Graph and Subgraph Isomorphism Using GNNs

An overview of the essential concepts in Stanford CS224W (Lectures 9 and 12)
with only oversimplified examples

Ng Yen Kaow

Graph Isomorphism

- Complexity of graph isomorphism is unknown
- Weisfeiler-Lehman graph kernel traditionally used to obtain graph-level embedding

WL color-refinement algorithm

1. Assign initial color $c^{(0)}(v)$ to each node v
2. Iteratively refine node colors by

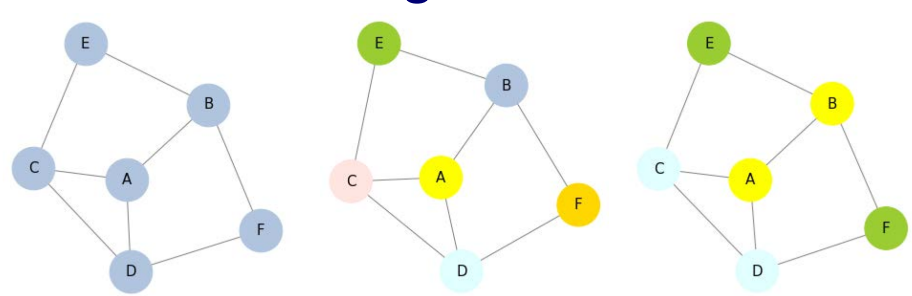
$$c^{(k+1)}(v) = \mathrm{HASH}\left(c^{(k)}(v), \{c^{(k)}(u)\}_{u \in N(v)}\right)$$

  - HASH function maps input to distinct values (colors)
  - After K steps, $c^{(K)}(v)$ summarizes the structure of the K-hop neighborhood

- To run as GNN, need to implement HASH as AGG
  - Need notion of distinguishing node embeddings

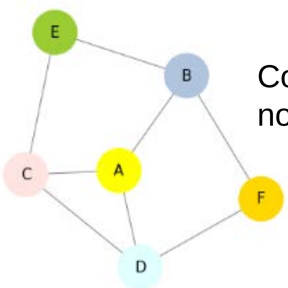
Distinguishing node embeddings

- Consider the task of keeping embeddings feature distinguishable
- Two factors affect embedding
  - (Initial) feature
    - Feature representation will affect whether features can be converted into each other
      - If $\begin{array}{|c|c|}\hline 1 & 0 \\ \hline\end{array}$, $\begin{array}{|c|c|}\hline 0 & 1 \\ \hline\end{array}$ and $\begin{array}{|c|c|}\hline 1 & 1 \\ \hline\end{array}$ represent three distinct features, then the sum of $\begin{array}{|c|c|}\hline 1 & 0 \\ \hline\end{array}$ and $\begin{array}{|c|c|}\hline 0 & 1 \\ \hline\end{array}$ would become $\begin{array}{|c|c|}\hline 1 & 1 \\ \hline\end{array}$, the third feature
    - To simplify this discussion assume that each distinct feature corresponds to one distinct dimension in the feature vector
  - Neighborhood structure
- Nodes with the same (initial) **feature** and **neighborhood structure** should be assigned the same embedding, and vice versa



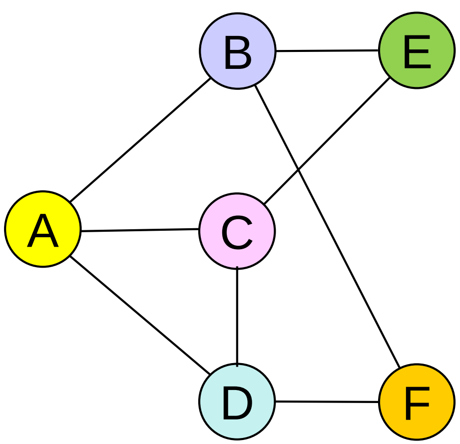
Computing node embeddings

- Recall that given a GCN of 2 layers, the embedding of A is computed through the computation graph as follows

