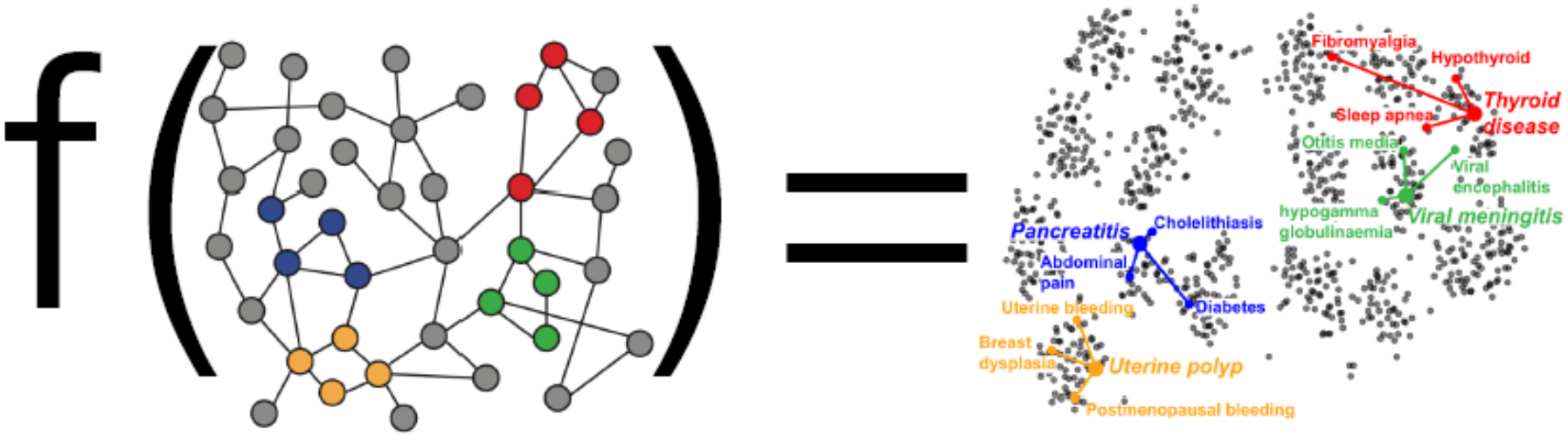
Graph Neural Networks

Slides adapted from Jure Leskovec's CS224W lecture on Machine Learning on Graphs

Recap – Node Embeddings

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



Input graph

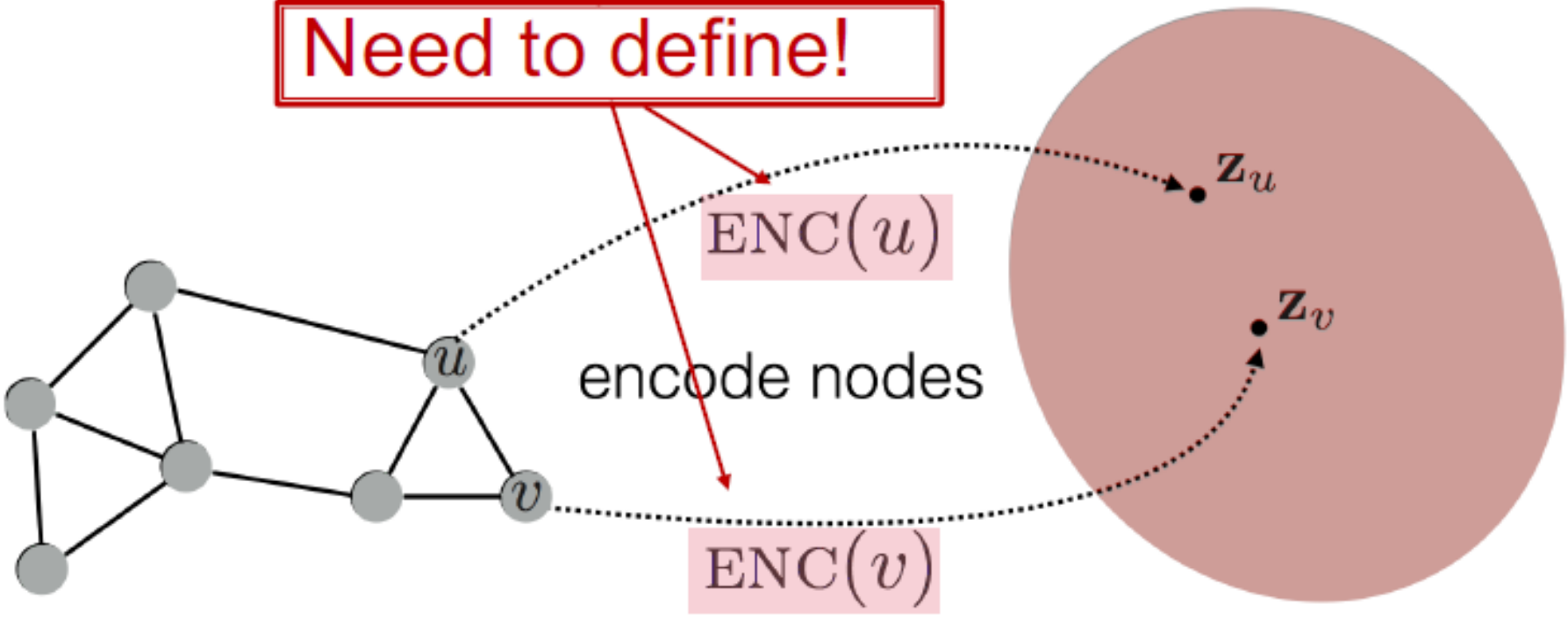
2D node embeddings

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

Recap – Node Embeddings

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

Need to define!



Recap – Node Embeddings

- **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

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

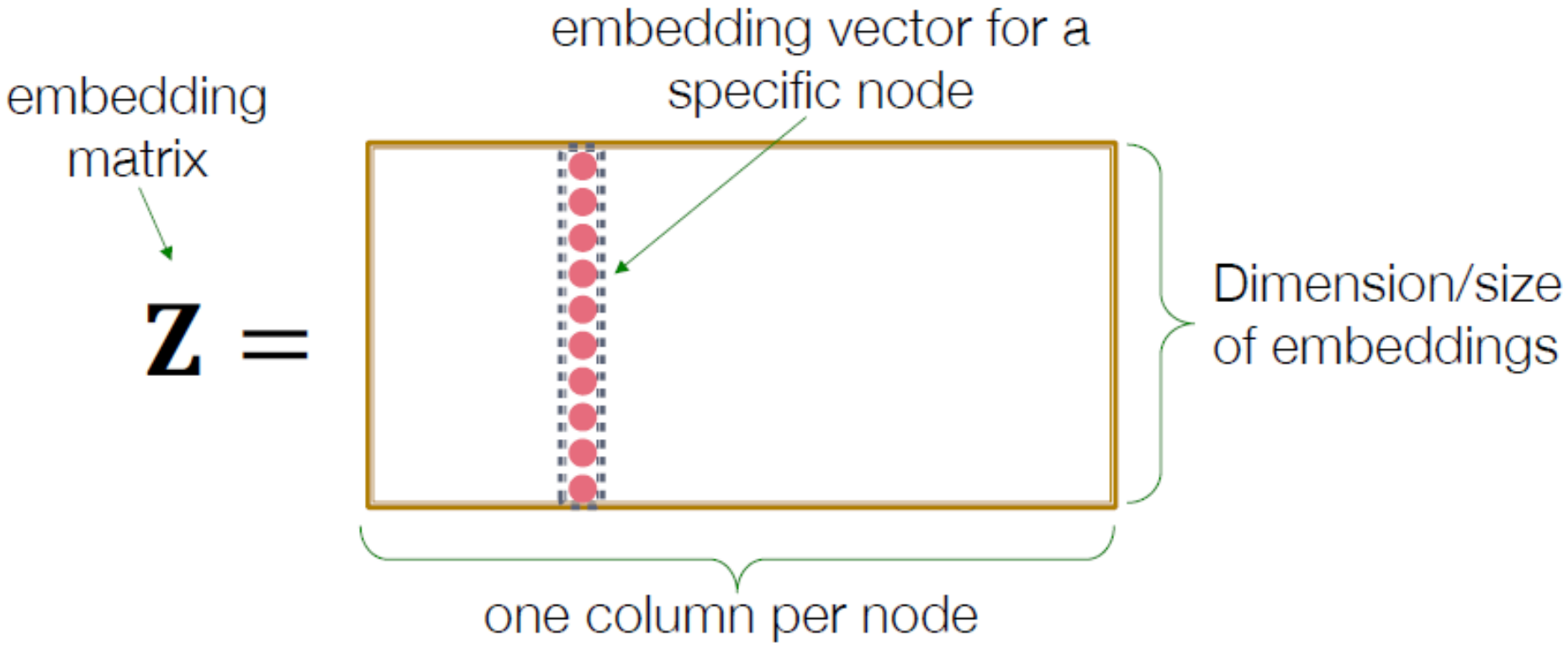
Decoder

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

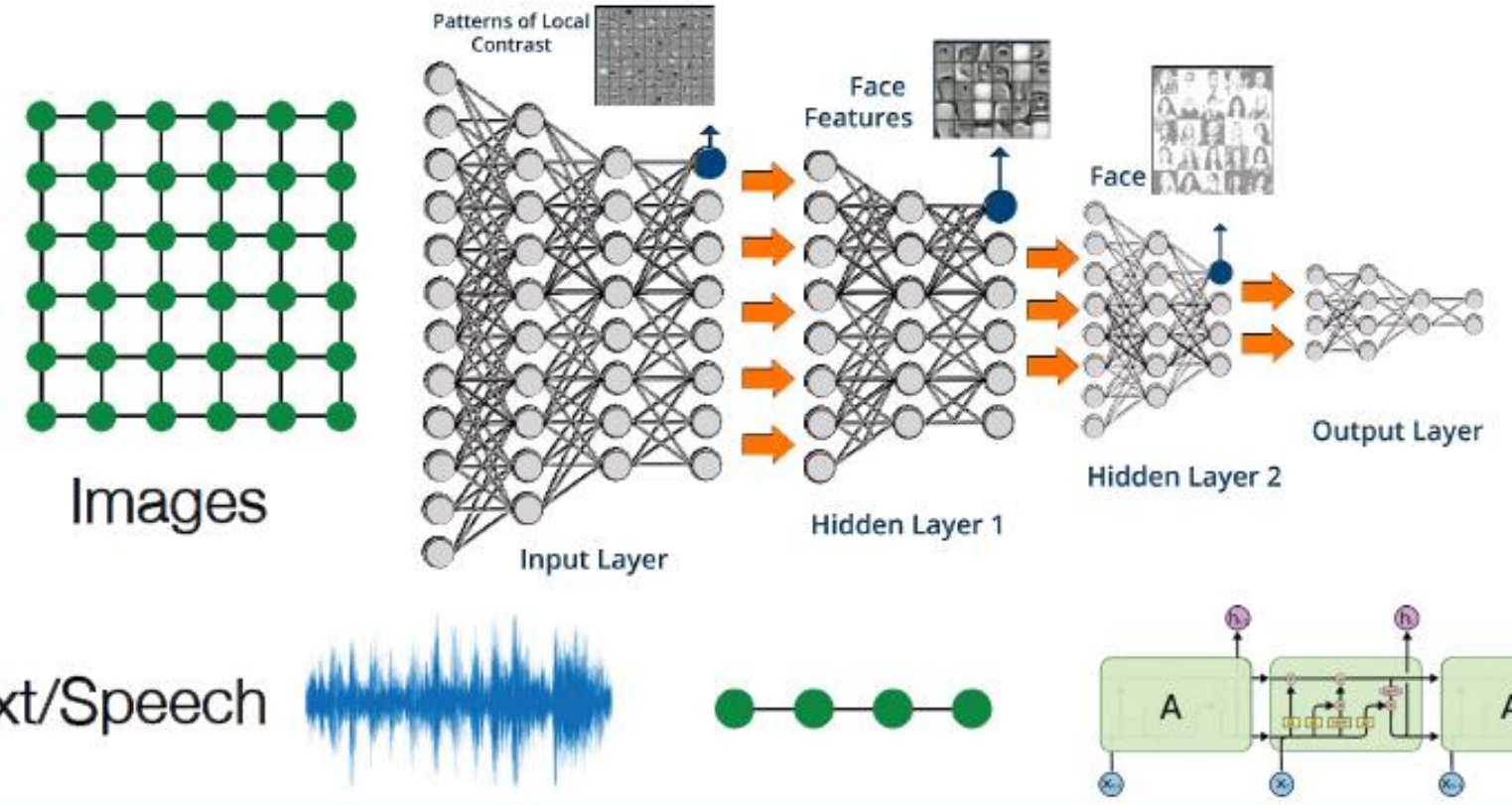
- **Limitations** of shallow embedding methods:
  - $O(|V|)$ **parameters are needed**:
    - No sharing of parameters between nodes
    - Every node has its own unique embedding
  - **Inherently "transductive"**:
    - Cannot generate embeddings for nodes that are not seen during training
  - **Do not incorporate node features**:
    - Many graphs have features that we can and should leverage

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

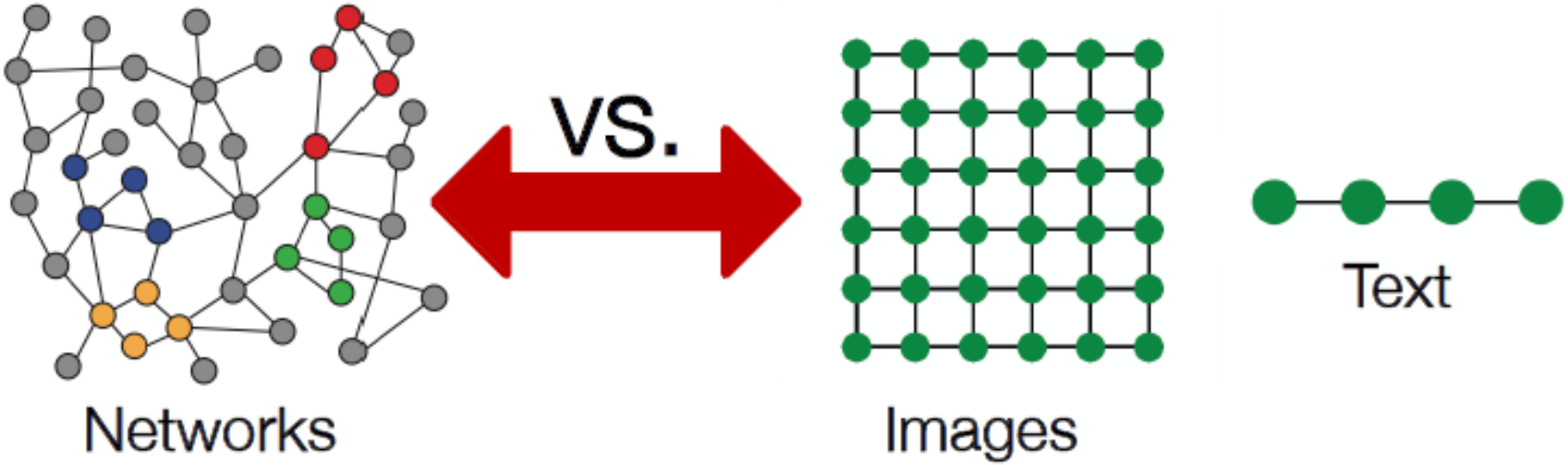


Modern deep learning toolbox is designed for simple sequences & grids

Why deep learning on Graphs is 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

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

- 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

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

  - 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: $f(\boldsymbol{x})_i = \frac{e^{g(x)_i}}{\sum_{j=1}^{C} e^{g(x)_j}}$,

where C is the number of classes.

