

Graph Neural Networks Demystified

An overview of the essential concepts in Stanford CS224W (Lectures 1~9)
with oversimplified examples

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Embeddings

- Relatively small vectors associated with each object where similar objects have similar embeddings
- Using the embeddings of graph elements, various tasks can be performed
 - Cluster nodes in a graph
 - Predict properties of a node
 - Predict if two nodes may be connected
 - Classify entire graphs
- To perform each task, use the embedding with a suitable ML method
 - e.g. clustering can be performed with k -means

Obtaining embeddings

- Embeddings can be formed with or learned from features
 - Node-level features
 - Degree
 - Centrality (eigenvector/ betweenness/ closeness)
 - Clustering coefficient
 - Graphlets
 - Structure-based features
 - Link-level features
 - Distance-based features
 - Local/global neighborhood overlap
 - Graph-level features
 - Graph kernels
- Task-independent embeddings can be learned from unsupervised learning

Task-independent embeddings

- Unsupervised extraction by random walks

- **DeepWalk**

- Estimate pairwise distance between nodes (hence their co-occurrence probability)
 - Usable for finding product relatedness in recommender
- Node embeddings
 1. Estimate node distances with random walks
 2. Train a neural network (with node input and embedding output) such that distances between embeddings agree with estimated distances

- **Anonymous Walk**

- Embeddings for entire graphs

- **Simpler method: just add up neighbors**

Embeddings by adding neighbors

- Sum up the features of (self and) neighbor nodes
 - Features of nodes in close proximity will become similar

Example: Let h_i^j denote features of node i at iteration j and let $h_1^0 = (1 \ 0 \ 0)$, $h_2^0 = (0 \ 1 \ 0)$, and $h_3^0 = (0 \ 0 \ 1)$



- $h_1 \equiv h_2$ after only 1 iteration

Embeddings by adding neighbors

- To cluster nodes in a graph, will it work if we
 1. Start with a unique feature for each node, and
 2. Repeatedly add up neighboring features, and
 3. Finally, cluster the resultant features with some method like *k*-means?

