Yale

Beyond WL: More Expressive GNNs

CPSC483: Deep Learning on Graph-Structured Data

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Readings

- Readings are updated on the website (syllabus page)
- **Lecture 9 readings:**
  - Graph Isomorphism Network
  - Weisfeiler and Leman Go Neural: Higher-order Graph Neural Networks
- **Lecture 11 readings:**
  - Position-aware Graph Neural Networks
  - Identity-aware Graph Neural Networks

Content

- Limitation of Message Passing GNN

- Expressive GNNs beyond WL test
  - Position-aware GNN
  - Identity-aware GNN

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- Limitation of Message Passing GNN

- Expressive GNNs beyond WL test
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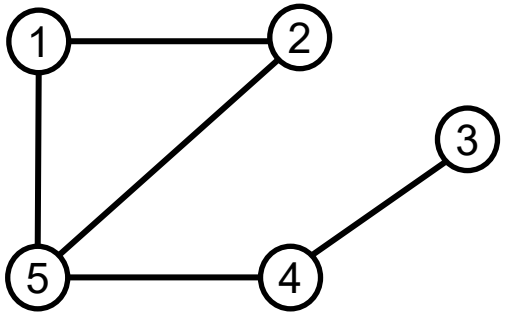
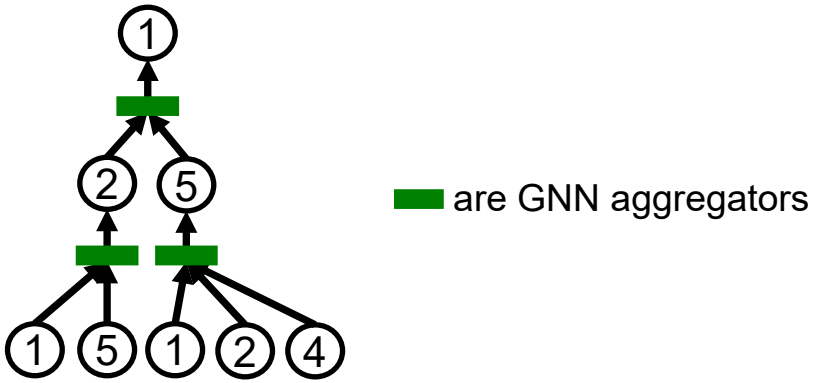
Recap: Computation Graph

- Consider how Message-passing GNN models work.
  - **Key concept: Computation Graphs**
- The local neighborhoods define the computation graphs
  - Example: computation graph of Node 1 with 2-layer GNN

Graph:



Computation Graph:

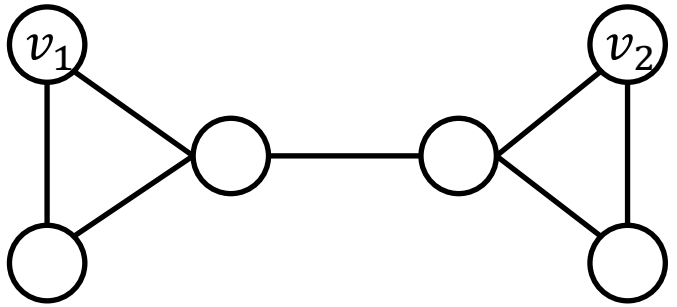


- A "perfect" GNN builds an **injective** function between neighborhood structure and node embedding, generating the same embedding for nodes with the same computation graph

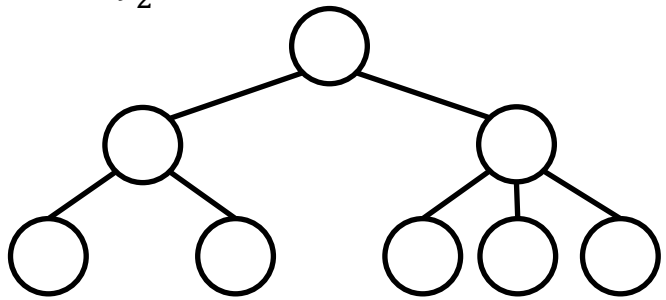
Limitations of GNNs (1)

- **Observation 1:** Message passing GNNs sometimes cannot capture positional information of nodes
  - Even though two nodes may have the same neighborhood structure, we may want to assign different embeddings to them
  - Because these nodes appear in different positions in graph

v_1 and v_2 have the same neighborhood structure but appear in different position



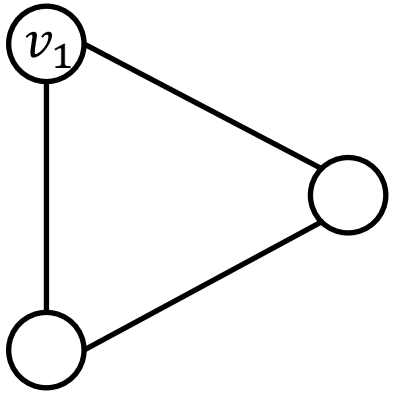
Computation graphs for nodes v_1 and v_2 are the same



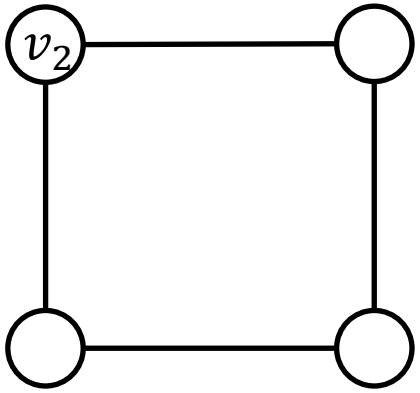
Limitations of GNNs (2)

- **Observation 2:** Different neighborhood structures sometimes create the same computation graph, thus leading to the same node embeddings.
- The GNNs we have introduced so far are **not perfect**
  - The expressive power of message-passing GNNs is upper bounded by WL test
    - Example: message passing GNNs cannot count cycle length

v_1 resides in a cycle with length 3

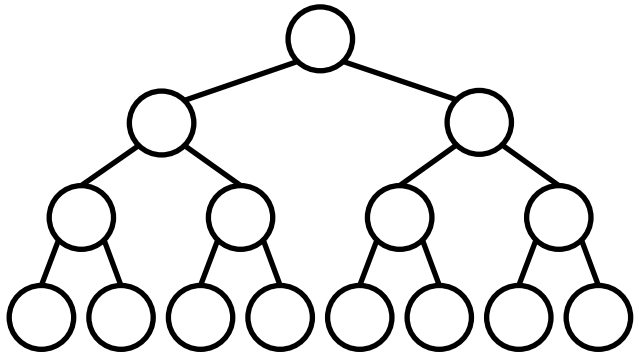


v_2 resides in a cycle with length 4



Computation graph

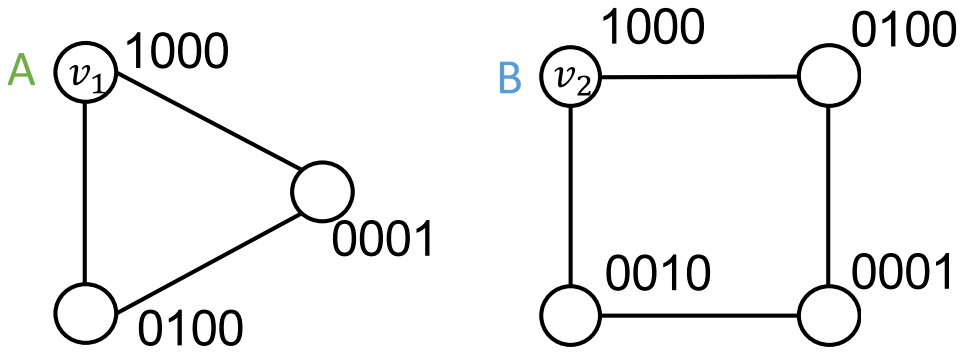
Computation graphs for nodes v_1 and v_2 are always the same



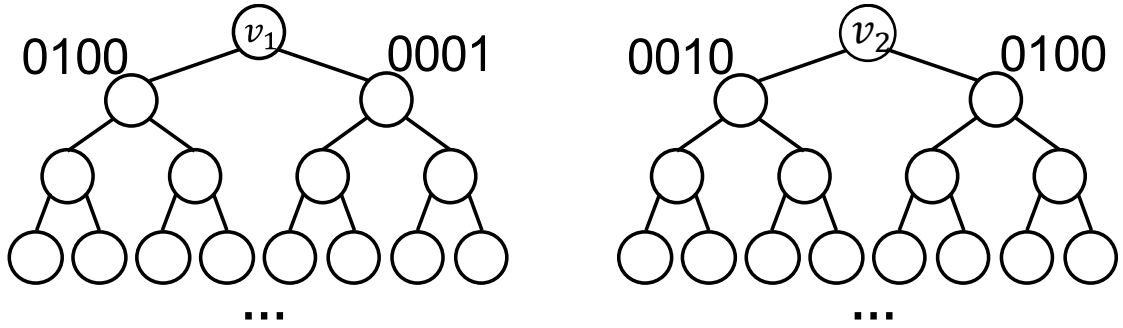
Naïve Solution is not Practical

- A naïve solution to assign different embeddings to nodes: **one-hot encoding**
  - Each node in the graph has a **different ID** (using one-hot encoding). Then we can always differentiate different nodes/edges/graphs.

Input graphs



Computation graphs of Node v_1 and v_2

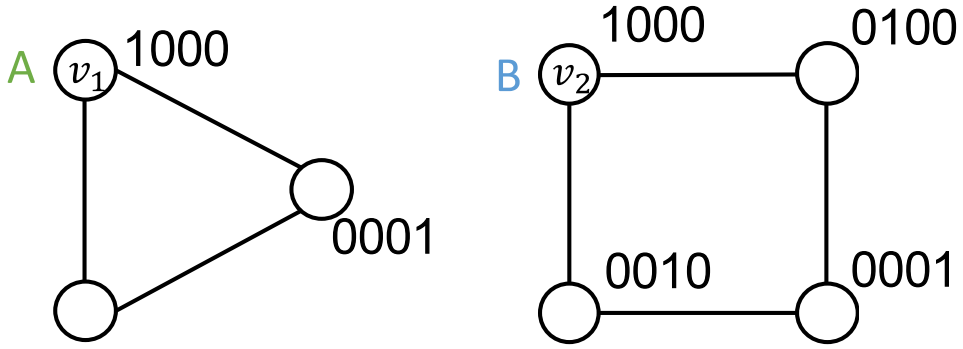


Computation graphs are clearly different if each node has a different ID

Naïve Solution is not Practical

- A naïve solution to assign different embeddings to nodes: **one-hot encoding**
  - Each node in the graph has a **different ID** (using one-hot encoding). Then we can always differentiate different nodes/edges/graphs.

Input graphs



  - **Limitations:**
    - **Not scalable**: Need $O(N)$ feature dimensions (N is the number of nodes)
    - **Not inductive:** Cannot generalize to new nodes/graphs
- **Goal:** Need to look for a **scalable, inductive** approach!

