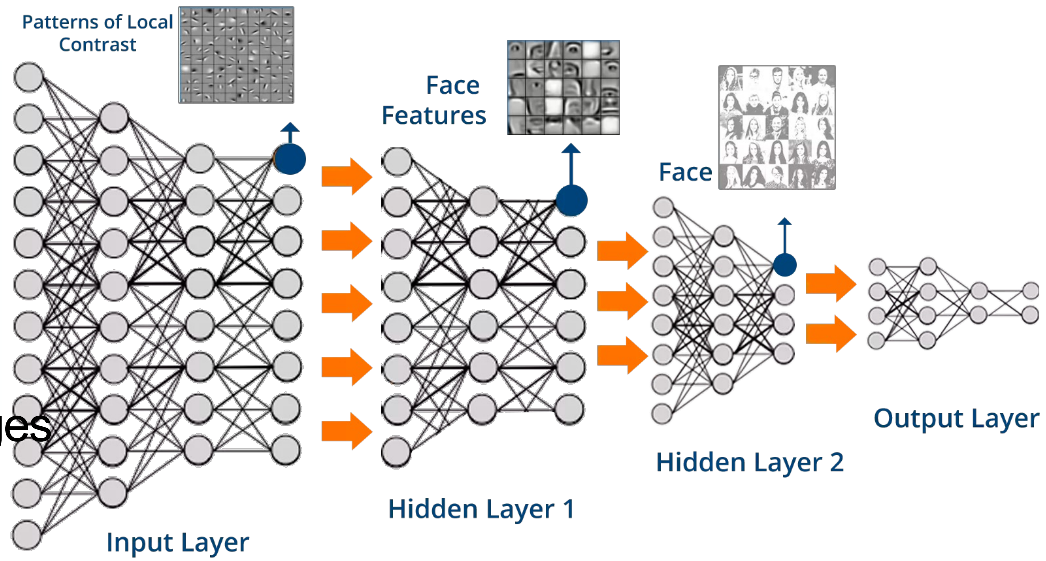


$\mathrm{ENC}(v) =$ **multiple layers of non-linear transformations based on graph structure**

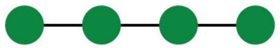
Modern ML Toolbox

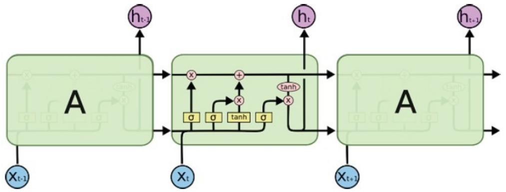


Images



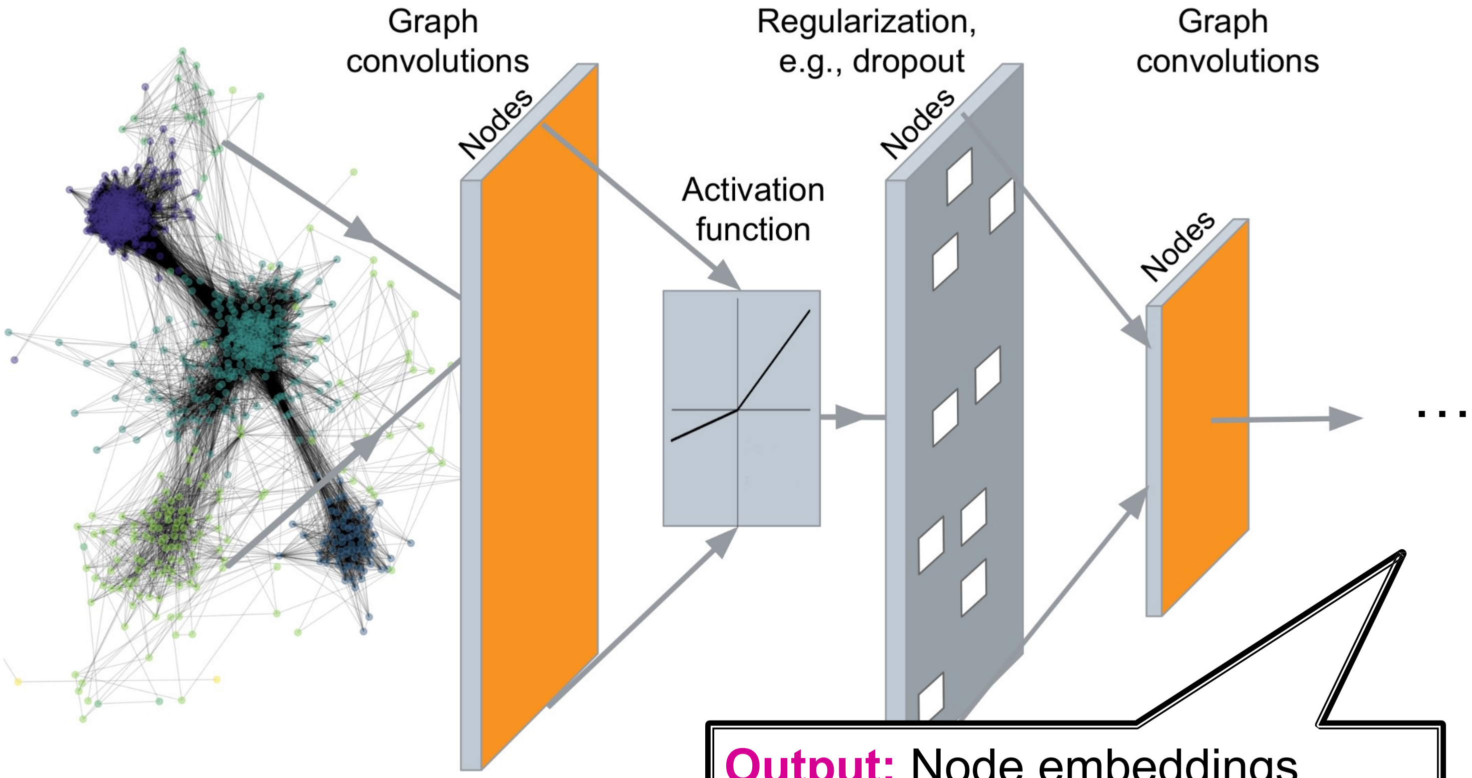
Text/Speech





Modern deep learning toolbox is designed for simple sequences & grids

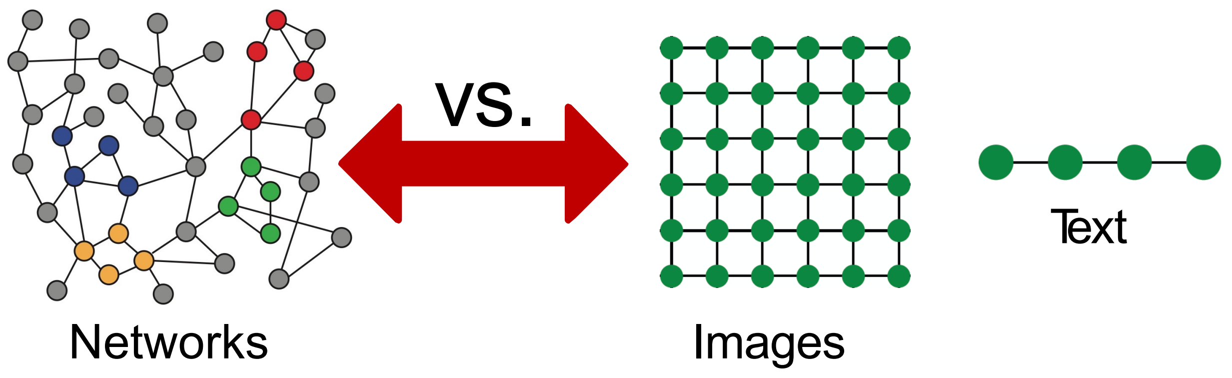
Deep Graph Encoders



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

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

Tasks on Networks

Tasks we will be able to solve:

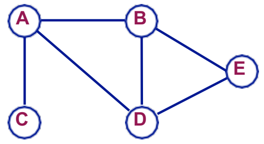
- Node classification
  - Predict a type of a given node
- Link prediction
  - Predict whether two nodes are linked
- Community detection
  - Identify densely linked clusters of nodes
- Network similarity
  - How similar are two (sub)networks

Setup

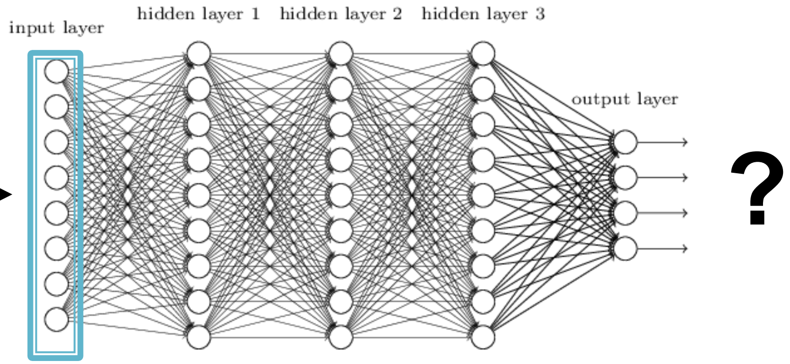
- **Assume we have a graph G:**
  - V is the **vertex set**
  - $\boldsymbol{A}$ is the **adjacency matrix** (assume binary)
  - $\boldsymbol{X} \in \mathbb{R}^{:m\times|V|}$ is a matrix of **node features**
  - v: a node in V; $N(v)$: the set of neighbors of v.
  - **Node features:**
    - Social networks: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



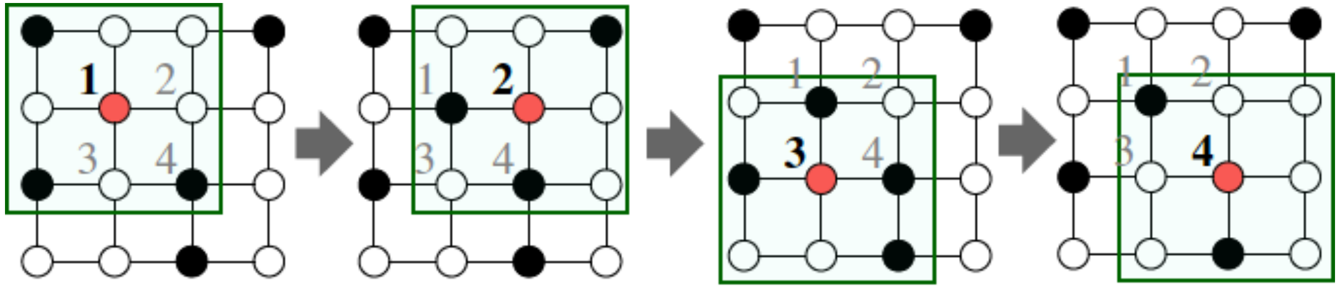
$$\begin{array}{c|ccccccc} & A & B & C & D & E & \text{Feat} & \\ \hline A & 0 & 1 & 1 & 1 & 0 & 1 & 0 \\ B & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ C & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\ D & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ E & 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{array}$$

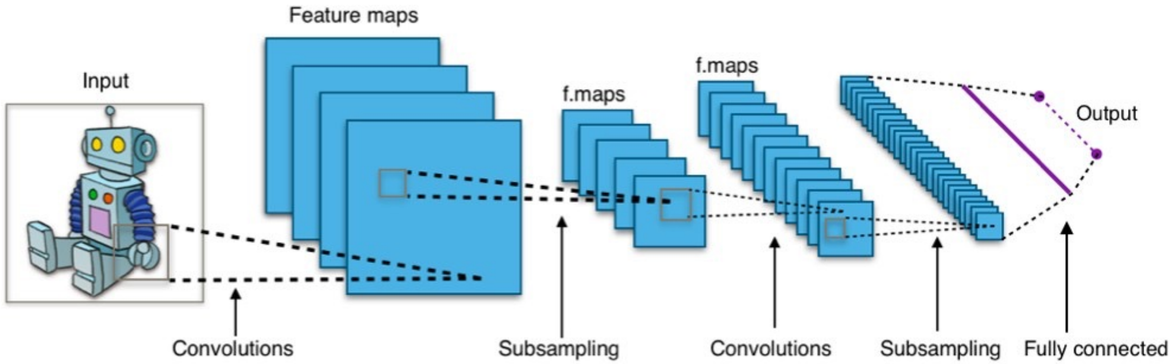


- Issues with this idea:
  - $O(|V|)$ parameters
  - Not applicable to graphs of different sizes
  - Sensitive to node ordering