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

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

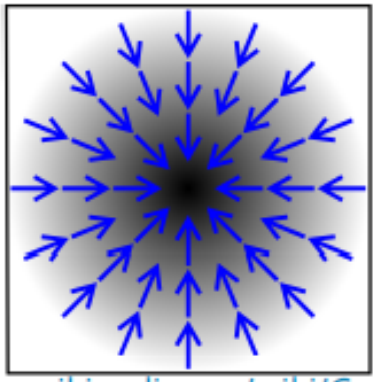
- $\text{CE}(\boldsymbol{y}, f(\boldsymbol{x})) = -\sum_{i=1}^{C}(y_i \log f(x)_i)$
  - $y_i, f(x)_i$ are the **actual** and **predicted** value of the i-th class.
  - **Intuition:** the lower the loss, the closer the prediction is to one-hot
- **Total loss over all training examples:**
  - $\mathcal{L}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

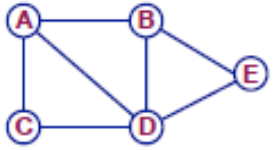
  - $\Theta_1, \Theta_2 \ldots$: components of Θ
- Recall **directional derivative** of a multi-variable function (e.g. $\mathcal{L}$) along a given vector represents the instantaneous rate of change of the function along the vector.
- Gradient is the directional derivative in the **direction of largest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

Setup

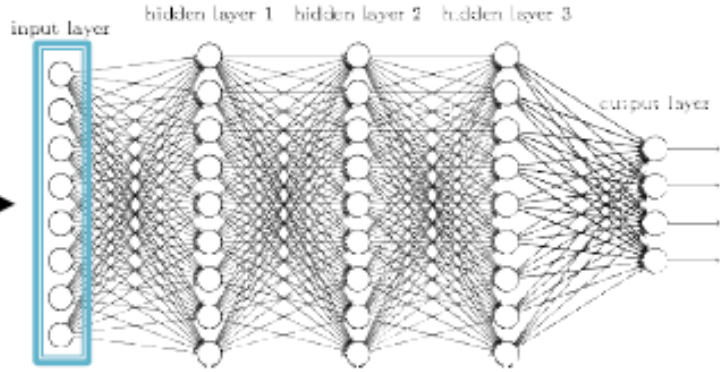
- **Assume we have a graph G:**
  - V is the **vertex set**
  - $\boldsymbol{A}$ is the **adjacency matrix** (assume binary)
  - $\boldsymbol{X} \in \mathbb{R}^{m \times |V|}$ is a matrix of **node features**
  - v: a node in V; $N(v)$: the set of neighbors of v.
  - **Node features:**
    - Social networks: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

Naïve Approach

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



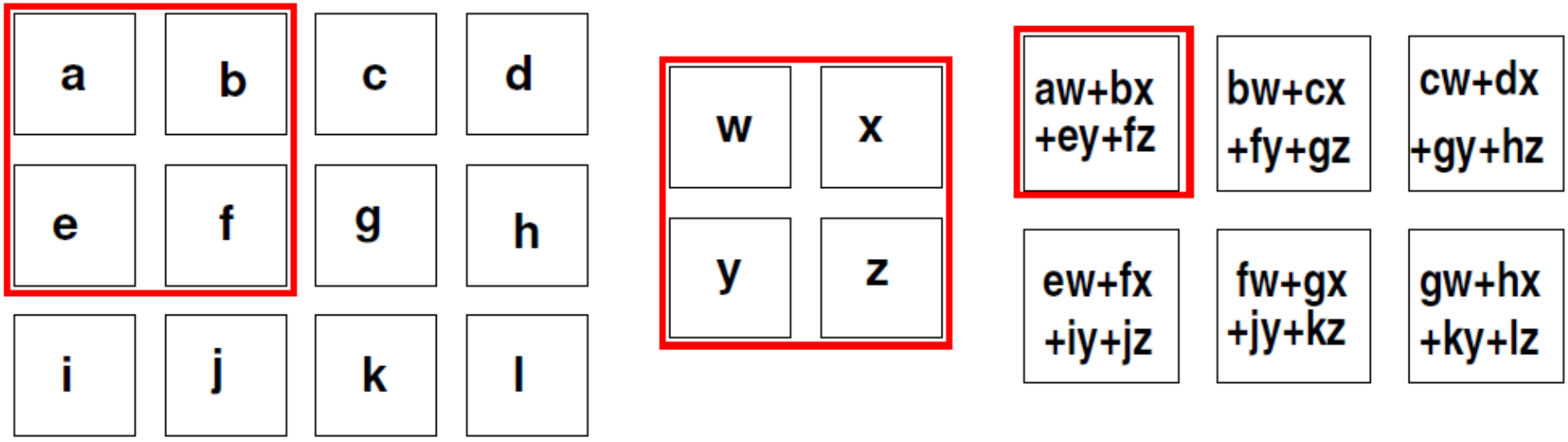
	A	B	C	D	E	Feat	
A	0	1	1	1	0	1	0
B	1	0	0	1	1	0	0
C	1	0	0	1	0	0	1
D	1	1	1	0	1	1	1
E	0	1	0	1	0	1	0



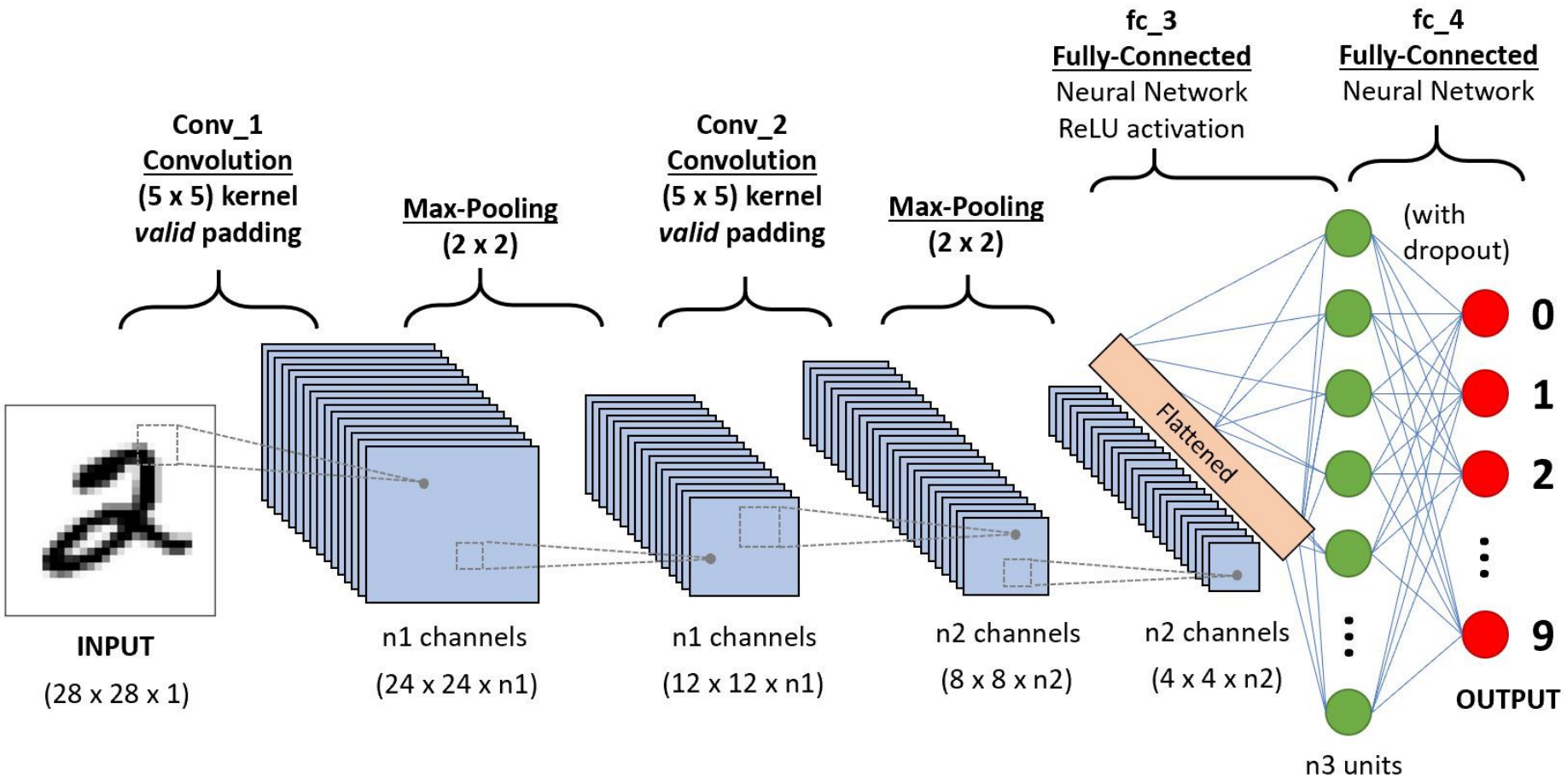
?

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

Idea – Use Convolution Networks



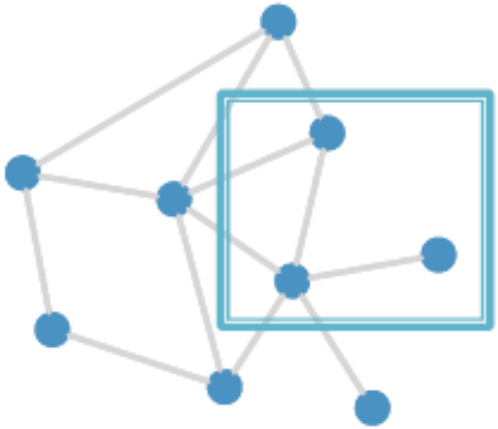
Idea – Use Convolution Neural Networks



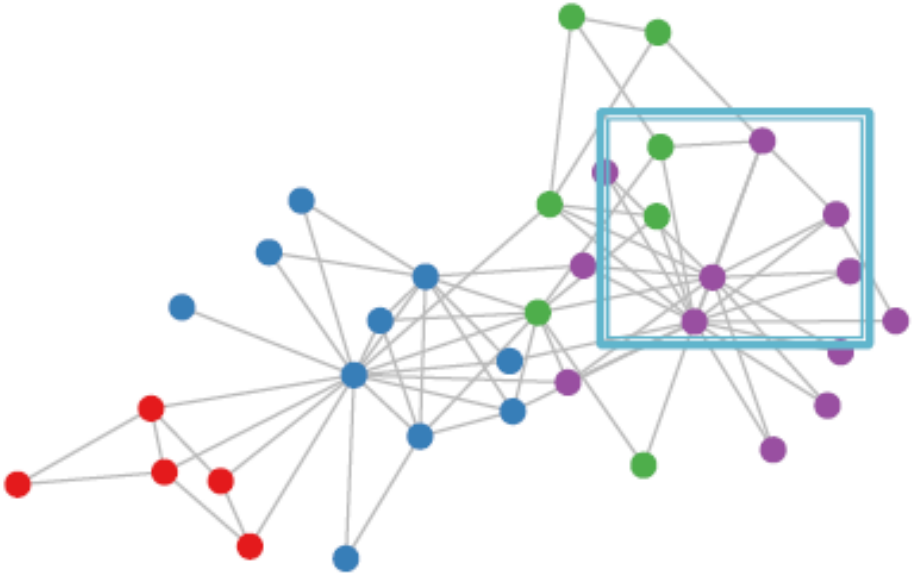
- Goal is to generalize convolutions beyond simple lattices
  - Leverage node feature attributes (texts and Images)

Real World Graphs

But our graphs look like this:



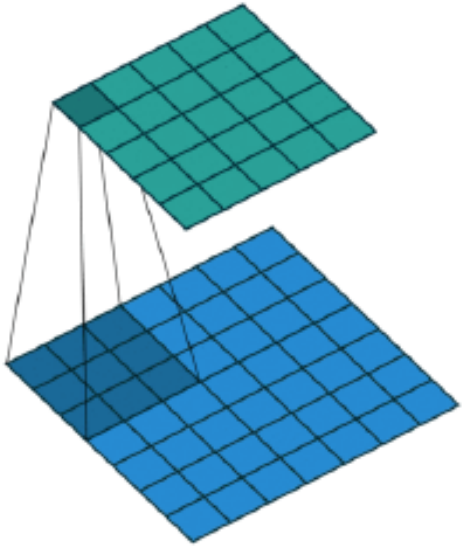
or this:



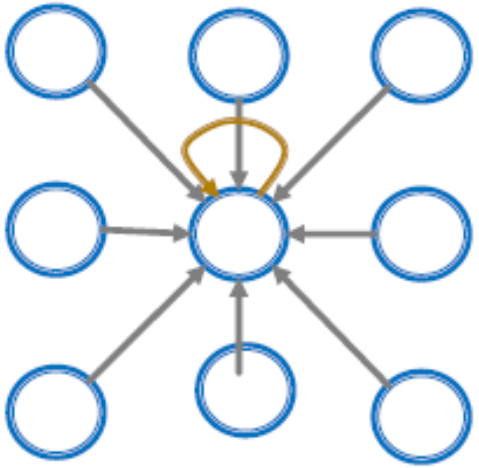
- There is no fixed notion of locality or sliding window on the graph
- Graph is permutation invariant

Applying CNNs for graphs

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



Image



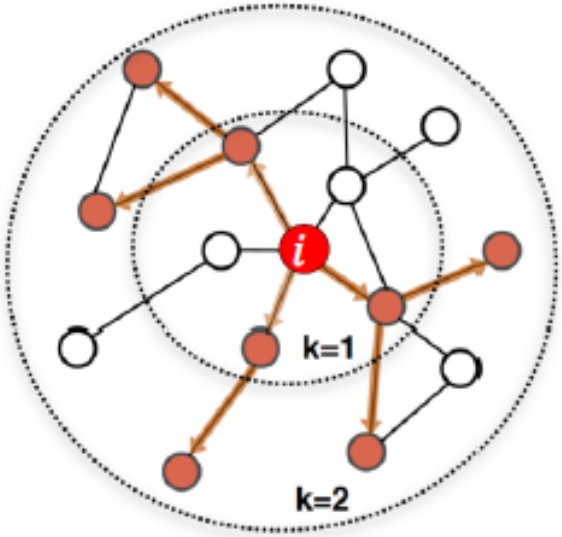
Graph

Idea: transform information at the neighbors and combine it:

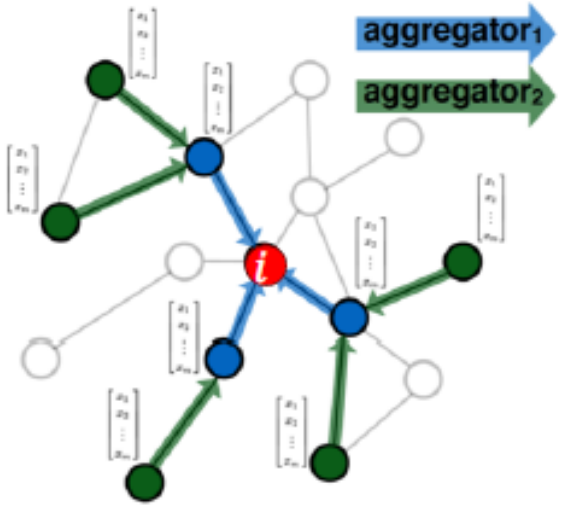
- Transform "messages" h_i from neighbors: $W_i\, h_i$
- Add them up: $\sum_i W_i\, h_i$

Graph Convolution Networks

Idea: Node's neighborhood defines a computation graph



Determine node computation graph

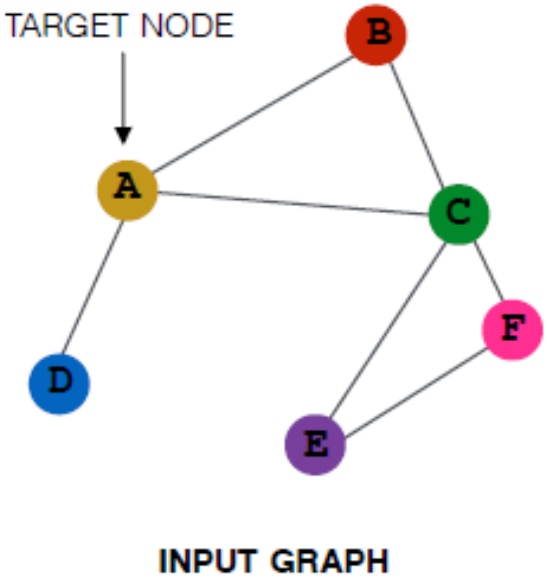


Propagate and transform information

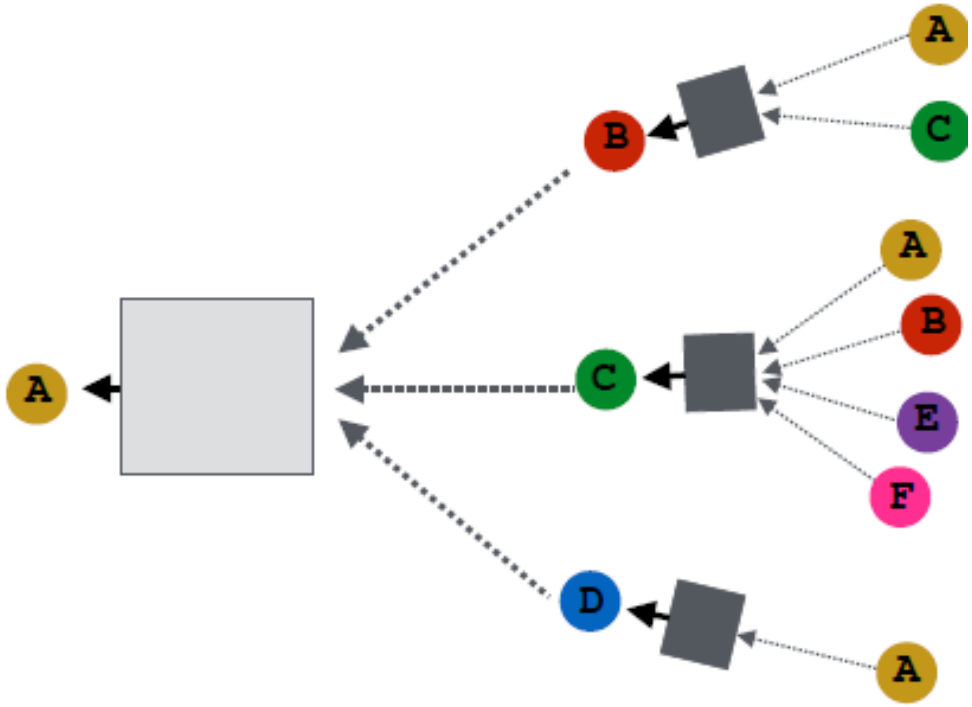
Learn how to propagate information across the graph to compute node features