Outline of Today's Lecture

- We will resolve **two limitations of GNNs** by building more expressive GNNs
- Fix issues in Observation 1:
  - Create node embeddings **based on their positions** in the graph
  - Example method: **Position-aware GNNs**
- Fix issues in Observation 2:
  - Build message passing GNNs that are **more expressive than WL test**
  - Example method: **Identity-aware GNNs**

Content

- Limitation of Message Passing GNN

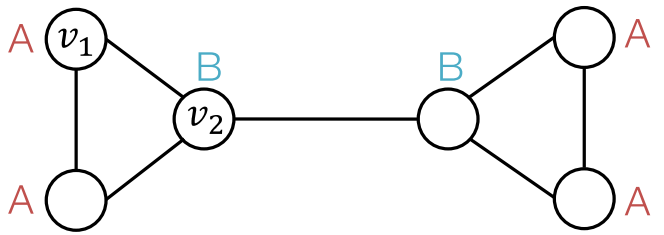
- Expressive GNNs beyond WL test
  - Position-aware GNN
  - Identity-aware GNN

Two Types of Tasks on Graphs

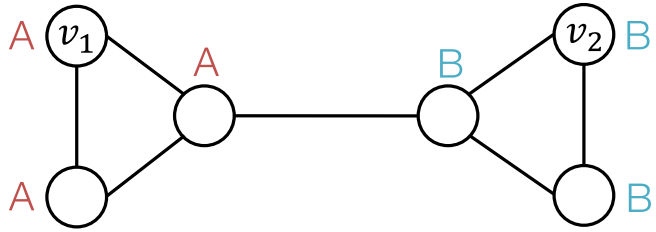
- **Structure-aware Task:** Nodes are labeled by their structural roles in the graph
  - v_1 and v_2 have **different labels** because their **different neighborhood structures**

- **Position-aware Task:** Nodes are labeled by their positions in the graph
  - v_1 and v_2 have the same neighborhood structures but the different labels, because they **appear in different positions in graph**

Structure-aware task



Position-aware task

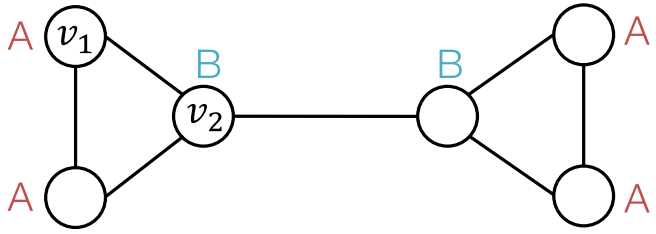


A and B denote different labels

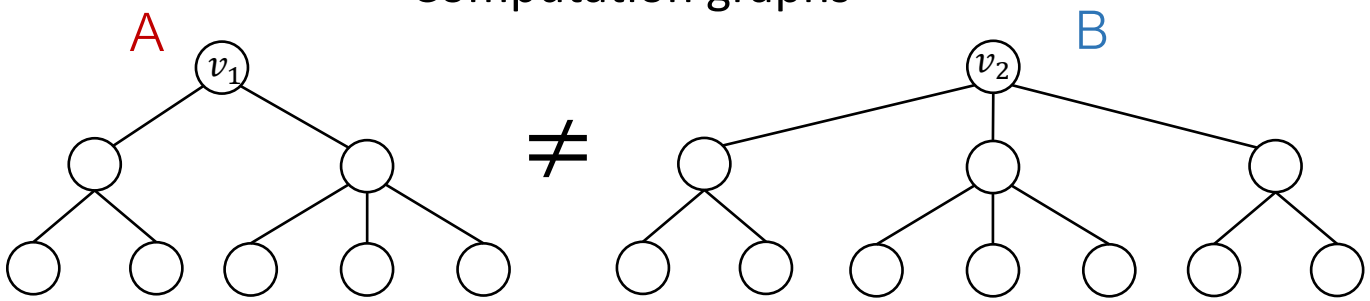
Structure-aware Tasks

- GNNs often work well for **structure-aware tasks**

Structure-aware task



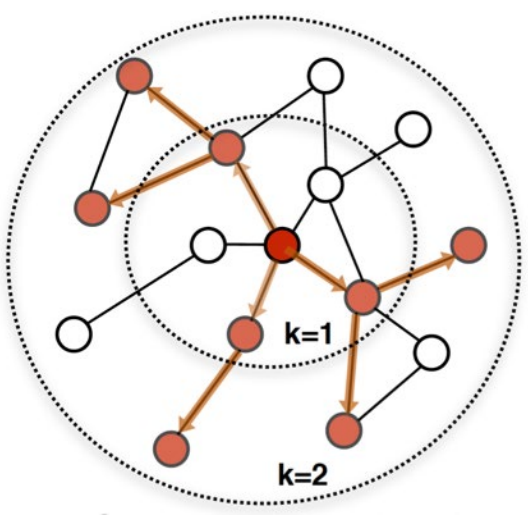
Computation graphs

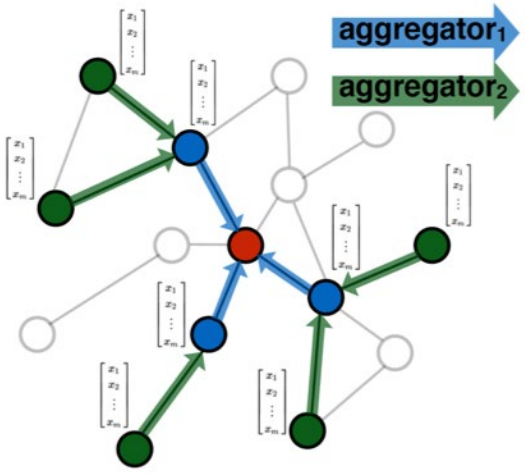


- Message passing GNNs can differentiate v_1 and v_2 by using different computation graphs

Structure-aware Embedding

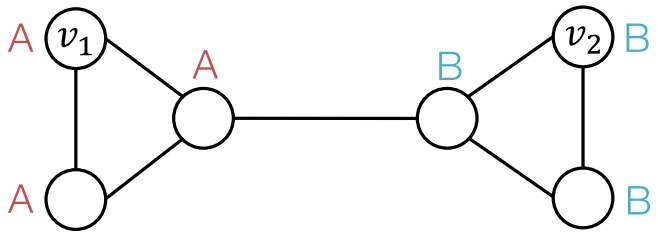
- **Structure-aware Embedding:**
  - Embedding $z_i = f_{s_q}(v_i)$ is **structure-aware** if it is **a function of up to q-hop neighbourhood** of node v_i.
  - GNNs that compute embedding by **aggregating q-hop neighborhood** information are **structure-aware**.



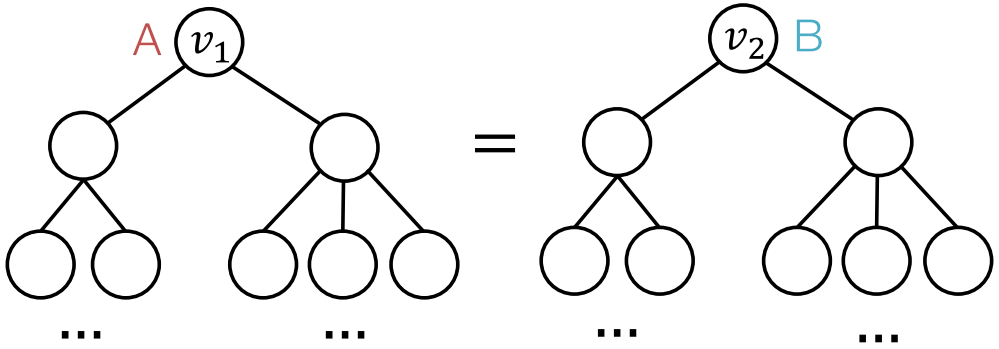


Position-aware Tasks

Position-aware task



Computation graphs

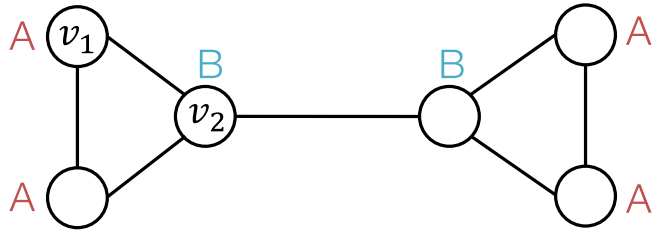


- Message-passing GNNs fail to distinguish v_1 and v_2 due to **the same computation graph.**
- **Observation**: v_1 and v_2 have a **symmetric** neighborhood structure in the graph
- **Key idea of Position-aware GNN**: break the symmetry by using **anchor-set to create difference**
  - Anchor set: a set of nodes that serve as reference points or "coordinates"

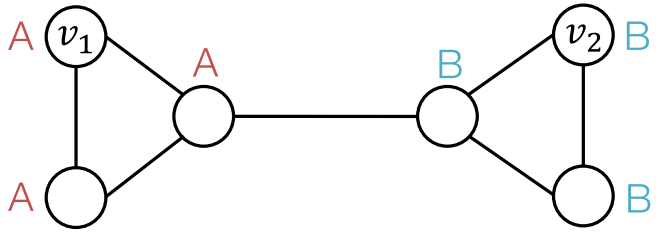
Position-aware Embedding

- **Position-aware Embedding:**
  - Embedding $z_i = f_p(v_i)$ is **position-aware** if there exists a function $g_p(\cdot,\cdot)$ such that $d_{sp}(v_i, v_j) = g_p(z_i, z_j)$.
  - $d_{sp}(\cdot,\cdot)$ is the **shortest path distance** in the graph
- Structure-aware embeddings **cannot** be mapped to position-aware embeddings.
- Structure-aware embeddings are not sufficient for tasks require node positional information
- P-GNN learns position-aware embedding!

Structure-aware task

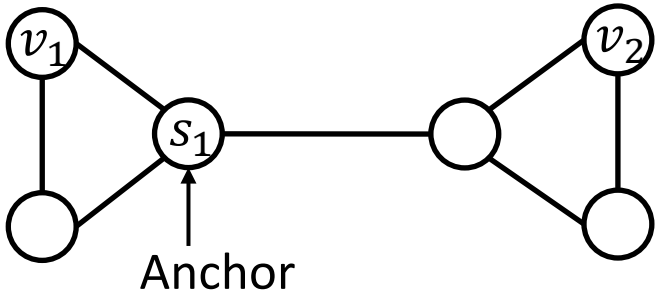


Position-aware task



Power of "Anchors"

- Randomly pick a node s_1 as an anchor node
- Represent v_1 and v_2 via their relative distance w.r.t. the the anchor s_1
  - Different relative distances create different representations
- Anchor node serves as a **coordinate axis** to locate the target node
  - Example: v_1 and v_2 have the symmetric position in graph but have different relative distance to the anchor s_1

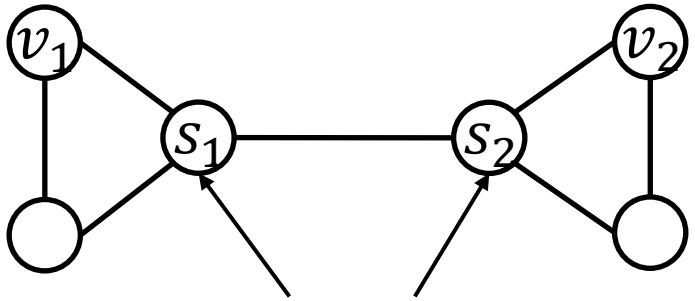


Relative Distances

	s_1
v_1	1
v_2	2

Power of "Anchors"

- Pick more nodes s_1 and s_2 as anchor nodes
- **Observation:** More anchor nodes locate the target node better
- Understand more anchors as more coordinate axes



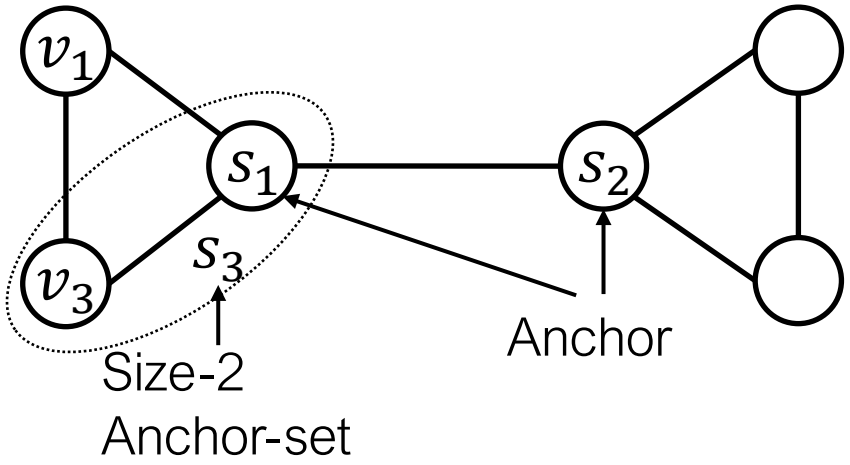
Relative Distances

	s_1	s_2
v_1	1	2
v_2	2	1

Intuitively, more anchor nodes characterize node position better.