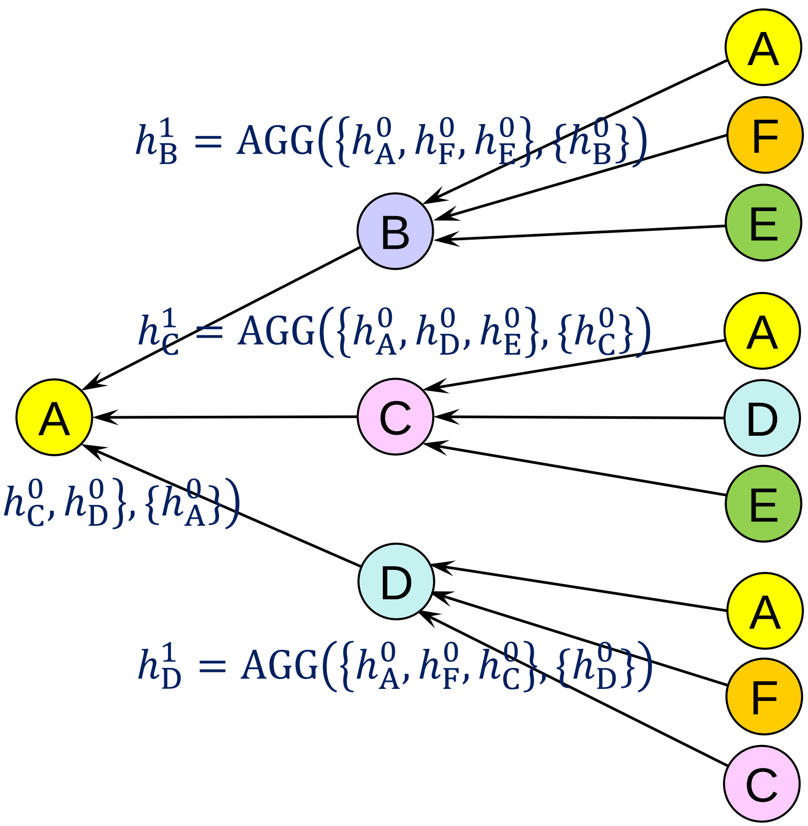


Consider the case where nodes have distinct features

Rearranged w.r.t. distance from A



Computation graph of A's embedding



$$h_{\mathrm{B}}^{1} = \mathrm{AGG}\left(\{h_{\mathrm{A}}^{0}, h_{\mathrm{F}}^{0}, h_{\mathrm{E}}^{0}\}, \{h_{\mathrm{B}}^{0}\}\right)$$

$$h_{\mathrm{C}}^{1} = \mathrm{AGG}\left(\{h_{\mathrm{A}}^{0}, h_{\mathrm{D}}^{0}, h_{\mathrm{E}}^{0}\}, \{h_{\mathrm{C}}^{0}\}\right)$$

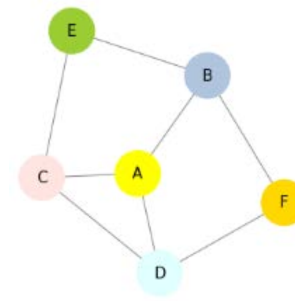
$$h_{\mathrm{A}}^{1} = \mathrm{AGG}\left(\{h_{\mathrm{B}}^{0}, h_{\mathrm{C}}^{0}, h_{\mathrm{D}}^{0}\}, \{h_{\mathrm{A}}^{0}\}\right)$$

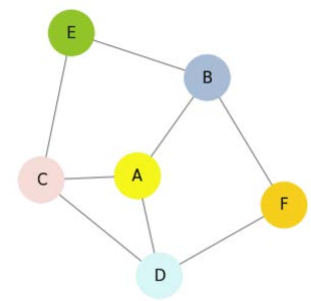
$$h_{\mathrm{D}}^{1} = \mathrm{AGG}\left(\{h_{\mathrm{A}}^{0}, h_{\mathrm{F}}^{0}, h_{\mathrm{C}}^{0}\}, \{h_{\mathrm{D}}^{0}\}\right)$$