Idea – Aggregate Neighbors

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

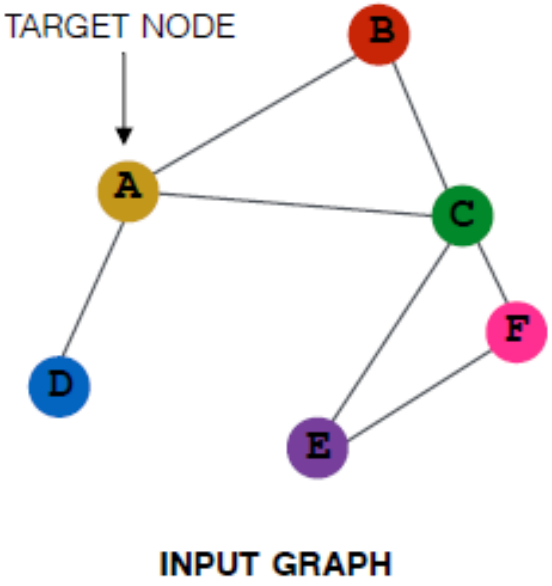


INPUT GRAPH

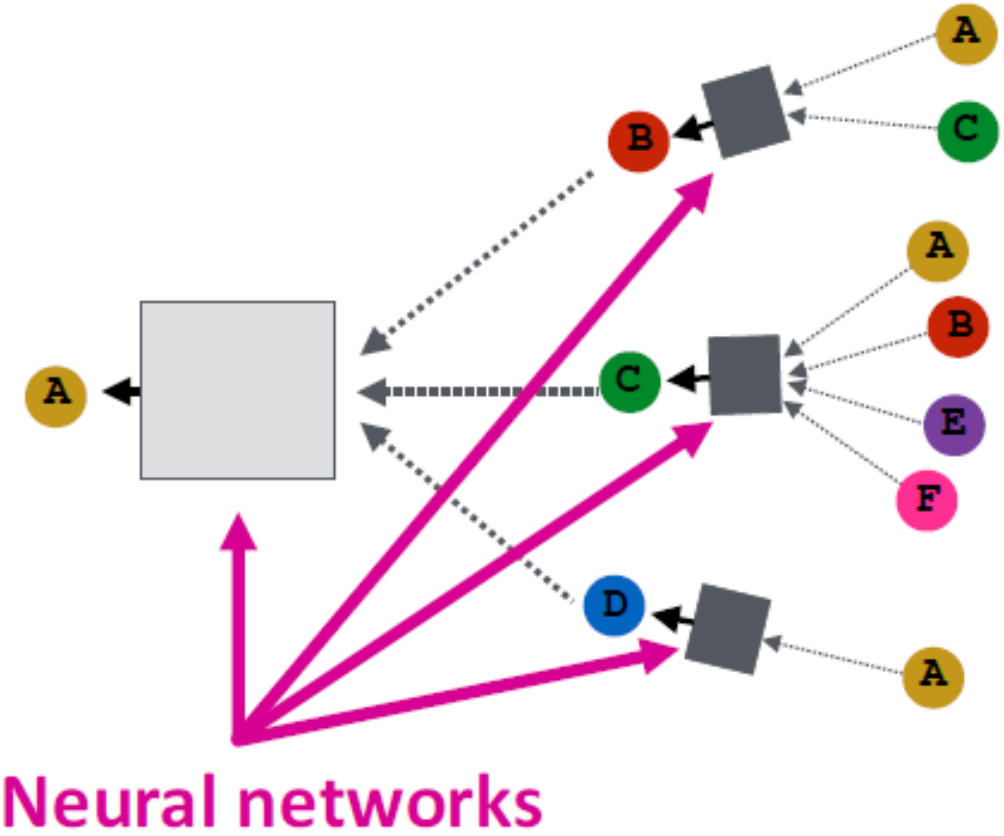


Idea – Aggregate Neighbors

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



INPUT GRAPH

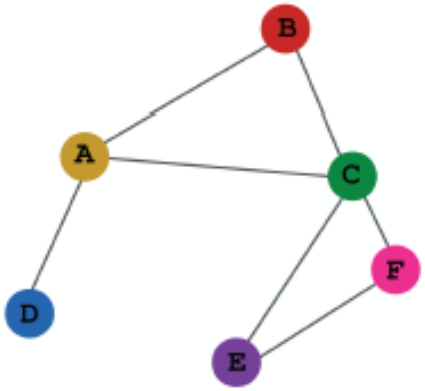


Neural networks

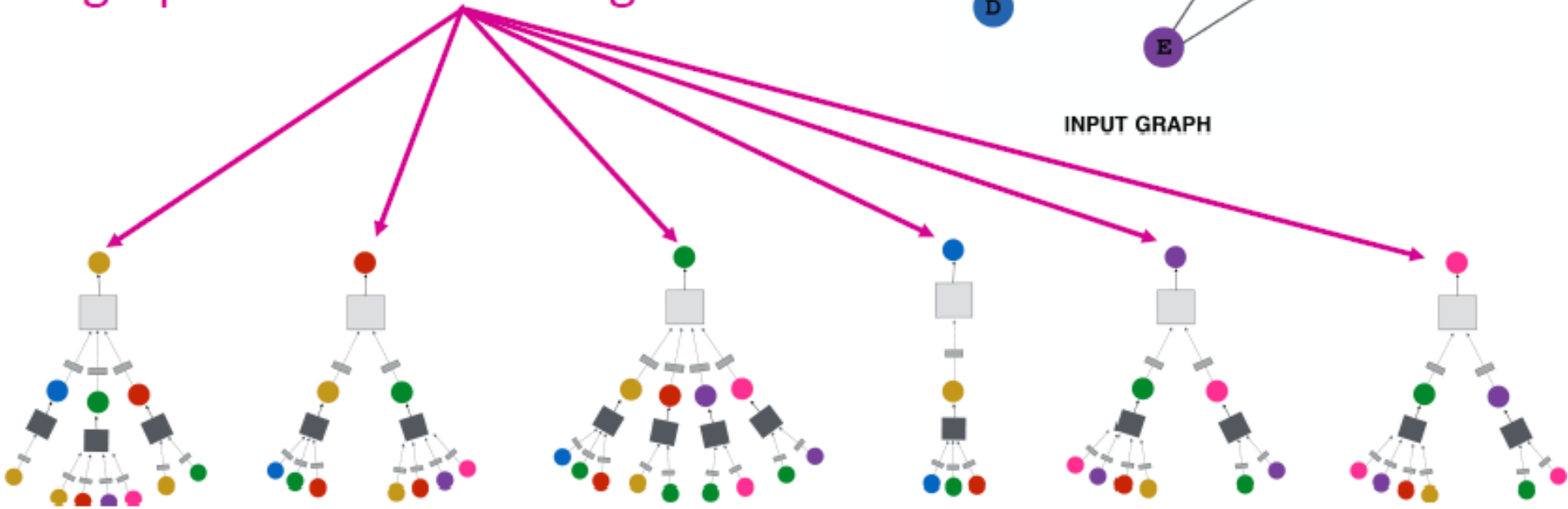
Key Idea – Aggregate Neighbors

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

Every node defines a computation graph based on its neighborhood!

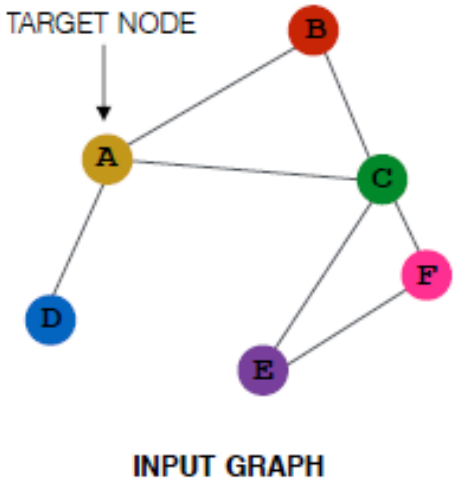


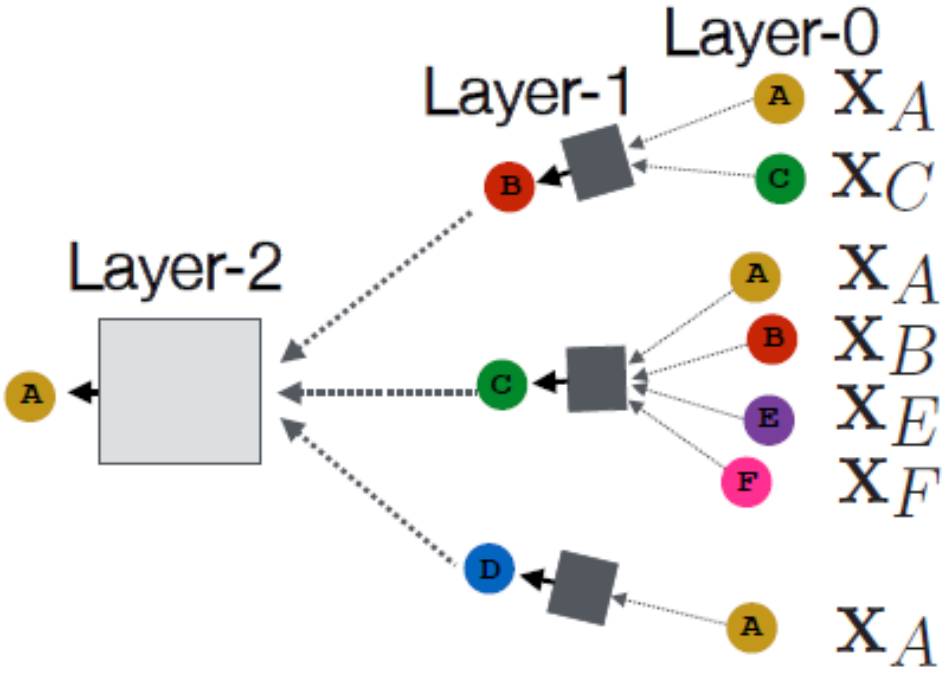
INPUT GRAPH



Deep Model – Many Layers

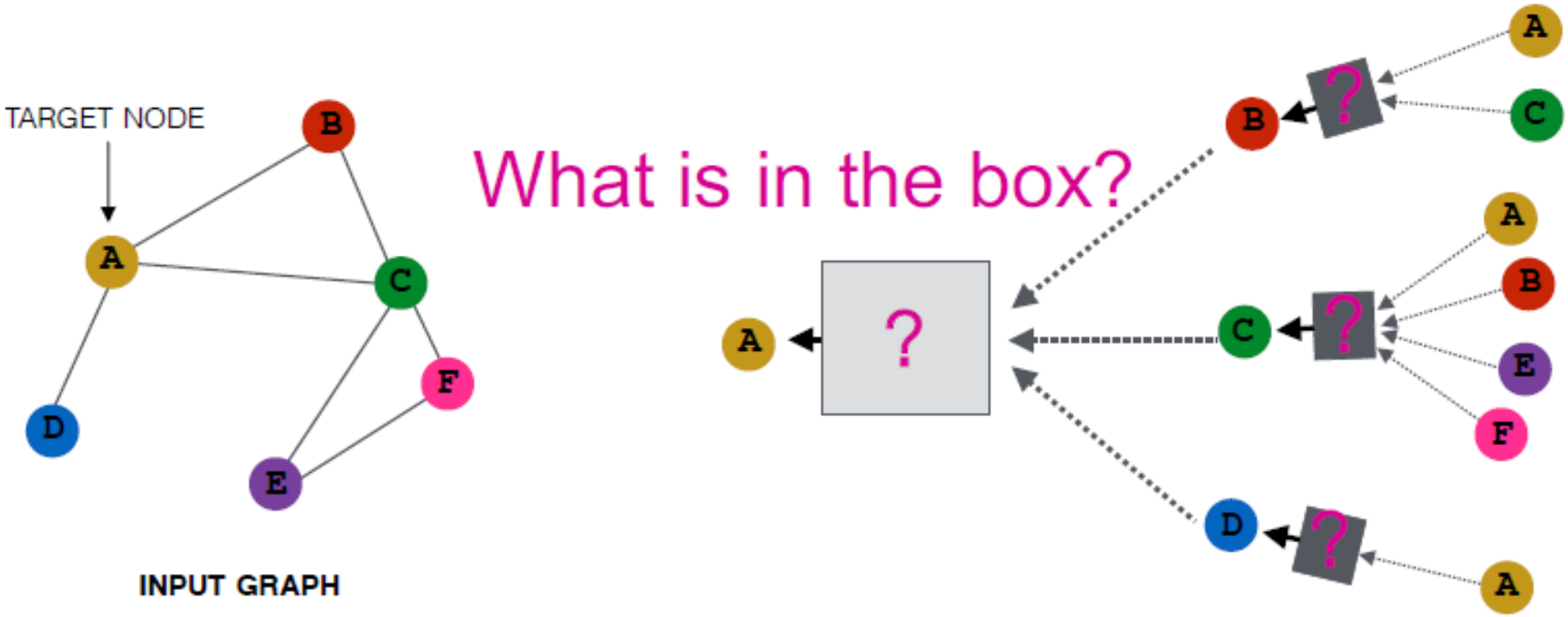
- Model can be of arbitrary depth:
  - Nodes have embeddings at each layer
  - Layer-0 embedding of node u is its input feature, x_u
  - Layer-k embedding gets information from nodes that are K hops away





