Stanford CS224W: GNN Theory 2, Breaking the Limits of the WL kernel

CS224W: Machine Learning with Graphs

Charilaos Kanatsoulis and Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Announcements

- **Homework 1 due Thursday, 10/17**
  - Late submissions accepted until end of day Monday, 10/21
- **Project Proposal due Tuesday, 10/22**
- **Colab 2 due Thursday, 10/24**

Response to high-resolution feedbacks

- **Move recitation time**

We will host our recitations in the evenings from now on to accommodate remote students. Recordings are also available via Ed posts.

- **Clarification on project feedbacks**

After project proposal, you will be assigned a TA to mentor your project for detailed feedbacks.

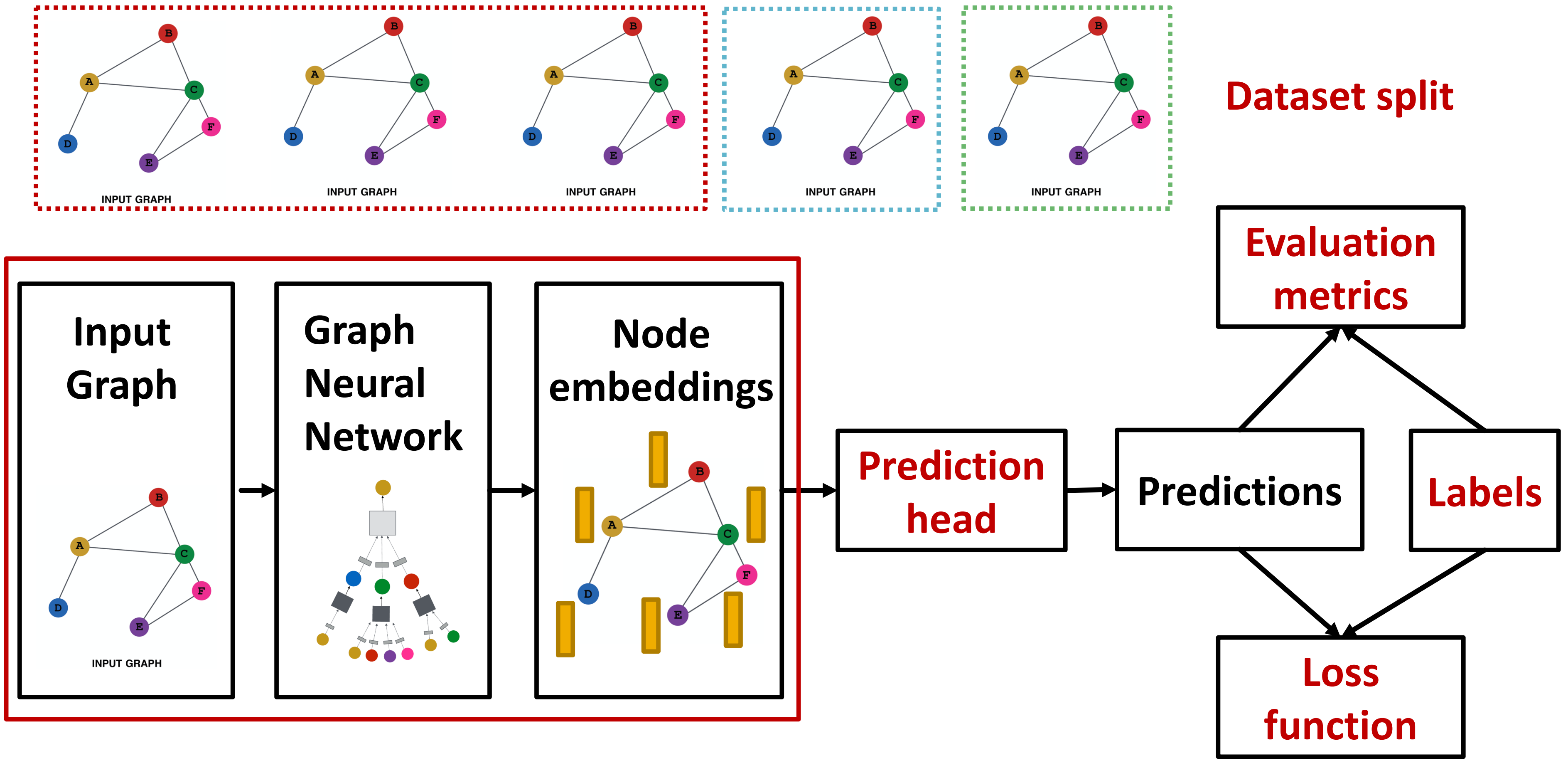
- **Lecture pace**

We will slow down the pace.

- **Individual questions around lecture content**

Please come to OH for in-depth QA.

Recap: GNN Training Pipeline



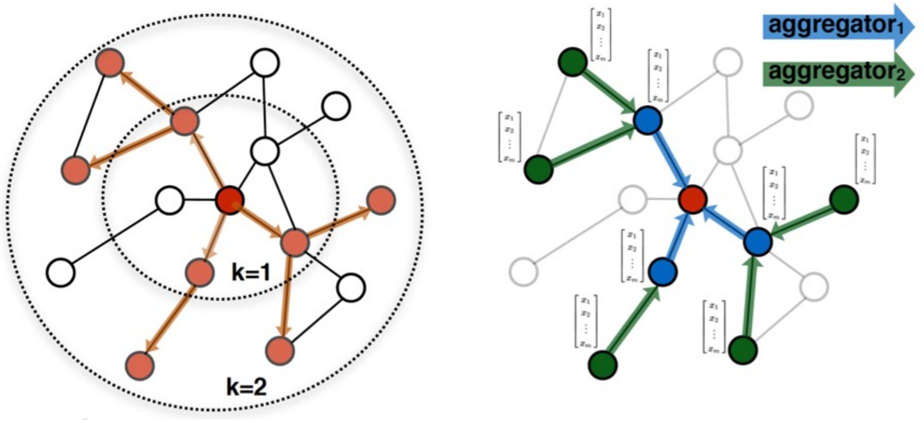
Today's lecture: Can we make GNN representation more expressive?

Stanford CS224W: Limitations of Graph Neural Networks

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

A "Perfect" GNN Model

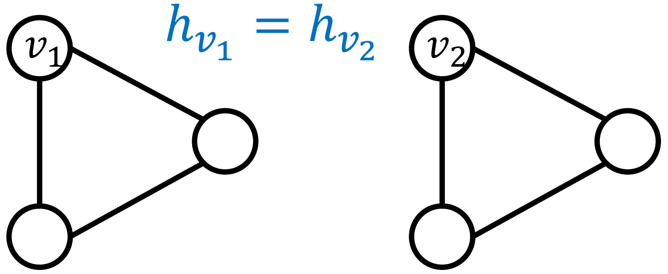
- **A thought experiment:** What should a perfect GNN do?
    - A k-layer GNN embeds a node based on the K-hop neighborhood structure



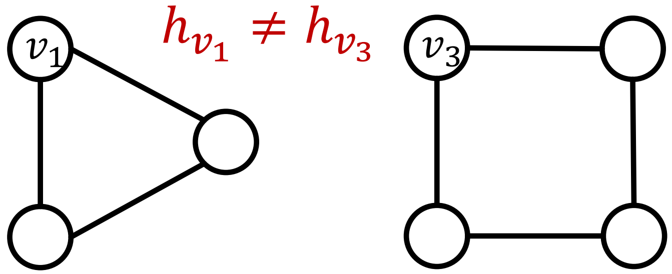
- A perfect GNN should build **an injective function** between neighborhood structure (regardless of hops) and node embeddings

A "Perfect" GNN Model

- **For a perfect GNN** **(ignore node attributes for now):**
  - **Observation 1:** If two nodes have the same neighborhood structure, they must have the same embedding



  - **Observation 2:** If two nodes have different neighborhood structure, they must have different embeddings

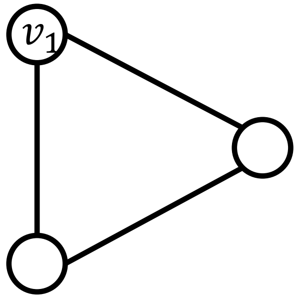


(Considering that attributes of all nodes are the same)

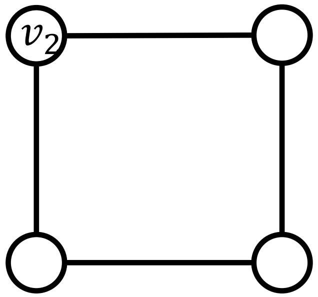
Imperfections of Existing GNNs

- **Observation 2 often cannot be satisfied:**
  - **The GNNs we have introduced so far are not perfect**
  - In previous lecture, we discussed that their expressive power is **upper bounded by the WL test**
  - For example, message passing GNNs **cannot count the cycle length:**

v_1 resides in a cycle with length 3

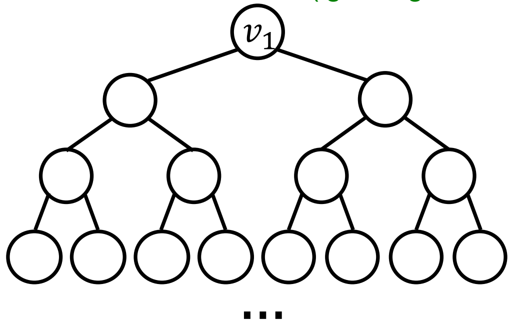


v_2 resides in a cycle with length 4



The computational graphs for nodes v_1 and v_2 are always the same

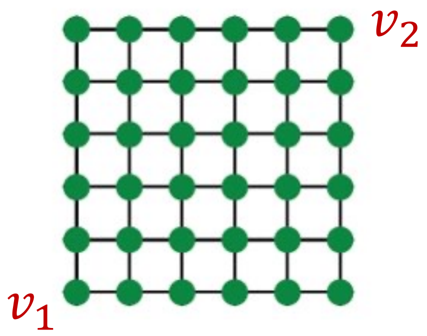
(ignoring node attributes)



