Stanford CS224W: How Expressive are Graph Neural Networks?

CS224W: Machine Learning with Graphs

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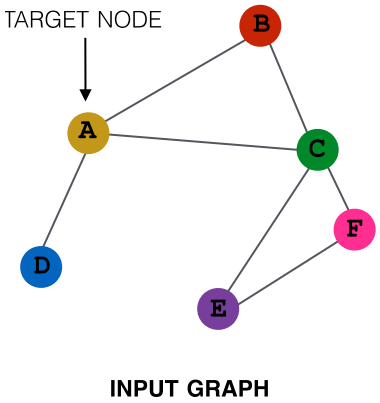
http://cs224w.stanford.edu

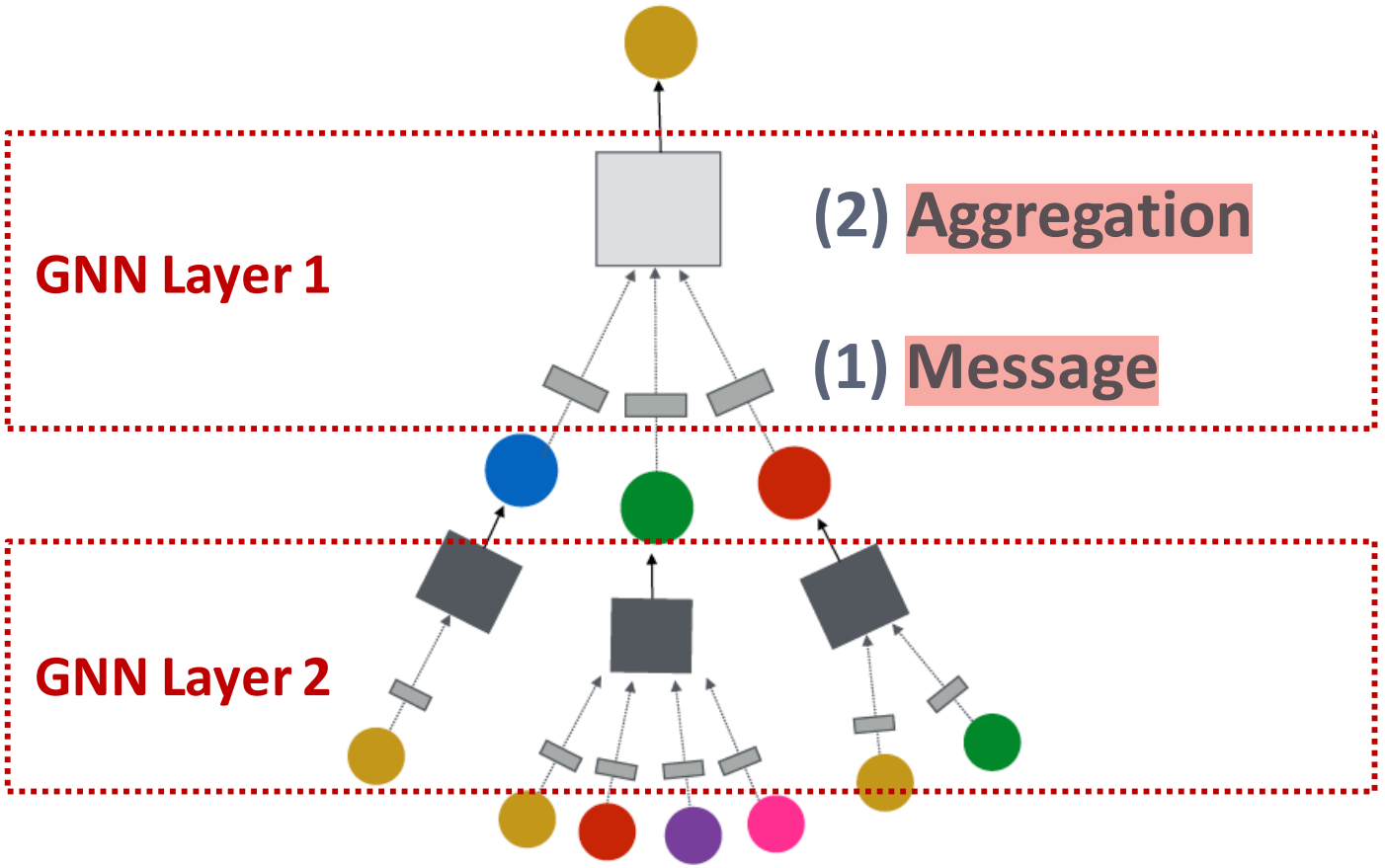
ANNOUNCEMENTS

- Homework 1 due on **Thursday** (2/2)
- Based on course feedback, we will hold in-person OHs every week on Wednesday 9-11 AM PT. Location will be updated on the OH calendar.

Recap: A General GNN Framework



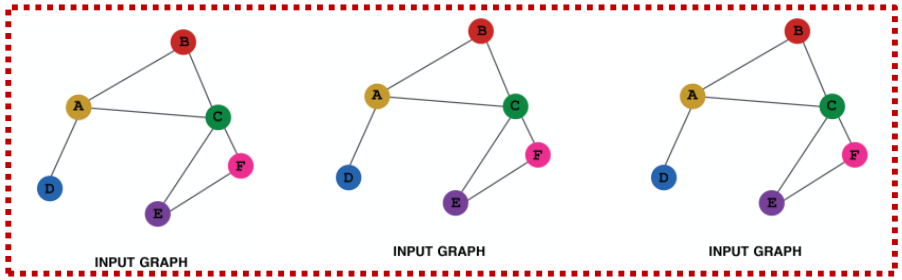
(5) Learning objective

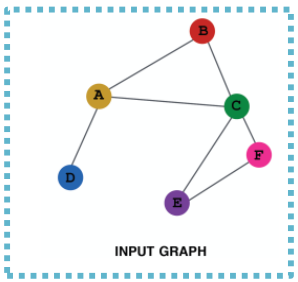


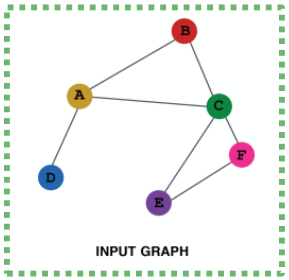
(3) Layer connectivity

(4) Graph augmentation

Recap: GNN Training Pipeline

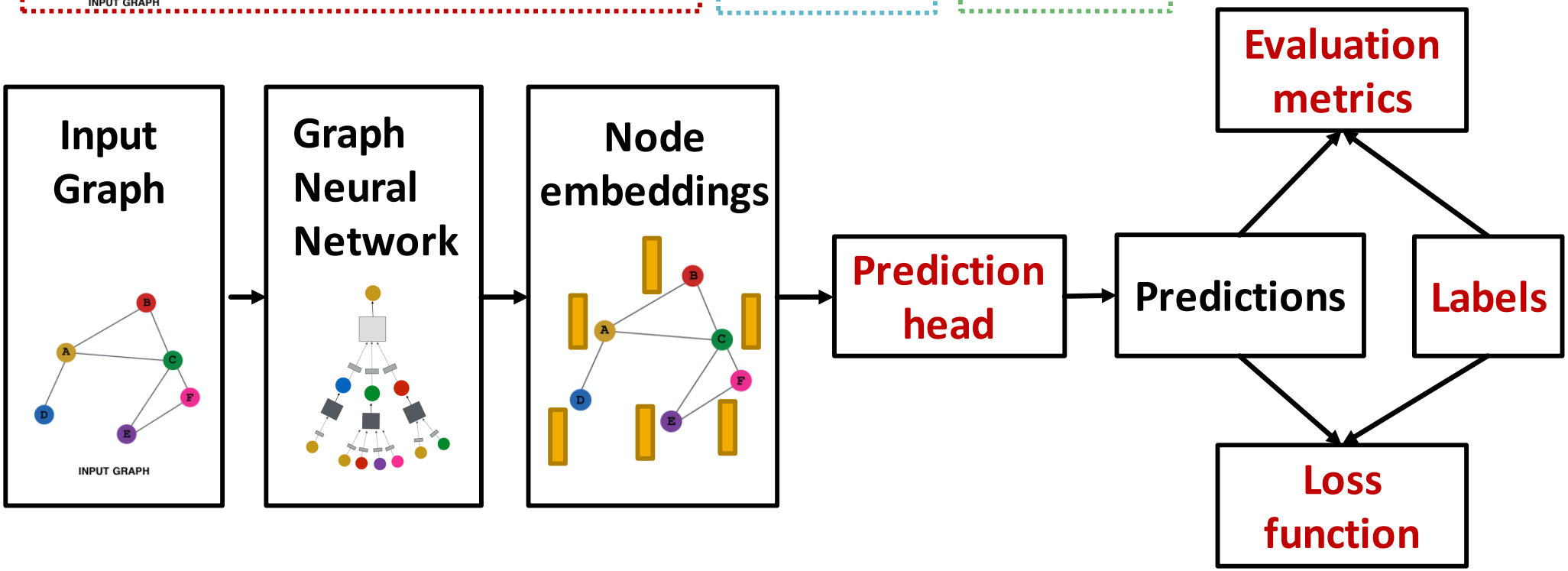






Dataset split

划分训练集和测试集



Implementation resources:

PyG provides core modules for this pipeline

GraphGym further implements the full pipeline to facilitate GNN design

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? GIN

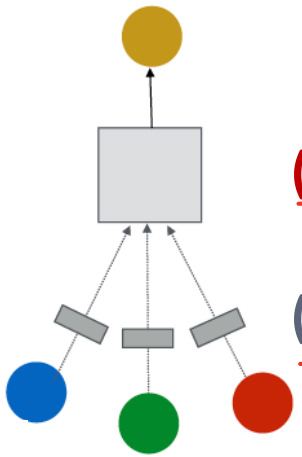
Background: A Single GNN Layer

- **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

$$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)}, u \in N(v)\right\}, \mathbf{m}_v^{(l)}\right)$$

