Stanford CS224W: How Expressive are Graph Neural Networks?

CS224W: Machine Learning with Graphs

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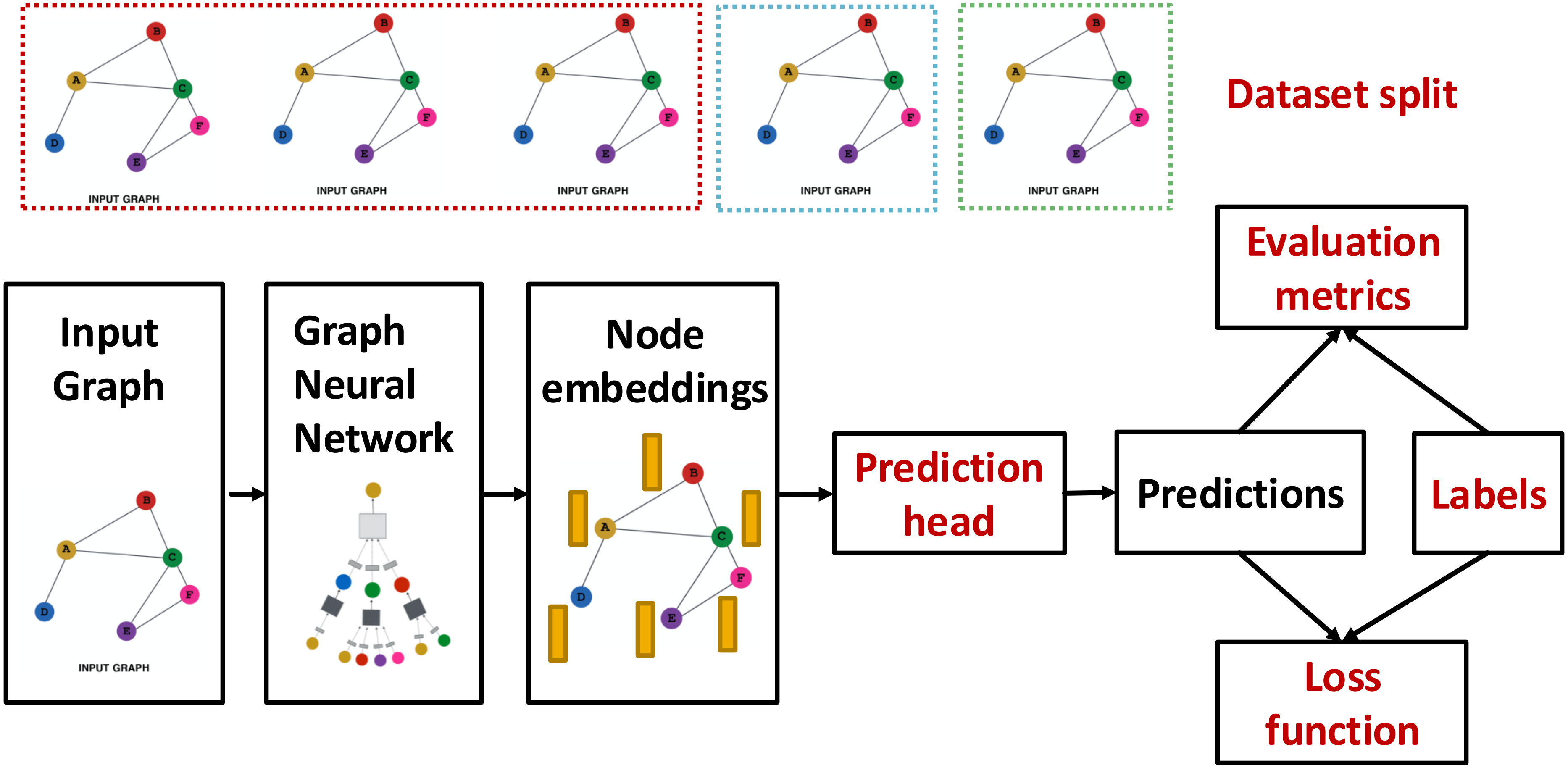
http://cs224w.stanford.edu

Announcements

- **Colab 1** due today at 11:59PM
- **Homework 1** due in 1 week (Thursday 10/16)
- **Colab 2** will be released today at 3PM
  - Due on Thursday 10/23 (2 weeks from now)
- **Project Proposal** is due Tuesday 10/21
  - Details on course website
  - To do a solo project, make a private post on Ed with your idea to get approval from course staff

Recap: GNN Training Pipeline



Implementation resources:

[PyG](#) provides core modules for this pipeline

[GraphGym](#) further implements the full pipeline to facilitate GNN design

Information modalities in Graphs

Image credit: Medium

Social Networks

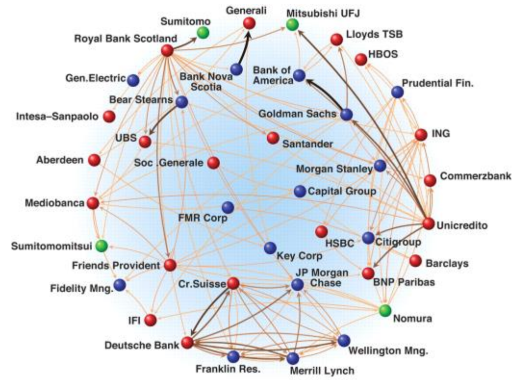
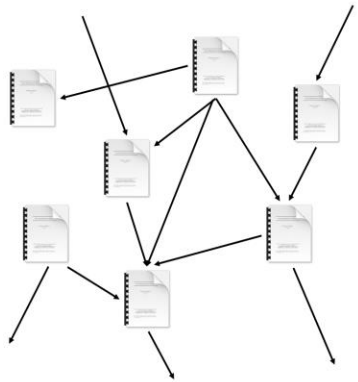


Image credit: Science

Economic Networks



Citation Networks

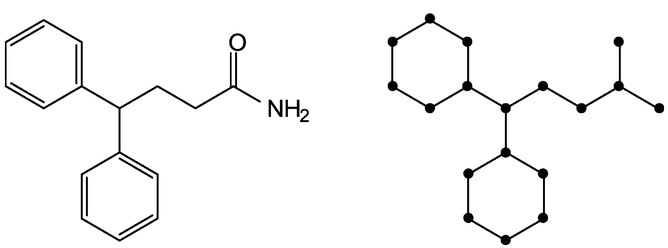


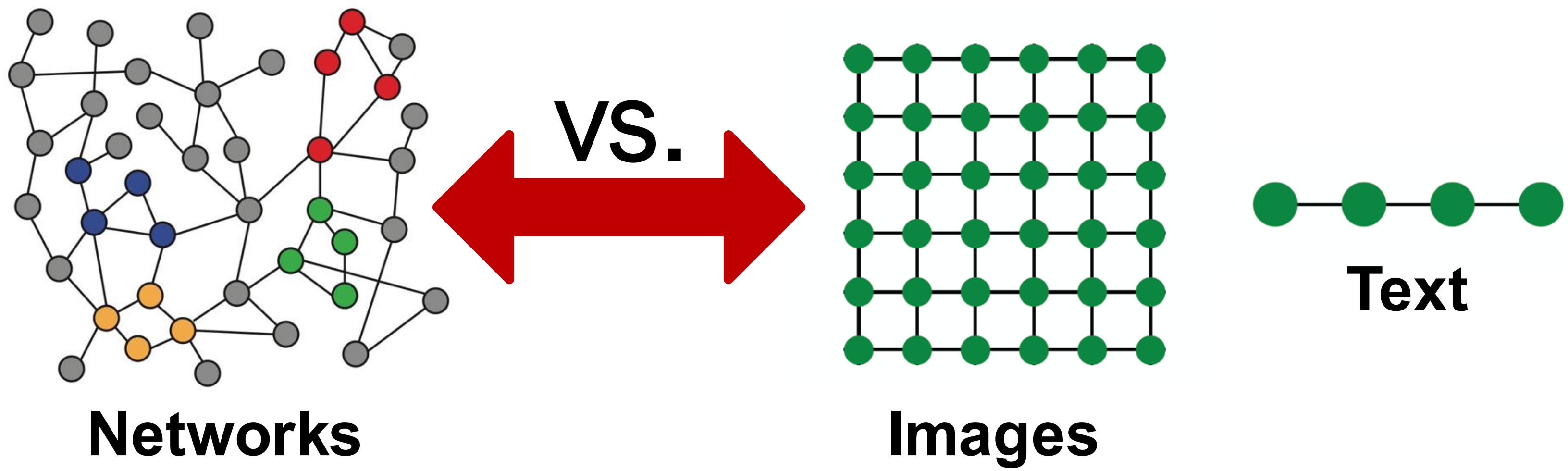
Image credit: MDPI

Molecules

Why is Graph Deep Learning Hard?

Graphs are complex.

- Complex topological structure (*i.e.*, no spatial locality like grids)



- No fixed node ordering or reference point

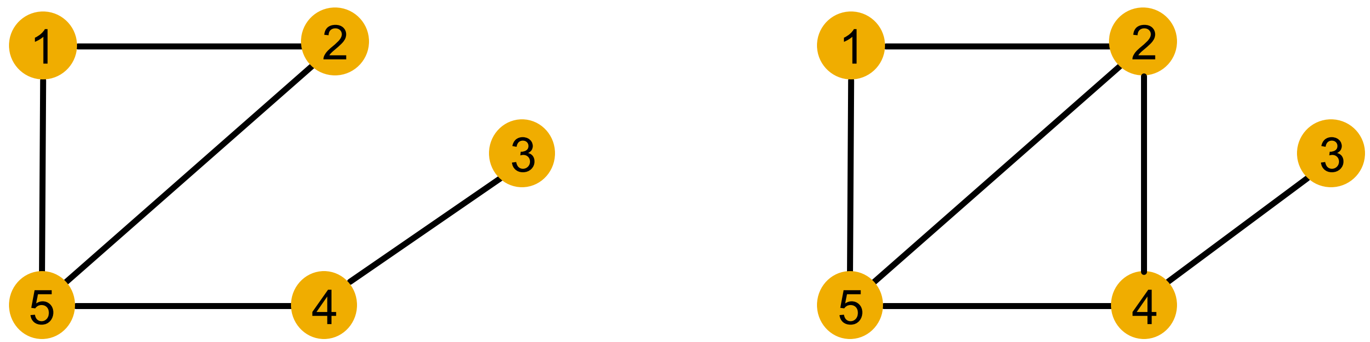
Theory of GNNs

How powerful are GNNs?

- **Many GNN models have been proposed (e.g., GCN, GAT, GraphSAGE, design space).**
- **What is the expressive power (ability to distinguish different graph structures) of these GNN models?**
- **How to design a maximally expressive GNN model?**

Graph Isomorphism problem

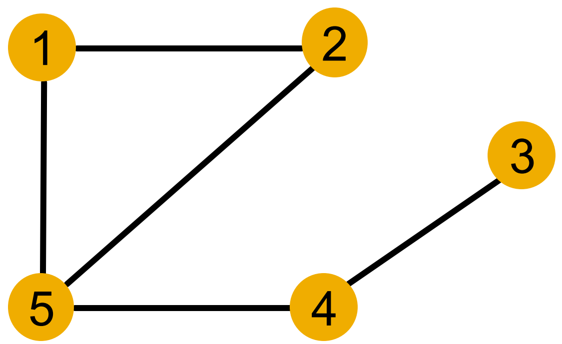
- **A classical expressivity test is graph isomorphism.**
  - **Given a pair of graphs, can we tell if they are isomorphic?**

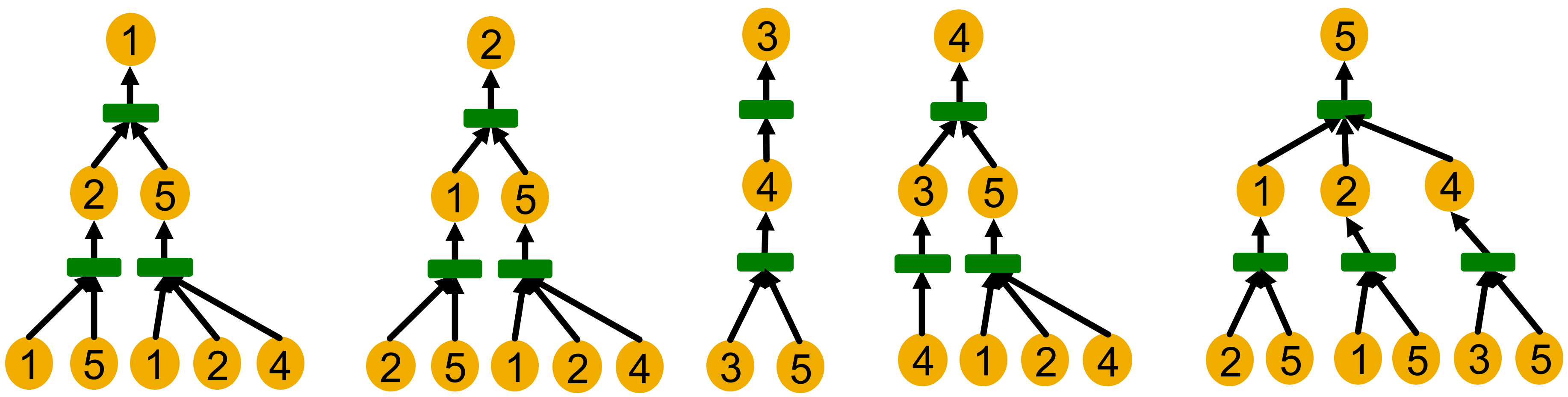


- **Open problem (a polynomial time algorithm does not exist, has not been proven NP-complete).**

A simpler problem

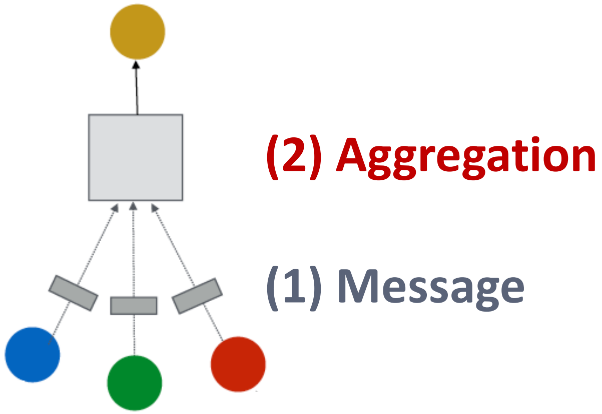
- **Given a pair of nodes with different neighborhood structures. Is there a GNN that can always tell them apart?**





