# Stanford CS224W: How Expressive are Graph Neural Networks?

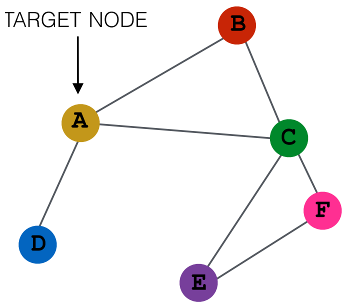
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

# 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.

J. You, R. Ying, J. Leskovec. Design Space of Graph Neural Networks, NeurIPS 2020

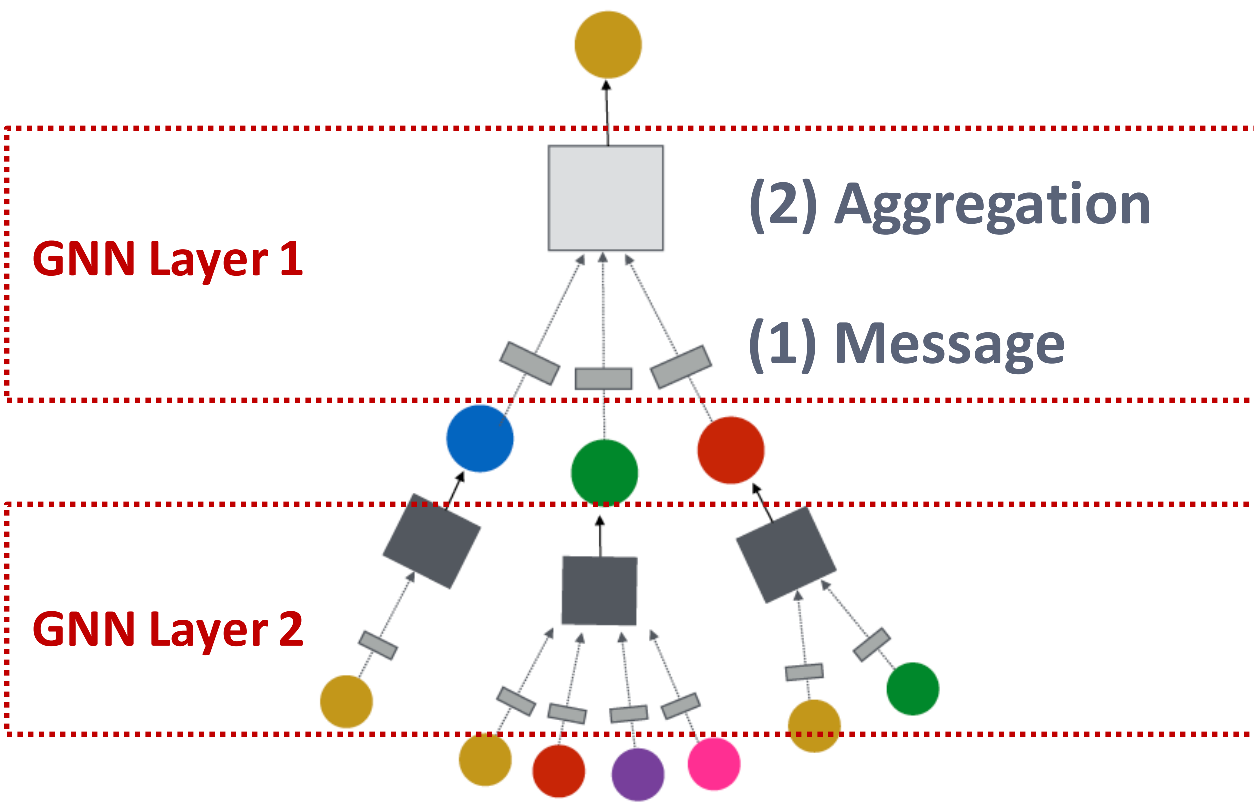
# Recap: A General GNN Framework




INPUT GRAPH

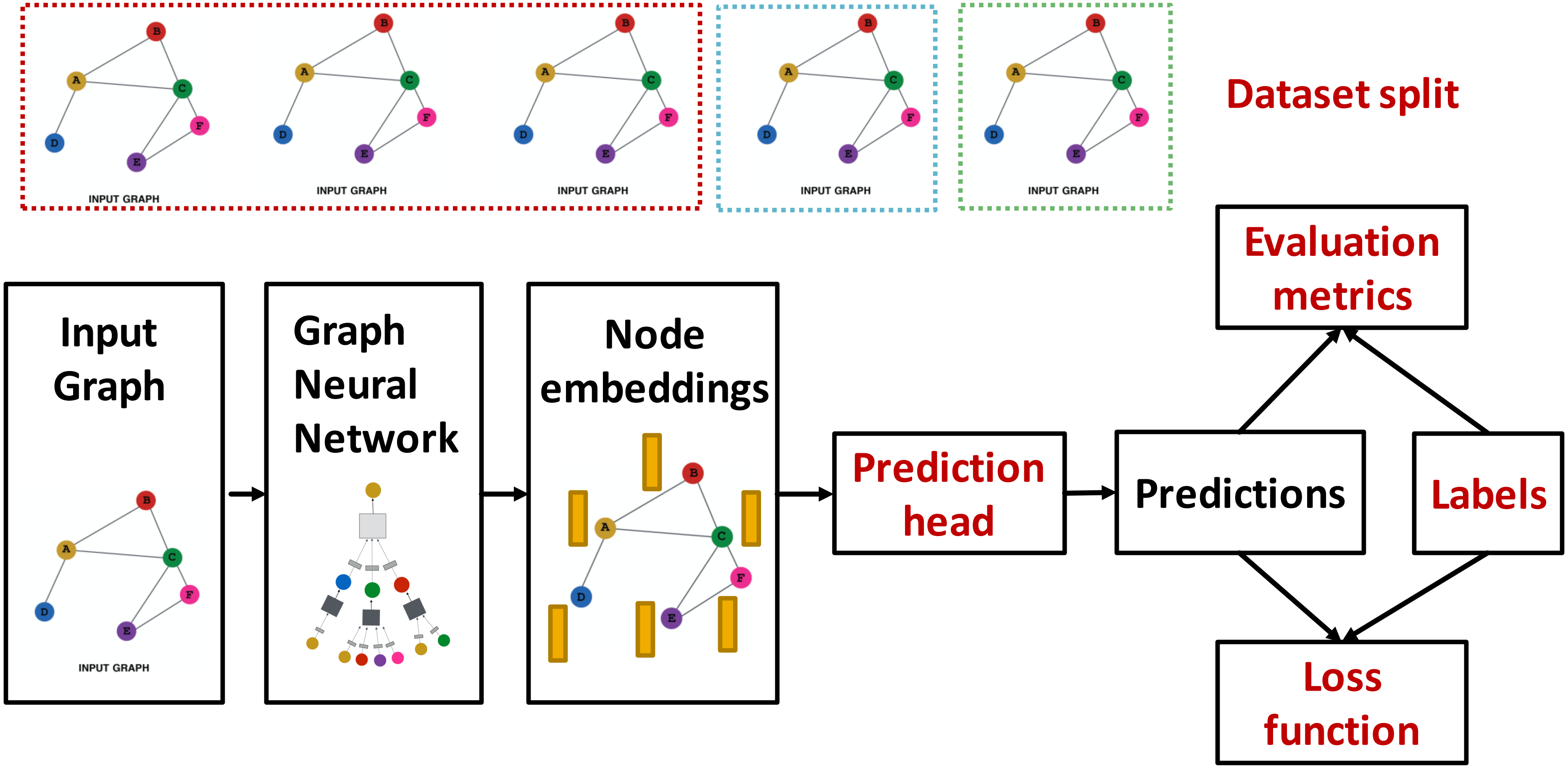
(5) Learning objective

(3) Layer connectivity




(4) Graph augmentation

# Recap: GNN Training Pipeline




**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).**

表达、学习、拟合、区分

- **What is the expressive power (ability to distinguish different graph structures) of these GNN models?**