Power of "Anchor-sets" (1)

- Generalize anchor from a single node to **a set of nodes** (we call Anchor-sets)
  - The distance to an anchor-set is defined as the minimum distance to all the nodes in this anchor-set.
- **Observation:** Large anchor-sets can sometimes provide more precise position estimate



Relative distances to anchor s_1 and s_2 are not sufficient to distinguish node v_1, v_3.

Relative Distances

	s_1	s_2	s_3
v_1	1	2	1
v_3	1	2	0

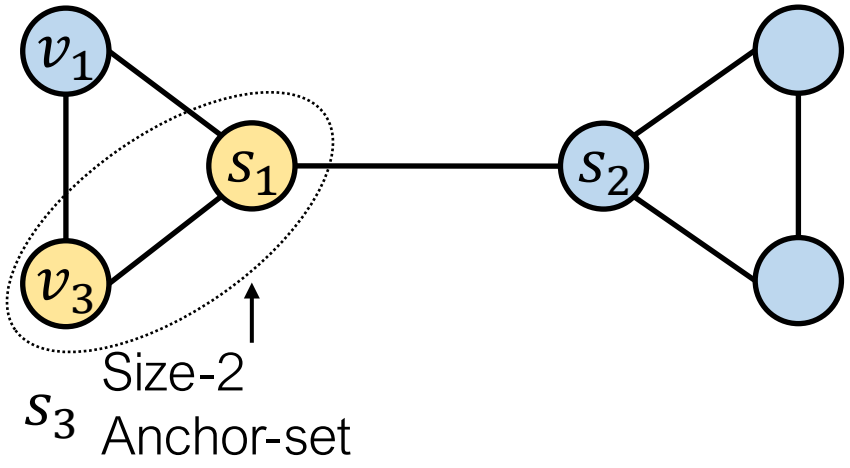
v_1's Position encoding [1,2,1]

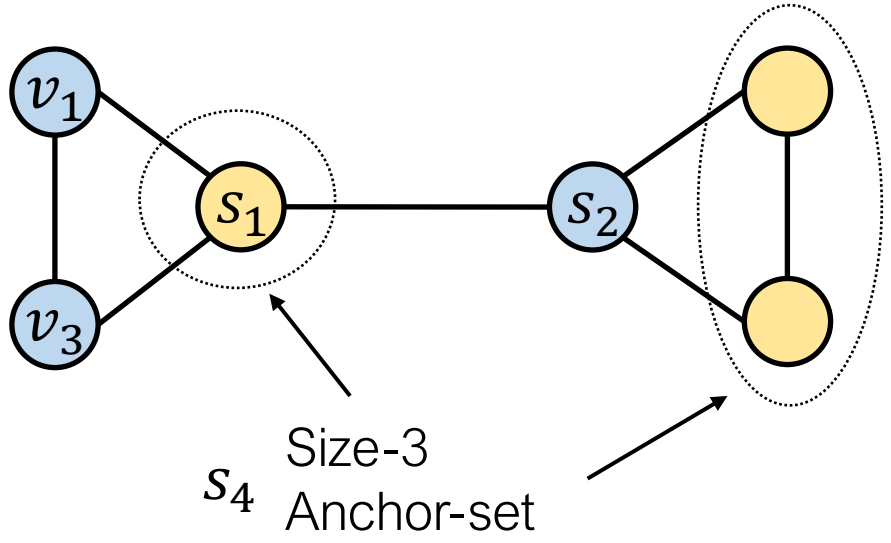
v_3's Position encoding [1,2,0]

anchor-set s_3 can distinguish node v_1, v_3.

Power of "Anchor-sets" (2)

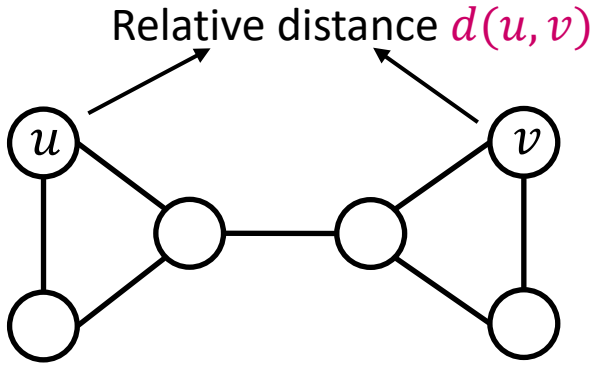
- Making every node as an anchor is very expensive
  - Embedding dimension is linear to the number of nodes
- Anchor sets allow us to divide the set of nodes into different categories
  - Smaller number of such sets can distinguish all nodes

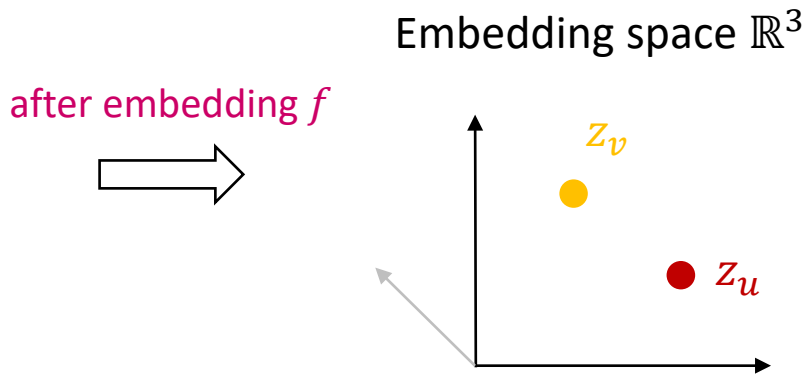




Anchor Set: Theory

- **Goal:** Embed **the metric space** $(\boldsymbol{V}, \boldsymbol{d})$ into the Euclidian space $\mathbb{R}^k$ and try to preserve the original distance metric.
- Node embedding should have **low distortion**.
  - **Distortion** measures the faithfulness of the embeddings in preserving distances when mapping from the original metric space to another metric space ($\mathbb{R}^k$)





u's position encoding z_u

v's position encoding z_v

Euclidean embedding distance $\boldsymbol{d'\big(f(u), f(v)\big) = \|z_u - z_v\|_2}$

$d(u,v)$ is close to $d'\big(f(u), f(v)\big)$ => low distortion!

Anchor Set: Theory

- **Definition:**

  The embedding f has distortion α if : $\frac{1}{\alpha} d(u,v) \leq d'\big(f(u), f(v)\big) \leq d(u,v)$, for any u, v in the graph.

- **Bourgain Theorem:**
  - Given any finite metric space (V, d) with $|V| = n$, there exists an embedding of (V, d) into $\mathbb{R}^k$ under any l_p metric, where $k = \mathcal{O}(\log^2 n)$, and the distortion α of the embedding is $\mathcal{O}(\log n)$.
  - k is the dimension of embedding space and n is the number of nodes.
  - In practice k is a **hyperparameter** controlling the budget for embedding dimensions
- We use **constructive proof** to prove Bourgain Theorem

Bourgain Theorem

- Consider the following embedding function f of node $v \in V$

$$f(v) = \left(\frac{d(v, S_{1,1})}{k}, \frac{d(v, S_{1,2})}{k}, \dots, \frac{d(v, S_{\log n, c \log n})}{k}\right)$$

- Where
  - c is a constant,
  - $S_{i,j} \subset V$ is chosen by including each node in V independently with probability $\frac{1}{2^i}$,
  - $d(v, S_{i,j}) = \min_{u \in S_{i,j}} d(v, u)$.
- Then, f is an embedding method satisfies Bourgain Theorem.
- The embedding distance produced by f is provably close to the original distance metric (V, d).

Position Information

- P-GNN follows the Bourgain theorem
  - Sample anchor sets $S_{i,j}$ for each graph
  - Embed each node v via

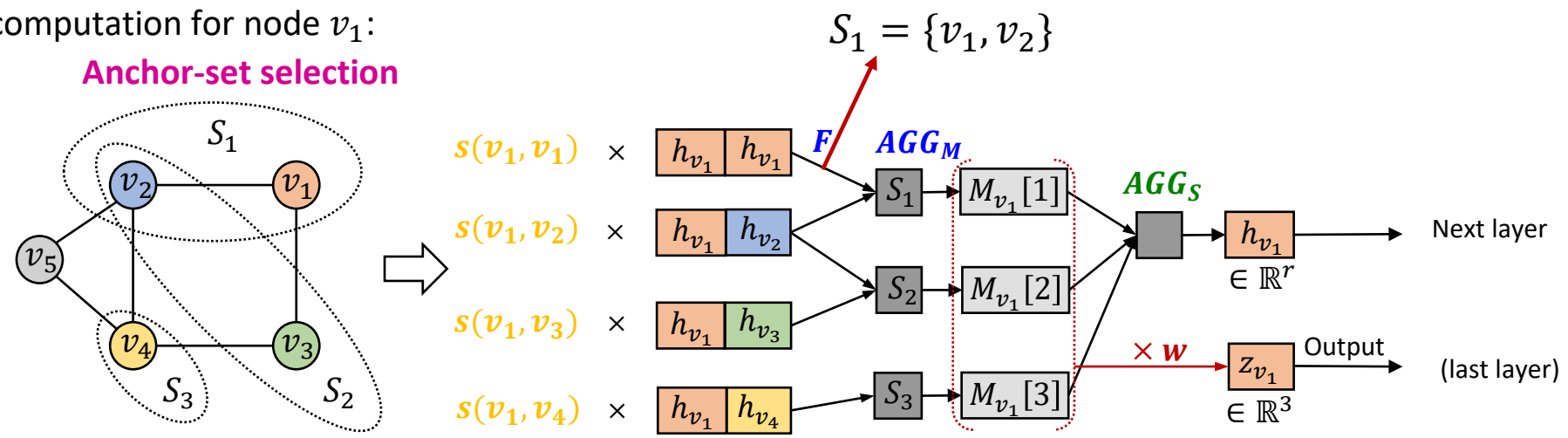
$$f(v) = \left(\frac{d(v,S_{1,1})}{k}, \frac{d(v,S_{1,2})}{k}, \dots, \frac{d(v,S_{\log n,\, c\log n})}{k}\right) \in \mathbb{R}^{c\log^2 n}$$