Graph Convolutional Networks

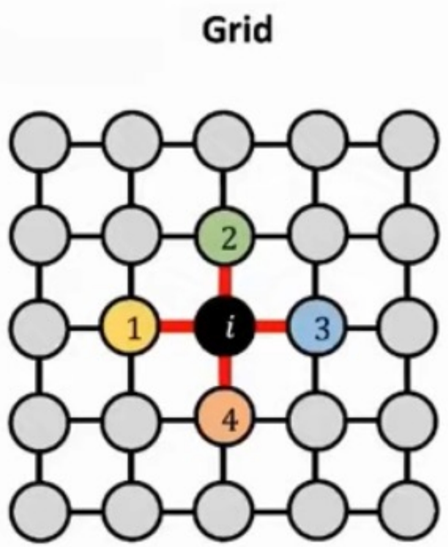
CNN on an image:





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

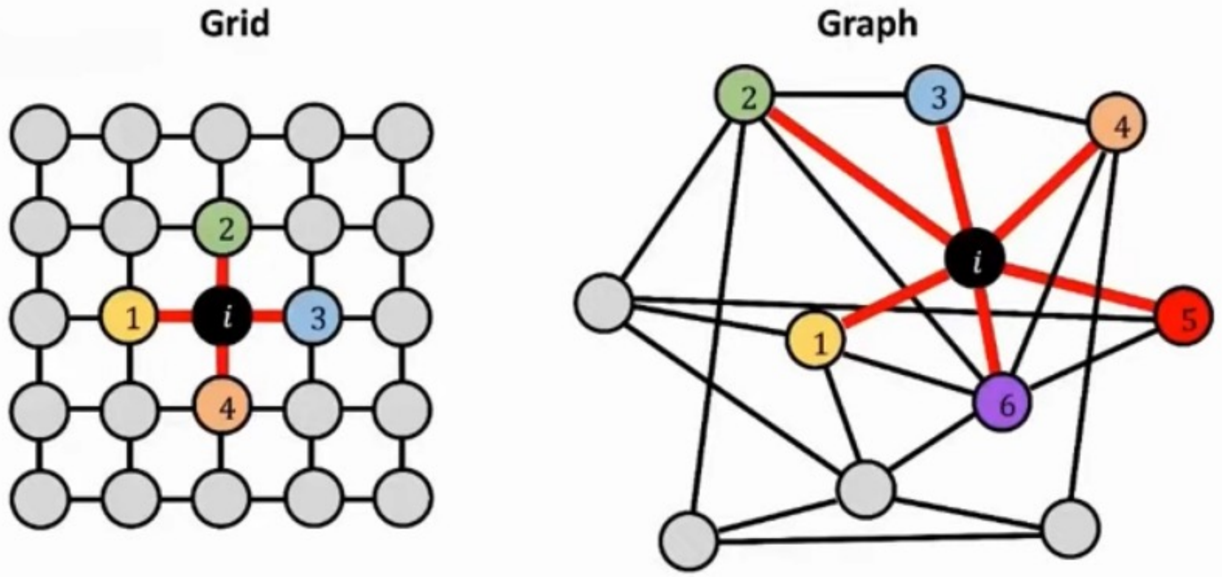
What about Graphs?



$$\mathbf{y}_i = w_1\mathbf{x}_{i,1} + \cdots + w_4\mathbf{x}_{i,4}$$

Talk on Deep learning on graphs: successes, challenges by Michael Bronstein

What about Graphs?

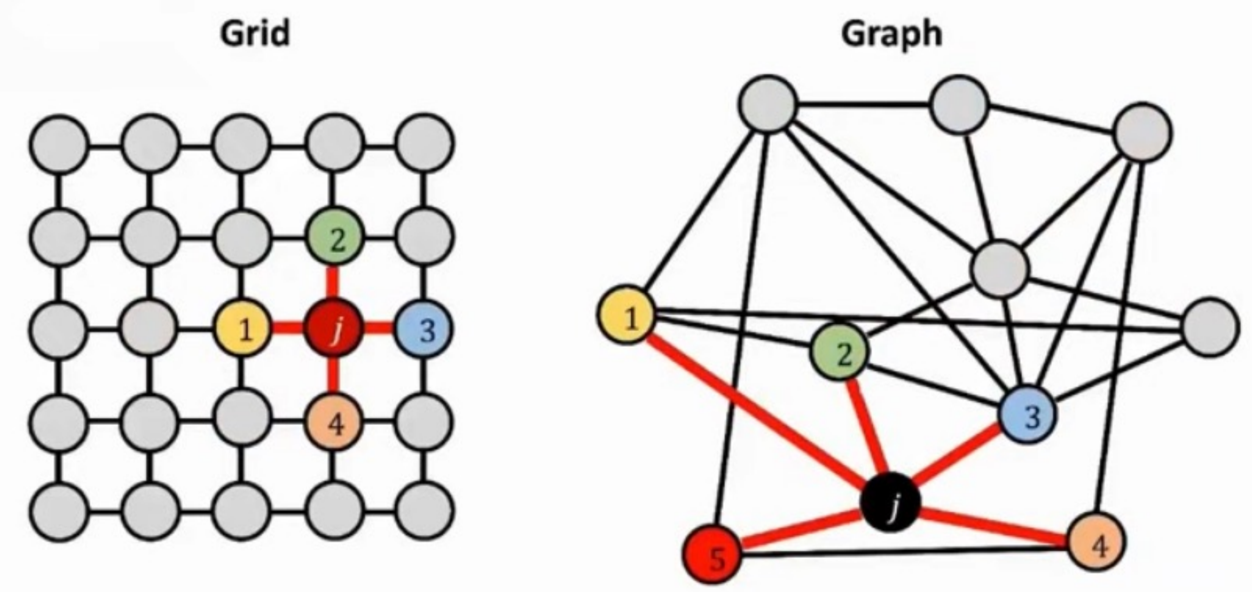


$$\mathbf{y}_i = w_1\mathbf{x}_{i,1} + \cdots + w_4\mathbf{x}_{i,4}$$

$$\mathbf{y}_i = w_1\mathbf{x}_{i,1} + \cdots + w_6\mathbf{x}_{i,6}$$

Talk on Deep learning on graphs: successes, challenges by Michael Bronstein

What about Graphs?



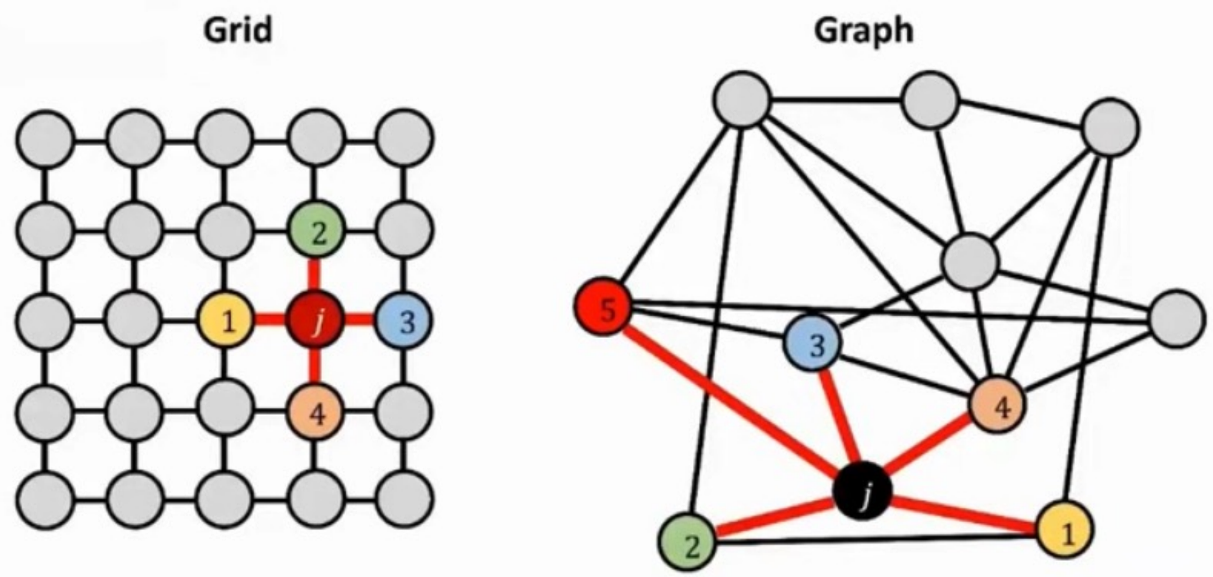
$$\mathbf{y}_j = w_1\mathbf{x}_{j,1} + \cdots + w_4\mathbf{x}_{j,4}$$

- Constant number of neighbors

$$\mathbf{y}_j = w_1\mathbf{x}_{j,1} + \cdots + w_5\mathbf{x}_{j,5}$$

- Different number of neighbors

What about Graphs?



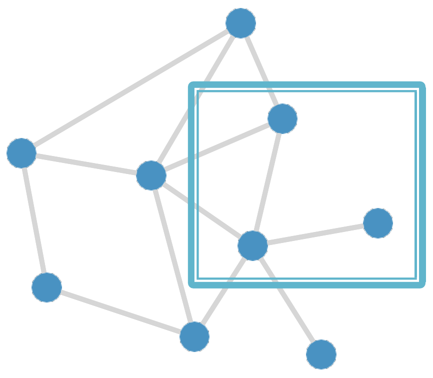
$\mathbf{y}_j = w_1 \mathbf{x}_{j,1} + \cdots + w_4 \mathbf{x}_{j,4}$

- Constant number of neighbors
- Fixed ordering of neighbors

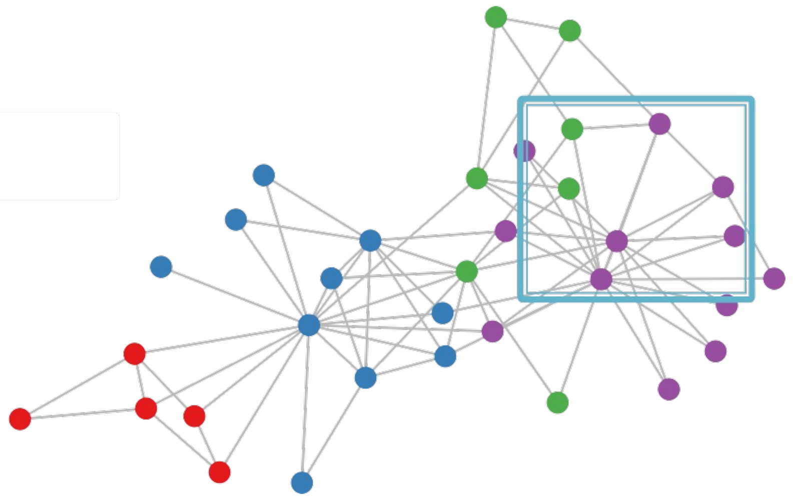
$\mathbf{y}_j = w_1 \mathbf{x}_{j,5} + \cdots + w_5 \mathbf{x}_{j,2}$