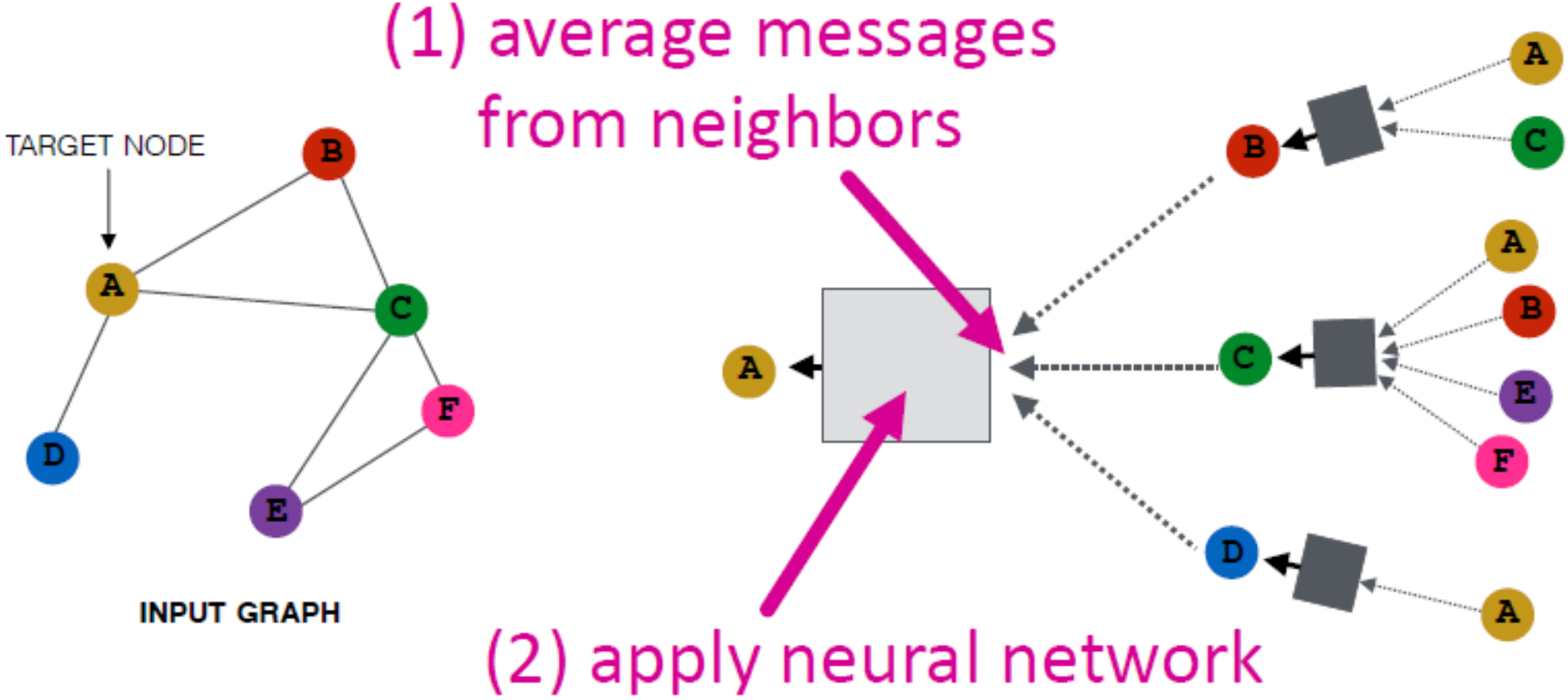
Neighborhood Aggregation

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



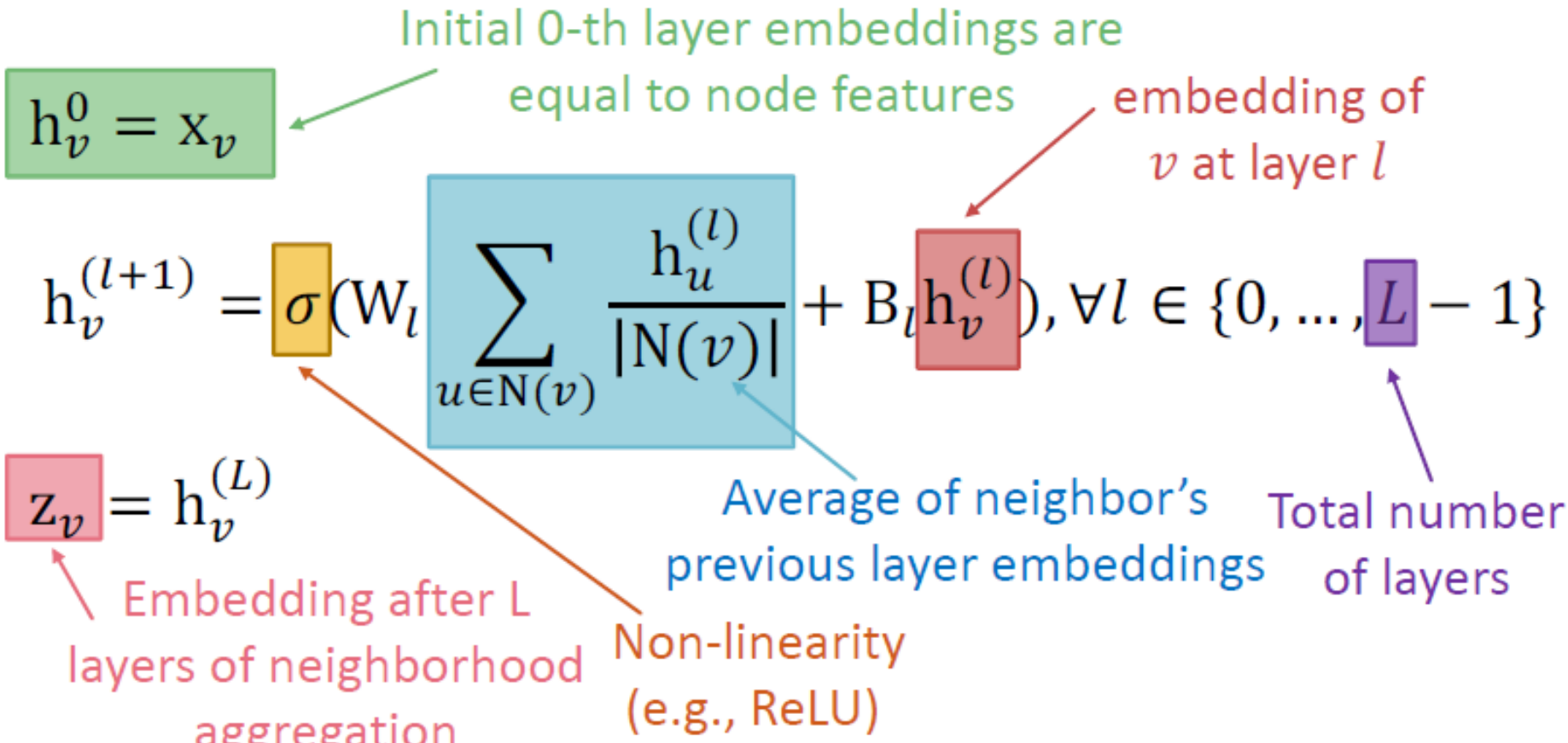
Neighborhood Aggregation

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



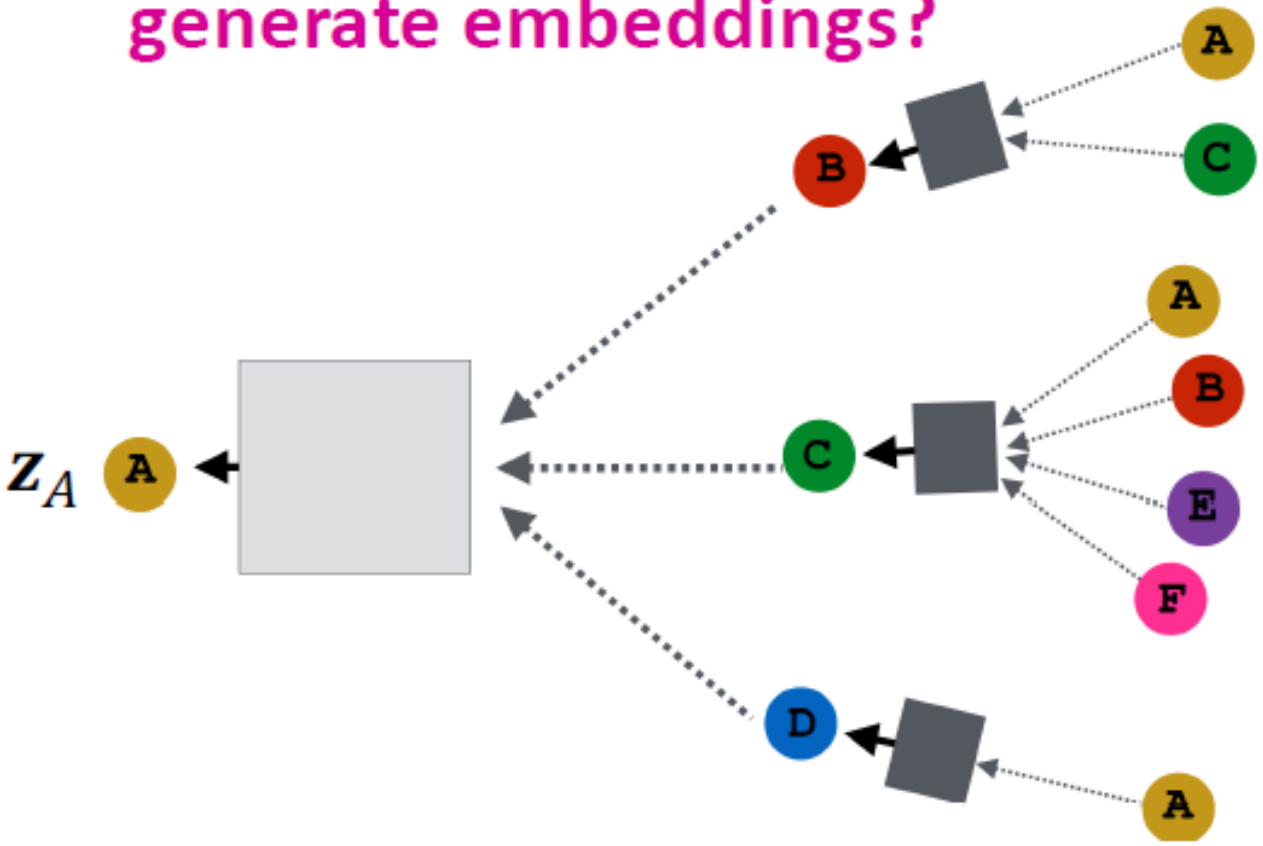
The maths behind the deep encoder

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



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)

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

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

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

Final node embedding

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

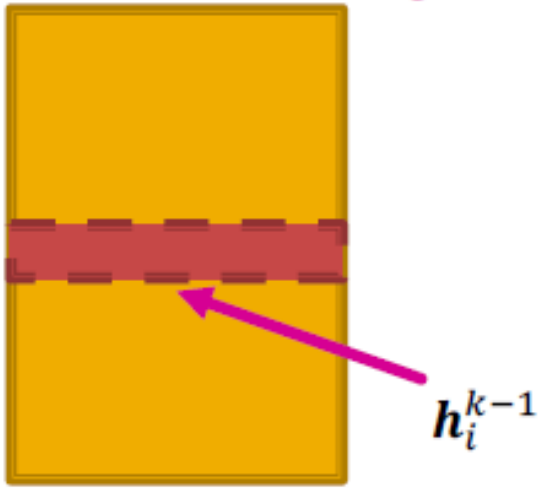
h_v^l: the hidden representation of node v at layer l

- 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,**

Matrix of hidden embeddings H^{k-1}



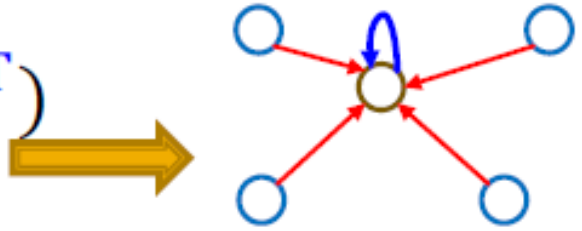
$$\sum_{u \in N(v)} \frac{h_u^{(l-1)}}{|N(v)|} \Rightarrow H^{(l+1)} = D^{-1}AH^{(l)}$$

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

Training the 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

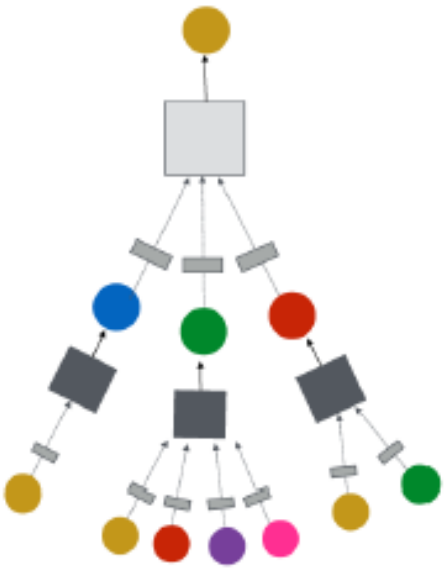
- **"Similar" nodes have similar embeddings**

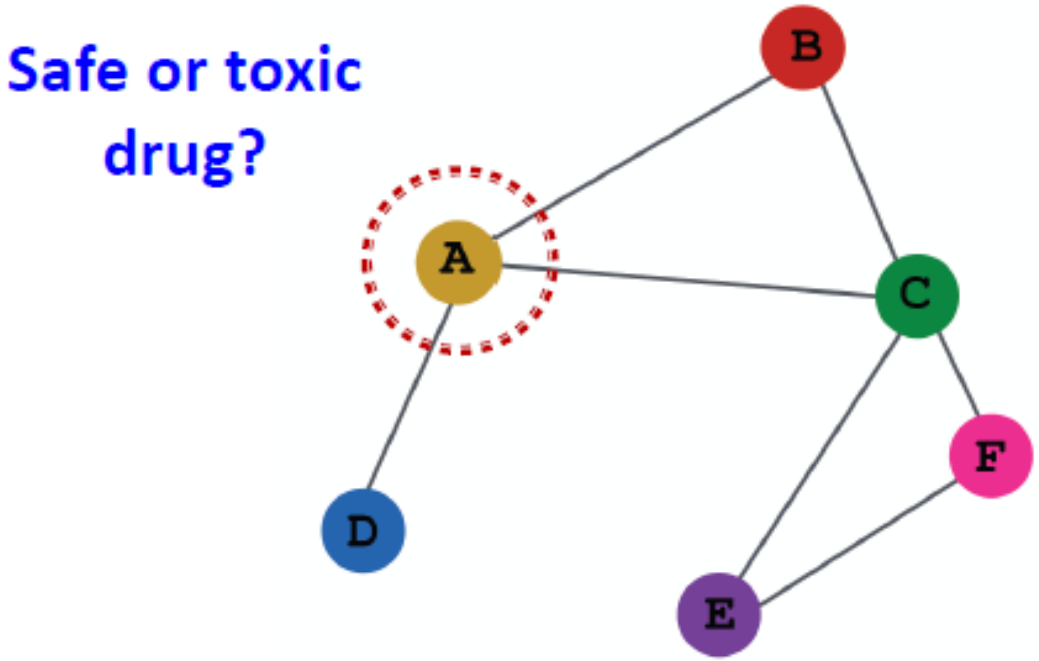
$$\mathcal{L} = \sum_{z_u, z_v} \mathrm{CE}(y_{u,v}, \mathrm{DEC}(z_u, z_v))$$

  - Where $y_{u,v} = 1$ when node u and v are **similar**
  - 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)





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)

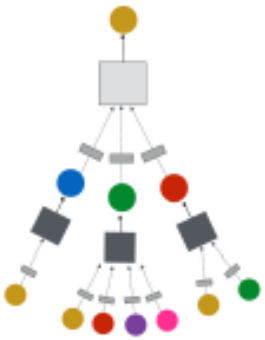
$$\mathcal{L} = \sum_{v \in V} y_v \log(\sigma(z_v^T \theta)) + (1 - y_v) \log(1 - \sigma(z_v^T \theta))$$

Encoder output: node embedding

Classification weights

Node class label

Safe or toxic drug?



Evaluation Metrics: Classification

- **Evaluate classification tasks on graphs:**
- **(1) Multi-class classification**
  - We simply report the accuracy

$$\frac{1\left[\operatorname{argmax}\left(\hat{\boldsymbol{y}}^{(i)}\right) = \boldsymbol{y}^{(i)}\right]}{N}$$

- **(2) Binary classification**
  - Metrics sensitive to classification threshold
    - Accuracy
    - Precision / Recall
    - If the range of prediction is $[0,1]$, we will use 0.5 as threshold
  - Metric Agnostic to classification threshold
    - **ROC AUC**

Metrics for Binary Classification

- **Accuracy:**

$$\frac{TP + TN}{TP + TN + FP + FN} = \frac{TP + TN}{|Dataset|}$$

- **Precision (P):**

$$\frac{TP}{TP + FP}$$

- **Recall (R):**

$$\frac{TP}{TP + FN}$$

- **F1-Score:**

$$\frac{2P * R}{P + R}$$

Confusion matrix

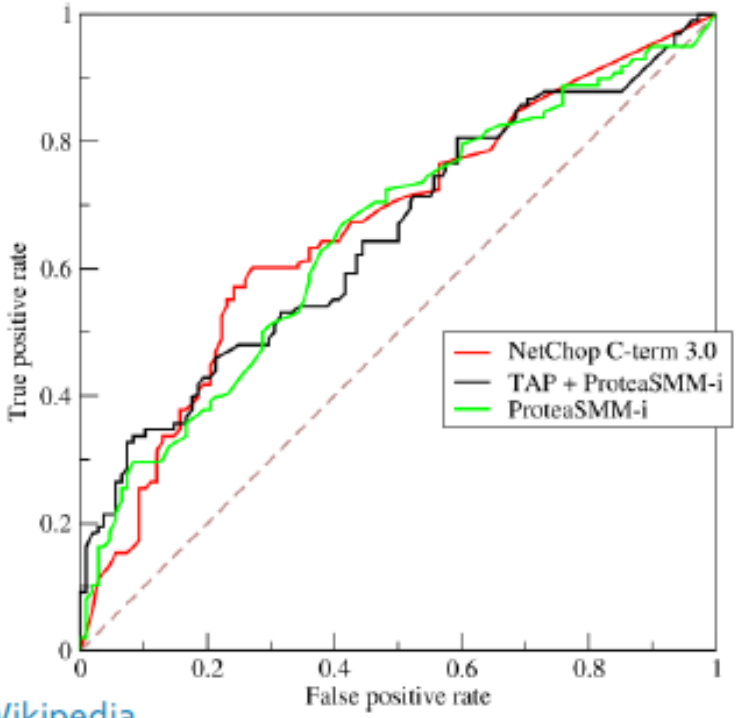
	Actually Positive (1)	Actually Negative (0)
Predicted Positive (1)	True Positives (TPs)	False Positives (FPs)
Predicted Negative (0)	False Negatives (FNs)	True Negatives (TNs)

Sklearn Classification Report

Evaluation Metrics

- **ROC Curve:** Captures the tradeoff in TPR and FPR **as the classification threshold is varied for a binary classifier.**

TPR



FPR

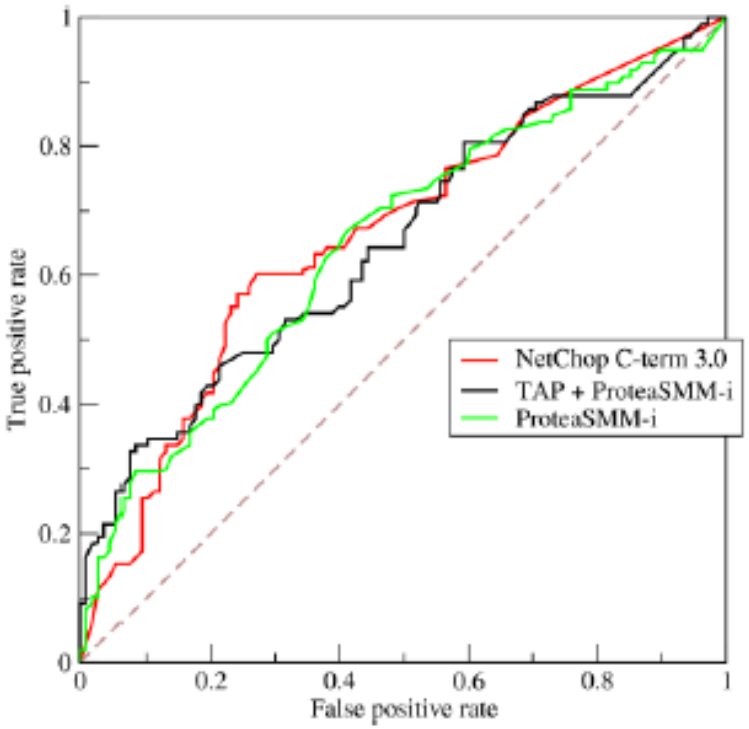
mage Credit: Wikipedia

$$\text{TPR} = \text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{FPR} = \frac{\text{FP}}{\text{FP} + \text{TN}}$$