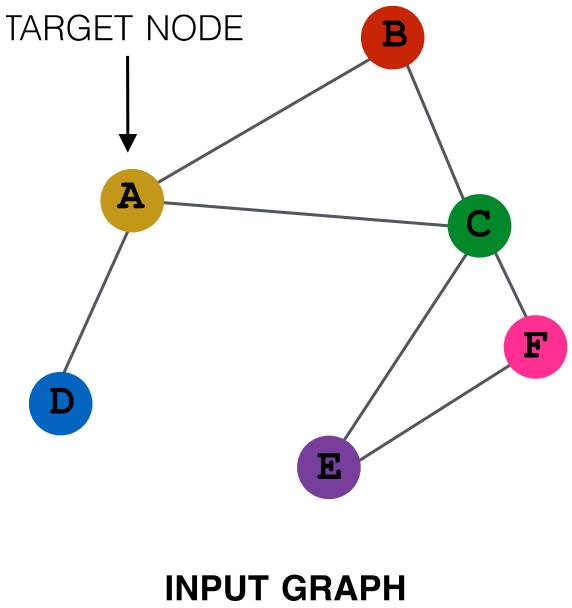


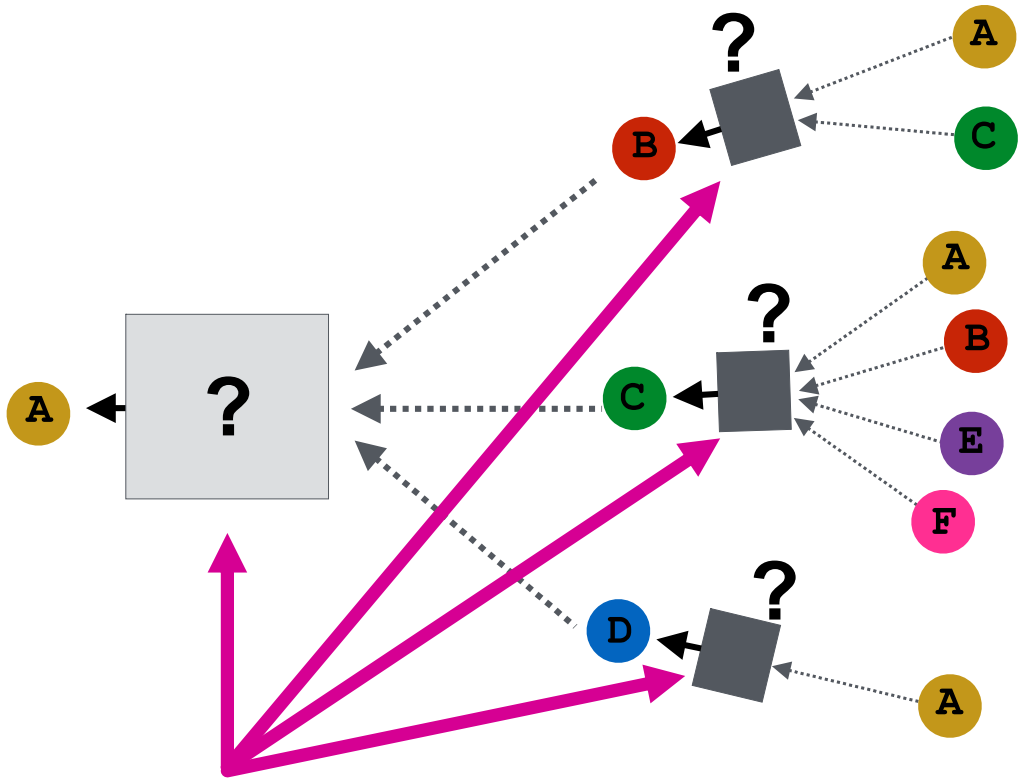
(2) Aggregation

(1) Message

Background: Many GNN Models

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

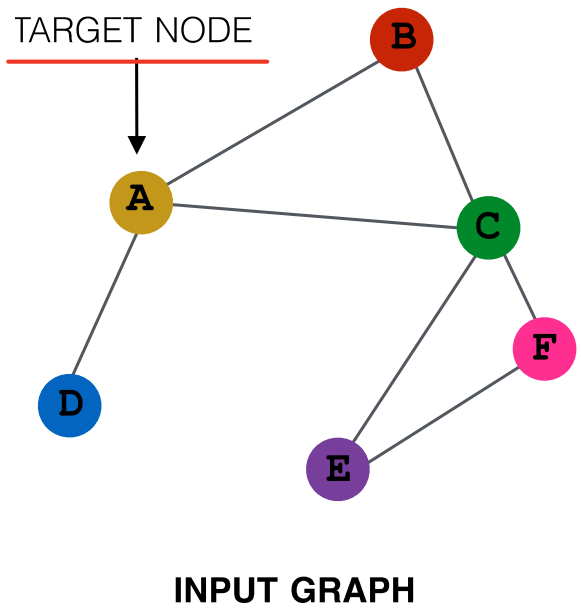




Different GNN models use different neural networks in the box

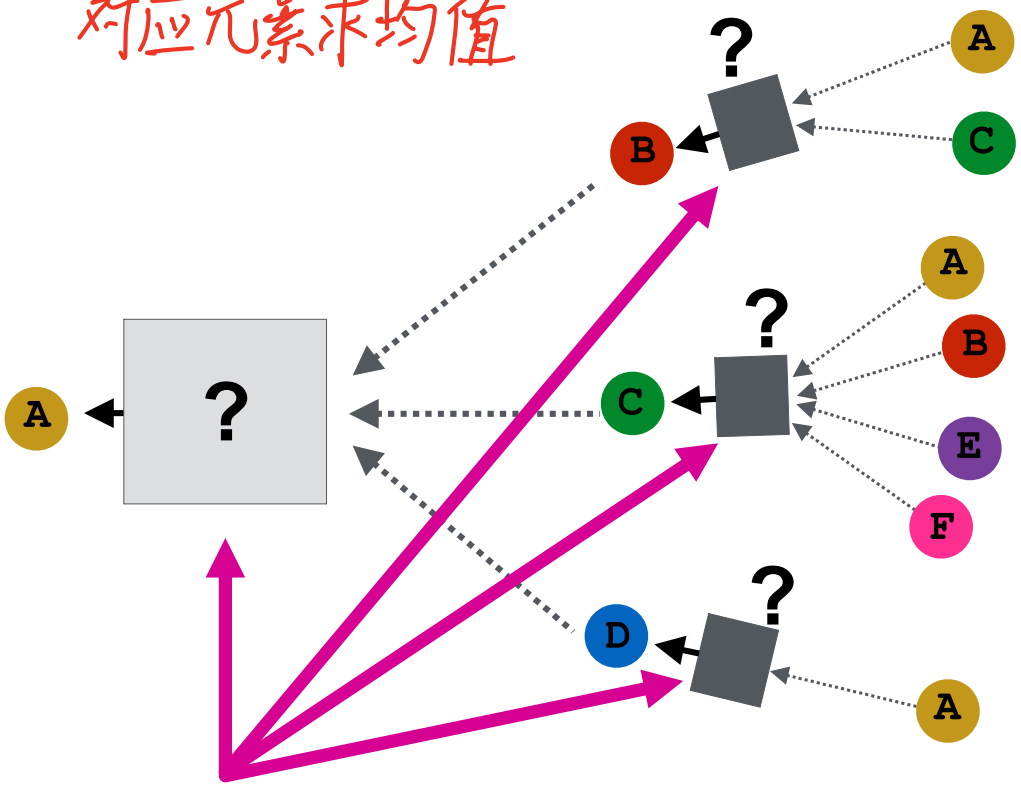
GNN Model Example (1)

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



INPUT GRAPH

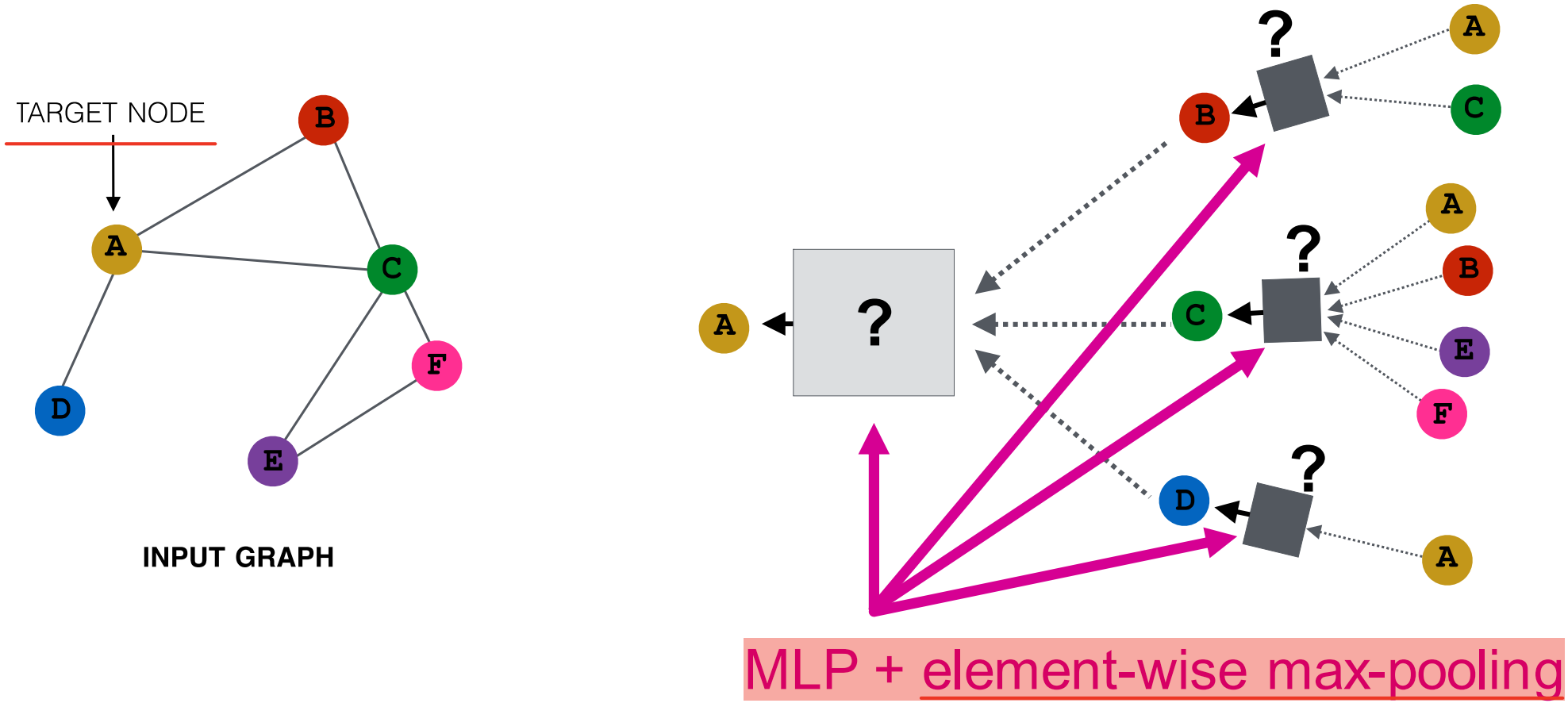
对应元素求均值



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

GNN Model Example (2)

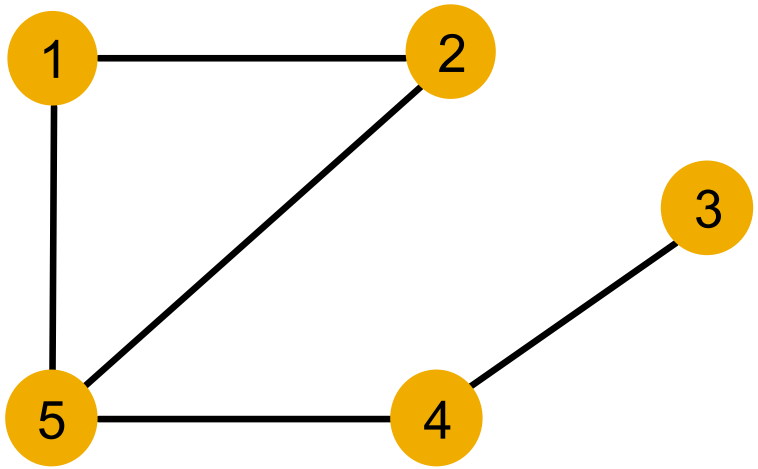
- **GraphSAGE (max-pool)** [Hamilton et al. NeurIPS 2017]



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. 节点属性特征：初始 embedding

只考虑图结构，因此假设所有属性一样.

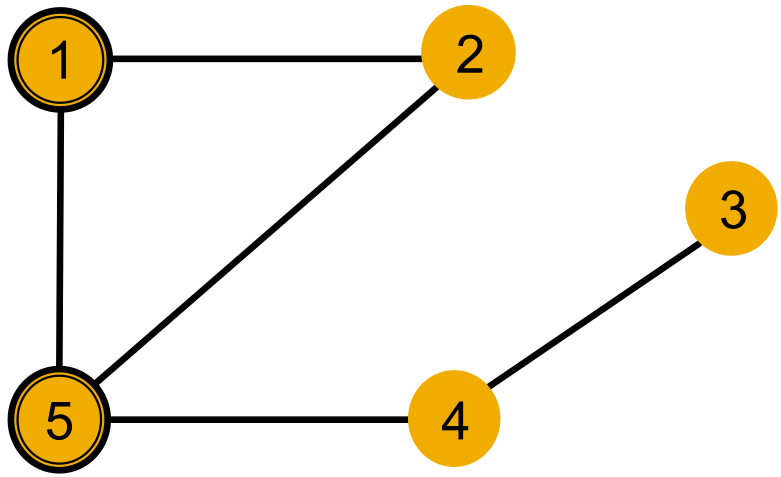


仅通过计算图（连接结构）区分不同节点

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

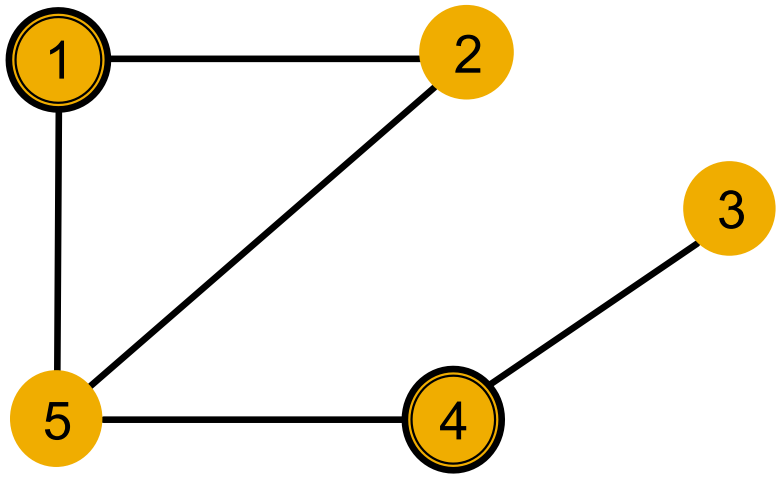
Local Neighborhood Structures

- 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.**



邻居连接数

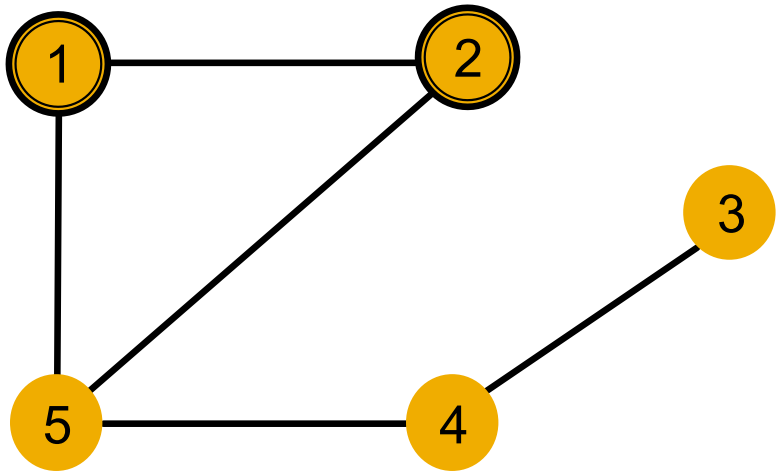
GNN中通过计算图体现

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.**

仅通过图的连接结构（GNN计算图），无法区分节点1和节点2（isomorphic同形）



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?