- Different number of neighbors
- No ordering of neighbors

Graphs look like this



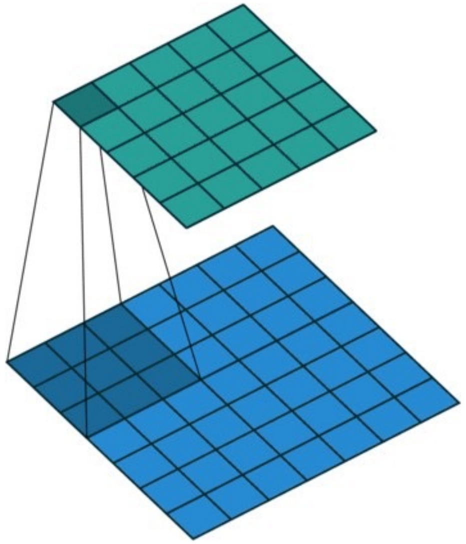
or this



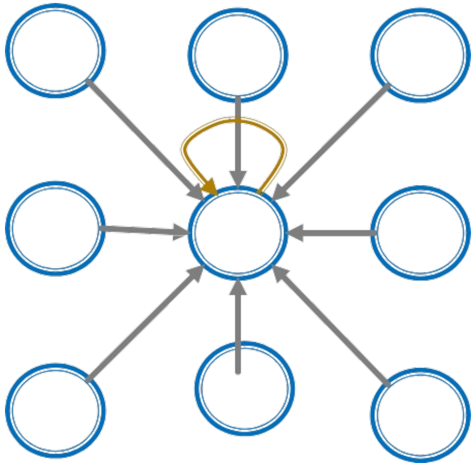
1. No fixed notion of locality or sliding window on the graph
2. Graph is permutation invariant

Convolutional layer with 3x3 filter

Image



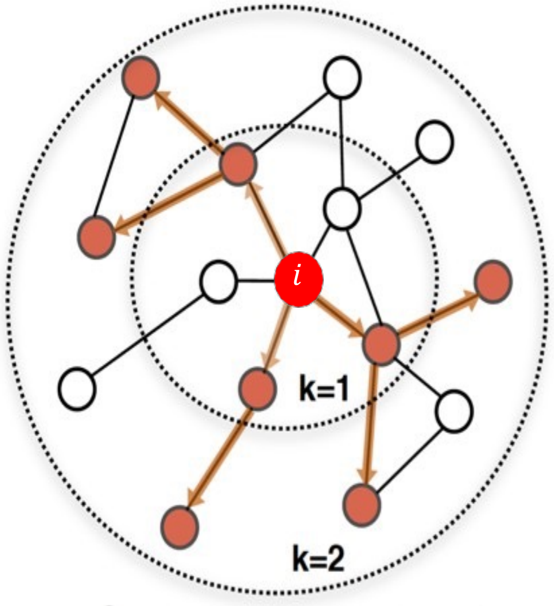
Graph



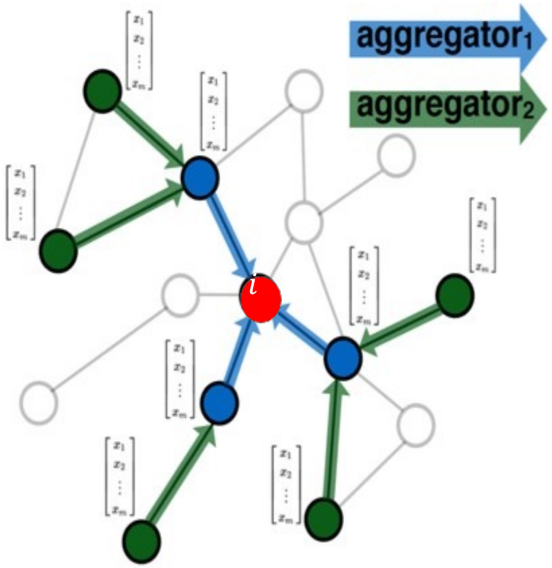
Idea: transform information at the neighbors and combine it:

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

A Computation Graph



Determine node computation graph

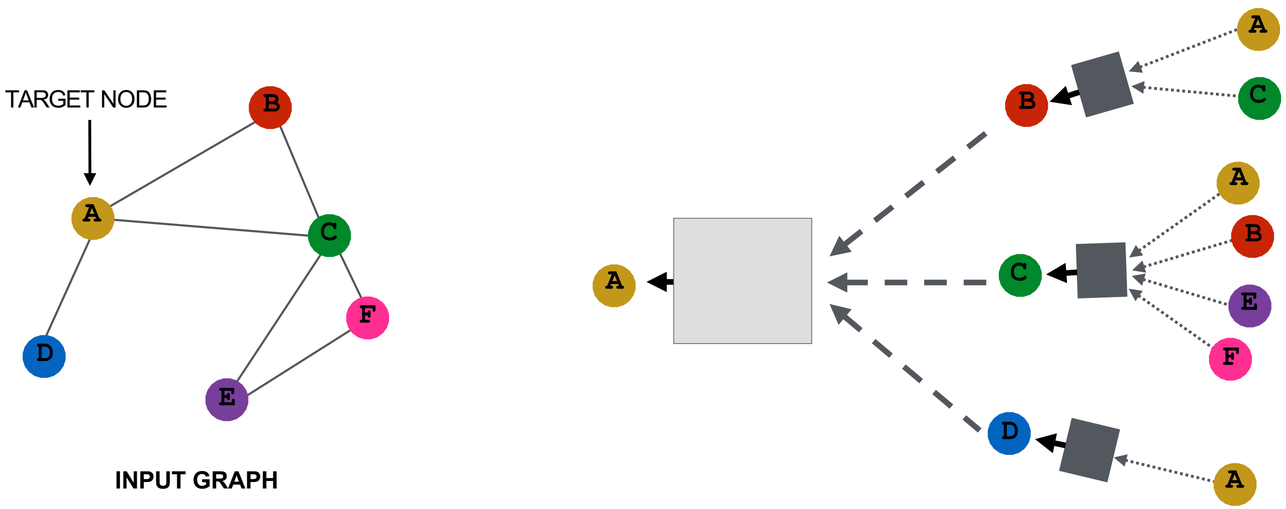


Propagate and transform information

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

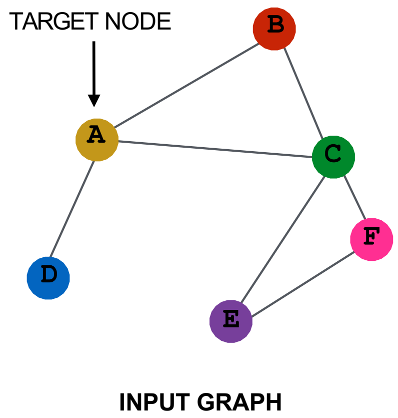
Aggregate Neighbors

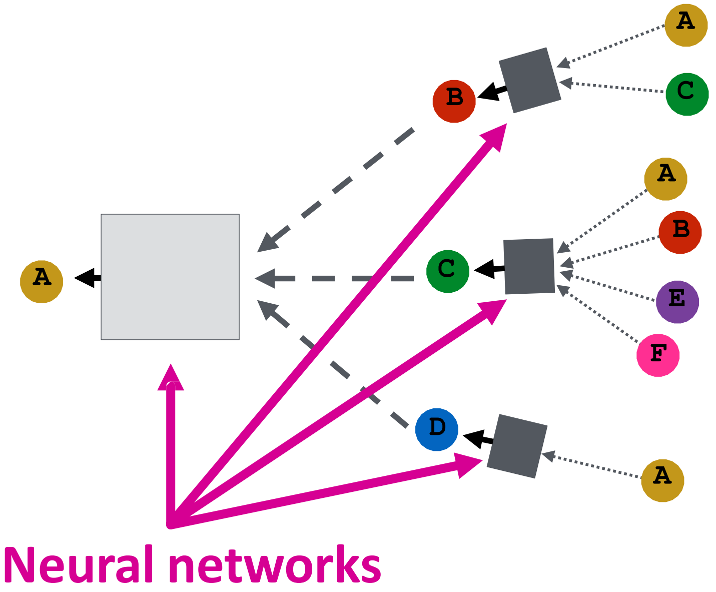
Key idea: Generate node embeddings based on **local network neighborhoods**



Aggregate Neighbors

Intuition: Nodes aggregate information from their neighbors using neural networks

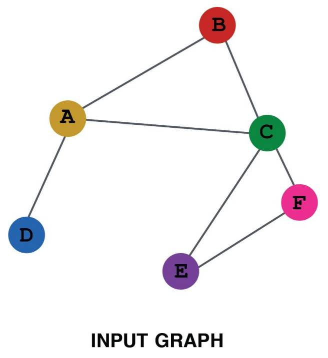


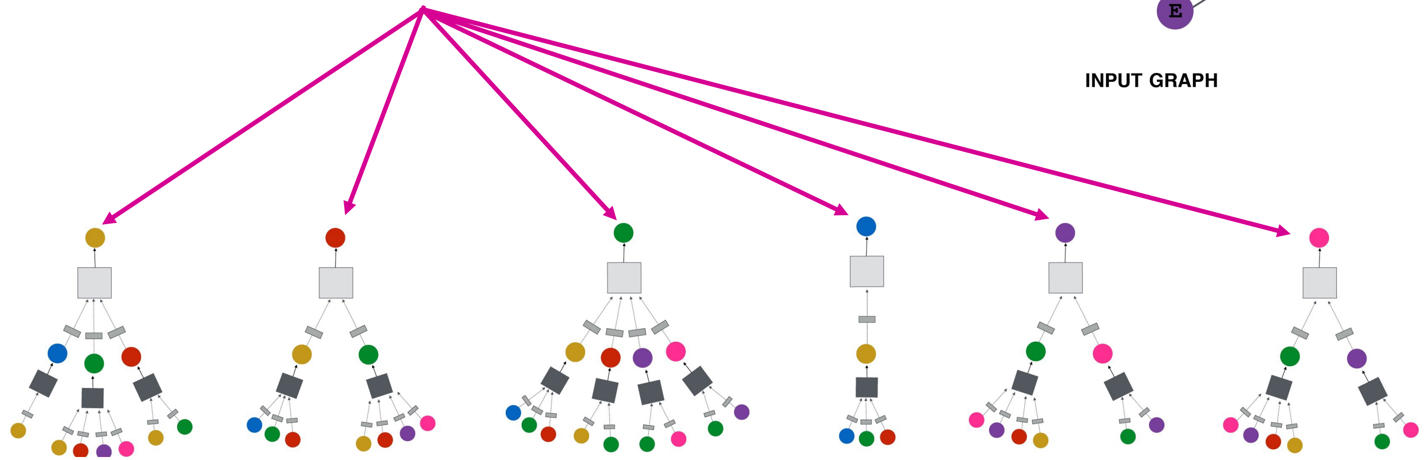


Aggregate Neighbors

Intuition: Network neighborhood defines a computation graph

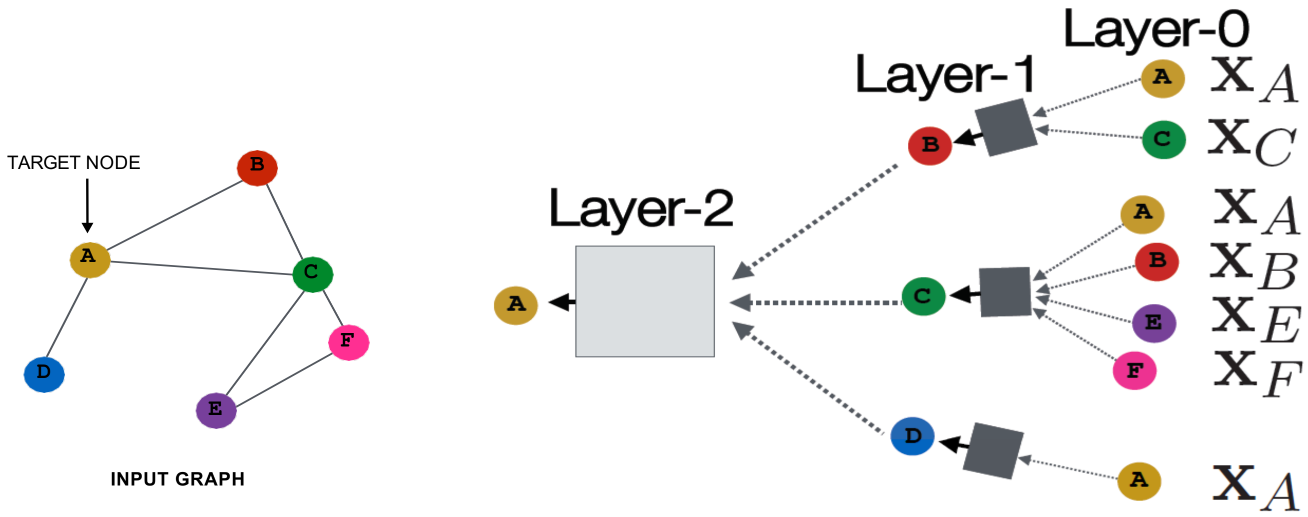
Every node defines a computation graph based on its neighborhood!