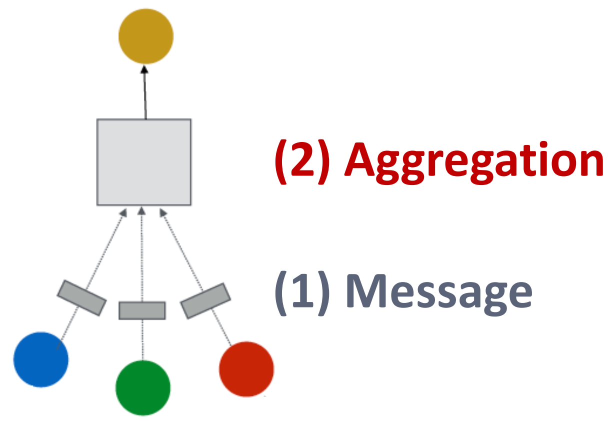
区分

- **How to design a maximally expressive GNN model?**

GIN

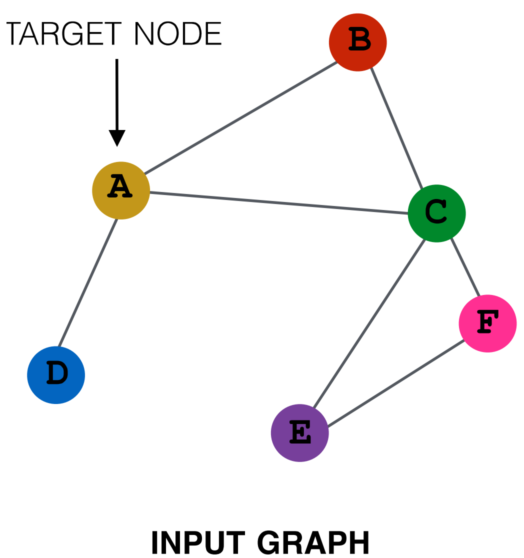
# Background: A Single GNN Layer

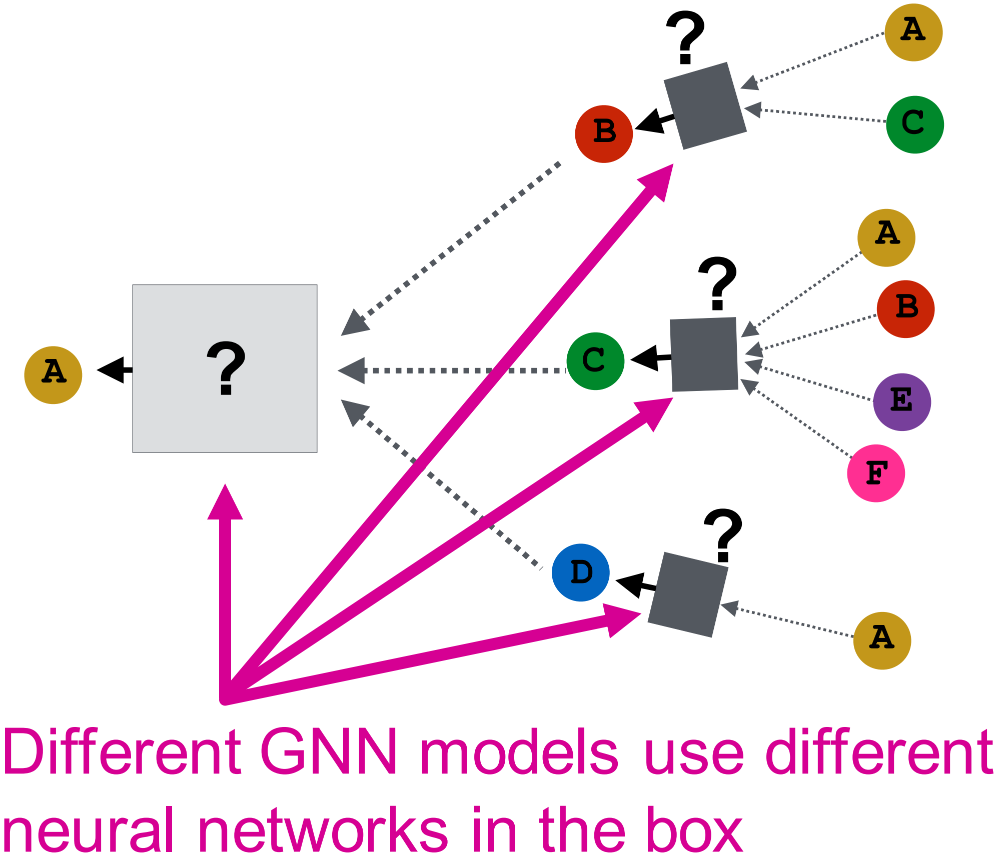
- **We focus on message passing GNNs:**
  - **(1) Message**: each node computes a message
    $$\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$
  - **(2) Aggregation**: aggregate messages from neighbors
    $$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)},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



# Background: Many GNN Models

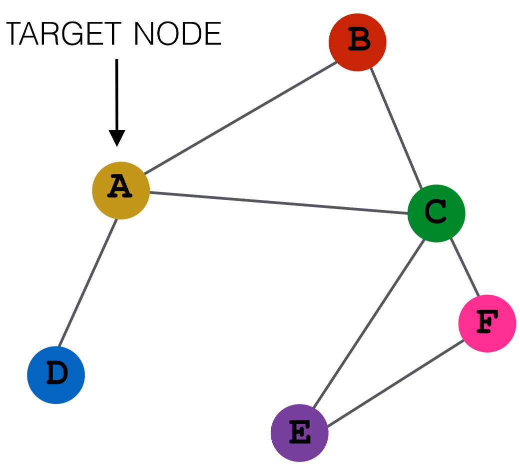
- Many GNN models have been proposed:
  - GCN, GraphSAGE, GAT, Design Space etc.