  - Each dimension of the position encoding is tied to an anchor-set
- P-GNN maintains the **inductive capability**
  - During training, new anchor sets are re-sampled every time.
  - At test time, given a new unseen graph, new anchor sets are sampled

Overview of Position-aware GNNs (P-GNNs)

- (a) Randomly select anchor-sets (Anchor-set selection)
- (b) Compute pairwise node distances $(s(v,u))$
- (c) Compute messages from anchor-sets (F, AGG_M)
- (d) Transform messages to embeddings (AGG_S, w)

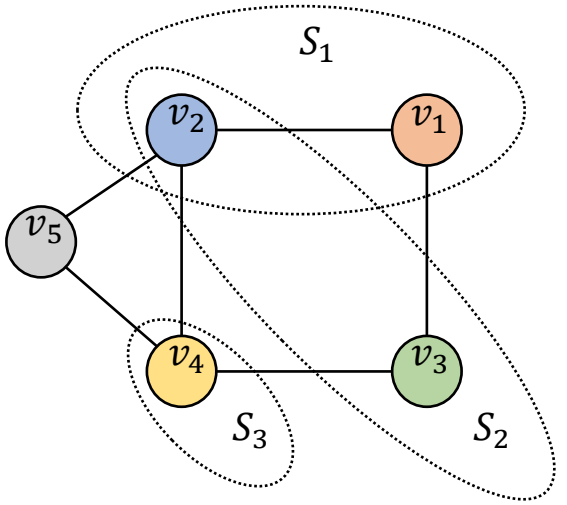
Steps of Embedding computation for node v_1:



Selection of Anchor-set

Step(a):

- Randomly choose anchor-sets with sizes from $1, 2, 4, \ldots, n/2$ ($\boldsymbol{\log n}$ number of sizes)
- For each size of anchor-set, repeat $\boldsymbol{c \log n}$ times
- In total, $\boldsymbol{k = c \log^2 n}$ anchors

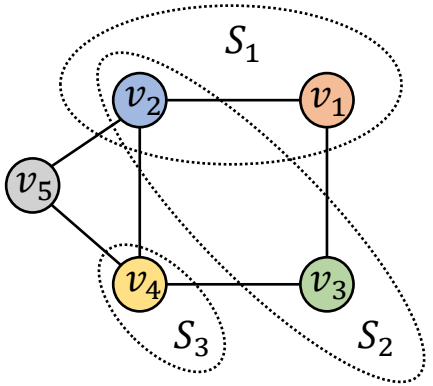


Pairwise Node Distance

Step(b):

- Compute pairwise node distances
- Position-based similarities: shortest path, personalized PageRank, etc.
- Use k-hop shortest path distance $d_{sp}^{k}(v_i, v_j)$ for fast computation

$$d_{sp}^{k}(v,u)=\begin{cases} d_{sp}(v,u), & \text{if } d_{sp}(v,u) \le k \\ \infty, & \text{otherwise} \end{cases}$$



$$s(v_i, v_j) = \frac{1}{d_{sp}^{k}(v_i, v_j) + 1}$$

pairwise node distances $s(v_i, v_j)$

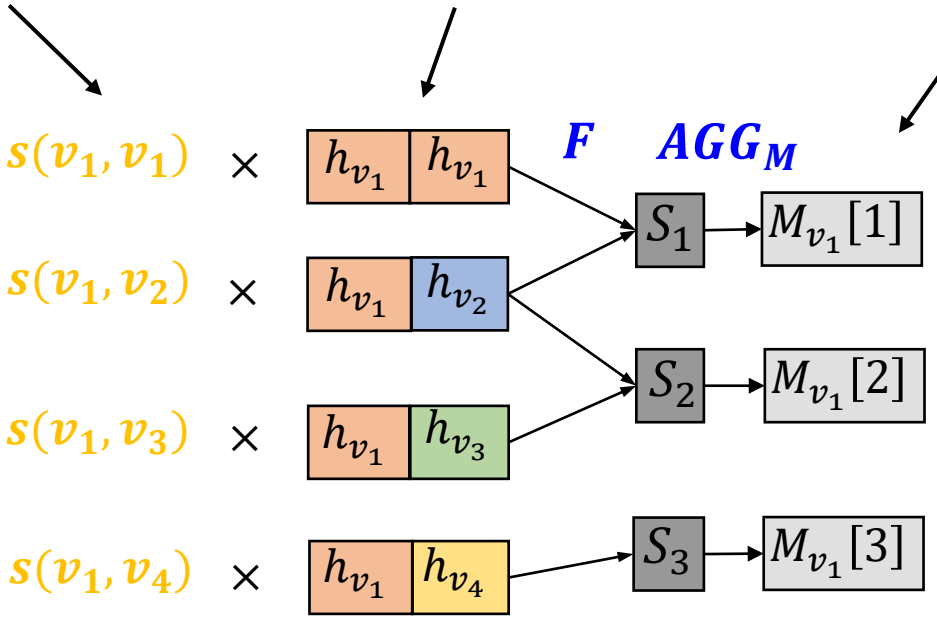
	v_1	v_2	v_3	v_4	v_5
v_1	1	0.5	0.5	0.3	0.3
v_2	0.5	1	0.3	0.5	0.5
v_3	0.5	0.3	1	0.5	0.3
v_4	0.3	0.5	0.5	1	0.5
v_5	0.3	0.5	0.3	0.5	1

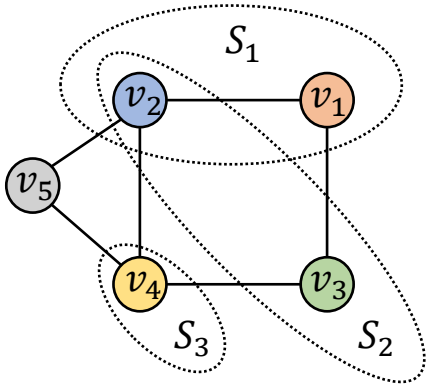
Messages from Anchor-set

Step(c):

- Compute messages from anchor-sets

Position info + Feature info → Messages from anchor-sets





(1) Combine position and feature

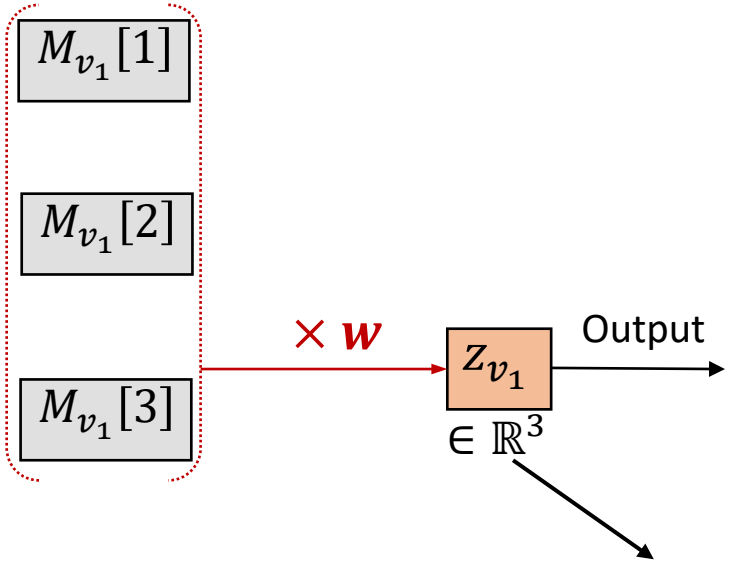
$$F(v, u, \mathbf{h}_v, \mathbf{h}_u) = s(v, u)\text{CONCAT}(\mathbf{h}_v, \mathbf{h}_u)$$

(2) GNN style aggregation
(over nodes in an anchor-set)

$$\text{AGG}_M(\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}) =$$
$$\mathbf{W}_2 \cdot \text{MEAN}(\{\sigma(\mathbf{W}_1 \cdot \mathbf{x}_i + \mathbf{b}_1\}) + \mathbf{b}_2$$

Transform to Embeddings

- **Step(d):**
- Transform messages to embeddings (2 parts)
  - Output component (position-aware embedding):

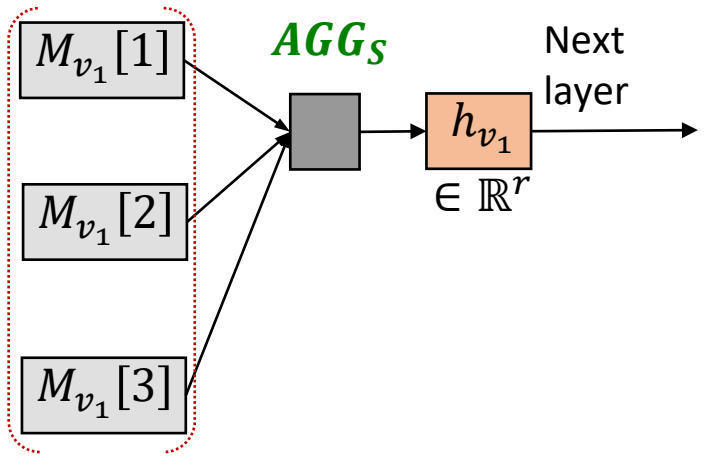


(1) Position-aware Embedding z_{v_1}:

- **Model's output for prediction**
- Transform message matrix to vector
- Each dimension is tied with an anchor-set, thus is position-aware

Transform to Embeddings

- **Step(d):**
- Transform messages to embeddings (2 parts)
  - Input to the next layer (structure-aware embedding):

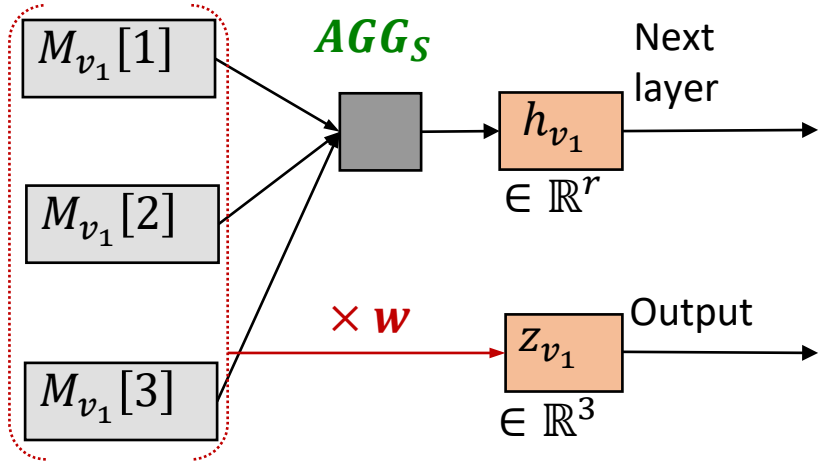


(2) Structure-aware Embedding h_{v_1}:

- **Fed into next layer of P-GNN**
- **Order-invariant message aggregation AGG_S** aggregates messages in GNN manner
- Each dimension is independent of anchor-set selection.

