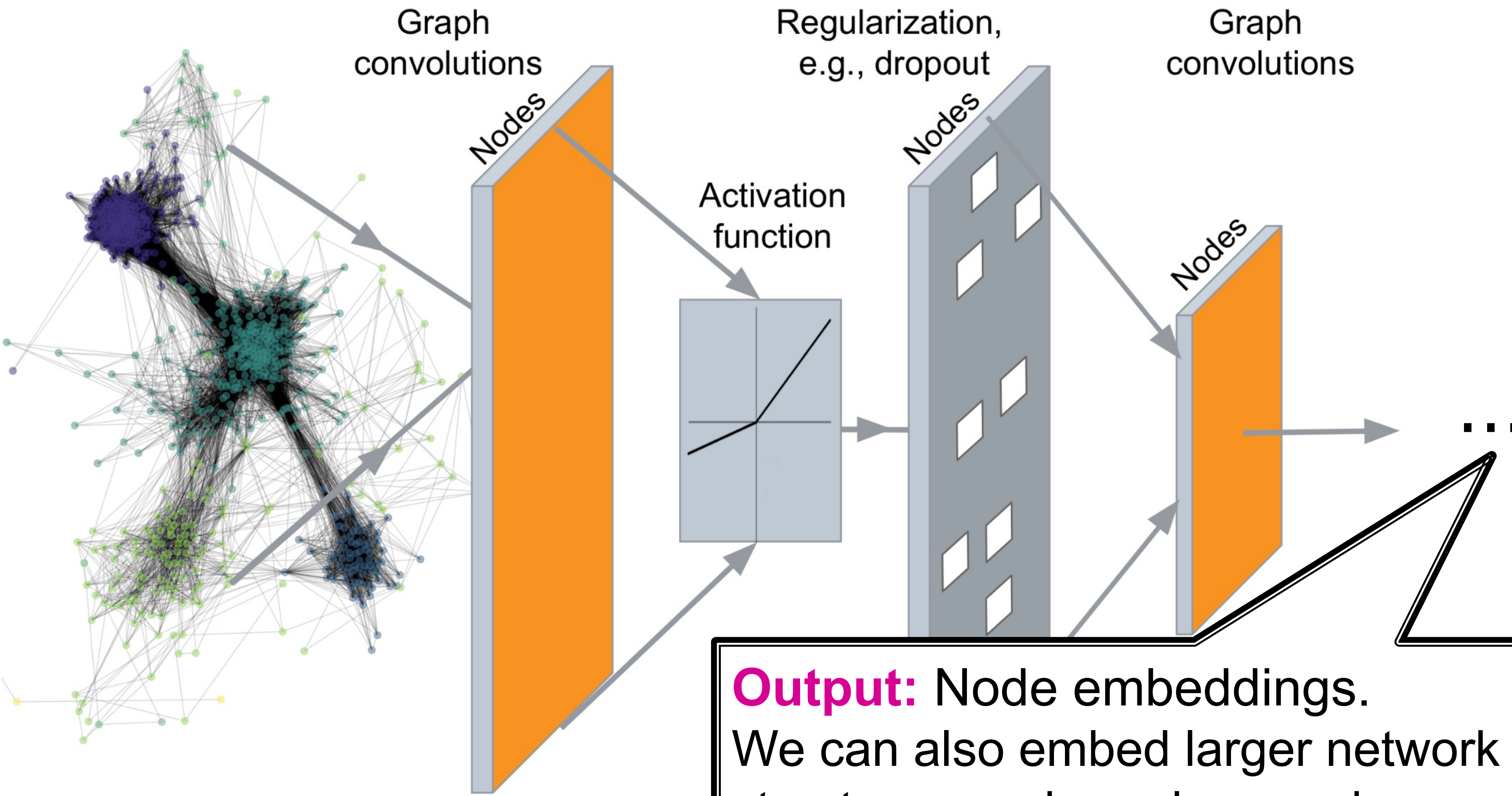
Stanford CS224W: Advanced Topics in Graph Neural Networks

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

UPCOMING EXAM

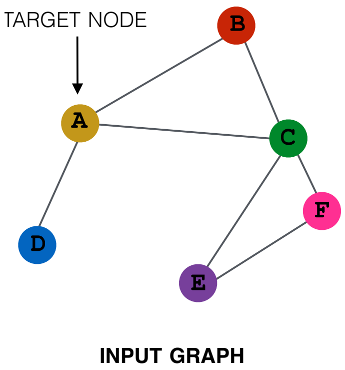
- **Exam coming up this Friday 11/19**
  - Make-up exam on Wed 11/17
  - Administered on Gradescope: open-book, take-home
  - Exam is open for 24 hours, you can take it in any 2-hour
  - If you need an extension (OAE), please request it now!
- **Highly recommend** looking over the **Exam Prep OH** slides and recording (see Ed for links)
  - We covered exam topics, format, and studying tips; reviewed three key concepts

Recap: Graph Neural Networks



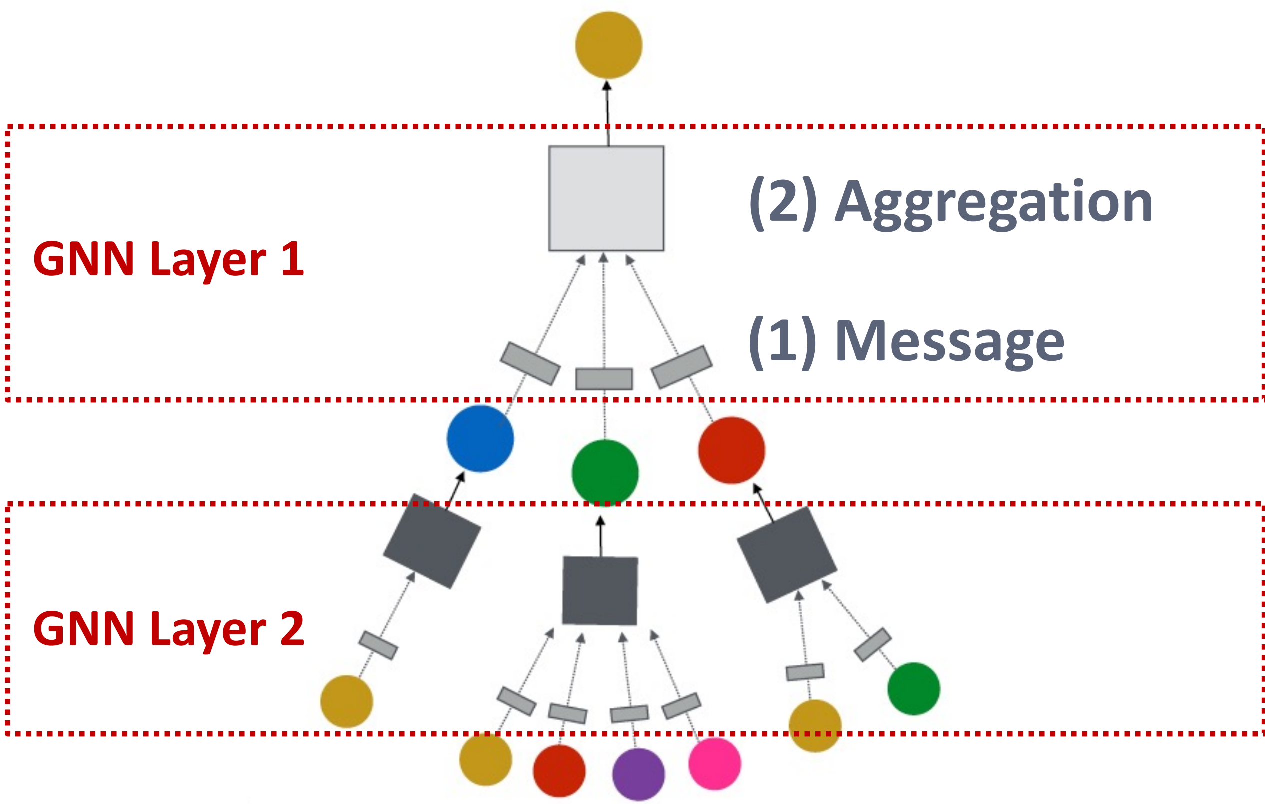
Output: Node embeddings.
We can also embed larger network structures, subgraphs, graphs

Recap: A General GNN Framework



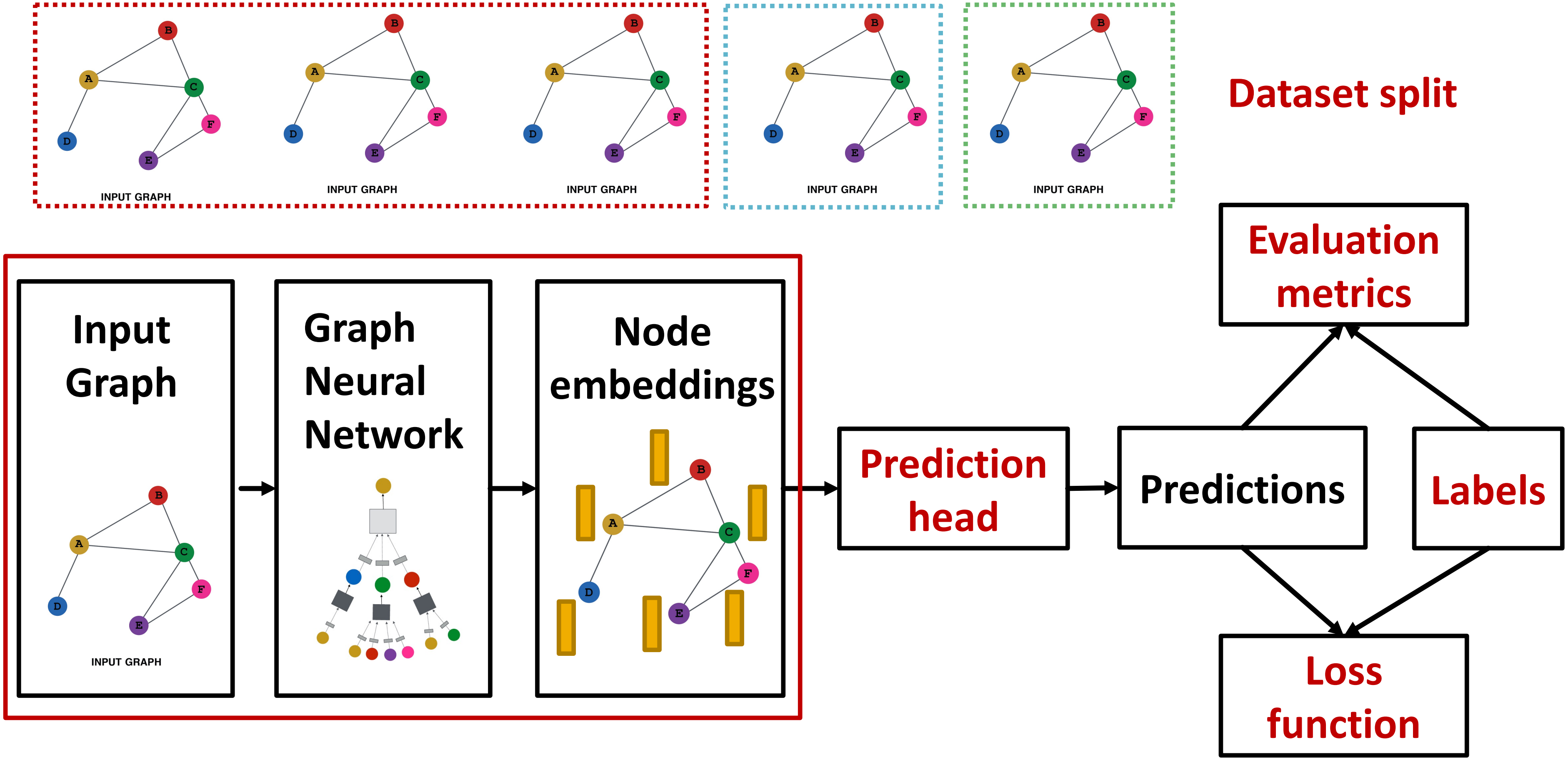
(5) Learning objective

(3) Layer connectivity



(4) Graph augmentation

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
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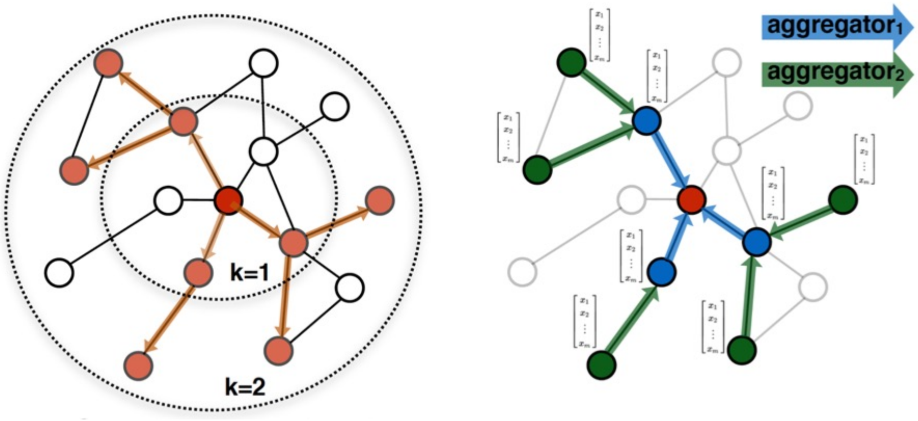
A "Perfect" GNN Model