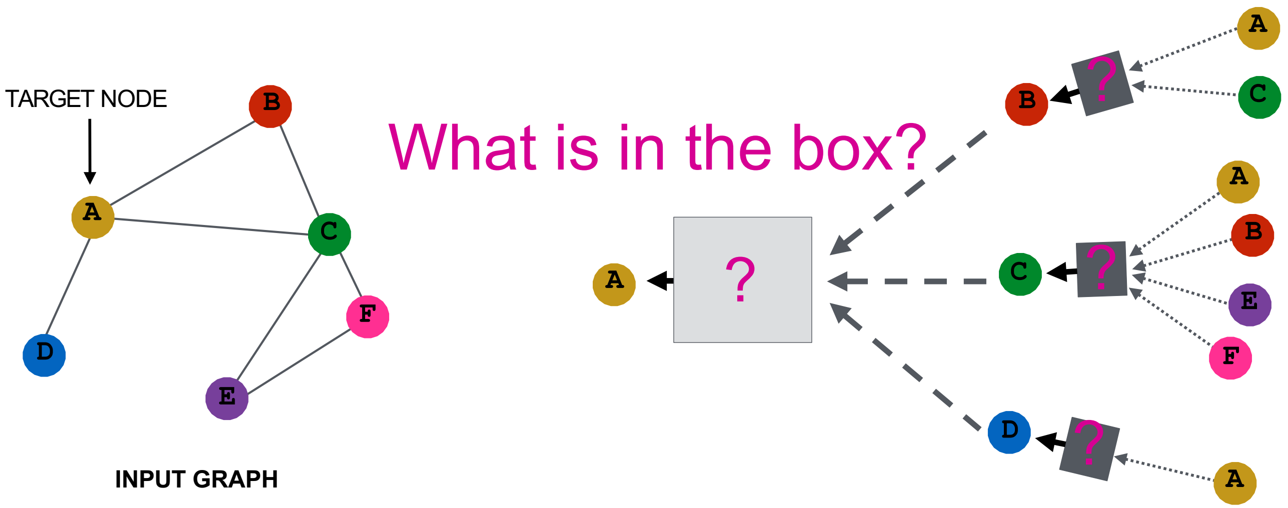
Deep: Many Layers

- 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



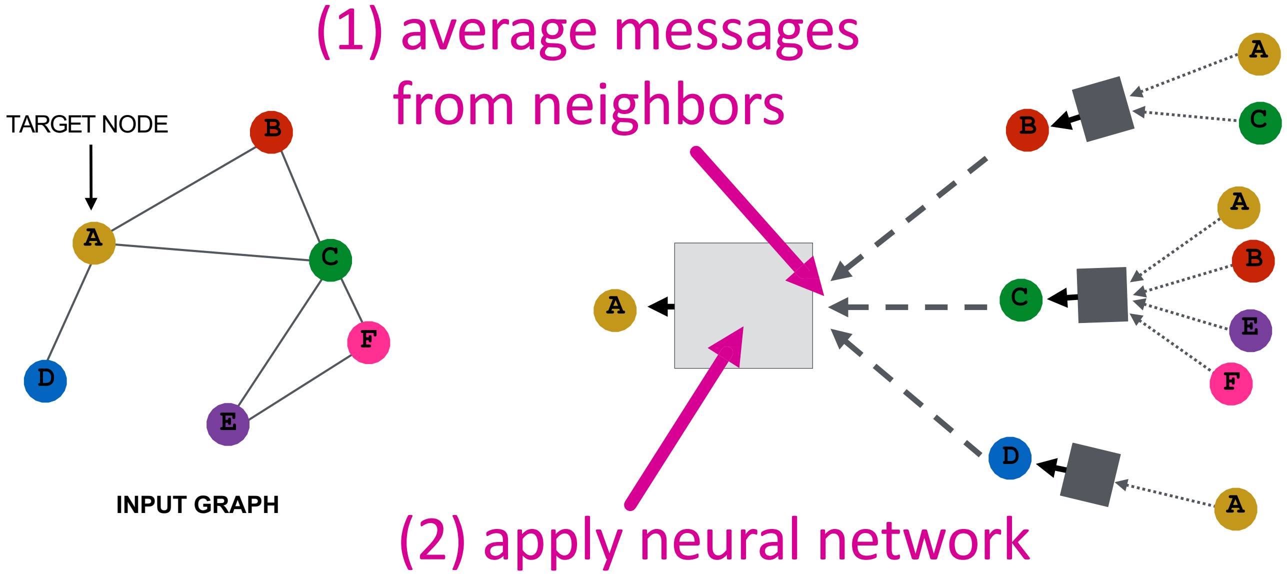
Neighborhood Aggregation

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



Neighborhood Aggregation

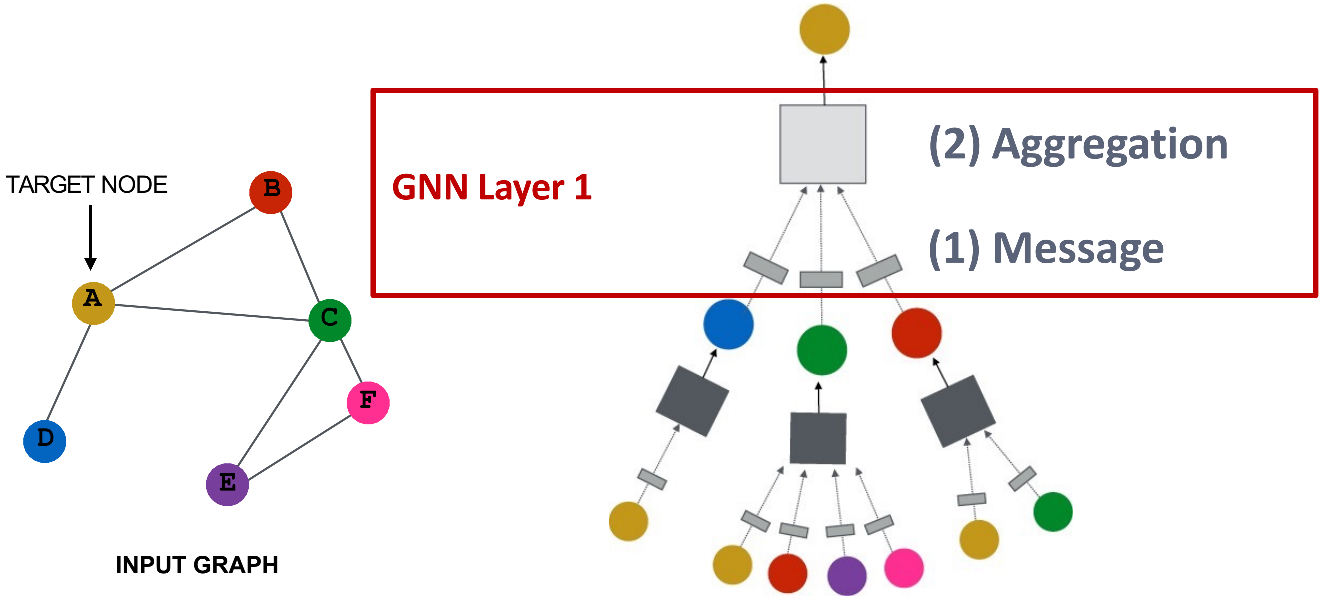
Basic approach: Average information from neighbors and apply a **neural network**



A GNN Layer

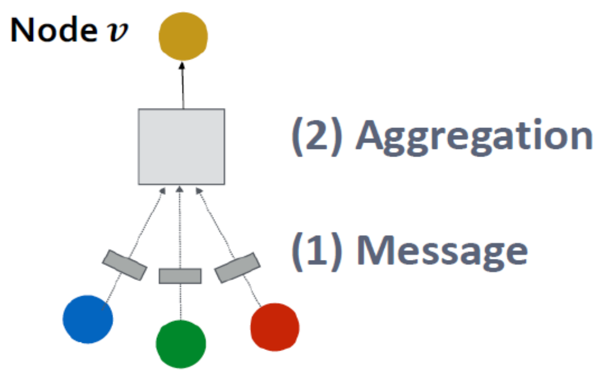
GNN Layer = Message + Aggregation

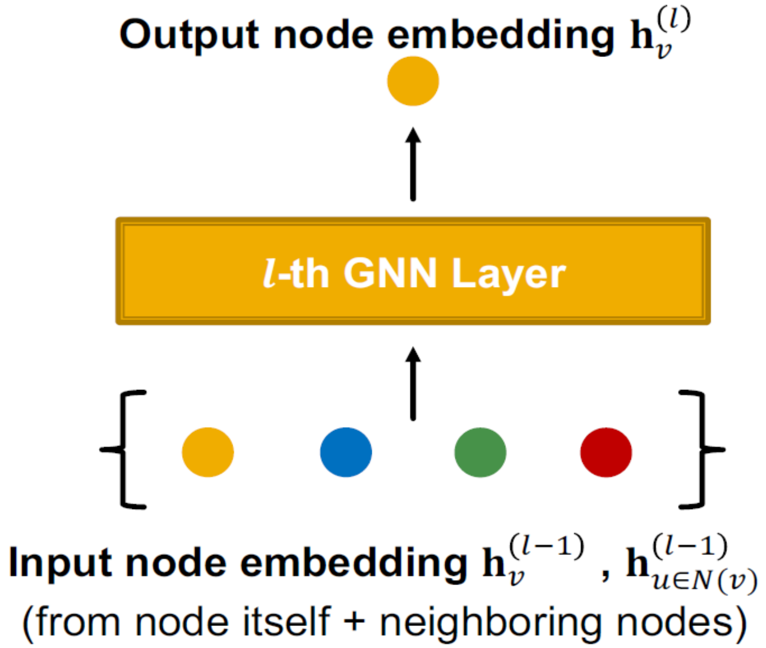
- **Different instantiations under this perspective**
- **GCN, GraphSAGE, GAT, …**



A Single GNN Layer

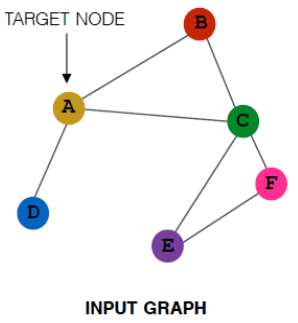
- **Idea of a GNN Layer:**
  - Compress a set of vectors into a single vector
  - **Two step process:**
    - **(1) Message**
    - **(2) Aggregation**

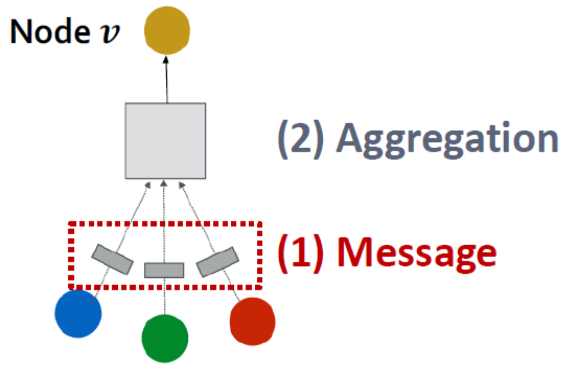




Message Computation

- (1) Message computation
  - **Message function:** $\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right)$
    - **Intuition:** Each node will create a message, which will be sent to other nodes later
    - **Example:** A Linear layer $\mathbf{m}_u^{(l)} = \mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}$
      - Multiply node features with weight matrix $\mathbf{W}^{(l)}$