Note: the dashed line represents **performance of a random classifier**

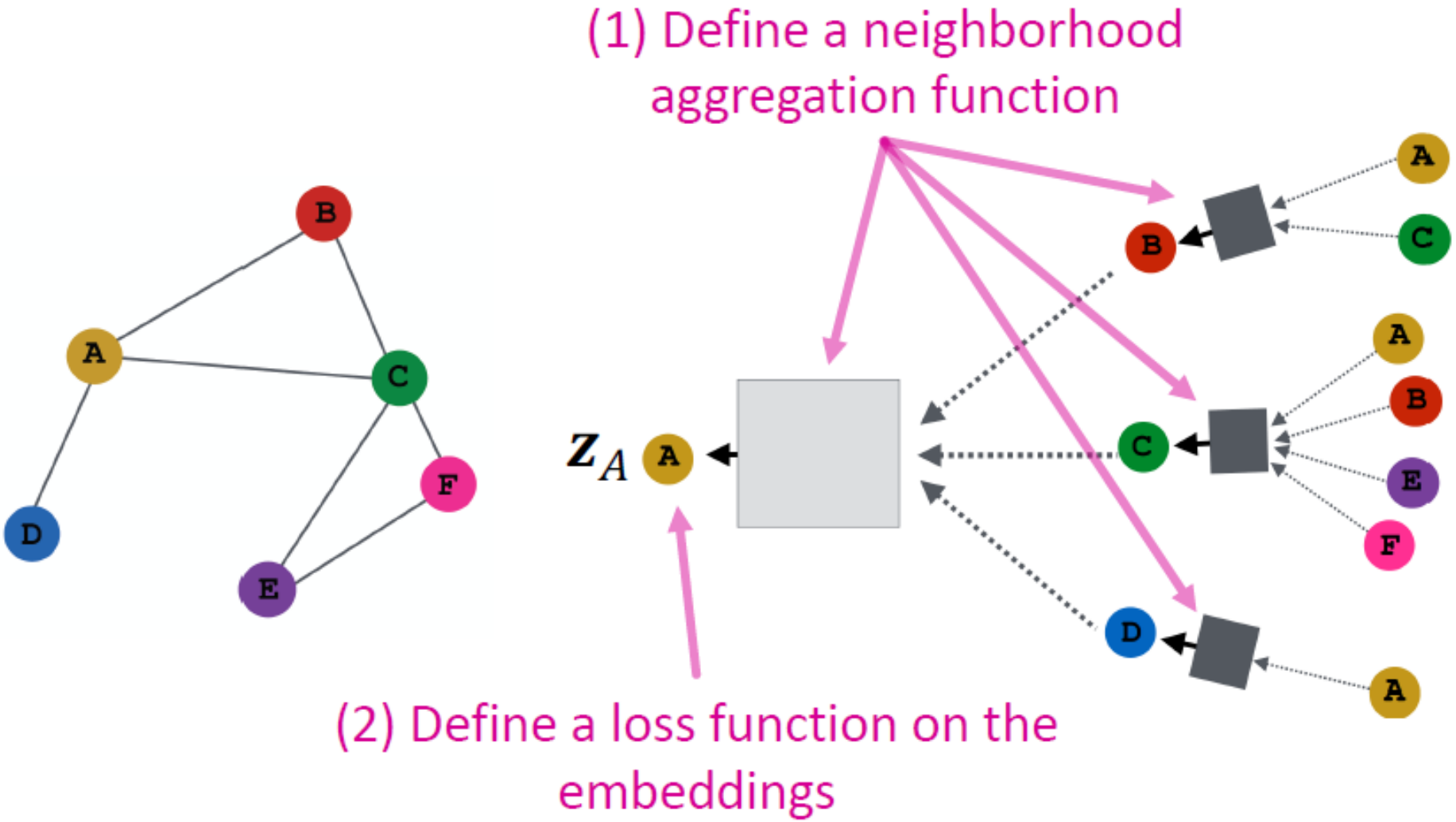
Evaluation Metrics



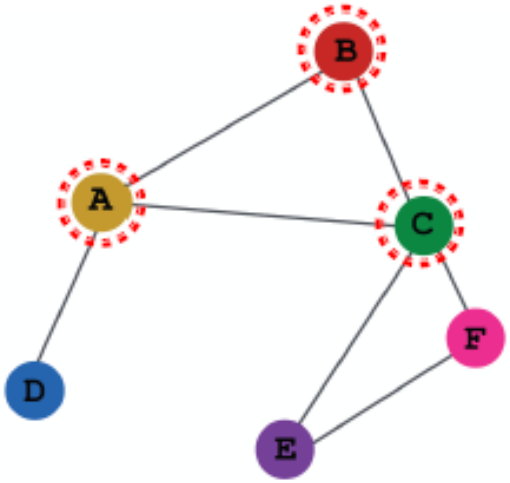
Content Credit: Wikipedia

- **ROC AUC: Area under the ROC Curve.**
- **Intuition:** The probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one

Model Design Overview

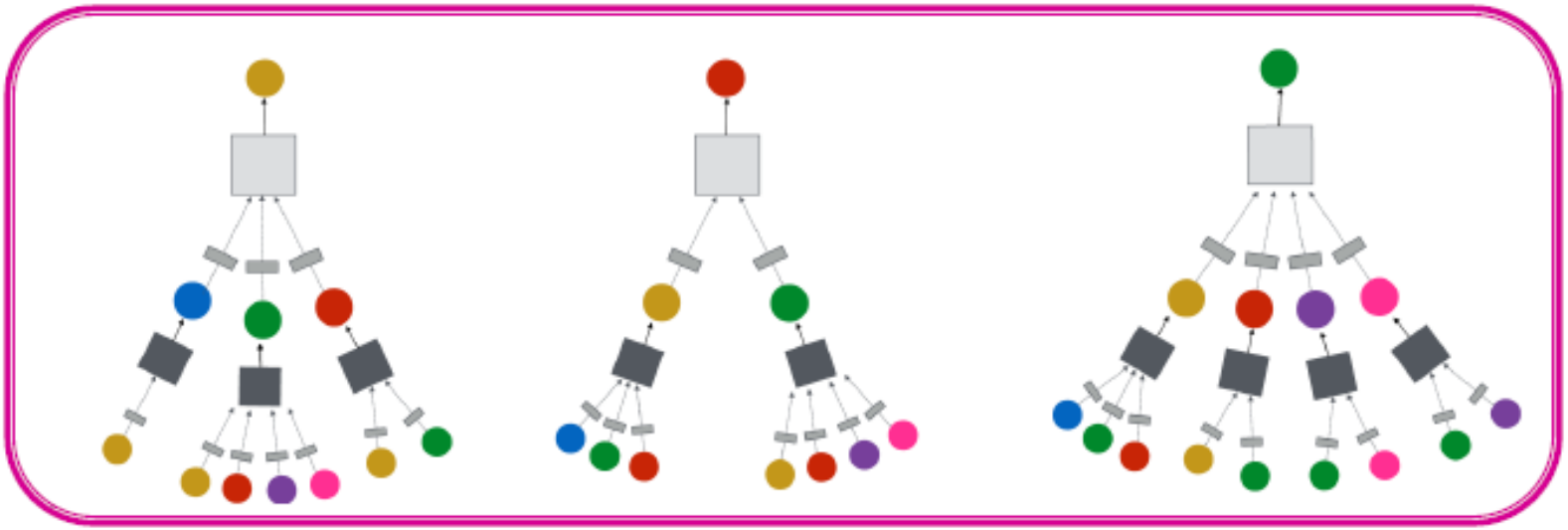


Model Design Overview

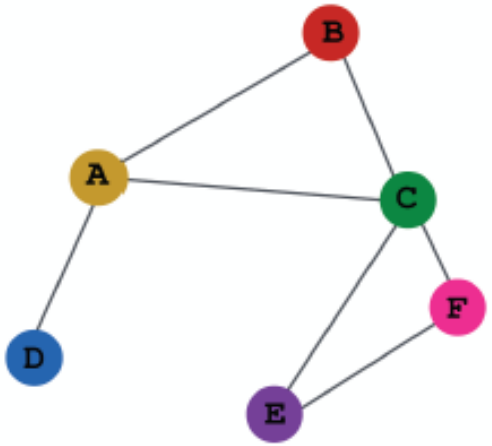


INPUT GRAPH

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



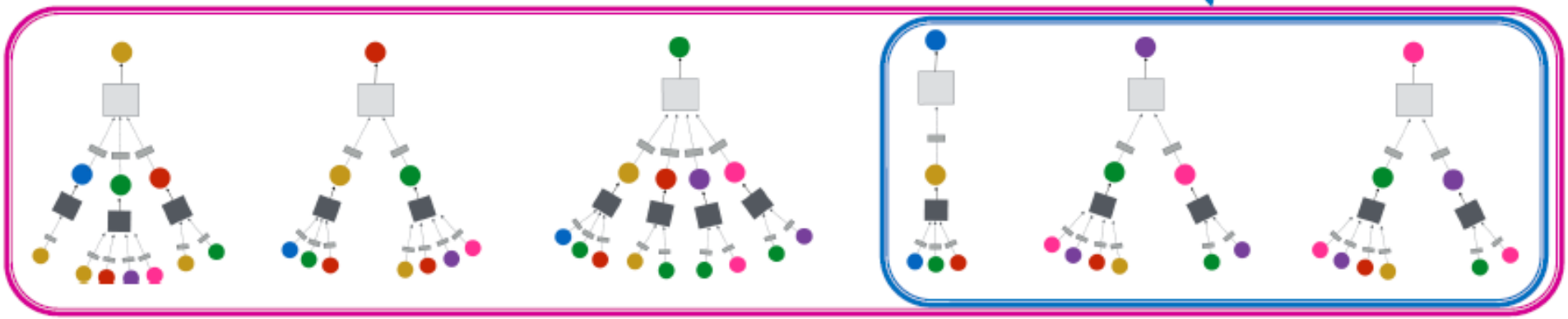
Model Design Overview



INPUT GRAPH

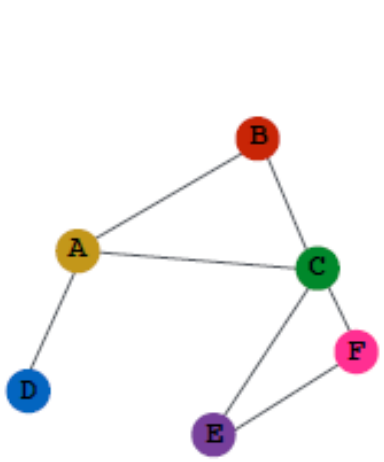
(4) Generate embeddings for nodes as needed

Even for nodes we never trained on!

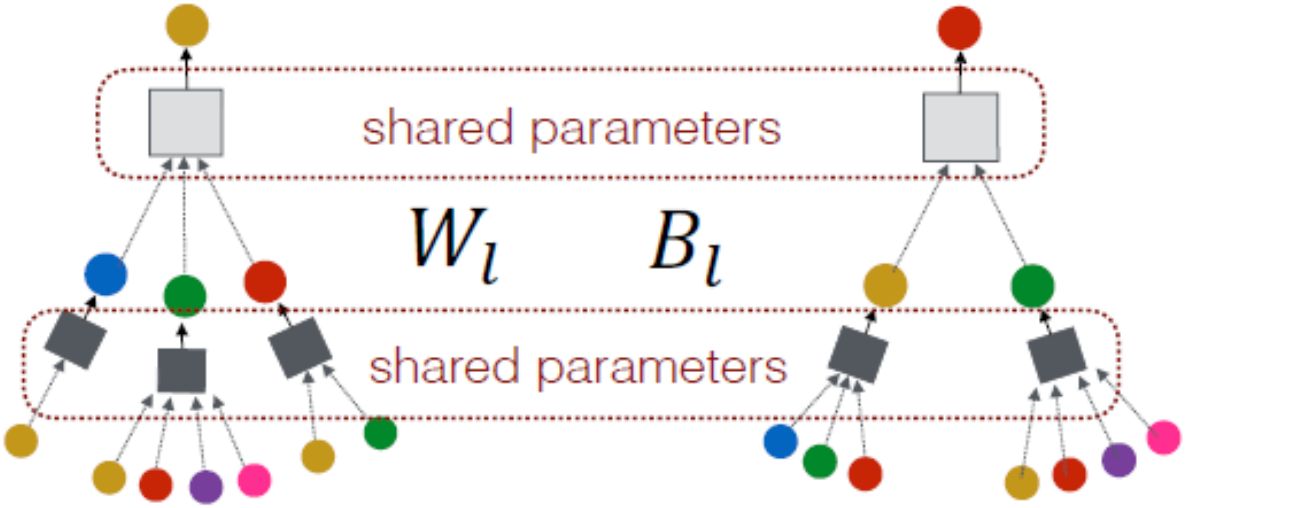


Inductive Capability

- **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**!



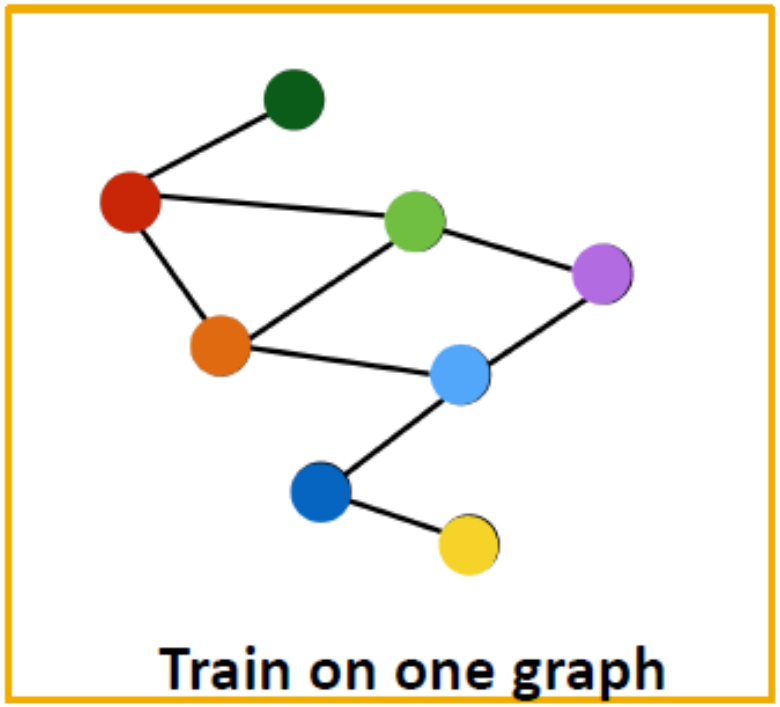
INPUT GRAPH



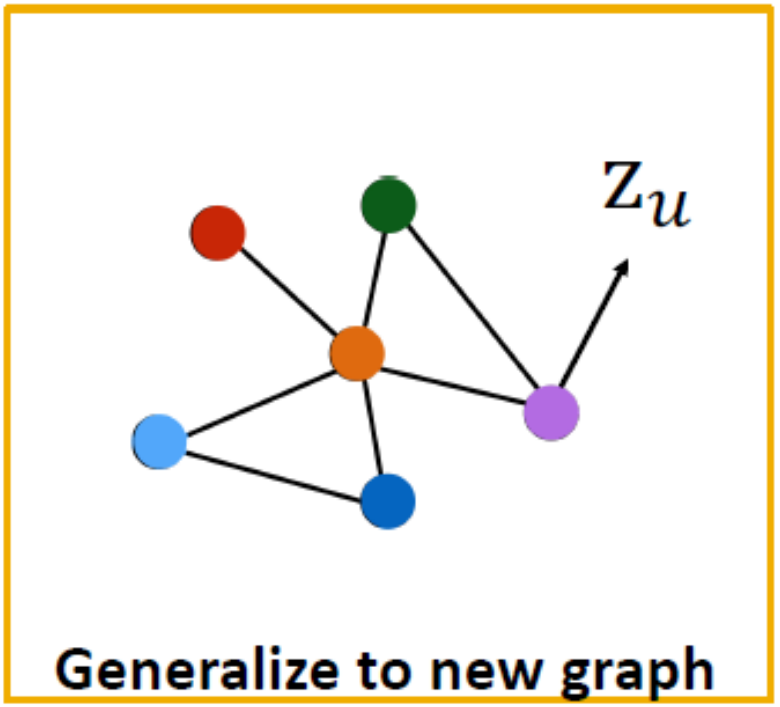
Compute graph for node A

Compute graph for node B

Inductive Capability on New Graphs



Train on one graph

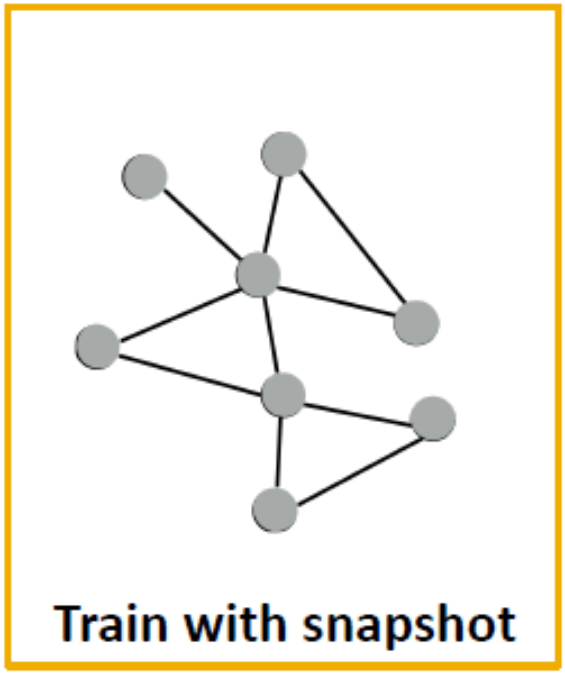


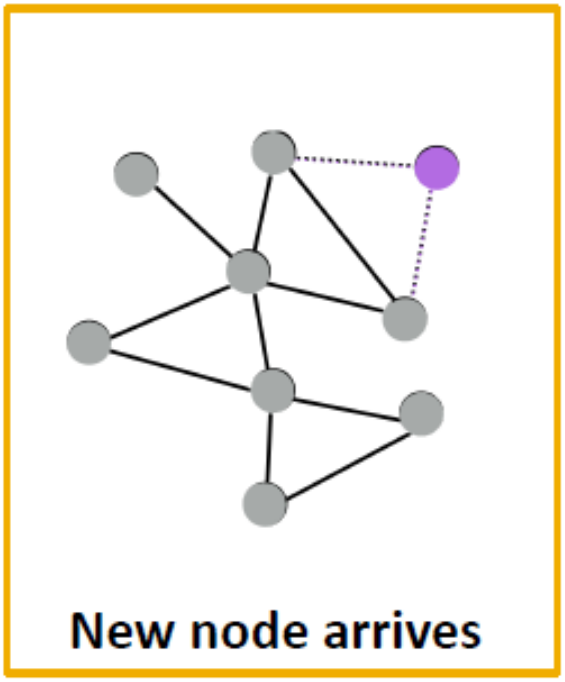
Generalize to new graph

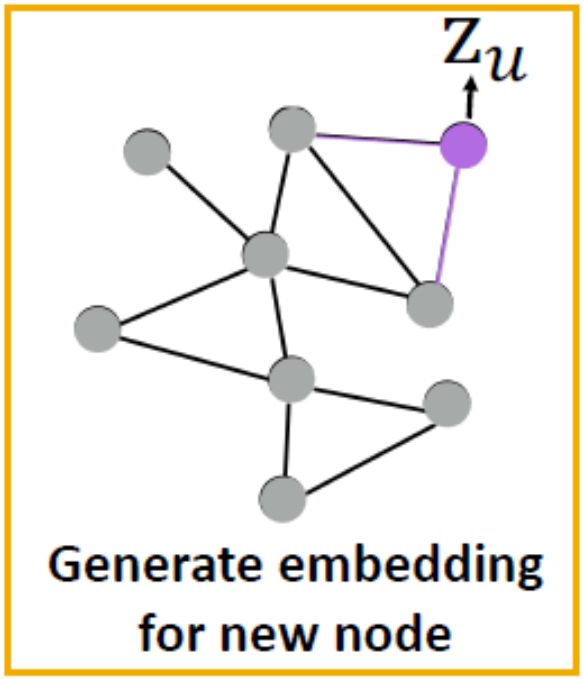
Inductive node embedding → Generalize to entirely unseen graphs