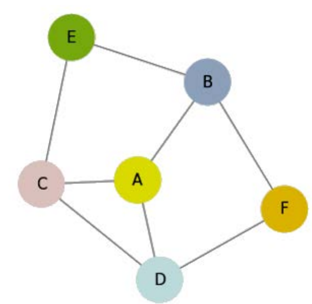
Distinguishability under **sum**

- Let AGG=**sum**, then for the GCN of 2 layers, the embeddings are as follows
  - Let h_{A}^0=$\begin{array}{|c|c|c|c|c|c|}\hline 1&0&0&0&0&0\\\hline\end{array}$, h_{B}^0=$\begin{array}{|c|c|c|c|c|c|}\hline 0&1&0&0&0&0\\\hline\end{array}$, h_{C}^0=$\begin{array}{|c|c|c|c|c|c|}\hline 0&0&1&0&0&0\\\hline\end{array}$, h_{D}^0=$\begin{array}{|c|c|c|c|c|c|}\hline 0&0&0&1&0&0\\\hline\end{array}$, h_{D}^0=$\begin{array}{|c|c|c|c|c|c|}\hline 0&0&0&0&1&0\\\hline\end{array}$, h_{D}^0=$\begin{array}{|c|c|c|c|c|c|}\hline 0&0&0&0&0&1\\\hline\end{array}$, and let AGG be **sum**. Then
    - $h_{\mathrm{B}}^1 = \mathrm{AGG}\left(\{h_{\mathrm{A}}^0, h_{\mathrm{F}}^0, h_{\mathrm{E}}^0\}, \{h_{\mathrm{B}}^0\}\right) = \begin{array}{|c|c|c|c|c|c|}\hline 1&1&0&0&1&1\\\hline\end{array}$
    - $h_{\mathrm{C}}^1 = \mathrm{AGG}\left(\{h_{\mathrm{A}}^0, h_{\mathrm{D}}^0, h_{\mathrm{E}}^0\}, \{h_{\mathrm{C}}^0\}\right) = \begin{array}{|c|c|c|c|c|c|}\hline 1&0&1&1&1&0\\\hline\end{array}$
    - $h_{\mathrm{D}}^1 = \mathrm{AGG}\left(\{h_{\mathrm{A}}^0, h_{\mathrm{F}}^0, h_{\mathrm{C}}^0\}, \{h_{\mathrm{D}}^0\}\right) = \begin{array}{|c|c|c|c|c|c|}\hline 1&0&1&1&0&1\\\hline\end{array}$
    - $h_{\mathrm{A}}^1 = \mathrm{AGG}\left(\{h_{\mathrm{B}}^0, h_{\mathrm{C}}^0, h_{\mathrm{D}}^0\}, \{h_{\mathrm{A}}^0\}\right) = \begin{array}{|c|c|c|c|c|c|}\hline 1&1&1&1&0&0\\\hline\end{array}$
  - Finally the embedding of A is
    - $h_{\mathrm{A}}^2 = \mathrm{AGG}\left(\{h_{\mathrm{B}}^1, h_{\mathrm{C}}^1, h_{\mathrm{D}}^1\}, \{h_{\mathrm{A}}^1\}\right) = \begin{array}{|c|c|c|c|c|c|}\hline 4&2&3&3&2&2\\\hline\end{array}$
  - Similarly,

$$\left.\begin{aligned} h_{\mathrm{B}}^2 &= \begin{array}{|c|c|c|c|c|c|}\hline 2&4&2&2&2&2\\\hline\end{array} \\ h_{\mathrm{C}}^2 &= \begin{array}{|c|c|c|c|c|c|}\hline 3&2&4&3&2&1\\\hline\end{array} \\ h_{\mathrm{D}}^2 &= \begin{array}{|c|c|c|c|c|c|}\hline 3&2&3&4&1&2\\\hline\end{array} \\ h_{E}^2 &= \begin{array}{|c|c|c|c|c|c|}\hline 2&2&2&1&3&1\\\hline\end{array} \\ h_{F}^2 &= \begin{array}{|c|c|c|c|c|c|}\hline 2&2&1&2&1&3\\\hline\end{array} \end{aligned}\right\} \text{Distinct embeddings}$$