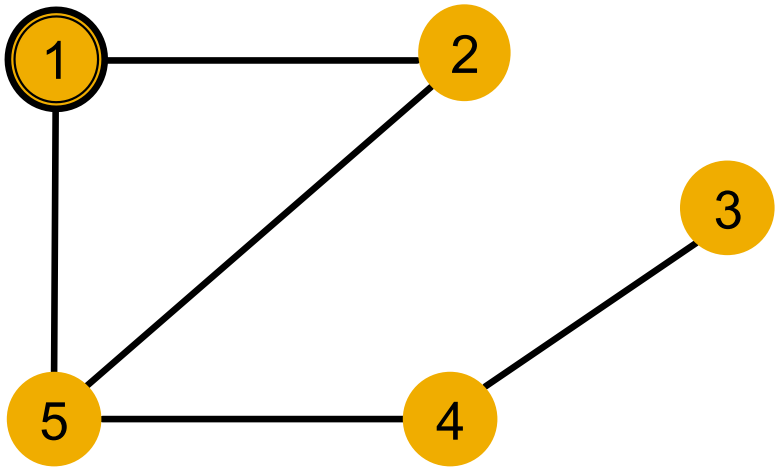
不同的节点是否能学到不同的 embedding.

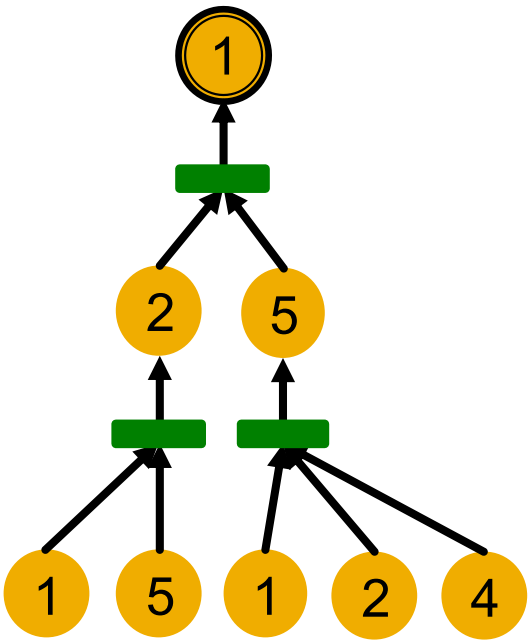
- **Next**: **We need to understand how a GNN captures local neighborhood structures.**
  - **Key concept**: **Computational graph**

GNN的表达能力 = 区分计算图根节点 embedding 的能力

Computational Graph (1)

- **In each layer, a GNN aggregates neighboring node embeddings.** 邻域消息传递计算图
- A GNN generates node embeddings through a computational graph defined by the neighborhood.
  - **Ex:** Node 1's computational graph (2-layer GNN)



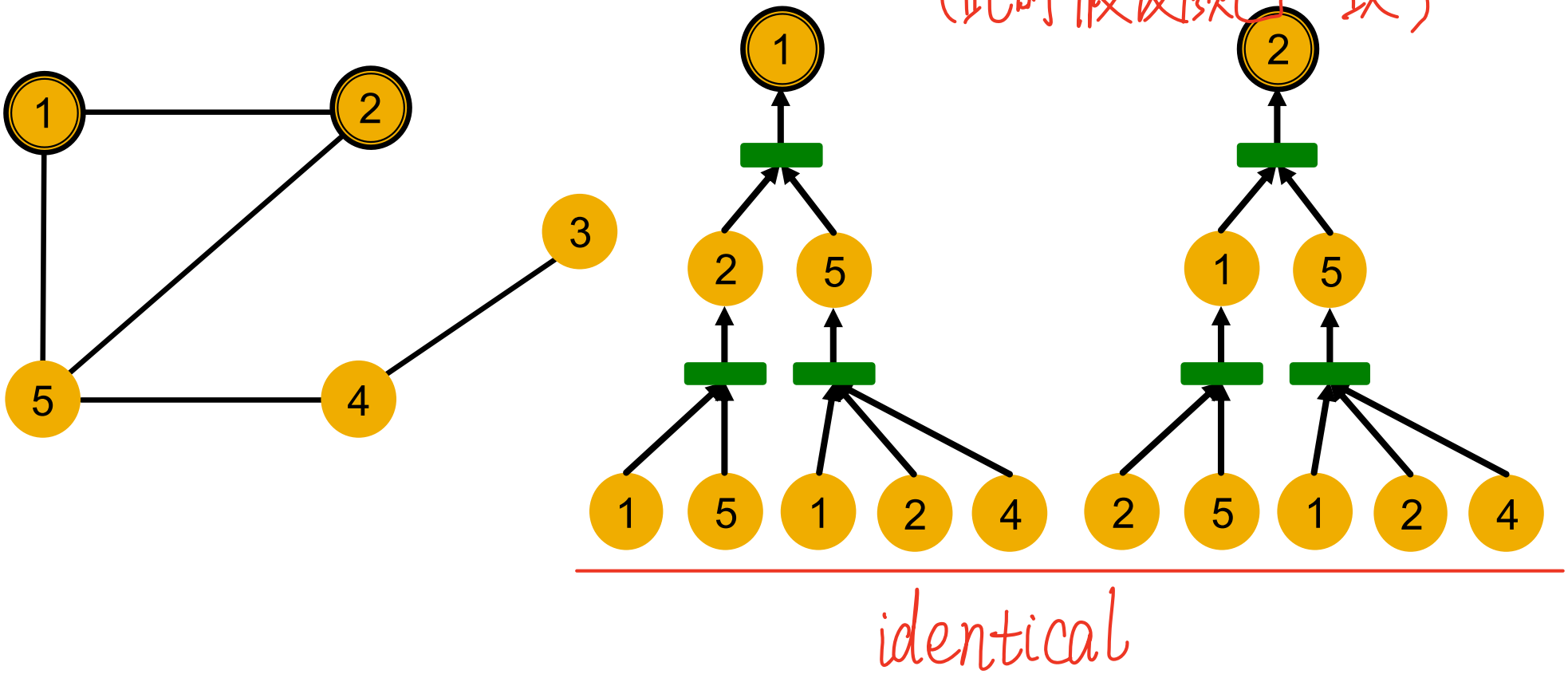


Computational Graph (2)

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

编号无意义，连接长度无意义，颜色有意义

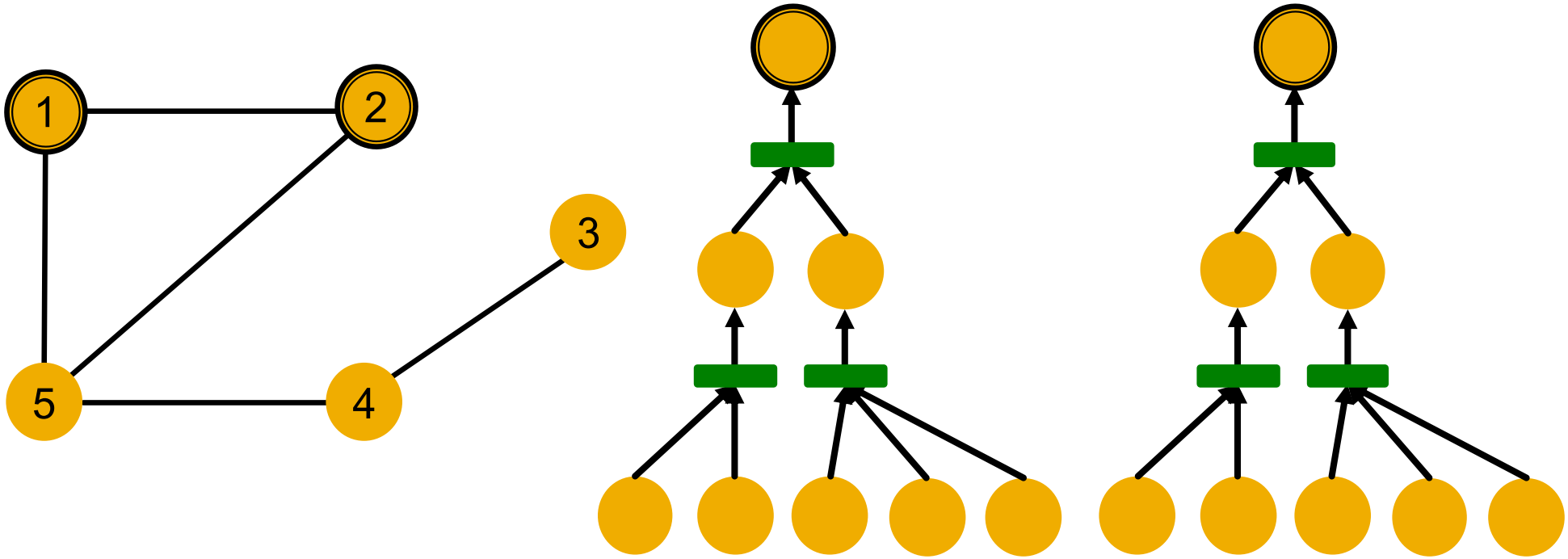
（此时假设颜色一致）



Computational Graph (3)

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

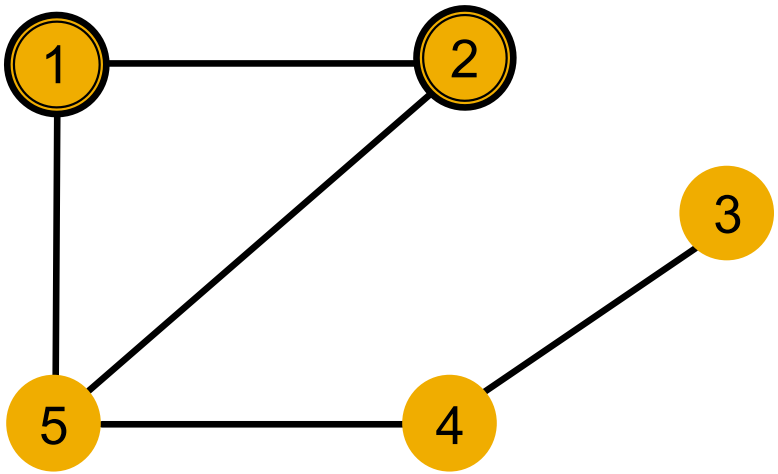
GNN眼中计算图相同 → 无法区分

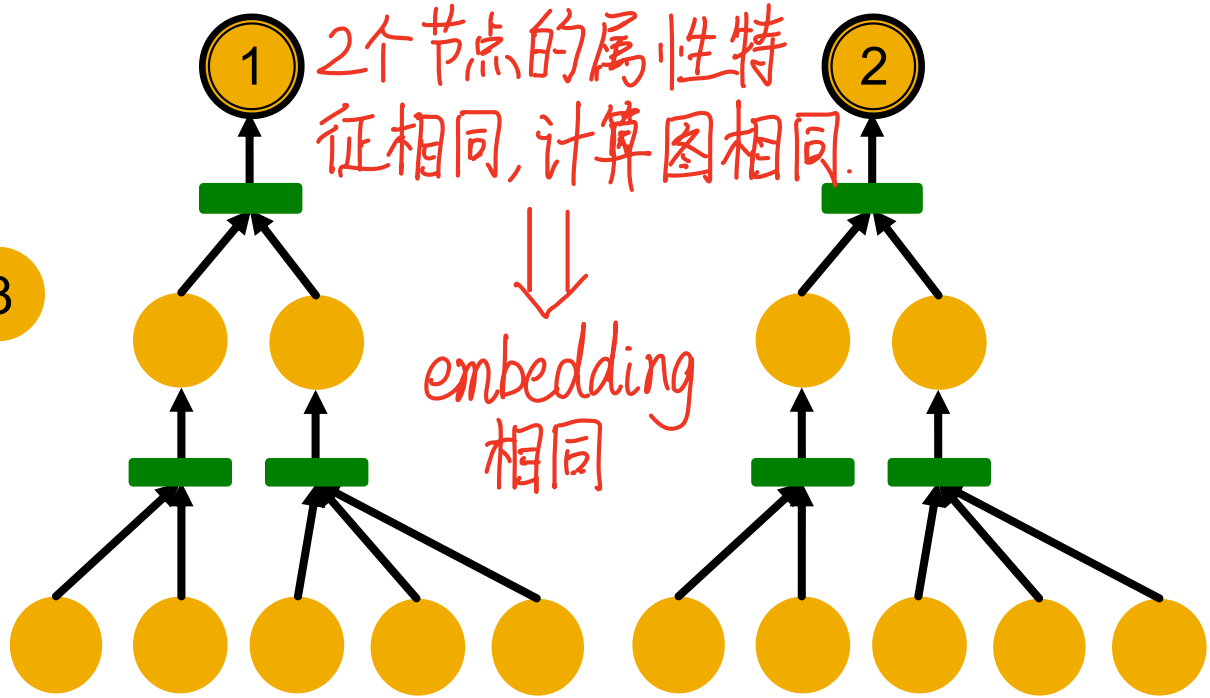


Computational Graph (4)

- **A GNN will generate the same embedding 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.