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

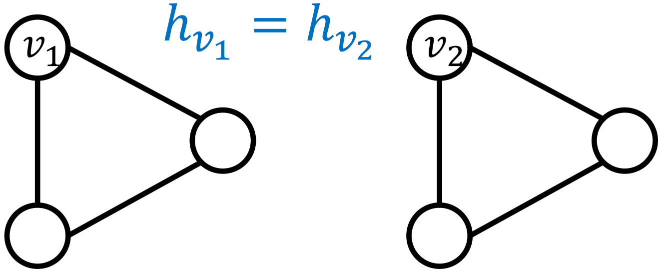


  - A perfect GNN should build **an injective function** between neighborhood structure (regardless of hops) and node embeddings

A "Perfect" GNN Model

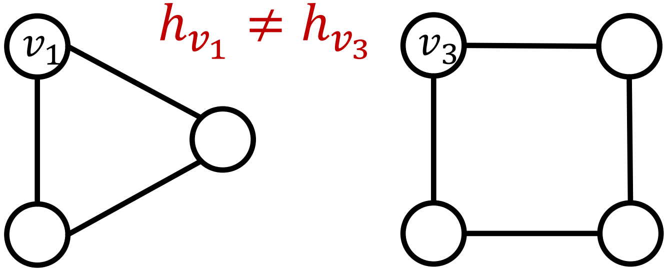
- **Therefore, for a perfect GNN:**
  - **Observation 1:** If two nodes have the same neighborhood structure, they must have the same embedding

$$h_{v_1} = h_{v_2}$$



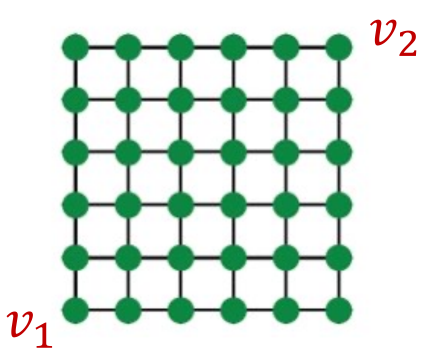
  - **Observation 2:** If two nodes have different neighborhood structure, they must have different embeddings

$$h_{v_1} \neq h_{v_3}$$



Imperfections of Existing GNNs

- **However, Observations 1 & 2 are imperfect**
- **Observation 1 could 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

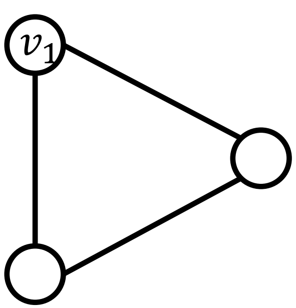
NYC road network

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

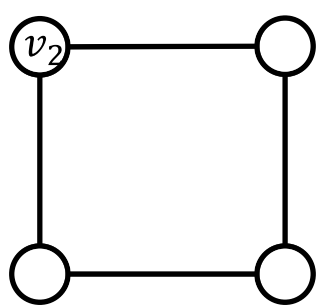
Imperfections of Existing GNNs

- **Observation 2 often cannot be satisfied:**
  - **The GNNs we have introduced so far are not perfect**
  - In Lecture 9, we discussed that their expressive power is **upper bounded by the WL test**
  - For example, message passing GNNs **cannot count cycle length:**

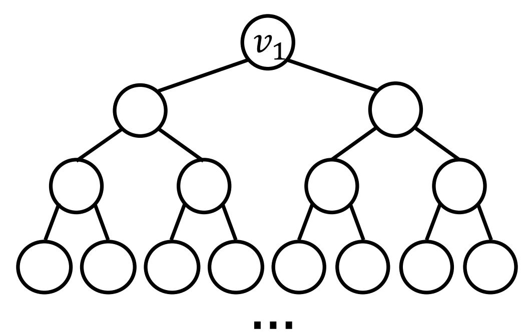
v_1 resides in a cycle with length 3



v_2 resides in a cycle with length 4



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

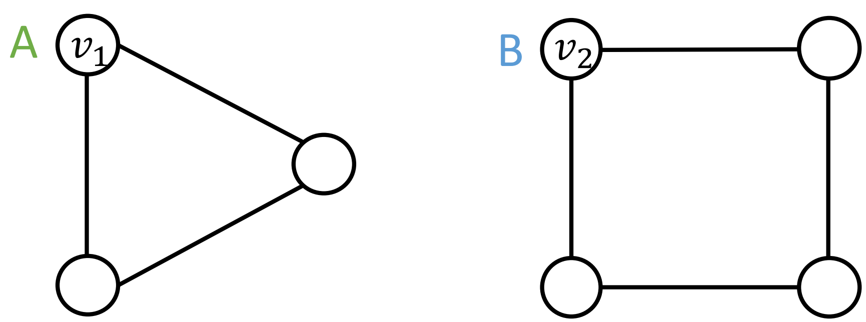


Plan for the Lecture

- We will resolve both issues 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

Our Approach

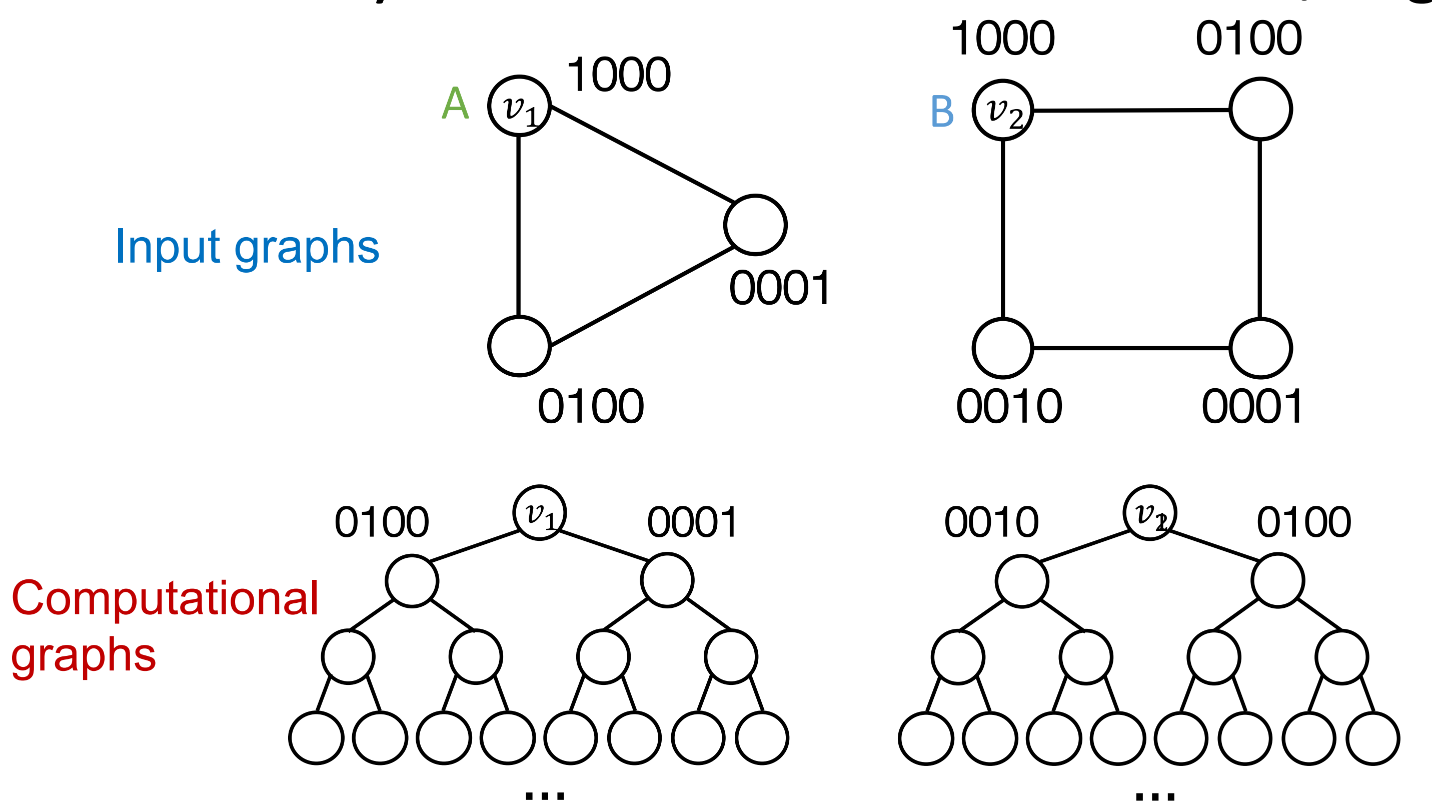
- **We use the following thinking:**
  - Two different inputs (nodes, edges, graphs) are labeled differently
  - A "failed" model will always assign the same embedding to them
  - A "successful" model will assign different embeddings to them
  - **Embeddings are determined by GNN computational graphs:**



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

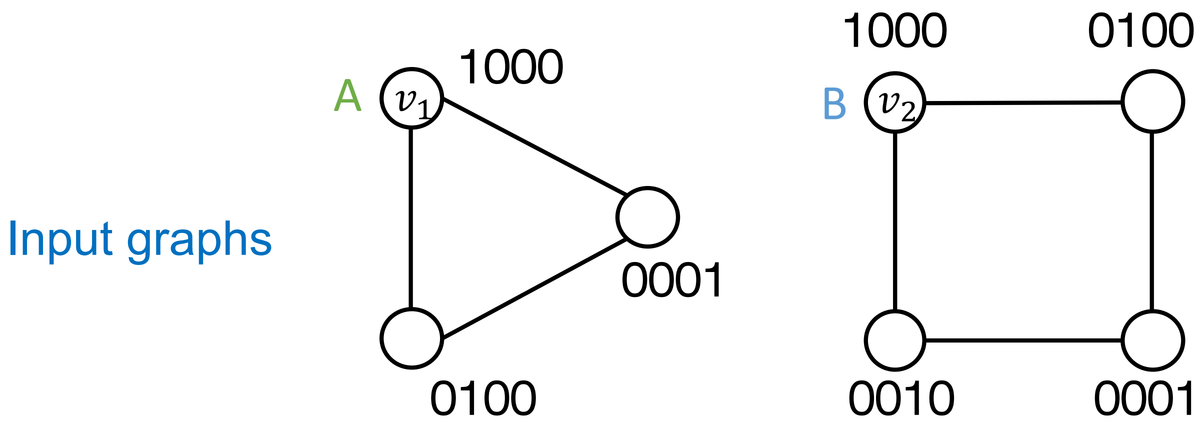
- **A naïve solution:** One-hot encoding
  - Encode each node with a different ID, then we can always differentiate different nodes/edges/graphs



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

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



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

Stanford CS224W: Position-aware Graph Neural Networks

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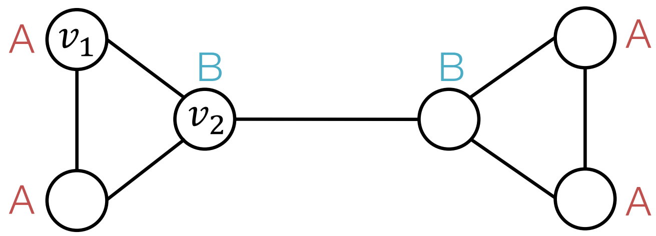
Two Types of Tasks on Graphs

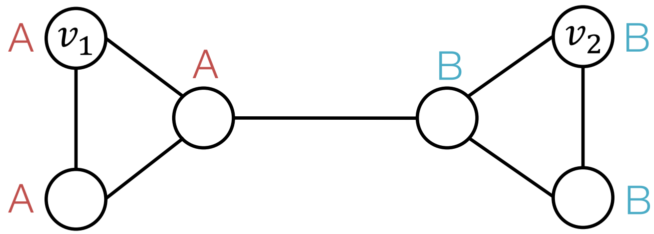
- **There are two types of tasks on graphs**