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

Inductive Capability on New Nodes

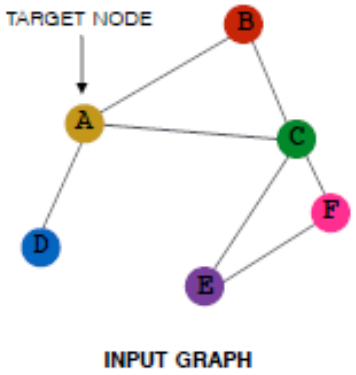






- Many application settings constantly encounter previously unseen nodes:
  - E.g., Reddit, YouTube, Google Scholar
- Need to generate new embeddings "on the fly"

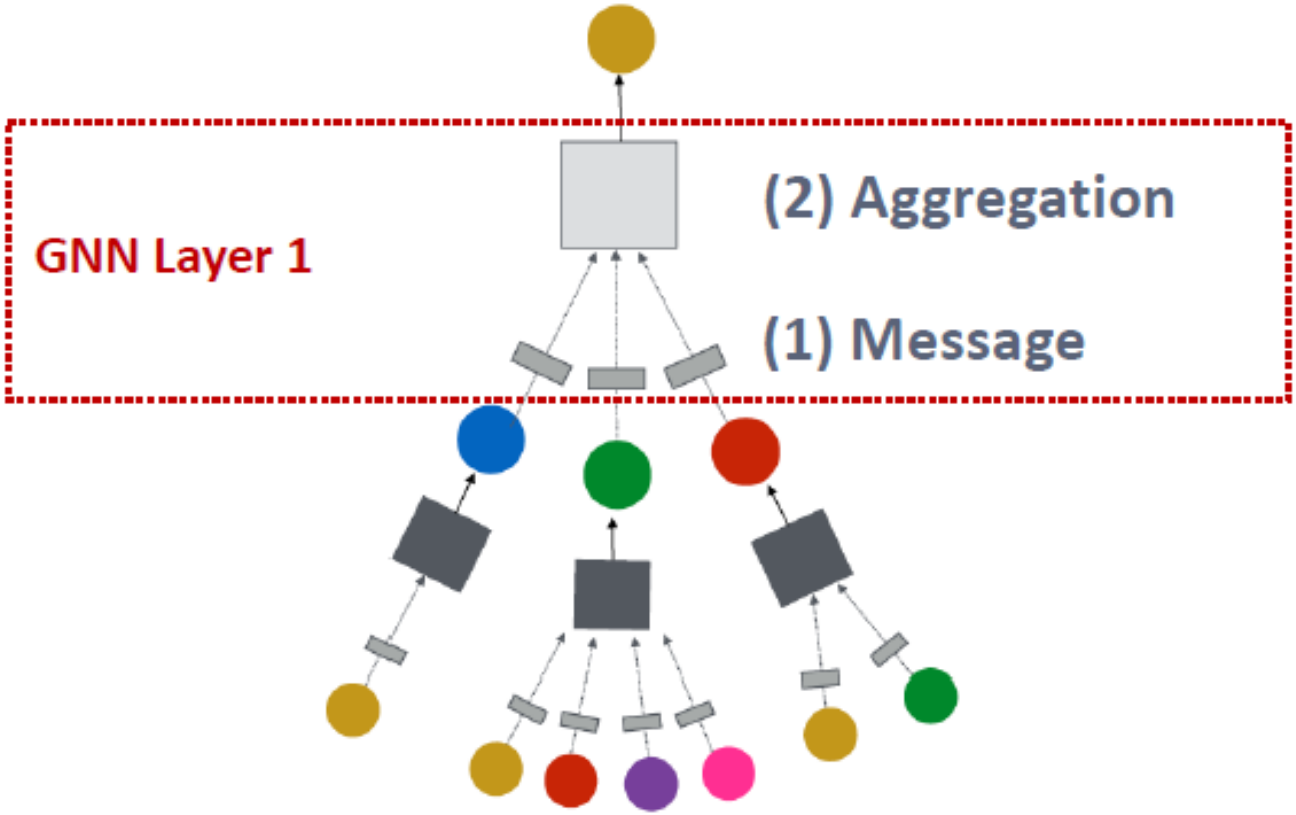
A Single GNN Layer



INPUT GRAPH

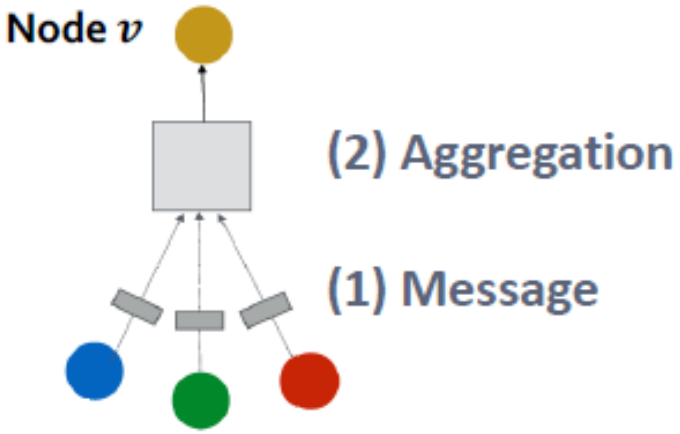
GNN Layer = Message + Aggregation

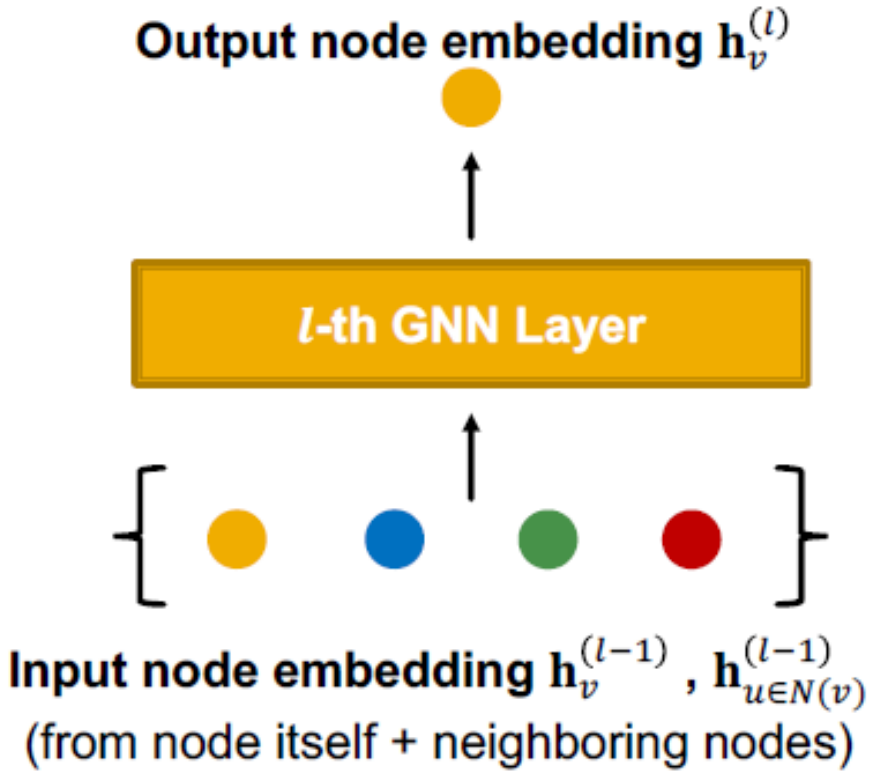
- **Different instantiations under this perspective**
- **GCN, GraphSAGE, GAT, …**



A Single GNN Layer

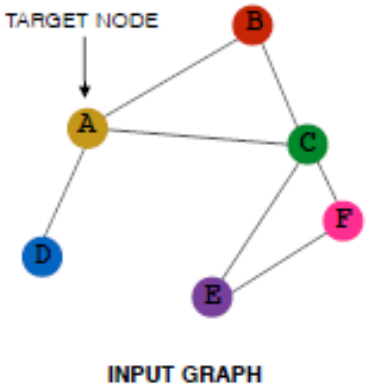
- **Idea of a GNN Layer:**
  - Compress a set of vectors into a single vector
  - **Two step process:**
    - **(1) Message**
    - **(2) Aggregation**

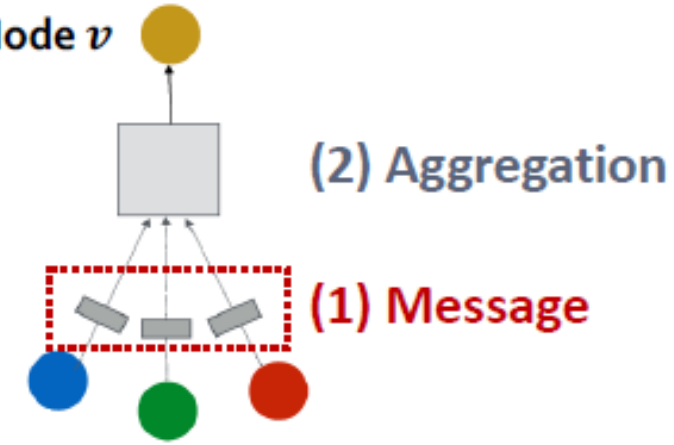




Message Computation

- **(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 $\mathbf{W}^{(l)}$



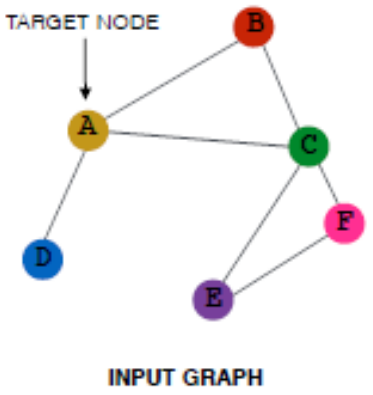


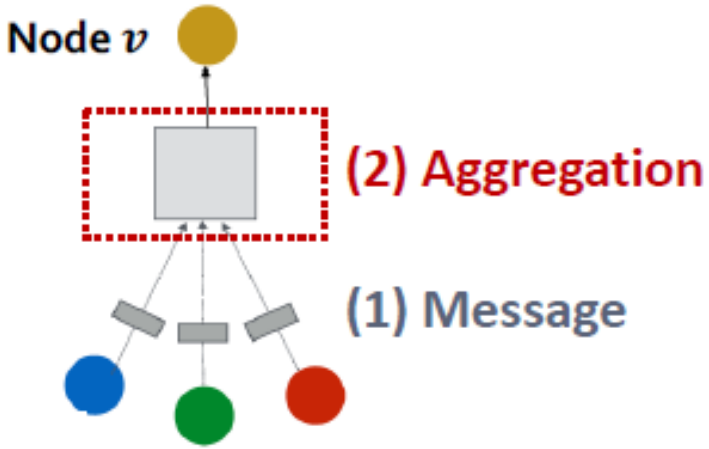
Message Aggregation

- **(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
    - $\mathbf{h}_v^{(l)} = \mathrm{Sum}(\{\mathbf{m}_u^{(l)}, u \in N(v)\})$



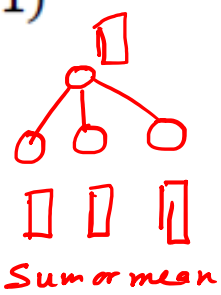


Message Aggregation Issue

- **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

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

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



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

Then aggregate from node itself

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

First aggregate from neighbors

A Single GNN Layer

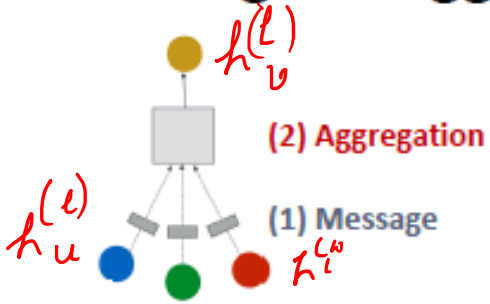
- **Putting things together:**
  - **(1) Message**: each node computes a message

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

  - **(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**



Different GNN layers

- **(1) Graph Convolutional Networks (GCN)**

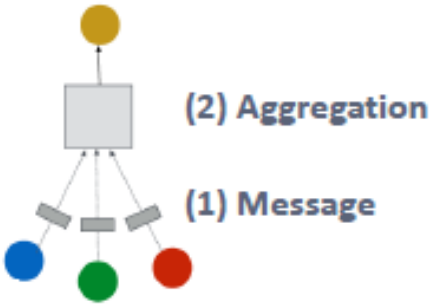
$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}^{(l)} \sum_{u \in N(v)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}\right)$$

- **How to write this as Message + Aggregation?**

Message

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

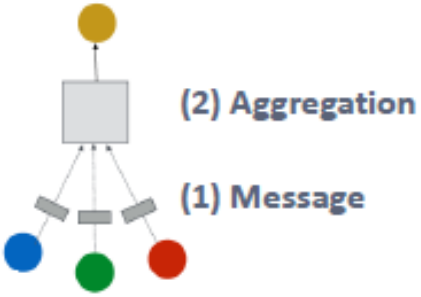
Aggregation



Different GNN Layers

- **(1) Graph Convolutional Networks (GCN)**

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



- **Message:**
  - Each Neighbor: $\mathbf{m}_u^{(l)} = \frac{1}{|N(v)|}\mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}$

Normalized by node degree
(In the GCN paper they use a slightly different normalization)

- **Aggregation:**
  - **Sum** over messages from neighbors, then apply activation
  - $\mathbf{h}_v^{(l)} = \sigma\left(\text{Sum}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}\right)\right)$

Different GNN Layers: GraphSage

- **(2) GraphSAGE**

$$\mathbf{h}_v^{(l)} = \sigma\left(\mathbf{W}^{(l)} \cdot \mathrm{CONCAT}\left(\mathbf{h}_v^{(l-1)}, \mathrm{AGG}\left(\left\{\mathbf{h}_u^{(l-1)}, \forall u \in N(v)\right\}\right)\right)\right)$$

- **How to write this as Message + Aggregation?**
  - **Message** is computed within the $\mathrm{AGG}(\cdot)$
  - **Two-stage aggregation**
    - **Stage 1:** Aggregate from node neighbors

$$\mathbf{h}_{N(v)}^{(l)} \leftarrow \mathrm{AGG}\left(\left\{\mathbf{h}_u^{(l-1)}, \forall u \in N(v)\right\}\right)$$

    - **Stage 2:** Further aggregate over the node itself

$$\mathbf{h}_v^{(l)} \leftarrow \sigma\left(\mathbf{W}^{(l)} \cdot \mathrm{CONCAT}(\mathbf{h}_v^{(l-1)}, \mathbf{h}_{N(v)}^{(l)})\right)$$

GraphSAGE Neighbor Aggregation

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

$$\text{AGG} = \sum_{u \in N(v)} \frac{\mathbf{h}_u^{(l-1)}}{|N(v)|}$$

Aggregation — Message computation

- **Pool:** Transform neighbor vectors and apply symmetric vector function $\text{Mean}(\cdot)$ or $\text{Max}(\cdot)$

$$\text{AGG} = \text{Mean}(\{\text{MLP}(\mathbf{h}_u^{(l-1)}), \forall u \in N(v)\})$$

Aggregation — Message computation

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

$$\text{AGG} = \text{LSTM}([\mathbf{h}_u^{(l-1)}, \forall u \in \pi(N(v))])$$

Aggregation

GraphSAGE L2 normalization

- **ℓ_2 Normalization:**
  - **Optional:** Apply ℓ_2 normalization to $\mathbf{h}_v^{(l)}$ at every layer
  - $\mathbf{h}_v^{(l)} \leftarrow \frac{\mathbf{h}_v^{(l)}}{\left\|\mathbf{h}_v^{(l)}\right\|_2} \forall v \in V$ where $\|u\|_2 = \sqrt{\sum_i u_i^2}$ (ℓ_2-norm)
  - Without ℓ_2 normalization, the embedding vectors have different scales (ℓ_2-norm) for vectors
  - In some cases (not always), normalization of embedding results in performance improvement
  - After ℓ_2 normalization, all vectors will have the same ℓ_2-norm

Graph Attention (GAT)

- **(3) Graph Attention Networks**

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \alpha_{vu} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

Attention weights

- **In GCN / GraphSAGE**
  - $\alpha_{vu} = \frac{1}{|N(v)|}$ is the **weighting factor (importance)** of node u's message to node v
  - $\Longrightarrow \alpha_{vu}$ is defined **explicitly** based on the structural properties of the graph (node degree)
  - $\Longrightarrow$ All neighbors $u \in N(v)$ are equally important to node v

Graph Attention (GAT)

- **(3) Graph Attention Networks**

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \alpha_{vu} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

Attention weights

Not all node's neighbors are equally important

- **Attention** is inspired by cognitive attention.
- The **attention** α_{vu} focuses on the important parts of the input data and fades out the rest.
  - **Idea:** the NN should devote more computing power on that small but important part of the data.
  - Which part of the data is more important depends on the context and is learned through training.

Graph Attention Networks

Can we do better than simple neighborhood aggregation?

Can we let weighting factors α_{vu} to be learned?

