Contents

Overview

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

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

Stepup: vertex set, adjacency matrix, node features

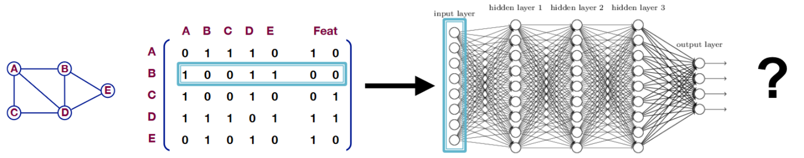
- **Assume we have a graph G:**
  - V is the vertex set
  - A is the adjacency matrix (assume binary)
  - $X \in \mathbb{R}^{m \times |V|}$ is a matrix of node features
  - v: a node in V; $N(v)$: the set of neighbors of v.
  - **Node features:**
    - Social networks: User profile, User image
    -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

Naive Approach: append node feaetures to adjacency matrix

3 problems: parameter size, graph size, node ordering

1. Parameter size
   a. One training example per node but for each node there are N + X (node features) number of features
   b. Training unstable / easy to overfit
2. Graph with different size
   - E.g. If 5 nodes, hard to fit in input size of 7
3. Node ordering
   - If the column order change, then the adjacency matrix changes
     - Rows & cols permuted thou the info is the same
   - For images, the ordering can be top left pixel to bottom right
   - but for graphs, there is no fix node ordering i.e. unclear how to sort the graph to put them as input in the matrix
   - Has to be **invariant** to **node ordering**

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



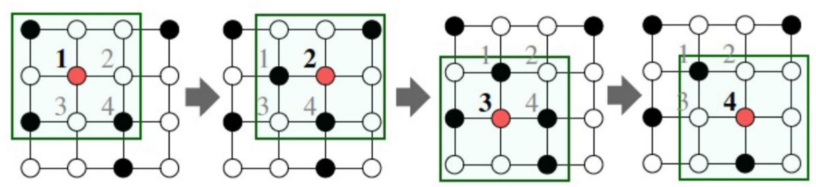
- Issues with this idea:
  - $O(|V|)$ parameters
  - Not applicable to graphs of different sizes
  - Sensitive to node ordering

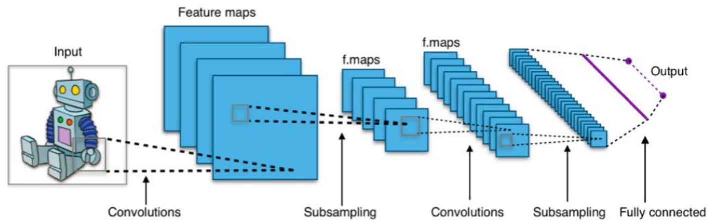
Adopt CNN

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

CNN = Sliding windows & locality.

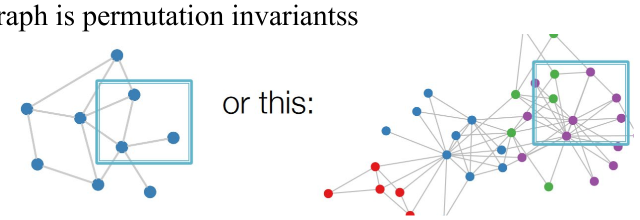
CNN on an image:





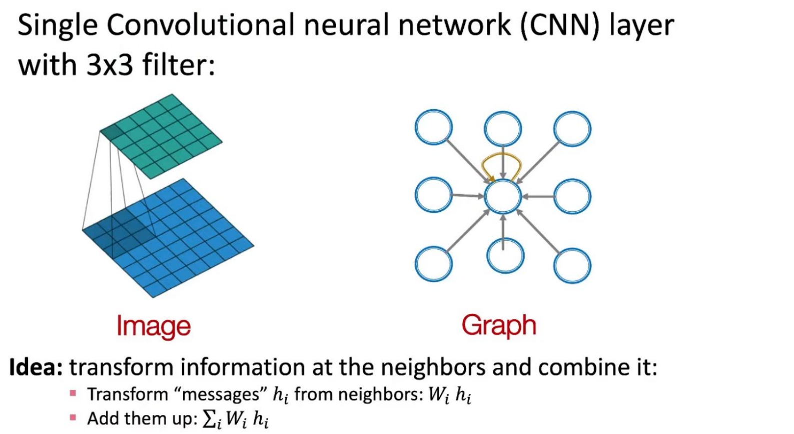
Problem

- no fixed notion of locality or sliding window on the graph
  - L: covers 3 nodes
  - R: covers more nodes
- Graph is permutation invariantss



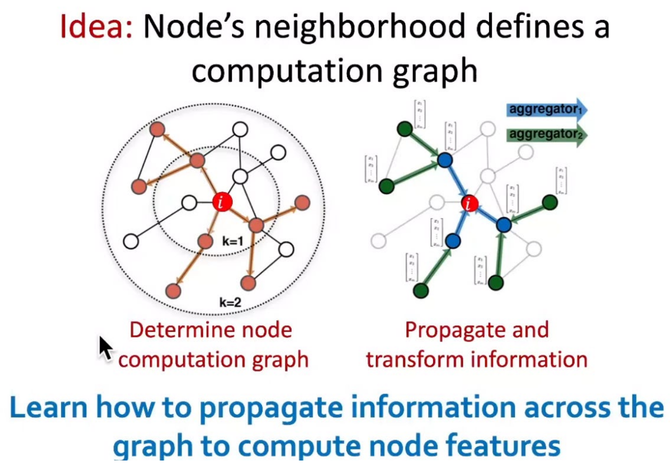
Solutions

- Aggregate information about a node based on its neighbouring nodes



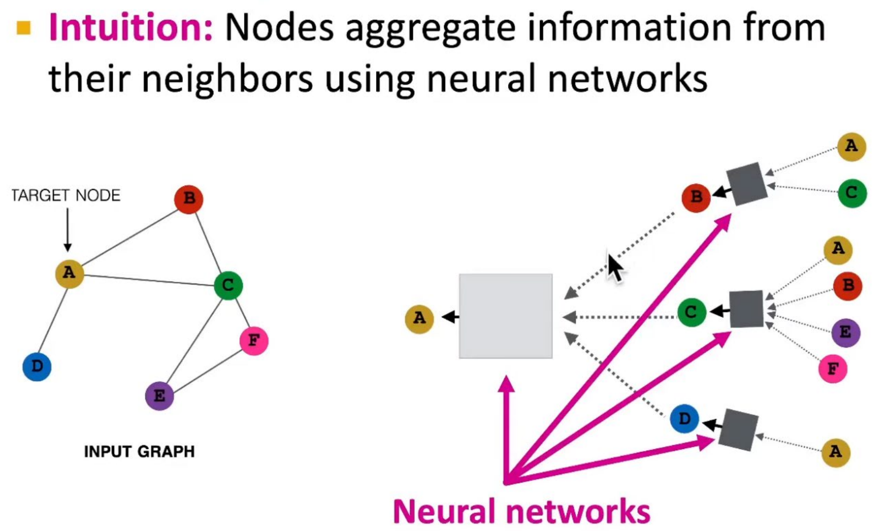
Kipf & Welling, ICLR 2017

- Neighbour nodes takes the message from the node and propagate. Steps
  1. Determine node computation graph
  2. Propagate & transform information