Structure-aware task



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

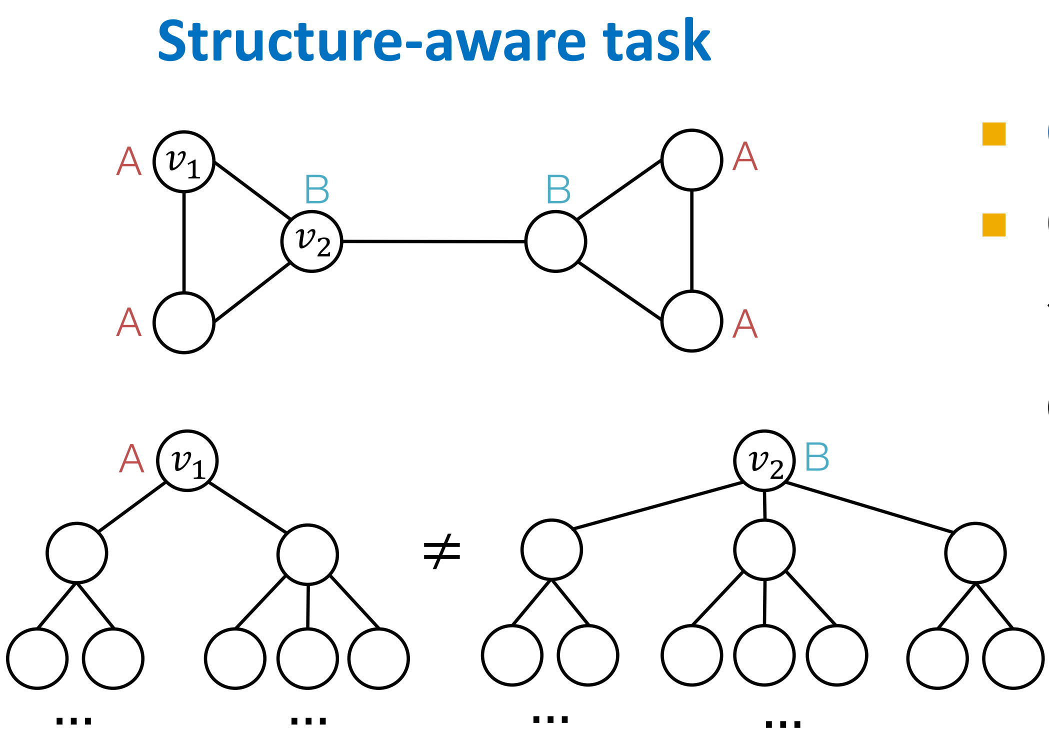
Position-aware task



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

Structure-aware Tasks

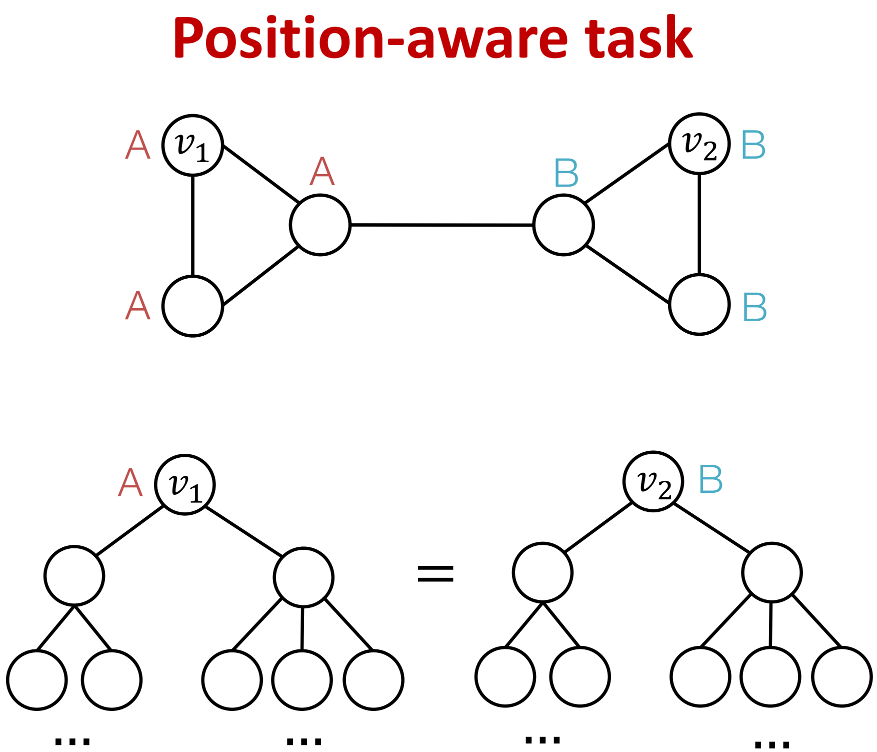
- **GNNs often work well for structure-aware tasks**



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

Position-aware Tasks

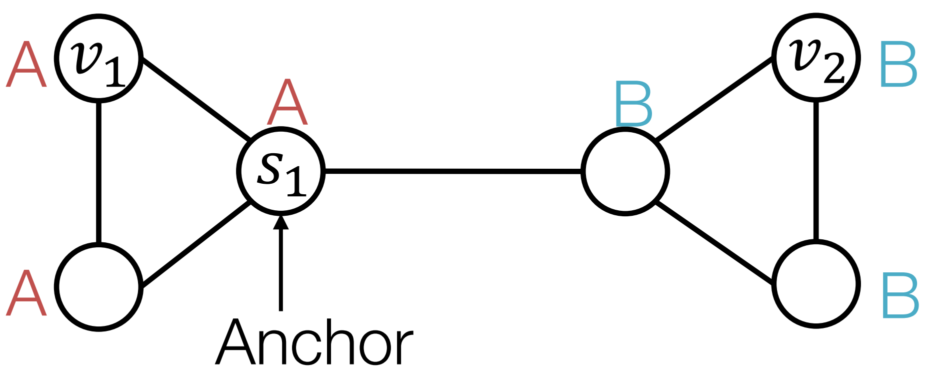
- **GNNs will always fail for position-aware tasks**



- 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**

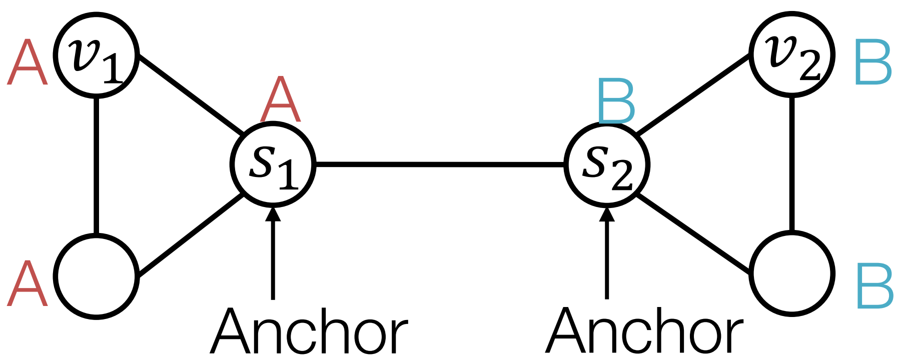


Relative Distances

	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

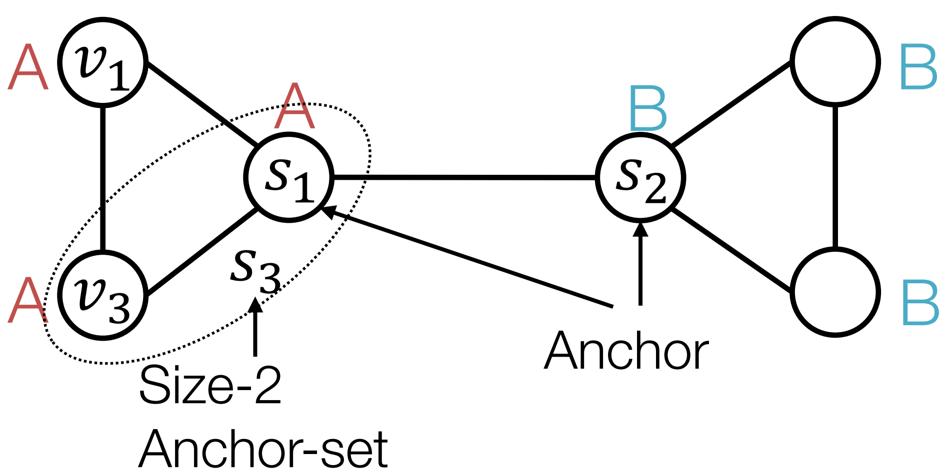


Relative Distances

	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 $v \in V$.

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

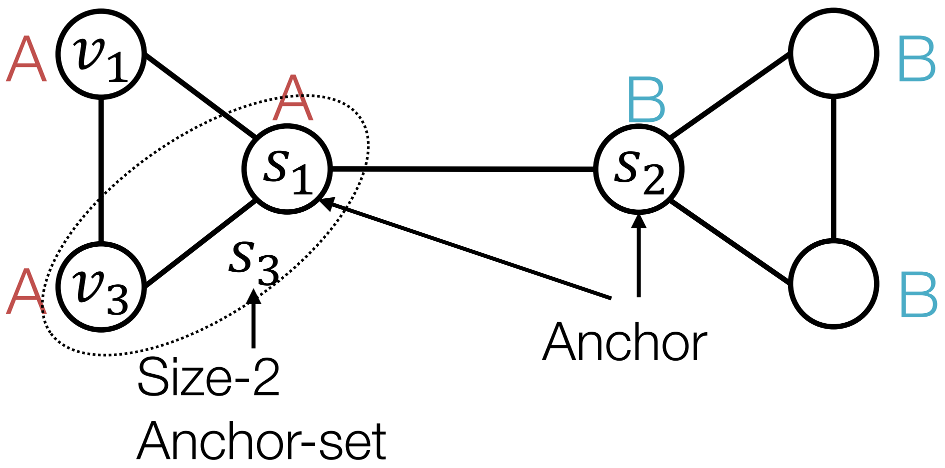
  - where
    - c is a constant.
    - $S_{i,j} \subset V$ is chosen by including each node in V independently with probability $\frac{1}{2^i}$.
    - $d_{\min}(v, S_{i,j}) \equiv \min_{u \in S_{i,j}} d(v, u)$.
  - **The embedding distance produced by f is provably close to the original distance metric (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 $\left(d_{\min}(v, S_{1,1}), d_{\min}(v, S_{1,2}), \dots, d_{\min}(v, S_{\log n, c\log n})\right) \in \mathbb{R}^{c\log^2 n}$.
- **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
  - Refer to the Position-aware GNN paper for more details

Stanford CS224W: Identity-Aware Graph Neural Networks

CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
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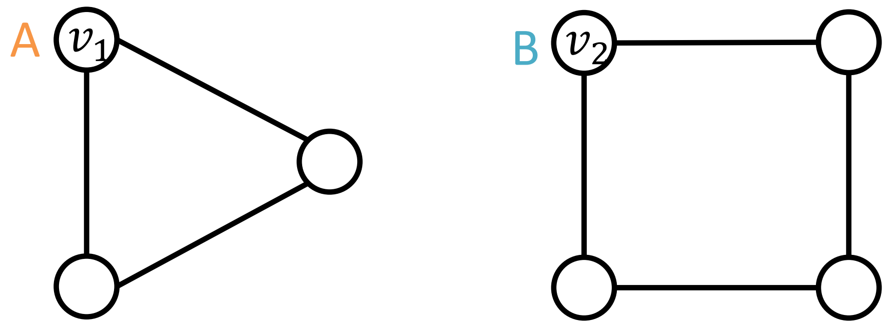
More Failure Cases for GNNs

- We learned that **GNNs would fail for position-aware tasks**
- **But can GNN perform perfectly in structure-aware tasks?**
  - Unfortunately, **NO.**
- GNNs exhibit three levels of failure cases in structure-aware tasks:
  - Node level
  - Edge level
  - Graph level