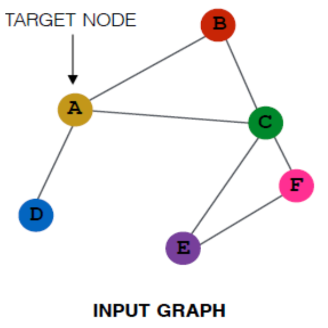


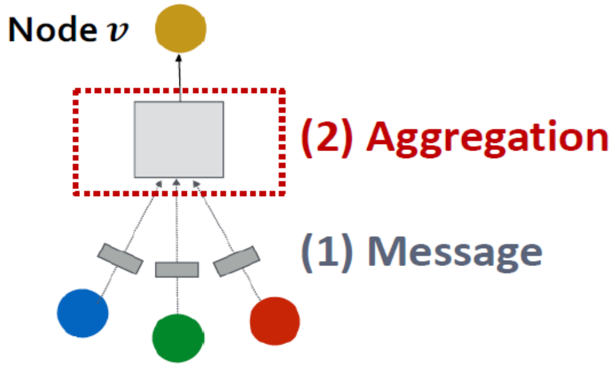
Message Aggregation

- (2) Aggregation
  - **Intuition:** Each node will aggregate the messages from node v's neighbors

$$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}\right)$$

  - **Example:** $\mathrm{Sum}(\cdot)$, $\mathrm{Mean}(\cdot)$ or $\mathrm{Max}(\cdot)$ aggregator
    - $\mathbf{h}_v^{(l)} = \mathrm{Sum}(\{\mathbf{m}_u^{(l)}, u \in N(v)\})$





Message Aggregation Issue

- **Issue:** Information from node v itself **could get lost**
  - Computation of $\mathbf{h}_v^{(l)}$ does not directly depend on $\mathbf{h}_v^{(l-1)}$
- **Solution:** Include $\mathbf{h}_v^{(l-1)}$ when computing $\mathbf{h}_v^{(l)}$
  - (1) Message: **compute message from node v itself**
    - Usually, a **different message computation** will be performed

$$\mathbf{m}_u^{(l)} = \mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)} \qquad \mathbf{m}_v^{(l)} = \mathbf{B}^{(l)}\mathbf{h}_v^{(l-1)}$$

  - (2) Aggregation: After aggregating from neighbors, we can **aggregate the message from node v itself**
    - Via concatenation **or** summation

Then aggregate from node itself

$$\mathbf{h}_v^{(l)} = \mathrm{CONCAT}\left(\mathrm{AGG}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}\right), \mathbf{m}_v^{(l)}\right)$$

First aggregate from neighbors

A Single GNN Layer

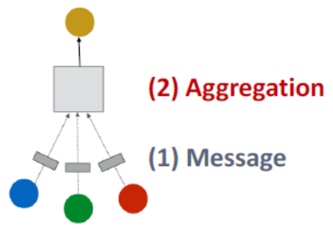
- **Putting things together:**
  - **(1) Message**: each node computes a message

$$\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$

  - **(2) Aggregation**: aggregate messages from neighbors

$$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}, \mathbf{m}_v^{(l)}\right)$$

  - **Nonlinearity (activation):** Adds expressiveness
    - Often written as $\sigma(\cdot)$: $\mathrm{ReLU}(\cdot)$, $\mathrm{Sigmoid}(\cdot)$, …
    - Can be added to **message or aggregation**



Activation (Non-linearity)

Apply activation to i-th dimension of embedding $\mathbf{x}$

- **Rectified linear unit (ReLU)**

  $$\mathrm{ReLU}(\mathbf{x}_i) = \max(\mathbf{x}_i, 0)$$

  - Most commonly used
- **Sigmoid**

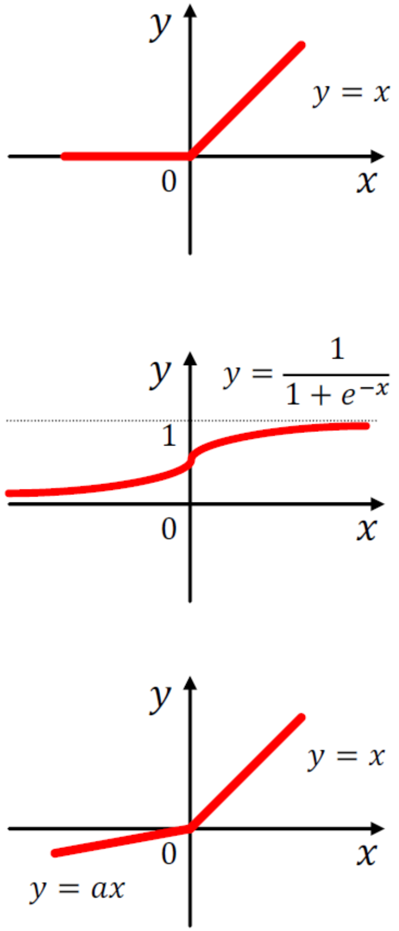
  $$\sigma(\mathbf{x}_i) = \frac{1}{1 + e^{-\mathbf{x}_i}}$$

  - Used only when you want to restrict the range of your embeddings
- **Parametric ReLU**

  $$\mathrm{PReLU}(\mathbf{x}_i) = \max(\mathbf{x}_i, 0) + a_i \min(\mathbf{x}_i, 0)$$

  a_i is a trainable parameter

  - Empirically performs better than ReLU



The Maths: Deep Encoder

Basic approach: Average neighbor messages and apply a neural network

Initial 0-th layer embeddings are equal to node features

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

embedding of v at layer l

$$h_v^{(l+1)} = \boxed{\sigma}\left(W_l \boxed{\sum_{u \in N(v)} \frac{h_u^{(l)}}{|N(v)|}} + B_l \boxed{h_v^{(l)}}\right), \forall l \in \{0, \ldots, \boxed{L} - 1\}$$

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

Average of neighbor's previous layer embeddings

Total number of layers

Embedding after L layers of neighborhood aggregation

Non-linearity (e.g., ReLU)

Model Parameters

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

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

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

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

Final node embedding

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

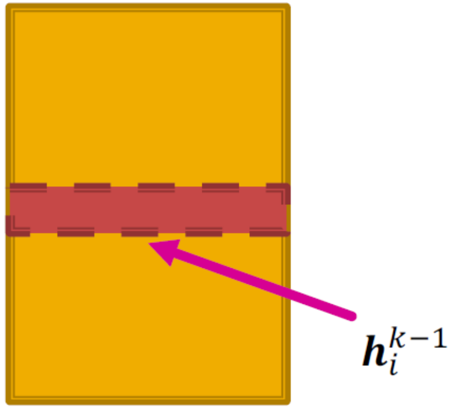
- h_v^l :the hidden representation of node v at layer l
- W_k:weight matrix for neighborhood aggregation
- B_k: weight matrix for transforming hidden vector of self

Matrix Formulation

- **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,**

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

Matrix of hidden embeddings H^{k-1}

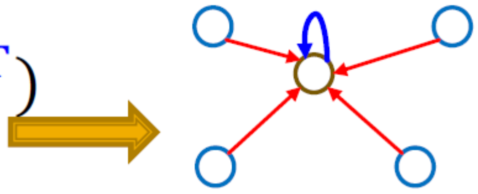


Matrix Formulation

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



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

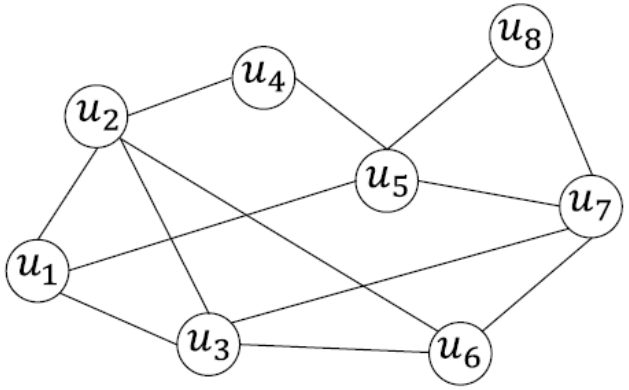
  - Red: neighborhood aggregation
  - Blue: self transformation

- 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

Example

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

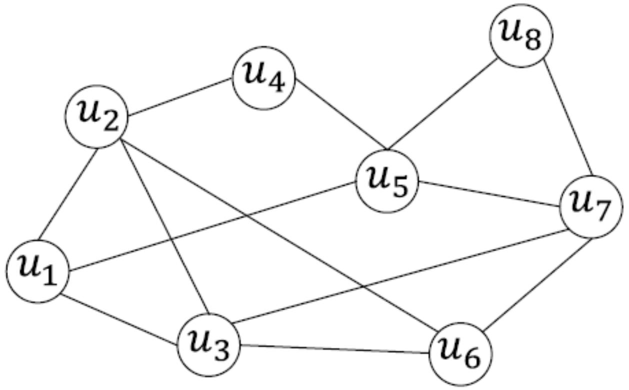


Compute the output of the first graph convolutional layer based on the above formula

$$H_0 = \begin{bmatrix} 0.20 & 0.60 & 0.30 & -0.40 \\ 0.40 & 0.30 & -0.20 & -0.60 \\ 0.20 & -0.60 & 0.50 & -0.30 \\ -0.40 & 0.20 & 0.20 & -0.40 \\ 0.70 & -0.90 & 0.10 & -0.50 \\ 0.30 & 0.50 & -0.30 & -0.70 \\ 0.90 & -0.60 & 0.20 & -0.80 \\ -0.10 & 0.70 & 0.10 & -0.90 \end{bmatrix} \quad W^0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad B^0 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

Example

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



The matrix D^{-1}:

Adjacent matrix A:

```
[[0 1 1 0 1 0 0 0]
 [1 0 1 1 0 1 0 0]
 [1 1 0 0 0 1 1 0]
 [0 1 0 0 1 0 0 0]
 [1 0 0 1 0 0 1 1]
 [0 1 1 0 0 0 1 0]
 [0 0 1 0 1 1 0 1]
 [0 0 0 0 1 0 1 0]]
```

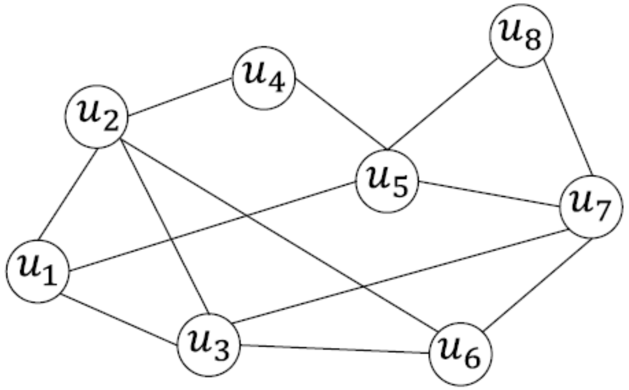
```
[[0.33333334 0.         0.         0.         0.         0.         0.         0.        ]
 [0.         0.25       0.         0.         0.         0.         0.         0.        ]
 [0.         0.         0.25       0.         0.         0.         0.         0.        ]
 [0.         0.         0.         0.5        0.         0.         0.         0.        ]
 [0.         0.         0.         0.         0.25       0.         0.         0.        ]
 [0.         0.         0.         0.         0.         0.33333334 0.         0.        ]
 [0.         0.         0.         0.         0.         0.         0.25       0.        ]
 [0.         0.         0.         0.         0.         0.         0.         0.5       ]]
```

The matrix $D^{-1}A$:

```
[[0.         0.33333334 0.33333334 0.         0.33333334 0.         0.         0.        ]
 [0.25       0.         0.25       0.25       0.         0.25       0.         0.        ]
 [0.25       0.25       0.         0.         0.         0.25       0.25       0.        ]
 [0.         0.5        0.         0.         0.5        0.         0.         0.        ]
 [0.25       0.         0.         0.25       0.         0.         0.25       0.25      ]
 [0.         0.33333334 0.33333334 0.         0.         0.         0.33333334 0.        ]
 [0.         0.         0.25       0.         0.25       0.25       0.         0.25      ]
 [0.         0.         0.         0.         0.5        0.         0.5        0.        ]]
```