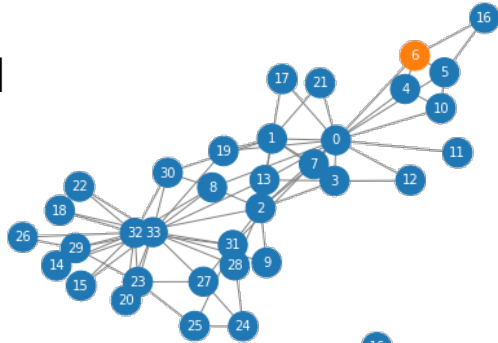


Let's try with karate club network

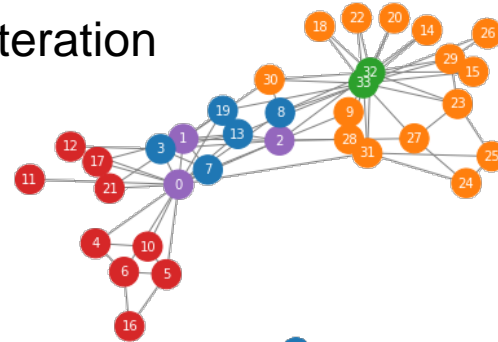
Embeddings by adding neighbors

□ Karate club

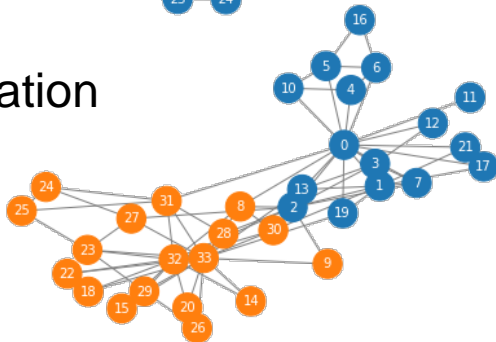
Initial



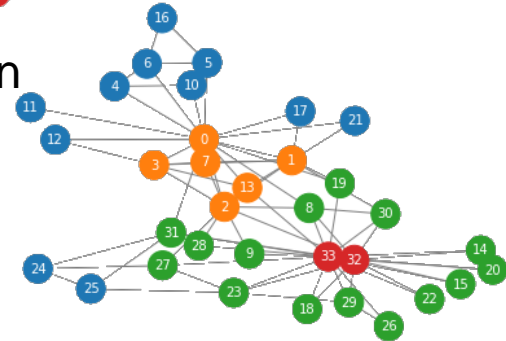
3rd iteration



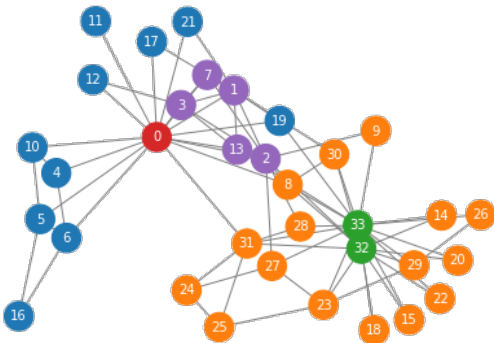
1st iteration



4th iteration



2nd iteration



5th iteration



(converged)

Adding neighbors w/ linear algebra

- Let matrix H be a matrix where each row is a node and each column is a feature
 - H have $\dim |V| \times d$
- Let A be an adjacency matrix
 - Let $\hat{A} = A + I$ where I is the identity matrix
- Then, **sum** is simply $\hat{A}H$

Note that node order is not important

$$\begin{pmatrix} a & b & c \\ \dots & & \\ \dots & & \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \begin{pmatrix} ah_1 + bh_2 + ch_3 \\ \dots \\ \dots \end{pmatrix}$$

e.g.



$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \begin{pmatrix} h_1 + h_2 \\ h_1 + h_2 \\ h_3 \end{pmatrix}$$

Adding neighbors w/ linear algebra

- Let matrix H be a matrix where each row is a node and each column is a feature
 - H have $\dim |V| \times d$
- Let A be an adjacency matrix
 - Let $\hat{A} = A + I$ where I is the identify matrix
- Further **normalize** each row of \hat{A} to sum to 1

$$\begin{pmatrix} 1/3 & 1/3 & 1/3 \\ & \dots & \\ & & \dots \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \begin{pmatrix} (h_1 + h_2 + h_3)/3 \\ & \dots & \\ & & \dots \end{pmatrix}$$

Note that
normalize
does the same
thing as **mean**

e.g.



$$\begin{pmatrix} .5 & .5 & 0 \\ .5 & .5 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ h_3 \end{pmatrix} = \begin{pmatrix} (h_1 + h_2)/2 \\ (h_1 + h_2)/2 \\ h_3 \end{pmatrix}$$

Adding neighbors w/ linear algebra

- Let matrix H be a matrix where each row is a node and each column is a feature
 - H have dim $|V| \times d$
- Let A be an adjacency matrix
 - Let $\hat{A} = A + I$ where I is the identify matrix
- Further **normalize** each row of \hat{A} to sum to 1
 - To perform this normalization, it suffices that we let $\hat{A} \leftarrow D^{-1}\hat{A}$ where D is the diagonal node degree matrix

- In PyTorch, use `torch.nn.functional.normalize(A, p=1, dim=1)`

- Or, use $\hat{A} \leftarrow D^{-\frac{1}{2}}\hat{A}D^{-\frac{1}{2}}$, the spectral variant

- In PyTorch, use

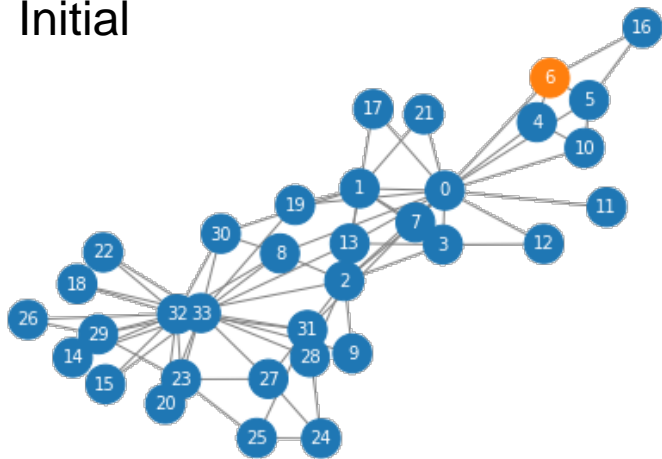
- ```
D = torch.diag(torch.sum(A, 1)).inverse().sqrt()
D = torch.mm(torch.mm(D, A), D)
```