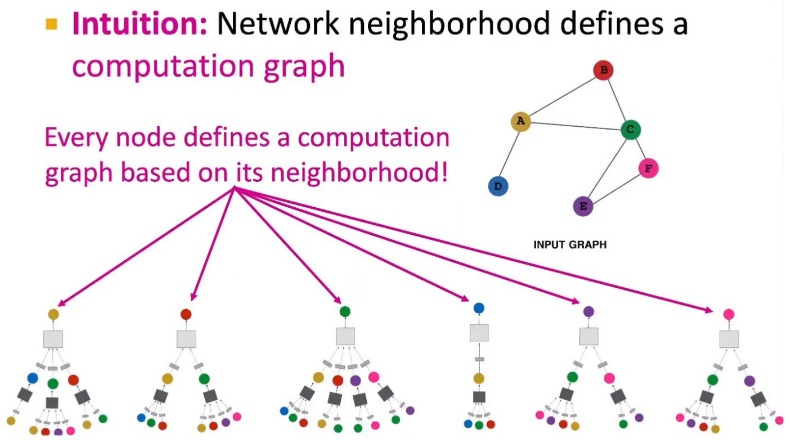
Explain – transformation & aggregation

1. To decide node A informatino, we collect from its neighbours {B, C, D}, in which their info are based on their neighbours.
2. The message passing is then from the leaf to root
   a. First, transform the info from leaf
   b. Second, aggregate them in the parent node
   c. Repeat

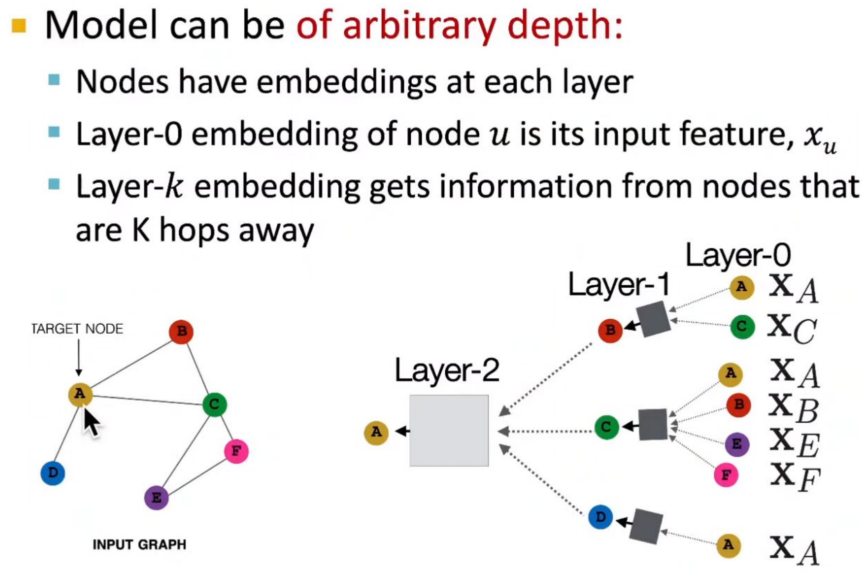


Explain – each node has a computational graph

- Every node has its own computation graph / architecture
- The structure depends on other structure
- Different to classical DL

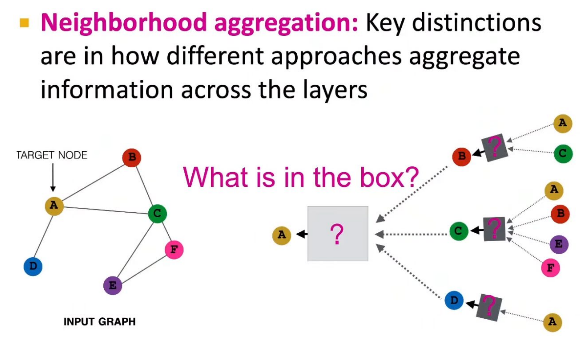


Many layers – k-hops



Neighbourhood aggregation

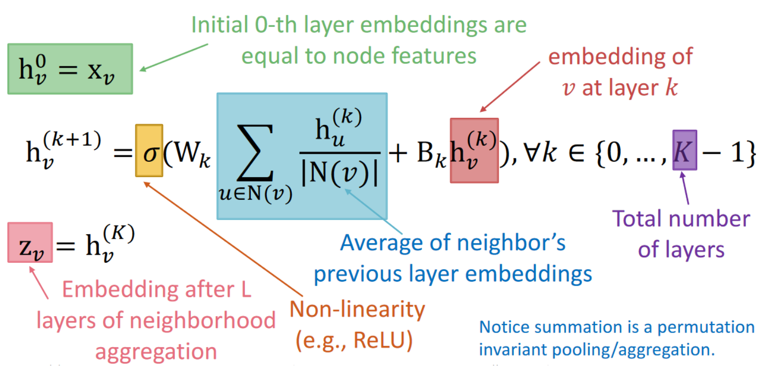
- The aggregation result is the same regardless of the ordering