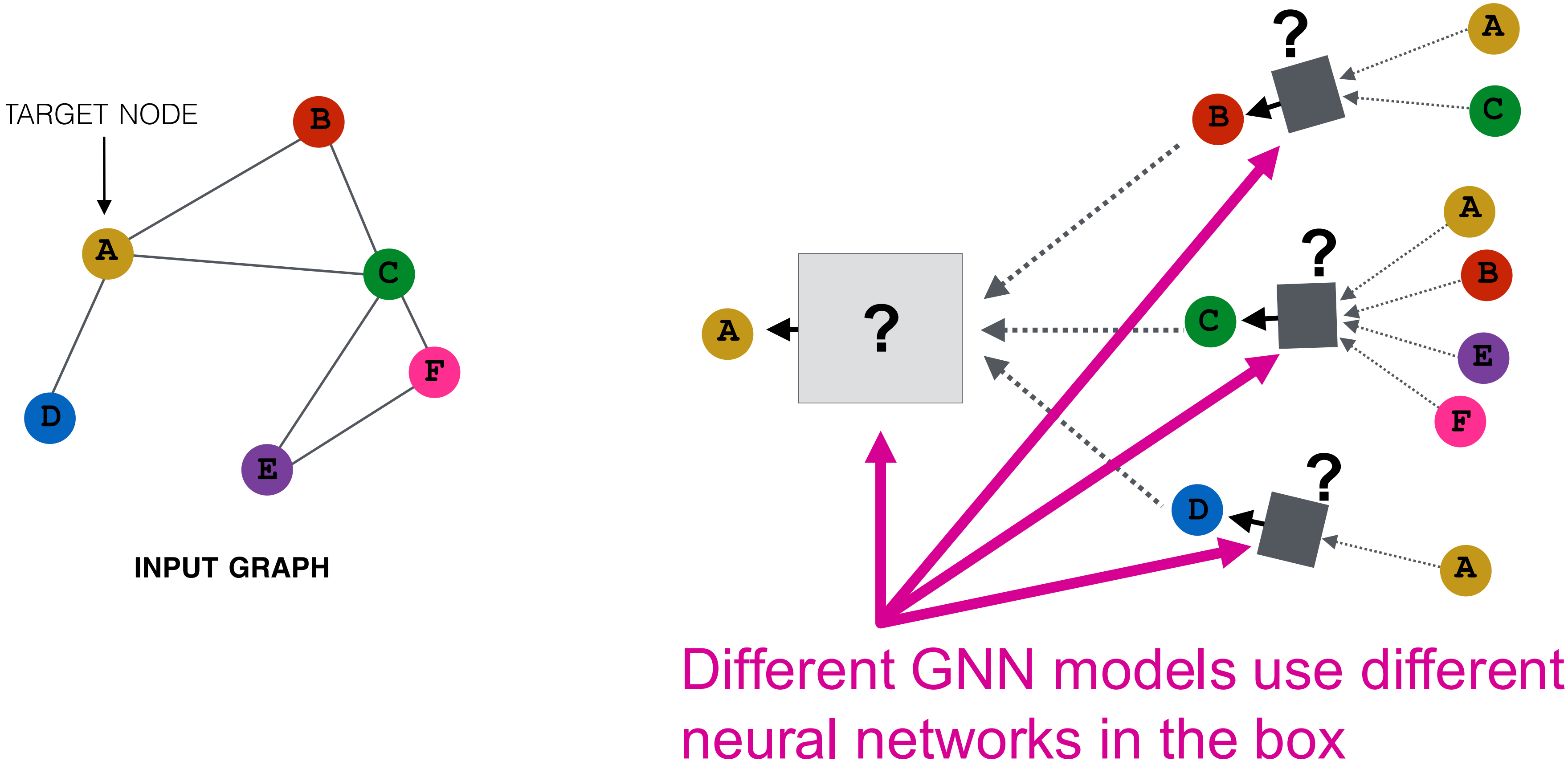
Background: A Single GNN Layer

- **We focus on message passing GNNs:**
  - **(1) Message**: each node computes a message
    $$\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$
  - **(2) Aggregation**: aggregate messages from neighbors
    $$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}, \mathbf{m}_v^{(l)}\right)$$



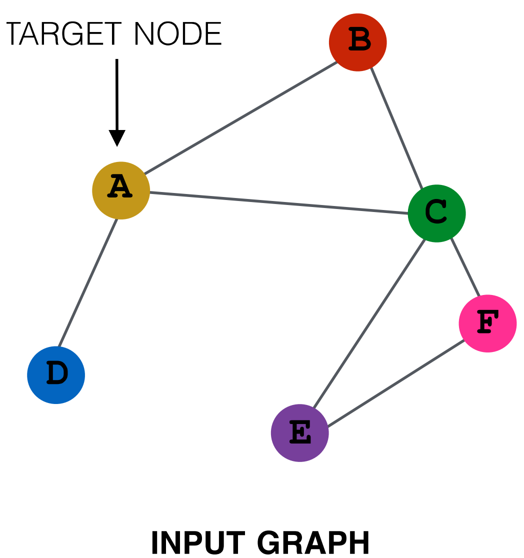
Background: Many GNN Models

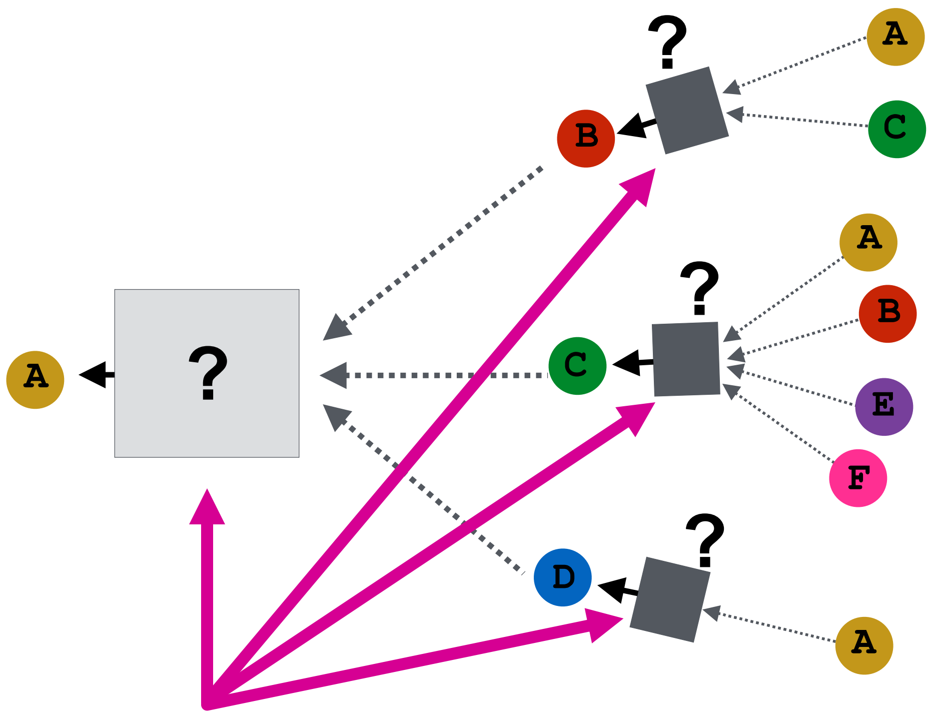
- Many GNN models have been proposed:
  - GCN, GraphSAGE, GAT, Design Space etc.



GNN Model Example (1)

- **GCN (mean-pool)** [Kipf and Welling ICLR 2017]

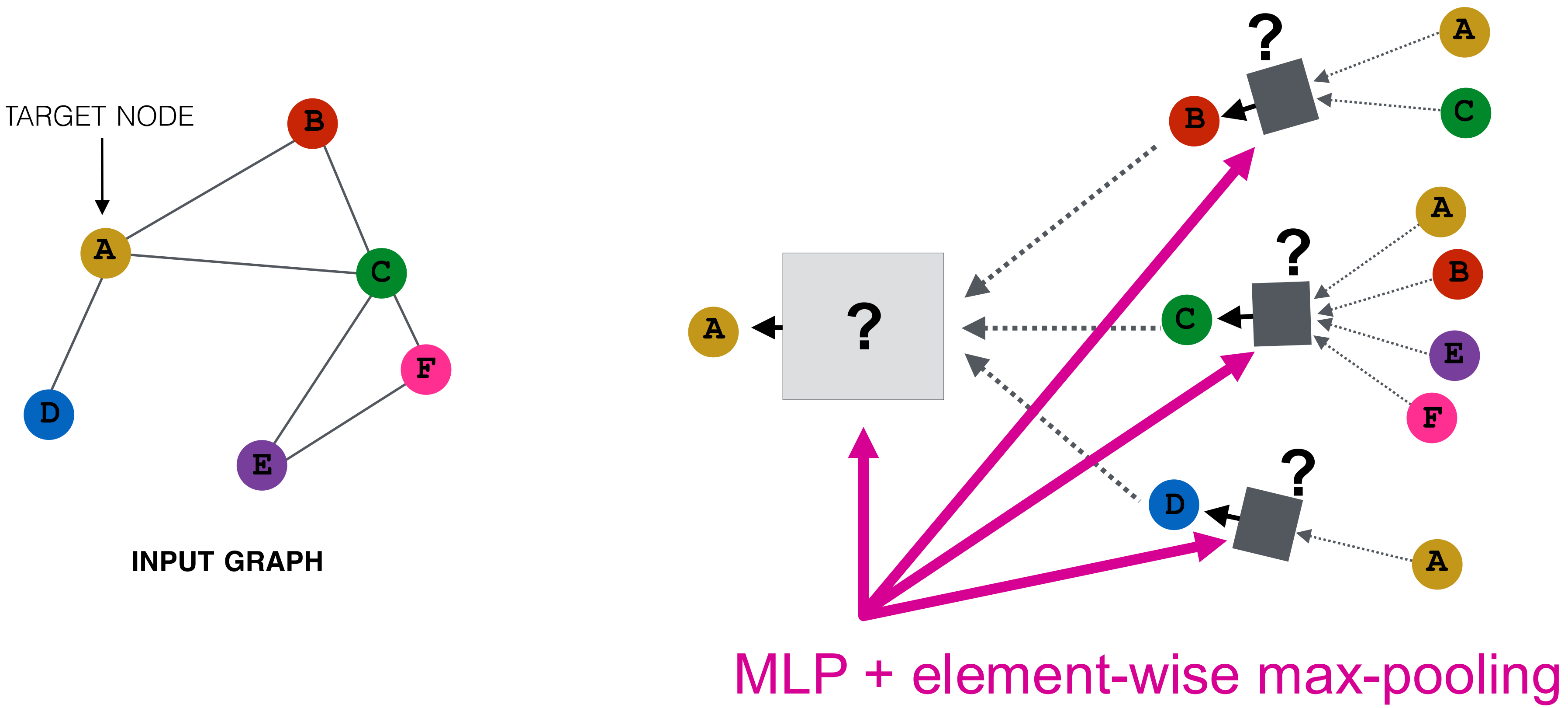




Element-wise mean pooling + Linear + ReLU non-linearity

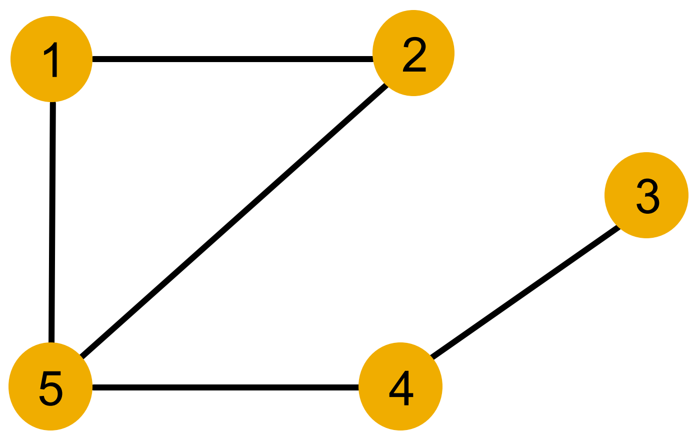
GNN Model Example (2)

- **GraphSAGE (max-pool)** [Hamilton et al. NeurIPS 2017]



Note: Node Colors

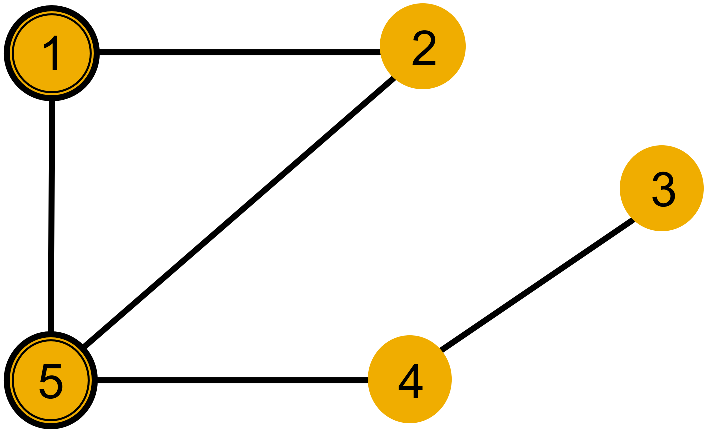
- We use node same/different **colors** to represent nodes with same/different features.
  - For example, the graph below assumes all the nodes share the same feature.



- Key question: **How well can a GNN distinguish different graph structures?**

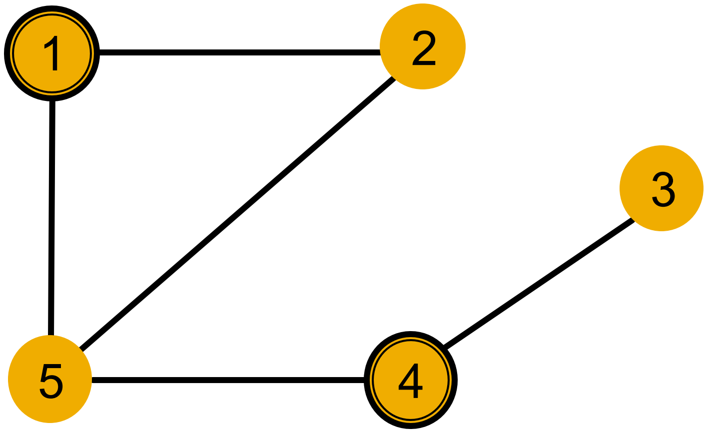
Local Neighborhood Structures

- We specifically consider **local neighborhood structures** around each node in a graph.
  - **Example:** Nodes 1 and 5 have **different** neighborhood structures because they have different node degrees.