Normalized  $\hat{A}$   
is in general  
**not symmetric**

# Adding neighbors w/ linear algebra

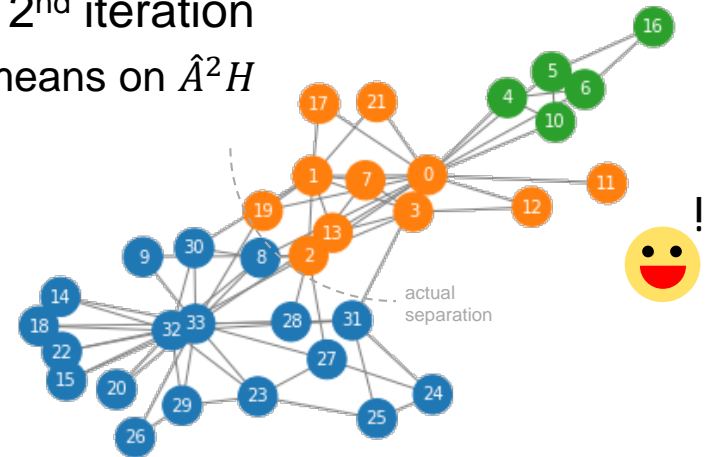
- Redo karate club with normalized  $\hat{A} \leftarrow D^{-1}\hat{A}$

Initial



2<sup>nd</sup> iteration

$k$ -means on  $\hat{A}^2 H$



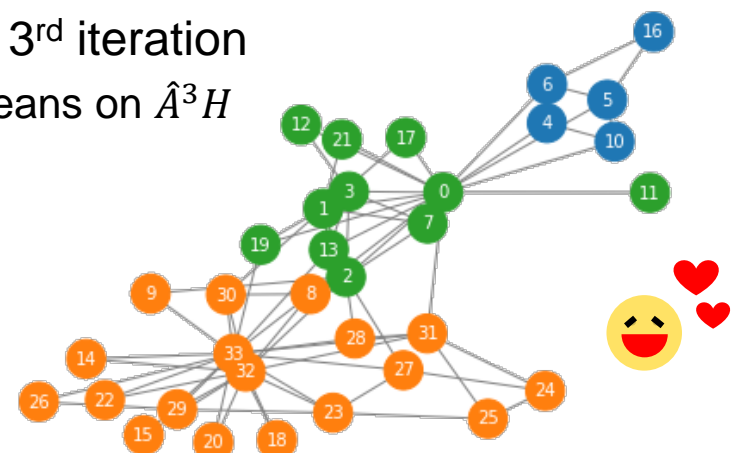
1<sup>st</sup> iteration

$k$ -means on  $\hat{A} H$



3<sup>rd</sup> iteration

$k$ -means on  $\hat{A}^3 H$



(no change)

# Adding neighbors: evaluation

## □ Why do we need normalization

- Without normalization, feature values for the nodes of high centrality would quickly add up, making them distinct from the nodes of low centrality

## □ How many iterations should be used?

- Each iteration would “bunch up” neighboring features of 1 hop away (receptive field)
- With that in mind, we should determine the number of iterations by the nature of the graph
- The earliest (RNN-like) GNNs are iterated until convergence but these ideas were quickly replaced by (CNN-like) GNNs where the number of iterations is fixed as defined by the number of layers

# Relationship to PageRank

For simplicity consider eigenvector centrality problem, that is, the undirected version of PageRank

- Problem Statement. Suppose each node  $v$  corresponds to a value  $x_v$  which is the sum of its neighbors' values

$$x_v = \frac{1}{\lambda} \sum_{u \in N(v)} x_u$$

where  $\lambda$  is some given constant and positive factor

Given adjacency matrix  $A$  of a graph  $G$ , solve  $x_v$  for all  $v \in G$

- Problem is equivalent to that of finding vector  $x$  such that

$$\lambda x = Ax$$

- Solutions are all the eigenvectors that maximize  $x^T Ax$

- Problem is also equivalent to that of **adding up all neighboring single-valued features, but excluding that of self, until convergence**