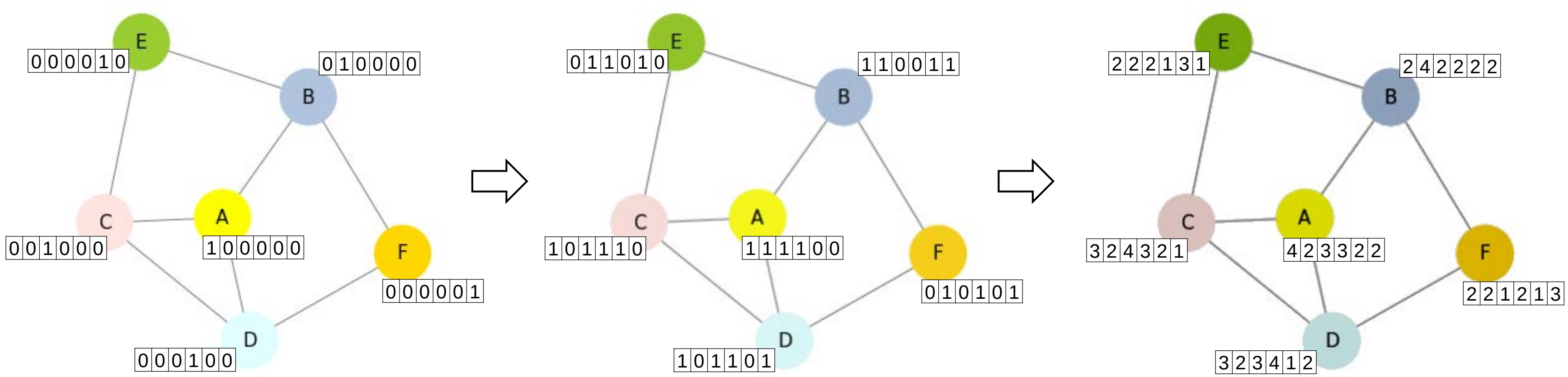


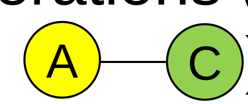


Distinguishability under **sum**

- Let AGG=**sum**, then for the GCN of 2 layers, the embeddings are as follows

Summarized

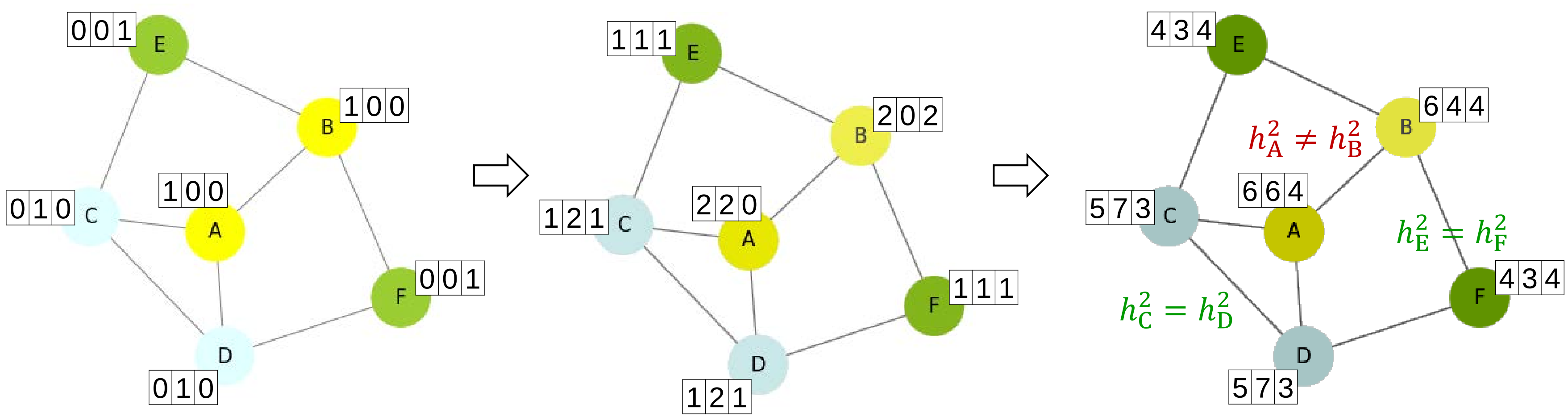


- By induction on the respective distinct feature dimension, the embeddings will be distinct for subsequent iterations
- **If every node has distinct feature, then they have distinct embeddings under sum** regardless of neighborhood structure or iterations (with the exception of the graph of only two nodes 

)

Distinguishability under **sum**

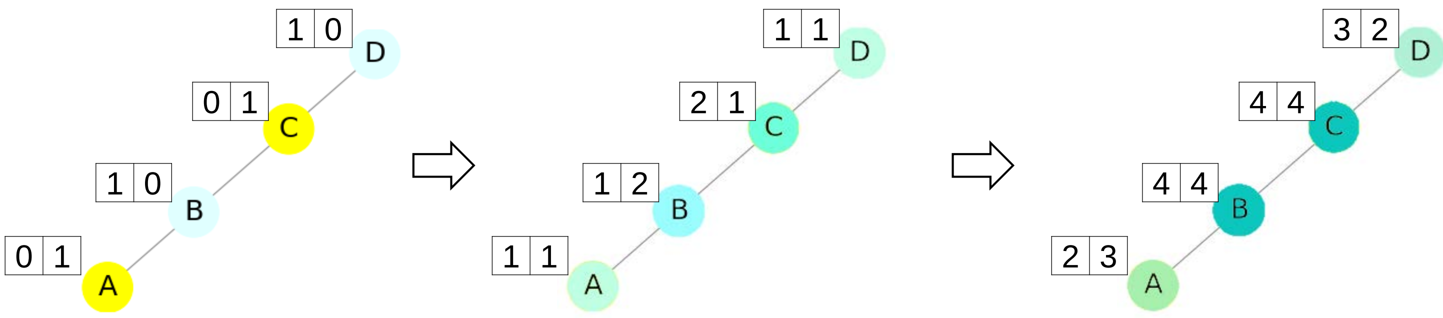
- **If some nodes have the same features?**
  - Let $h_A^0 = h_B^0 = \boxed{1|0|0}$, $h_C^0 = h_D^0 = \boxed{0|1|0}$, $h_E^0 = h_F^0 = \boxed{0|0|1}$, and let AGG be **sum**. Then, as can be seen from the following example