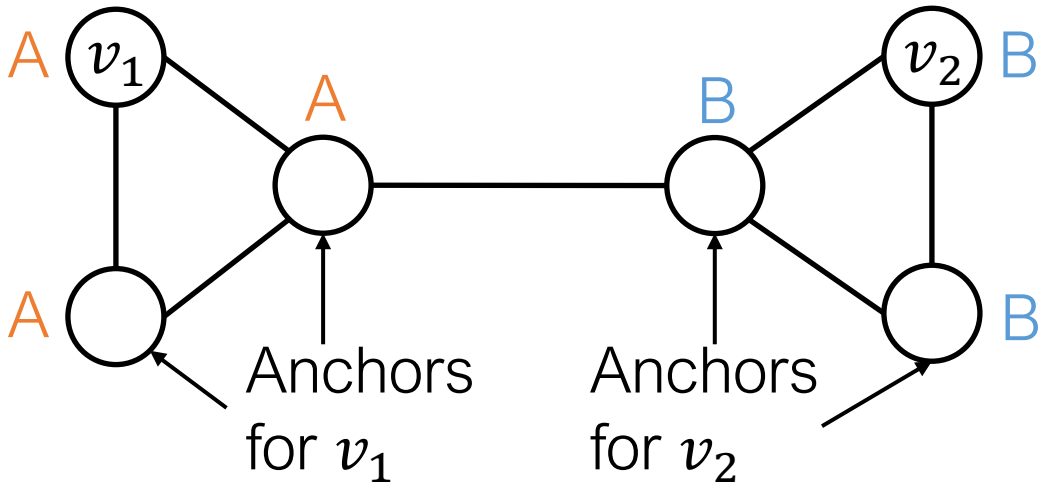
Transform to Embeddings

- The resulting model can potentially **capture both structure and position information**
- Model outputs **position-aware embedding z_{v_i}** for downstream tasks
- **Structure-aware embedding h_{v_i}** is fed to the next layer of model



Connection to GNNs

- Anchor: What you refer to when you compute (position-aware) embeddings
- Normal GNNs are special cases where each node **independently** selects **its own anchors** to aggregate information
  - Example: GNNs look at the k-hop neighbor nodes when compute an embedding
  - $s(v_i, v_j) = 1$ iff $d_{sp}^k(v_i, v_j) = k$ for k-hop GNNs.

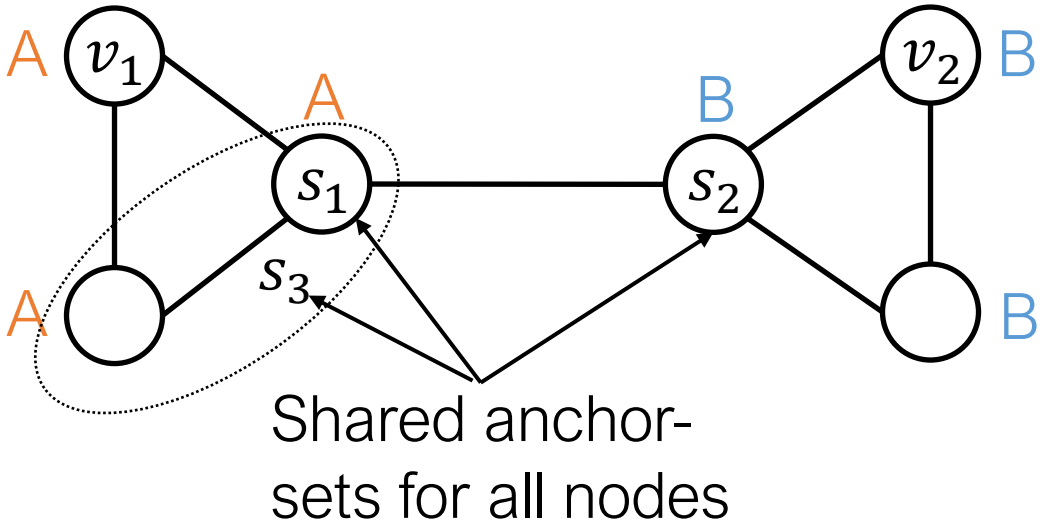


$$s(v_i, v_j) = \frac{1}{d_{sp}^k(v_i, v_j) + 1}$$

	v_1	v_2	v_3	v_4	v_5
v_1	1	0.5	0.5	0.3	0.3
v_2	0.5	1	0.3	0.5	0.5
v_3	0.5	0.3	1	0.5	0.3
v_4	0.3	0.5	0.5	1	0.5
v_5	0.3	0.5	0.3	0.5	1

Connection to GNNs

- While for P-GNNs, each node aggregates information from **shared** anchor-sets
- That's why anchor-sets can serve as **coordinate axes**
  - Example: P-GNNs look at shared anchor sets to aggregate neighborhood information



Ways to Use Position Information

- **The simple way:**
  - Use position encoding as an augmented node feature (works well in practice)
- **Issue:** since each dimension of position encoding is tied to a random anchor set, dimensions of positional encoding can be randomly permuted, without changing its meaning
- Imagine you permute the input dimensions of a normal NN, the output will surely change!

Ways to Use Position Information

- **The rigorous solution:**
  - requires a special NN that can maintain the permutation invariant property of position encoding
  - Permuting the input feature dimension will only result in the permutation of the output dimension, the value in each dimension won't change
  - Refer to the Position-aware GNN paper for more details

P-GNN vs. GNN

- Two families of models

	P-GNNs	**GNNs**
Message aggregation	Mean, Sum, Attention, …	
Neighborhood selection	**Shared** anchor selection	**Independent** anchor selection
Embedding computation	Each dimension is **tied to an anchor**	Each dimension is **aggregated across anchors**
Embedding property	**Position**-aware	**Structure**-aware

Position-aware GNNs: Summary

- **Position-aware GNNs:** A new class of GNNs that incorporate node positional information
- **Key idea:** select shared anchor-sets as coordinate axes for all the nodes
- Position-aware GNNs work well for position-aware tasks

Content

- Limitation of Message Passing GNN

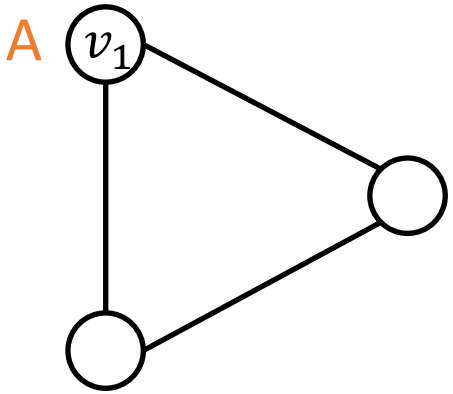
- Expressive GNNs beyond WL test
  - Position-aware GNN
  - Identity-aware GNN

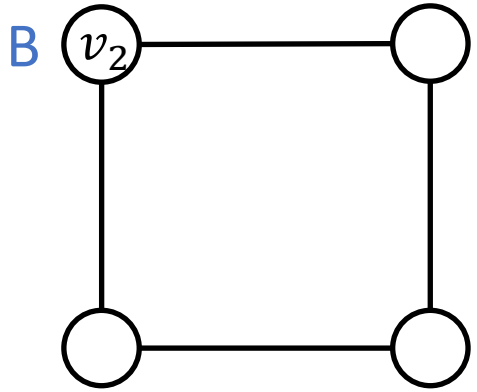
Limitation of GNNs

- We learned that GNNs would fail for position-aware tasks
- Question: Can GNN always perform perfectly in structure-aware tasks?
  - **No!** The expressive power of GNNs we have introduced so far is **upper bounded by WL test.** (lecture 9)
- GNNs exhibit (at least) three levels of failure cases in structure-aware tasks
  - Node level
  - Edge level
  - Graph level
- Main cause of failure cases: **the same computation graph**

GNN Failure 1: Node-level Tasks

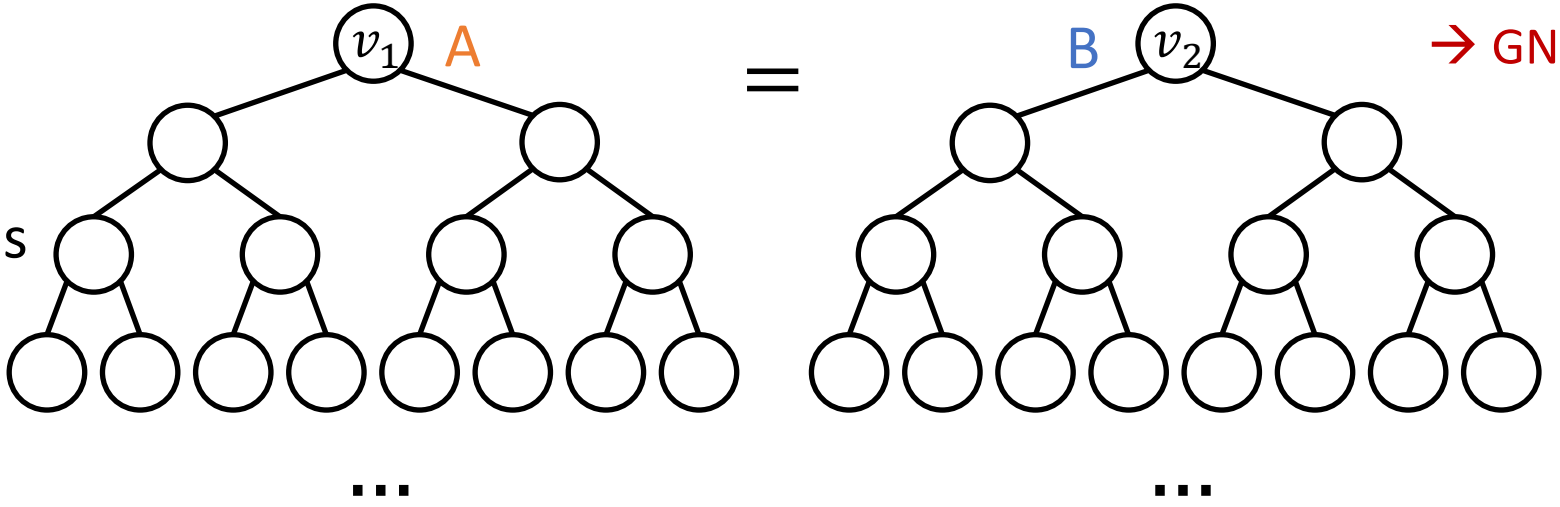
Example input graphs





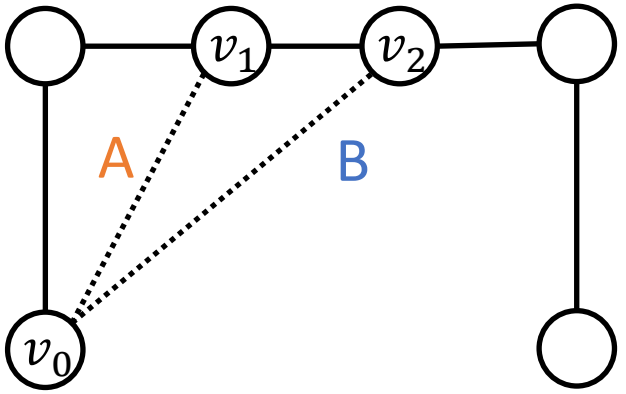
Different Inputs but the same computation graph → GNN fails