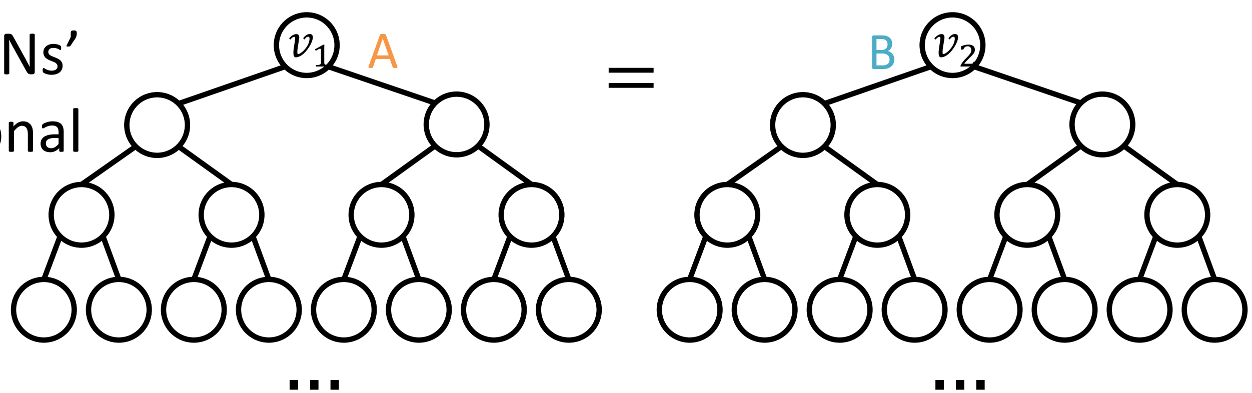
GNN Failure 1: Node-level Tasks

Different Inputs but the same computational graph → GNN fails

Example input graphs



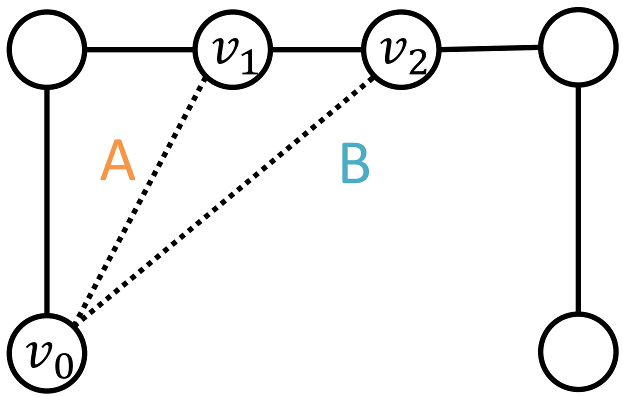
Existing GNNs' computational graphs



GNN Failure 2: Edge-level Tasks

Different Inputs but the same computational graph → GNN fails

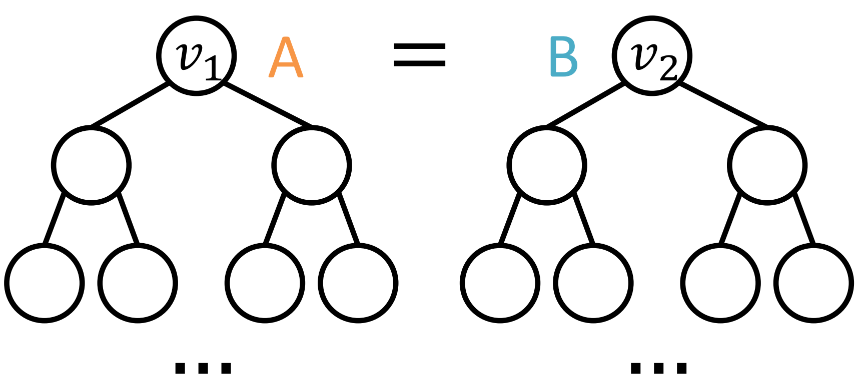
Example input graphs



Edge A and B share node v_0

We look at embeddings for v_1 and v_2

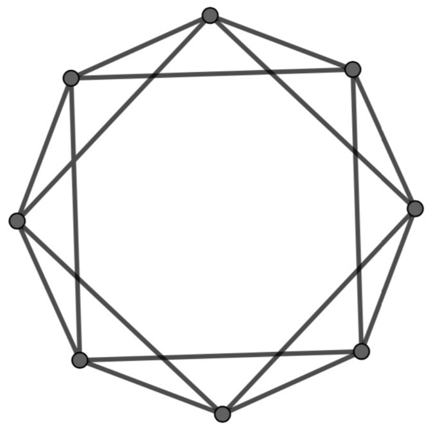
Existing GNNs' computational graphs



GNN Failure 3: Graph-level Tasks

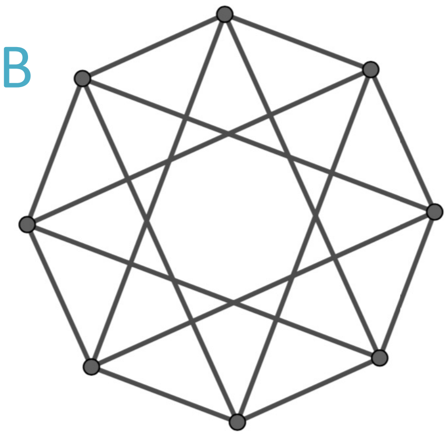
Different Inputs but the same computational graph → GNN fails

Example input graphs



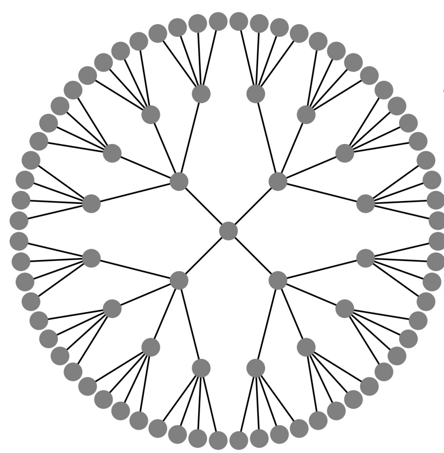
A

B



We look at embeddings for each node

For each node:



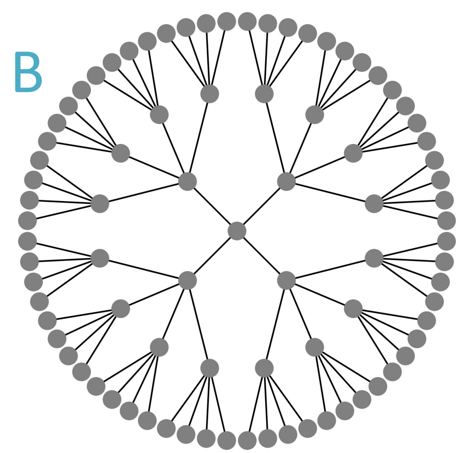
A

Existing GNNs' computational graphs

=

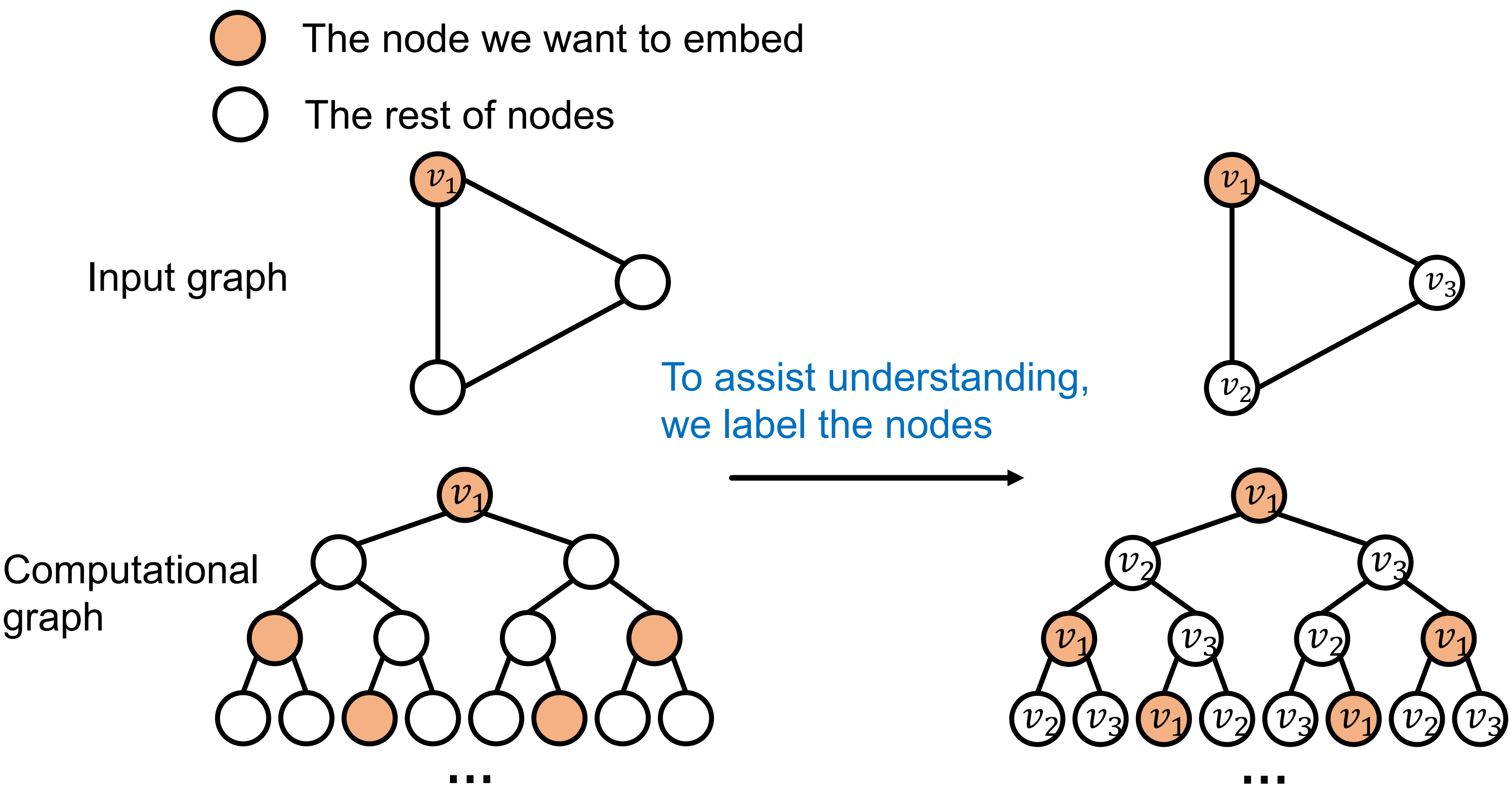
For each node:

B



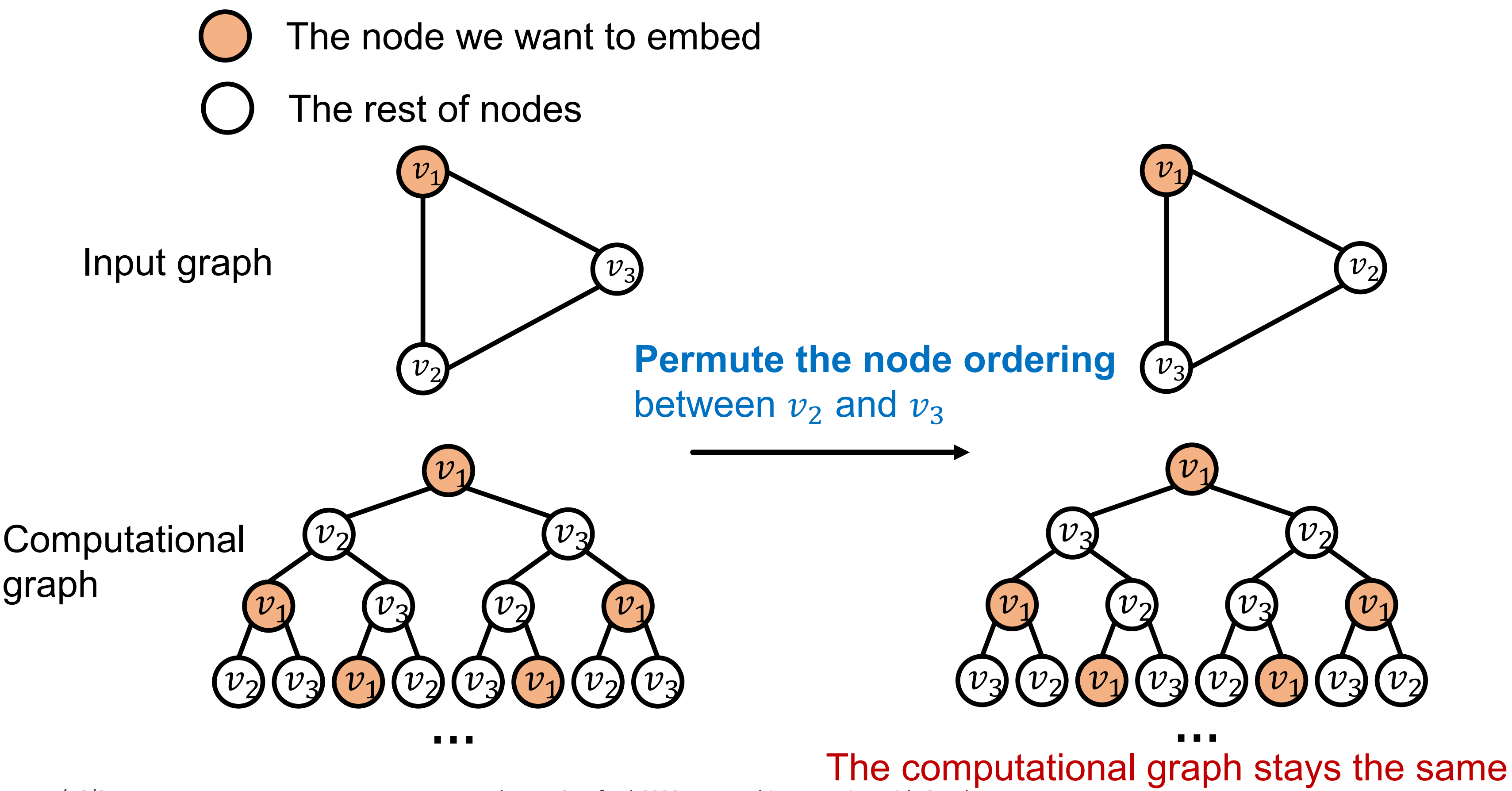
Idea: Inductive Node Coloring

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



Idea: Inductive Node Coloring

- This coloring is **inductive**:
  - It is invariant to node ordering/identities