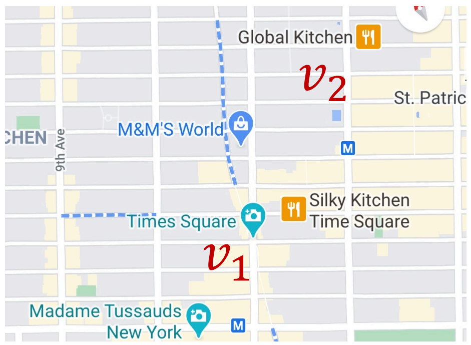
J. You, R. Ying, J. Leskovec. Postion-aware Graph Neural Networks, ICML 2019

Imperfections of Existing GNNs

- **Observation 1 could also have issues:**
  - 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 the graph**
  - We call these tasks **Position-aware tasks**
  - **Even a perfect GNN will fail for these tasks:**



A grid graph



NYC road network

Plan for the Lecture

We will resolve both issues by **building more expressive GNNs**

- **Fix issues in Observation 2:**
  - Build message passing GNNs that are more expressive than WL test
  - Example method: **Structurally-aware GNNs**
- **Fix issues in Observation 1:**
  - Create node embeddings based on their positions in the graph
  - Example method: **Position-aware GNNs**

Stanford CS224W: A Spectral Perspective of message-passing GNNs

CS224W: Machine Learning with Graphs

Charilaos Kanatsoulis and Jure Leskovec, Stanford University

http://cs224w.stanford.edu

J. You, J. Gomes-Selman, R. Ying, J. Leskovec. Identity-aware Graph Neural Networks, AAAI 2021

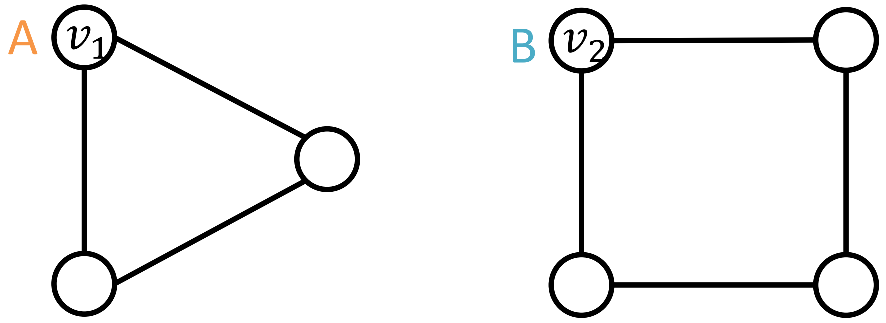
More Failure Cases for GNNs

- GNNs exhibit three levels of failure cases in structure-aware tasks:
  - Node level
  - Edge level
  - Graph level

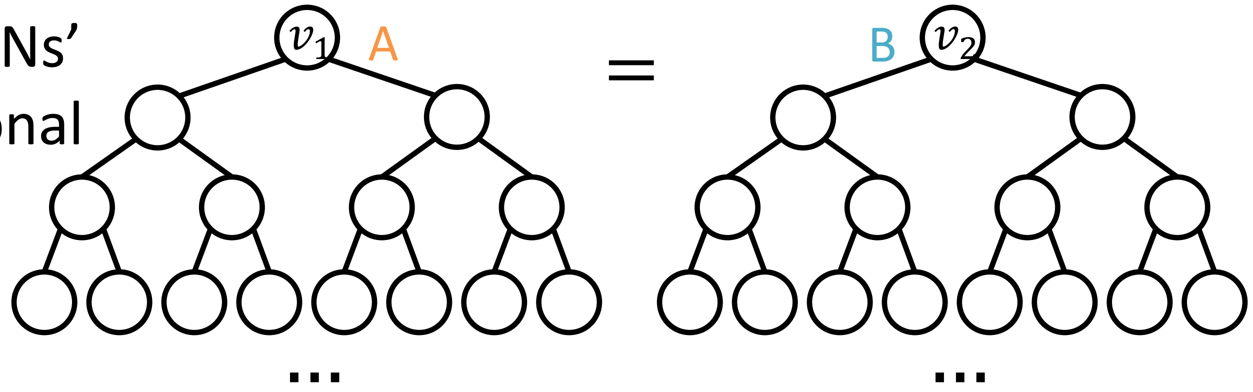
GNN Failure 1: Node-level Tasks

Different Inputs but the same computational graph → GNN fails

Example input graphs



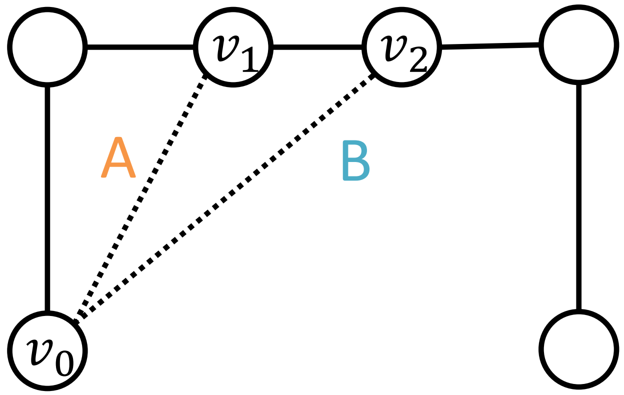
Existing GNNs' computational graphs



GNN Failure 2: Edge-level Tasks

Different Inputs but the same computational graph → GNN fails

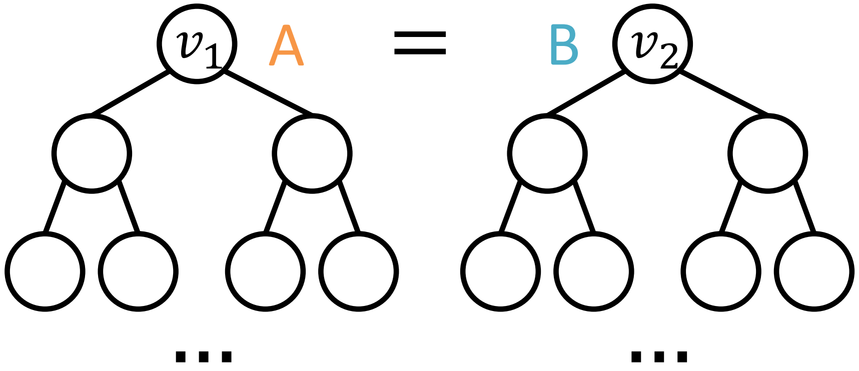
Example input graphs



Edge A and B share node v_0

We look at embeddings for v_1 and v_2

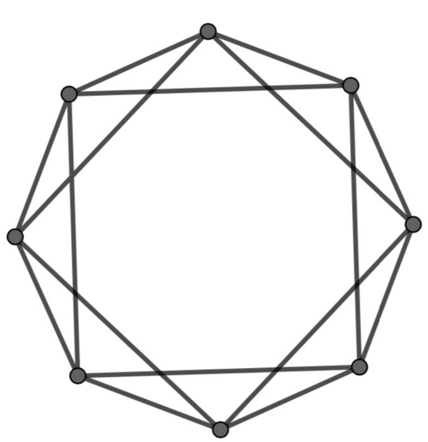
Existing GNNs' computational graphs

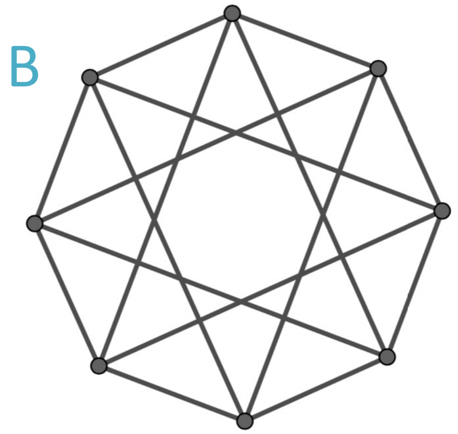


GNN Failure 3: Graph-level Tasks

Different Inputs but the same computational graph → GNN fails

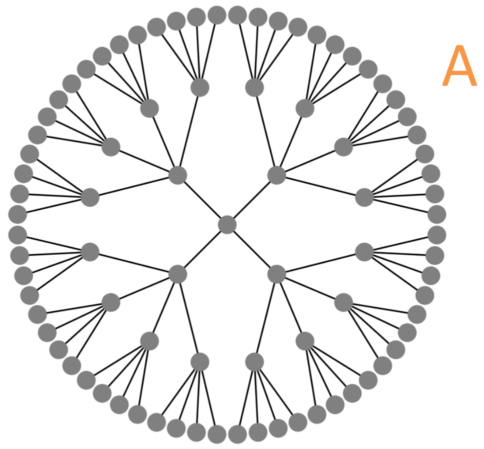
Example input graphs





We look at embeddings for each node

For each node:



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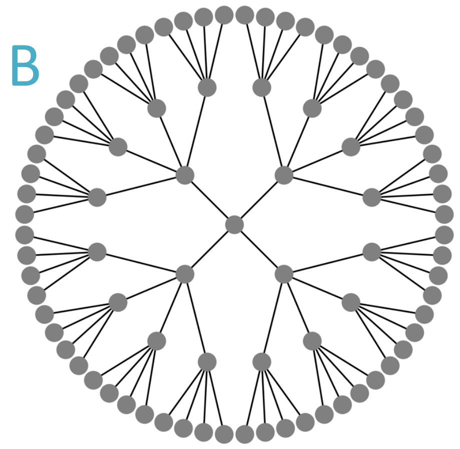
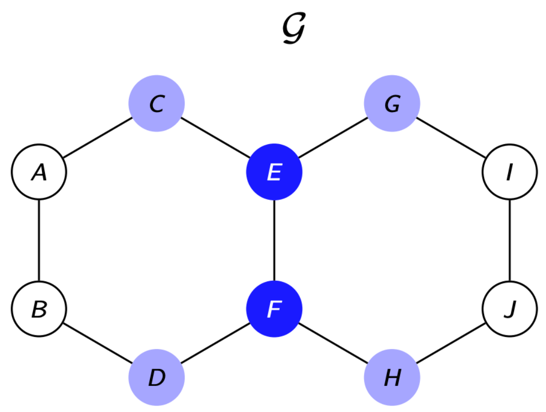
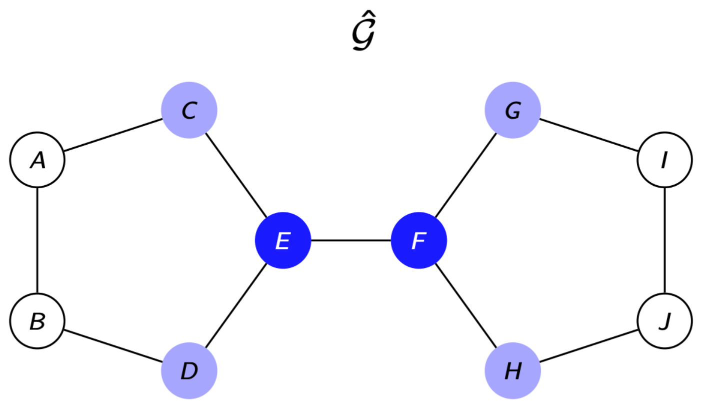
For each node:



Existing GNNs' computational graphs

Limitation of the WL kernel





- **The WL kernel** colors **inherit the graph symmetries**.
- **Symmetric colors** are associated with limitations involving the **spectral decomposition of the graph**.

Matrix representation of GIN

- **Recall the GIN update:**

$$\boldsymbol{c}_v^{(l+1)} = \mathrm{MLP}\left((1+\epsilon)\,\boldsymbol{c}_v^{(l)} + \sum_{u\in\mathcal{N}(v)} \boldsymbol{c}_u^{(l)}\right)$$

  - We can unroll the first MLP layer:

$$\boldsymbol{c}_v^{(l+1)} = \mathrm{MLP}_{-1}\left(\sigma\left(\boldsymbol{W}^{(l)}\,(1+\epsilon)\,\boldsymbol{c}_v^{(l)} + \sum_{u\in\mathcal{N}(v)} \boldsymbol{W}^{(l)}\boldsymbol{c}_u^{(l)}\right)\right)$$

  - MLP_{-1} denotes all the MLP layers except the first.

Matrix representation of GIN

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Matrix representation of GIN

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$$\boldsymbol{c}_v^{(l+1)} = \mathrm{MLP}_{-1}\left(\sigma\left(\boldsymbol{W}_0^{(l)}\boldsymbol{c}_v^{(l)} + \sum_{u\in\mathcal{N}(v)} \boldsymbol{W}_1^{(l)}\boldsymbol{c}_u^{(l)}\right)\right)$$

  - We can write the color update in a matrix form:

$$\boldsymbol{C}^{(l+1)} = \mathrm{MLP}_{-1}\left(\sigma\left(\boldsymbol{C}^{(l)}\boldsymbol{W}_0^{(l)} + \boldsymbol{A}\boldsymbol{C}^{(l)}\boldsymbol{W}_1^{(l)}\right)\right) = \mathrm{MLP}_{-1}\left(\sigma\left(\sum_{k=0}^{1}\boldsymbol{A}^k\boldsymbol{C}^{(l)}\boldsymbol{W}_k^{(l)}\right)\right)$$

  - $\boldsymbol{C}^{(l)} \in \mathbb{R}^{N\times d}, \quad \boldsymbol{C}^{(l)}[v,:] = \boldsymbol{c}_v^{(l)}$
  - Where $A\epsilon\{0,1\}^{N\times N}$ is the adjacency matrix of the graph, i.e., $A[u,v] = 1$ if (u,v) is an edge and $A[u,v] = 0$ if (u,v) is not an edge.

Spectral Graph Representation

- **Let's compute the eigenvalue decomposition of the graph adjacency matrix A.**

$$\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$$

- $\boldsymbol{V} = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n]$ is the orthonormal matrix of eigenvectors
- $\boldsymbol{\Lambda}$ is the diagonal matrix of eigenvalues $\{\lambda_n\}_{n=1}^{N}$
  - The eigenvalue (**spectral**) decomposition of the adjacency is a **universal characterization** of the graph.
  - **Different graphs have different spectral decompositions**
  - The **number of cycles** in a graph can be viewed as **functions of eigenvalues and eigenvectors**, e.g.,

$$\#\text{triangles} = \text{diag}\left(\boldsymbol{A}^3\right) = \sum_{n=1}^{N} \lambda_n^3 \left|\boldsymbol{v}_n\right|^2$$

GNN as functions of eigenvectors

- **We can interpret GIN layers as MLPs operating on the eigenvectors:**

$$\boldsymbol{C}^{(l+1)} = \mathrm{MLP}_{-1}\left(\sigma\left(\boldsymbol{C}^{(l)}\boldsymbol{W}_0^{(l)} + \boldsymbol{A}\boldsymbol{C}^{(l)}\boldsymbol{W}_1^{(l)}\right)\right) = \mathrm{MLP}_{-1}\left(\sigma\left(\sum_{k=0}^{1}\boldsymbol{A}^k\boldsymbol{C}^{(l)}\boldsymbol{W}_k^{(l)}\right)\right)$$

- **If we replace A with the spectral decomposition** $\boldsymbol{A} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^T$

$$\boldsymbol{C}^{(l+1)} = MLP\left(\boldsymbol{V}\right) = MLP_{-1}\left(\sigma\left(\boldsymbol{V}\boldsymbol{W}\right)\right)$$

$$\boldsymbol{W}[n,f] = \sum_{i=1}^{d}\sum_{k=0}^{1}\lambda_n^k\boldsymbol{W}_k[i,f]\langle\boldsymbol{v}_n,\boldsymbol{C}^{(l)}[:,i]\rangle$$

- The weights of the first MLP layer depend on the eigenvalues and the **dot product between the eigenvectors and the colors at the previous level**.

GNN with uniform initial colors

- **We can interpret GIN layers as MLPs operating on the eigenvectors:**

$$\boldsymbol{C}^{(1)} = \mathrm{MLP}\left(\boldsymbol{V}\right) = \mathrm{MLP}_{-1}\left(\sigma\left(\boldsymbol{V}\boldsymbol{W}\right)\right)$$

$$\boldsymbol{W}\left[n, f\right] = \sum_{k=0}^{1} \lambda_n^k \boldsymbol{W}_k[i, f]\langle \boldsymbol{v}_n, \boldsymbol{1}\rangle \qquad \alpha_f\left(\lambda_n\right) = \sum_{k=0}^{1} \lambda_n^k \boldsymbol{W}_k[i, f]$$

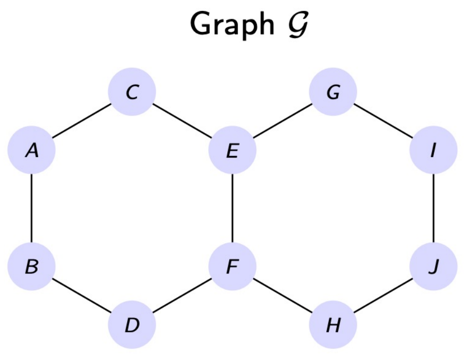
- **If we zoom in**

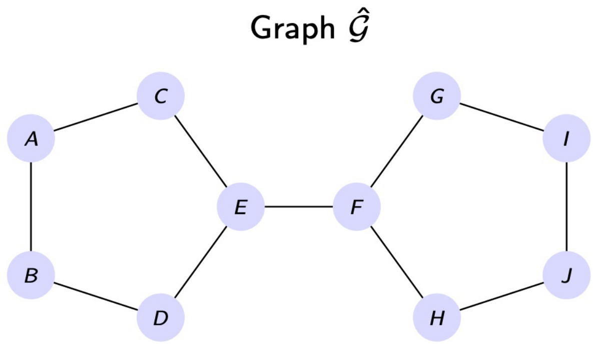
$$\left(\boldsymbol{V}\boldsymbol{W}\right)[:, f] = \sum_{n=1}^{N} \boldsymbol{W}\left[n, f\right]\boldsymbol{v}_n = \sum_{n=1}^{N} \alpha_f\left(\lambda_n\right)\langle \boldsymbol{v}_n, \boldsymbol{1}\rangle \boldsymbol{v}_n$$