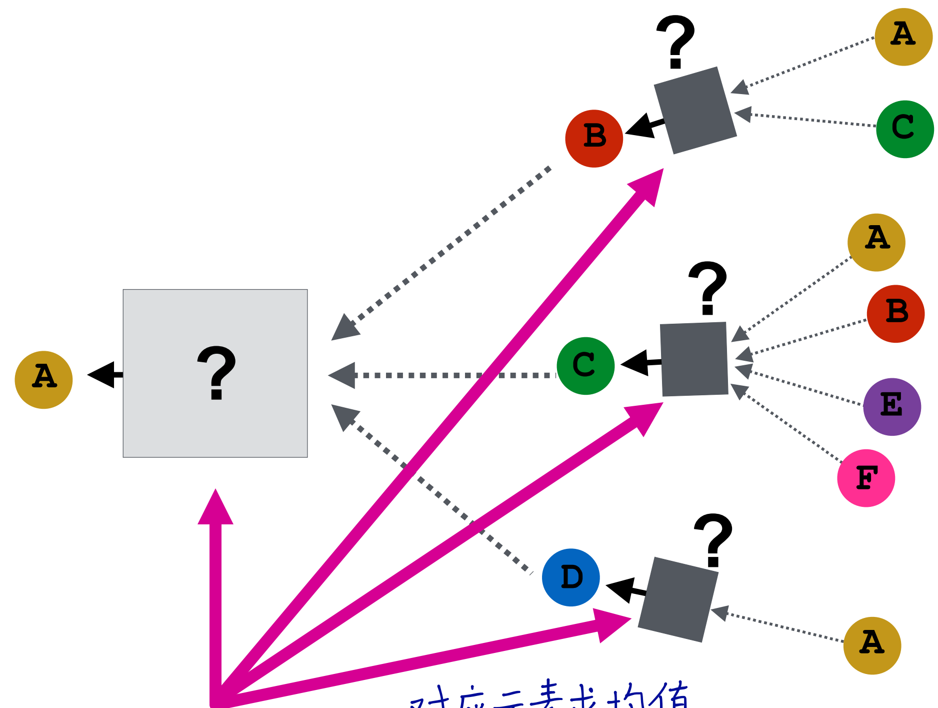



# GNN Model Example (1)

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




**INPUT GRAPH**

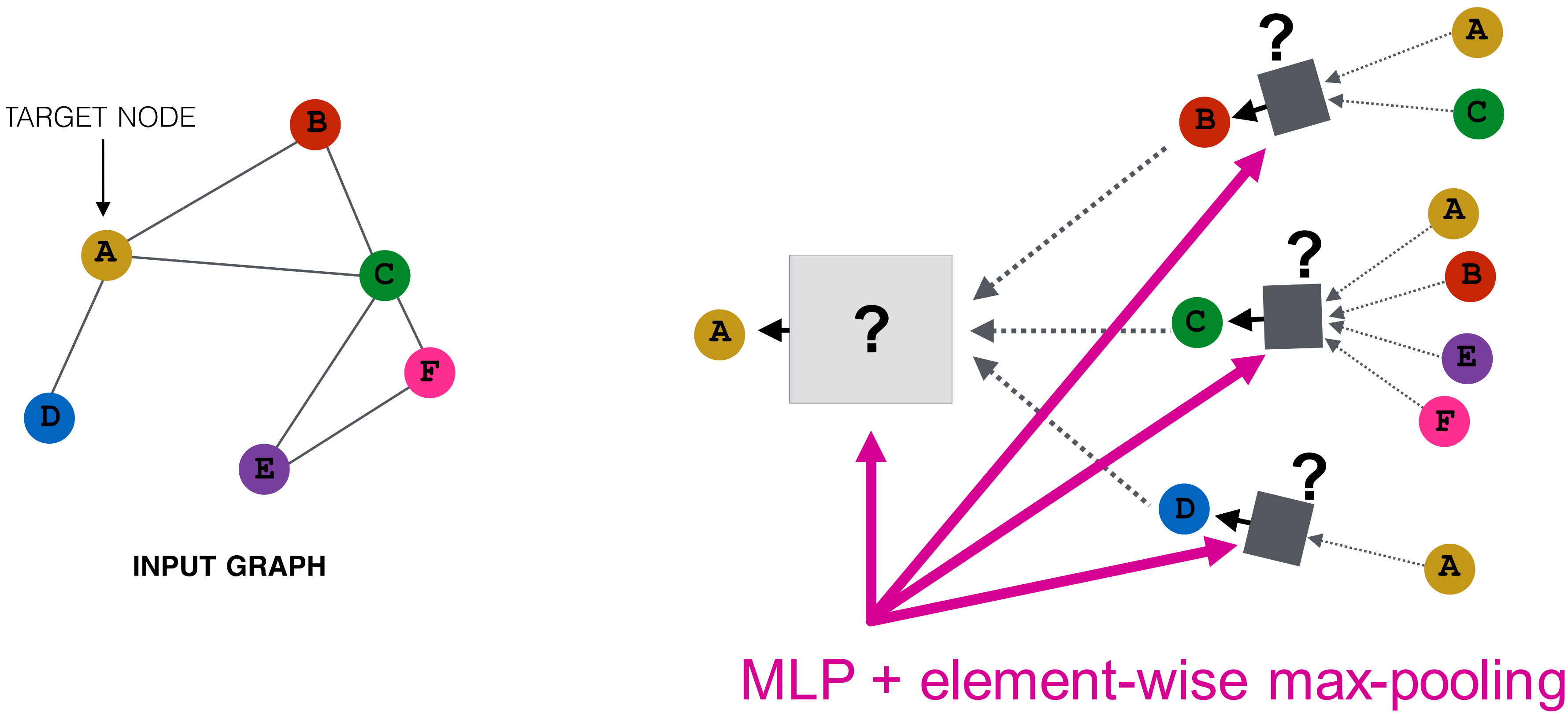



对应元素求均值

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

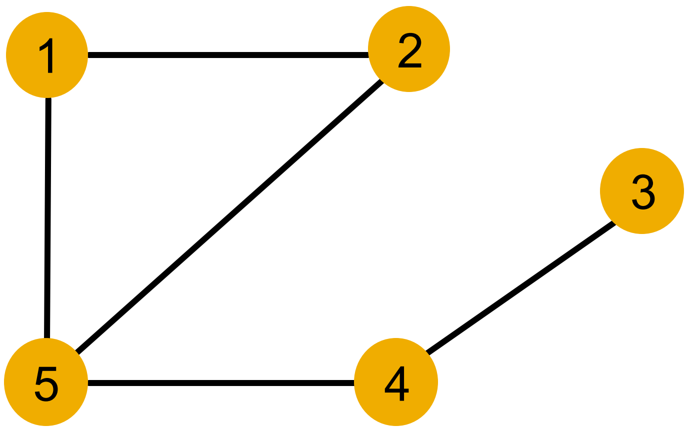
# GNN Model Example (2)

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



# Note: Node Colors

- We use node same/different **colors** to represent nodes with same/different features. 用不同颜色表示不同Embedding
  - For example, the graph below assumes all the nodes share the same feature. 节点属性特征 初始Embedding