Local Neighborhood Structures

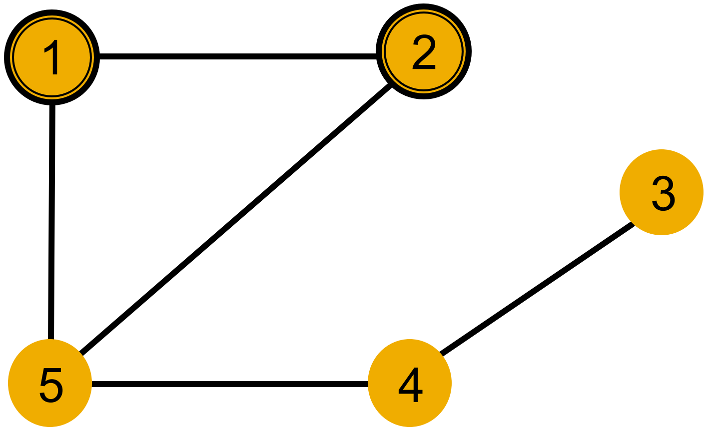
- We specifically consider **local neighborhood structures** around each node in a graph.
  - **Example:** Nodes 1 and 4 both have the same node degree of 2. However, they still have **different** neighborhood structures because **their neighbors have different node degrees.**



Node 1 has neighbors of degrees 2 and 3.
Node 4 has neighbors of degrees 1 and 3.

Local Neighborhood Structures

- We specifically consider **local neighborhood structures** around each node in a graph.
  - **Example:** Nodes 1 and 2 have the **same** neighborhood structure because **they are symmetric within the graph.**



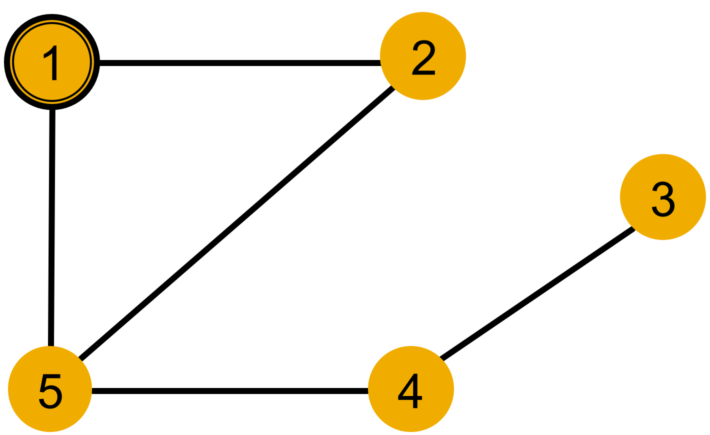
Node 1 has neighbors of degrees 2 and 3.
Node 2 has neighbors of degrees 2 and 3.
And even if we go a step deeper to 2nd hop neighbors, both nodes have the same degrees (Node 4 of degree 2)

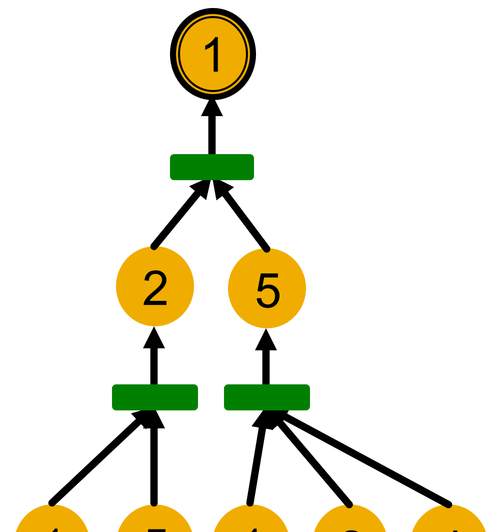
Local Neighborhood Structures

- **Key question: Can GNN node embeddings distinguish different node's local neighborhood structures?**
  - If so, when? If not, when will a GNN fail?
- **Next: We need to understand how a GNN captures local neighborhood structures.**
  - **Key concept: Computational graph**

Computational Graph (1)

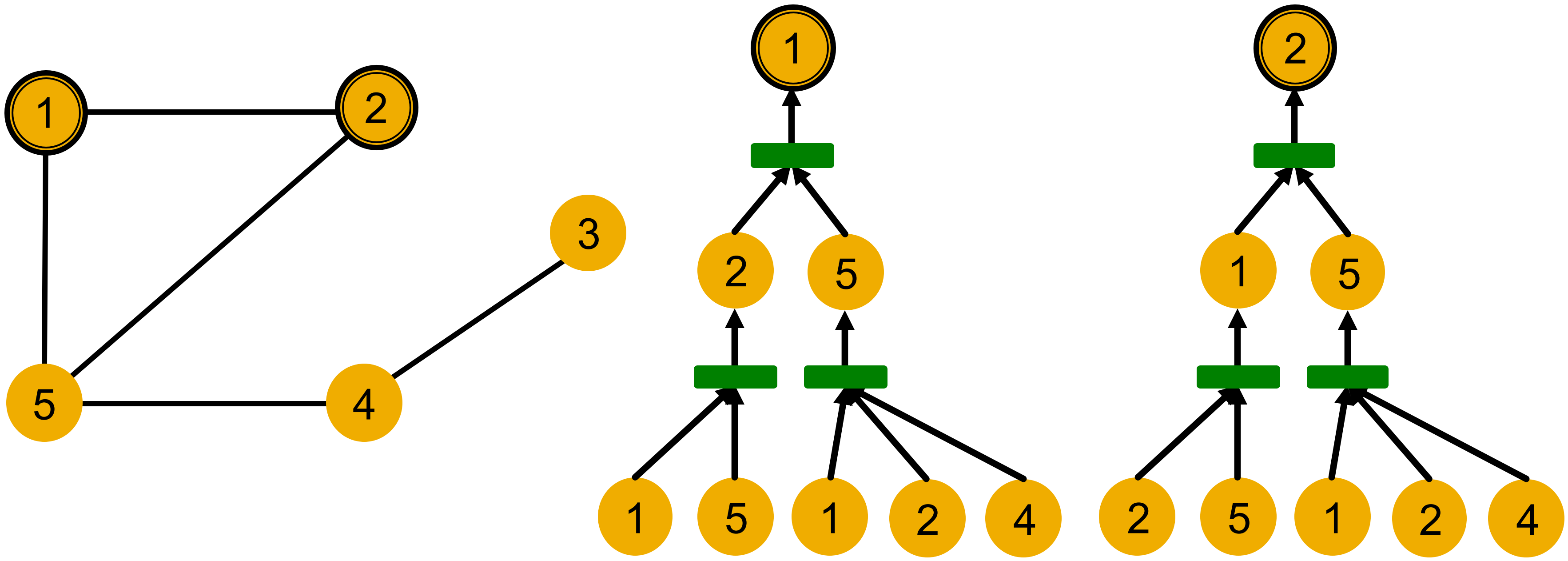
- **In each layer, a GNN aggregates neighboring node embeddings.**
- A GNN generates node embeddings through a computational graph defined by the neighborhood.
  - **Ex:** Node 1's computational graph (2-layer GNN)





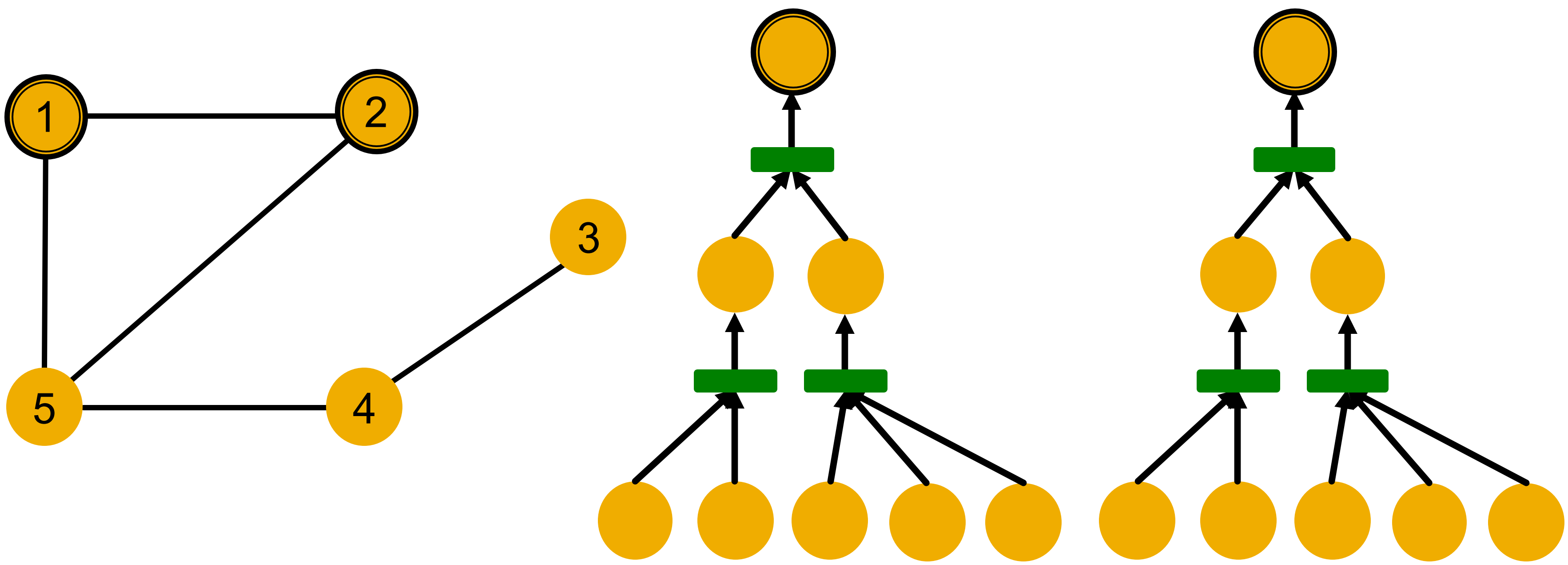
Computational Graph (2)

- **Ex:** Nodes 1 and 2's computational graphs.



Computational Graph (3)

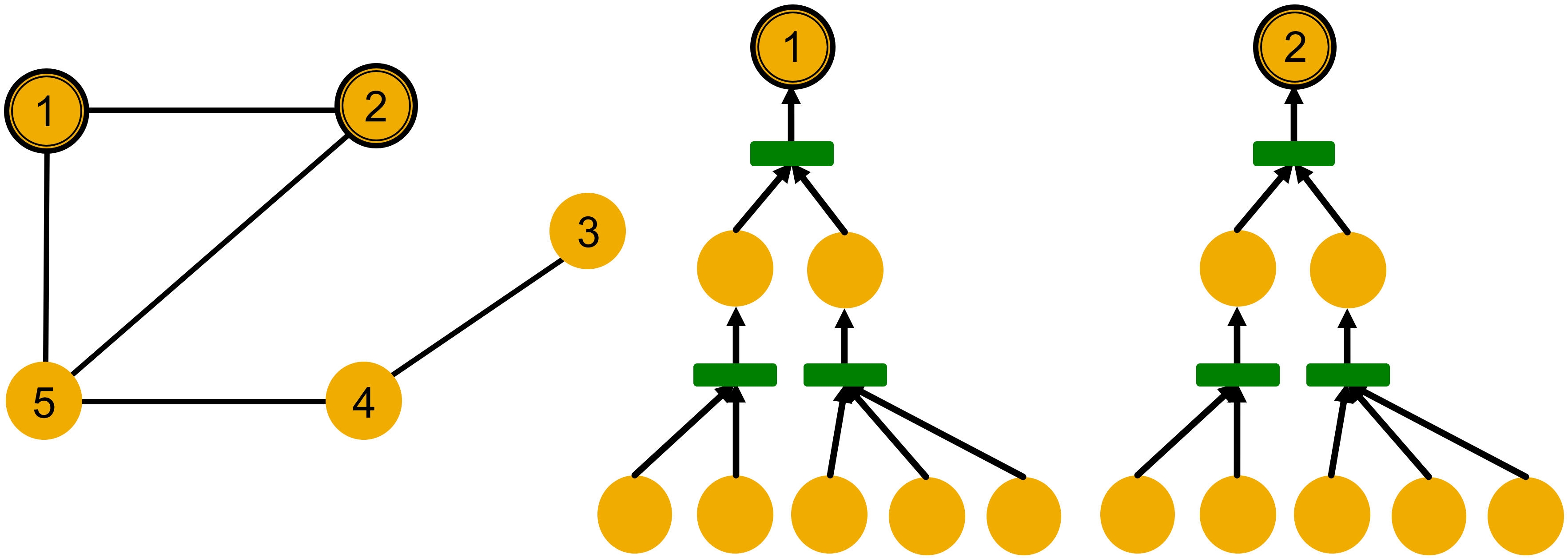
- **Ex:** Nodes 1 and 2's computational graphs.
- **But GNN only sees node features (not IDs):**



Computational Graph (4)

- **A GNN will generate <u>the same embedding</u> for nodes 1 and 2 because:**
  - Computational graphs are the same.
  - Node features (colors) are identical.

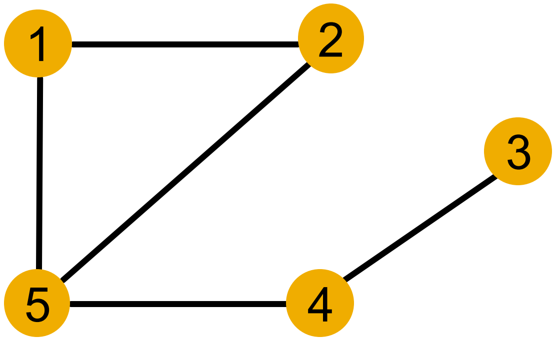
Note: GNN does not care about node ids, it just aggregates features vectors of different nodes.