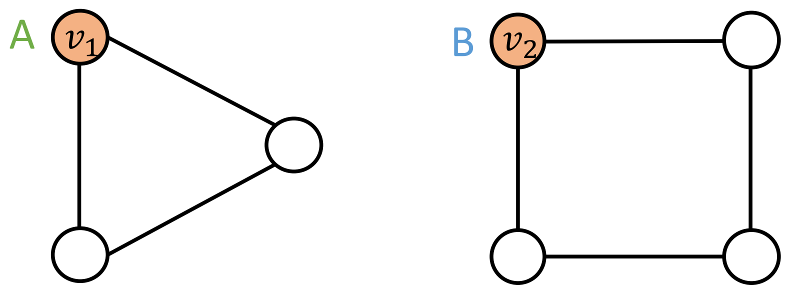


Inductive Node Coloring – Node level

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

Node classification

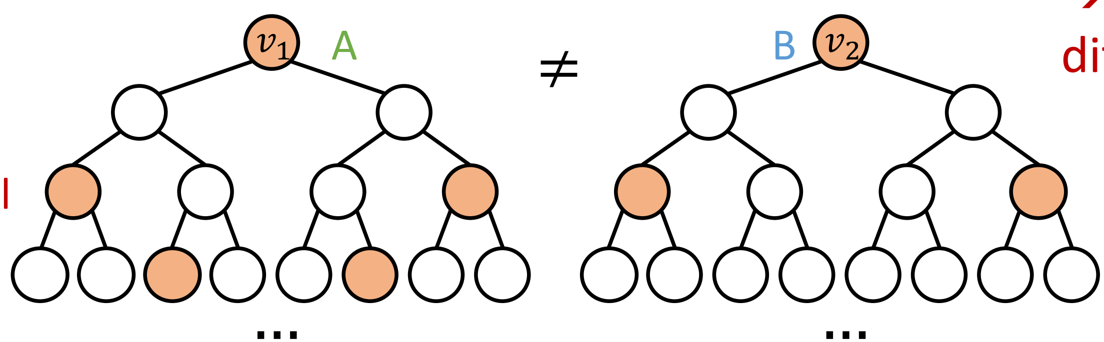
Example input graphs



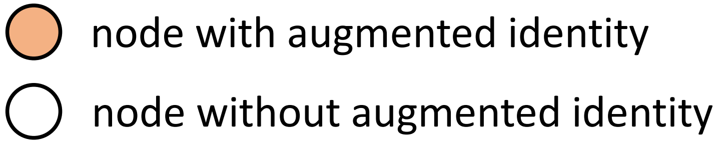
Different computational graphs → Successfully differentiate nodes

We color root nodes with identity

ID-GNNs' computational graphs



Two types of nodes:

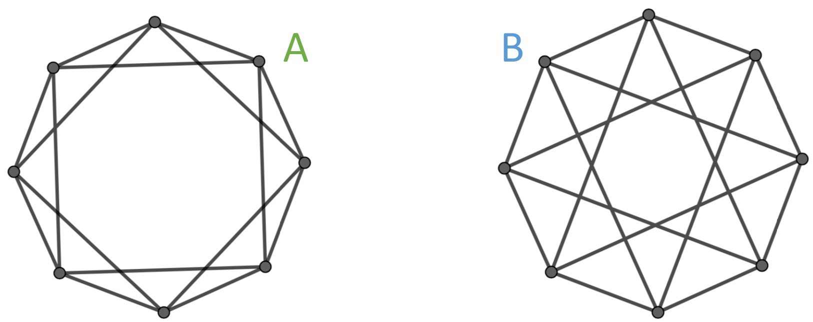


Inductive Node Coloring – Graph Level

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

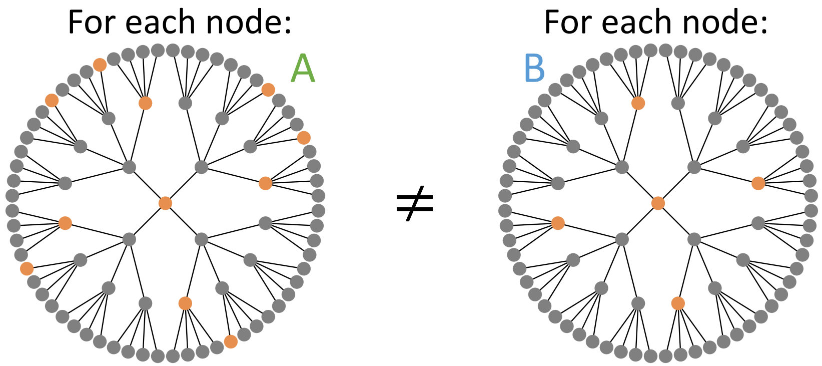
Graph classification

Example input graphs



We color root nodes with identity

ID-GNNs' computational graphs



Different computational graphs → Successful differentiate graphs

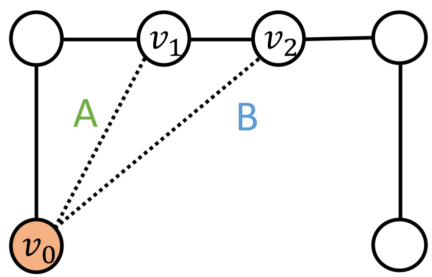
Two types of nodes:
node with augmented identity
node without augmented identity

Inductive Node Coloring – Edge Level

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

Link prediction

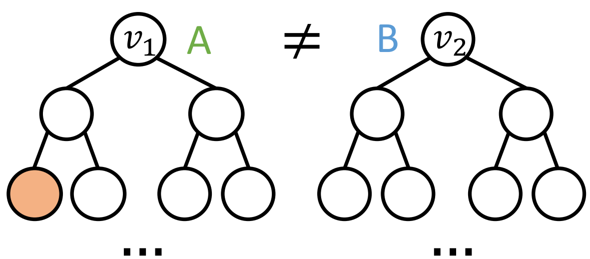
Example input graphs



An edge-level task involves classifying a pair of nodes:

1. We color one of the node (v_0)
2. We then embed the other node in the node pair (v_1 or v_2)
3. We use the node embedding for v_1 or v_2 conditioned on v_0 being colored or not to make edge-level prediction

ID-GNNs' computational graphs



Different computational graphs → Successfully differentiate edges

Two types of nodes:

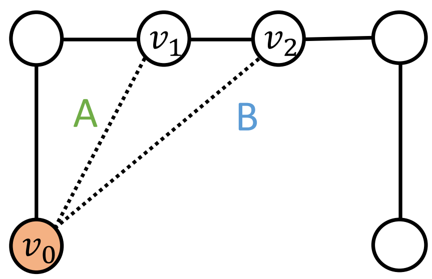
- node with augmented identity
- node without augmented identity

Inductive Node Coloring – Edge Level

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

Link prediction

Example input graphs



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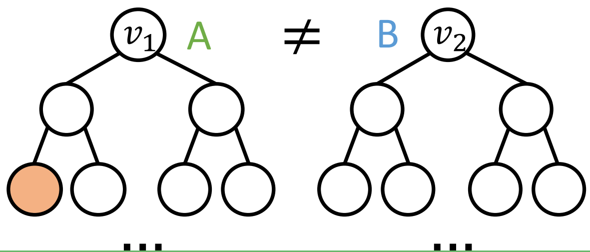
ID-GNNs' computational graphs



Different

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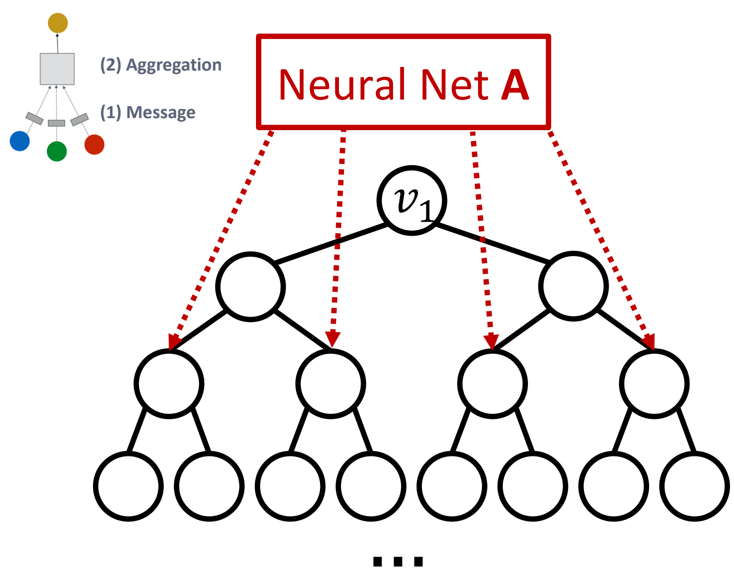
Two

How to build a GNN using node coloring?

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

Identity-aware GNN

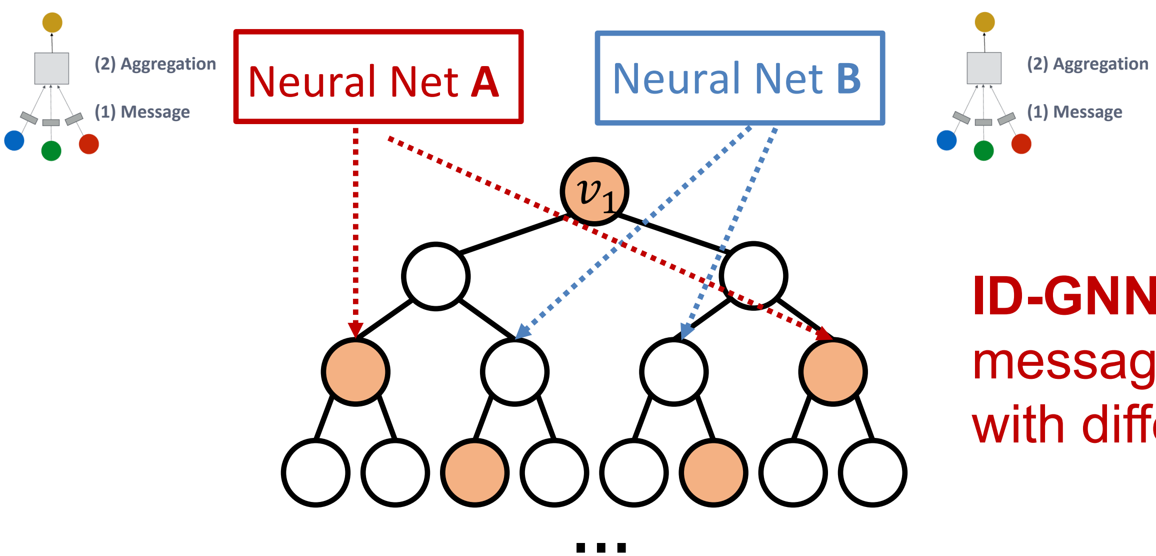
- **Utilize inductive node coloring** in embedding computation
  - **Idea: Heterogenous message passing**
    - Normally, a GNN applies **the same message/aggregation computation to all the nodes**



GNN: At a given layer, we apply the same message/aggregation to each node

Identity-aware GNN

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



ID-GNN: At a given layer, different message/aggregation to nodes with different colorings

Identity-aware GNN

- **Output**: Node embedding $\boldsymbol{h}_v^{(K)}$ for $v \in \mathcal{V}$.
- **Step 1**: Extract the ego-network
  - $\mathcal{G}_v^{(K)}$: K-hop neighborhood graph around v
  - Set the initial node feature
    - For $u \in \mathcal{G}_v^{(K)}$, $\boldsymbol{h}_u^{(0)} \leftarrow \boldsymbol{x}_u$ (input node feature)