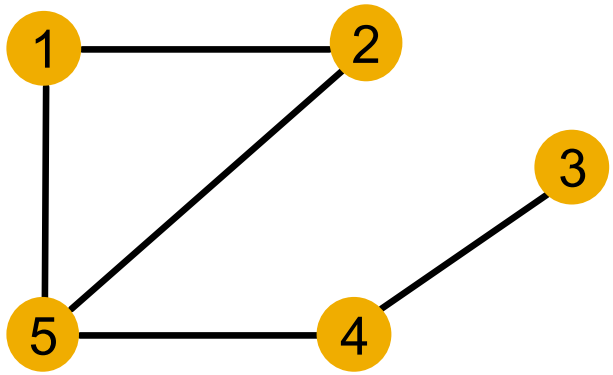




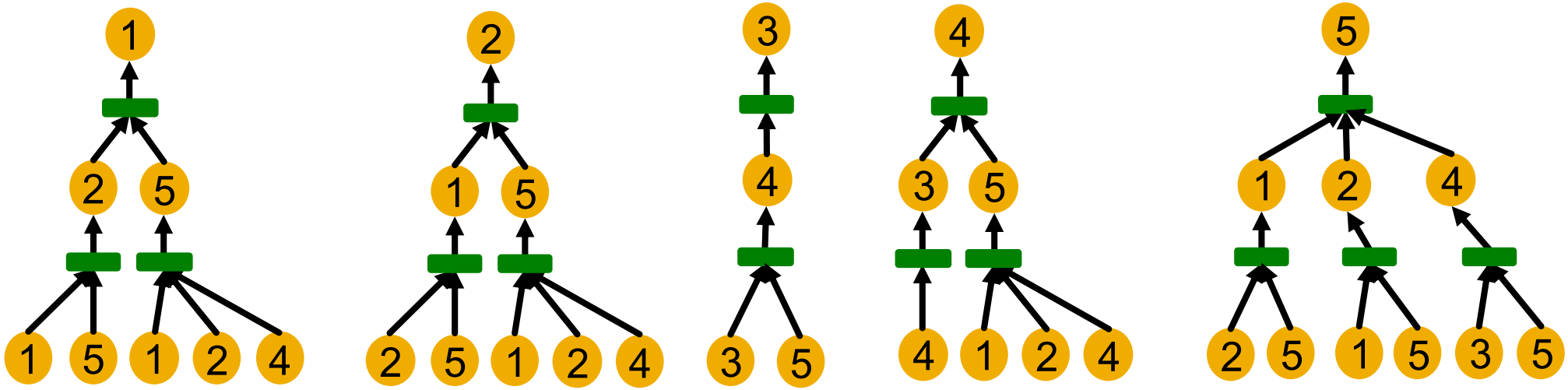
GNN won't be able to distinguish nodes 1 and 2

Computational Graph

- In general, different local neighborhoods define different computational graphs