# Adding neighbors: evaluation

## □ Benefits of strategy

- Simplicity
- Efficiently computed with adjacency matrix

## □ Disadvantage of strategy

- Embeddings produced are of size of the number of nodes in the graph

⇒ Learn a **transformation matrix**

$$W: R^{|V|} \rightarrow R^d \text{ for some smaller } d$$

# Transformation matrix $W$

- $W$  is typically a linear transformation layer of size  $|V| \times d$  where  $d$  is the target dimensionality of the embeddings
- Combined with the adjacency matrix  $\hat{A}$ , we now have a complete matrix formulation for computing embedding  $h_v$  of a node  $v$  from (itself and) its neighbors, in the form of

$$h_v \leftarrow (\hat{A})_v HW$$

where

- $(\hat{A})_v$  is the row in  $\hat{A}$  for the node  $v$ , and
- $H$  is a matrix containing the features/embeddings of all the nodes (of course, only the rows in  $H$  with non-zero entries in  $(\hat{A})_v$  are needed for computing  $h_v$ )



**Variations in this formula lead to various frameworks**

# Variations

- Message-aggregation (MSG-AGG)
  - First transform features/embeddings (MSG), then aggregate transformed embeddings (AGG)

$$h_v \leftarrow \underbrace{(\hat{A})_v}_{\text{aggregate}} \overbrace{(HW)}^{\text{message}}$$

- Separate computation of self and neighbors
  - Exclude entry for  $v$  from  $(\hat{A})_v$ , and let

$$h_v \leftarrow \text{AGG} \left( \overbrace{(\hat{A})_v HW}^{\text{Aggregate only neighbors}}, \overbrace{h_v W'}^{\text{Self}} \right)$$

Learn a different transformation for self

Also denoted as  $B$

where  $\text{AGG}$  is, for instance, concatenation



# Frameworks

## □ Graph Convolutional Network (GCN)

$$h_v \leftarrow (\hat{A})_v (HW) \quad (\text{basically just MSG-AGG})$$

## □ GraphSAGE

- Exclude entry for  $v$  from  $(\hat{A})_v$

$$h_v \leftarrow \underbrace{\left( \underbrace{\text{CONCAT} \left( \underbrace{\text{AGG} \left( (\hat{A})_v H \right)}_{\text{Aggregate neighbors}}, \underbrace{h_v}_{\text{Self}} \right)}_{\text{Concatenate self \& aggregated neighbors}} \right)}_{\text{Transform}} W$$

AGG can be one of many options including MLP, LSTM, *etc.*

(Why use these? See Graph Isomorphism Network)

$\Rightarrow$  AGG is learnable

# GraphSAGE

$$\square h_v \leftarrow \left( \text{CONCAT} \left( \text{AGG} \left( (\hat{A})_v H \right), h_v \right) \right) W$$

- As mentioned **AGG** is learnable

- $\hat{A}$  is also learnable

- Generalize adjacency to **attention weights**  $\alpha_{uv}$

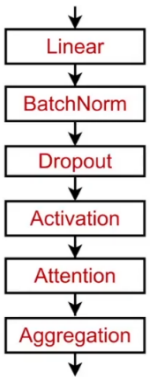
$$\alpha_{vu} = \frac{\exp(e_{vu})}{\sum_{x \in N(v)} \exp(e_{vx})}$$

where  $e_{vu}$  is a measure of how related  $u$  and  $v$  are,  
usually computed as  $\text{LINEAR}(\text{CONCAT}(h_v W, h_u W))$

- PyTorch Geometric (PyG) has implementations of these frameworks (GCN, GraphSAGE)

# In practical use

- At this point we have not mentioned activation function or other elements of DL
  - For activation function just let  $\sigma(h_v) \leftarrow h_v$
  - Mix and match as you like
- Embeddings can be used for many downstream tasks
  - We have earlier used  $k$ -means for clustering the final output
  - Better performed by constructing a neural network directly with the GNN layers



# In practical use

## □ Adding graph elements

### ■ Features

- Similar to feature engineering

### ■ Virtual nodes

- Connecting all the nodes in a sparse but apparent subgraph to a virtual node will allow those nodes to better communicate