- The new node colors **only depend** on the **eigenvectors that are not orthogonal to 1**.
- **Graphs with symmetries** admit **eigenvectors orthogonal to 1.**

Spectral limitation of the WL kernel

- **The WL kernel cannot distinguish between some basic graph structures, e.g.,**





$\mathcal{G}$	λ_n	2.303	1.618	1.303	1	0.618	-2.303	-1.618	-0.618	-1	-1.303
$\hat{\mathcal{G}}$	$\hat{\lambda}_n$	2.303	1.861	1	0.618	0.618	0.254	-1.303	-1.618	-1.618	-2.115

Spectral limitation of the WL kernel

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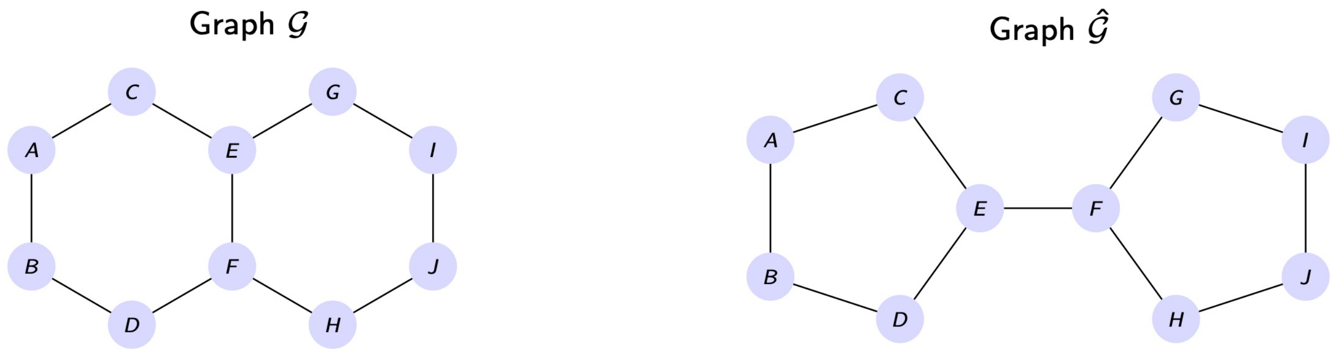

$\mathcal{G}$	λ_n	2.303	1.618	1.303	1	0.618	-2.303	-1.618	-0.618	-1	-1.303
	$\langle \boldsymbol{v}_n, \mathbf{1} \rangle$	3.048	0	0	-0.816	0	0	0	0	0	-0.210
$\hat{\mathcal{G}}$	$\hat{\lambda}_n$	2.303	1.861	1	0.618	0.618	0.254	-1.303	-1.618	-1.618	-2.115
	$\langle \hat{\boldsymbol{v}}_n, \mathbf{1} \rangle$	3.048	0	-0.816	0	0	0	-0.210	0	0	0

Spectral limitation of the WL kernel

- **The WL kernel cannot count basic graph structures:**

$$\#\text{triangles} = \text{diag}\left(\boldsymbol{A}^3\right) = \sum_{n=1}^{N} \lambda_n^3 \left|\boldsymbol{v}_n\right|^2$$

$\mathcal{G}$	λ_n	2.303	1.618	1.303	1	0.618	-2.303	-1.618	-0.618	-1	-1.303
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$\hat{\mathcal{G}}$	$\hat{\lambda}_n$	2.303	$\boxed{1.861}$	1	0.618	0.618	0.254	-1.303	-1.618	-1.618	-2.115
	$\langle \hat{\boldsymbol{v}}_n, \mathbf{1} \rangle$	3.048	$\boxed{0}$	-0.816	0	0	0	-0.210	0	0	0

Limitations of the WL kernel

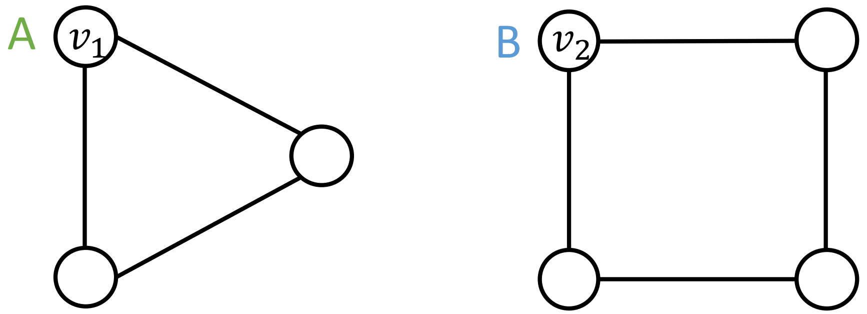
- **Summary: The limitations of the WL kernel are limitations of the initial node color.**
  - These limitations are well understood in the **spectral domain**.
    - Constant node colorings are orthogonal with adjacency eigenvectors and **critical spectral components** (eigenvalues and eigenvectors) **are omitted**.
  - In a high level, colors generated by the WL kernel obey the **same symmetries as graph structure**.
  - These joint symmetries **lock** the message-passing operations to limited representations.

Stanford CS224W: Feature Augmentation: Structurally-Aware GNNs

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Our Approach

- **We use the following thinking:**
  - Two different inputs (nodes, edges, graphs) are labeled differently
  - A "failed" model will always assign the same embedding to them
  - A "successful" model will assign different embeddings to them
  - **Embeddings are determined by GNN computational graphs:**

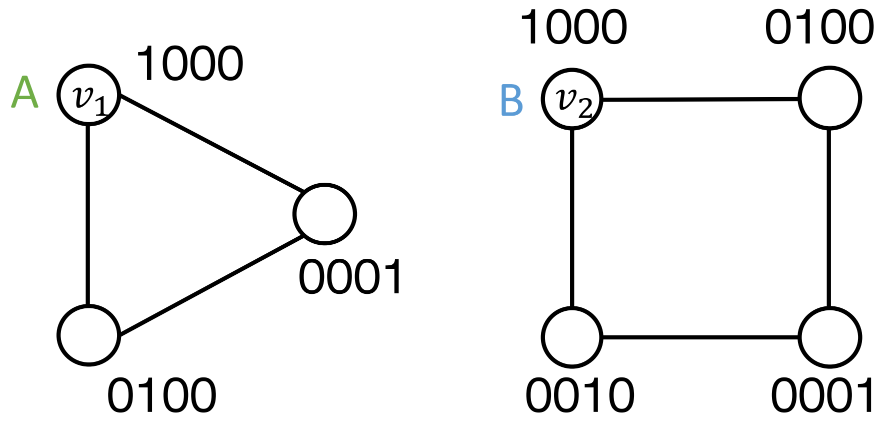


Two inputs: nodes v_1 and v_2
Different labels: A and B
Goal: assign different embeddings to v_1 and v_2

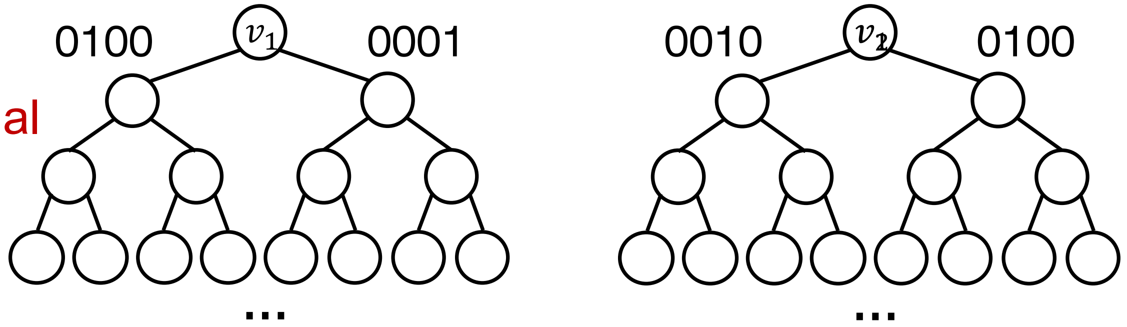
Naïve Solution is not Desirable

- **A naïve solution:** One-hot encoding
  - Encode each node with a different ID, then we can always differentiate different nodes/edges/graphs

Input graphs



Computational graphs



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

Naïve Solution is not Desirable

- **A naïve solution:** One-hot encoding
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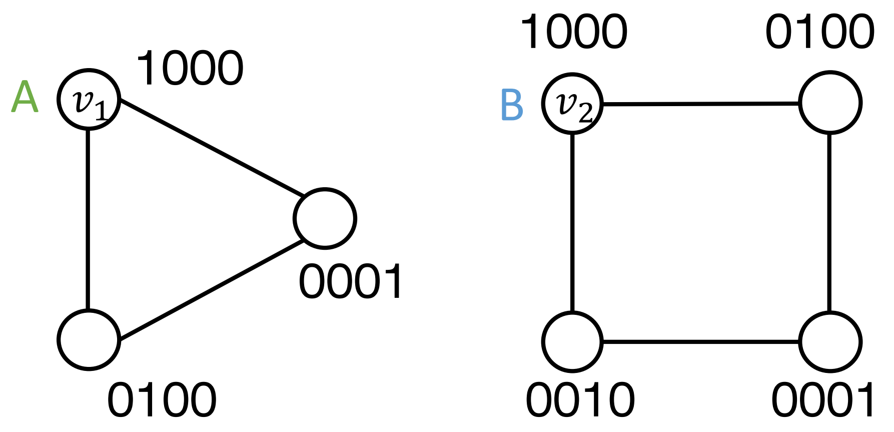
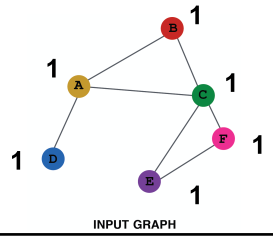
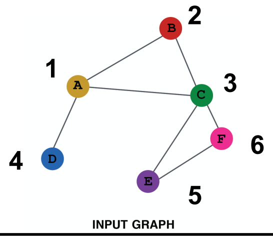
Input graphs