Example

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



Matrix H^0 :

$$H_0 = \begin{bmatrix} 0.20 & 0.60 & 0.30 & -0.40 \\ 0.40 & 0.30 & -0.20 & -0.60 \\ 0.20 & -0.60 & 0.50 & -0.30 \\ -0.40 & 0.20 & 0.20 & -0.40 \\ 0.70 & -0.90 & 0.10 & -0.50 \\ 0.30 & 0.50 & -0.30 & -0.70 \\ 0.90 & -0.60 & 0.20 & -0.80 \\ -0.10 & 0.70 & 0.10 & -0.90 \end{bmatrix}$$

Matrix $D^{-1}A$:

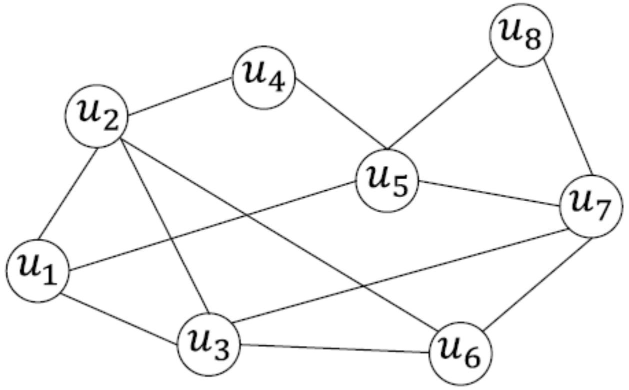
```
[[0.         0.33333334 0.33333334 0.         0.33333334 0.         0.         0.        ]
 [0.25       0.         0.25       0.25       0.         0.25       0.         0.        ]
 [0.25       0.25       0.         0.         0.         0.25       0.25       0.        ]
 [0.         0.5        0.         0.         0.5        0.         0.         0.        ]
 [0.25       0.         0.         0.25       0.         0.         0.25       0.25      ]
 [0.         0.33333334 0.33333334 0.         0.         0.         0.33333334 0.        ]
 [0.         0.         0.25       0.         0.25       0.25       0.         0.25      ]
 [0.         0.         0.         0.         0.5        0.         0.5        0.        ]]
```

Matrix $D^{-1}AH$:

```
[[ 0.43333335 -0.40000001  0.13333334 -0.46666668]
 [ 0.075       0.175       0.175      -0.1       ]
 [ 0.45        0.2         0.         -0.275     ]
 [ 0.55       -0.3        -0.05       -0.55      ]
 [ 0.15        0.225       0.2        -0.625     ]
 [ 0.50000001 -0.30000001  0.16666667 -0.56666668]
 [ 0.275      -0.075       0.1        -0.25      ]
 [ 0.8        -0.75        0.15       -0.65      ]]
```

Example

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



Matrix $D^{-1}AH$:

```
[[ 0.43333335 -0.40000001  0.13333334 -0.46666668]
 [ 0.075       0.175       0.175      -0.1       ]
 [ 0.45        0.2         0.         -0.275     ]
 [ 0.55       -0.3        -0.05       -0.55      ]
 [ 0.15        0.225       0.2        -0.625     ]
 [ 0.50000001 -0.30000001  0.16666667 -0.56666668]
 [ 0.275      -0.075       0.1        -0.25      ]
 [ 0.8        -0.75        0.15       -0.65      ]]
```

Matrix W^0 :

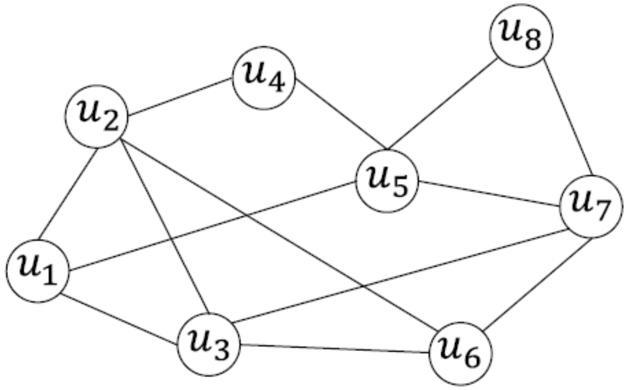
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Matrix $D^{-1}AHW^T$:

```
[[ 0.43333335  0.03333333  0.16666667 -0.30000001]
 [ 0.075       0.25        0.425       0.325     ]
 [ 0.45        0.65        0.65        0.375     ]
 [ 0.55        0.25        0.2        -0.35      ]
 [ 0.15        0.375       0.575      -0.05      ]
 [ 0.50000001  0.20000001  0.36666668 -0.20000001]
 [ 0.275       0.2         0.3         0.05      ]
 [ 0.8         0.05        0.2        -0.45      ]]
```

Example

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



Matrix B^0 :

$$\begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

Matrix H^0 :

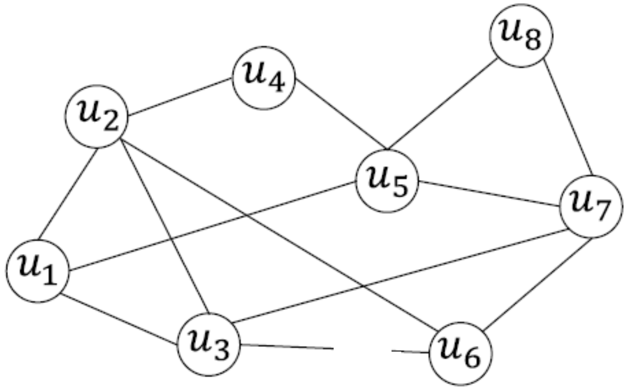
$$\begin{bmatrix} 0.20 & 0.60 & 0.30 & -0.40 \\ 0.40 & 0.30 & -0.20 & -0.60 \\ 0.20 & -0.60 & 0.50 & -0.30 \\ -0.40 & 0.20 & 0.20 & -0.40 \\ 0.70 & -0.90 & 0.10 & -0.50 \\ 0.30 & 0.50 & -0.30 & -0.70 \\ 0.90 & -0.60 & 0.20 & -0.80 \\ -0.10 & 0.70 & 0.10 & -0.90 \end{bmatrix}$$

Matrix HB^T :

```
[[-0.2  0.5 -0.1  0.5]
 [-0.2  0.2 -0.8  0.2]
 [-0.1  0.7  0.2  0.7]
 [-0.8 -0.2 -0.2 -0.2]
 [ 0.2  0.8 -0.4  0.8]
 [ 1.   0.   0.4  0. ]
 [ 0.1  1.1 -0.6  1.1]
 [-1.   0.  -0.8  0. ]]
```

Example

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



Matrix $D^{-1}AHW^T$:

```
[[ 0.43333335  0.03333333  0.16666667 -0.30000001]
 [ 0.075       0.25        0.425       0.325     ]
 [ 0.45        0.65        0.65        0.375     ]
 [ 0.55        0.25        0.2        -0.35      ]
 [ 0.15        0.375       0.575      -0.05      ]
 [ 0.50000001  0.20000001  0.36666668 -0.20000001]
 [ 0.275       0.2         0.3         0.05      ]
 [ 0.8         0.05        0.2        -0.45      ]]
```

Matrix HB^T :

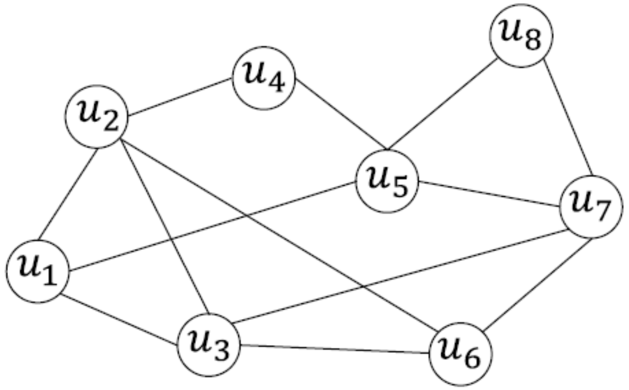
```
[[-0.2  0.5 -0.1  0.5]
 [-0.2  0.2 -0.8  0.2]
 [-0.1  0.7  0.2  0.7]
 [-0.8 -0.2 -0.2 -0.2]
 [ 0.2  0.8 -0.4  0.8]
 [ 1.   0.   0.4  0. ]
 [ 0.1  1.1 -0.6  1.1]
 [-1.   0.  -0.8  0. ]]
```

Matrix $D^{-1}AHW^T + HB^T$:

```
[[ 0.23333335  0.53333333  0.06666667  0.19999999]
 [-0.125       0.45       -0.375       0.525     ]
 [ 0.35        1.35        0.85        1.075     ]
 [-0.25        0.05        0.         -0.55      ]
 [ 0.35        1.175       0.175       0.75      ]
 [ 1.50000001  0.20000001  0.76666668 -0.20000001]
 [ 0.375       1.3        -0.3         1.15      ]
 [-0.2         0.05       -0.6        -0.45      ]]
```

Example

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



Matrix $D^{-1}AHW^T + HB^T$:

```
[[ 0.23333335  0.53333333  0.06666667  0.19999999]
 [-0.125       0.45       -0.375       0.525     ]
 [ 0.35        1.35        0.85        1.075     ]
 [-0.25        0.05        0.         -0.55      ]
 [ 0.35        1.175       0.175       0.75      ]
 [ 1.50000001  0.20000001  0.76666668 -0.20000001]
 [ 0.375       1.3        -0.3         1.15      ]
 [-0.2         0.05       -0.6        -0.45      ]]
```

Matrix $\sigma(D^{-1}AHW^T + HB^T)$:

```
[[0.23333335 0.53333333 0.06666667 0.19999999]
 [0.         0.45       0.         0.525     ]
 [0.35       1.35       0.85       1.075     ]
 [0.         0.05       0.         0.        ]
 [0.35       1.175      0.175      0.75      ]
 [1.50000001 0.20000001 0.76666668 0.        ]
 [0.375      1.3        0.         1.15      ]
 [0.         0.05       0.         0.        ]]
```

Train a GNN

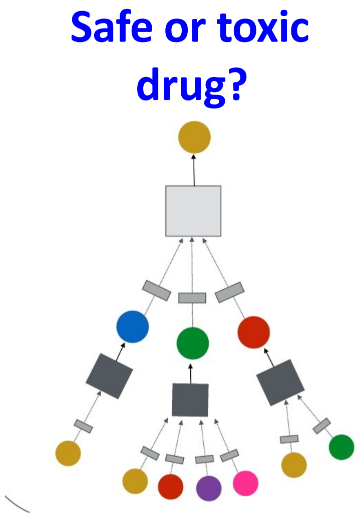
- Node embedding $\boldsymbol{z}_v$ is a function of input graph
- **Supervised setting**: we want to minimize the loss $\mathcal{L}$:

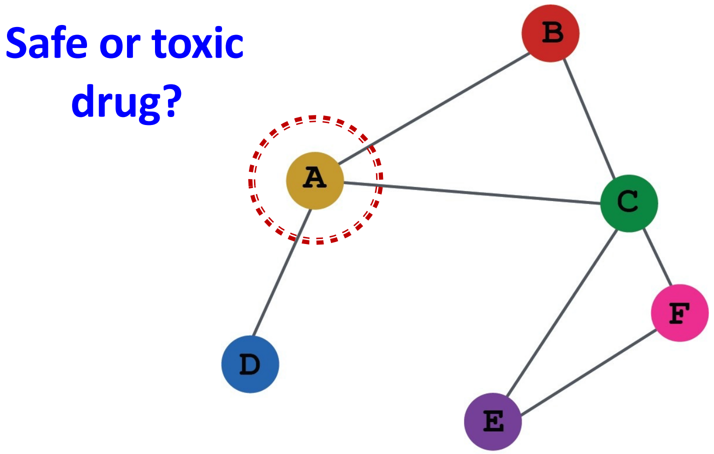
$$\min_{\Theta} \mathcal{L}(\boldsymbol{y}, f(\boldsymbol{z}_v))$$

  - $\boldsymbol{y}$: 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!**

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

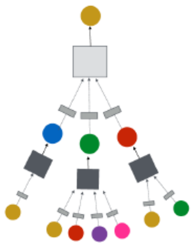
$$\mathcal{L} = -\sum_{v\in V} \boxed{y_v}\log(\sigma(\boxed{\mathrm{z}_v^{\mathrm{T}}}\boxed{\theta})) + (1-\boxed{y_v})\log(1-\sigma(\boxed{\mathrm{z}_v^{\mathrm{T}}}\boxed{\theta}))$$

Encoder output:
node embedding

Classification
weights

Node class
label

Safe or toxic drug?