### ■ Virtual edges

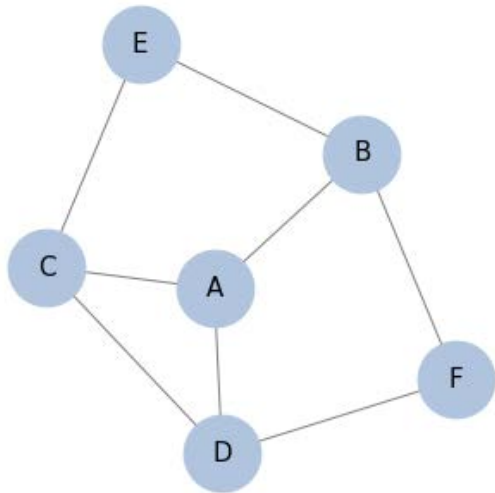
- Create new graph by systematically adding edges
- Example: Given a bipartite graph, breaking the graph into two of only nodes of the same type is good for some analyses
  - Let  $A$  be the adjacency matrix of the bipartite graph  $G$
  - $A^2$  then gives the number of paths of distance 2 between nodes in  $G$ 
    - ⇒ an adjacency matrix between nodes of the same type
    - ⇒ allows us to separate  $G$  into two graphs, each of same node type
  - $A + A^2$  can form an adjacency matrix with heterogeneous edges

# Training GNNs

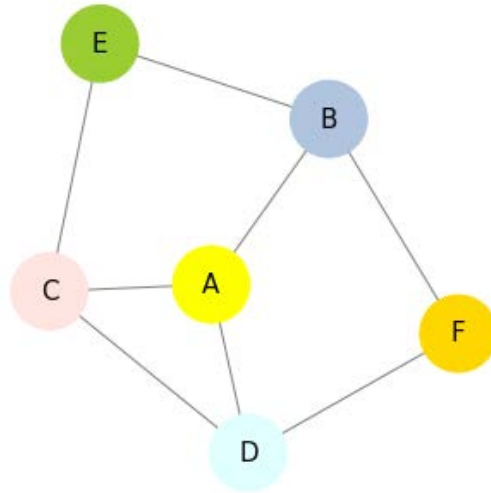
- Using node embeddings as input to a prediction function
  - Embedding of 1 node can be used directly
  - Embedding of 2 nodes can be
    - Concatenated to form an edge embedding
    - Projected on each other to get their similarity
  - Embeddings of nodes of the entire graph can be
    - Summed, averaged, searched for max/min, *etc.*
    - Clustered, then the clusters summed, average, *etc.*, in a hierarchical fashion
- Using edge embeddings
  - Relational GCN

# Distinguishing node embeddings

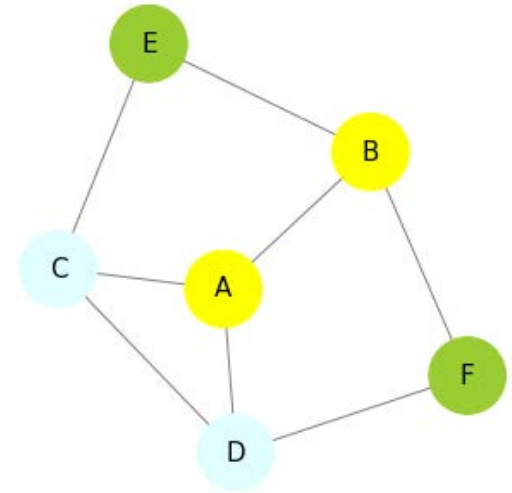
- Should C and D have the same embedding in the following graphs? Given that features are given by the colors and mutually exclusive (orthogonal)



Yes?



No?

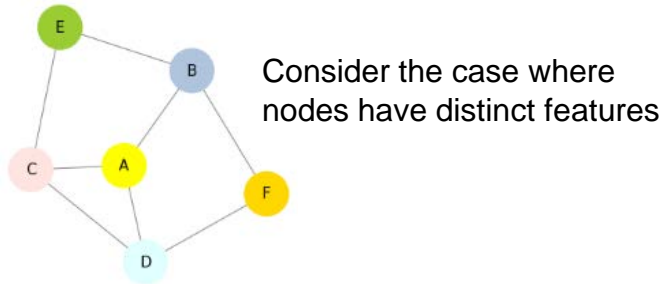


Should?