Existing GNNs' computation graphs

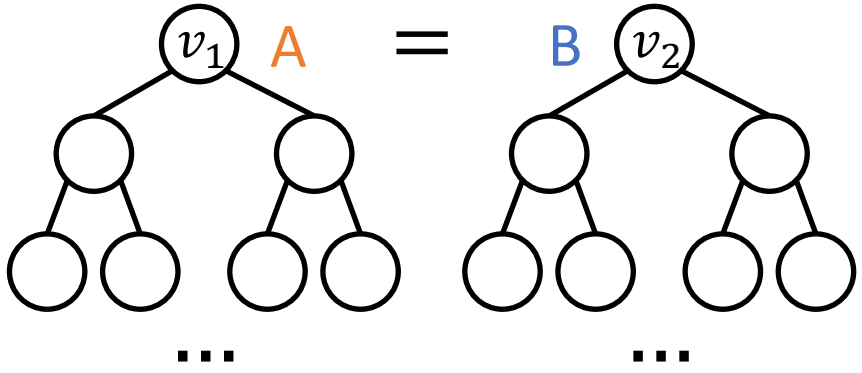


GNN Failure 2: Edge-level Tasks

Example input graph



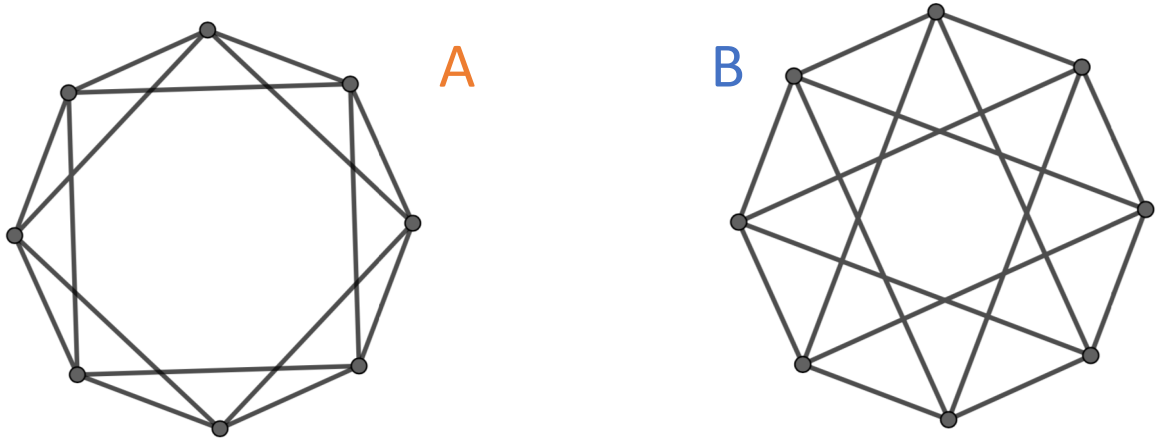
Existing GNNs' computation graphs



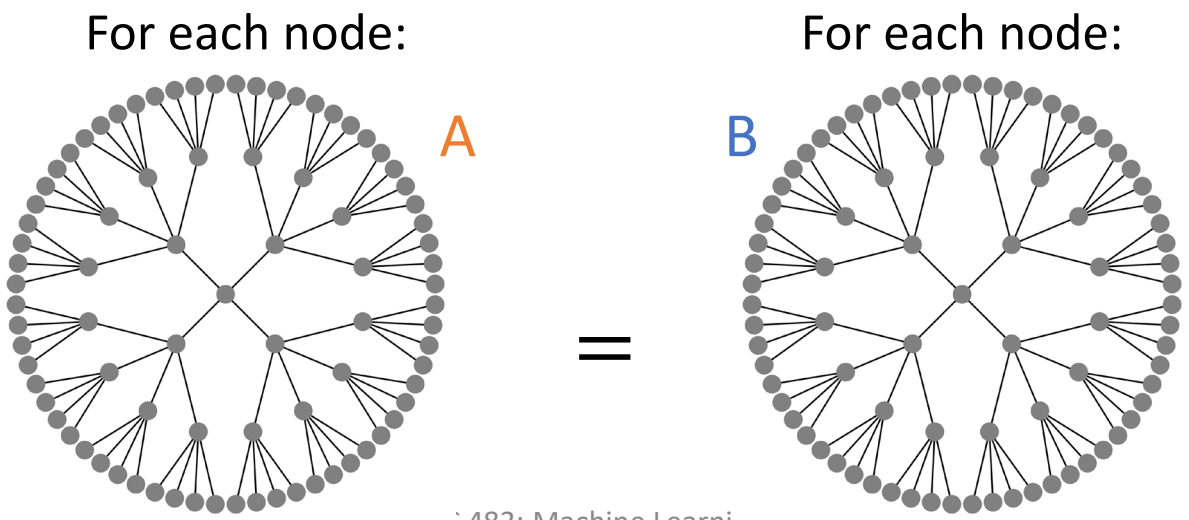
Different Inputs but the same computation graph → GNN fails

GNN Failure 3: Graph-level Tasks

Example input graph



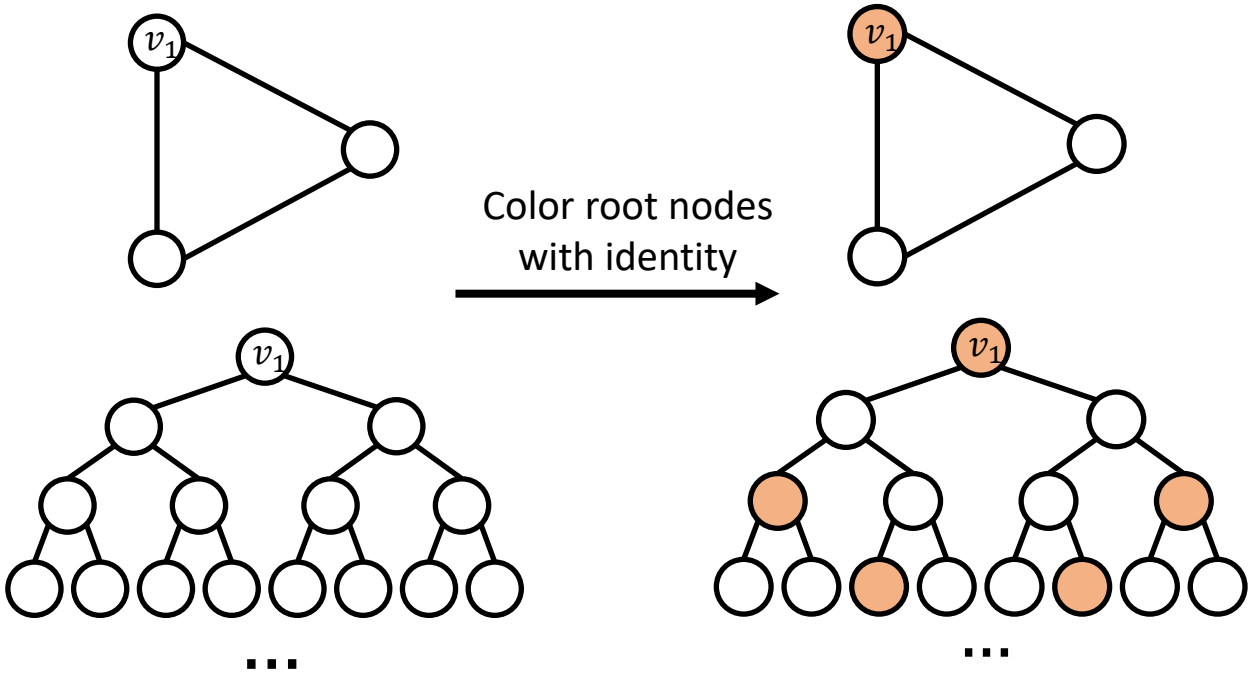
Existing GNNs' computation graphs

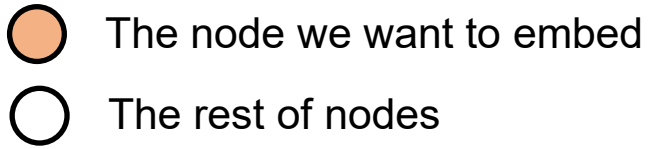


Different Inputs but the same computation graph → GNN fails

Idea of Identity-aware GNN

- Idea: assign a color to the node we want to embed

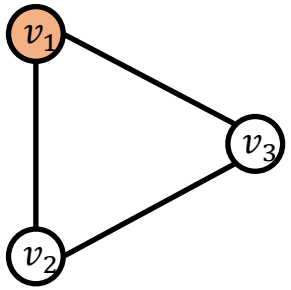




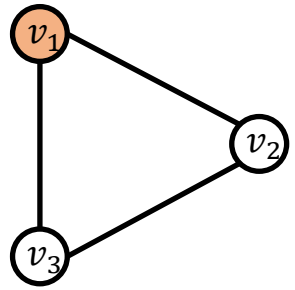
Inductive Node Coloring

- This coloring is **inductive**:
  - It is invariant to node ordering/identities
  - Easily generalize to unseen graphs

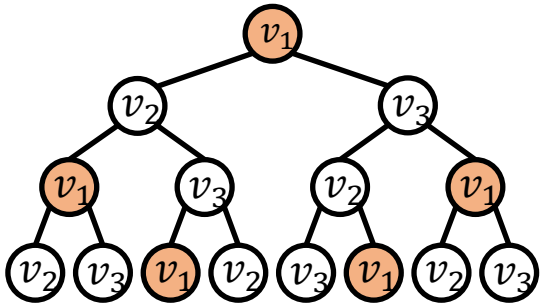
Example inputs graphs

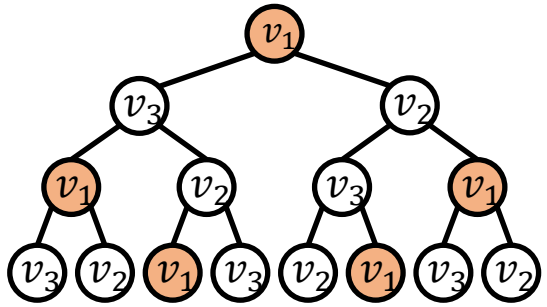


Permute the node ordering between v_2 and v_3



Computation graph of colored graph



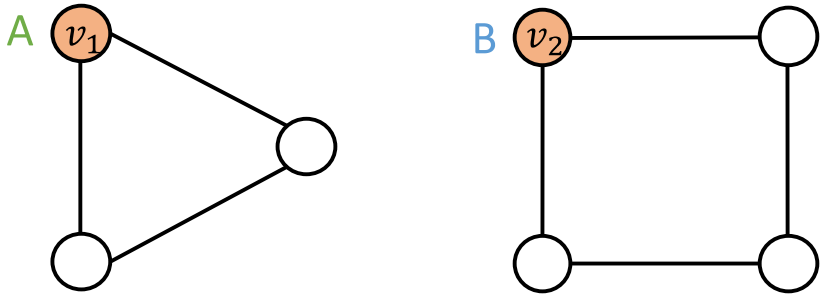


The computation graph stays the same

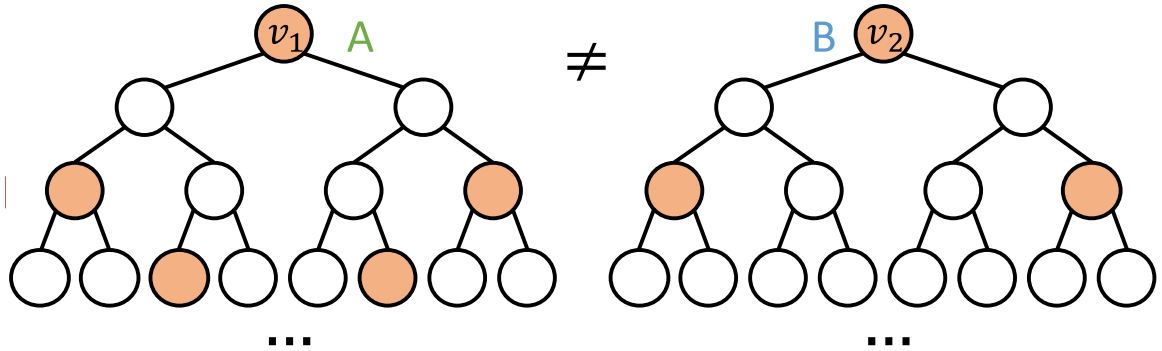
Inductive Node Coloring – Node level

- Inductive node coloring can help **node classification**
  - We color root nodes with identity