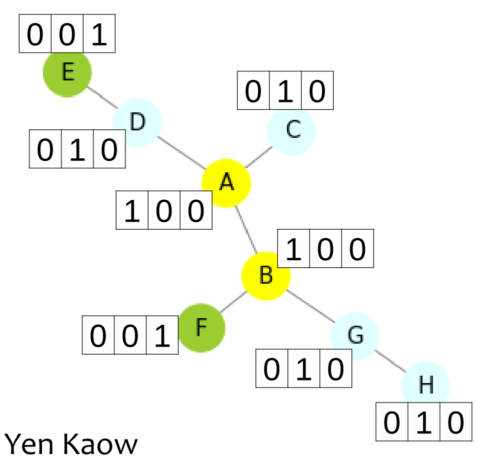
- Two nodes with the **same feature** will have the same embedding under **sum** if they have the same **neighborhood structure**
  - However different features and neighborhood structure cannot guarantee distinct embeddings

Distinguishability under **sum**

- **If some nodes have the same features?**
  - Different features and neighborhood structure cannot guarantee distinct embeddings for various reasons
    - Complementary neighborhood structure



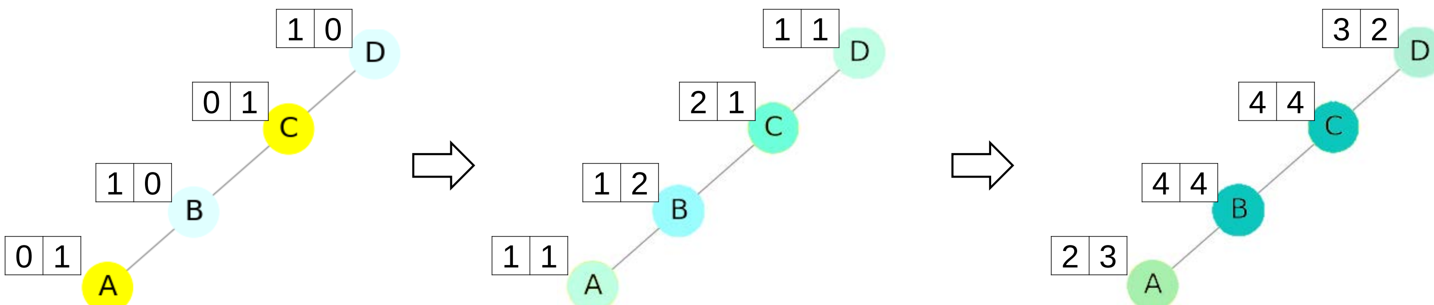
    - Hard-to-predict cases



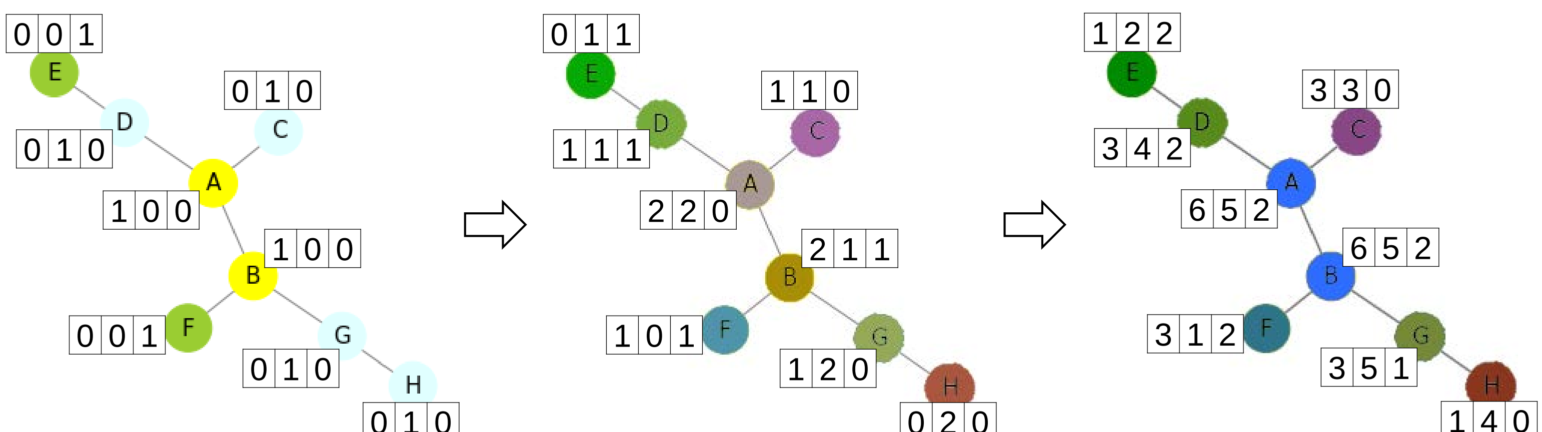
Will A and B ever become the same again after the first step?

Distinguishability under **sum**

- **If some nodes have the same features?**
  - Different features and neighborhood structure cannot guarantee distinct embeddings for various reasons
    - Complementary neighborhood structure