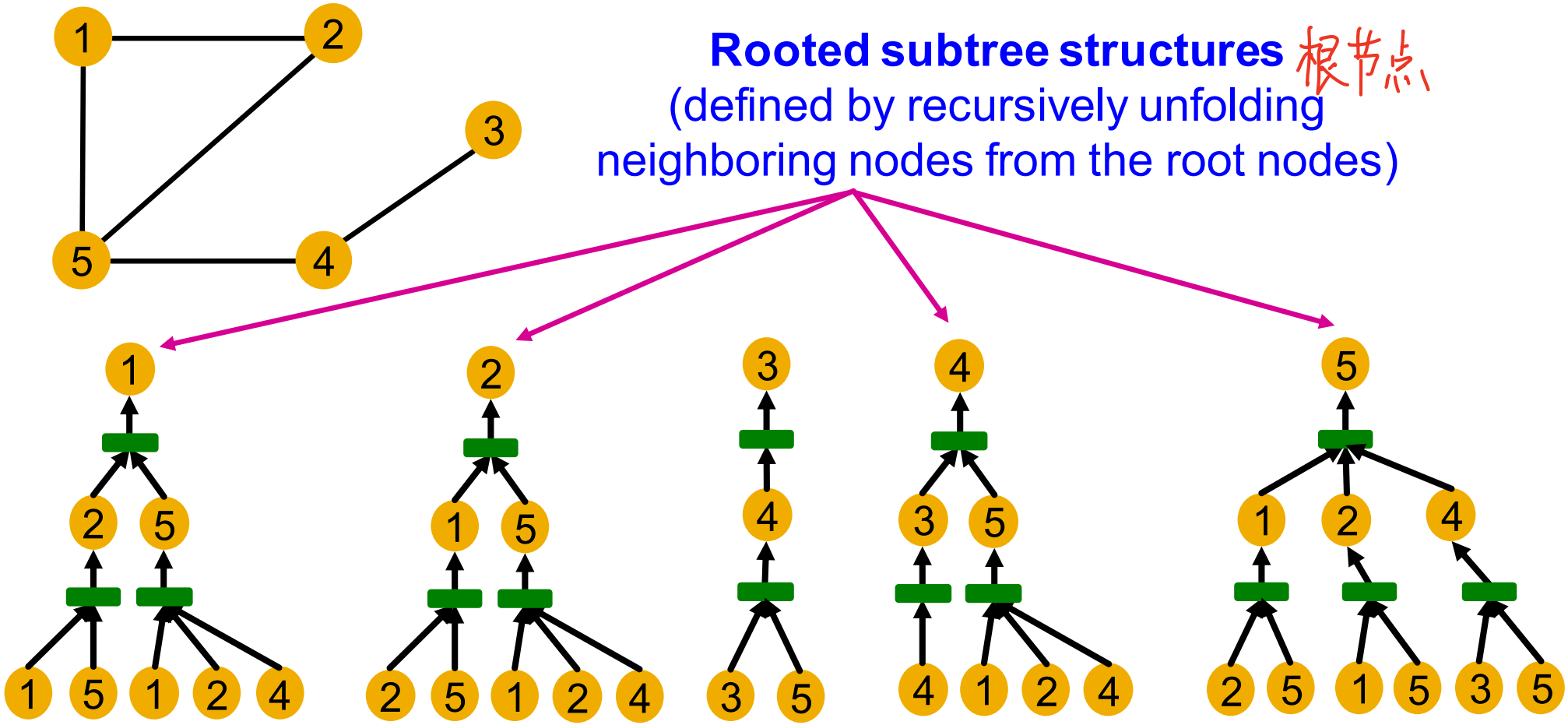


即使计算图不同，
GNN就能区分3和4了吗？



Computational Graph

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

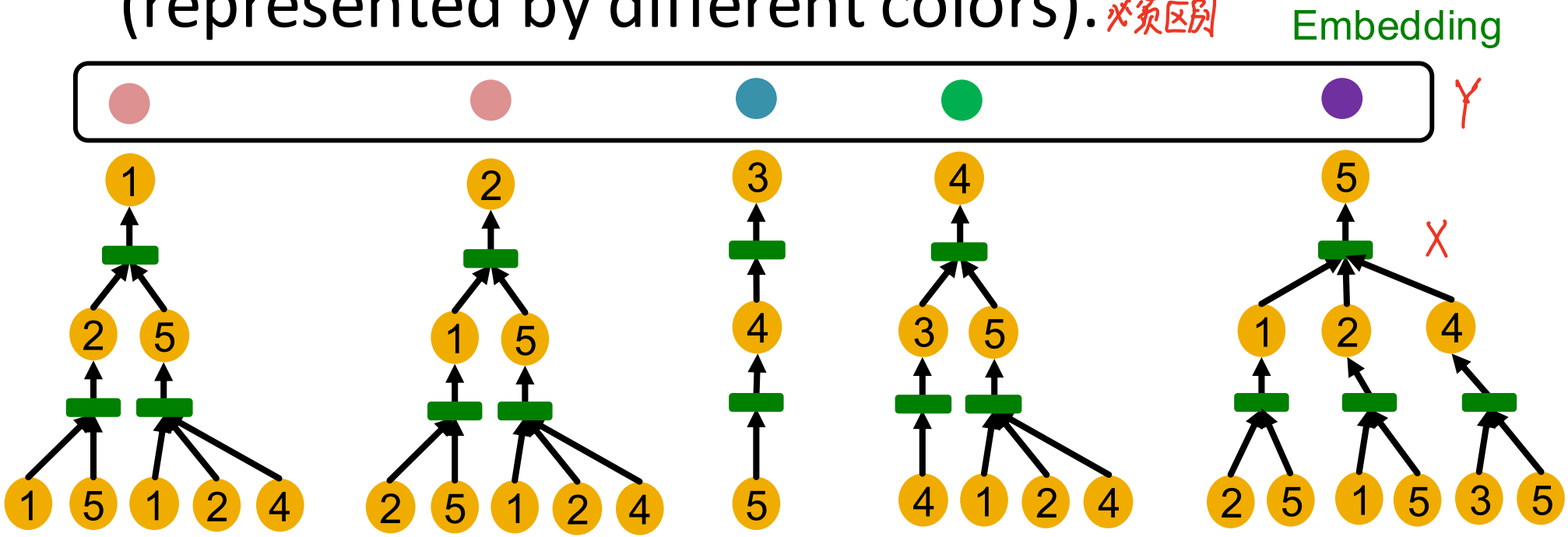


Computational Graph

GNN的表达能力 = 区分计算图根节点embedding的能力

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

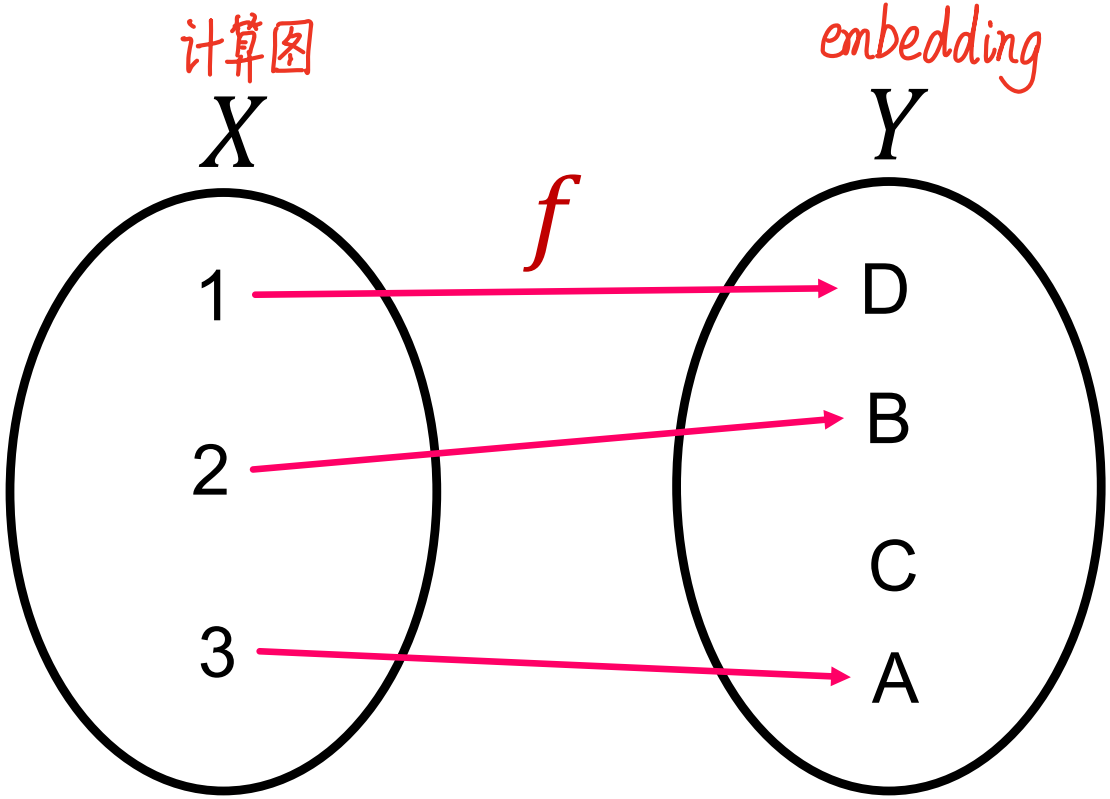
1和2可以无法区分，但3,4,5必须区别

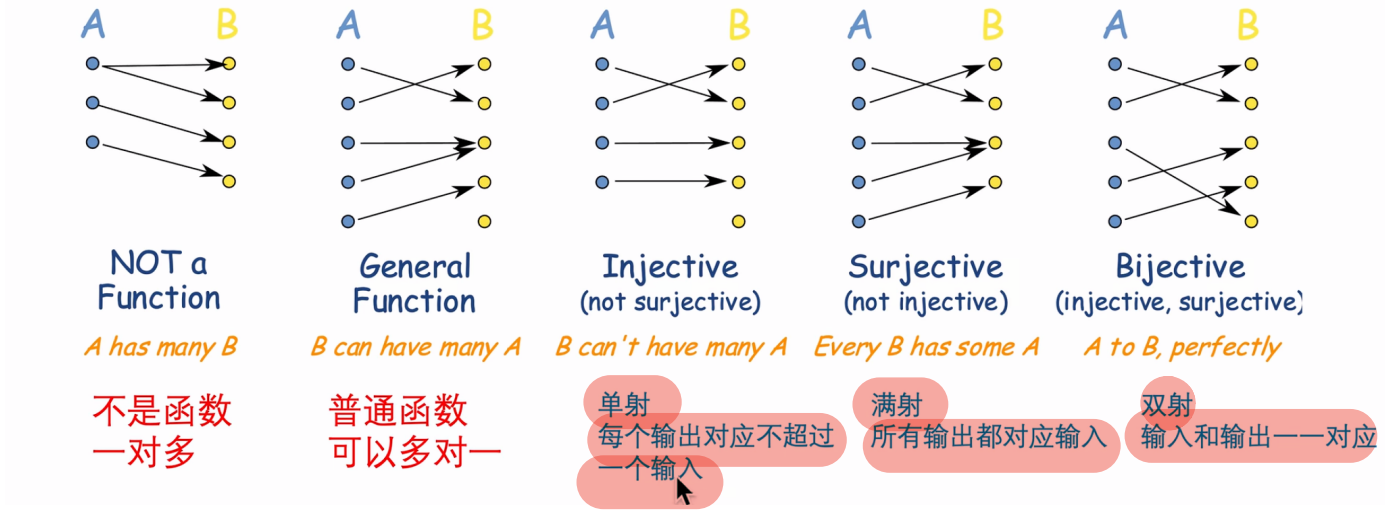


Recall: Injective Function

单射：每个输入对应唯一输出

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

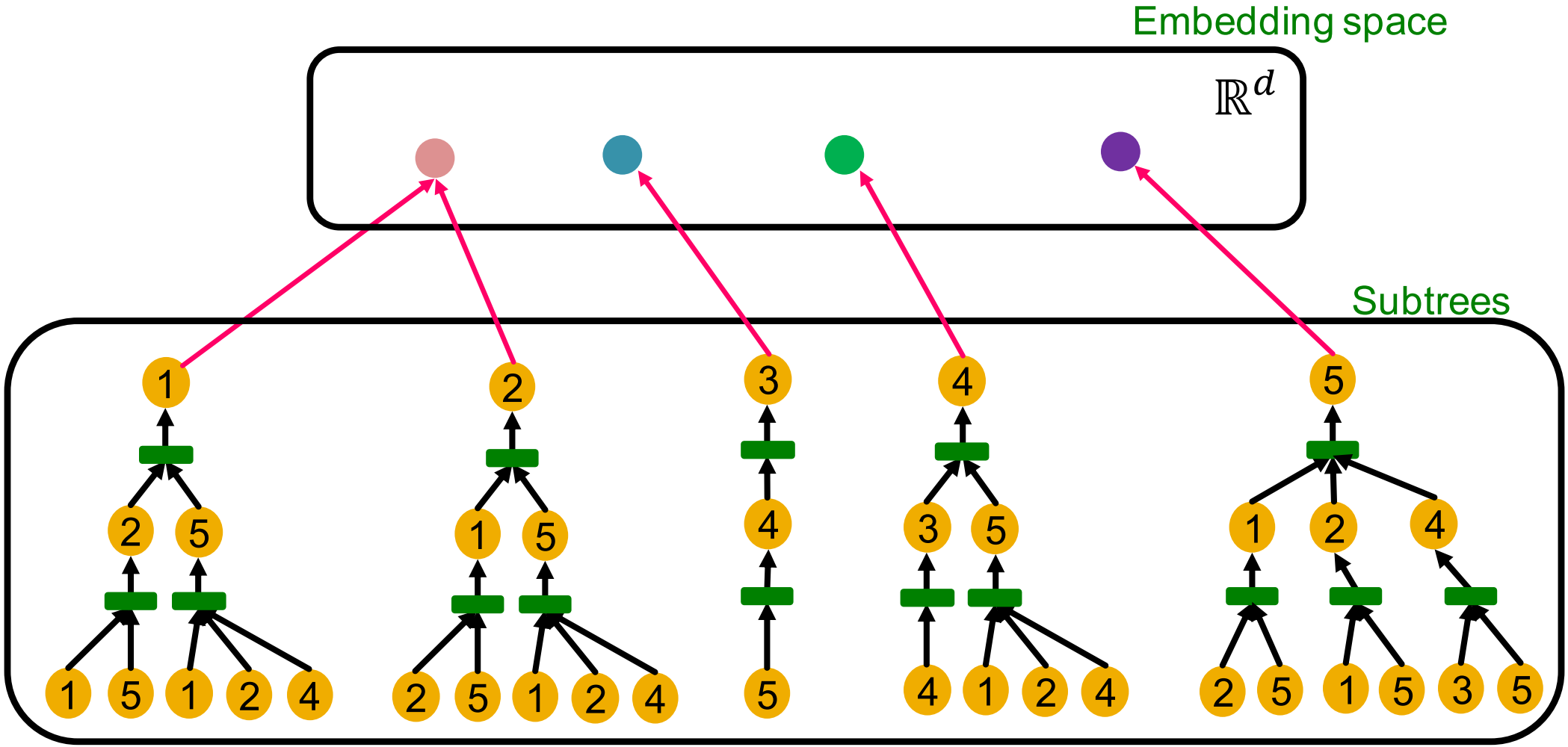



A
B
NOT a Function
A has many B
不是函数
一对多
General Function
B can have many A
普通函数
可以多对一
Injective
(not surjective)
B can't have many A
单射
每个输出对应不超过一个输入
Surjective
(not injective)
Every B has some A
满射
所有输出都对应输入
Bijective
(injective, surjective)
A to B, perfectly
双射
输入和输出一一对应

(函数是单射)

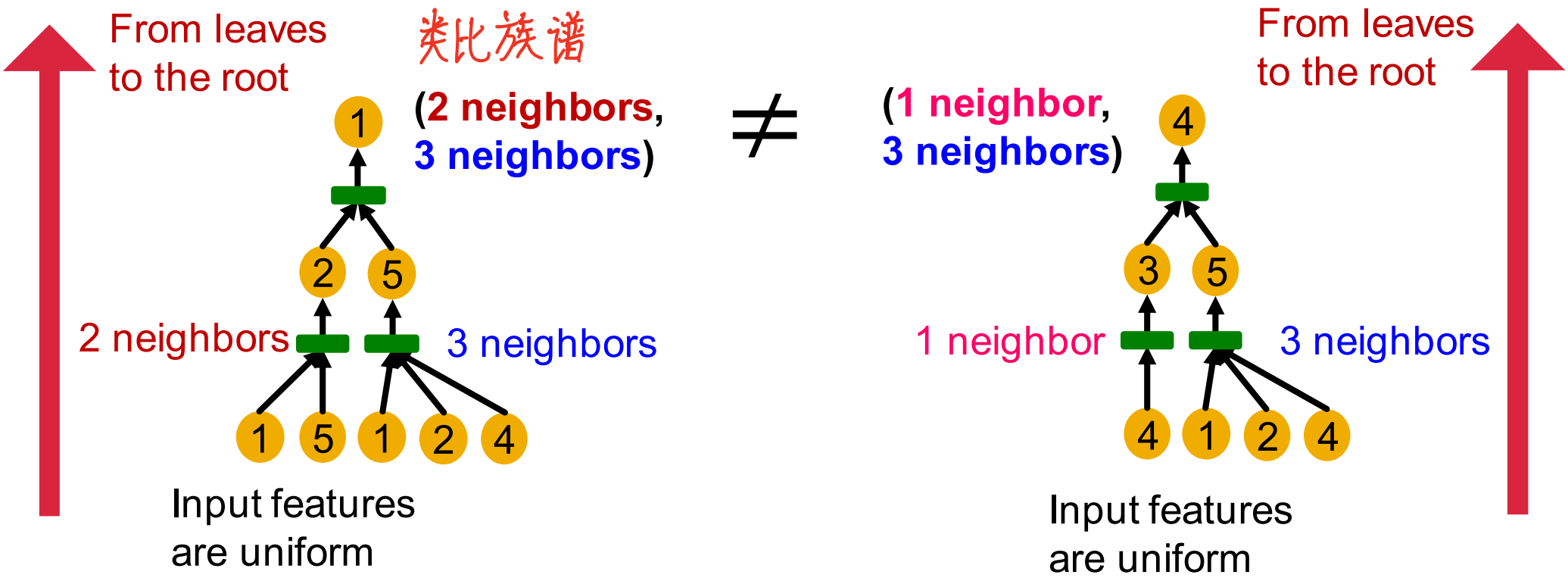
How Expressive is a GNN?

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



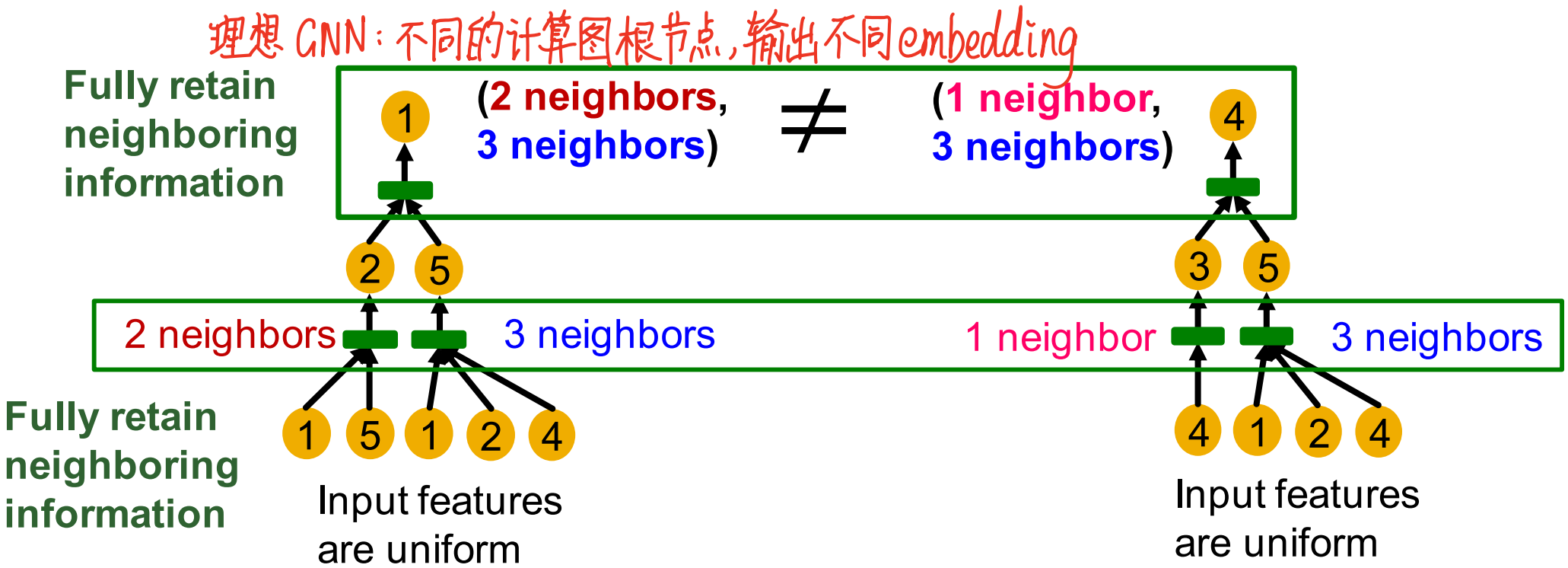
How Expressive is a GNN?

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



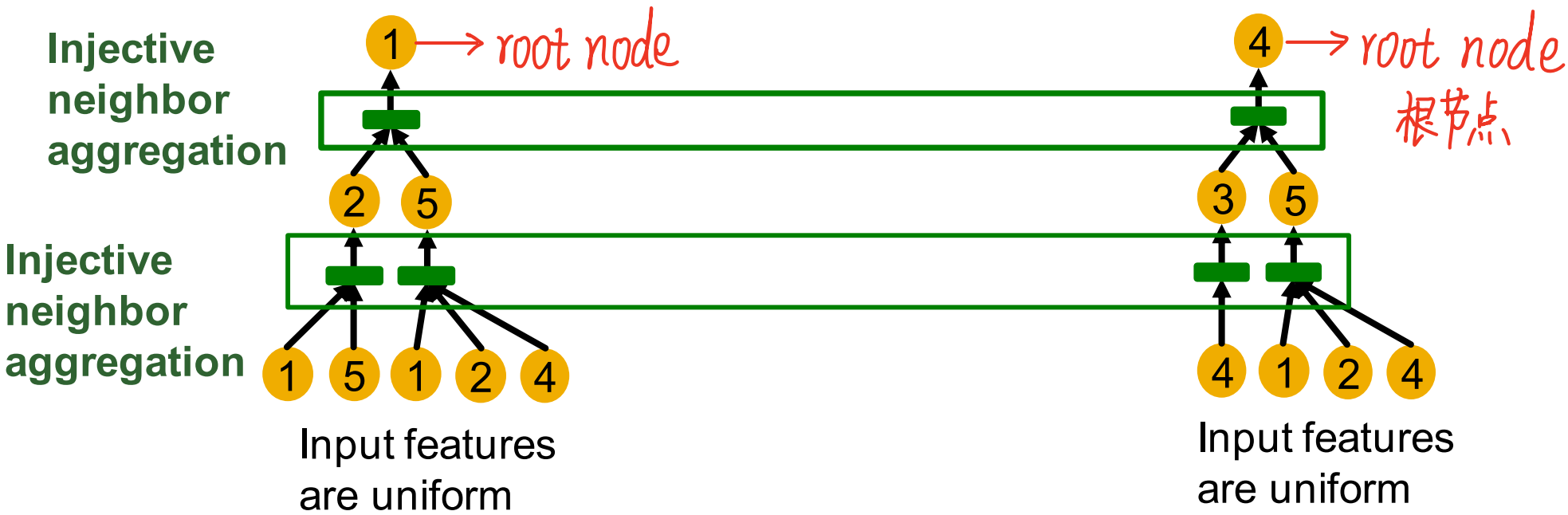
How Expressive is a GNN?