  - **Issues:**
    - **Not scalable**: Need $O(N)$ feature dimensions (N is the number of nodes)
    - **Not inductive:** Cannot generalize to new nodes/graphs

Feature Augmentation on Graphs

- Feature augmentation: **constant** vs. **one-hot**

	Constant node feature 	**One-hot node feature** 
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a unique ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple to generalize to new nodes: we assign constant feature to them, then apply our GNN	**Low**. Cannot generalize to new nodes: new nodes introduce new IDs, GNN doesn't know how to embed unseen IDs
Computational cost	**Low**. Only 1 dimensional feature	**High**. High dimensional feature, cannot apply to large graphs
Use cases	Any graph, inductive settings (generalize to new nodes)	Small graph, transductive settings (no new nodes)

J. You, J. Gomes-Selman, R. Ying, J. Leskovec. Identity-aware Graph Neural Networks, AAAI 2021

Feature Augmentation on Graphs

Why do we need feature augmentation?

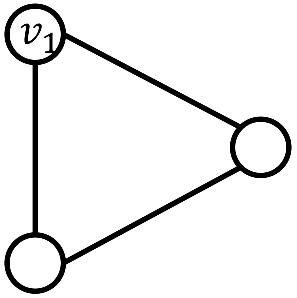
- **(2) Certain structures are hard to learn by GNN**
- **Solution:**
  - We can use cycle count as augmented node features

We start from cycle with length 0

Augmented node feature for v_1

[0, 0, 0, 1, 0, 0]

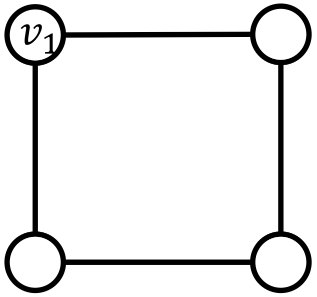
v_1 resides in a cycle with length 3



Augmented node feature for v_1

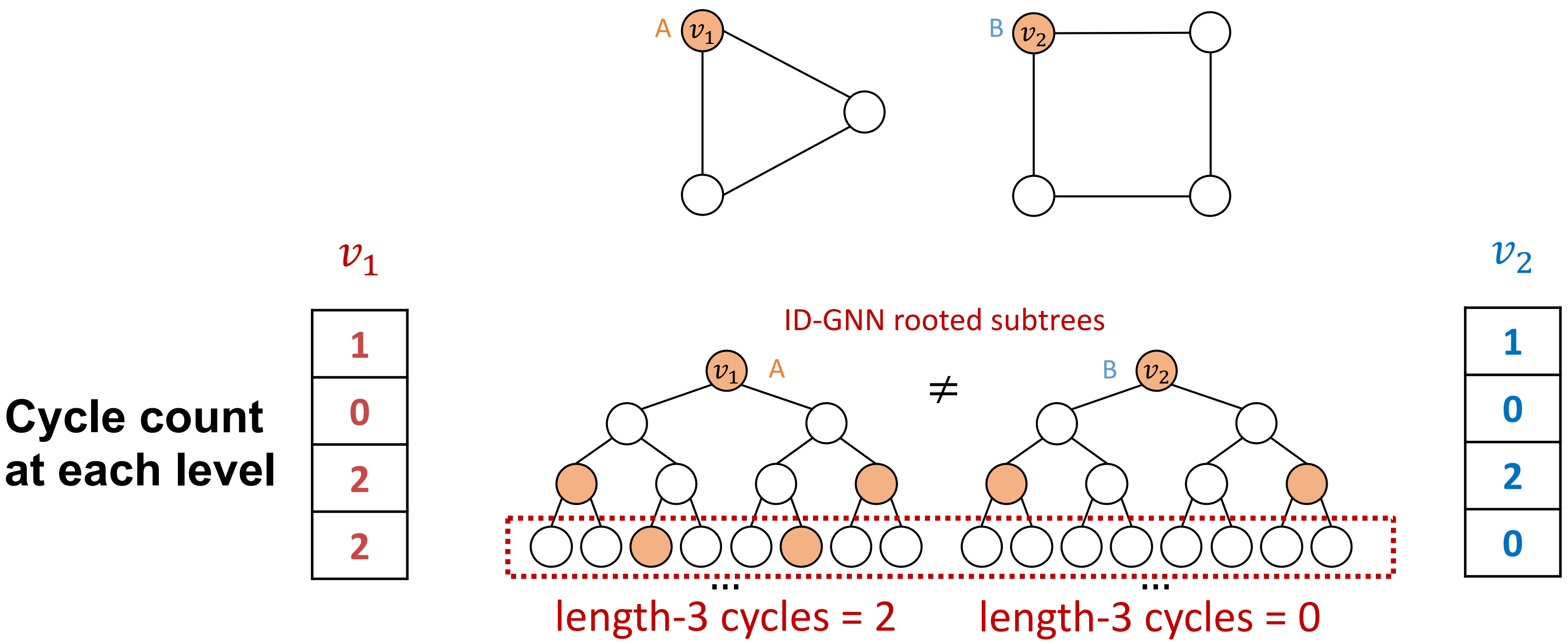
[0, 0, 0, 0, 1, 0]

v_1 resides in a cycle with length 4



J. You, J. Gomes-Selman, R. Ying, J. Leskovec. Identity-aware Graph Neural Networks, AAAI 2021

ID-GNN-Fast



- Idea: Count cycles originating from a given node, use it as initial feature.
  - Include identity information as an **augmented node feature**
  - **Use cycle counts in each layer as an augmented node feature**. Also can be used together with **any GNN**

C. Kanatsoulis, A. Ribeiro. Graph Neural Network Are More Powerful Than we Think, ICASSP 2024

Closed loops as node features

- We can also use the **diagonals of the adjacency powers** as augmented node features.
- They correspond to the **closed loops** each node is involved in.

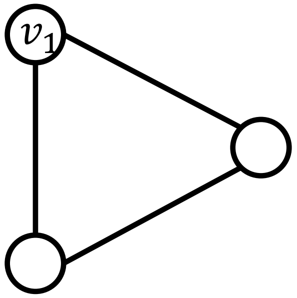
$$C^{(0)} = \left[\operatorname{diag}\left(A^0\right), \operatorname{diag}\left(A^1\right), \operatorname{diag}\left(A^2\right), \operatorname{diag}\left(A^3\right), \ldots, \operatorname{diag}\left(A^{D-1}\right)\right] \in \mathbb{N}_0^{N \times D}$$

Augmented node feature for v_1

[1, 0, 2, 2, 6, 8]

$\uparrow$

v_1 resides in a cycle with length 3

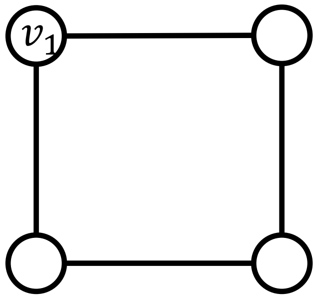


Augmented node feature for v_1

[1, 0, 2, 0, 8, 0]

$\uparrow$

v_1 resides in a cycle with length 4



C. Kanatsoulis, A. Ribeiro. Graph Neural Network Are More Powerful Than we Think, ICASSP 2024

Expressive Power

- **Theorem:** If two graphs have adjacency matrices with **different eigenvalues**, there exists a GNN with closed-loop initial node features that can **always tell them apart.**

- GNNs with **structural initial node features** can produce different representations for **almost all real-world graphs**.

- GIN with structural initial node features is **strictly more powerful** than the WL-kernel.

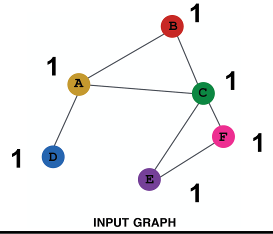
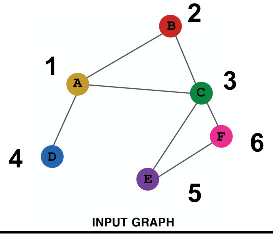
Feature Augmentation on Graphs

Why do we need feature augmentation?