Example inputs graphs



Computation graph of colored graph

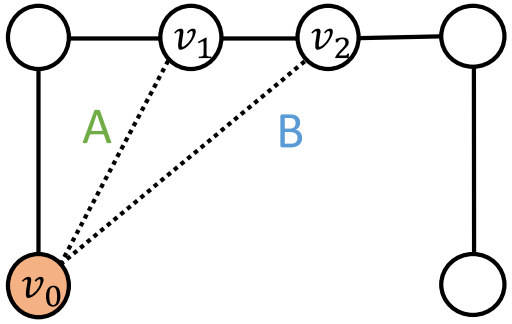


Different computation graphs
Successfully differentiate nodes

Inductive Node Coloring – Edge level

- Inductive node coloring can help **link prediction**

Example inputs graphs



Edge A and B share node v_0.
We look at embeddings for v_1 and v_2.

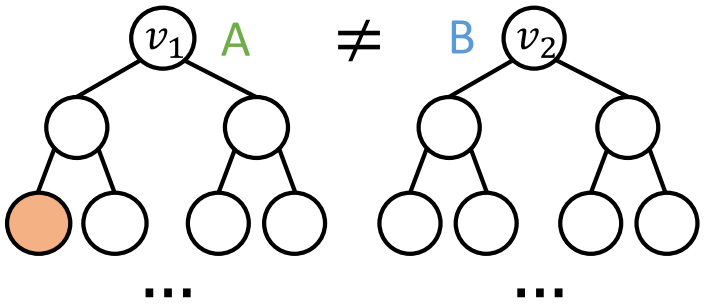
Without node coloring:

- the computation graphs of v_1 and v_2 are the same.

With node coloring (v_0):

- We embed the other node in the node pair (v_1 or v_2)
- We use the node embedding for v_1 or v_2 conditioned on v_0 being colored or not to make edge-level prediction

Computation graph of colored graph

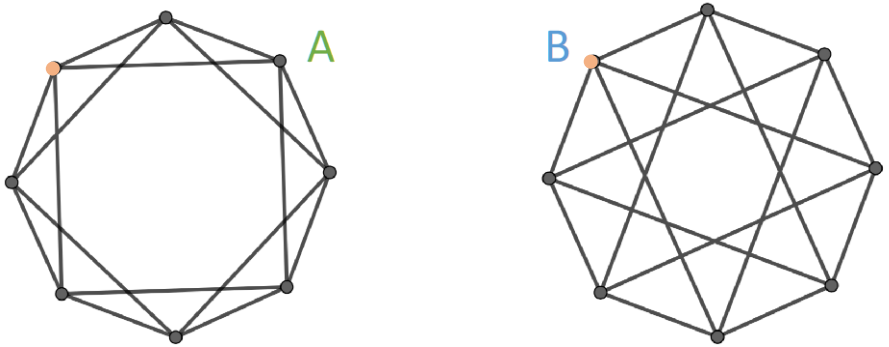


Different computation graphs successfully differentiate edges

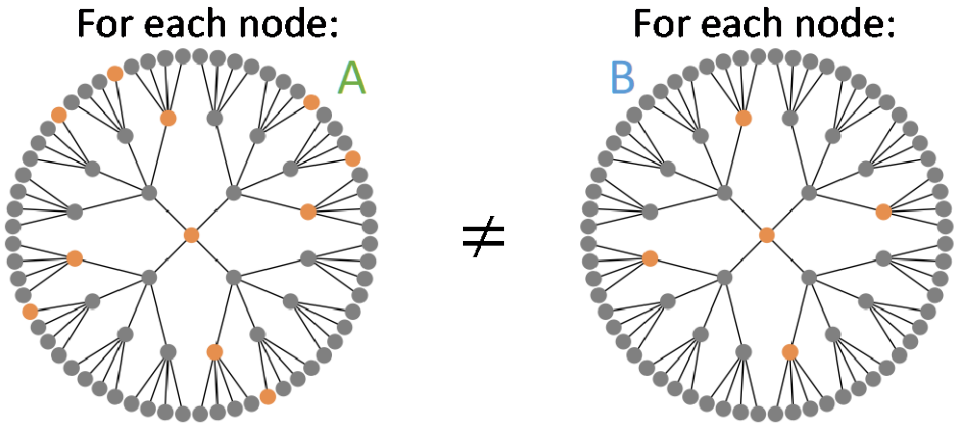
Inductive Node Coloring – Graph Level

- Inductive node coloring can help **graph classification**

Example inputs graphs



Computation graph of colored graph

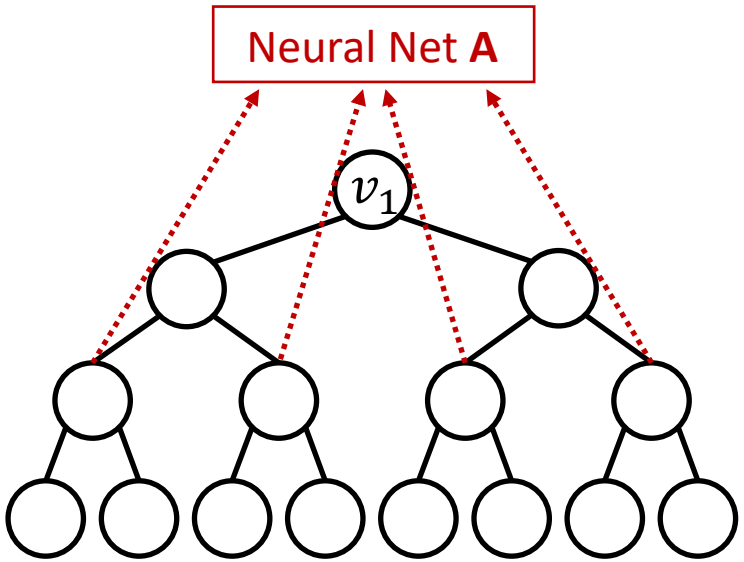


Different computation graphs
Successful differentiate graphs

Heterogenous Message Passing

- How to build a GNN using node coloring?
- **Idea:** Heterogenous message passing
  - Normally, a GNN applies the same message/aggregation computation to all the nodes

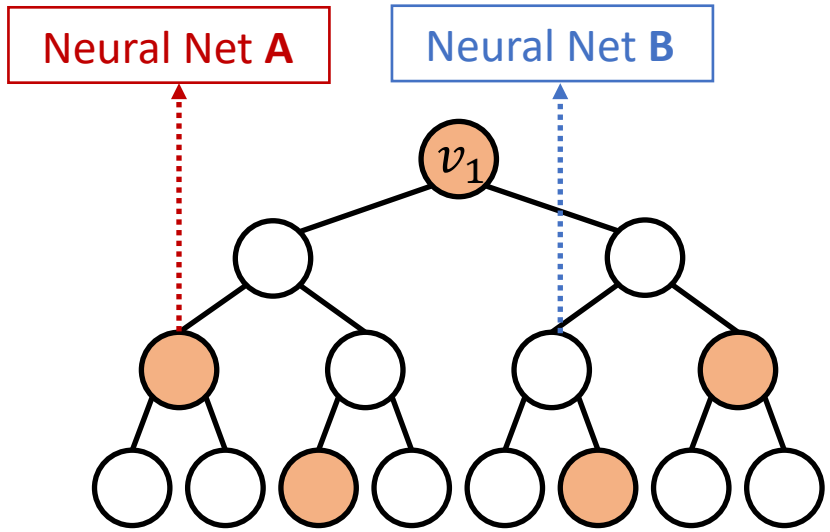
GNN:



Heterogenous Message Passing

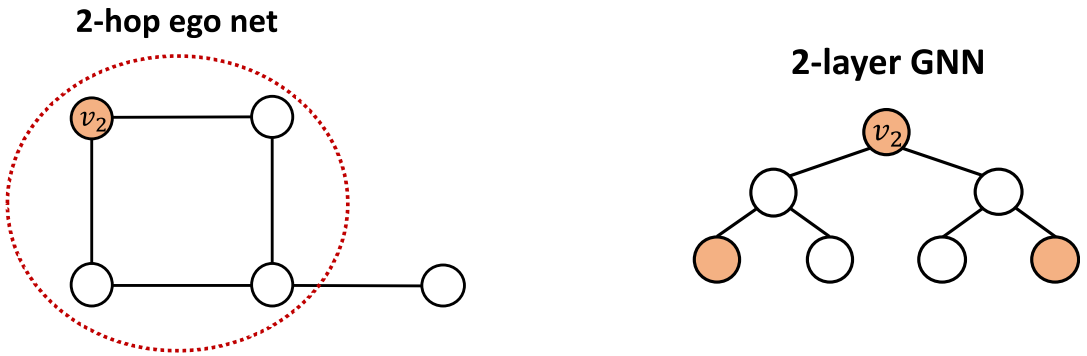
- **Idea:** Heterogenous message passing
  - **Heterogenous:** different types of message passing is applied to different nodes
  - An ID-GNN applies different neural networks to nodes with different colorings

ID-GNN



Identity-aware GNN Algorithm

- **Computation of Node v embedding:**
- **Step 1: extract the ego-network**
  - $\mathcal{G}_v^{(K)}$: K-hop neighborhood graph around v
  - Set the initial node feature to each node in $\mathcal{G}_v^{(K)}$
  - Example:



- We extract the ego net for each node, and initialize node embedding by raw node features.
- Ego net can be used to determine the GNN computation graph for a node

Identity-aware GNN Algorithm

- **Computation of Node v embedding:**
- **Step 2: Heterogeneous message passing**
  - For $k = 1, \dots K$ do
    - For $u \in \mathcal{G}_v^{(K)}$ do

$$h_u^{(k)} = \mathrm{AGG}^{(k)}\left(\left\{\mathrm{MSG}_{\mathbb{I}[s=v]}^{(k)}\left(h_s^{(k-1)}\right), s \in \mathcal{N}(u)\right\}, h_u^{(k-1)}\right)$$

- $h_u^{(k)}$ is the embedding of node u at the k-th layer.
- $\mathrm{AGG}^{(k)}$ is the aggerator of the k-th layer.
- $\mathbb{I}[s = v] = 0$ if $s = v$ else 0.
- Message passing equation $\mathrm{MSG}_0^{(k)}$ for nodes with identy coloring and $\mathrm{MSG}_1^{(k)}$ for the rest of nodes.
- $\mathcal{N}(u)$ is the set of neighborhood nodes of u.