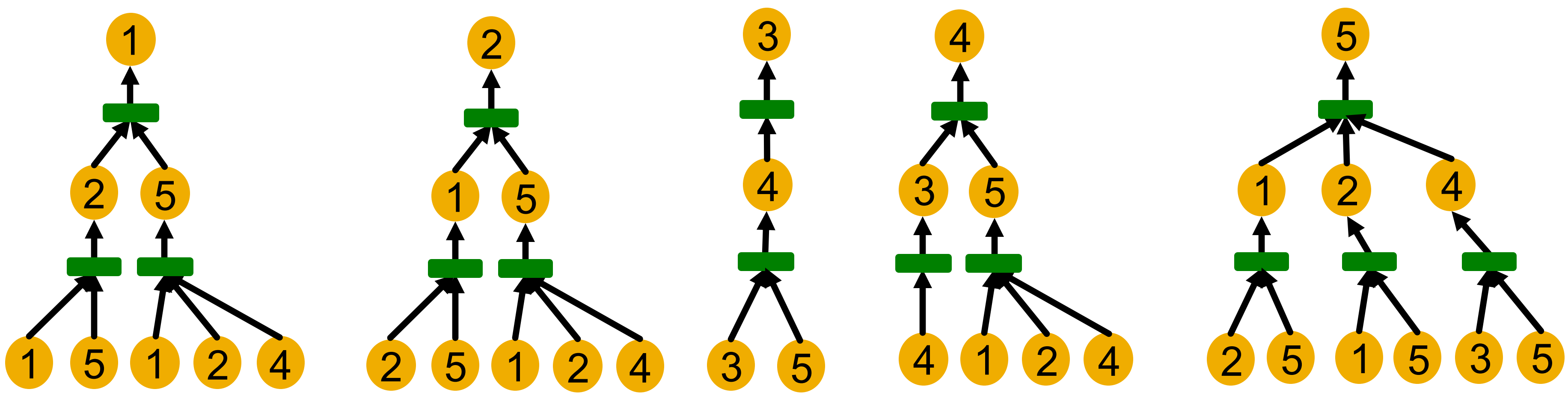


GNN won't be able to distinguish nodes 1 and 2

Computational Graph

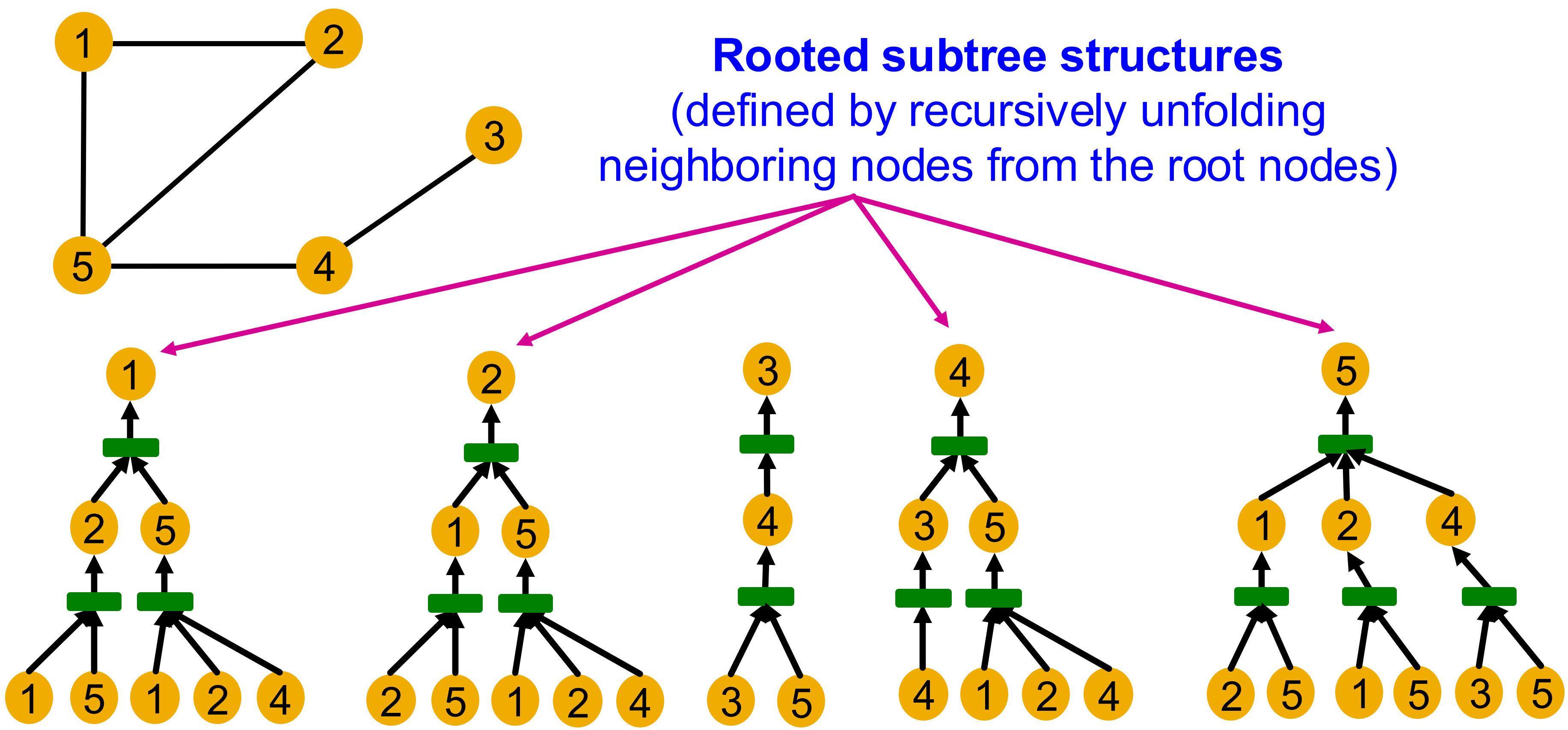
- **In general, different local neighborhoods define different computational graphs**





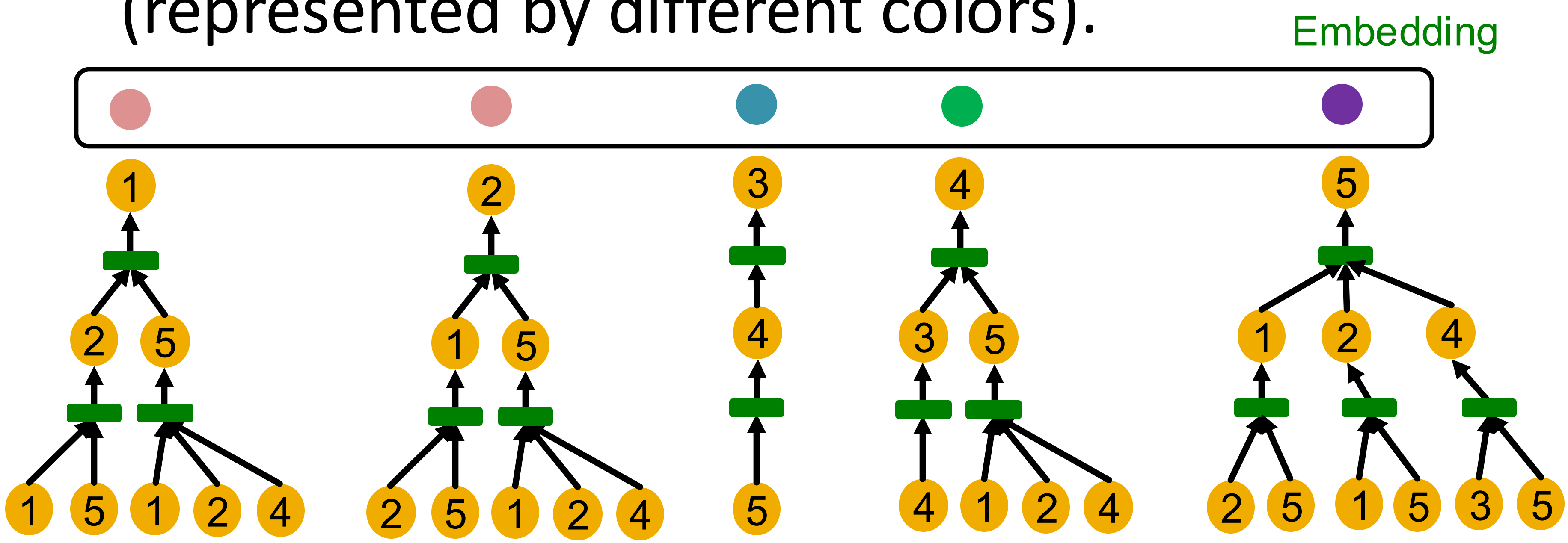
Computational Graph

- Computational graphs are identical to **rooted subtree structures** around each node.



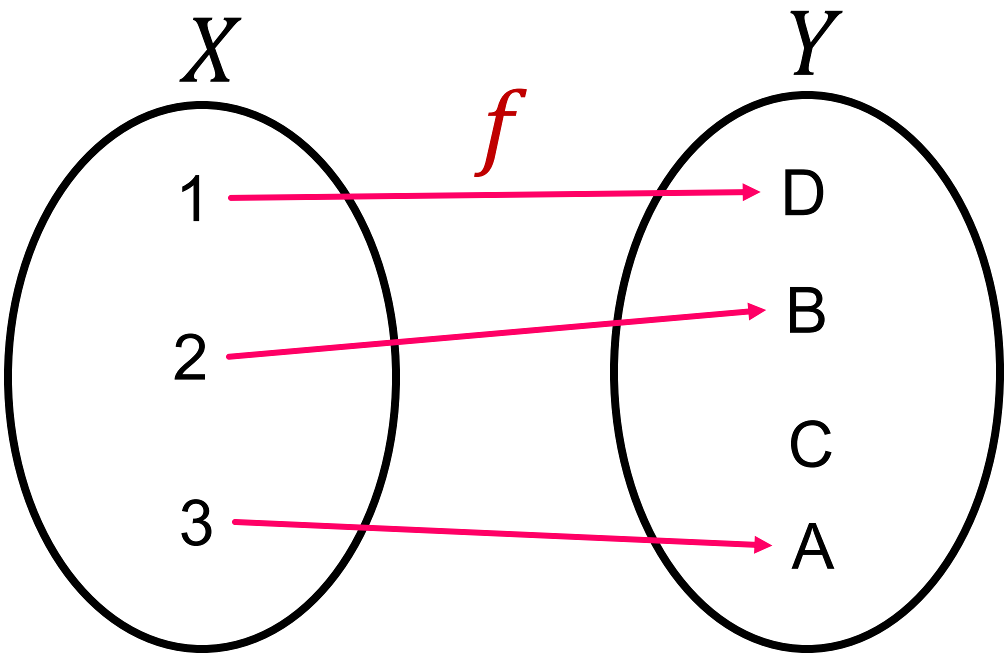
Computational Graph

- GNN's node embeddings capture rooted subtree structures.
- Most expressive GNN maps different rooted subtrees into different node embeddings (represented by different colors).



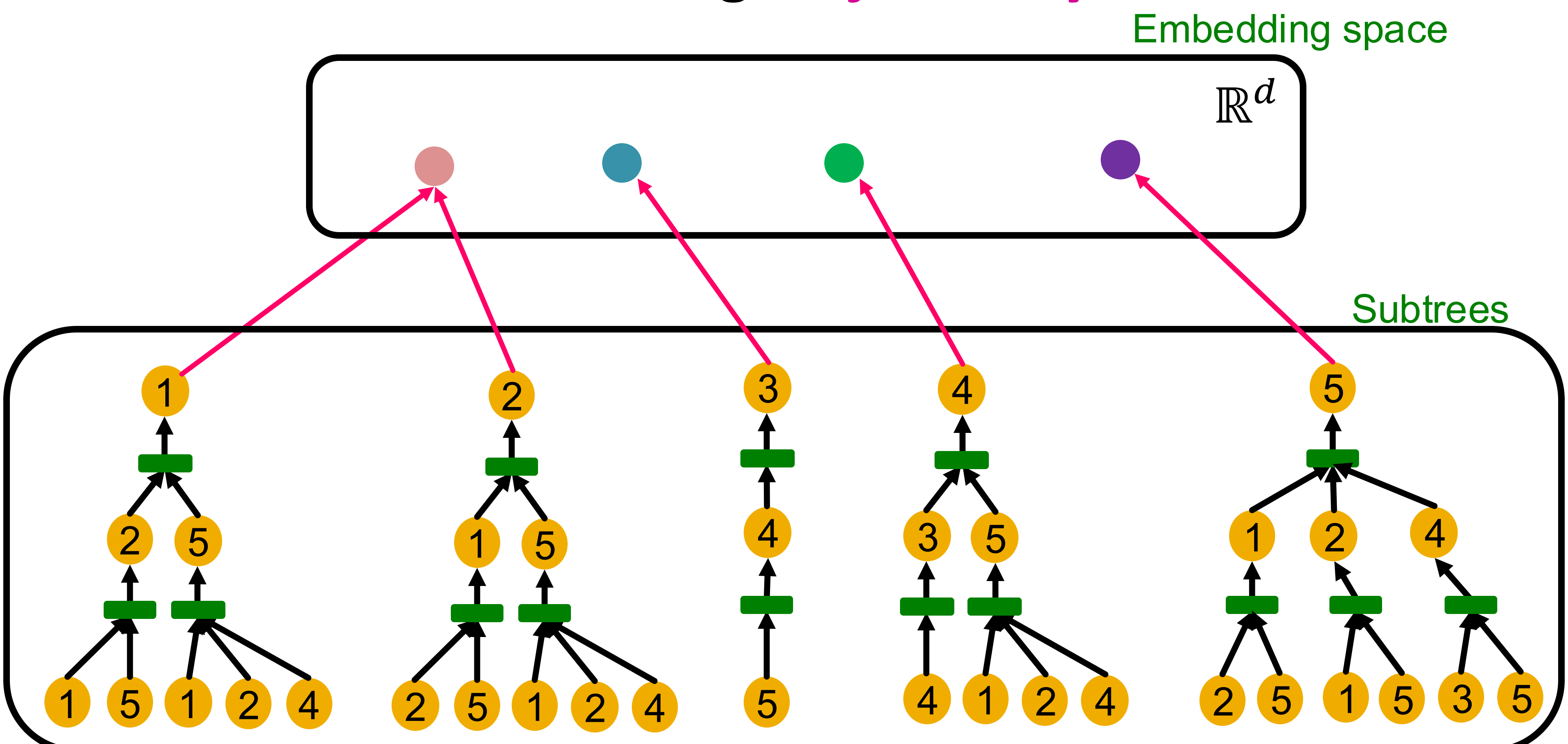
Recall: Injective Function

- **Function** $f: X \to \mathrm{Y}$ is **injective** if it maps different elements into different outputs.
- **Intuition:** f retains all the information about input.