- **(2) Certain structures are hard to learn by GNN**
- Other commonly used augmented features:
  - **Clustering coefficient**
  - **PageRank**
  - **Centrality**
  - **…**
- Any **feature we have introduced in Lecture 1 can be used!**

Feature Augmentation on Graphs

- Feature augmentation: **constant** vs. **Structure**

	Constant node feature 	**Structure-aware node feature** 
Expressive power	**Medium**. All the nodes are identical, but GNN can still learn from the graph structure	**High**. Each node has a structure-aware ID, so node-specific information can be stored
Inductive learning (Generalize to unseen nodes)	**High**. Simple to generalize to new nodes: we assign constant feature to them, then apply our GNN	**High**. Simple to generalize to new nodes: can count triangles or closed loops for any graph
Computational cost	**Low**. Only 1 dimensional feature	**Low/High**. Depending on the structures we are counting
Use cases	Any graph, inductive settings (generalize to new nodes)	Any graph, inductive settings (generalize new nodes)

Stanford CS224W: Counting Graph Substructures with GNNs

CS224W: Machine Learning with Graphs

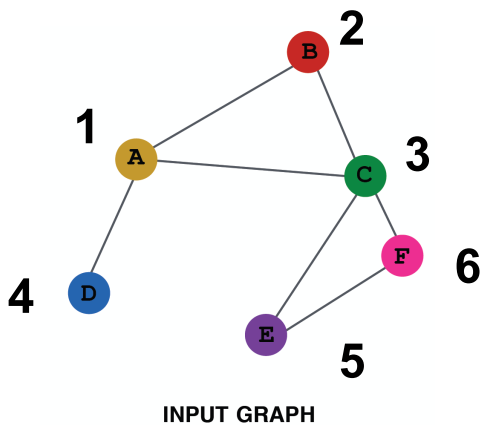
Charilaos Kanatsoulis and Jure Leskovec, Stanford University

http://cs224w.stanford.edu

Random samples as node ID's

Can we count graph substructures with GNNs only?

- **Assign unique IDs to nodes**
  - These IDs are represented by **random samples**
  - **Each node will be represented by a different set of random variables**



Random samples for node 3

$$\underbrace{[0.2, 1.5, -2.3, -10.1]}_{\text{Total number of random samples = 4}}$$

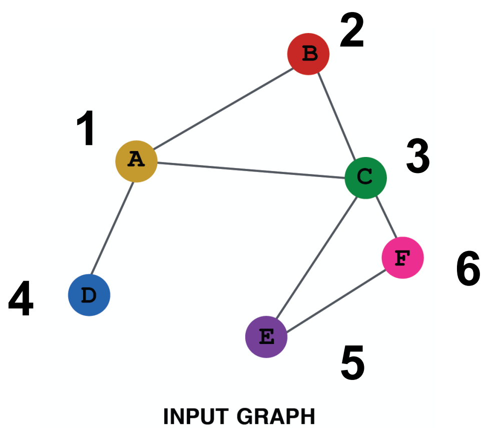
Designing a simple GNN

- **We design a simple GNN**
  - With SUM Aggregations and Linear Message Functions.
  - **We add a square pointwise nonlinearity** $\sigma(\cdot) = (\cdot)^2$ **in the last layer.**

$$\boldsymbol{c}_v^{(l+1)} = \texttt{Linear}\left((1+\epsilon)\, \boldsymbol{c}_v^{(l)} + \sum_{u \in \mathcal{N}(v)} \boldsymbol{c}_u^{(l)} \right)$$

$$\boldsymbol{c}_v^{(L)} = \sigma\left(\texttt{Linear}\left((1+\epsilon)\, \boldsymbol{c}_v^{(L-1)} + \sum_{u \in \mathcal{N}(v)} \boldsymbol{c}_u^{(L-1)} \right) \right)$$

Independent Processing of samples



Node 1 [3.3, -1.7, -1.2, -0.1]

Node 2 [-0.1, -5.4, 3.0, -9.8]

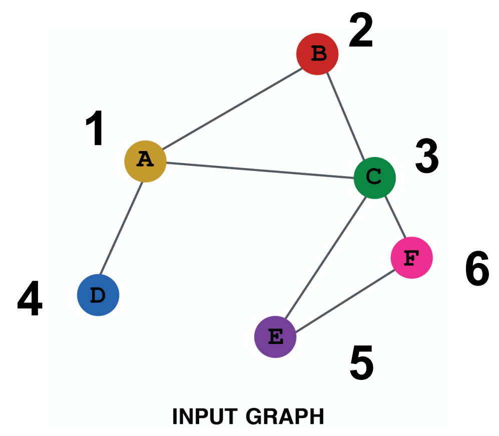
Node 3 [0.2, 1.5, -2.3, -10.1]

Node 4 [0.5, 1.9, -12.7, 11.1]

Node 5 [5.1, -0.7, -2.9, -13.5]

Node 6 [-1.2, 7.5, -0.3, -7.9]

Independent Processing of samples



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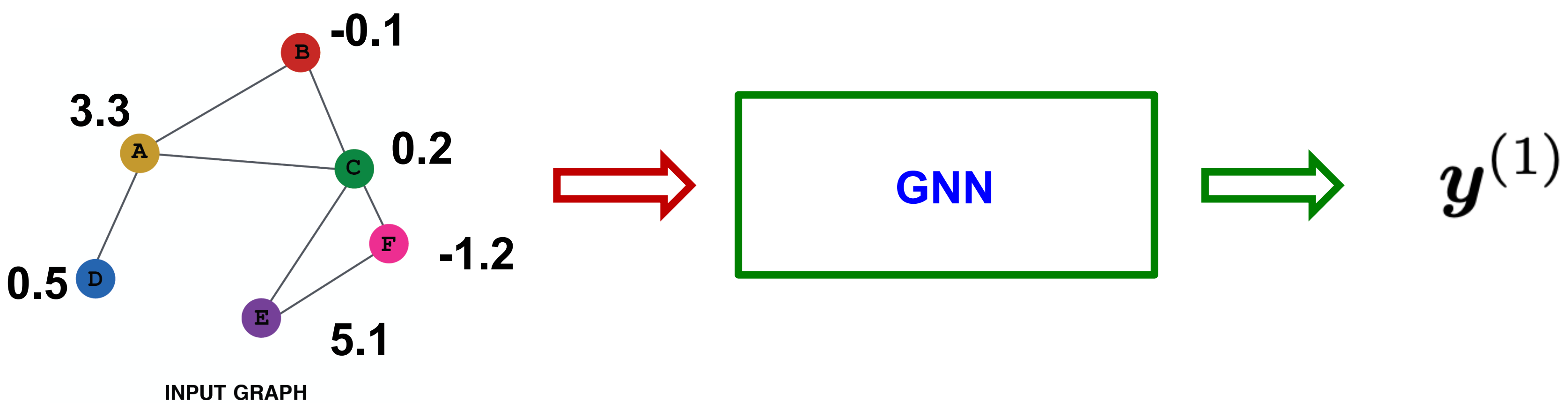

$\boldsymbol{y}^{(1)}$

Independent Processing of samples

Node 1 [3.3, -1.7, -1.2, -0.1]
Node 2 [-0.1, -5.4, 3.0, -9.8]
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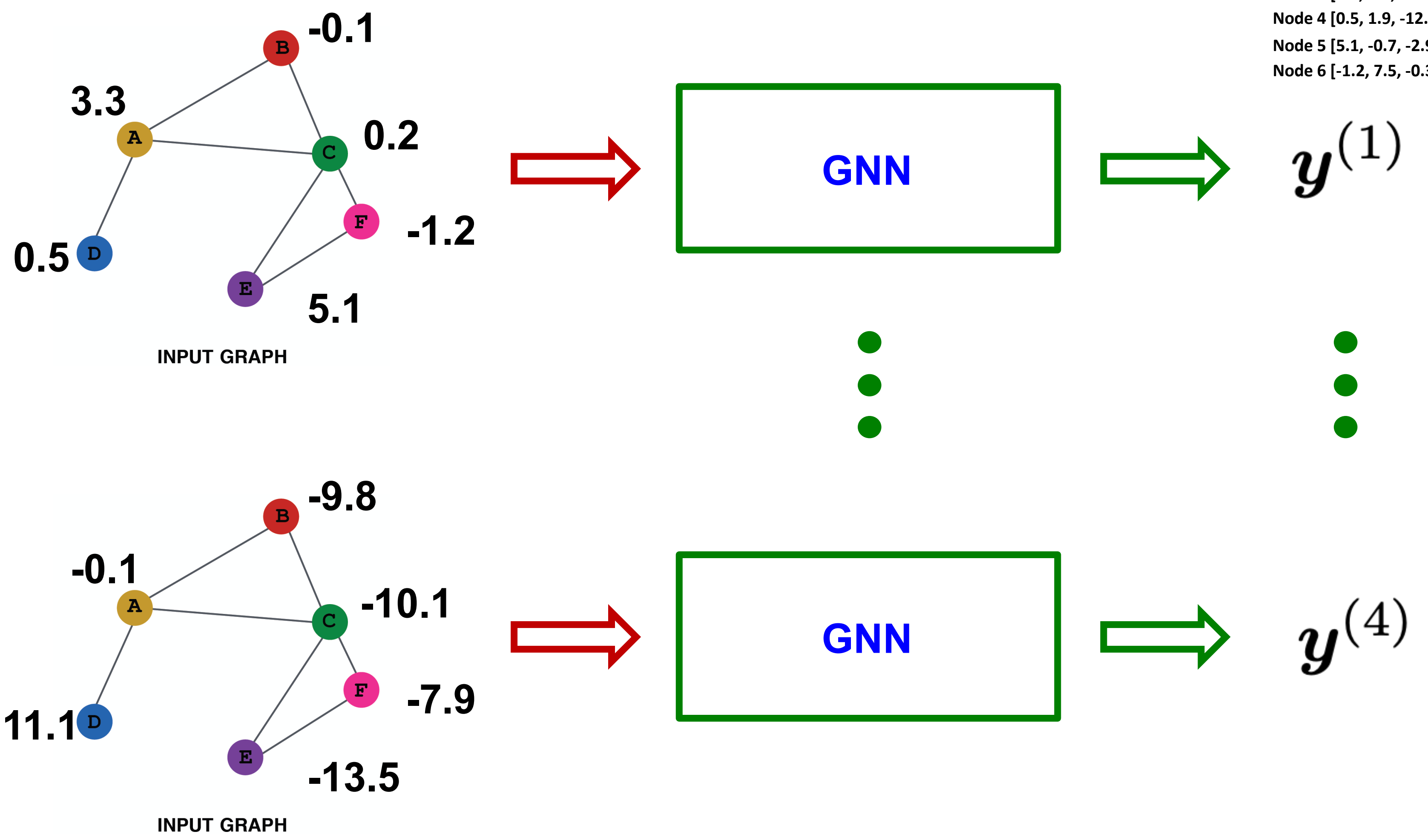