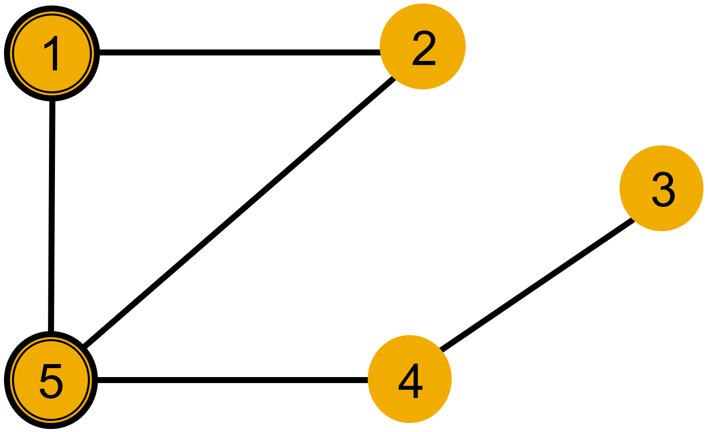



（计算图）
通过连接结构区分不同节点

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

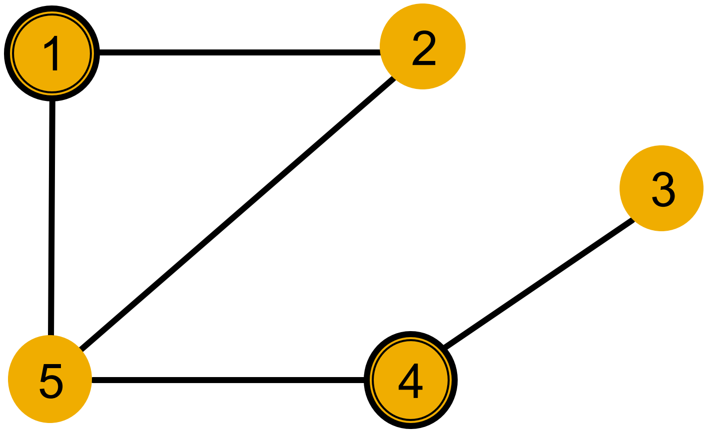
# Local Neighborhood Structures

- 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.**

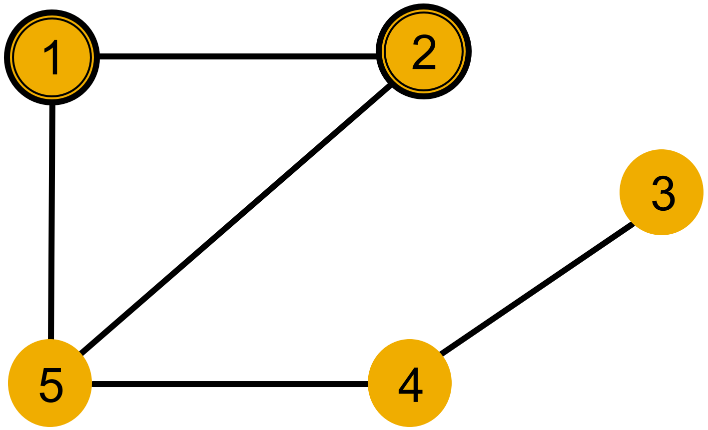



Node 1 has neighbors of degrees 2 and 3.
Node 4 has neighbors of degrees 1 and 3.

# 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** 对称 **symmetric within the graph.**

仅通过图的连接结构
无法区分节点1和节点2




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

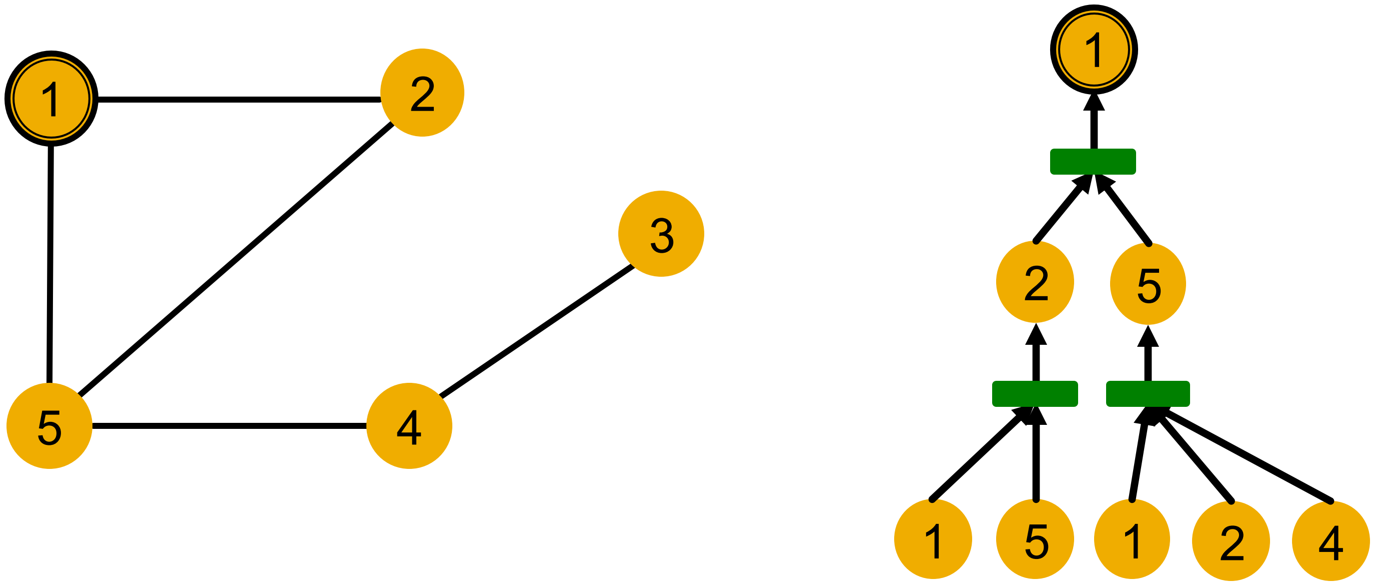
- **Key question: Can GNN node embeddings distinguish different node's local neighborhood structures?**
  - If so, when? If not, when will a GNN fail?
- **Next: We need to understand how a GNN captures local neighborhood structures.**
  - **Key concept: Computational graph**