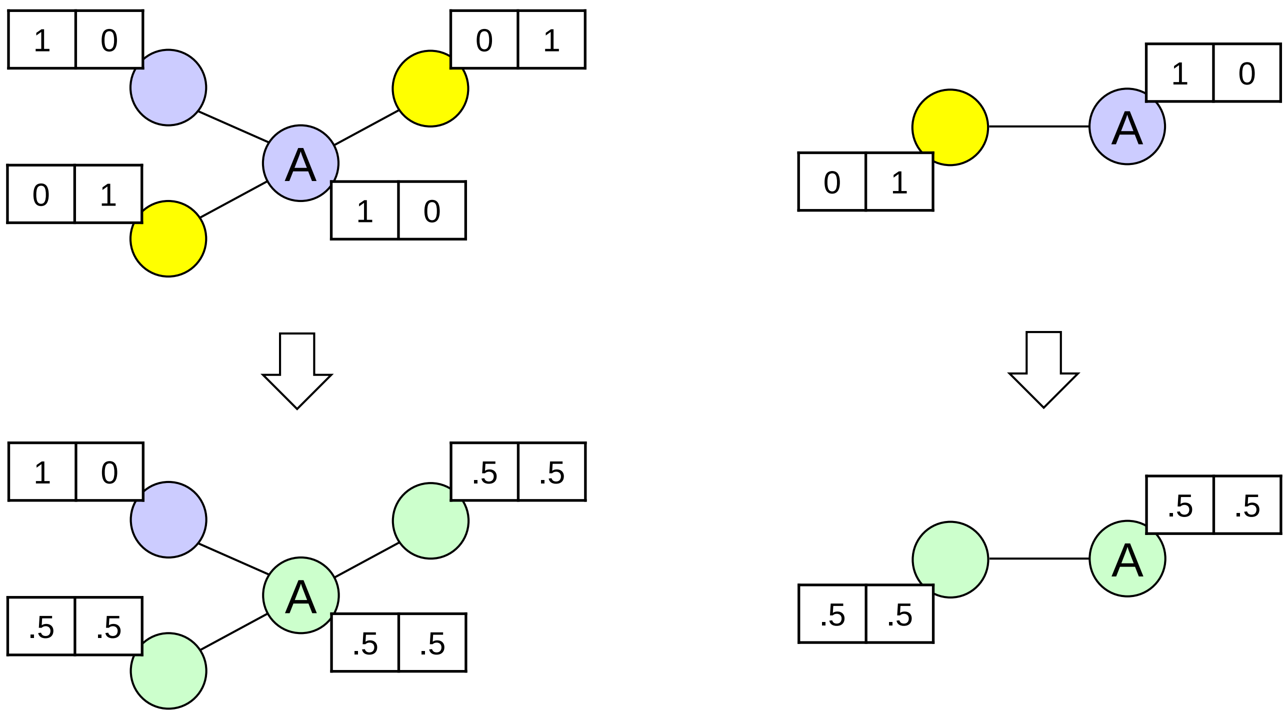


    - Hard-to-predict cases



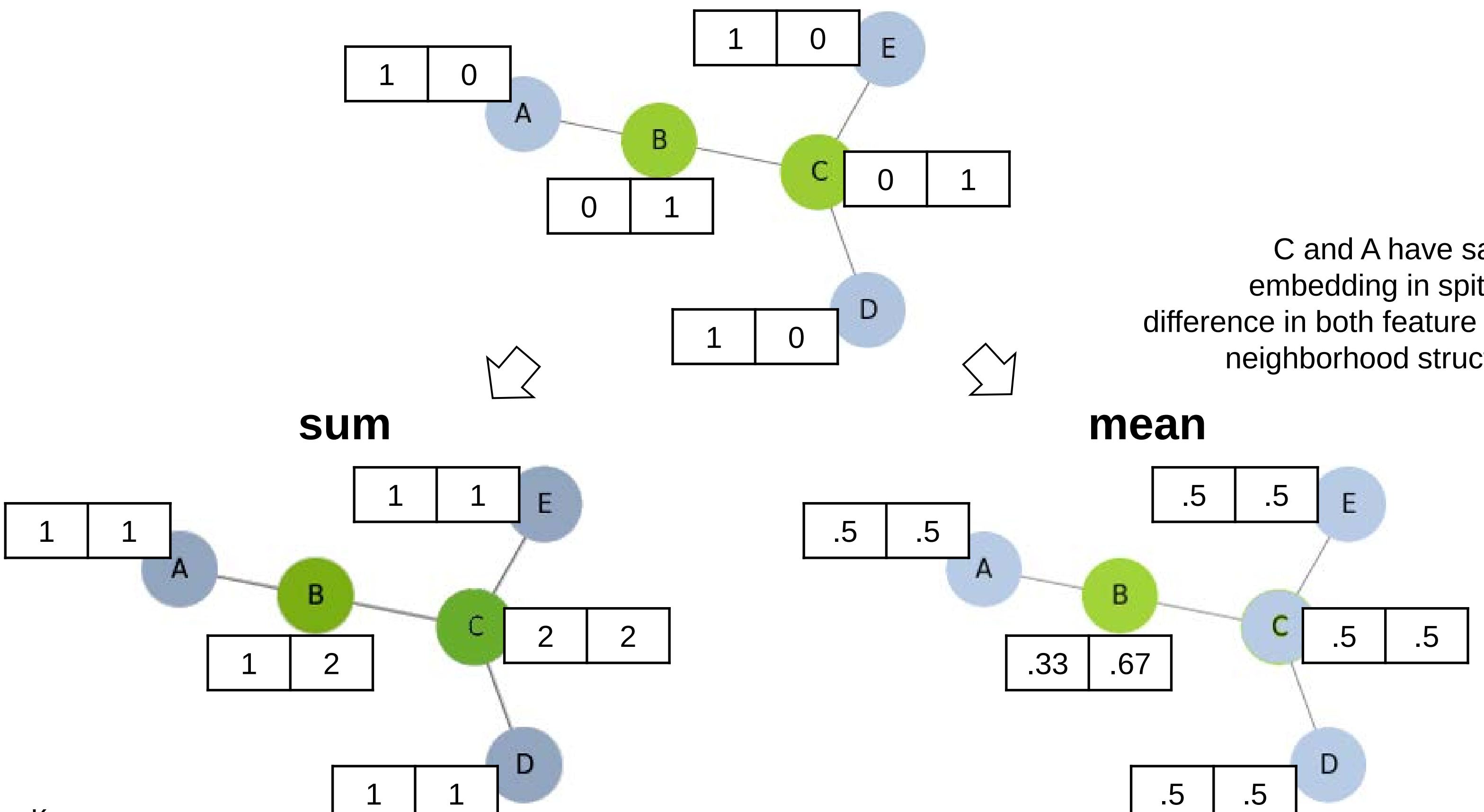
Distinguishability under **mean**

- Using **mean** as AGG results in even less desirable behavior
  - For instance, node A in both graphs below would give the same embedding under **mean** with one iteration



Distinguishability under **mean**

- Using **mean** as AGG results in even less desirable behavior
  - The following example shows **sum** to result in more consistent embeddings than **mean**



C and A have same embedding in spite of difference in both feature and neighborhood structure