Identity-aware GNN

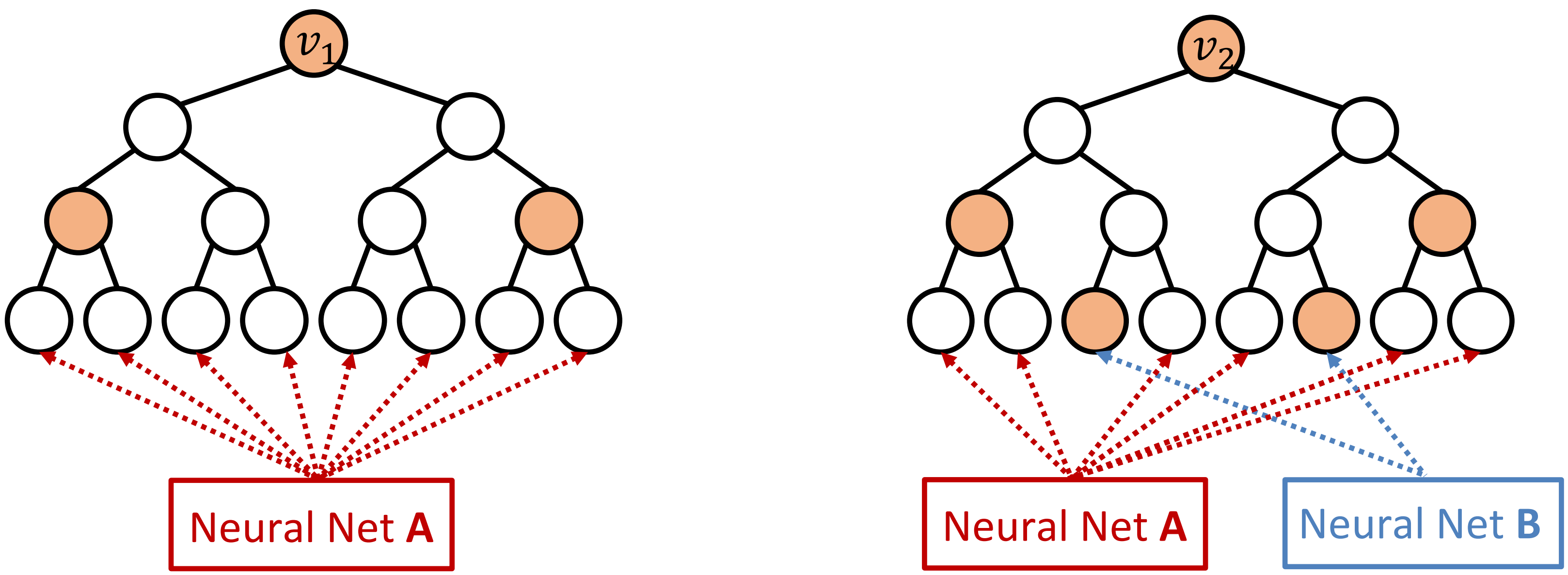
- **Step 2**: Heterogeneous message passing
  - For $k = 1, \dots, K$ do
    - For $u \in \mathcal{G}_v^{(K)}$ do

$$\boldsymbol{h}_{\boldsymbol{u}}^{(\boldsymbol{k})} \leftarrow AGG^{(k)}\left(\left\{\mathrm{MSG}_{\mathbf{1}[s=v]}^{(k)}\left(\boldsymbol{h}_s^{(k-1)}\right), s \in N(u)\right\}, \boldsymbol{h}_u^{(k-1)}\right)$$

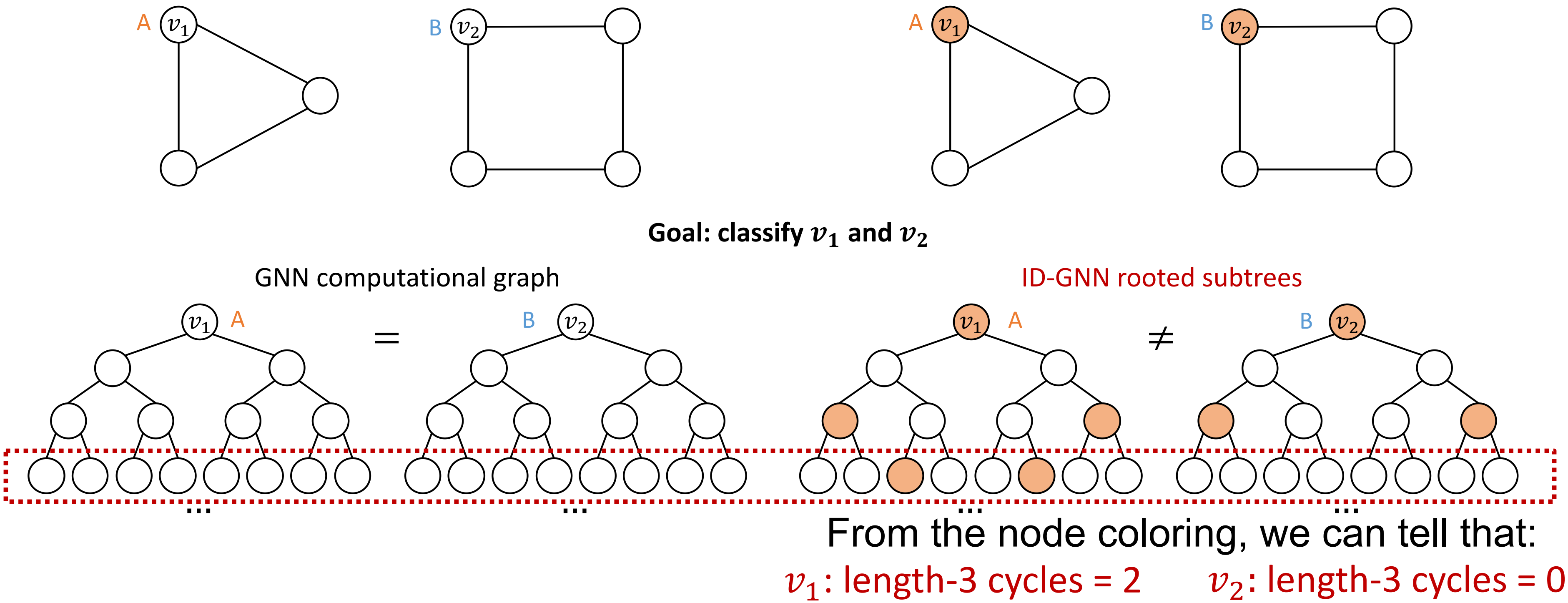
Depending on whether $s = v$ (s is the center node v) or not, we use different neural network functions to transform $\boldsymbol{h}_s^{(k-1)}$.

Identity-aware GNN

- **Why does heterogenous message passing work:**
  - Suppose two nodes v_1, v_2 have the same computational graph structure, but have different node colorings
  - Since we will apply different neural network for embedding computation, their embeddings will be different

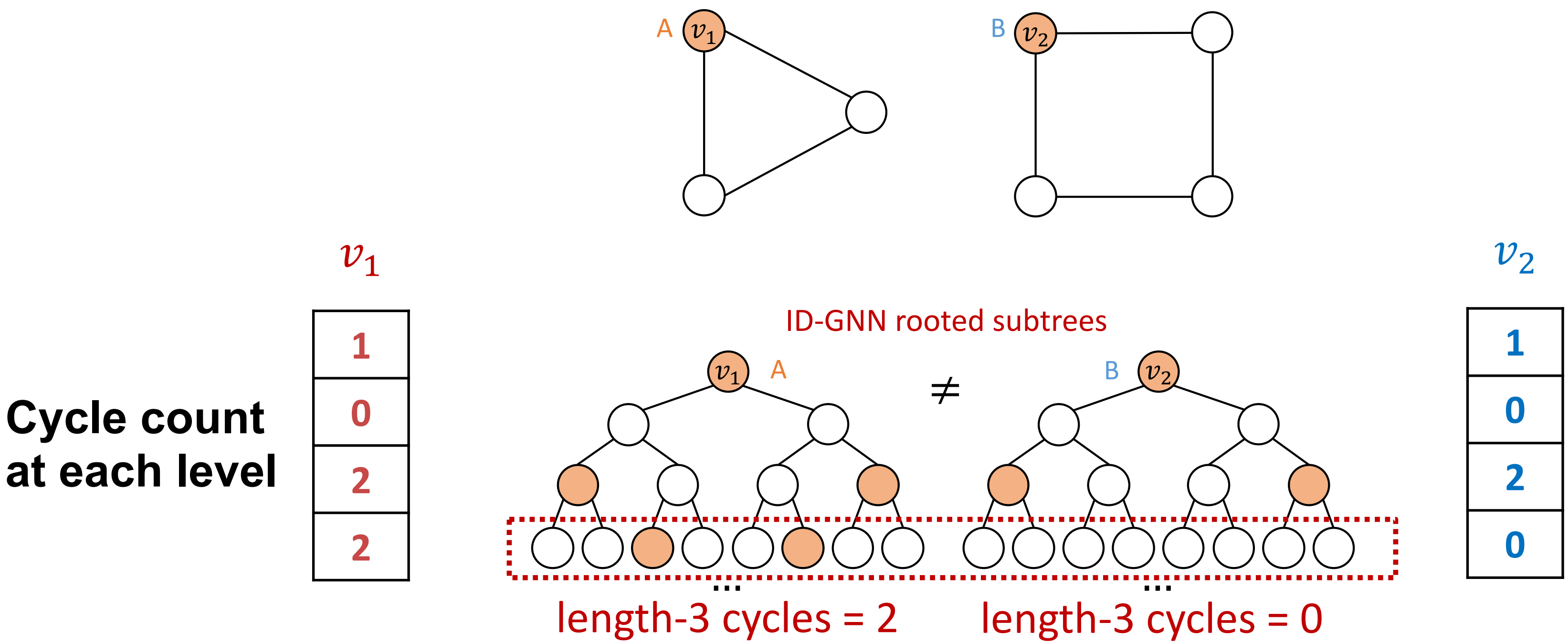


GNN vs ID-GNN



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

Simplified Version: ID-GNN-Fast



- Based on the intuition, we propose 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**

Identity-aware GNN

- **Summary of ID-GNN: A general and powerful extension to GNN framework**
  - We can apply ID-GNN on **any** message passing GNNs (GCN, GraphSAGE, GIN, …)
    - ID-GNN provides **consistent performance gain** in node/edge/graph level tasks
  - ID-GNN is more expressive than their GNN counterparts. ID-GNN is the first message passing GNN that is more expressive than 1-WL test
  - We can easily implement ID-GNN using popular GNN tools (PyG, DGL, …)

Stanford CS224W: Robustness of Graph Neural Networks

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

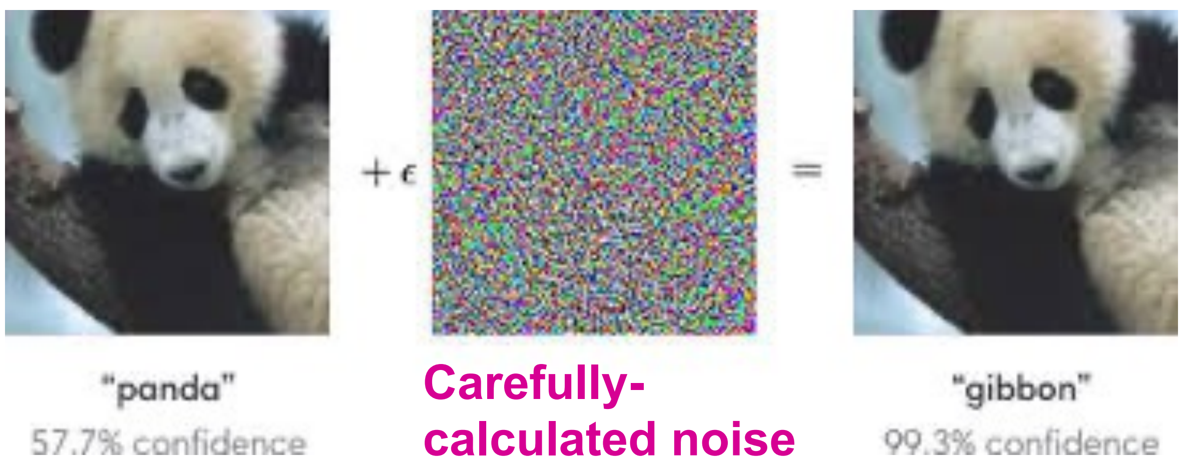
http://cs224w.stanford.edu

Deep Learning Performance

- Recent years have seen **impressive performance of deep learning models in a variety of applications.**
  - Ex) In computer vision, **deep convolutional networks** have achieved human-level performance on ImageNet (image category classification)
- **Are these models ready to be deployed in real world?**

Adversarial Examples

- Deep convolutional neural networks are vulnerable to **adversarial attacks:**
  - Imperceptible noise changes the prediction.



Carefully-calculated noise

Adversarial example

Adopted from Goodfellow et al. ICLR 2015

- Adversarial examples are also reported in natural language processing [Jia & Liang et al. EMNLP 2017] and audio processing [Carlini et al. 2018] domains.