计算图

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

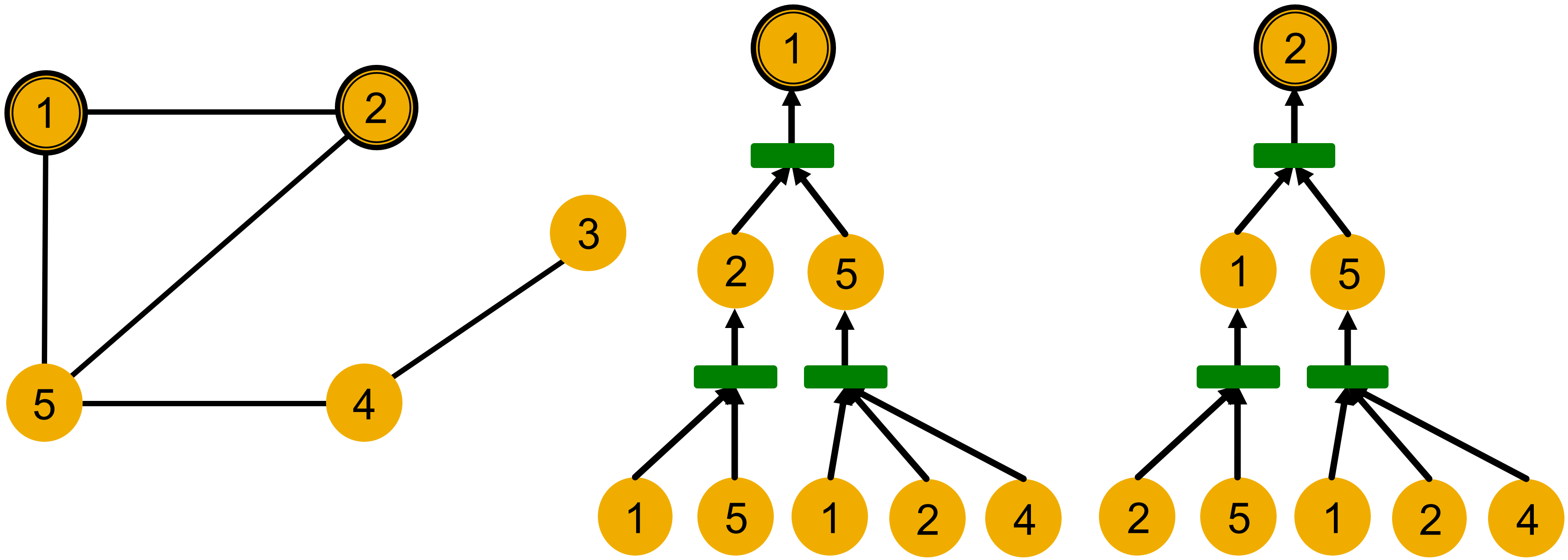


# Computational Graph (2)

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

编号无意义　连接长度无意义

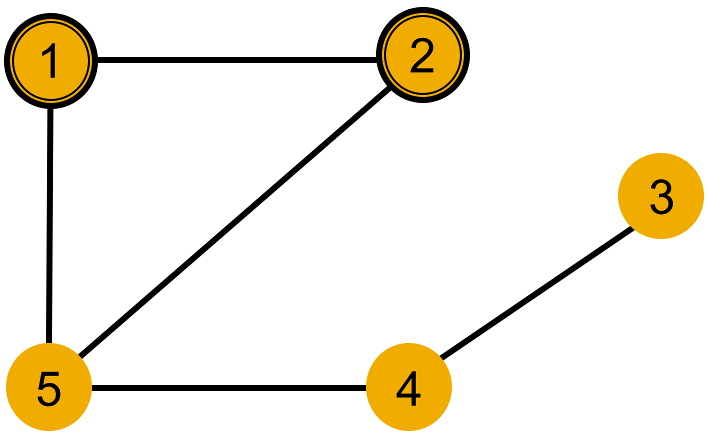
颜色有意义

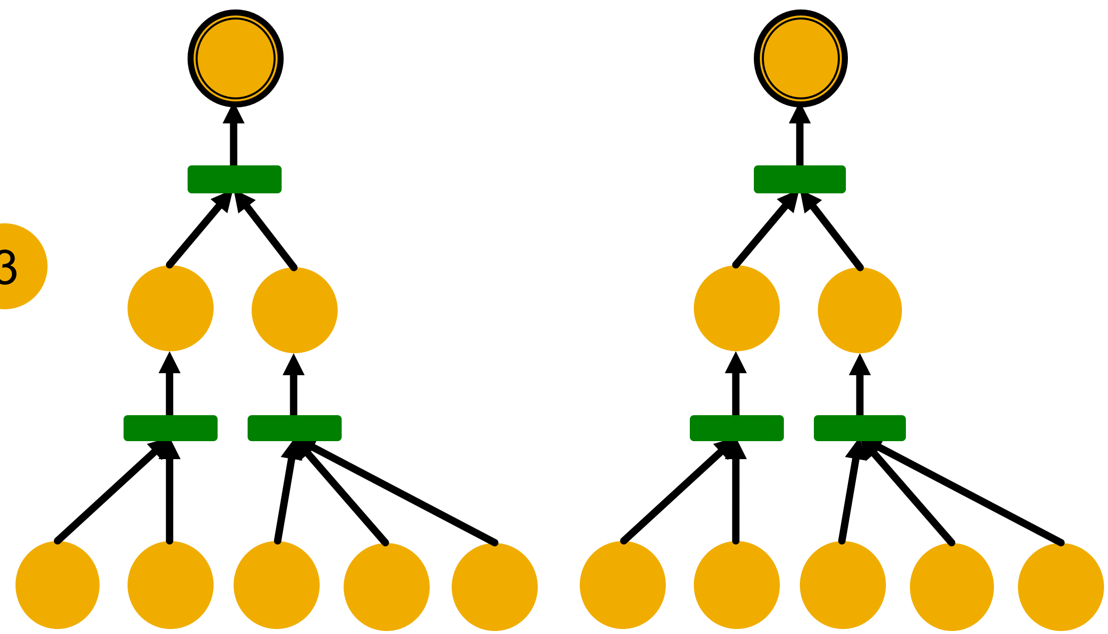


# Computational Graph (3)

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

GNN眼中的计算图

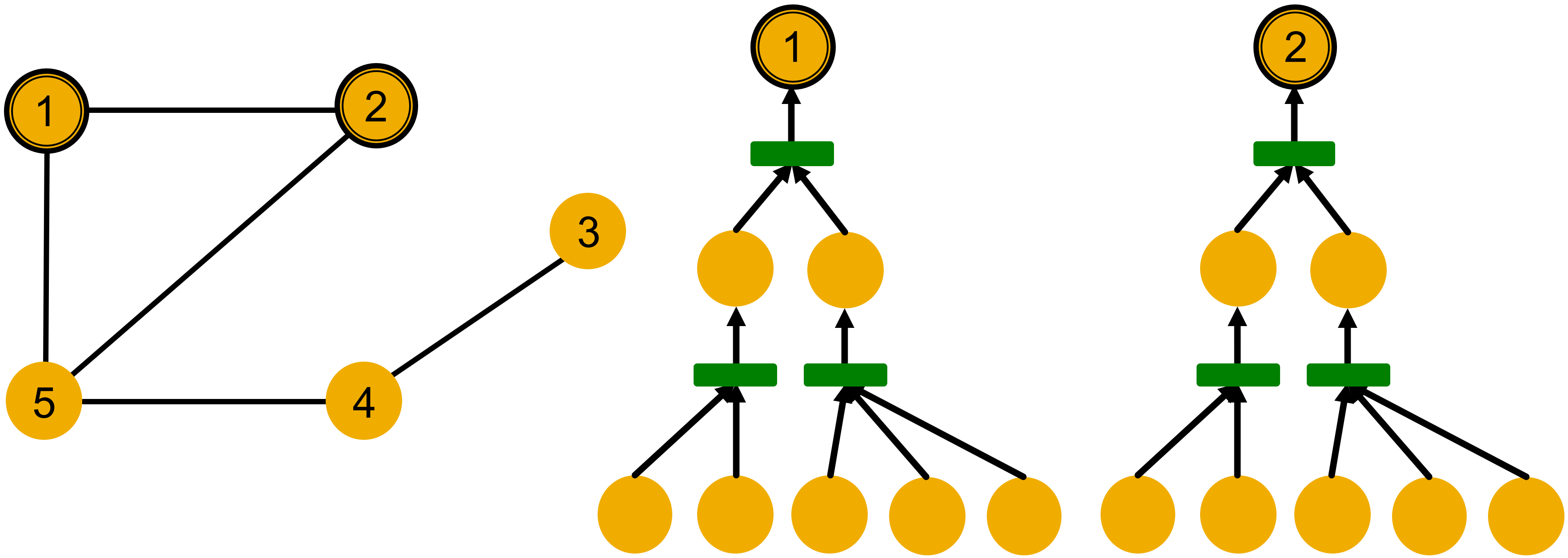


# Computational Graph (4)

- **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.