Identity-aware GNN Algorithm

- **Computation of Node v embedding:**
- **Step 2: Heterogeneous message passing**
  - For $k = 1, \dots K$ do
    - For $u \in \mathcal{G}_v^{(K)}$ do

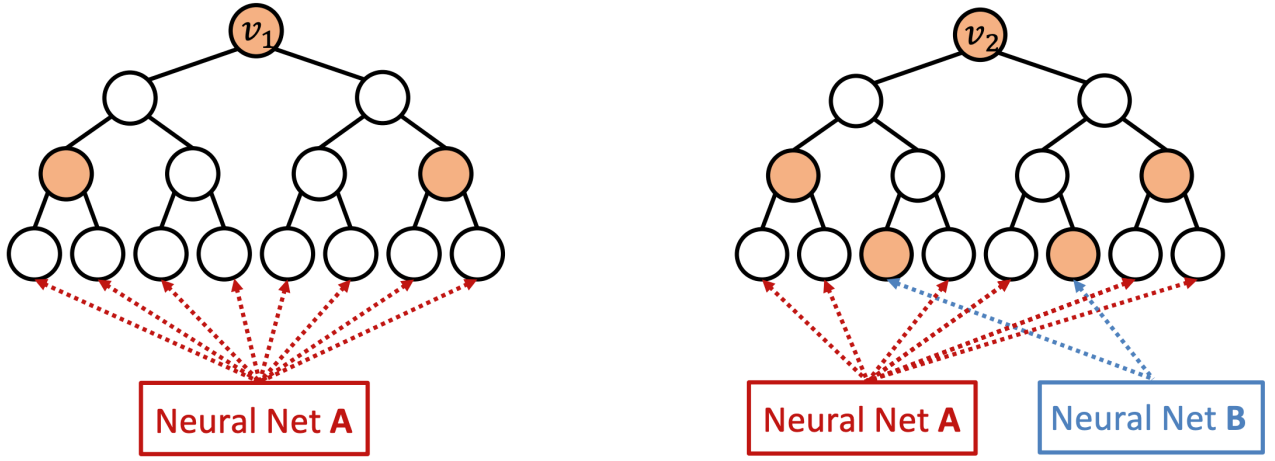
Depending on whether $s = v$ (s is the center node v) or not, we use different neural network functions to transform $h_s^{(k-1)}$.
$MSG_1^{(k)}$ for central node v and $MSG_0^{(k)}$ for others.

$$h_u^{(k)} = \mathrm{AGG}^{(k)}\left(\left\{\mathrm{MSG}_{\mathbb{I}[s=v]}^{(k)}\left(h_s^{(k-1)}\right), s \in \mathcal{N}(u)\right\}, h_u^{(k-1)}\right)$$

- $h_u^{(k)}$ is the embedding of node u at the k-th layer.
- $\mathrm{AGG}^{(k)}$ is the aggerator of the k-th layer.
- $\mathbb{I}[s = v] = 0$ if $s = v$ else 0.
- Message passing equation $\mathrm{MSG}_0^{(k)}$ for nodes with identy coloring and $\mathrm{MSG}_1^{(k)}$ for the rest of nodes.
- $\mathcal{N}(u)$ is the set of neighborhood nodes of u.

Identity-aware GNN

- **Why does heterogenous message passing work?**
  - Suppose two nodes v_1, v_2 have the same computation graph structure, but have different node colorings
  - Since we will apply different neural network for embedding computation, their embeddings will be different (implement via $\boldsymbol{MSG}^{(k)}_{\mathbb{I}[s=v]}$)
  - Thus can distinguish nodes even with the same computation graphs



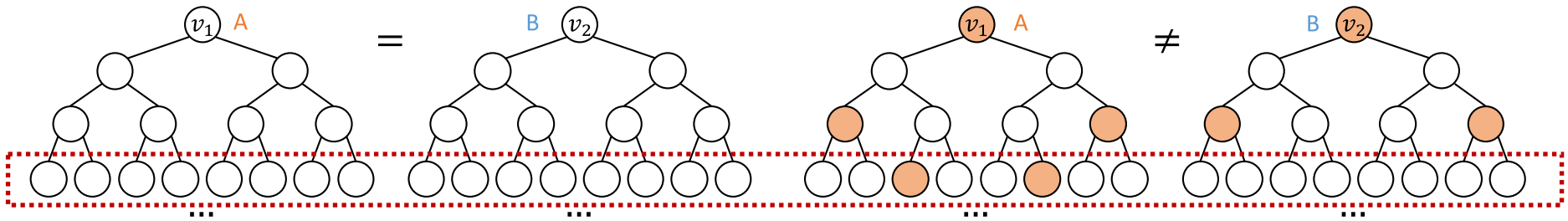
GNN vs Identity-aware GNN

- **Why does ID-GNN work better than GNN?**
- **Intuition:** ID-GNN can count cycles originating from a given node, but GNN cannot

Goal: classify v_1 and v_2

GNN computational graph

ID-GNN rooted subtrees

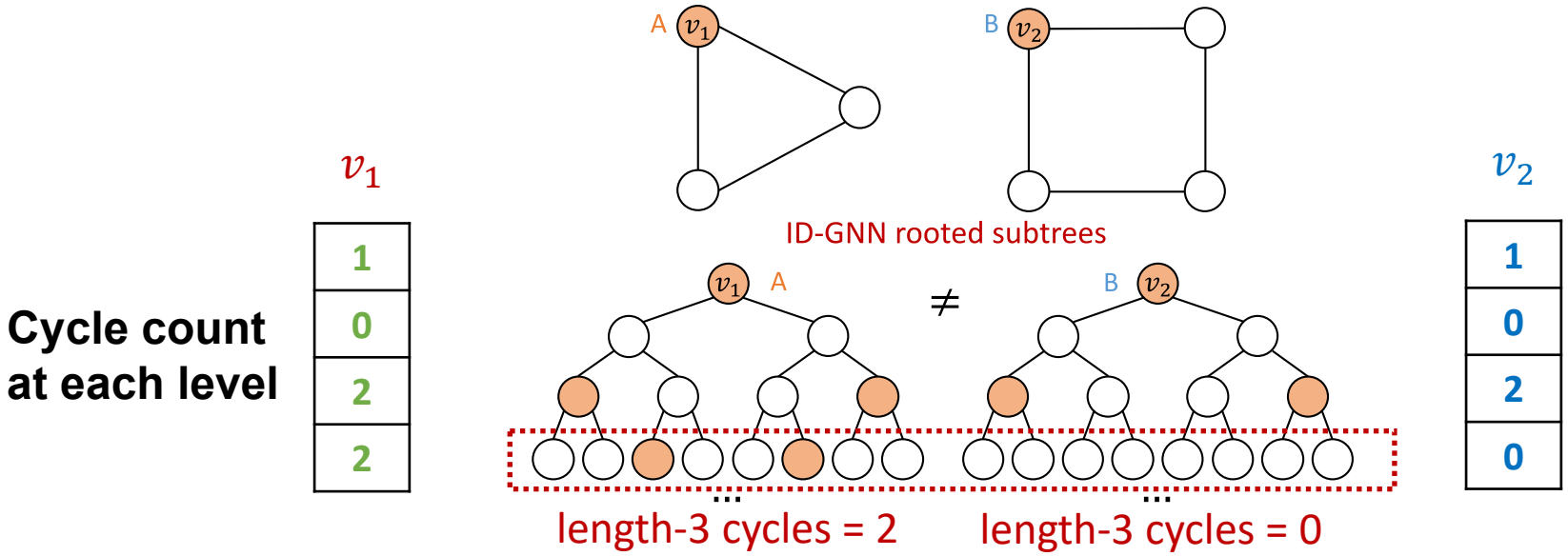


From the node coloring, we can tell that:

v_1: length-3 cycles = 2 v_2: length-3 cycles = 0

Simplified Version: ID-GNN-Fast

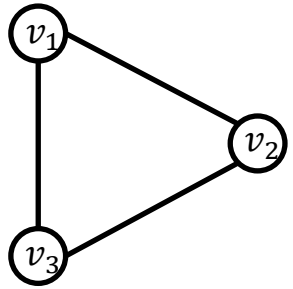
- Based on the intuition, we can write a simplified version **ID-GNN-Fast**
  - Include identity information as an **augmented node feature** (no need to do heterogenous message passing)
  - **Use cycle counts in each layer as an augmented node feature.** Also can be used together with **any GNN**



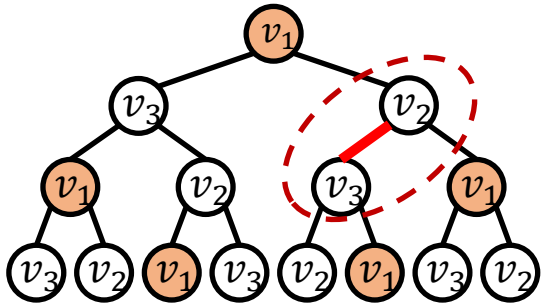
Limitation of Identity-aware GNN

- ID-GNN usually must be implemented with **minibatch training**.
  - The root of one computation tree is no longer the root of another computation tree
  - ID-GNN uses heterogeneous message passing
  - Message type of the same edge is different for different computation trees
  - Less efficient compared to full batch matrix multiplication

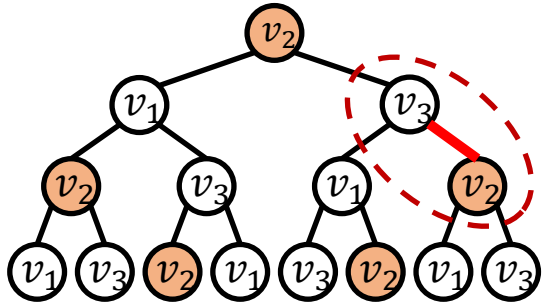
Original graph



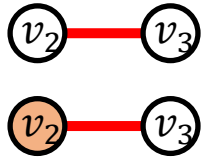
Computation graph of Node v_1



Computation graph of Node v_2



Same edge, but different message types in different computation graphs



Identity-aware GNN: Summary

- **ID-GNN:** A general and powerful extension to GNN framework
  - We can apply ID-GNN on any message passing GNNs (GCN, GraphSAGE, GIN, …)
  - We can easily implement ID-GNN using popular GNN tools (PyG, DGL, …)
- **ID-GNN:** A general solution to the limitations of expressive power in existing message passing GNNs
  - ID-GNN has expressive power beyond 1-WL test.
  - ID-GNN can count cycles originating from a given node, but GNN cannot
- Key idea of ID-GNN: assign a color to the node we want to embed and apply heterogenous message passing to nodes with different colorings

More Expressive GNNs

- Provably expressive graph neural networks
- Improving graph neural network expressivity via subgraph isomorphism counting
- Building powerful and equivariant graph neural networks with structural message-passing
- Relational pooling for graph representations
- Distance encoding: Design provably more powerful neural networks for graph representation learning
- Reconstruction for powerful graph representations
- Ego-GNNs: Exploiting ego structures in graph neural networks
- Weisfeiler and Lehman Go Cellular: CW Networks
- Weisfeiler and Lehman Go Topological: Message Passing Simplicial Networks