Implication of Adversarial Examples

- **The existence of adversarial examples prevents the reliable deployment of deep learning models to the real world.**
  - Adversaries may try to actively hack the deep learning models.
  - The model performance can become much worse than we expect.
- **Deep learning models are often not robust.**
  - In fact, it is an active area of research to make these models robust against adversarial examples

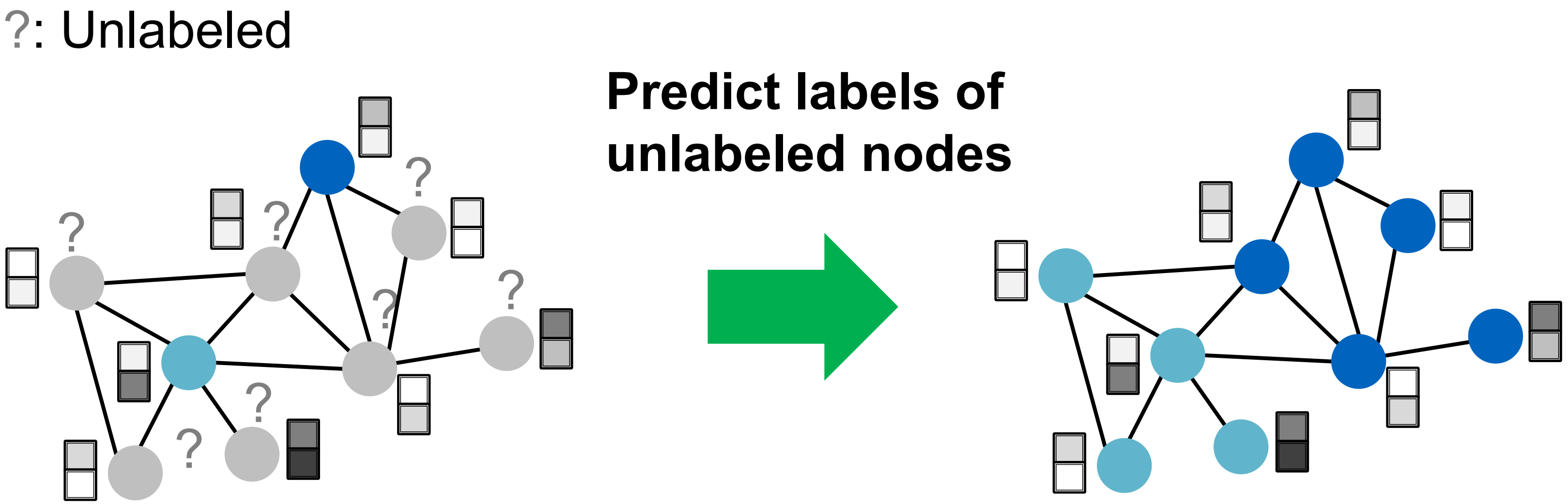
Zügner et al. Adversarial Attacks on Neural Networks for Graph Data, KDD 2018

Robustness of GNNs

- **This lecture: How about GNNs? Are they robust to adversarial examples?**
- **Premise**: Common applications of GNNs involve **public platforms** and **monetary interests**.
  - Recommender systems
  - Social networks
  - Search engines
- Adversaries **have the incentive to** manipulate input graphs and hack GNNs' predictions.

Setting to Study GNNs' Robustness

- To study the robustness of GNNs, we specifically consider the following setting:
  - **Task**: Semi-supervised node classification
  - **Model**: GCN [Kipf & Welling ICLR 2017]

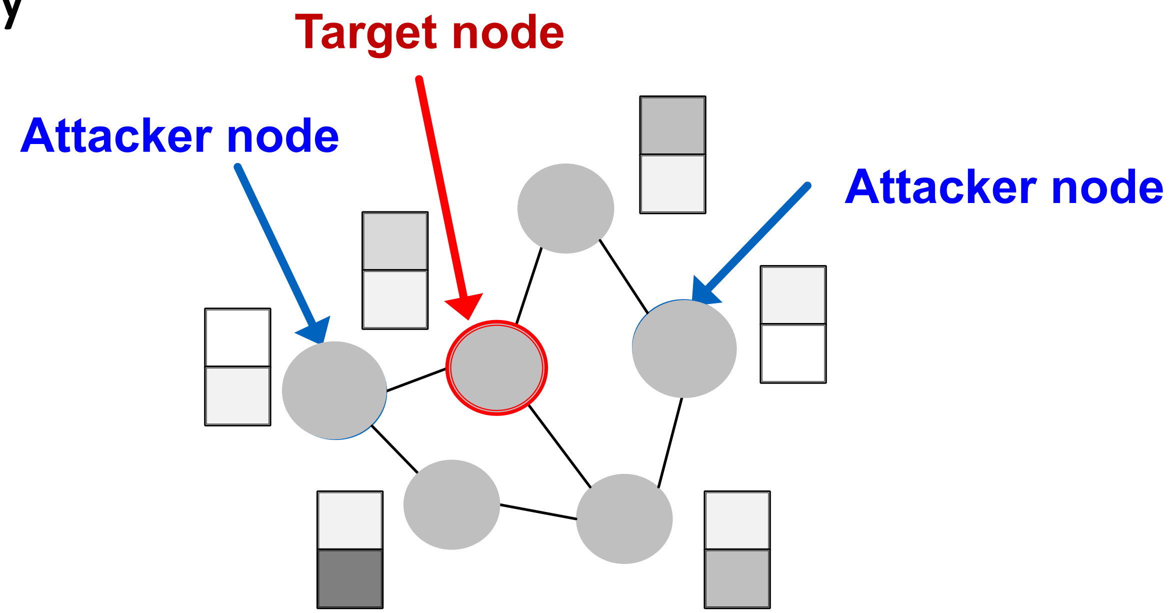


Roadmap

- We first describe several real-world **adversarial attack possibilities**.
- We then review the GCN model that we are going to attack (**knowing the opponent**).
- We mathematically **formalize the attack problem as an optimization problem.**
- **We empirically see how vulnerable GCN's prediction is to the adversarial attack.**

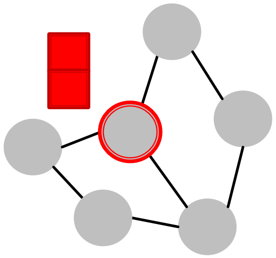
Attack Possibilities

- What are the attack possibilities in real world?
  - **Target node $t \in V$:** node whose label prediction we want to change
  - **Attacker nodes $S \subset V$:** nodes the attacker can modify

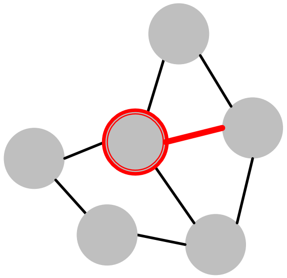


Attack Possibilities: Direct Attack

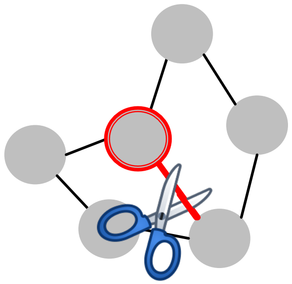
- **Direct Attack: Attacker node is the target node:** $S = \{t\}$
- Modify **target** node feature
  - Ex) Change website content



- Add connections to **target**
  - Ex) Buy likes/followers

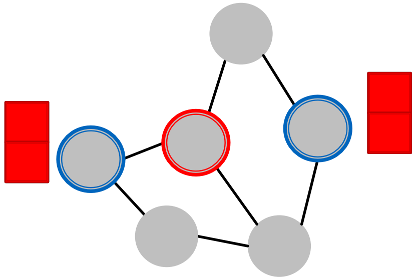


- Remove connections from **target**
  - Ex) Unfollow users

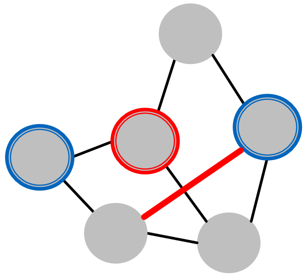


Attack Possibilities: Indirect Attack

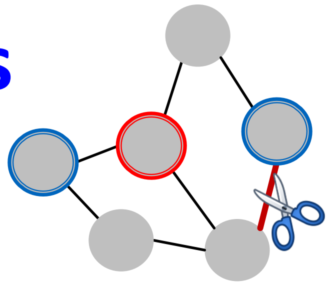
- **Indirect Attack:** **The target node is not in the attacker nodes:** $t \notin S$
- Modify **attacker** node features
  - Ex) Hijack friends of targets



- Add connections to **attackers**
  - Ex) Create a link, link farm



- Remove connections from **attackers**
  - Ex) Delete undesirable link

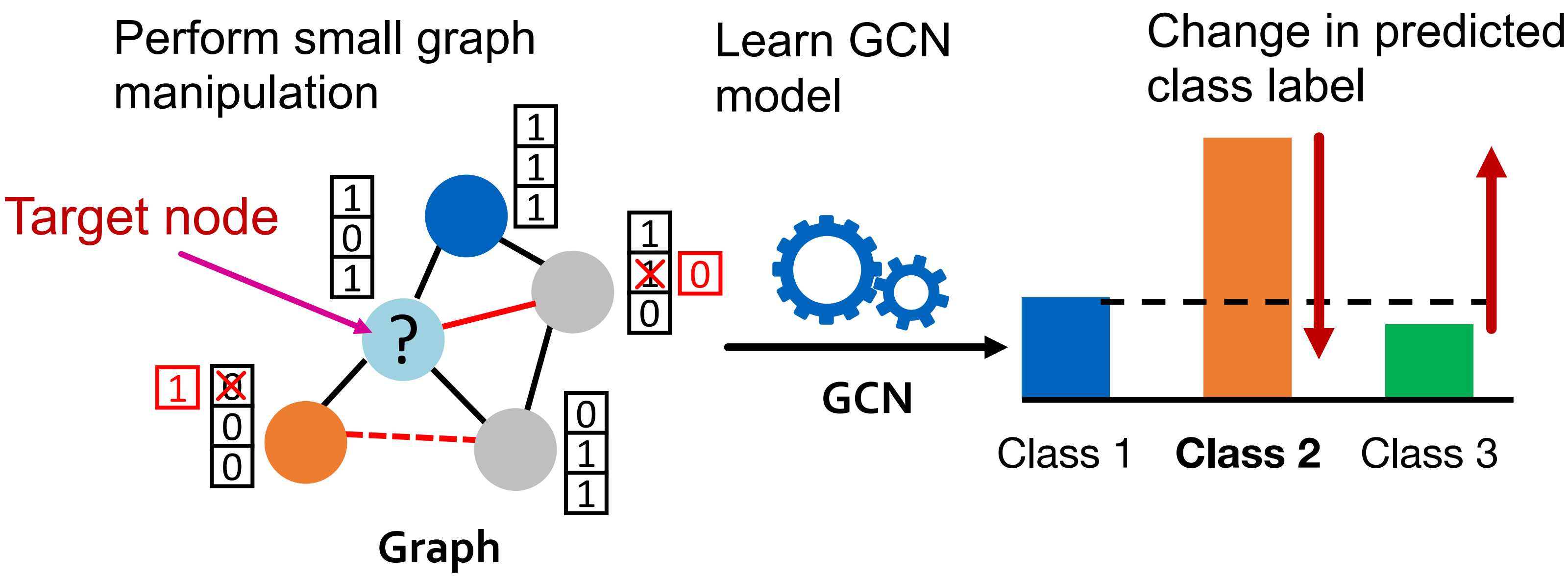


Formalizing Adversarial Attacks

- **Objective for the attacker**:

Maximize (change of target node label prediction)
Subject to (graph manipulation is small)

If graph manipulation is too large, it will easily be detected. Successful attacks should change the target prediction with "unnoticeably-small" graph manipulation.



Mathematical Formulation (1)

- **Original graph**:
  - $\boldsymbol{A}$: adjacency matrix, $\boldsymbol{X}$: feature matrix
- **Manipulated graph (after adding noise):**
  - $\boldsymbol{A}'$: adjacency matrix, $\boldsymbol{X}'$: feature matrix
- **Assumption**: $(\boldsymbol{A}', \boldsymbol{X}') \approx (\boldsymbol{A}, \boldsymbol{X})$
  - Graph manipulation is **unnoticeably small.**
    - Preserving basic graph statistics (e.g,. degree distribution) and feature statistics.
  - Graph manipulation is either **direct** (changing the feature/connection of target nodes) or **indirect**.

Mathematical Formulation (2)

- Overview of the attack framework
  - Original adjacency matrix $\boldsymbol{A}$, node features $\boldsymbol{X}$, node labels $\boldsymbol{Y}$.
  - $\boldsymbol{\theta}^*$: Model parameter learned over $\boldsymbol{A}, \boldsymbol{X}, \boldsymbol{Y}$.
    - c_v^*: class label of node v predicted by GCN with $\boldsymbol{\theta}^*$
  - **An attacker has access to $\boldsymbol{A}, \boldsymbol{X}, \boldsymbol{Y}$, and the learning algorithm.**
  - **The attacker modifies $(\boldsymbol{A}, \boldsymbol{X})$ into $(\boldsymbol{A}', \boldsymbol{X}')$.**
  - $\boldsymbol{\theta}^{*\prime}$: Model parameter learned over $\boldsymbol{A}', \boldsymbol{X}', \boldsymbol{Y}$.
    - $c_v^{*\prime}$: class label of node v predicted by GCN with $\boldsymbol{\theta}^{*\prime}$
  - The goal of the attacker is to make $c_v^{*\prime} \neq c_v^*$.