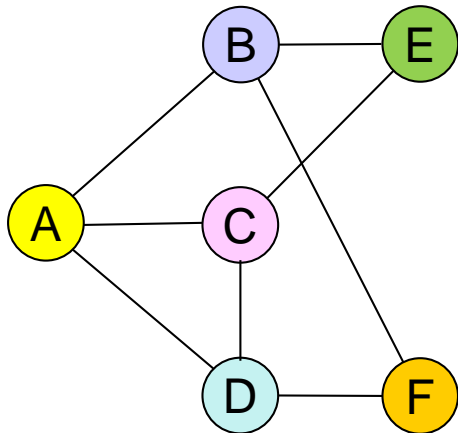
- How about A and B?
- Idea:** Two nodes should have the same **embedding** if they have the same **feature** and **neighborhood structure**, and vice versa

# Distinguishing node embeddings

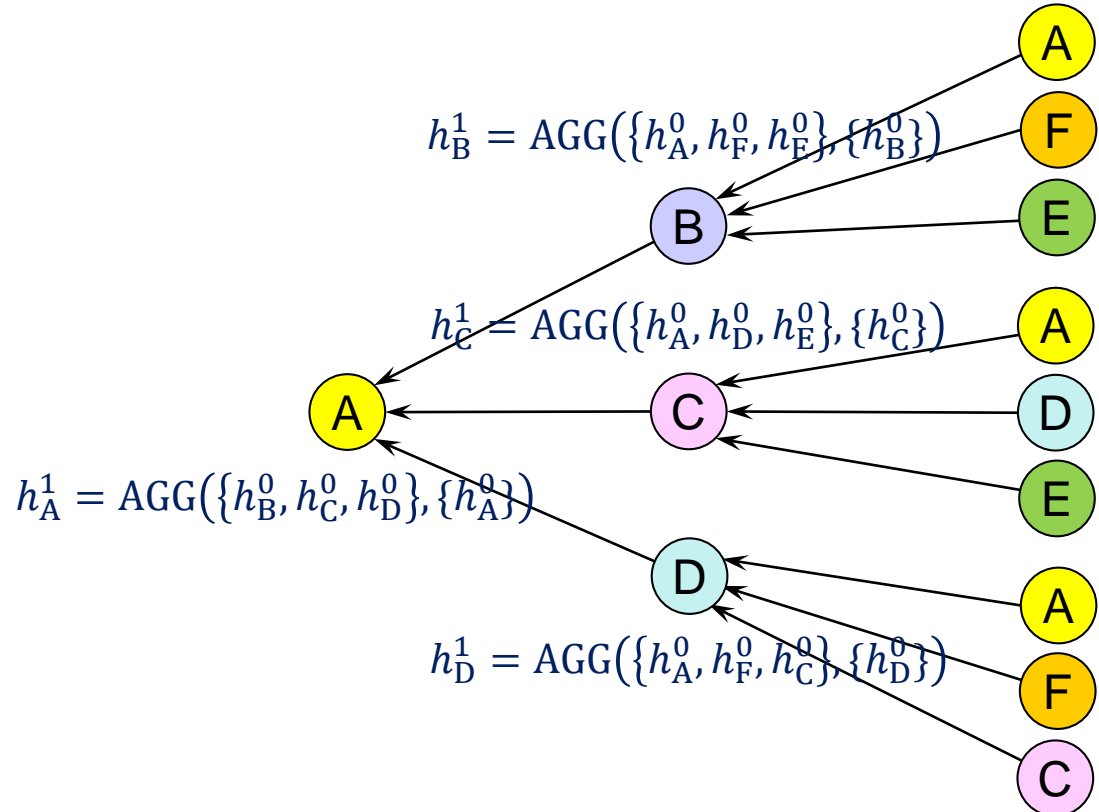
- Given a GCN of 2 layers, the embedding of A is computed as follows