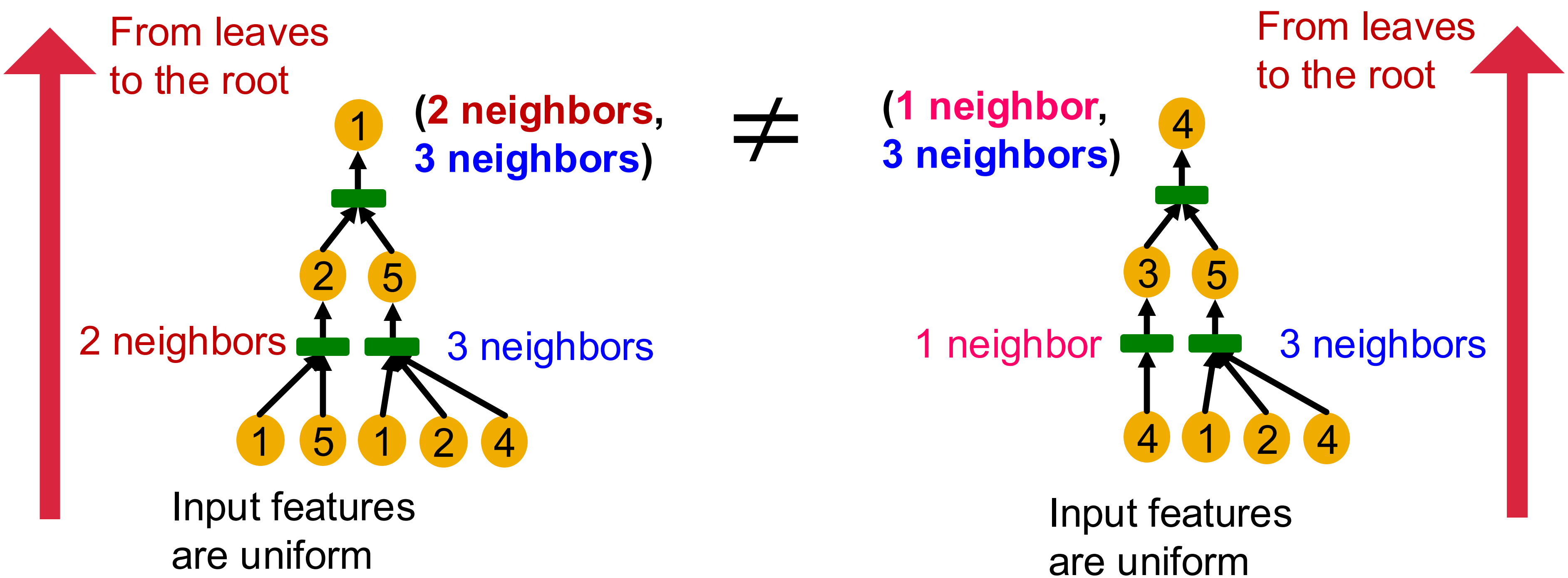
How Expressive is a GNN?

- Most expressive GNN should map subtrees to the node embeddings **injectively**.



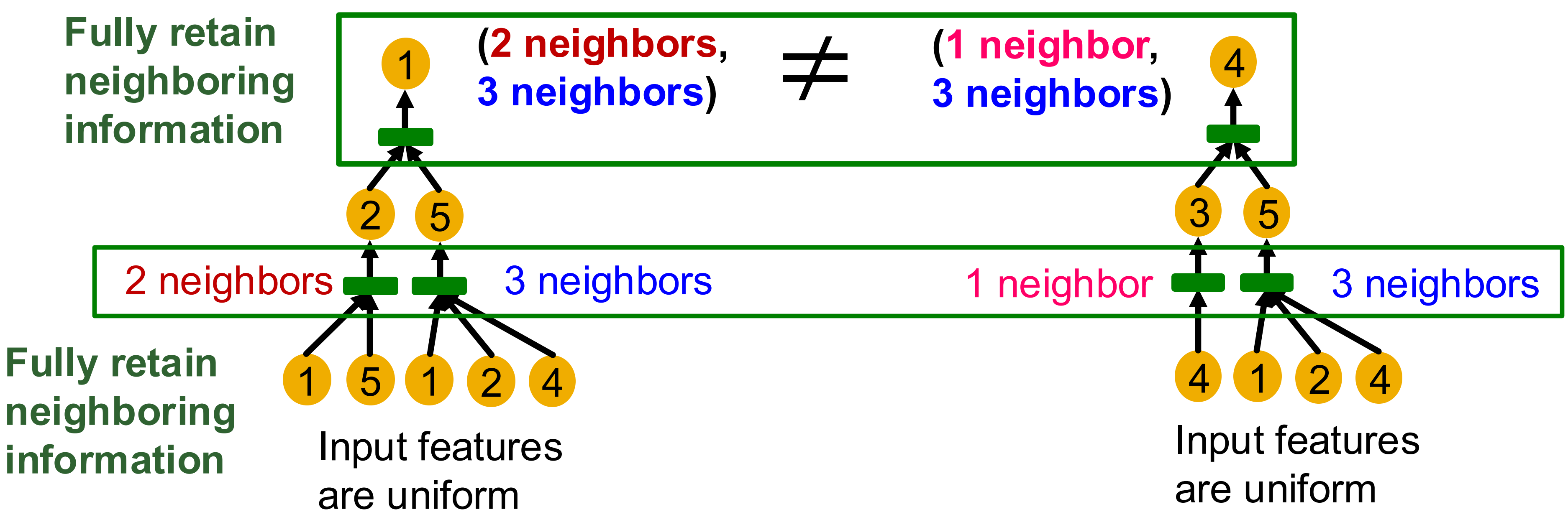
How Expressive is a GNN?

- **Key observation**: Subtrees of the same depth can be recursively characterized from the leaf nodes to the root nodes.



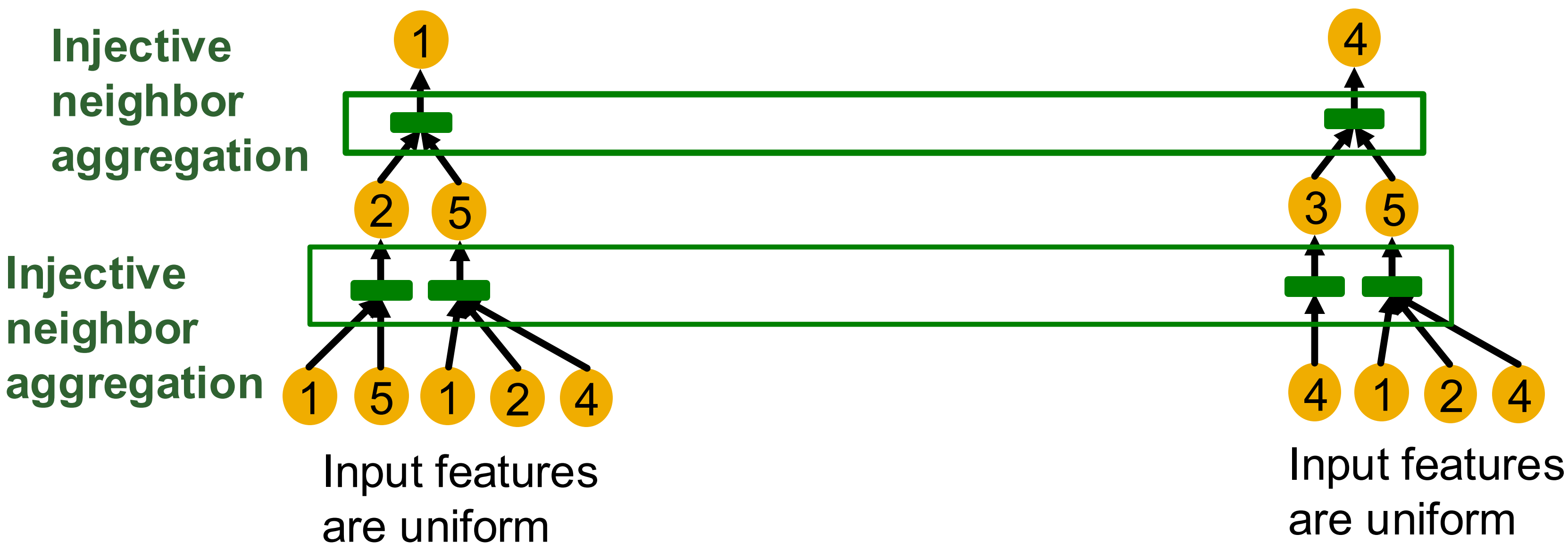
How Expressive is a GNN?

- If each step of GNN's aggregation **can fully retain the neighboring information**, the generated node embeddings can distinguish different rooted subtrees.



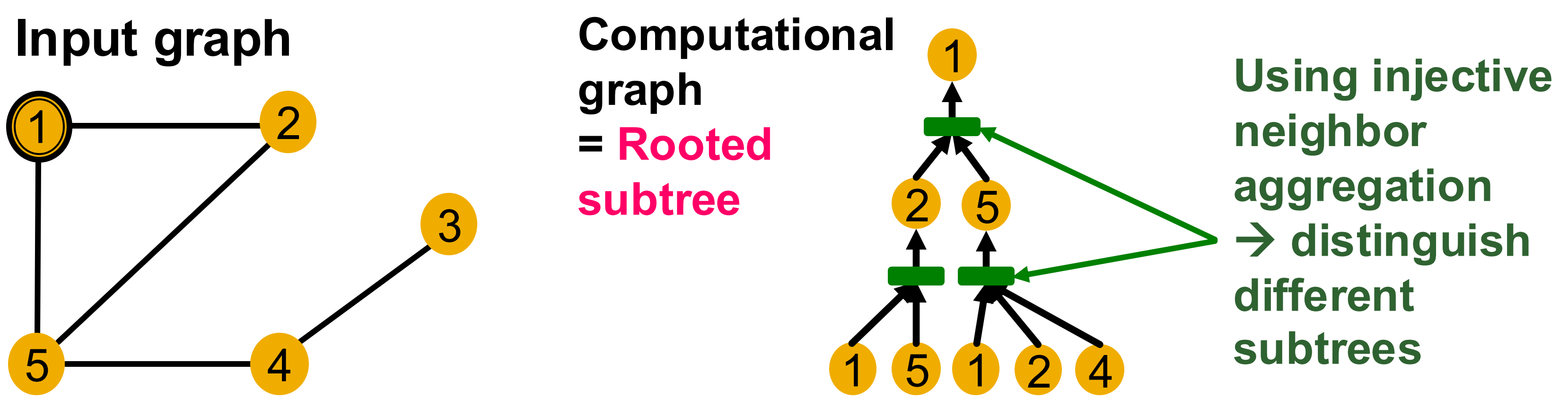
How Expressive is a GNN?

- In other words, most expressive GNN would use an **injective neighbor aggregation** function at each step.
  - Maps different neighbors to different embeddings.



How Expressive is a GNN?

- **Summary so far**
  - To generate a node embedding, GNNs use a computational graph corresponding to a subtree rooted around each node.



  - GNN can fully distinguish different subtree structures if **every step of its neighbor aggregation is injective.**

Stanford CS224W: Designing the Most Powerful Graph Neural Network

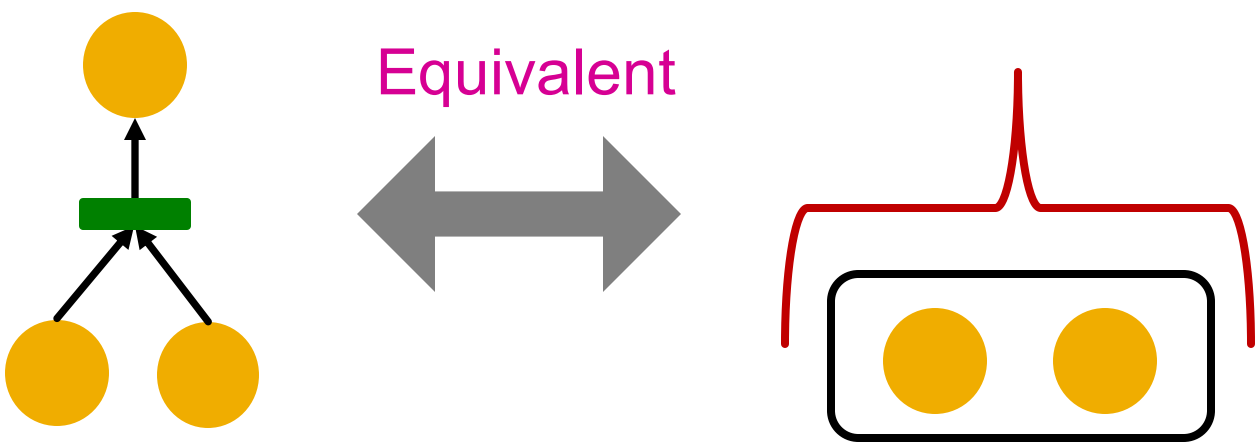
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Expressive Power of GNNs

- **Key observation: Expressive power of GNNs can be characterized by that of neighbor aggregation functions they use.**
  - A more expressive aggregation function leads to a more expressive GNN.
  - Injective aggregation function leads to the most expressive GNN.
- **Next:**
  - Theoretically analyze expressive power of aggregation functions.

Neighbor Aggregation

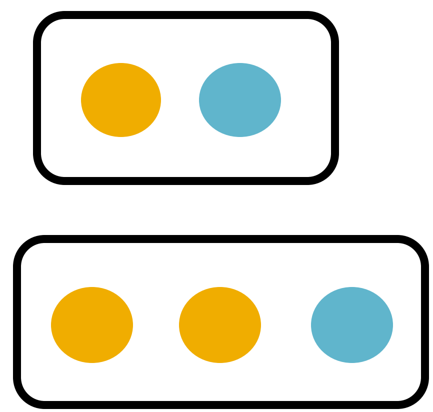
- **Observation**: **Neighbor aggregation** can be abstracted as **a function over a multi-set** (a set with repeating elements).