Mathematical Formulation (3)

- **Target node**: $v \in V$
- GCN learned over the **original graph**

$$\boldsymbol{\theta}^* = \text{argmin}_{\boldsymbol{\theta}} \mathcal{L}_{train}(\boldsymbol{\theta}; \boldsymbol{A}, \boldsymbol{X})$$

- GCN's original prediction on the target node:

$$c_v^* = \textbf{argmax}_c f_{\boldsymbol{\theta}^*}(\boldsymbol{A}, \boldsymbol{X})_{v,c}$$

Predict the class c_v^* of vertex v that has the highest predicted probability

Mathematical Formulation (4)

- GCN learned over the **manipulated graph**

$$\boldsymbol{\theta}^{*\prime} = \operatorname{argmin}_{\boldsymbol{\theta}} \mathcal{L}_{train}(\boldsymbol{\theta}; \boldsymbol{A}', \boldsymbol{X}')$$

- GCN's prediction on the **target node v**:

$$c_v^{*\prime} = \operatorname{argmax}_c f_{\boldsymbol{\theta}^{*\prime}}(\boldsymbol{A}', \boldsymbol{X}')_{v,c}$$

- **We want the prediction to change after the graph is manipulated:**

$$c_v^{*\prime} \neq c_v^{*}$$

Mathematical Formulation (5)

- **Change of prediction on target node v:**

$$\Delta(v; \boldsymbol{A}', \boldsymbol{X}') =$$

$$\log f_{\boldsymbol{\theta}^{*\prime}}(\boldsymbol{A}', \boldsymbol{X}')_{v, c_v^{*\prime}} - \log f_{\boldsymbol{\theta}^{*\prime}}(\boldsymbol{A}', \boldsymbol{X}')_{v, c_v^{*}}$$

Predicted (log) probability of the newly-predicted class $c_v^{*\prime}$

Predicted (log) probability of the originally-predicted class c_v^{*}

Want to increase this term

Want to decrease this term

Mathematical Formulation (6)

- **Final optimization objective:**

$$\text{argmax}_{A',X'} \Delta(v; A', X')$$
$$\text{subject to } (A', X') \approx (A, X)$$

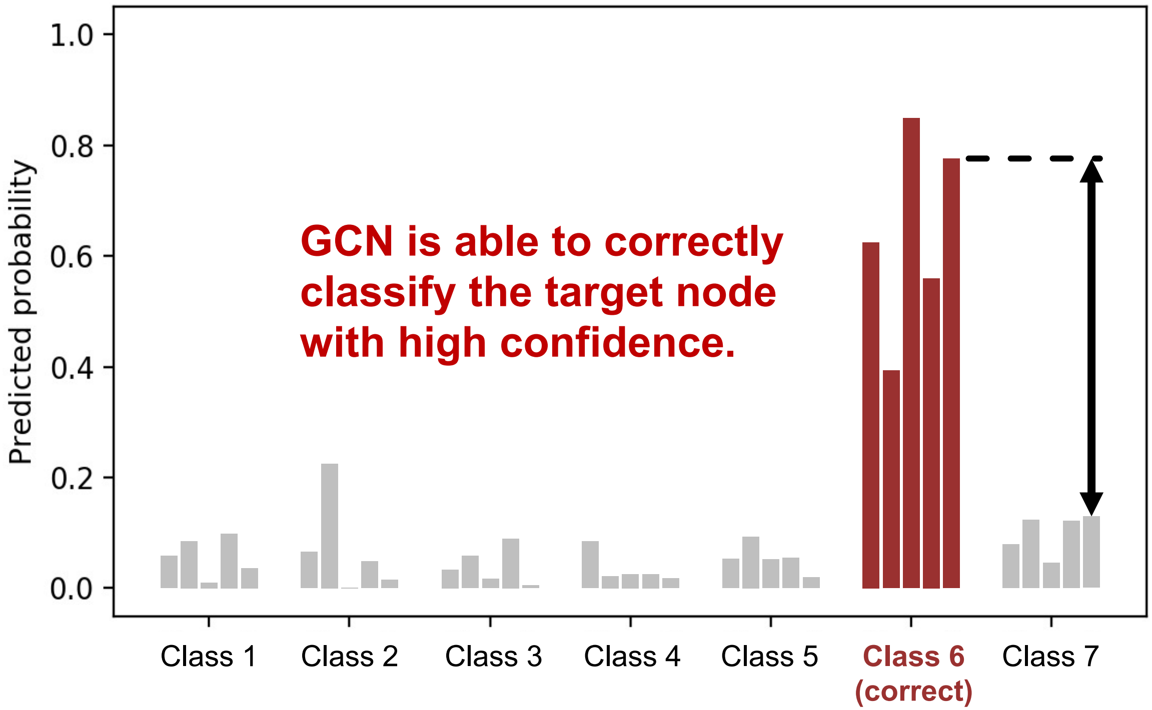
- **Challenges in optimizing the objective**
  - Adjacency matrix $\boldsymbol{A}'$ is a discrete object: gradient-based optimization cannot be used.
  - For every modified graph $\boldsymbol{A}'$ and $\boldsymbol{X}'$, GCN needs to be re-trained (this is computationally expensive):
    - $\boldsymbol{\theta}^{*\prime} = \text{argmin}_{\boldsymbol{\theta}} \mathcal{L}_{train}(\boldsymbol{\theta}; \boldsymbol{A}', \boldsymbol{X}')$
- Several approximations are proposed to make the optimization tractable [Zügner et al. KDD2018].

Experiments: Setting

- **Setting:** Semi-supervised node classification with GCN
- **Graph:** Paper citation network (2,800 nodes, 8,000 edges).
- **Attack type:** Edge modification (addition or deletion of edges)
- **Attack budget on node v:** $d_v + 2$ modifications (d_v: degree of node v).
  - **Intuition**: It is harder to attack a node with a larger degree.
- Model is trained and attacked 5 times using different random seeds.

Experiments: Adversarial Attack

Predicted probabilities of a target node v over 5 re-trainings (each bar represents a single trial)
(without graph manipulation, i.e., clean graph)

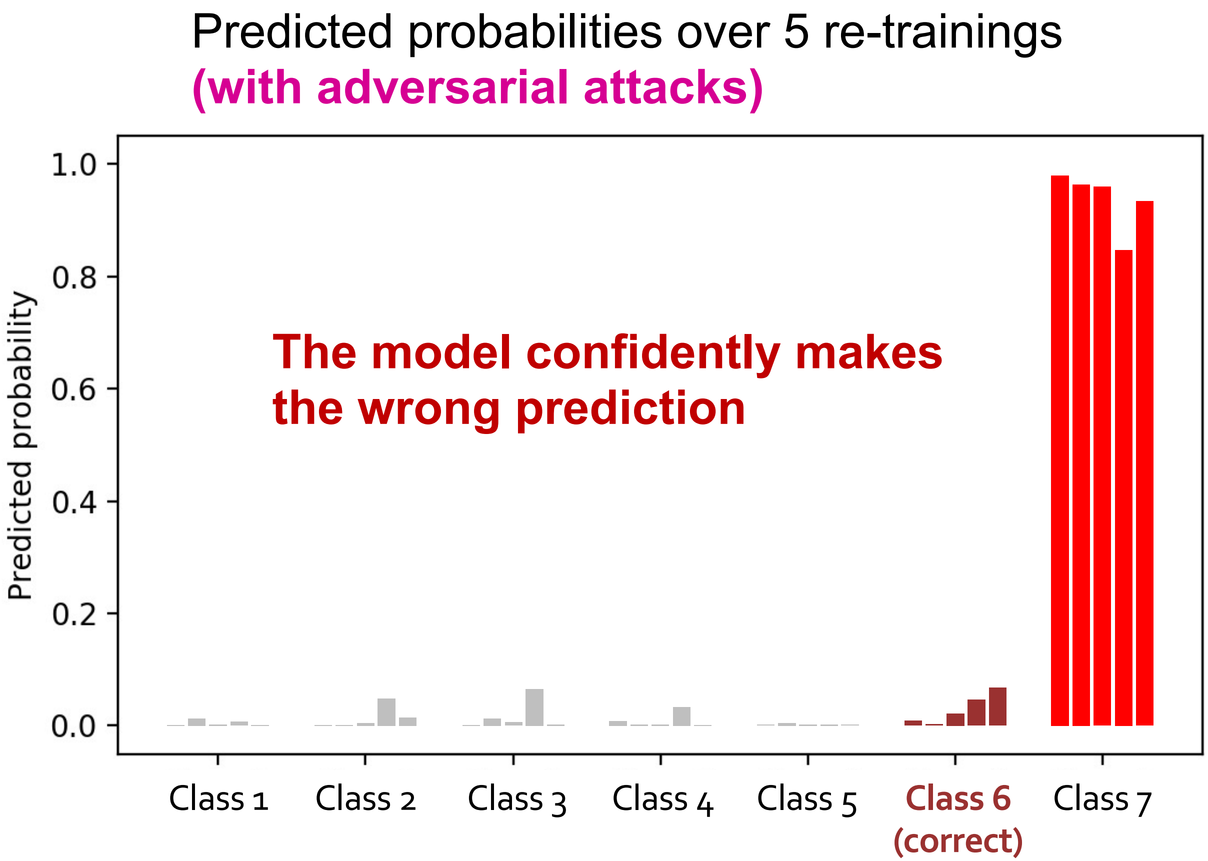


Classification margin
> 0: Correct classification
< 0: Incorrect classification

7-class classification

Experiments: Adversarial Attack

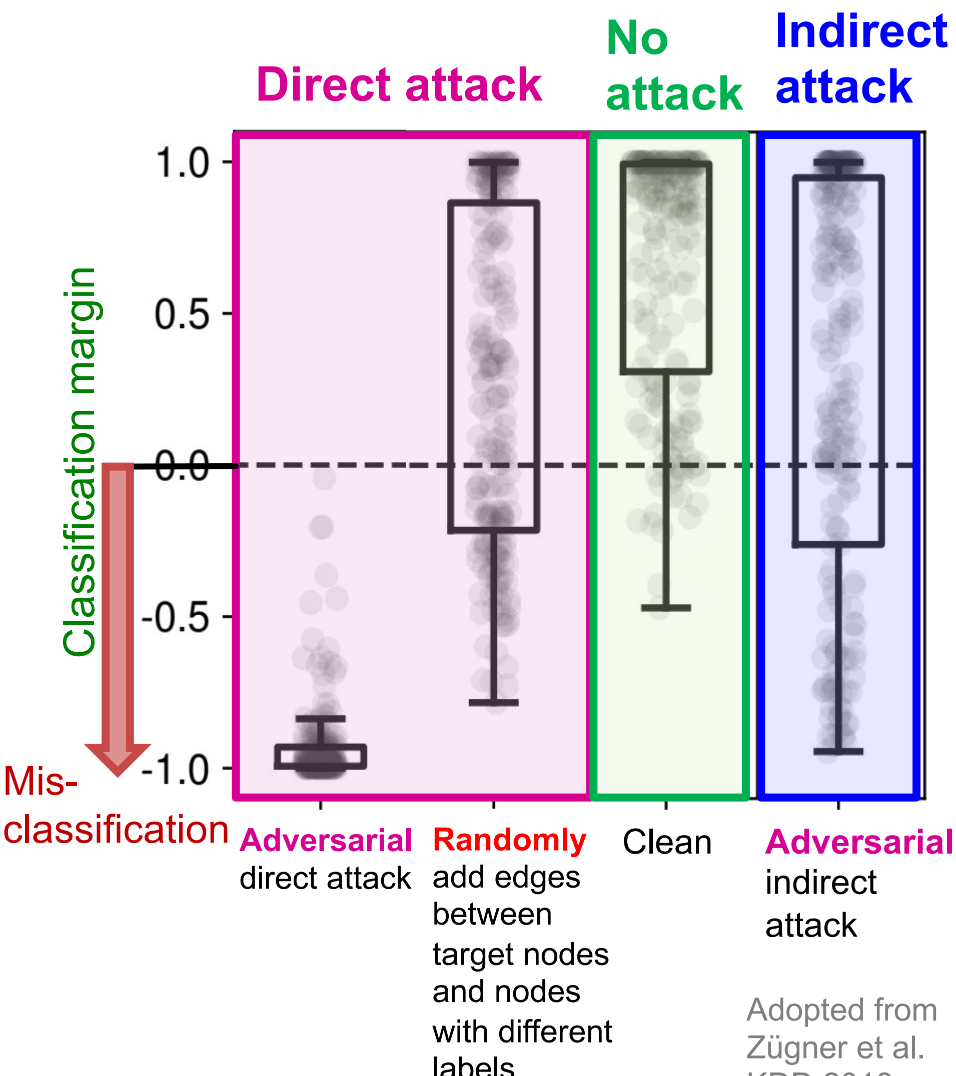
GCN's prediction after modifying 5 edges attached to the target node (direct adversarial attack).



Experiments: Attack Comparison

- **Adversarial direct attack** is the strongest attack, significantly worsening GCN's performance (compared to **no attack**).
- **Random** attack is much weaker than **adversarial** attack.
- **Indirect attack** is more challenging than direct attack.

Each dot indicates one attack trial.



Adopted from Zügner et al. KDD 2018

Summary

- We study the adversarial robustness of GCN applied to semi-supervised node classification.
- We consider different **attack possibilities on graph-structured data.**
- We mathematically **formulate the adversarial attack as an optimization problem**.
- We empirically demonstrate that GCN's prediction performance can be significantly harmed by adversarial attacks.
- **GCN is *not* robust to adversarial attacks but it is somewhat robust to indirect attacks and random noise.**