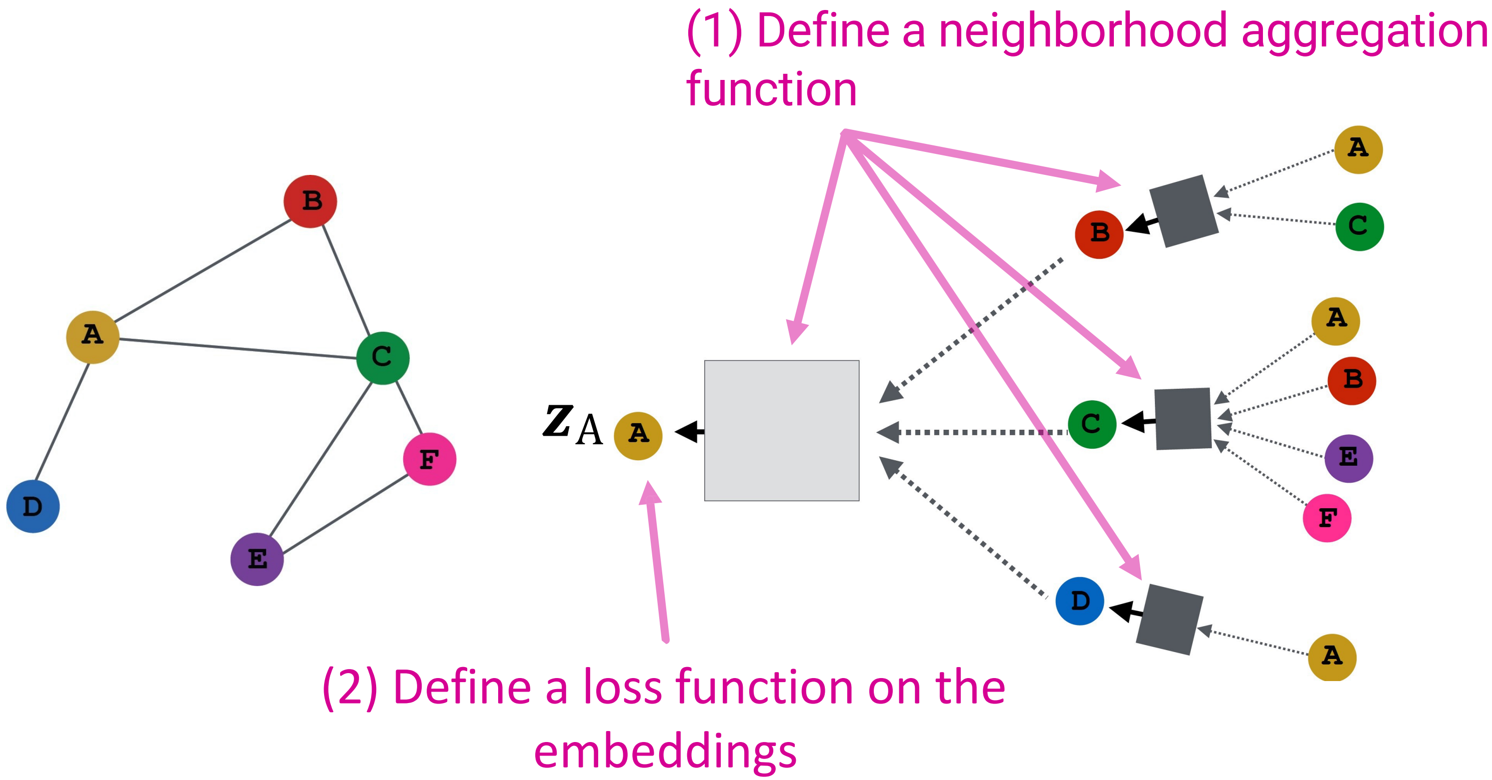
Unsupervised Training

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

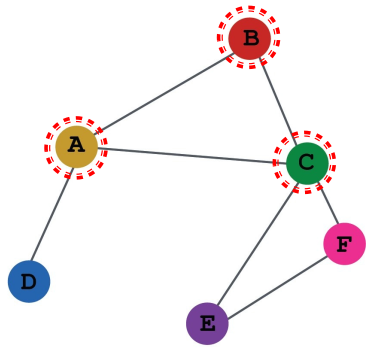
$$\mathcal{L} = \sum_{z_u, z_v} \mathrm{CE}(y_{u,v}, \mathrm{DEC}(z_u, z_v))$$

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

Model Design: Overview

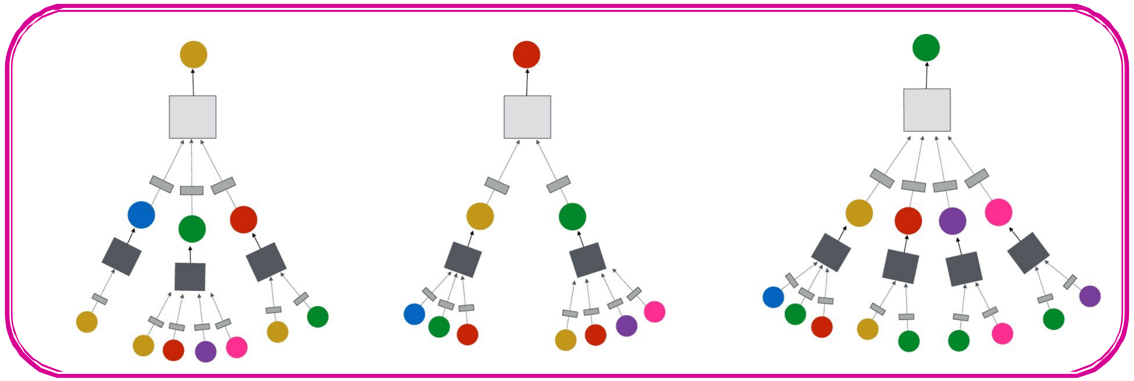


Model Design: Overview

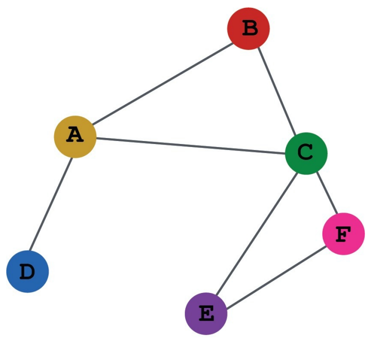


INPUT GRAPH

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



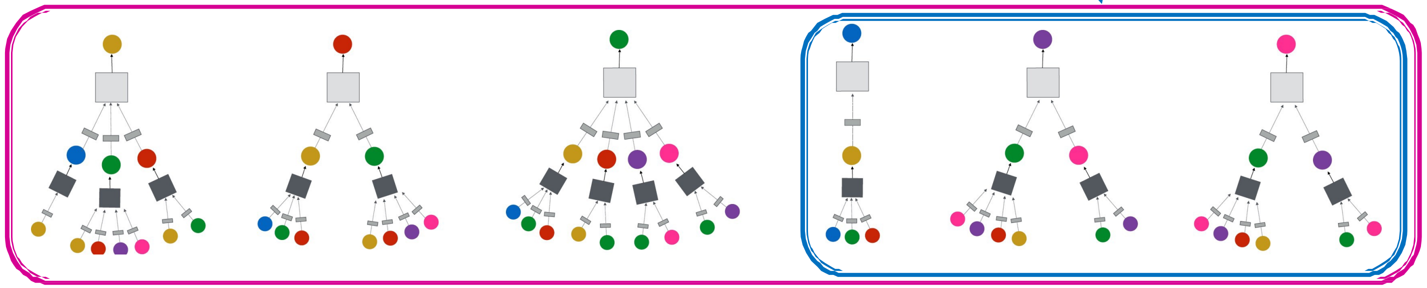
Model Design: Overview



INPUT GRAPH

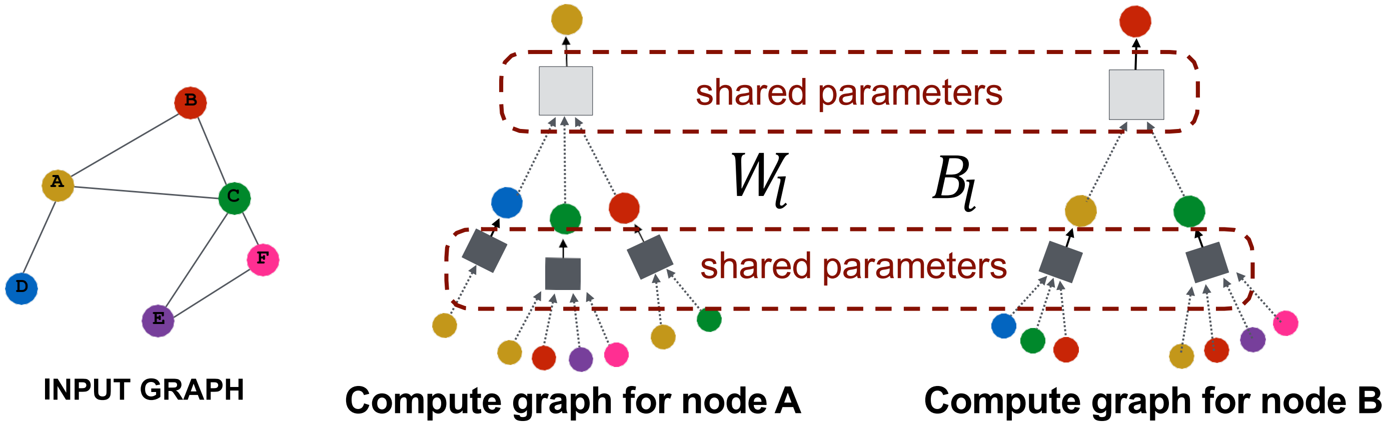
(4) Generate embeddings for nodes as needed

Even for nodes we never trained on!

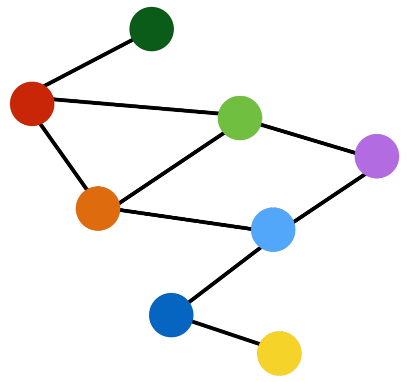


Inductive Capability

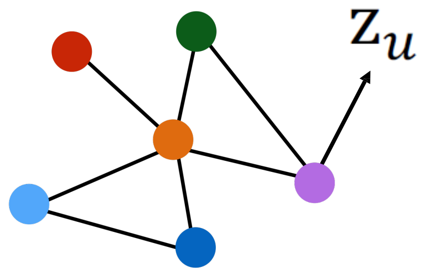
- **The same aggregation parameters are shared for all nodes:**
  - The number of model parameters is sublinear in $|V|$ and we can **generalize to unseen nodes**!