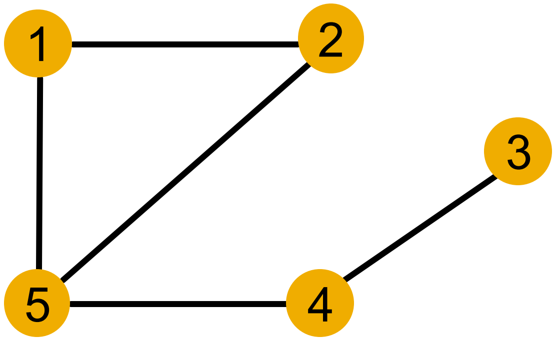
Note: GNN does not care about node ids, it just aggregates features vectors of different nodes.

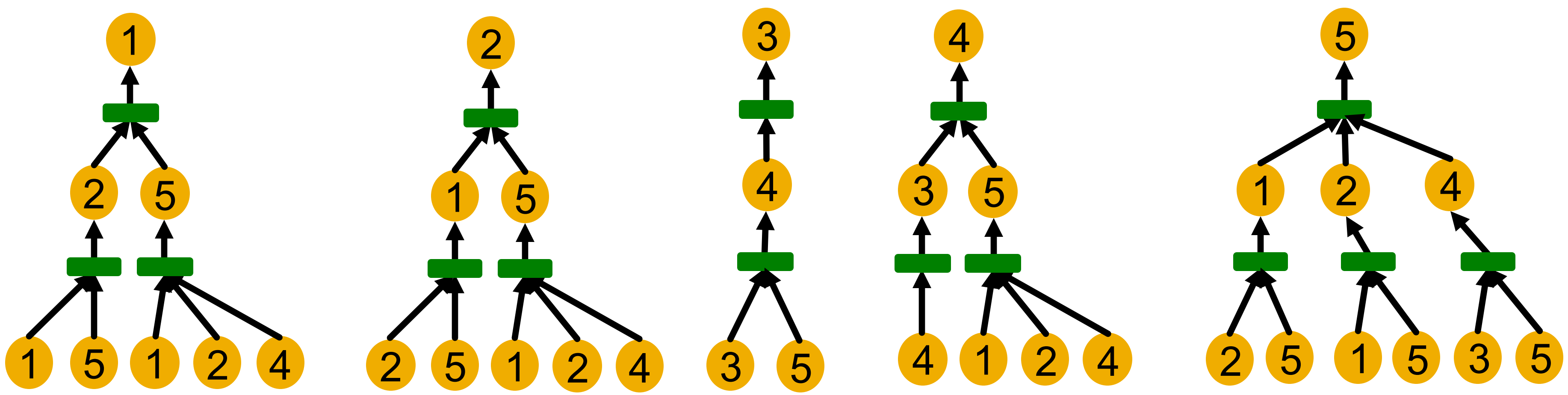



GNN won't be able to distinguish nodes 1 and 2

# Computational Graph

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

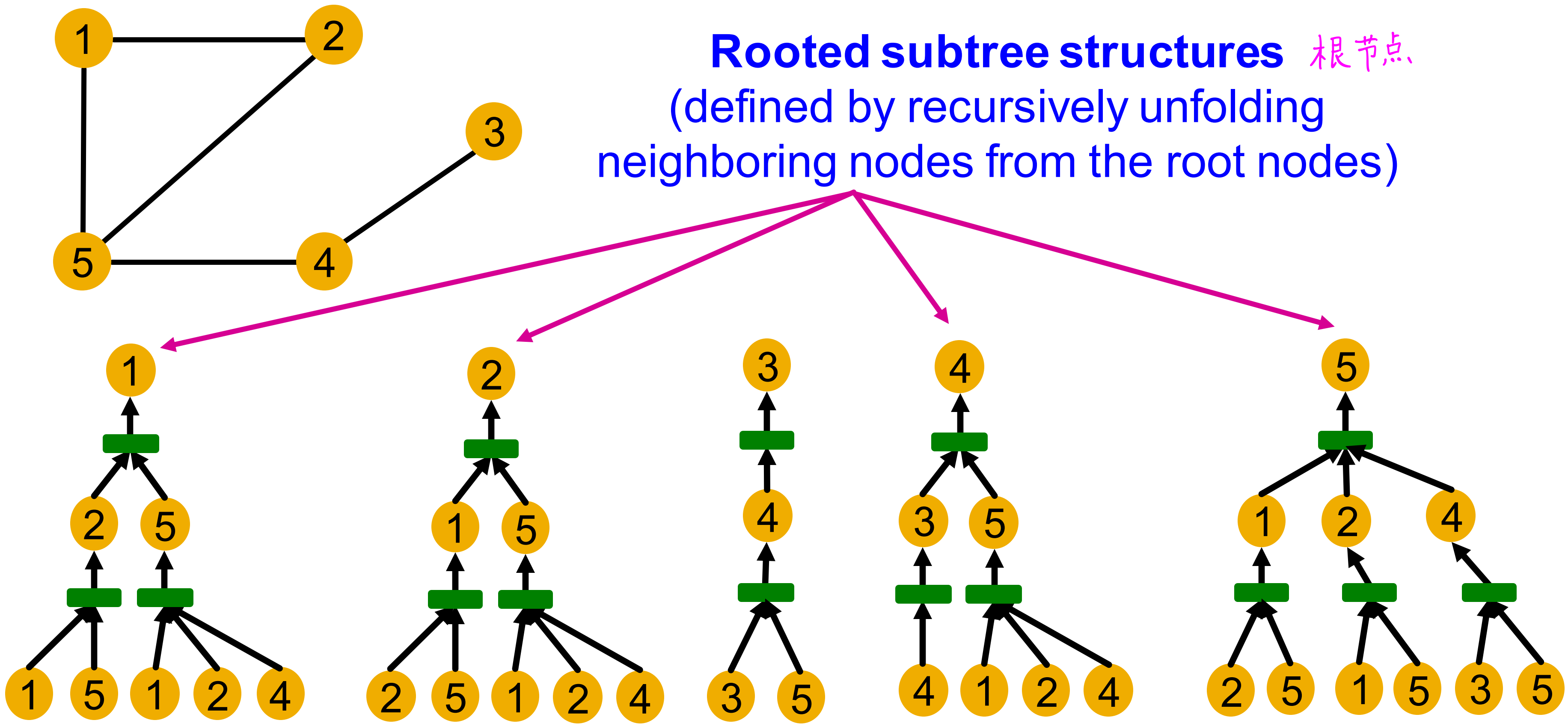


# Computational Graph

相同