Neighbor aggregation

Multi-set function

Examples of multi-set



Same color indicates the same features.

Neighbor Aggregation

- **Next: We analyze aggregation functions of two popular GNN models**
  - **GCN** (mean-pool) [Kipf & Welling, ICLR 2017]
    - Uses **element-wise** mean pooling over neighboring node features

$$\mathrm{Mean}(\{x_u\}_{u \in N(v)})$$

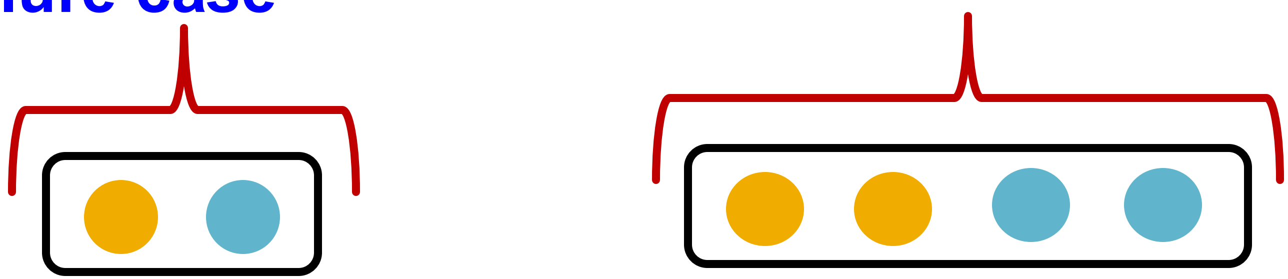
  - **GraphSAGE** (max-pool) [Hamilton et al. NeurIPS 2017]
    - Uses **element-wise** max pooling over neighboring node features

$$\mathrm{Max}(\{x_u\}_{u \in N(v)})$$

Neighbor Aggregation: Case Study

- **GCN (mean-pool)** [Kipf & Welling ICLR 2017]
  - Take **element-wise mean**, followed by linear function and ReLU activation, i.e., $\max(0, x)$.
  - **Theorem** [Xu et al. ICLR 2019]
    - GCN's aggregation function **cannot distinguish different multi-sets with the same color proportion.**

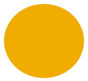
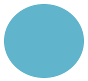
Failure case



- **Why?**

Neighbor Aggregation

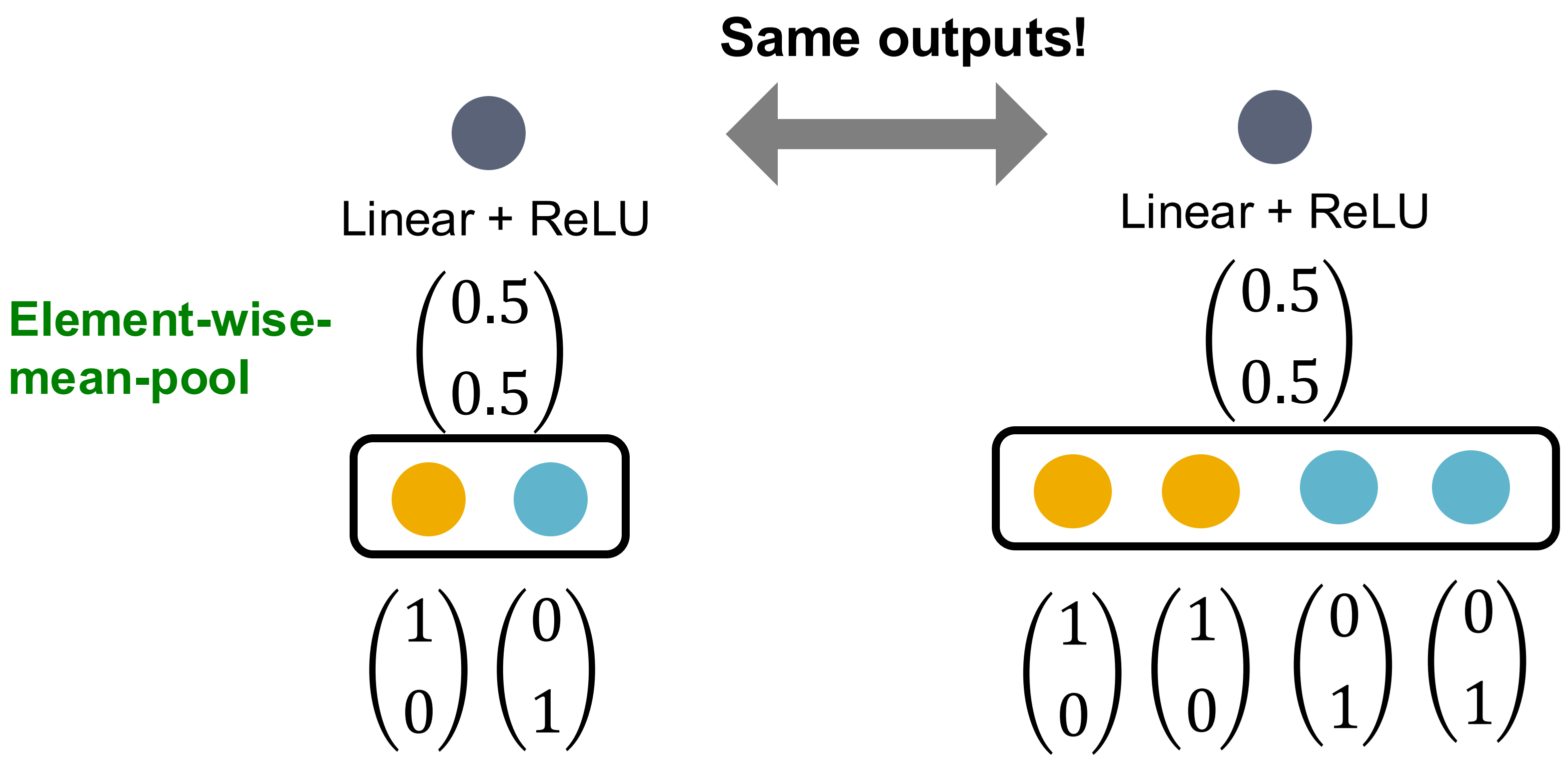
- For simplicity, we assume node features (colors) are represented by **one-hot encoding**.
  - **Example:** If there are two distinct colors:

 $= \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  $= \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

  - This assumption is sufficient to illustrate how GCN fails.

Neighbor Aggregation: Case Study

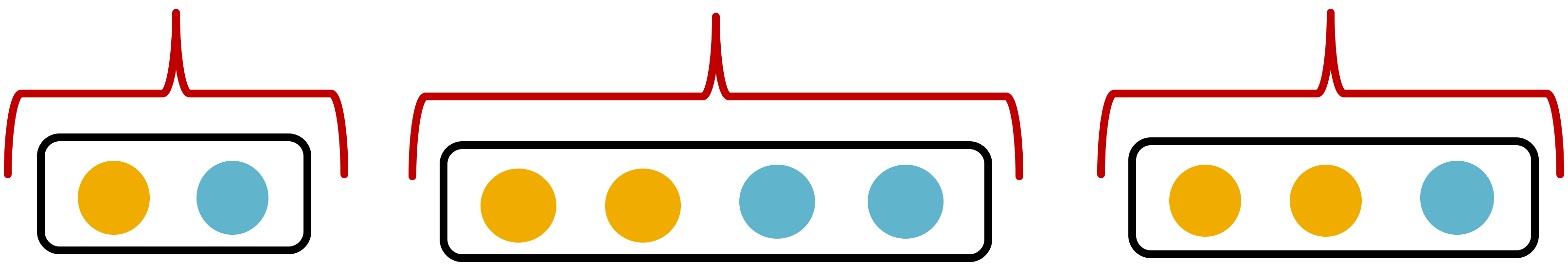
- **GCN (mean-pool)** [Kipf & Welling ICLR 2017]
  - **Failure case illustration**



Neighbor Aggregation: Case Study

- **GraphSAGE (max-pool)** [Hamilton et al. NeurIPS 2017]
  - Apply an MLP, then take **element-wise max.**
  - **Theorem** [Xu et al. ICLR 2019]
    - GraphSAGE's aggregation **function cannot distinguish different multi-sets with the same set of distinct colors.**

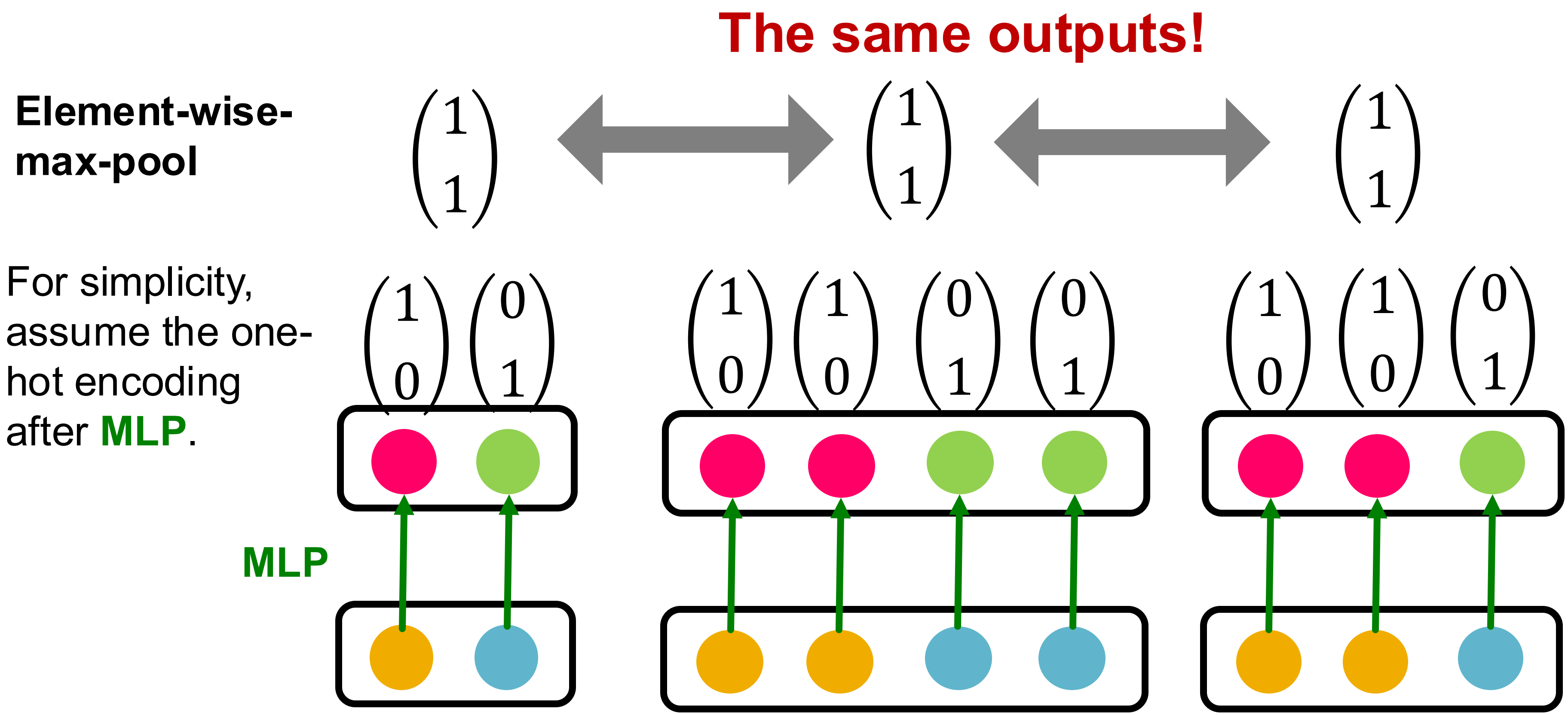
Failure case



- **Why?**

Neighbor Aggregation: Case Study

- **GraphSAGE (max-pool)** [Hamilton et al. NeurIPS 2017]
  - **Failure case illustration**



Summary So Far

- We analyzed the **expressive power of GNNs.**
- **Main takeaways**:
  - Expressive power of GNNs can be characterized by that of the neighbor aggregation function.
  - Neighbor aggregation is a function over multi-sets (sets with repeating elements)
  - GCN and GraphSAGE's aggregation functions fail to distinguish some basic multi-sets; hence **not injective**.
  - Therefore, GCN and GraphSAGE are **not** maximally powerful GNNs.