- 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?

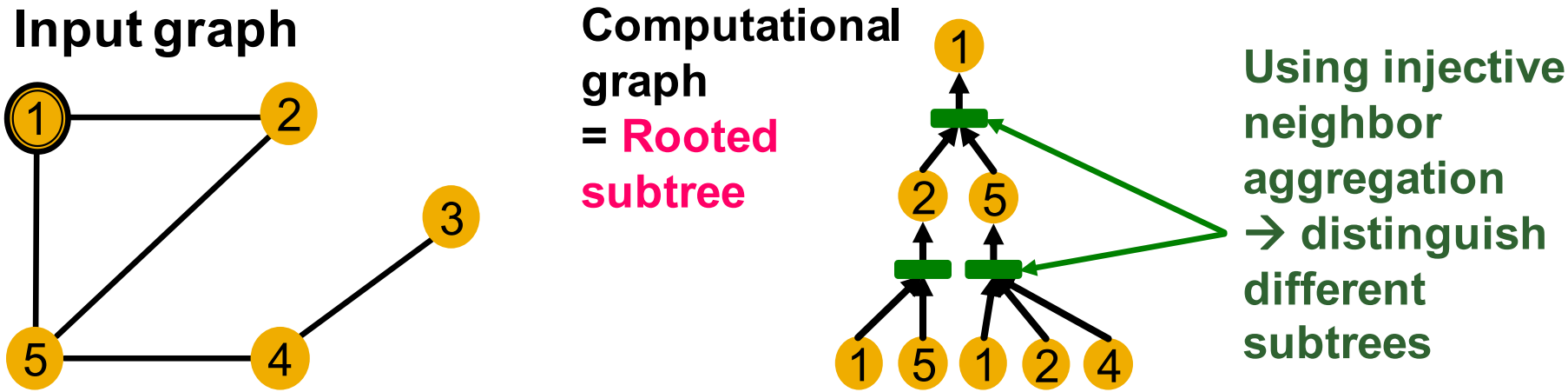
- In other words, most expressive GNN would use an **injective neighbor aggregation** function at each step. 聚合操作应该单射 最完美的单射聚合操作：哈希 Hash
  - Maps different neighbors to different embeddings.



How Expressive is a GNN?

GNN的表达能力 = 区分计算图根节点embedding的能力

- **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.**

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Expressive Power of GNNs

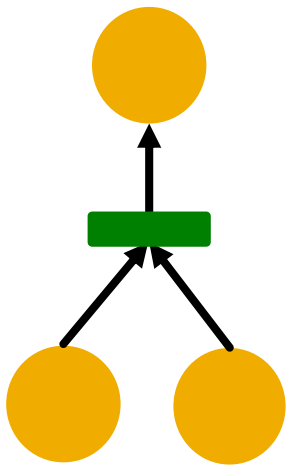
- **Key observation: Expressive power of GNNs can be characterized by that of neighbor aggregation functions they use.**
  - A more expressive aggregation function leads to a more expressive a GNN.
  - Injective aggregation function leads to the most expressive GNN. 聚合函数应该是单射的(单射重集函数)
- **Next:**
  - 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).

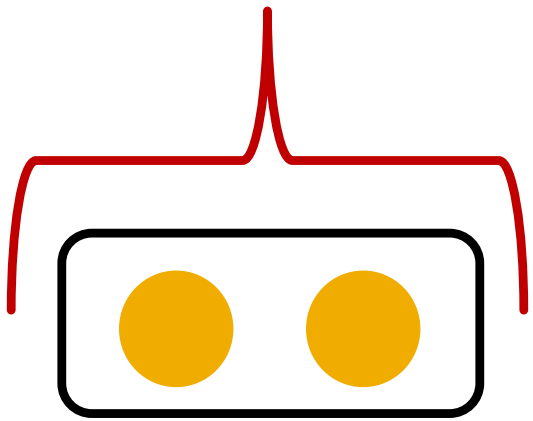
重集

重复的元素



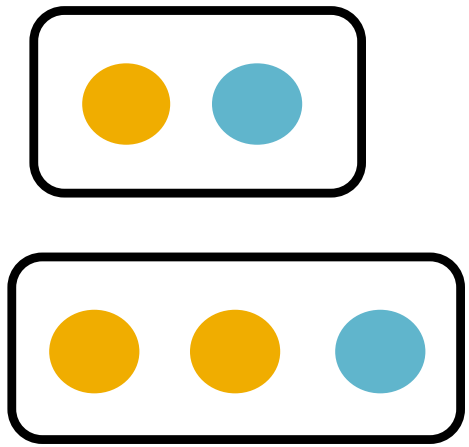
Neighbor aggregation

Equivalent



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 逐元素求平均

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

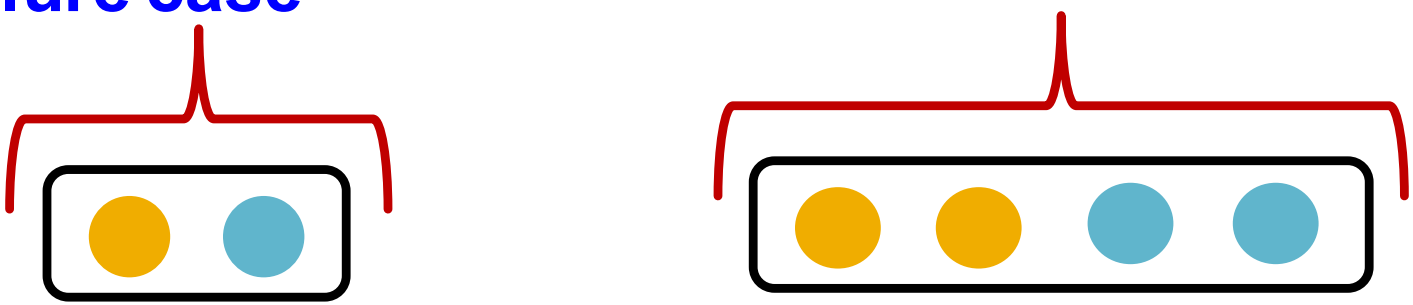
  - **GraphSAGE** (max-pool) [Hamilton et al. NeurIPS 2017]
    - Uses **element-wise** max pooling over neighboring node features 逐元素求最大值

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

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?**

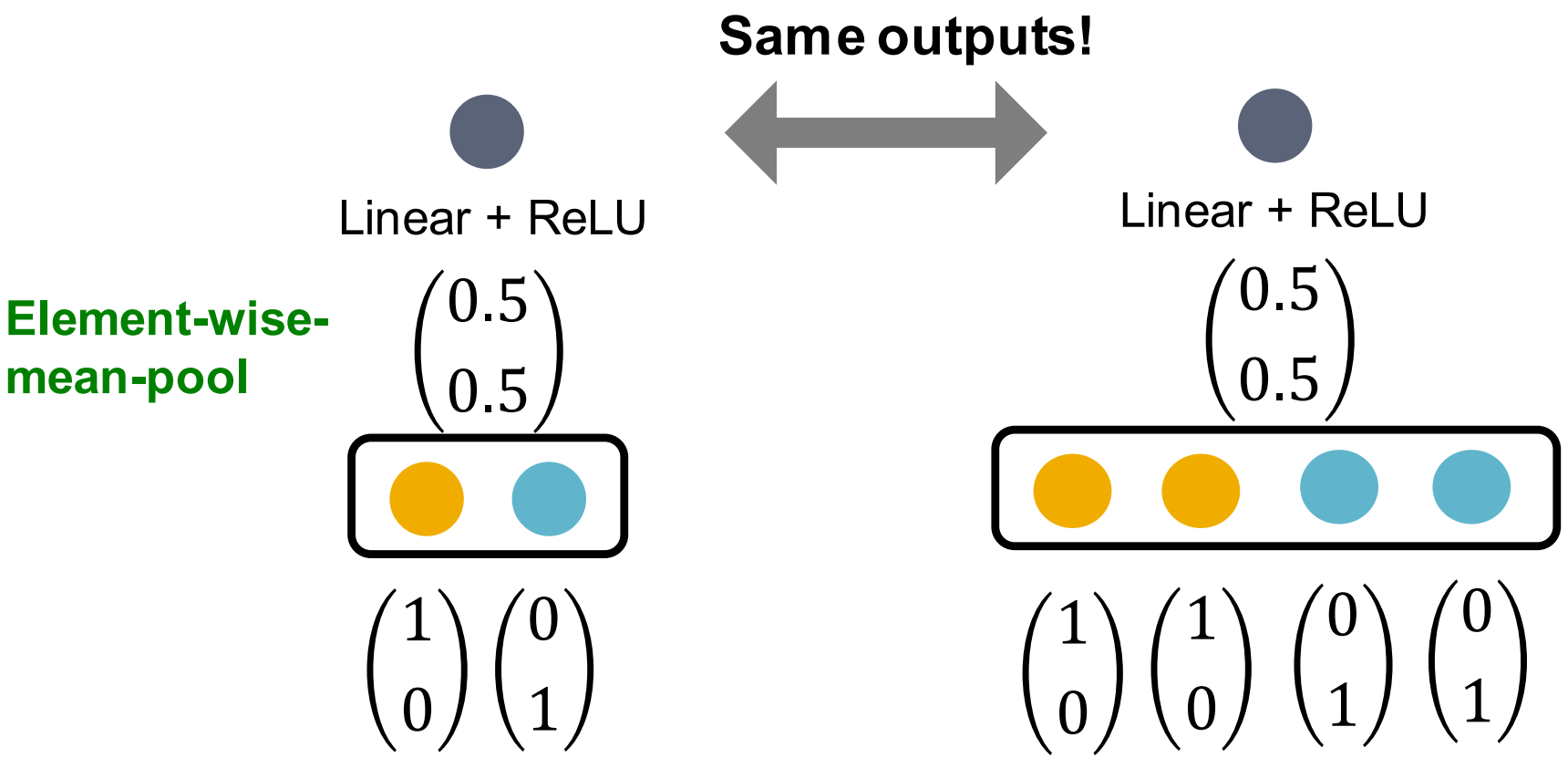
Neighbor Aggregation

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

  - This assumption is sufficient to illustrate how GCN fails.

Neighbor Aggregation: Case Study

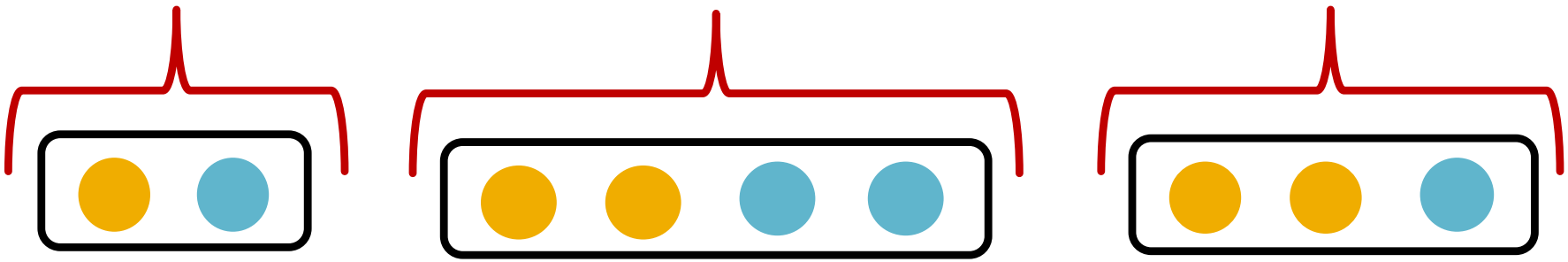
- **GCN (mean-pool)** [Kipf & Welling ICLR 2017]
  - **Failure case illustration**



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**.