Transformation choice – average embedding

- Ordering invariant
- Examples
  - Average messages
  - Apply NN
    - Apply linear transformation
    - Follow by non-linearity

- Transform current layer features + aggregated previous child nodes messages



Model Parameters: W, B; neighborhood aggregation, transformation

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

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

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

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

Final node embedding

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

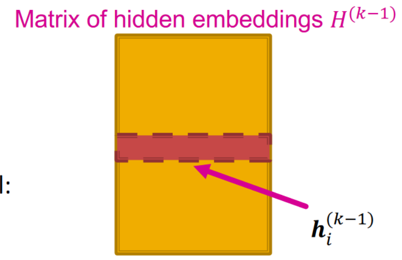
h_v^k: the hidden representation of node v at layer k
- W_k: weight matrix for neighborhood aggregation
- B_k: weight matrix for transforming hidden vector of self

Matrix Formulation - efficient sparse matrix

Averging of neighbour embedding

- Many aggregations can be performed **efficiently** by (sparse) matrix operations
- Then
  - Node embedding is the avage of the neighbour embedding
  - i.e. the adjacency matrix * embedding spaces at a layer
- in short
  - averging of neighbour embedding
    - summing and averagign can be rewritten as
    - **matrix multiplication (dot prodct)**
  - the drawing is what correspond to what

- Let $H^{(k)} = [h_1^{(k)} \dots h_{|V|}^{(k)}]^T$
- Then: $\sum_{u \in N_v} h_u^{(k)} = A_{v,:} H^{(k)}$
- Let D be diagonal matrix where $D_{v,v} = \text{Deg}(v) = |N(v)|$
  - The inverse of D: D^{-1} is also diagonal: $D_{v,v}^{-1} = 1/|N(v)|$
- **Therefore,**



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

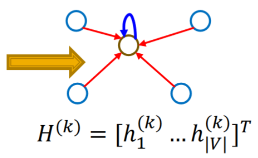
Re-writing update function in matrix form

- 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**

- Re-writing update function in matrix form:

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

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



- Red: neighborhood aggregation
- Blue: self transformation

How to train GNN: supervised & unsupervised setting

- Node embedding z_v is a function of input graph
- **Supervised setting**: we want to minimize the loss $\mathcal{L}$ (see also Slide 15):

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

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

Unsupervised Training

- No labels

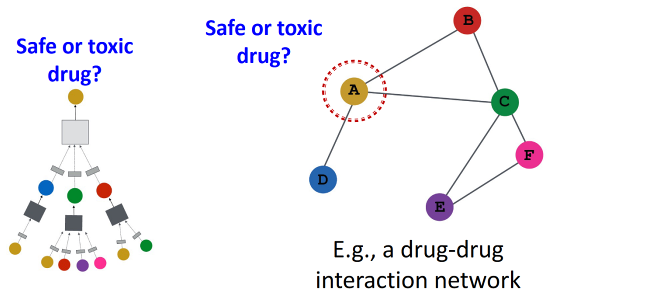
- **"Similar" nodes have similar embeddings**