Designing Most Expressive GNNs

- **Our goal: Design maximally powerful GNNs in the class of message-passing GNNs.**
- This can be achieved by designing **injective neighbor aggregation function over multi-sets**.
- **Here, we design a neural network that can model injective multiset function.**

Injective Multi-Set Function

Theorem [Xu et al. ICLR 2019]

Any injective multi-set function can be expressed as:

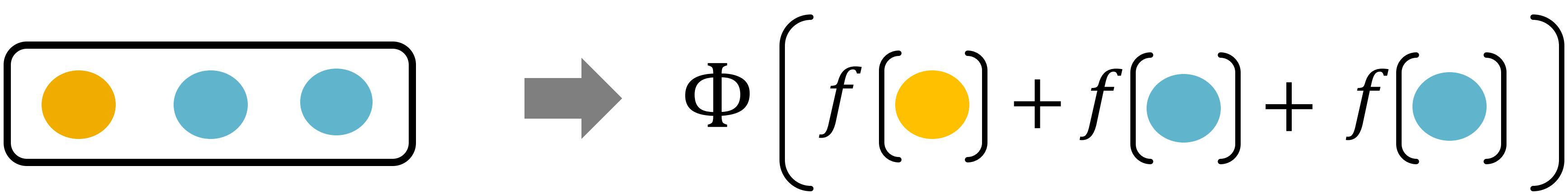
Some non-linear function

Some non-linear function

$$\Phi\left(\sum_{x\in S} f(x)\right)$$

Sum over multi-set

S : multi-set



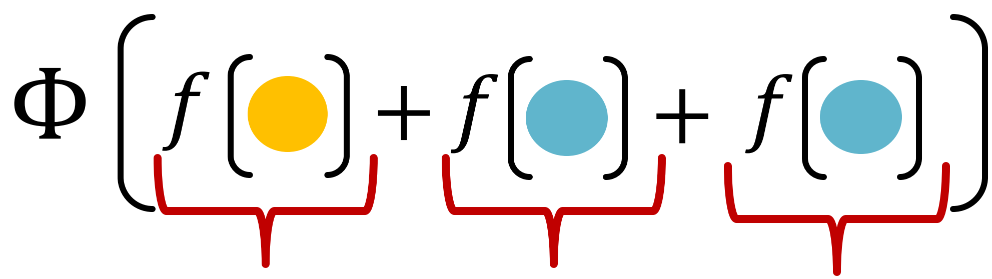
Injective Multi-Set Function

Proof Intuition: [Xu et al. ICLR 2019]

f produces one-hot encodings of colors. Summation of the one-hot encodings retains all the information about the input multi-set.

$$\Phi\left(\sum_{x\in S} f(x)\right)$$

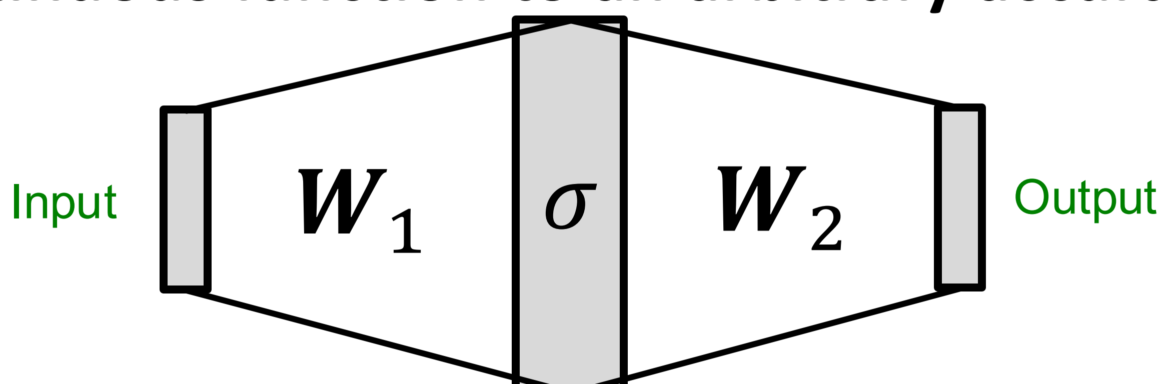
Example:



One-hot $\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\\2\end{pmatrix}$

Universal Approximation Theorem

- **How to model $\boldsymbol{\Phi}$ and $\boldsymbol{f}$ in $\boldsymbol{\Phi}\left(\sum_{x \in S} \boldsymbol{f}(\boldsymbol{x})\right)$?**
- We use a Multi-Layer Perceptron (MLP).
- **Theorem: Universal Approximation Theorem**
  [Hornik et al., 1989]
  - 1-hidden-layer MLP with sufficiently-large hidden dimensionality and appropriate non-linearity $\sigma(\cdot)$ (including ReLU and sigmoid) can **approximate any continuous function to an arbitrary accuracy**.



Injective Multi-Set Function

- **We have arrived at a neural network that can model any injective multiset function.**

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

  - In practice, MLP hidden dimensionality of 100 to 500 is sufficient.

Most Expressive GNN

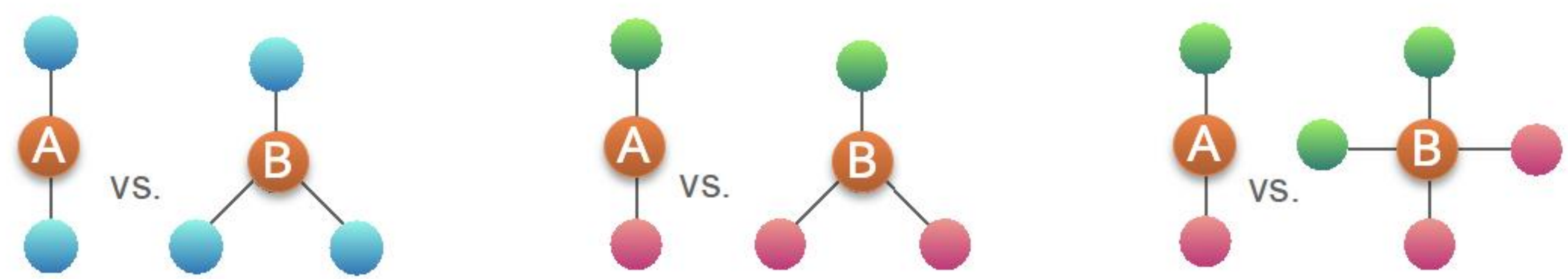
- **Graph Isomorphism Network (GIN)** [Xu et al. ICLR 2019]
  - Apply an MLP, element-wise **sum**, followed by another MLP.

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

- **Theorem** [Xu et al. ICLR 2019]
  - GIN's neighbor aggregation function is injective.
- **No failure cases!**
- **GIN is THE most expressive GNN in the class of message-passing GNNs we have introduced!**

Discussion: The Power of Pooling

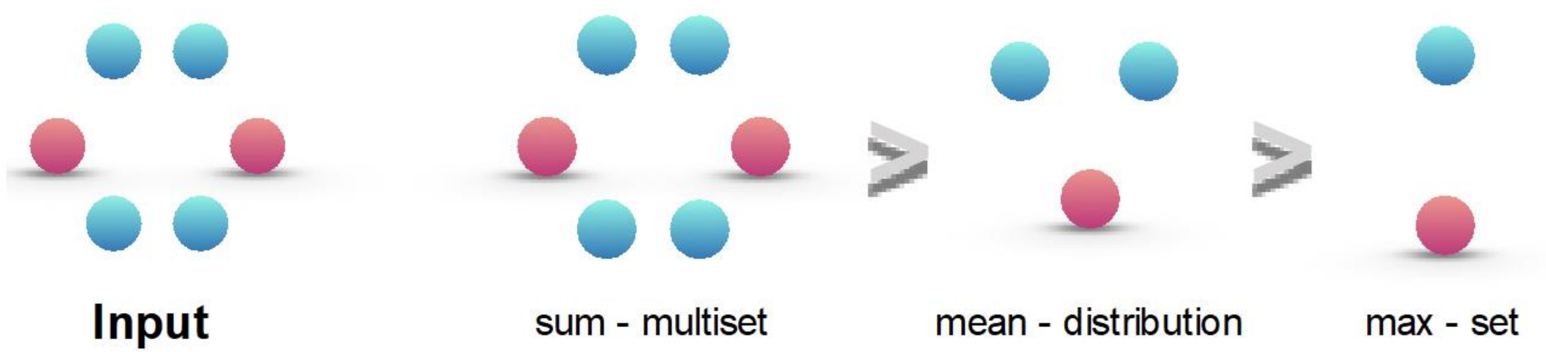
Failure cases for mean and max pooling:



(a) Mean and Max both fail (b) Max fails (c) Mean and Max both fail

Colors represent feature values

Ranking by discriminative power:



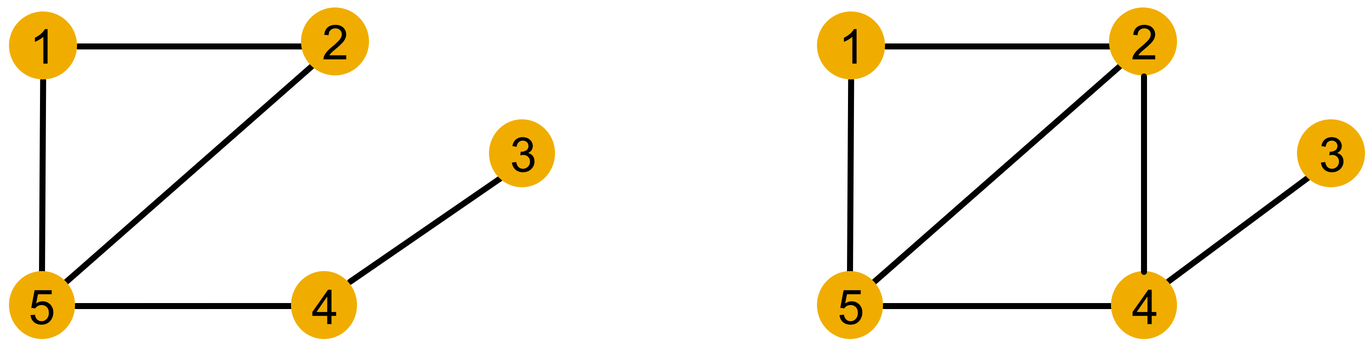
Full Model of GIN

- **So far:** **We have described the neighbor aggregation part of GIN.**

- We now describe the full model of GIN by relating it to **WL graph kernel** (traditional way of obtaining graph-level features).
  - We will see how GIN is a "neural network" version of the WL graph kernel.

Graph Isomorphism problem

- **A classical expressivity test is Graph isomorphism.**
  - **Given a pair of graphs, can we tell if they are isomorphic?**



- **Open problem (a polynomial time algorithm does not exist, has not been proven NP-complete)**

Relation to WL Graph Kernel

Color refinement algorithm in WL kernel.

- **Given:** A graph G with a set of nodes V.
  - Assign an initial color $c^{(0)}(v)$ to each node v.
  - Iteratively refine node colors by

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

where HASH maps different inputs to different colors.

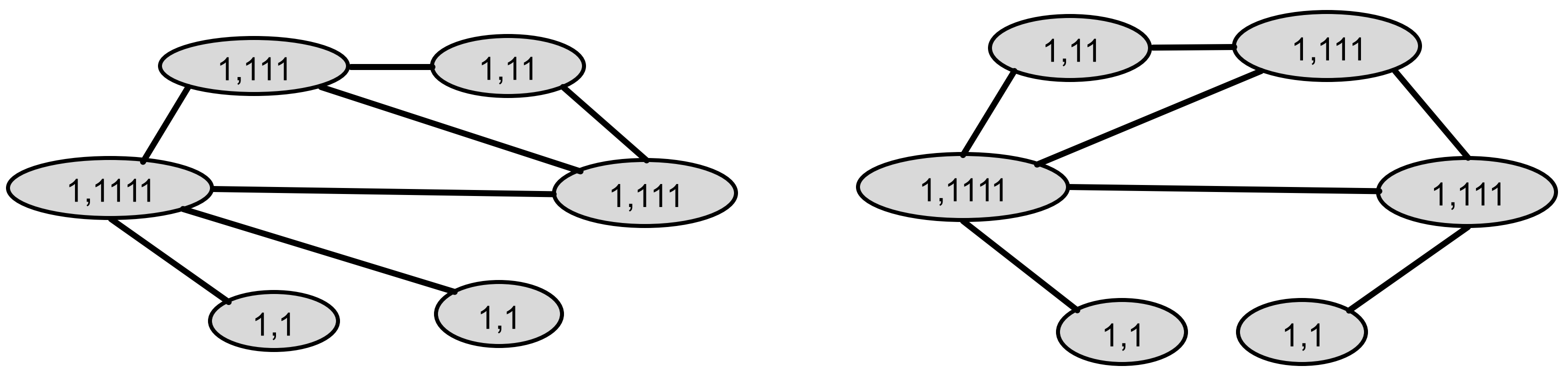
  - After K steps of color refinement, $c^{(K)}(v)$ summarizes the structure of K-hop neighborhood

Color Refinement (1)

Example of color refinement given <u>two graphs</u>

- Assign initial colors

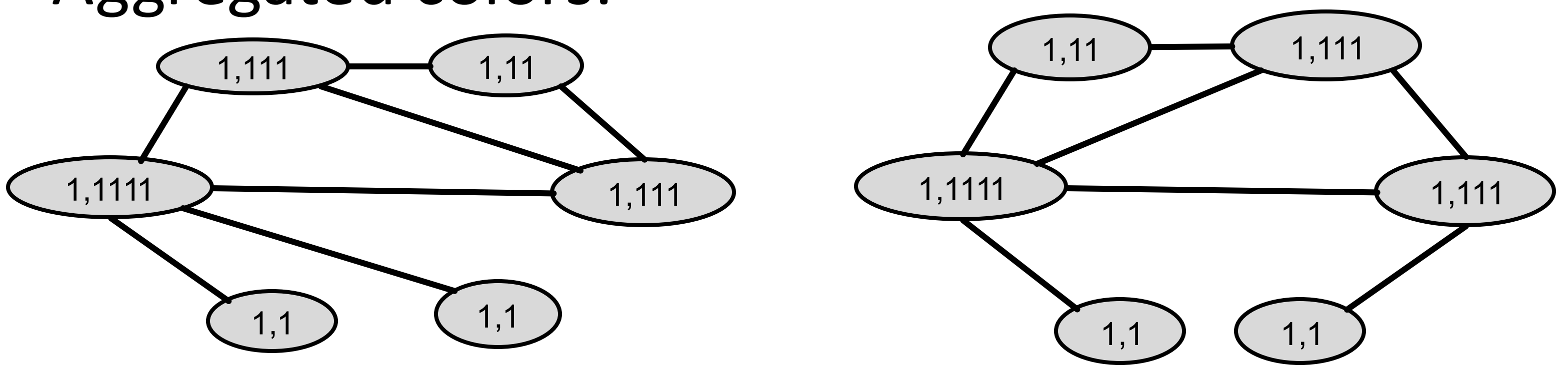
- Aggregate neighboring colors



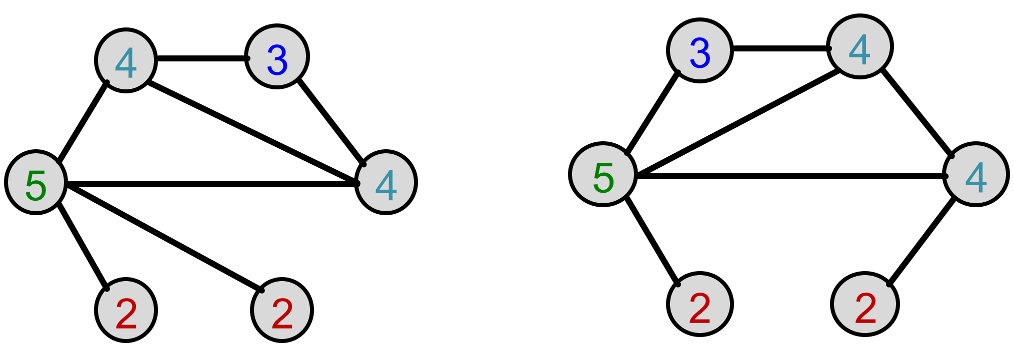
Color Refinement (2)