Injective function for isomorphism

- An **injective** function will output distinguishable embeddings for nodes of distinct feature and neighborhood structure
  - **sum**, **mean**, and **max** are not injective
- **Theorem** (Xu *et al.* 2019). Any **injective** AGG function can be expressed as $\Phi(\sum_{x \in S} f(x))$ for some non-linear Φ and linear f
- Since MLP is able to approximate any function, we can learn Φ and f with non-linear MLP_Φ and linear MLP_f

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

$\Rightarrow$ **Graph Isomorphism Network (GIN)**

Subgraph Isomorphism

- Subgraph isomorphism is NP-complete
  $\Rightarrow$ Compare **neighborhood around each node**
- The k**-hop neighborhood around node** $u \in Q$ is
  1. All the nodes within k hops from u, and
  2. All the edges in between those nodes
  - Such a neighborhood is a subgraph of Q
    - However, not every subgraph of Q is a neighborhood of some node $u \in Q$
      - At most $k|V|$ neighborhoods for each k
- If P is a subgraph of Q, then every neighborhood of P is a subgraph of some neighborhood of Q

Order embedding space

- Idea: We want an d-dimensional embedding space z such that for every neighborhoods $p \in P$ and $q \in Q$

$$q \subseteq p \Leftrightarrow \forall_{i=1}^{d} z_q[i] \leq z_p[i]$$

- With embedding space, we can test subgraph isomorphism through the following

For each neighborhood $p \in P$ and $q \in Q$

If $(\exists i)\left[z_q[i] \leq z_p[i]\right]$, return false

Return true

Order embedding space

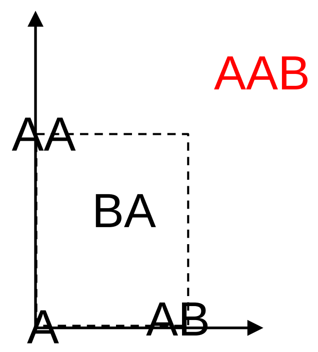
- Idea: We want an d-dimensional embedding space z such that for every neighborhoods $p \in P$ and $q \in Q$

$$q \subseteq p \Leftrightarrow \forall_{i=1}^{d} z_q[i] \leq z_p[i]$$

- Whether such an embedding space exist depends on D and the class of graphs
  - Even for substring relation ($\preccurlyeq$) with only alphabet {A, B}, a 2D embedding space is insufficient for

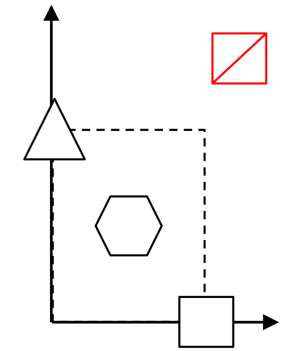
$$q \preccurlyeq p \Leftrightarrow \forall_{i=1}^{2} z_q[i] \leq z_p[i]$$

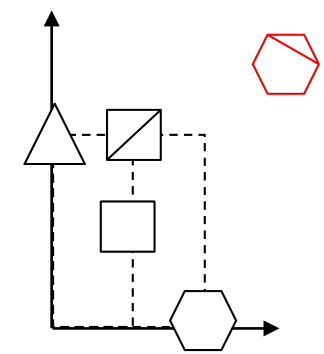
    - AAB needs to cover the dotted box (since it includes both AA and AB)
    - On the other hand, BA cannot be brought out of the dotted box (otherwise it would cover AA or AB)



Order embedding space

- 2D embedding space example for graph
  - needs to cover the dotted box (since it must cover both triangle and square) but that would cover
    - On the other hand, cannot be brought out of the dotted box (otherwise it would cover or)
  - Toggling hexagon and square will allow to be placed, but now cannot be placed
- Assume that d is sufficiently large for reasonable embeddings





Training order embedding space

- Use a **node embedding space of** k-hop
- Denote the embedding of a node u as z_u
- Use the loss function
  $$\text{loss}(u, v) = \sum_{i=1}^{d} \max(0, z_u[i] - z_v[i])^2$$
  It is clear that
  - $\text{loss}(u, v) = 0$ when $\forall_{i=1}^{d}(z_u[i] \leq z_v[i])$
  - $\text{loss}(u, v) > 0$ otherwise
- Generate random pair of graphs P, Q and train GNN such that embeddings of $u_P \in P$ and $u_Q \in Q$ has
  - $\text{loss}(u_Q, u_P) = 0$ when $u_Q \subseteq u_P$, and
  - $\text{loss}(u_Q, u_P) > 0$ otherwise