Counting Cycles with GNNs

- **To maintain inductive capability the final output:**

$$\boldsymbol{y} = \mathbb{E}\left[\boldsymbol{y}^{(m)}\right]$$

  - Which in practice is computed as:

$$\boldsymbol{y} = \frac{1}{M}\sum_{m=1}^{M} \boldsymbol{y}^{(m)}$$

  - We can show that the previous procedure **computes the closed loops of a graph:**

$$\boldsymbol{C}^{(0)} = \left[\operatorname{diag}\left(\boldsymbol{A}^{0}\right), \operatorname{diag}\left(\boldsymbol{A}^{1}\right), \operatorname{diag}\left(\boldsymbol{A}^{2}\right), \operatorname{diag}\left(\boldsymbol{A}^{3}\right), \ldots, \operatorname{diag}\left(\boldsymbol{A}^{D-1}\right)\right] \in \mathbb{N}_0^{N\times D}$$

  - **And a GNN can break the limits of the WL kernel and count important substructures in the graph.**

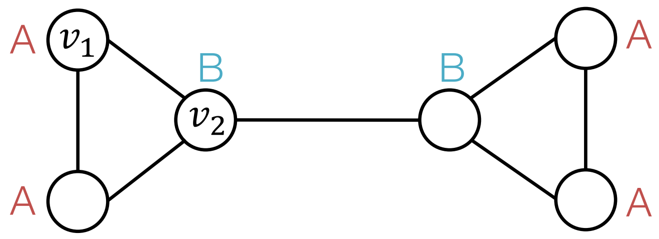
Stanford CS224W: Position-aware Graph Neural Networks

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Two Types of Tasks on Graphs

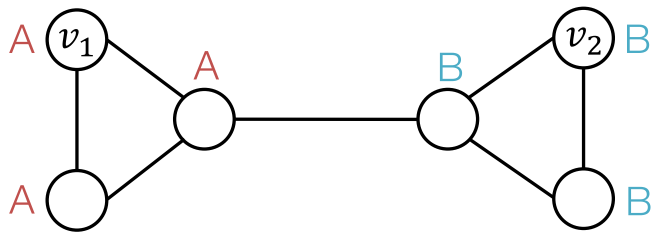
- **There are two types of tasks on graphs**

Structure-aware task



- Nodes are labeled by their **structural roles** in the graph

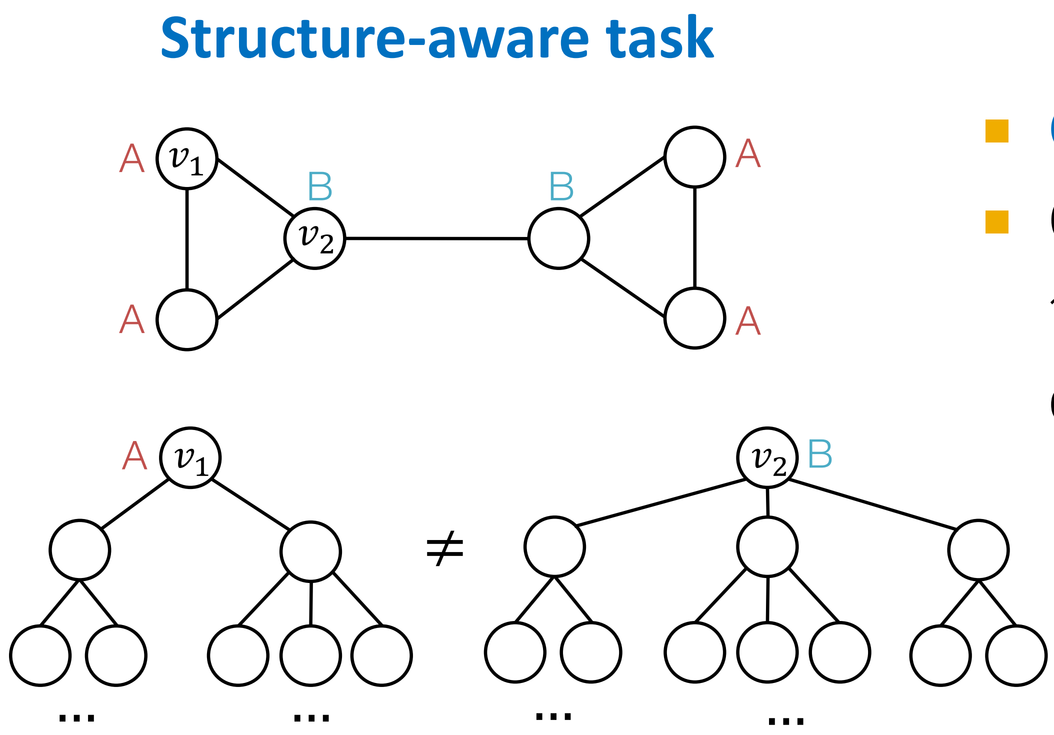
Position-aware task



- Nodes are labeled by their **positions** in the graph

Structure-aware Tasks

- **We showed how to design GNNs to work well for structure-aware tasks**

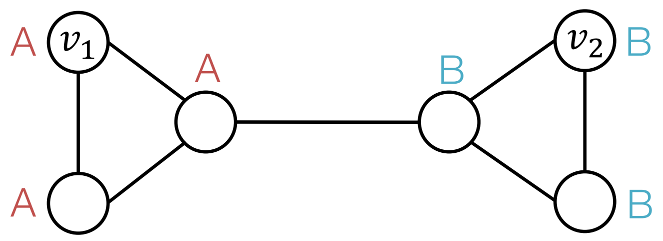


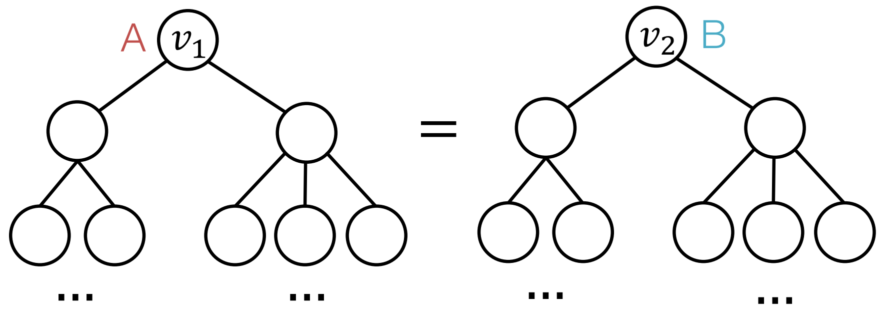
- GNNs work ☺
- Can differentiate v_1 and v_2 by using different computational graphs

Position-aware Tasks

- **GNNs will always fail for position-aware tasks**

Position-aware task

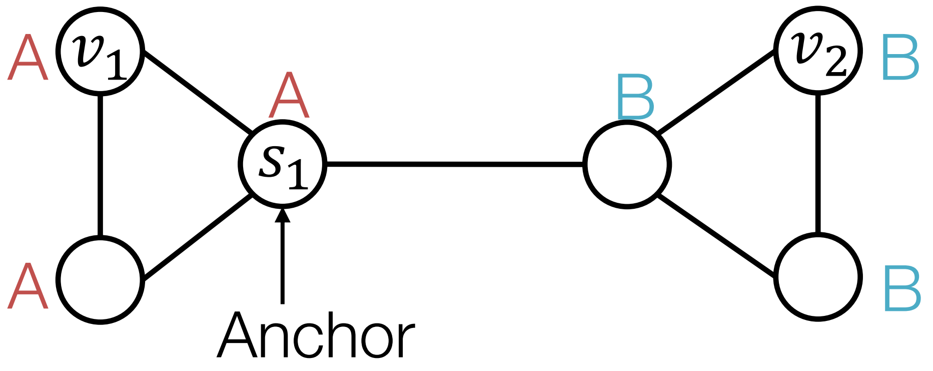




- GNNs fail ☹
- v_1 and v_2 will always have the same computational graph, **due to structure symmetry**
- **Can we define deep learning methods that are position-aware?**

Power of "Anchor"

- Randomly pick a node s_1 as an **anchor node**
- Represent v_1 and v_2 via their relative distances w.r.t. the anchor s_1, **which are different**
- An anchor node serves as **a coordinate axis**
  - Which can be used to **locate nodes in the graph**