Rearranged w.r.t. distance from A



Computational graph of A's embedding



# Distinguishing node embeddings

- Given a GCN of 2 layers, the embedding of A is computed as follows

- Let  $h_A^0 = [1|0|0|0|0|0]$ ,  $h_B^0 = [0|1|0|0|0|0]$ ,  $h_C^0 = [0|0|1|0|0|0]$ ,  $h_D^0 = [0|0|0|1|0|0]$ ,  $h_E^0 = [0|0|0|0|1|0]$ ,  $h_F^0 = [0|0|0|0|0|1]$ , and let AGG be **addition**. Then

- $h_B^1 = \text{AGG}(\{h_A^0, h_F^0, h_E^0\}, \{h_B^0\}) = 1|1|0|0|1|1$
- $h_C^1 = \text{AGG}(\{h_A^0, h_D^0, h_E^0\}, \{h_C^0\}) = 1|0|1|1|1|0$
- $h_D^1 = \text{AGG}(\{h_A^0, h_F^0, h_C^0\}, \{h_D^0\}) = 1|0|1|1|0|1$
- $h_A^1 = \text{AGG}(\{h_B^0, h_C^0, h_D^0\}, \{h_A^0\}) = 1|1|1|1|0|0$

Compute  $\text{AGG}(X)$  as  $AH$ , where  $A$  is the adjacency matrix (with self loop), and  $H$  is a matrix containing all the embeddings in  $X$

- Finally the embedding of A is
  - $h_A^2 = \text{AGG}(\{h_B^1, h_C^1, h_D^1\}, \{h_A^1\}) = 4|2|3|3|2|2$
- Similarly,
  - $h_B^2 = 2|4|2|2|2|2$
  - $h_C^2 = 3|2|4|3|2|1$
  - $h_D^2 = 3|2|3|4|1|2$
  - $h_E^2 = 2|2|2|1|3|1$
  - $h_F^2 = 2|2|1|2|1|3$

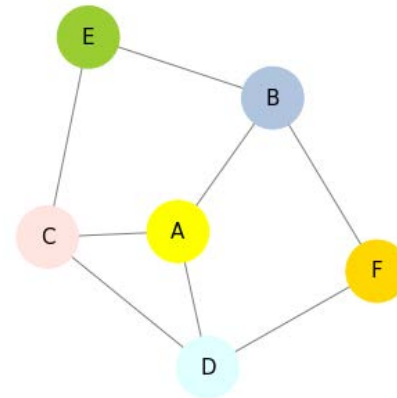


# Distinguishing node embeddings

- Given a GCN of 2 layers, the embedding of A is computed as follows

- Let  $h_A^0 = [1\ 0\ 0\ 0\ 0\ 0]$ ,  $h_B^0 = [0\ 1\ 0\ 0\ 0\ 0]$ ,  $h_C^0 = [0\ 0\ 1\ 0\ 0\ 0]$ ,  $h_D^0 = [0\ 0\ 0\ 1\ 0\ 0]$ ,  $h_E^0 = [0\ 0\ 0\ 0\ 1\ 0]$ ,  $h_F^0 = [0\ 0\ 0\ 0\ 0\ 1]$ , and let AGG be **addition**. Then

- $h_A^2 = 4\ 2\ 3\ 3\ 2\ 2$   
 $h_B^2 = 2\ 4\ 2\ 2\ 2\ 2$   
 $h_C^2 = 3\ 2\ 4\ 3\ 2\ 1$   
 $h_D^2 = 3\ 2\ 3\ 4\ 1\ 2$   
 $h_E^2 = 2\ 2\ 2\ 1\ 3\ 1$   
 $h_F^2 = 2\ 2\ 1\ 2\ 1\ 3$



By induction they will be distinct for all subsequent iterations

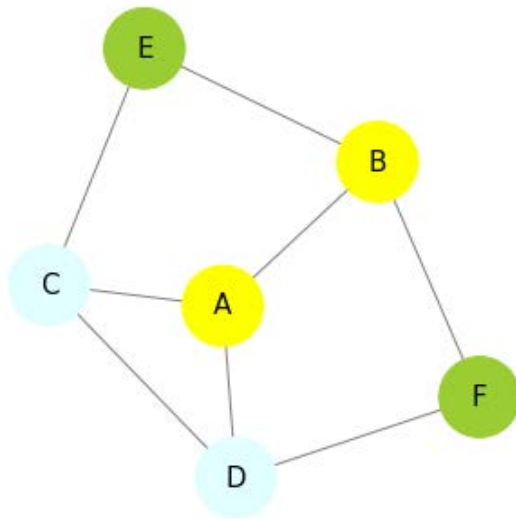
- For a graph with **distinct node features**, the embeddings will be distinct under **addition** regardless of **neighborhood structure** or **iterations**