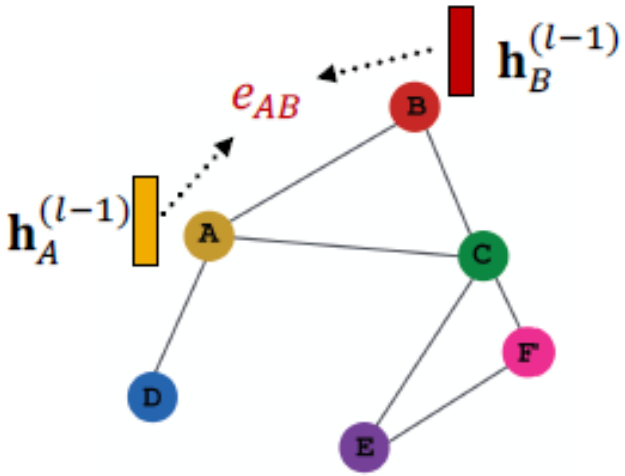
- **Goal:** Specify **arbitrary importance** to different neighbors of each node in the graph
- **Idea:** Compute embedding $\boldsymbol{h}_v^{(l)}$ of each node in the graph following an **attention strategy:**
  - Nodes attend over their neighborhoods' message
  - Implicitly specifying different weights to different nodes in a neighborhood

Attention Mechanism

- Let α_{vu} be computed as a byproduct of an **attention mechanism a:**
  - (1) Let a compute **attention coefficients e_{vu}** across pairs of nodes u, v based on their messages:

$$e_{vu} = a(\mathbf{W}^{(l)}\mathbf{h}_u^{(l-1)}, \mathbf{W}^{(l)}\boldsymbol{h}_v^{(l-1)})$$

    - **e_{vu} indicates the importance of $u's$ message to node v**



$$e_{AB} = a(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)})$$

Attention Mechanism

- **Normalize** e_{vu} into the **final attention weight** α_{vu}
  - Use the **softmax** function, so that $\sum_{u \in N(v)} \alpha_{vu} = 1$:

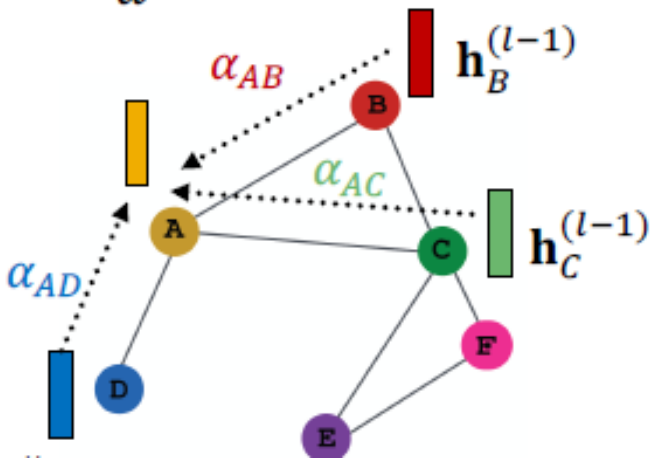
$$\alpha_{vu} = \frac{\exp(e_{vu})}{\sum_{k \in N(v)} \exp(e_{vk})}$$

- **Weighted sum** based on the **final attention weight** α_{vu}

$$\mathbf{h}_v^{(l)} = \sigma\left(\sum_{u \in N(v)} \alpha_{vu} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

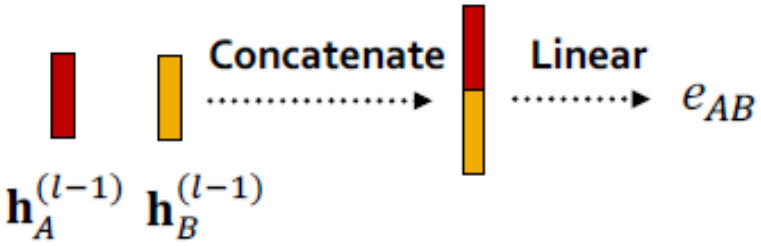
Weighted sum using α_{AB}, α_{AC}, α_{AD}:

$$\mathbf{h}_A^{(l)} = \sigma(\alpha_{AB}\mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)} + \alpha_{AC}\mathbf{W}^{(l)}\mathbf{h}_C^{(l-1)} + \alpha_{AD}\mathbf{W}^{(l)}\mathbf{h}_D^{(l-1)})$$



Attention Mechanism

- **What is the form of attention mechanism a?**
  - The approach is agnostic to the choice of a
    - E.g., use a simple single-layer neural network
      - a have trainable parameters (weights in the Linear layer)



$$e_{AB} = a\left(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)}\right)$$
$$= \text{Linear}\left(\text{Concat}\left(\mathbf{W}^{(l)}\mathbf{h}_A^{(l-1)}, \mathbf{W}^{(l)}\mathbf{h}_B^{(l-1)}\right)\right)$$

  - Parameters of a are trained jointly:
    - Learn the parameters together with weight matrices (i.e., other parameter of the neural net $\mathbf{W}^{(l)}$) in an end-to-end fashion

Multihead Attention

- **Multi-head attention:** Stabilizes the learning process of attention mechanism
  - **Create multiple attention scores** (each replica with a different set of parameters):

$$\mathbf{h}_v^{(l)}[1] = \sigma\left(\sum_{u \in N(v)} \alpha_{vu}^{1} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

$$\mathbf{h}_v^{(l)}[2] = \sigma\left(\sum_{u \in N(v)} \alpha_{vu}^{2} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

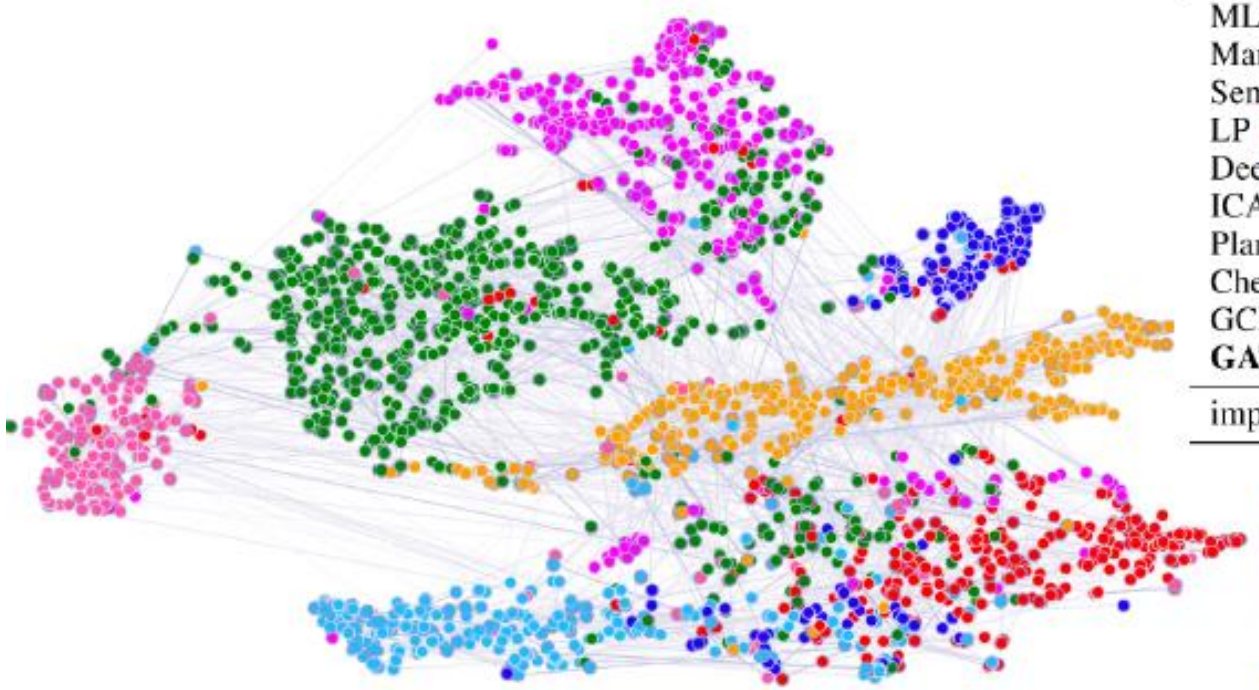
$$\mathbf{h}_v^{(l)}[3] = \sigma\left(\sum_{u \in N(v)} \alpha_{vu}^{3} \mathbf{W}^{(l)} \mathbf{h}_u^{(l-1)}\right)$$

  - **Outputs are aggregated:**
    - By concatenation or summation
    - $\mathbf{h}_v^{(l)} = \mathrm{AGG}(\mathbf{h}_v^{(l)}[1], \mathbf{h}_v^{(l)}[2], \mathbf{h}_v^{(l)}[3])$

Benefits of GAT

- **Key benefit:** Allows for (implicitly) specifying **different importance values** (α_{vu}) **to different neighbors**
- **Computationally efficient**:
  - Computation of attentional coefficients can be parallelized across all edges of the graph
  - Aggregation may be parallelized across all nodes
- **Storage efficient**:
  - Sparse matrix operations do not require more than $O(V + E)$ entries to be stored
  - **Fixed** number of parameters, irrespective of graph size
- **Localized**:
  - Only **attends over local network neighborhoods**
- **Inductive capability**:
  - It is a shared *edge-wise* mechanism
  - It does not depend on the global graph structure

GAT Example Cora Citation Net



Method	Cora
MLP	55.1%
ManiReg (Belkin et al., 2006)	59.5%
SemiEmb (Weston et al., 2012)	59.0%
LP (Zhu et al., 2003)	68.0%
DeepWalk (Perozzi et al., 2014)	67.2%
ICA (Lu & Getoor, 2003)	75.1%
Planetoid (Yang et al., 2016)	75.7%
Chebyshev (Defferrard et al., 2016)	81.2%
GCN (Kipf & Welling, 2017)	81.5%
GAT	**83.3%**
improvement w.r.t GCN	1.8%

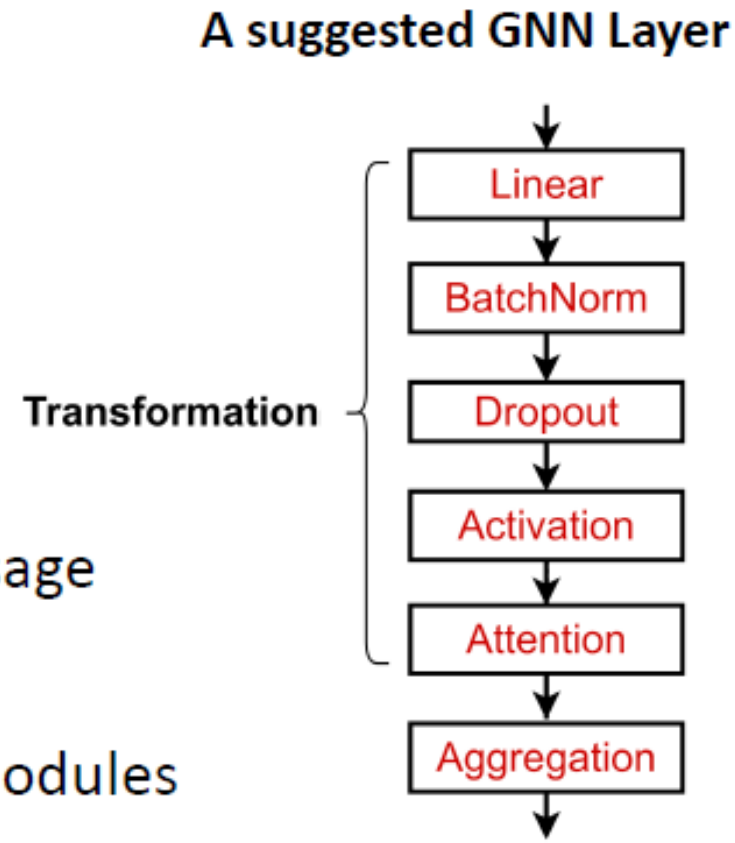
Attention mechanism can be used with many different graph neural network models

In many cases, attention leads to performance gains

- **t-SNE plot of GAT-based node embeddings:**
  - Node color: 7 publication classes
  - Edge thickness: Normalized attention coefficients between nodes i and j, across eight attention heads, $\sum_k (\alpha_{ij}^k + \alpha_{ji}^k)$

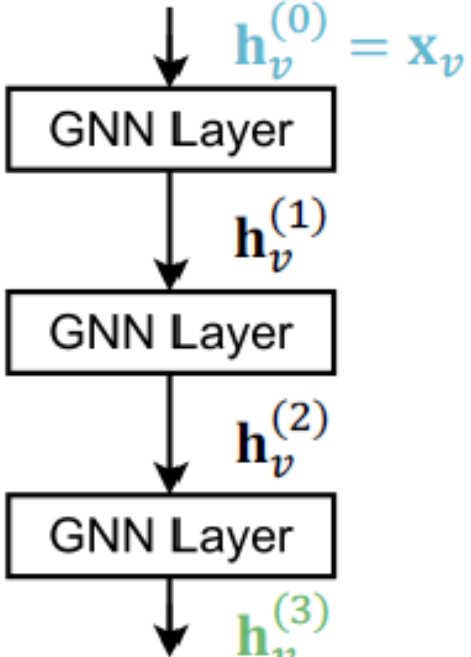
GNN Layers in practice

- **Many modern deep learning modules can be incorporated into a GNN layer**
  - **Batch Normalization:**
    - Stabilize neural network training
  - **Dropout:**
    - Prevent overfitting
  - **Attention/Gating:**
    - Control the importance of a message
  - **More:**
    - Any other useful deep learning modules



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



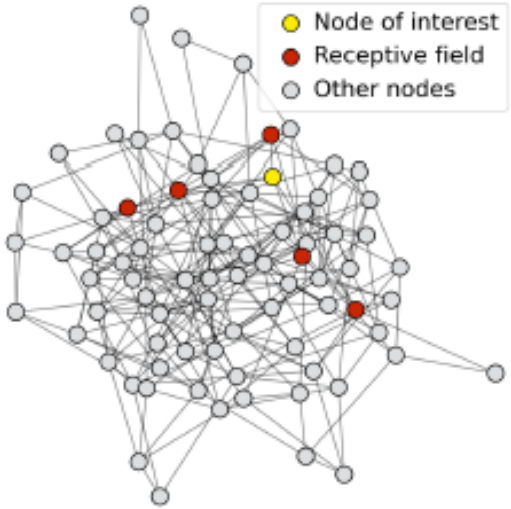
The over-smoothing problem

- **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?**

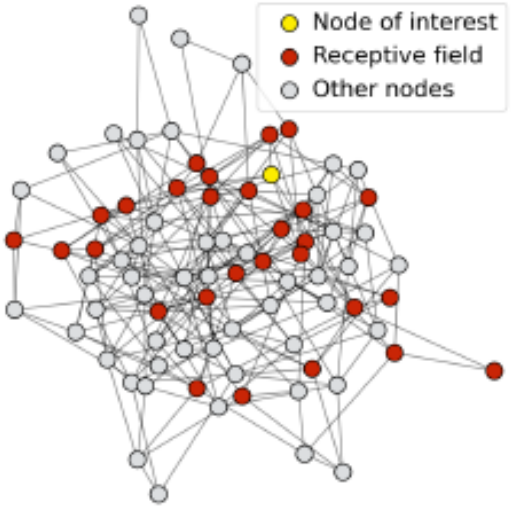
Receptive fields of GNNs

- **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**

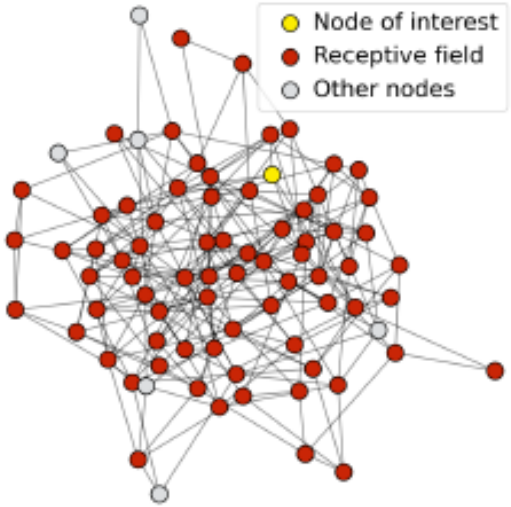
Receptive field for 1-layer GNN



Receptive field for 2-layer GNN



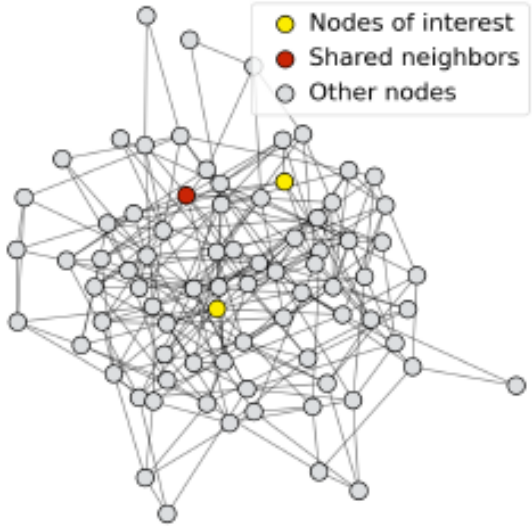
Receptive field for 3-layer GNN



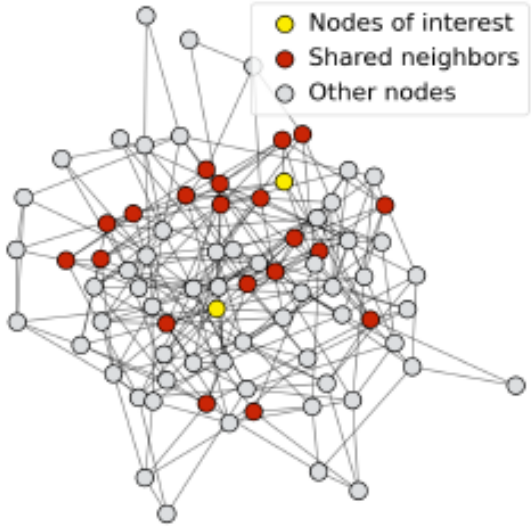
Receptive fields of GNNs

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

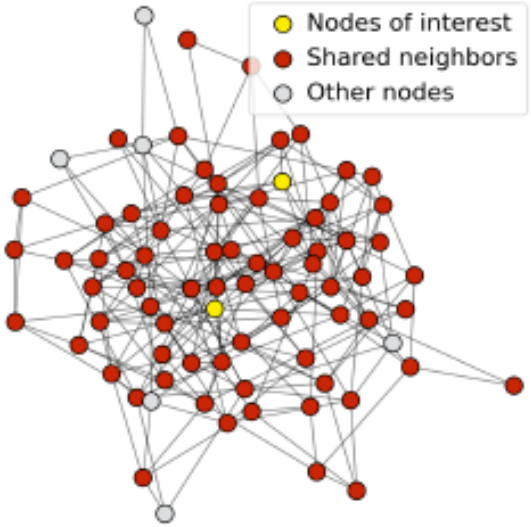
1-hop neighbor overlap
Only 1 node



2-hop neighbor overlap
About 20 nodes



3-hop neighbor overlap
Almost all the nodes!