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



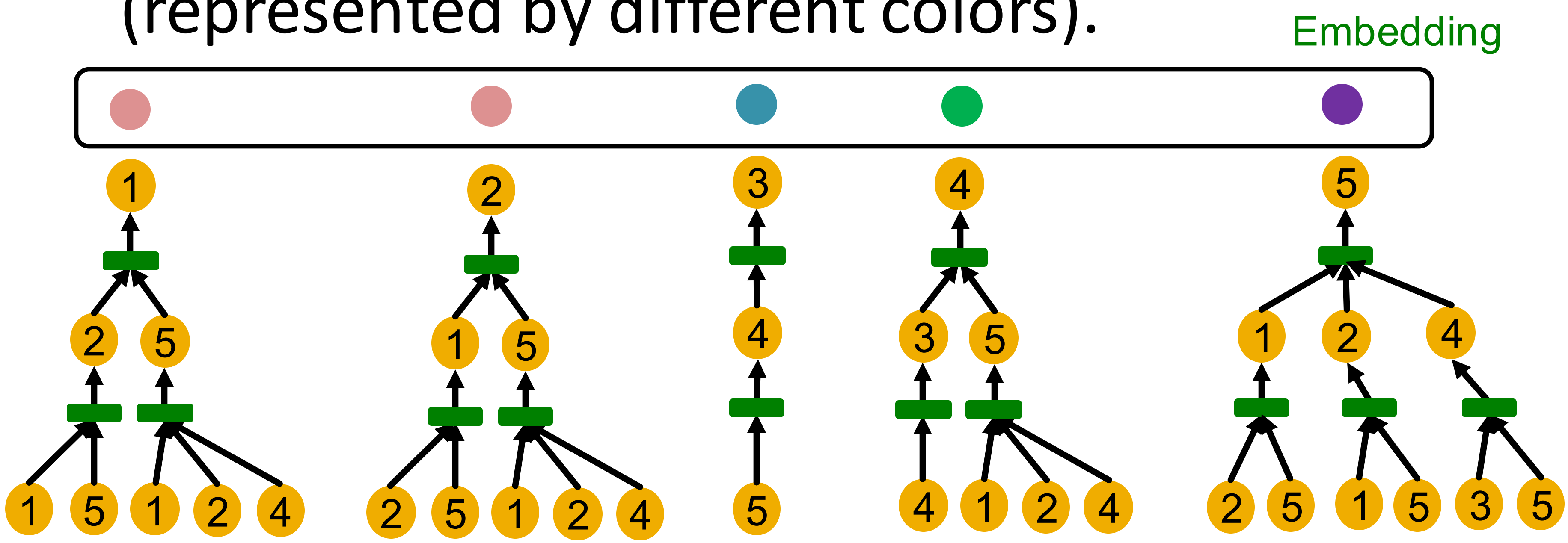
# Computational Graph

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**. 理想GNN: 不同的计算图根节点, 输出不同Embedding

但仍旧无法区分节点1和节点2

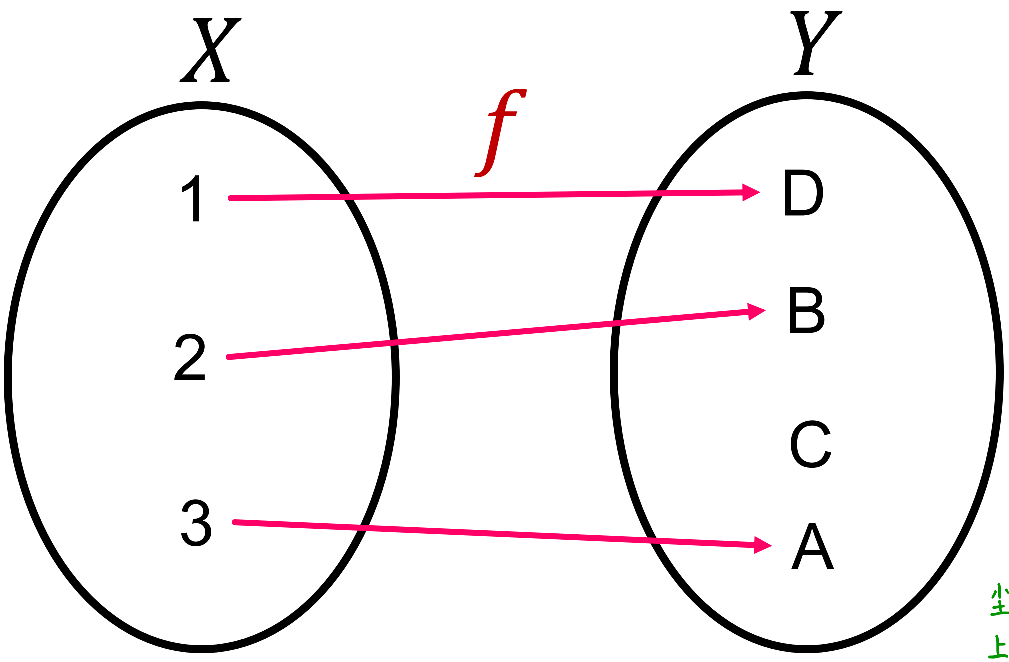
- Most expressive GNN maps different **rooted subtrees** into different node embeddings (represented by different colors).