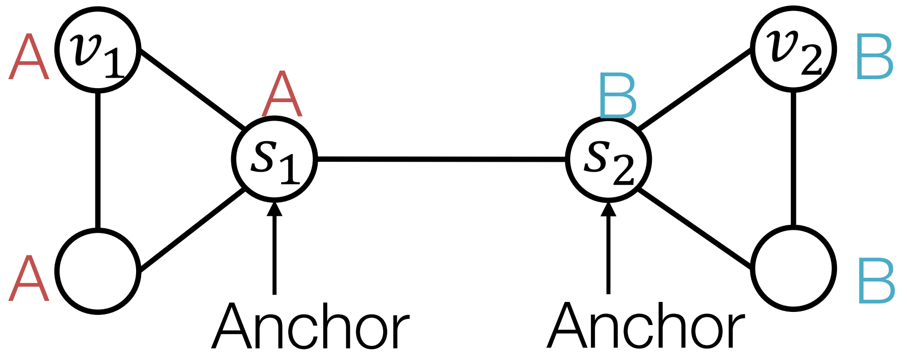


Relative Distances

	s_1
v_1	1
v_2	2

Power of "Anchors"

- Pick more nodes s_1, s_2 as **anchor nodes**
- **Observation:** More anchors can better characterize node position in different regions of the graph
- Many anchors –> Many coordinate axes

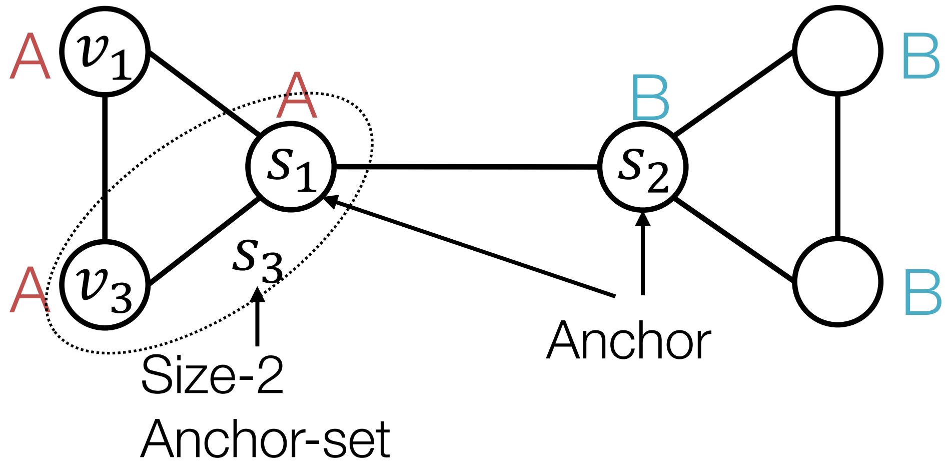


Relative Distances

	s_1	s_2
v_1	1	2
v_2	2	1

Power of “Anchor-sets”

- Generalize anchor from a single node to **a set of nodes**
  - We define distance to an anchor-set as the minimum distance to all the nodes in the ancho-set
- **Observation:** Large anchor-sets can sometimes provide more precise position estimate
  - We can save the total number of anchors



Relative Distances

	s_1	s_2	s_3
v_1	1	2	1
v_3	1	2	0

Anchor s_1, s_2 cannot differentiate node v_1, v_3, but anchor-set s_3 can

Anchor Set: Theory

- **Goal:** Embed the metric space (V, d) into the Euclidian space $\mathbb{R}^k$ such that the original distance metric is preserved.
  - For every node pairs $u, v \in V$, the Euclidian embedding distance $||\boldsymbol{z}_u - \boldsymbol{z}_v||_2$ is close to the original distance metric $d(u, v)$.

Anchor Set: Theory

- Bourgain Theorem [Informal] [Bourgain 1985]
  - Consider the following embedding function of node $v \in V$.

$$f(v) = \left(d_{\min}(v, S_{1,1}), d_{\min}(v, S_{1,2}), \ldots, d_{\min}(v, S_{\log n, c \log n})\right) \in \mathbb{R}^{c \log^2 n}$$

  - where
    - c is a constant.
    - $S_{i,j} \subset V$ is chosen by including each node in V independently with probability $\frac{1}{2^i}$.
    - $d_{\min}(v, S_{i,j}) \equiv \min_{u \in S_{i,j}} d(v, u)$.
  - **The embedding distance produced by f is provably close to the original distance metric (V, d).**

Anchor Set: Theory

P-GNN follows the theory of Bourgain theorem

- First samples $O(\log^2 n)$ anchor sets $S_{i,j}$.
- Embed each node v via

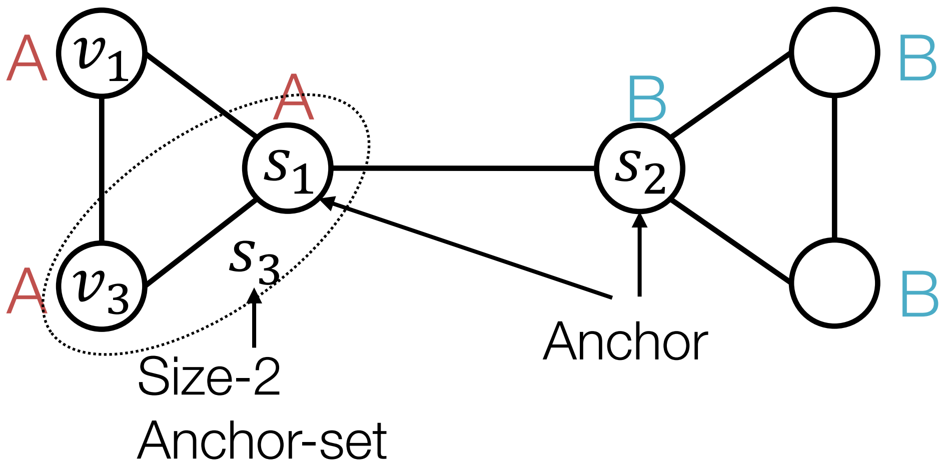
$$\left(d_{\min}(v, S_{1,1}), d_{\min}(v, S_{1,2}), \ldots, d_{\min}(v, S_{\log n, c\log n})\right) \in \mathbb{R}^{c \log^2 n}.$$

P-GNN maintains the inductive capability

- During training, new anchor sets are *re-sampled* every time.
- P-GNN is learned to operate over the new anchor sets.
- At test time, given a new unseen graph, new anchor sets are sampled.

Position Information: Summary

- **Position encoding for graphs:** Represent a node's position by its distance to randomly selected anchor-sets
  - Each dimension of the position encoding is tied to an anchor-set



	s_1	s_2	s_3
v_1	1	2	1
v_3	1	2	0

v_1's Position encoding

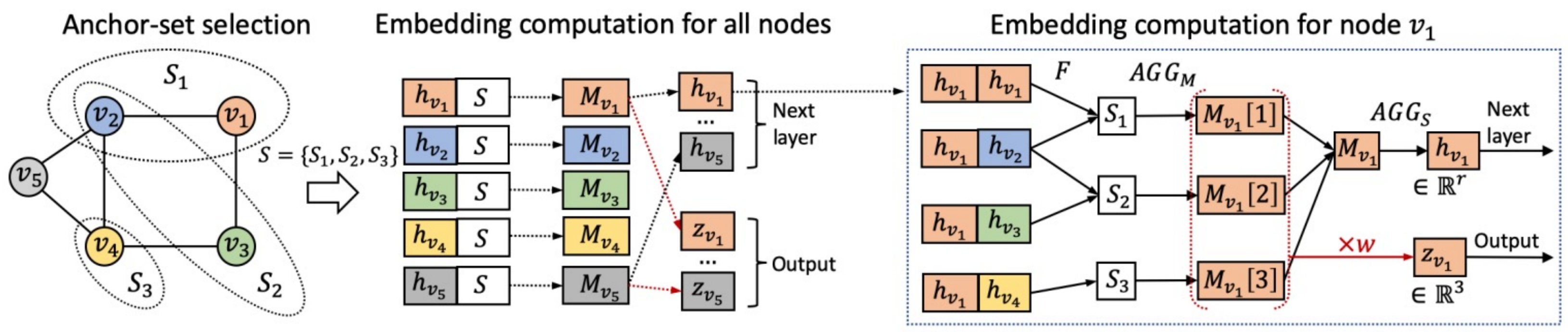
v_3's Position encoding

How 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

How 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
  - Position-aware GNN paper has more details


Anchor-set selection
S_1
v_1
v_2
v_3
v_4
v_5
S_2
S_3
$S = \{S_1, S_2, S_3\}$
Embedding computation for all nodes
h_{v_1} S M_{v_1}
h_{v_2} S M_{v_2}
h_{v_3} S M_{v_3}
h_{v_4} S M_{v_4}
h_{v_5} S M_{v_5}
h_{v_1} … h_{v_5}
Next layer
z_{v_1} … z_{v_5}
Output
Embedding computation for node v_1
F
AGG_M
h_{v_1} h_{v_1}
h_{v_1} h_{v_2}
h_{v_1} h_{v_3}
h_{v_1} h_{v_4}
S_1
S_2
S_3
$M_{v_1}[1]$
$M_{v_1}[2]$
$M_{v_1}[3]$
AGG_S
M_{v_1}
h_{v_1}
$\in \mathbb{R}^r$
Next layer
$\times w$
z_{v_1}
$\in \mathbb{R}^3$
Output