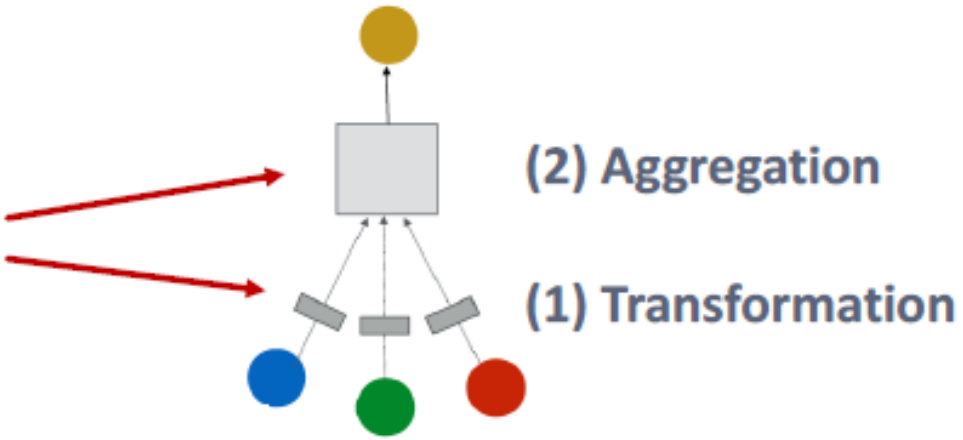
Mitigating Over-Smoothing Problem

- **What do we learn from the over-smoothing problem?**
- **Lesson 1: 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**!
- **Question:** How to enhance the expressive power of a GNN, if the number of GNN layers is small?

Solution - 1

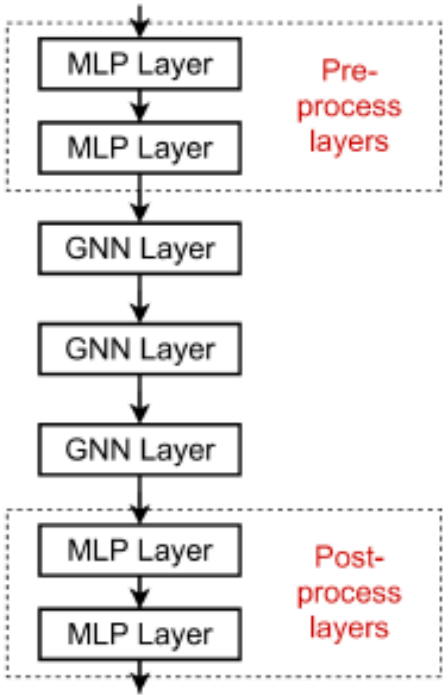
- **How to make a shallow GNN more expressive?**
- **Solution 1:** Increase the expressive power **within each GNN layer**
  - In our previous examples, each transformation or aggregation function only include one linear layer
  - We can **make aggregation / transformation become a deep neural network**!

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



Solution - 2

- **How to make a shallow GNN more expressive?**
- **Solution 2:** Add layers that do not pass messages
  - A GNN does not necessarily only contain GNN layers
    - E.g., we can add **MLP layers** (applied to each node) before and after GNN layers, as **pre-process layers** and **post-process layers**



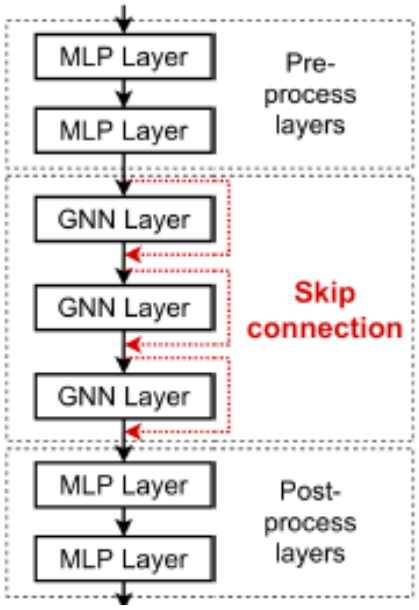
Pre-processing layers: Important when encoding node features is necessary.
E.g., when nodes represent images/text

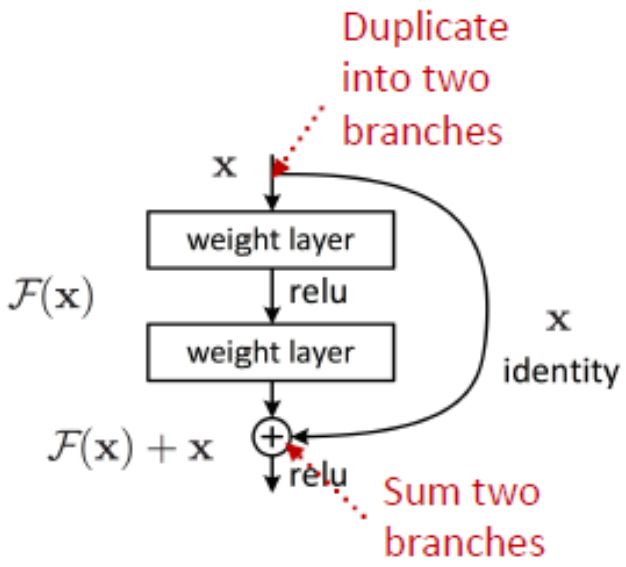
Post-processing layers: Important when reasoning / transformation over node embeddings are needed
E.g., graph classification, knowledge graphs

In practice, adding these layers works great!

Solution - 3

- **What if my problem still requires many GNN layers?**
- **Lesson 2: Add skip connections in GNNs**
  - **Observation from over-smoothing:** Node embeddings in earlier GNN layers can sometimes better differentiate nodes
  - **Solution:** We can increase the impact of earlier layers on the final node embeddings, **by adding shortcuts in GNN**





Idea of skip connections:

Before adding shortcuts:

$$\boldsymbol{F}(\mathbf{x})$$

After adding shortcuts:

$$\boldsymbol{F}(\mathbf{x}) + \mathbf{x}$$

Scaling up GCNs

- How to implement GCNs for large graphs

Problem with scale

- **Large-scale:**
  - #nodes ranges from 10M to 10B.
  - #edges ranges from 100M to 100B.
- **Tasks**
  - **Node-level**: User/item/paper classification.
  - **Link-level**: Recommendation, completion.
- **Todays' lecture**
  - **Scale up GNNs to large graphs!**

Why it is hard

- **Recall: How we usually train an ML model on large data (N=#data is large)**
- **Objective**: Minimize the averaged loss

$$\ell(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=0}^{N-1} \ell_i(\boldsymbol{\theta})$$

  - $\boldsymbol{\theta}$: model parameters, $\ell_i(\boldsymbol{\theta})$: loss for i-th data point.
- We perform **Stochastic Gradient Descent (SGD)**.
  - Randomly sample M $(<< N)$ data (**mini-batches**).
  - Compute the $\ell_{sub}(\boldsymbol{\theta})$ over the M data points.
  - Perform SGD: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \nabla\ell_{sub}(\boldsymbol{\theta})$

Methods

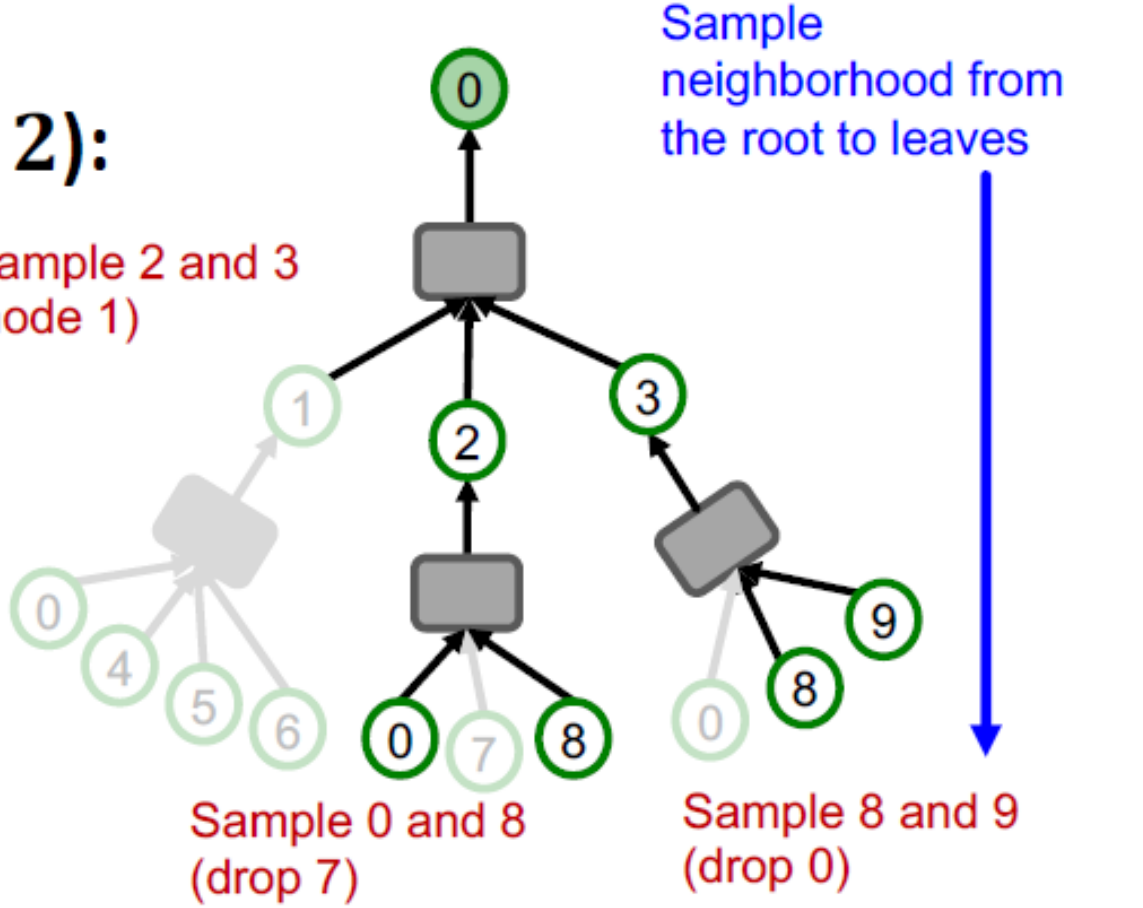
We introduce **three methods for scaling up GNNs:**

- Two methods perform message-passing over **small subgraphs in each mini-batch**; only the subgraphs need to be loaded on a GPU at a time.
  - **Neighbor Sampling** [Hamilton et al. NeurIPS 2017]
  - **Cluster-GCN** [Chiang et al. KDD 2019]
- One method **simplifies a GNN into feature-preprocessing operation** (can be efficiently performed even on a CPU)
  - **Simplified GCN** [Wu et al. ICML 2019]

Neighbor Sampling

Key idea: **Construct the computational graph** by (randomly) sampling at most H neighbors at each hop.

- **Example ($H = 2$):**



Issues

- **Remark 1: Trade-off in sampling number H**
  - Smaller H leads to more efficient neighbor aggregation, but results in more unstable training **due to the larger variance** in neighbor aggregation.
- **Remark 2: Computational time**
  - Even with neighbor sampling, **the size of the computational graph is still exponential with respect to number of GNN layers K.**
  - Increasing one GNN layer would make computation H times more expensive.

How to sample nodes?

- **Remark 3: How to sample the nodes**
  - **Random sampling:** fast but many times not optimal (may sample many "unimportant" nodes)
  - **Random Walk with Restarts:**
    - Natural graphs are "scale free", sampling random neighbors, samples many low degree "leaf" nodes.
    - Strategy to sample important nodes:
      - Compute Random Walk with Restarts score R_i starting at the **green** node
      - At each level sample H neighbors i with the highest R_i
    - This strategy works much better in practice.

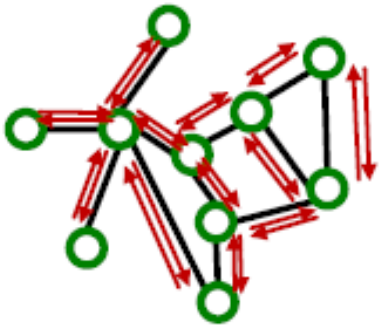
Subgraph Sampling

- **Key idea**: We can **sample a small subgraph of the large graph** and then perform the efficient **layer-wise** node embeddings update over the subgraph.

Large graph

Sampled subgraph (small enough to be put on a GPU)

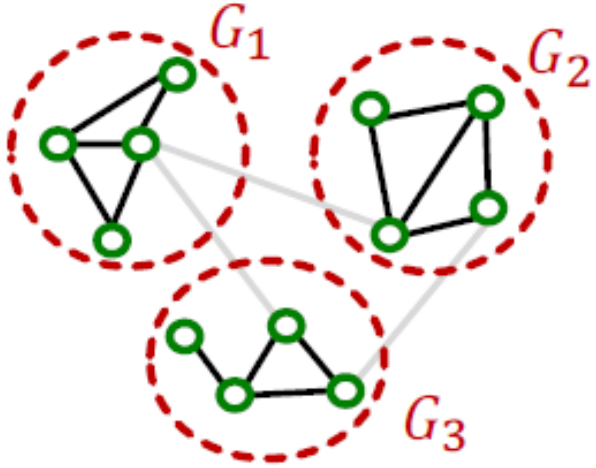
Layer-wise node embeddings update on the GPU



Cluster GCN

- Given a large graph $G = (V, E)$, **partition its nodes V into C groups: $V_1, \ldots, V_C$.**
  - We can use any scalable community detection methods, e.g., Louvain, METIS [Karypis et al. SIAM 1998].
- $V_1, \ldots, V_C$ **induces** C subgraphs, $G_1, \ldots, G_C$,
  - Recall: $G_c \equiv (V_c, E_c)$,
  - where $E_c = \{(u, v) | u, v \in V_c\}$

Notice: Between-group edges are *not* included in $G_1, \ldots, G_C$.



Simplifying GCN

- **We start from Graph Convolutional Network** (GCN) [Kipf & Welling ICLR 2017].
- We simplify GCN by **removing the non-linear activation** from the GCN [Wu et al. ICML 2019].
  - *Wu et al.* demonstrated that the performance on benchmark is not much lower by the simplification.
- Simplified GCN turns out to be extremely scalable by the model design.

GCN (Mean Pool)

- **Given**: Graph $G = (V, E)$ with input node features X_v for $v \in V$, where ***E* includes the self-loop:**
  - $(v, v) \in E$ **for all** $v \in V$.

- Set input node embeddings: $h_v^{(0)} = X_v$ for $v \in V$.
- For $k \in \{0, \ldots, K-1\}$:
  - For all $v \in V$, aggregate neighboring information as

$$h_v^{(k+1)} = \mathrm{ReLU}\left(\boldsymbol{W_k} \frac{1}{|N(v)|} \sum_{u \in N(v)} h_u^{(k)}\right)$$

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

Mean-pooling

- **Final node embedding**: $z_v = h_v^{(K)}$

Simplifying GCN

- **Simplify GCN by removing ReLU non-linearity:**

$$\boldsymbol{H}^{(k+1)} = \widetilde{\boldsymbol{A}}\boldsymbol{H}^{(k)}\boldsymbol{W}_{\boldsymbol{k}}^{\mathrm{T}}$$

- The final node embedding matrix is given as

$$\boldsymbol{H}^{(K)} = \widetilde{\boldsymbol{A}}\,\boldsymbol{H}^{(K-1)}\,\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}$$

$$= \widetilde{\boldsymbol{A}}\left(\widetilde{\boldsymbol{A}}\boldsymbol{H}^{(K-2)}\boldsymbol{W}_{\boldsymbol{K-2}}^{T}\right)\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}$$

$$\cdots = \widetilde{\boldsymbol{A}}\left(\widetilde{\boldsymbol{A}}\left(\cdots\left(\widetilde{\boldsymbol{A}}\,\boldsymbol{H}^{(0)}\,\boldsymbol{W}_{\boldsymbol{0}}^{\mathrm{T}}\right)\cdots\right)\boldsymbol{W}_{\boldsymbol{K-2}}^{\mathrm{T}}\right)\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}$$

$$= \widetilde{\boldsymbol{A}}^{K}\,\boldsymbol{X}\left(\boldsymbol{W}_{\boldsymbol{0}}^{\mathrm{T}}\cdots\boldsymbol{W}_{\boldsymbol{K-1}}^{\mathrm{T}}\right)$$

Composition of linear transformation is still linear!

$$= \widetilde{\boldsymbol{A}}^{K}\,\boldsymbol{X}\,\boldsymbol{W}^{\mathrm{T}} \quad \text{where } \boldsymbol{W} \equiv \boldsymbol{W}_{\boldsymbol{K-1}}\cdots\boldsymbol{W}_{\boldsymbol{0}}$$