Example of color refinement given two graphs

- Aggregated colors:



- **Injectively** HASH the aggregated colors



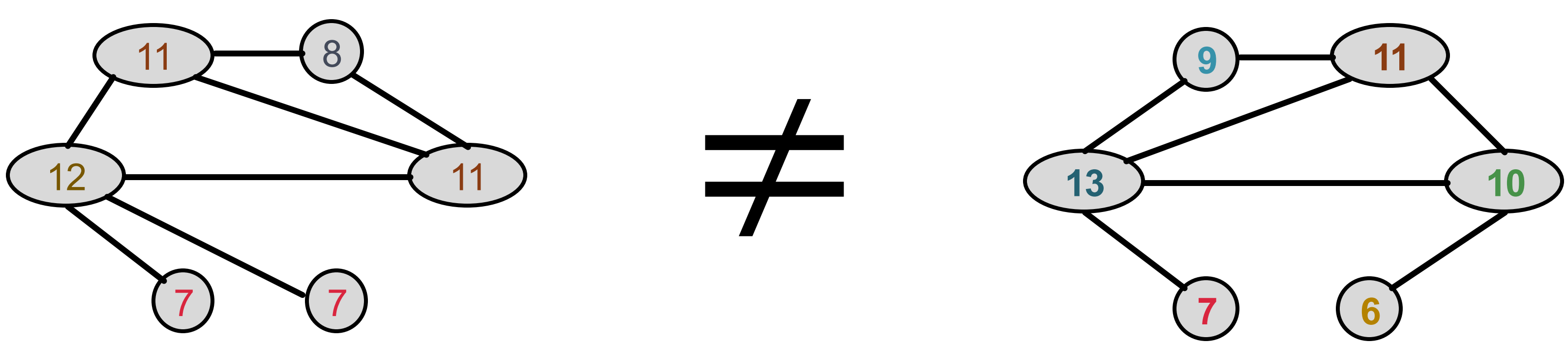
HASH table: **Injective!**

1,1	-->	2
1,11	-->	3
1,111	-->	4
1,1111	-->	5

Color Refinement (3)

Example of color refinement given two graphs

- Process continues until a stable coloring is reached
- Two graphs are considered **isomorphic** if they have the same set of colors.



The Complete GIN Model

- **GIN uses a neural network to model the injective HASH function.**

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

- Specifically, we will model the injective function over the tuple:

$$\left(\boxed{c^{(k)}(v)}, \boxed{\{c^{(k)}(u)\}_{u \in N(v)}}\right)$$

Root node features

Neighboring node colors

The Complete GIN Model

Theorem (Xu et al. ICLR 2019)

Any injective function over the tuple

Root node feature $\left(\boxed{c^{(k)}(v)}, \boxed{\{c^{(k)}(u)\}_{u \in N(v)}}\right)$ Neighboring node features

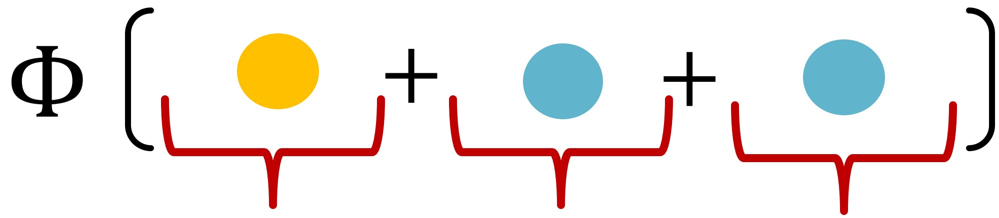
can be modeled as

$$\mathrm{MLP}_{\Phi}\left((1+\epsilon) \cdot \mathrm{MLP}_f(c^{(k)}(v))) + \sum_{u \in N(v)} \mathrm{MLP}_f(c^{(k)}(u))\right)$$

where ϵ is a learnable scalar.

The Complete GIN Model

- If input feature $c^{(0)}(v)$ is represented as one-hot, **direct summation is injective.**

Example: 

$$\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\\2\end{pmatrix}$$

- We only need Φ to ensure the injectivity.

$$\text{GINConv}\left(\boxed{c^{(k)}(v)}, \boxed{\left\{c^{(k)}(u)\right\}_{u\in N(v)}}\right) = \text{MLP}_{\Phi}\left((1+\epsilon)\cdot c^{(k)}(v) + \sum_{u\in N(v)} c^{(k)}(u)\right)$$

Root node features

Neighboring node features

This MLP can provide "one-hot" input feature for the next layer.

The Complete GIN Model

- **GIN's node embedding updates**
- Given: A graph G with a set of nodes V.
  - Assign an **initial vector** $c^{(0)}(v)$ to each node v.
  - Iteratively update node vectors by

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

Differentiable color HASH function

where GINConv maps different inputs to different embeddings.

  - After K steps of GIN iterations, $c^{(K)}(v)$ summarizes the structure of K-hop neighborhood.

GIN and WL Graph Kernel

- **GIN can be understood as differentiable neural version of the WL graph Kernel:**

	Update target	Update function
WL Graph Kernel	Node colors (one-hot)	HASH
GIN	Node embeddings (low-dim vectors)	GINConv

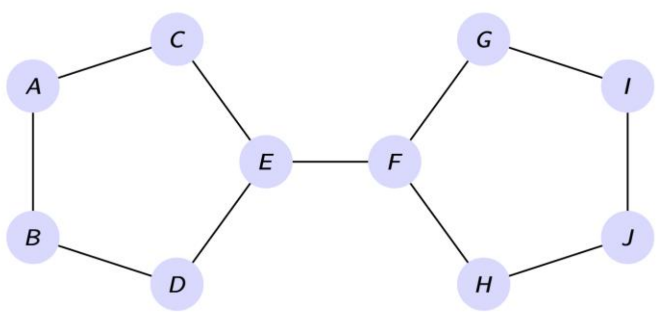
- **Advantages of GIN over the WL graph kernel are:**
  - Node embeddings are **low-dimensional**; hence, they can capture the fine-grained similarity of different nodes.
  - Parameters of the update function can be **learned for the downstream tasks.**

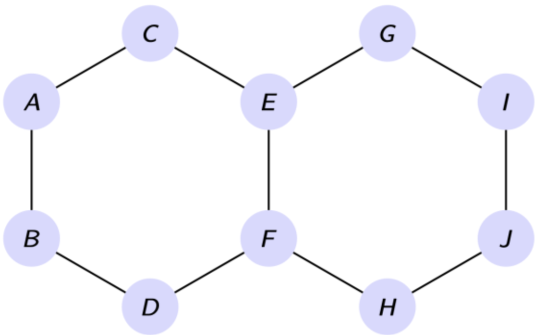
Expressive Power of GIN

- **Because of the relation between GIN and the WL graph kernel, their expressive is exactly the same.**
  - If two graphs can be distinguished by GIN, they can be also distinguished by the WL kernel, and vice versa.
- **How powerful is this?**
  - WL kernel has been both theoretically and empirically shown to distinguish most of the real-world graphs [Cai et al. 1992].
  - Hence, GIN is also powerful enough to distinguish most of the real graphs!

Some bad news

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

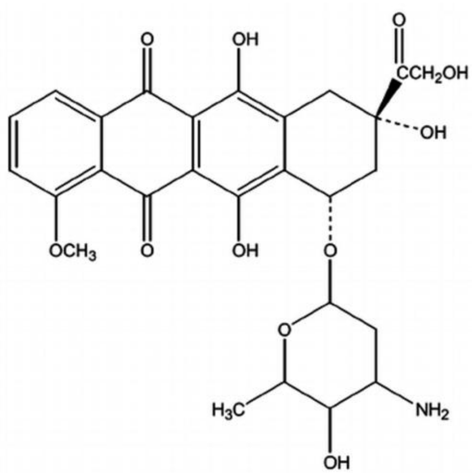




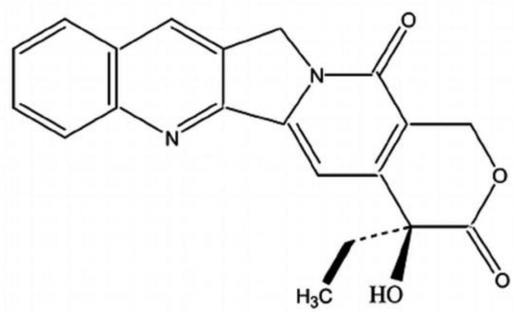
- **The WL kernel cannot count important sub-structures, e.g., cycles and cliques.**

Why do we care about cycles?

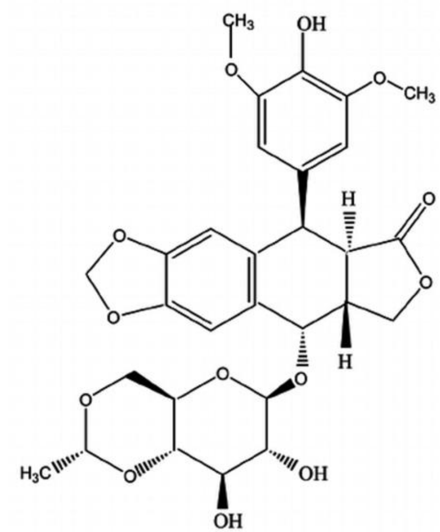
- The **bonds between different atoms** in chemical compounds form **cycles**.
- The hexagon is the **most common polygon** in organic compounds ⇒ yields stable materials.



Doxorubicin



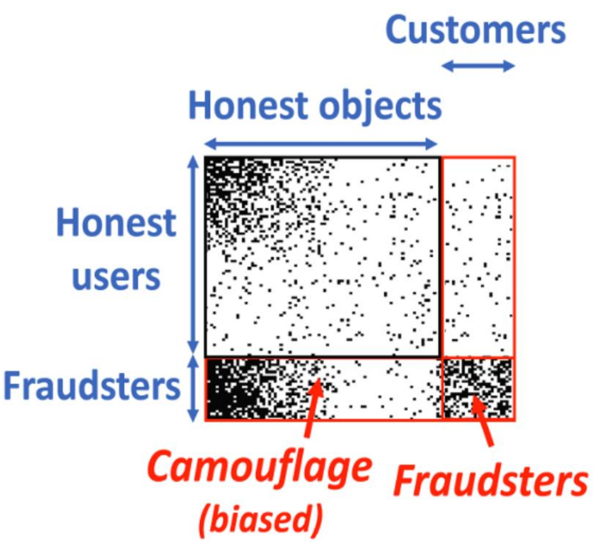
Camptothecin



Etoposide

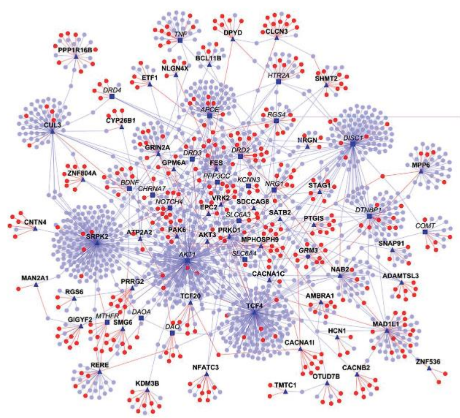
Why cliques and quasi-cliques?

Fraudster Detection in e-Commerce Networks



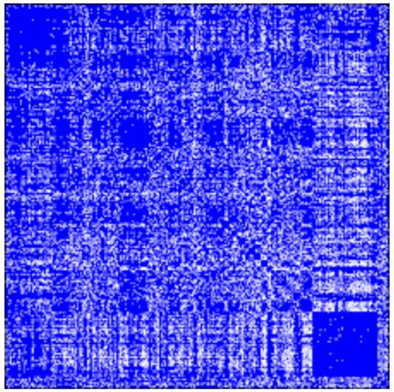
[Hooi et al. 2016]

Detection of Protein Complexes in PPI Networks



[Vlaic et al. 2017]

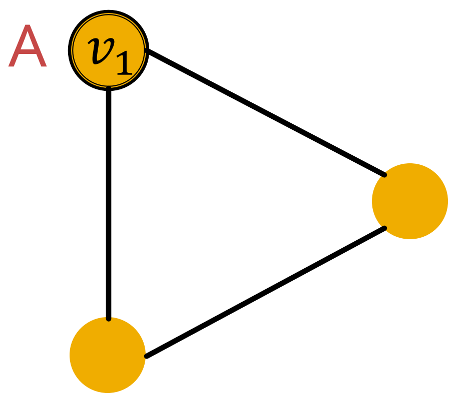
Graph Compression



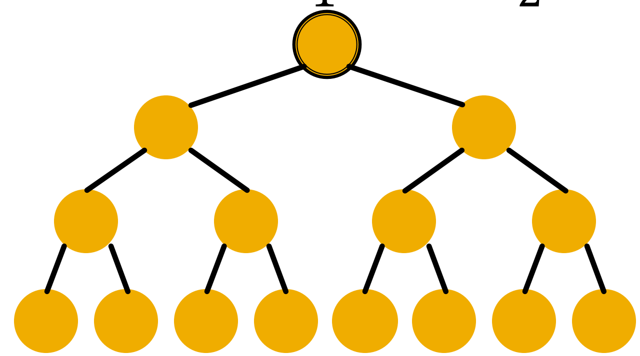
Dhulipala et al. 2017

Improving GNNs' Power

- **Can the expressive power of GNNs be improved?**
  - There are basic graph structures that existing GNN framework cannot distinguish, such as difference in cycles.



Computational graphs for nodes v_1 and v_2:



  - GNNs' expressive power **can be improved** to resolve the above problem. [You et al. AAAI 2021, Li et al. NeurIPS 2020, Kanatsoulis et al. ICLR 2024]

Summary of the Lecture

- We design a neural network that can model an injective multi-set function.
- We use the neural network for neighbor aggregation function and arrive at **GIN**---the most expressive GNN model.
- The key is to use **element-wise sum pooling**, instead of mean-/max-pooling.
- GIN is closely related to the WL graph kernel.
- Both GIN and WL graph kernel can distinguish most of the real graphs!