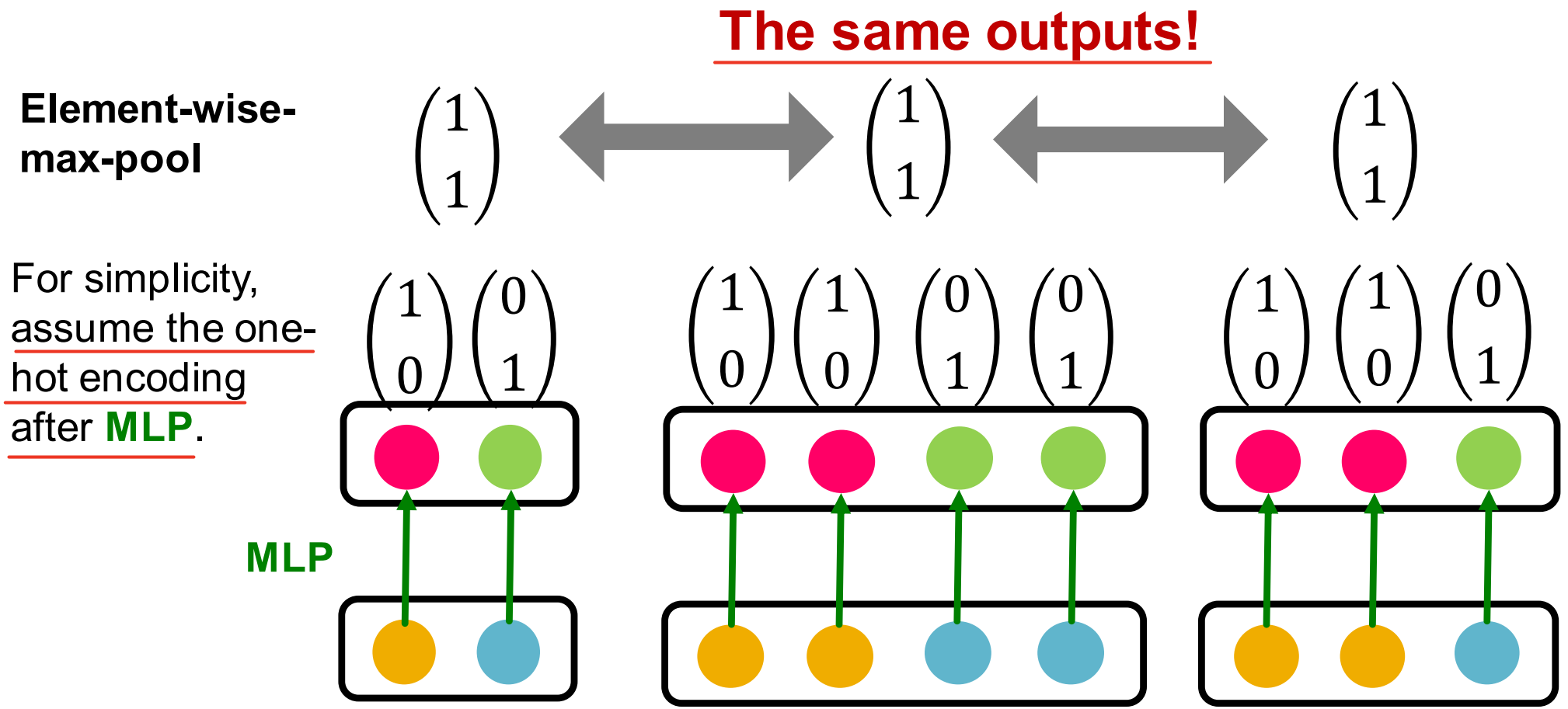
Failure case



- **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**.

用神经网络拟合单射函数

- **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:

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

Some non-linear function

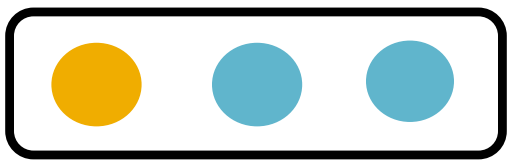
Some non-linear function

2个非线性函数

Sum over multi-set

逐元素求和

S : multi-set



$$\Phi\left(f(\bullet) + f(\bullet) + f(\bullet)\right)$$

Injective Multi-Set Function

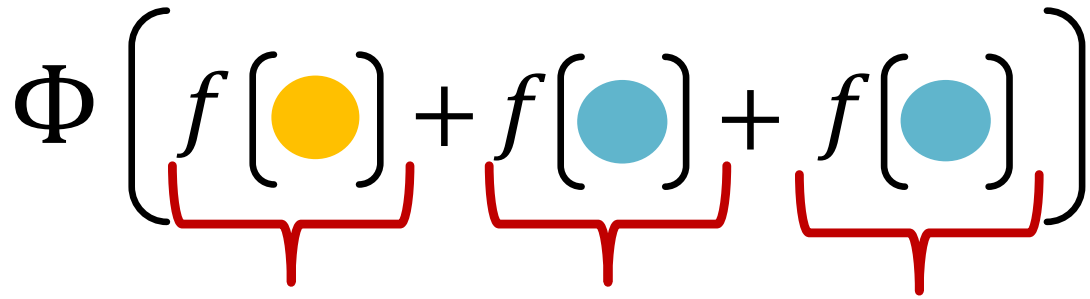
Proof Intuition: [Xu et al. ICLR 2019]

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

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

f: 产生"颜色"
求和: 记录颜色个数
Φ: 单射函数, 产生新"颜色"

Example:

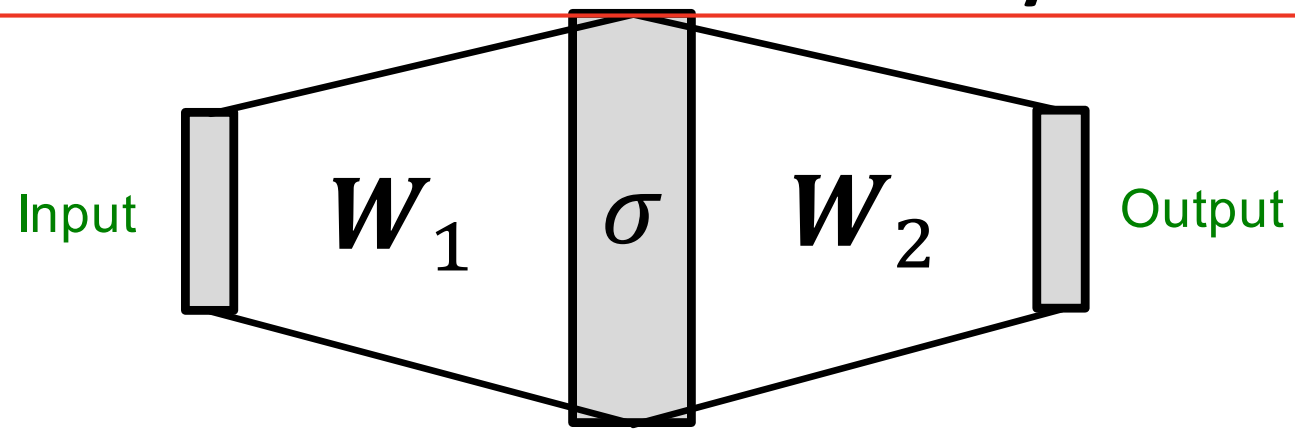


One-hot $\begin{pmatrix}1\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\\2\end{pmatrix}$

Universal Approximation Theorem

- **How to model Φ and f in $\Phi(\sum_{x \in S} f(x))$?**
- We use a Multi-Layer Perceptron (MLP).
- **Theorem: Universal Approximation Theorem**

  [Hornik et al., 1989] 万能近似定理（深度学习的理论基础和"上限"）
  - 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.**

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

  - 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.

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

- **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!**

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.

Weisfeiler-Lehman kernel

Relation to WL Graph Kernel

Recall: 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

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

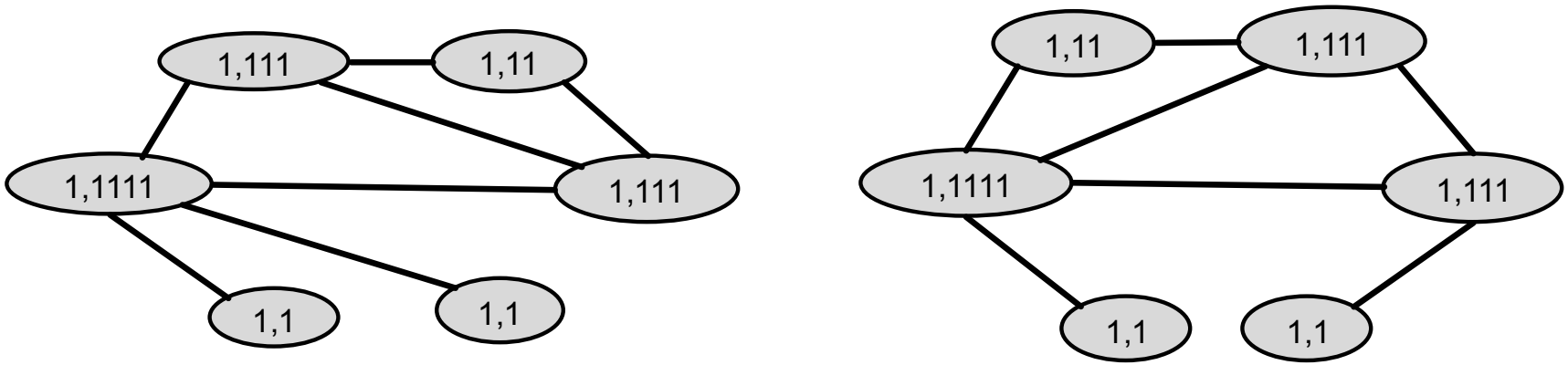
    where HASH maps different inputs to different colors.
  - After K steps of color refinement, $c^{(K)}(v)$ summarizes the structure of K-hop neighborhood

Color Refinement (1)

Example of color refinement given two graphs

- Assign initial colors

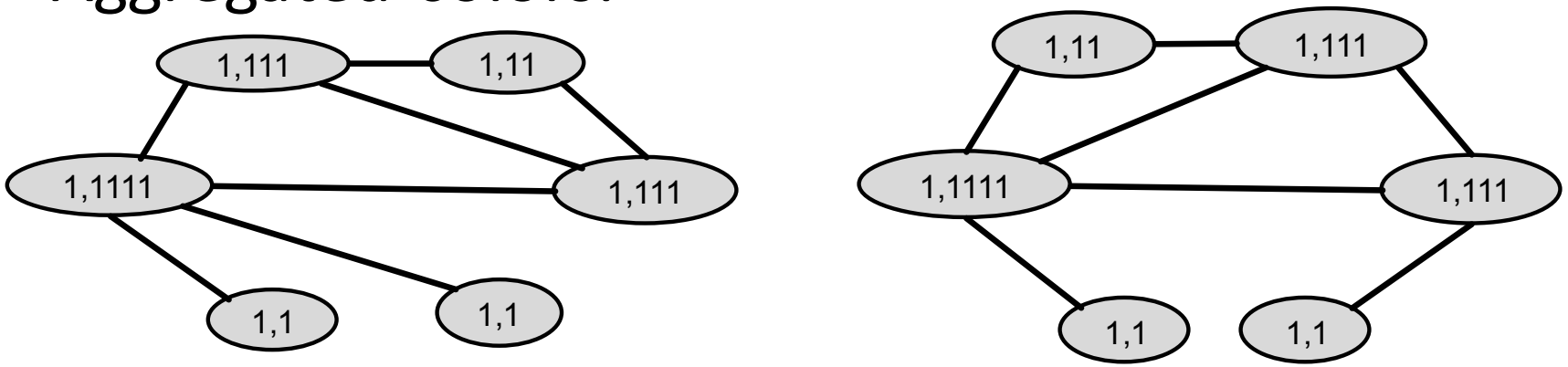
- Aggregate neighboring colors



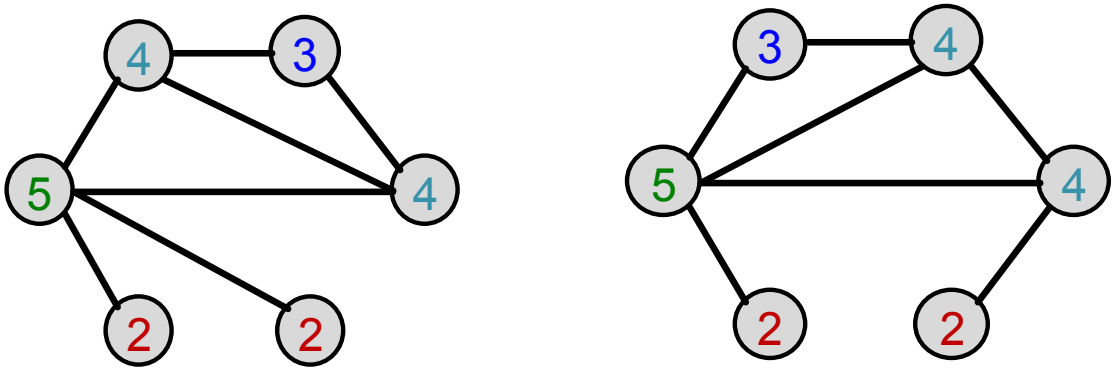
Color Refinement (2)

Example of color refinement given two graphs

- Aggregated colors:



- **Injectively** HASH the aggregated colors



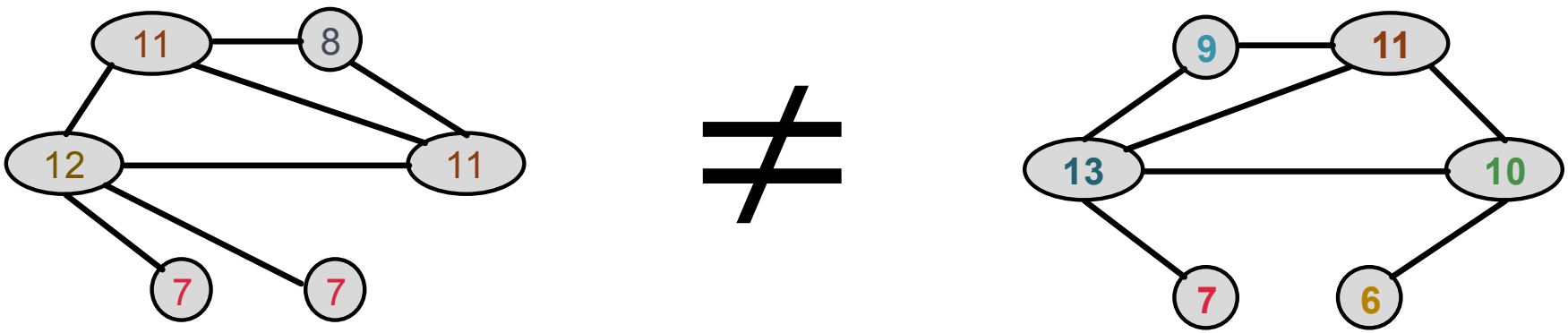
HASH table: **Injective!**

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.**

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

WL-kernel建立了Hash函数
GIN里用NN去拟合 Hash函数

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

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

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: $c^{(k)}(v)$

Neighboring node features: $\{c^{(k)}(u)\}_{u \in N(v)}$

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

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.

f和Φ的作用都是产生 one-hot encoding

The Complete GIN Model

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

Example: $\Phi\left(\begin{pmatrix}1\\0\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}+\begin{pmatrix}0\\1\end{pmatrix}\right)=\begin{pmatrix}1\\2\end{pmatrix}$

- We only need Φ to ensure the injectivity.