- With the exception of “twin nodes” that are connected only to each other (in which case they will become equal after the first iteration)

# Distinguishing node embeddings

- Given a GCN of 2 layers, the embedding of A is computed as follows

- Let  $h_A^0 = h_B^0 = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}$ ,  $h_C^0 = h_D^0 = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix}$ ,  $h_E^0 = h_F^0 = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}$ , and let AGG be **addition**. Then, for the following graph



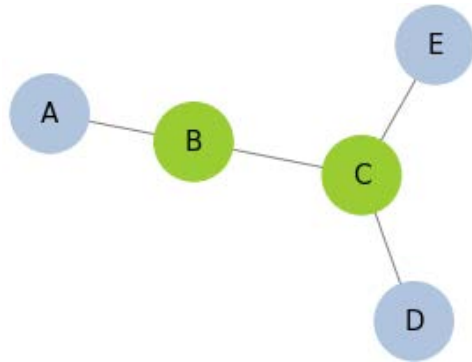
|                 |                 |                      |
|-----------------|-----------------|----------------------|
| $h_A^1 = 2 2 0$ | $h_A^2 = 6 6 4$ | } $h_A^2 \neq h_B^2$ |
| $h_B^1 = 2 0 2$ | $h_B^2 = 6 4 4$ |                      |
| $h_C^1 = 1 2 1$ | $h_C^2 = 5 7 3$ | } $h_C^2 = h_D^2$    |
| $h_D^1 = 1 2 1$ | $h_D^2 = 5 7 3$ |                      |
| $h_E^1 = 1 1 1$ | $h_E^2 = 4 3 4$ | } $h_E^2 = h_F^2$    |
| $h_F^1 = 1 1 1$ | $h_F^2 = 4 3 4$ |                      |

- Two nodes with the **same feature** will always have the same embedding under **addition** if and only if they have the same **neighborhood structure**
  - What about other AGG functions, e.g. **mean**?

# Distinguishing node embeddings

- Let  $h_A^0 = h_D^0 = h_E^0 = \begin{bmatrix} 1 & 0 \end{bmatrix}$ ,  $h_B^0 = h_C^0 = \begin{bmatrix} 0 & 1 \end{bmatrix}$ , and let AGG be **mean**.  
Then, for the following graph

Compute  $AGG(X)$  as  $\hat{A}H$



$$h_A^1 = 0.5 \mid 0.5$$

$$h_B^1 = 0.33 \mid 0.67$$

$$h_C^1 = 0.5 \mid 0.5$$

$$h_D^1 = 0.5 \mid 0.5$$

$$h_E^1 = 0.5 \mid 0.5$$

- As expected,  $h_A^1 = h_D^1 = h_E^1$  due to the same feature and neighborhood structure (within 1 hop)
- However,  $h_A^1 = h_C^1$  in spite of their differences in both features and neighborhood structure  
 $\Rightarrow$  **mean** cannot get distinct embeddings for distinct nodes
  - Even though this is true only for the first iteration in this example, similar examples can be obtained for any number of layers

# Distinguishing node embeddings

- While our earlier examples did not consider the transformation  $W$  or the activation function  $\sigma$ , the arguments are just as valid with them considered
- A function that can distinguish the nodes of distinct feature and neighborhood structure is one that is **injective**
  - **mean** and **max** are not injective
  - On the other hand, **sum** has problems as mentioned
- Theorem (Xu *et al.* 2019). Any injective AGG function can be expressed as  $\Phi(\sum_{x \in S} f(x))$  for some non-linear  $\Phi$  and linear  $f$
- Since MLP is able to approximate any function, we can learn  $\Phi$  and  $f$  with non-linear  $\text{MLP}_{\Phi}$  and linear  $\text{MLP}_f$

$$\text{AGG} = \text{MLP}_{\Phi} \left( \sum_{x \in S} \text{MLP}_f(x) \right)$$

⇒ **Graph Isomorphism Network (GIN)**