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

  - 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**

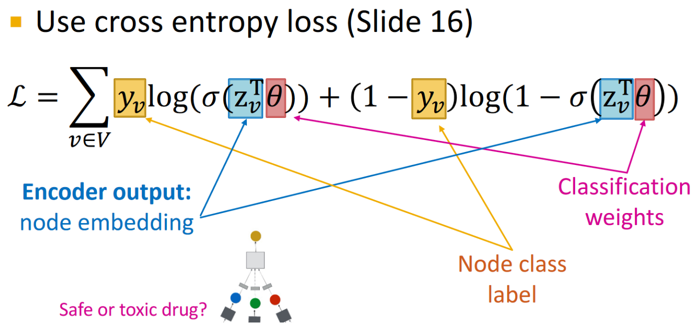
Supervised Training

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



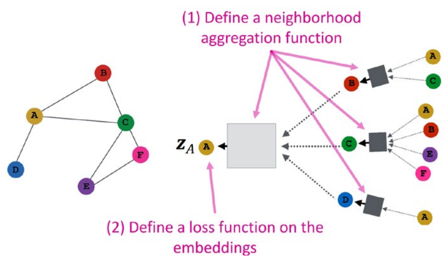
Cross entropy loss

- If label is 1, want output to be 1
- If 0, want 0

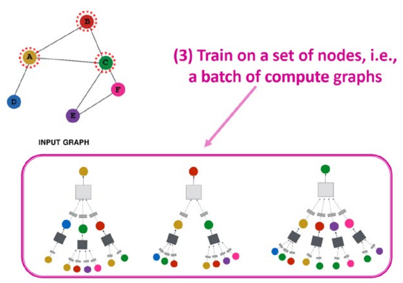


Model design

Step 1,2 - neighbour aggregation & loss function

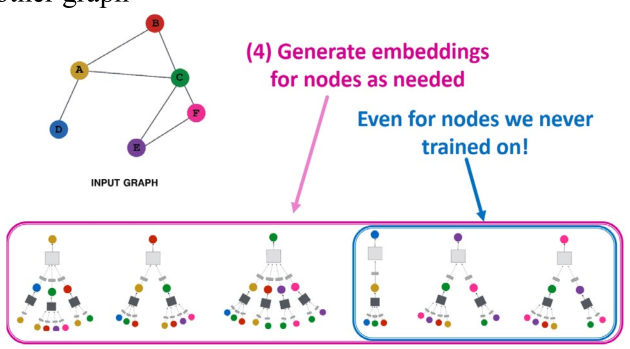


Step 3 – train on a batch



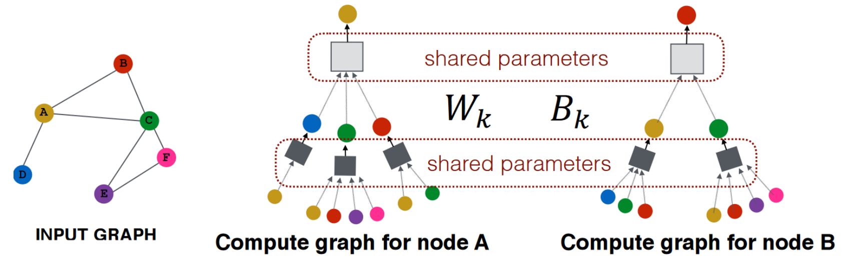
Step 4 - enerate embeddings for nodes as needed

- **Generalisability.** Train embedding for one graph and transfer to another graph

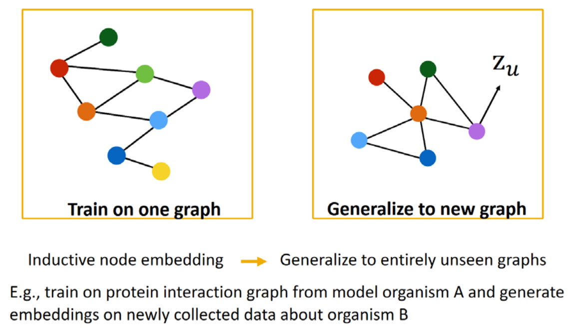


Inductive capcability

- The same aggregation parameters are **shared** for all nodes
- The number of model parameters is **sublinear** in $|V|$
- # model parameters **W & B**, depends on
  - #features / embedding dimensationality (since shared)
  - not the size of graph (#nodes)
- Thus, generalize to **unseen** nodes



New graph



New nodes

- One forward pass can generate new embedding for the new node as the graph evoluving