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

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

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

和WL-kernel非常类似

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.**

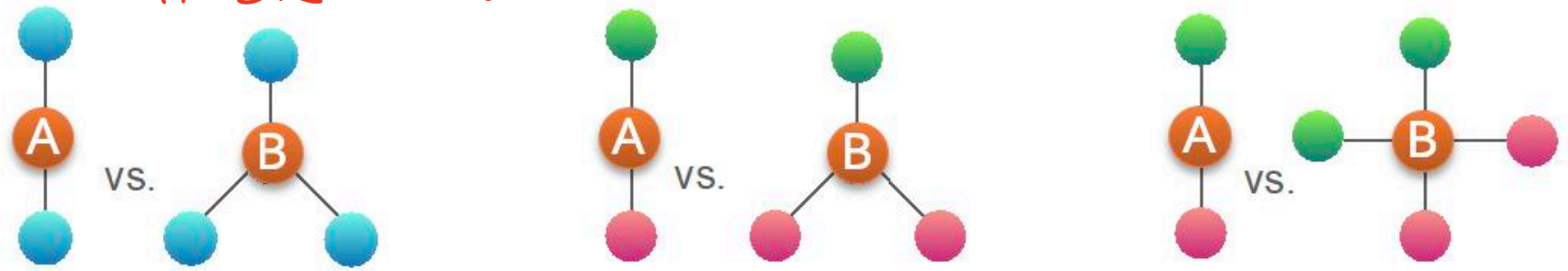
Expressive Power of GIN

- **Because of the relation between GIN and the WL graph kernel, their expressive is exactly the same.** WL-kernel是消息传递GNN表达能力的上界
  - 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!

Discussion: The Power of Pooling

Failure cases for mean and max pooling:

A和B是root node

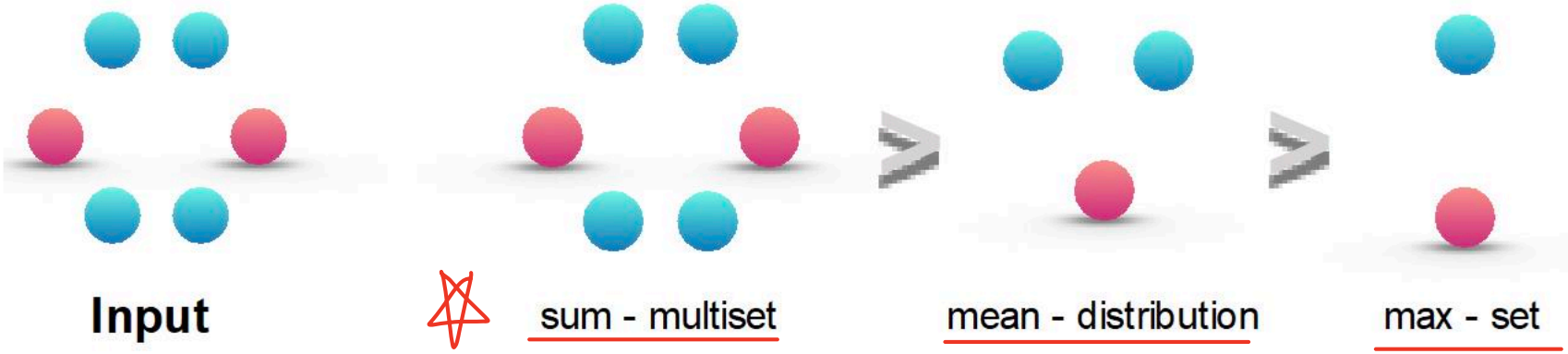


(a) Mean and Max both fail (b) Max fails (c) Mean and Max both fail

Colors represent feature values

Ranking by discriminative power:

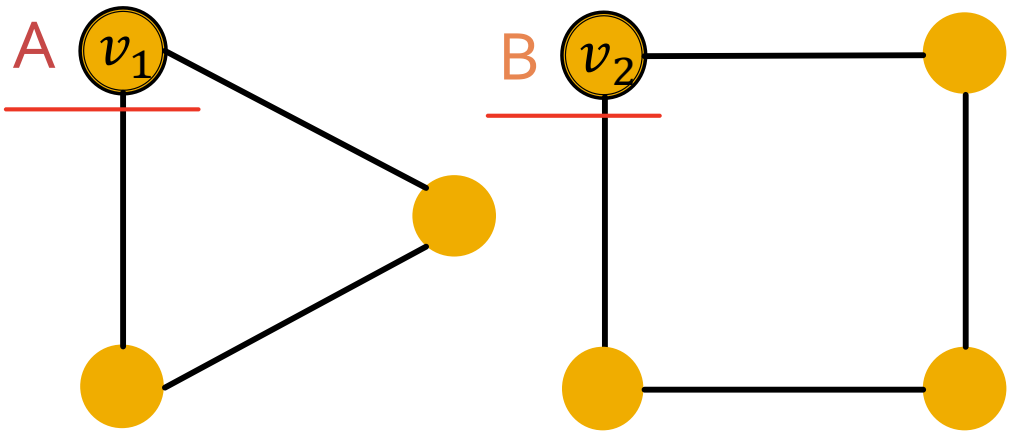
在保持"顺序不变性"的前提下:



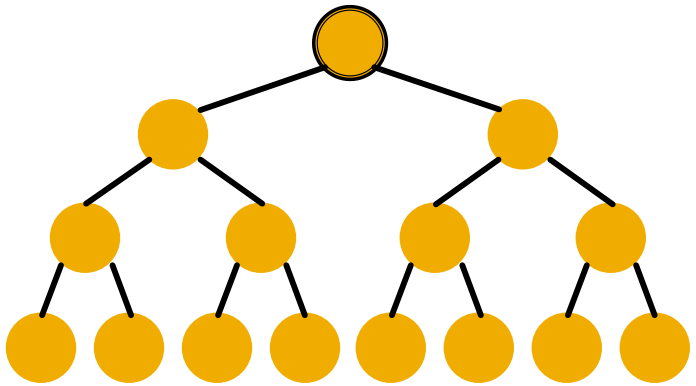
Improving GNNs' Power

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

Graphs



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]
    - Stay tuned for **Lecture 15: Advanced Topics in GNNs**

Summary of the Lecture

- We design a neural network that can model 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!

Stanford CS224W: When Things Don't Go As Planned

CS224W: Machine Learning with Graphs

Jure Leskovec, Stanford University

http://cs224w.stanford.edu

General Tips

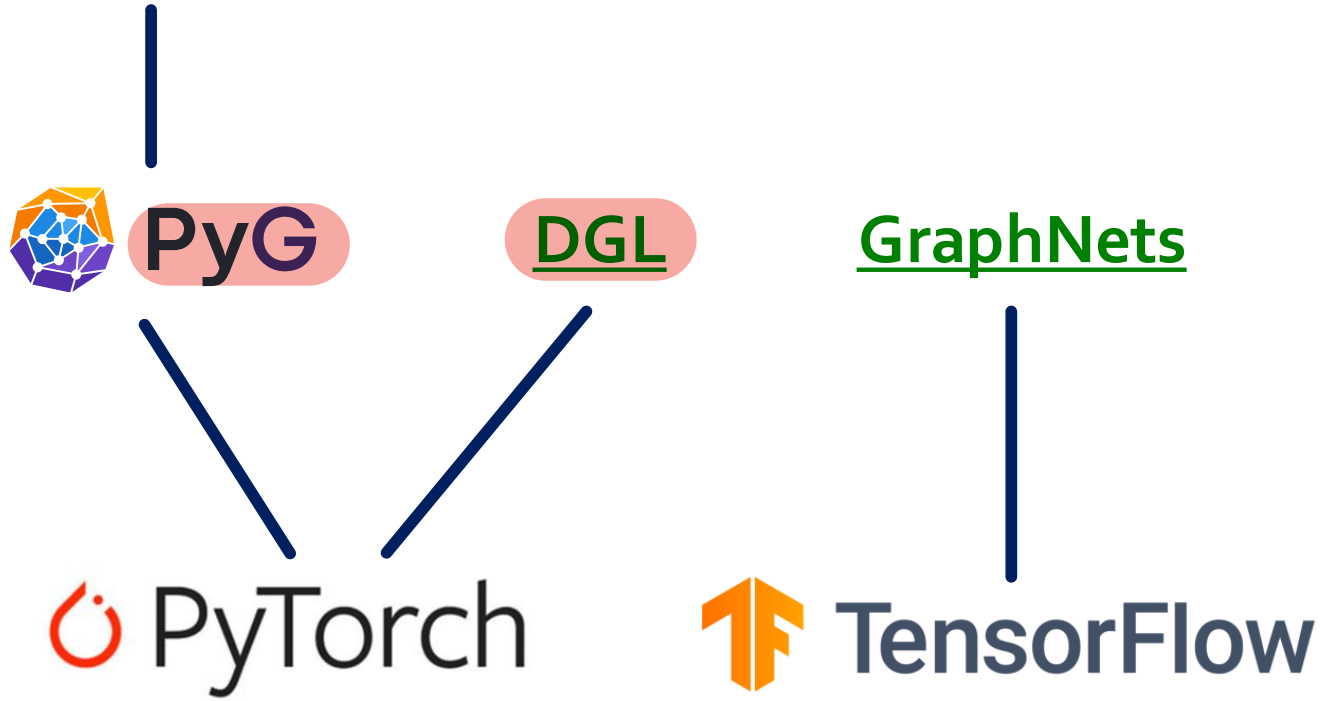
- **Data preprocessing is important:**
  - Node attributes can vary a lot! Use **normalization**
    - E.g. probability ranges $(0,1)$, but some inputs could have much larger range, say $(-1000, 1000)$
- **Optimizer:** ADAM is relatively robust to learning rate
- **Activation function**
  - ReLU activation function often works well
  - Other good alternatives: LeakyReLU, PReLU
  - No activation function at your output layer
  - Include bias term in every layer
- **Embedding dimensions:**
  - 32, 64 and 128 are often good starting points

Debugging Deep Networks

- **Debug issues:** Loss/accuracy not converging during training
  - Check pipeline (e.g. in PyTorch we need zero_grad)
  - Adjust hyperparameters such as learning rate
  - Pay attention to weight parameter initialization
  - **Scrutinize loss function!**
- **Important for model development:**
  - **Overfit on (part of) training data:** (early stop / 正则化)
    - With a small training dataset, loss should be essentially close to 0, with an expressive neural network
  - **Monitor the training & validation loss curve**

Resources on Graph Neural Networks

GraphGym:
Easy and flexible end-to-end GNN pipeline based on PyTorch Geometric (PyG)



GNN frameworks:
Implements a variety of GNN architectures

Auto-differentiation frameworks

Resources on Graph Neural Networks

Tutorials and overviews:
- Relational inductive biases and graph networks (Battaglia et al., 2018)
- Representation learning on graphs: Methods and applications (Hamilton et al., 2017)

Attention-based neighborhood aggregation:
- Graph attention networks (Hoshen, 2017; Velickovic et al., 2018; Liu et al., 2018)

Embedding entire graphs:
- Graph neural nets with edge embeddings (Battaglia et al., 2016; Gilmer et. al., 2017)
- Embedding entire graphs (Duvenaud et al., 2015; Dai et al., 2016; Li et al., 2018) and graph pooling (Ying et al., 2018, Zhang et al., 2018)
- Graph generation and relational inference (You et al., 2018; Kipf et al., 2018)
- How powerful are graph neural networks(Xu et al., 2017)

Embedding nodes:
- Varying neighborhood: Jumping knowledge networks (Xu et al., 2018), GeniePath (Liu et al., 2018)
- Position-aware GNN (You et al. 2019)

Spectral approaches to graph neural networks:
- Spectral graph CNN & ChebNet (Bruna et al., 2015; Defferrard et al., 2016)
- Geometric deep learning (Bronstein et al., 2017; Monti et al., 2017)

Other GNN techniques:
- Pre-training Graph Neural Networks (Hu et al., 2019)
- GNNExplainer: Generating Explanations for Graph Neural Networks (Ying et al., 2019)