Inductive Capability: New Graphs



Train on one graph

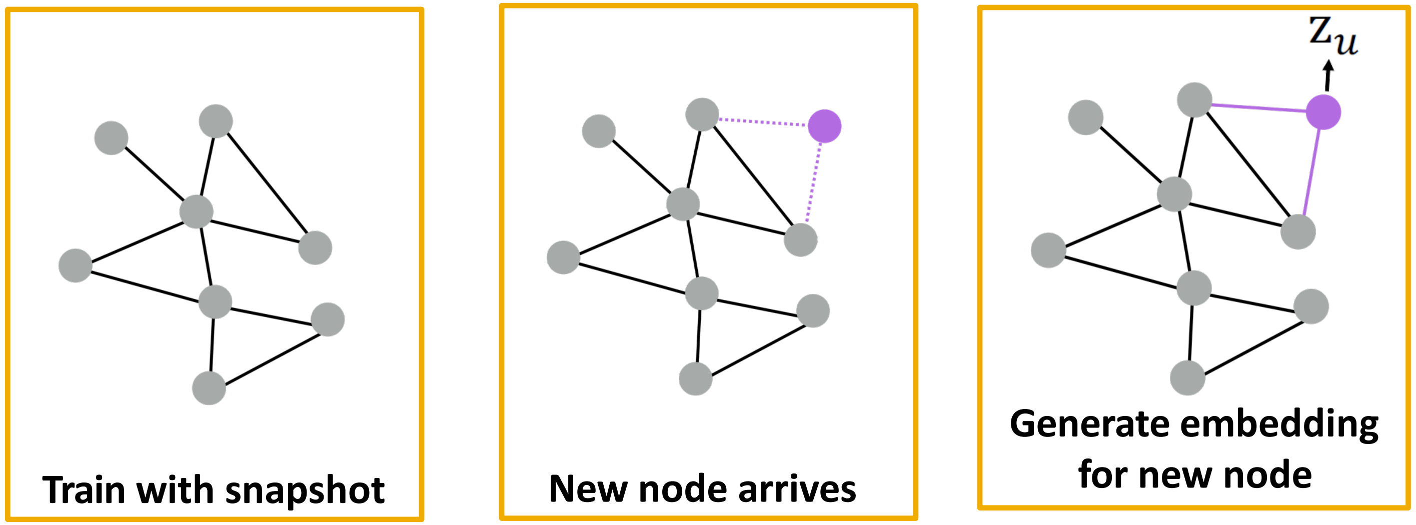


Generalize to new graph

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

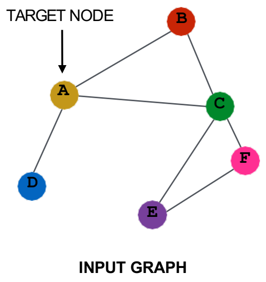


- Many application settings constantly encounter previously unseen nodes:
  - E.g., Reddit, YouTube, Google Scholar
- Need to generate new embeddings "on the fly"

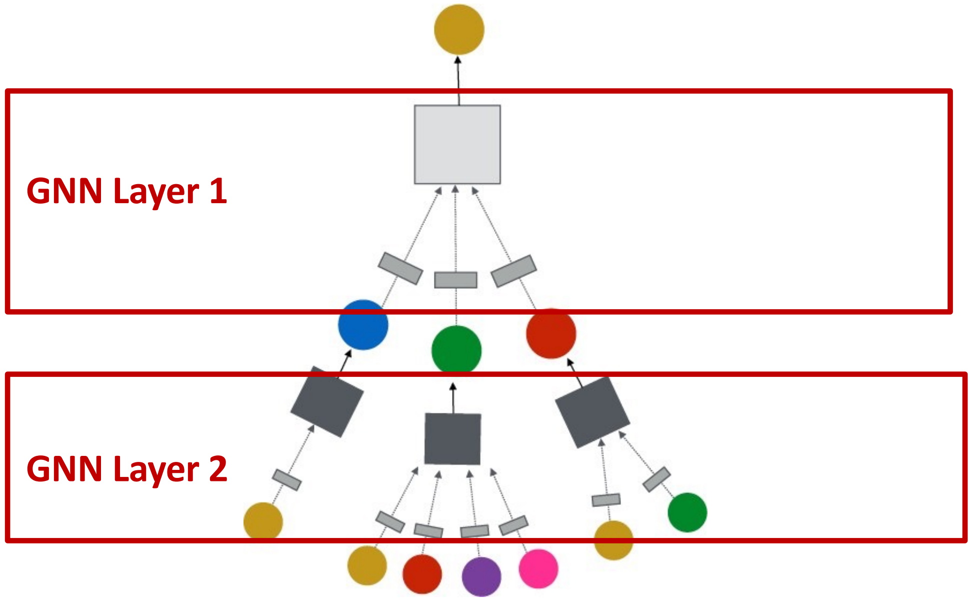
Stacking GNN Layers

How to connect GNN layers into a GNN?

1. Stack layers sequentially

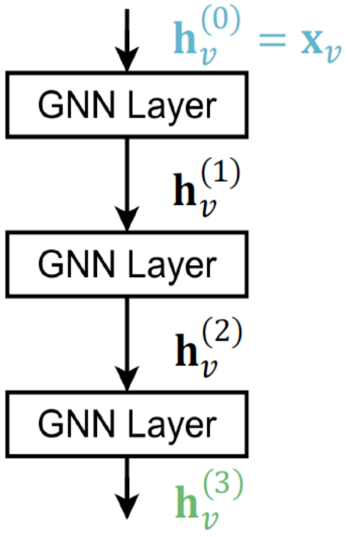


(3) Layer connectivity



Stacking GNN Layers

- **How to construct a Graph Neural Network?**
  - **The standard way:** Stack GNN layers sequentially
  - **Input:** Initial raw node feature $\mathbf{x}_v$
  - **Output:** Node embeddings $\mathbf{h}_v^{(L)}$ after L GNN layers

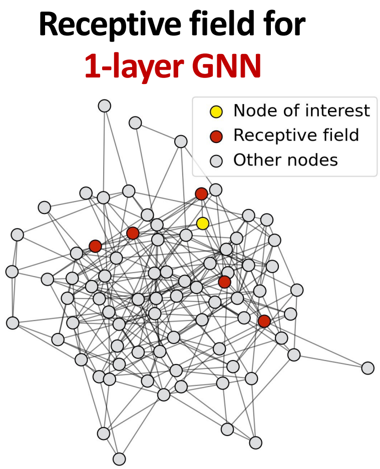


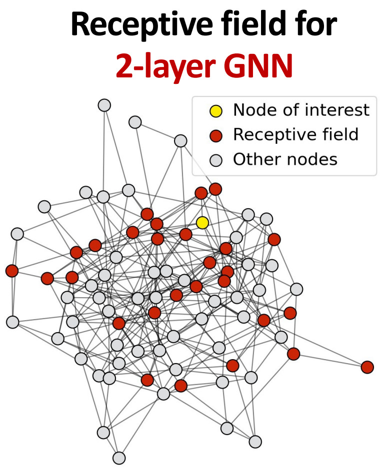
An Over-smoothing Problem

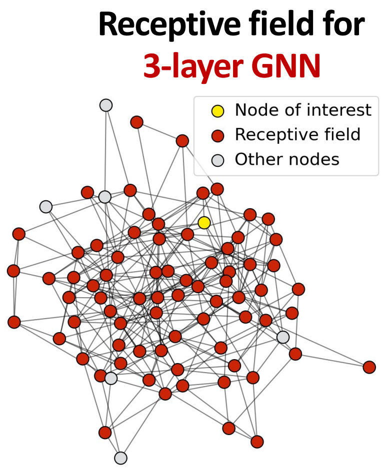
- The Issue of stacking many GNN layers
  - GNN suffers from **the over-smoothing problem**
- **The over-smoothing problem: all the node embeddings converge to the same value**
  - This is bad because we **want to use node embeddings to differentiate nodes**
- **Why does the over-smoothing problem happen?**

Receptive Field of a GNN

- **Receptive field:** the set of nodes that determine the embedding of a node of interest
  - **In a K-layer GNN, each node has a receptive field of K-hop neighborhood**



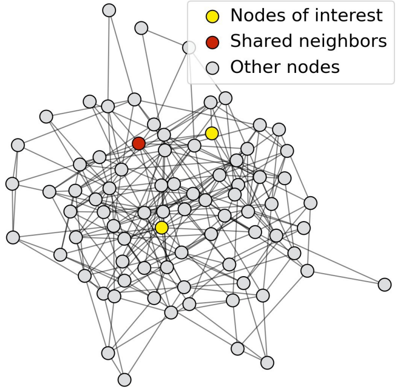




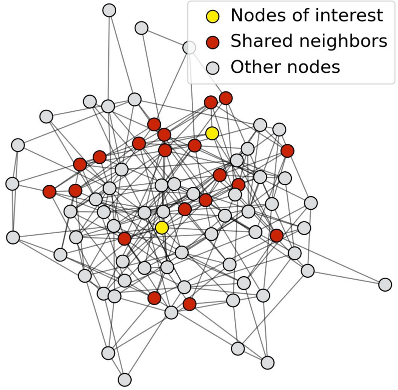
Receptive Field of a GNN

- Receptive field overlap for two nodes
  - **The shared neighbors quickly grows** when we increase the number of hops (num of GNN layers)

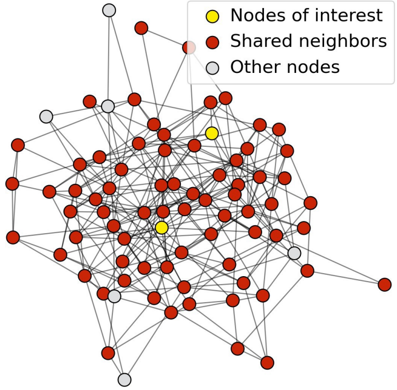
1-hop neighbor overlap Only 1 node



2-hop neighbor overlap About 20 nodes



3-hop neighbor overlap Almost all the nodes!



Receptive Field &Over-smoothing

- We can explain over-smoothing via the notion of receptive field
  - **The embedding of a node is determined by its** receptive field
    - If two nodes **have highly-overlapped receptive fields, then their embeddings are highly similar**
  - **Stack many GNN layers → nodes will have highly- overlapped receptive fields → node embeddings will be highly similar → suffer from the over- smoothing problem**
- **Next:** how do we overcome over-smoothing problem?

Over-smoothing

Model	2-Layer	4-Layer	8-Layer	16-Layer	32-Layer	64-Layer
GCN-res	88.18±1.59	86.50±1.87	84.83±1.93	78.60±4.28	59.82±7.74	39.71±5.15
PairNorm	79.98±3.80	82.32±2.79	81.52±3.66	82.29±2.62	81.91±2.45	81.72±2.82
NodeNorm	89.53±1.29	88.60±1.36	88.02±1.67	88.41±1.25	88.30±1.30	87.40±2.06

Typical results of node classification accuracy on CoautorCS dataset

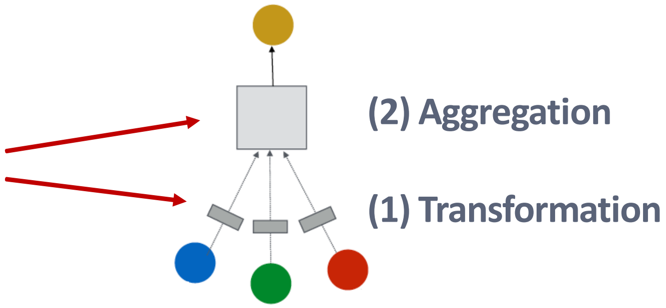
Design GNN Layer Connectivity

- What do we learn from the over-smoothing problem?
- Lesson: Be cautious when adding GNN layers
  - Unlike neural networks in other domains (CNN for image classification), **adding more GNN layers do not always help**
  - **Step 1: Analyze the necessary receptive field** to solve your problem. E.g., by computing the diameter of the graph
  - **Step 2:** Set number of GNN layers L to be a bit more than the receptive field we like. **Do not set L to be unnecessarily large**!

Expressive Power for Shallow GNNs

- **Question:** How to enhance the expressive power of a GNN, if the number of GNN layers is small?
- **Solution:** Increase the expressive power **within each GNN layer**
  - In our previous examples, each transformation or aggregation function only include one linear layer
  - We can **make aggregation / transformation become a deep neural network**!

If needed, each box could include a 3-layer MLP



Learning Outcome

- Generate node embeddings by aggregating neighborhood information
- Key distinctions are in how different approaches aggregate information across the layers