# 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.

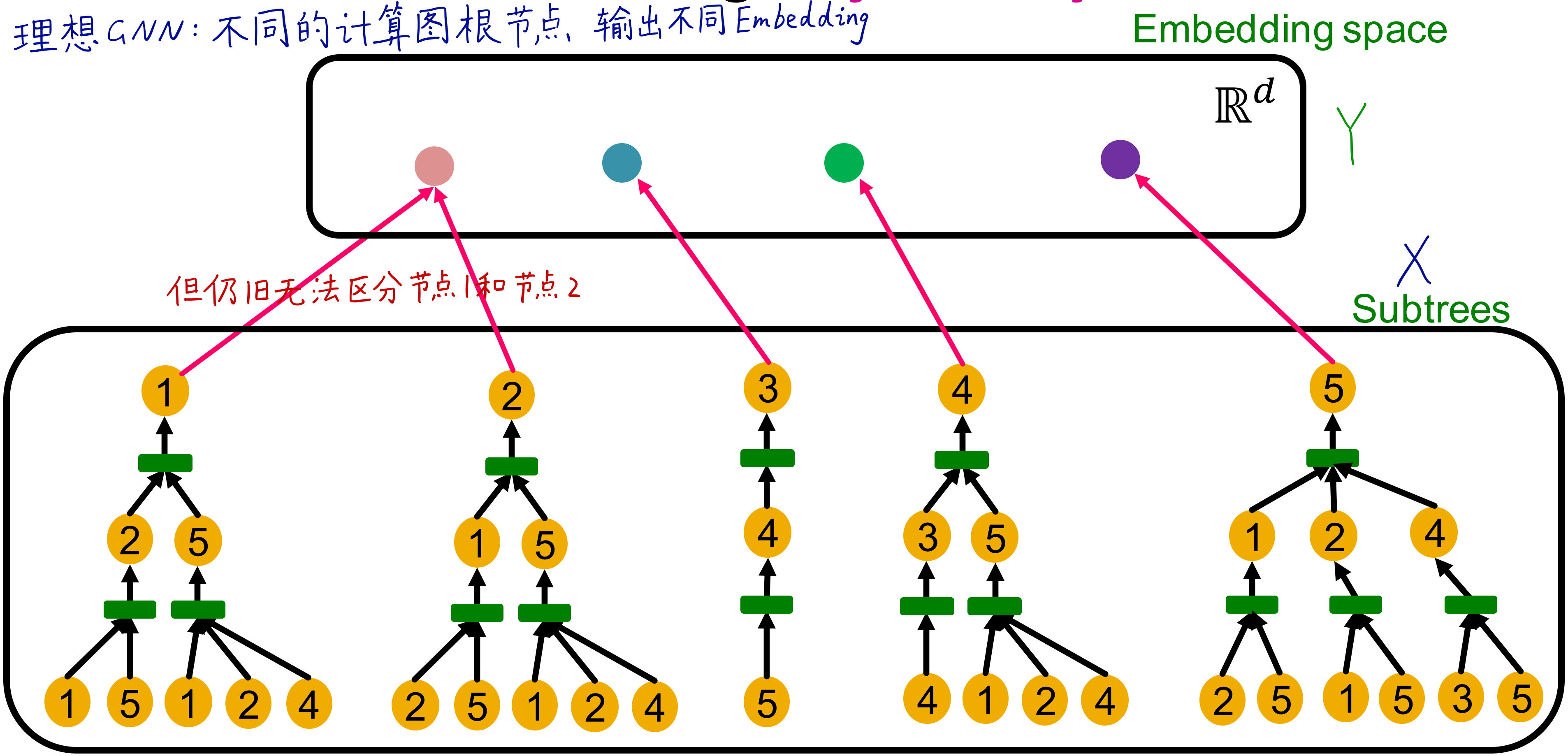



尘归尘，土归土
上帝的归上帝，凯撒的归凯撒

# How Expressive is a GNN?

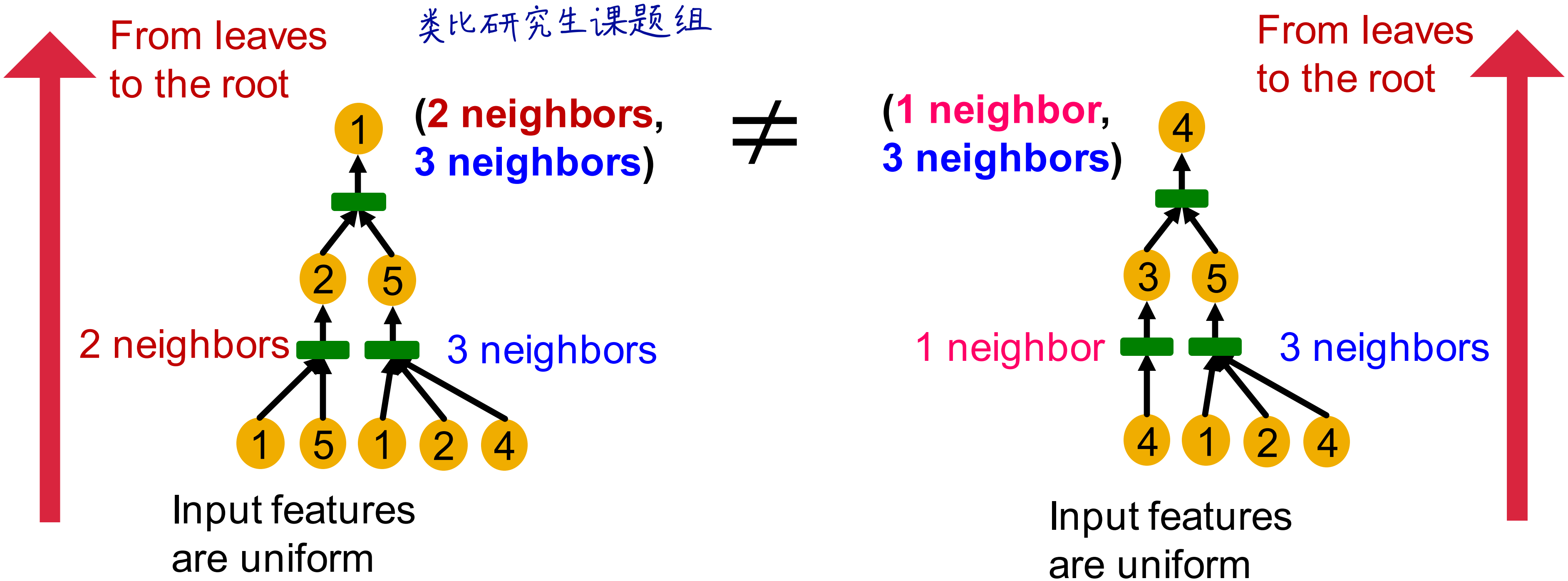
- Most expressive GNN should map subtrees to the node embeddings **injectively**.

理想GNN：不同的计算图根节点，输出不同Embedding



# How Expressive is a GNN?

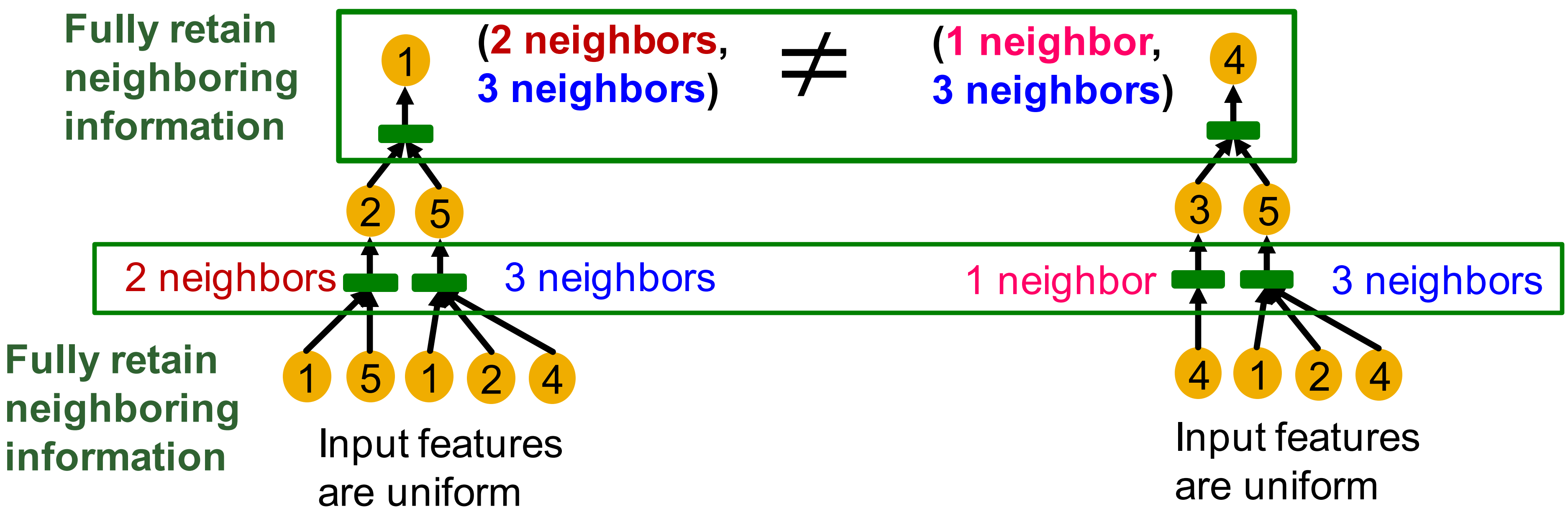
- **Key observation**: Subtrees of the same depth can be recursively characterized from the leaf nodes to the root nodes.



# How Expressive is a GNN?

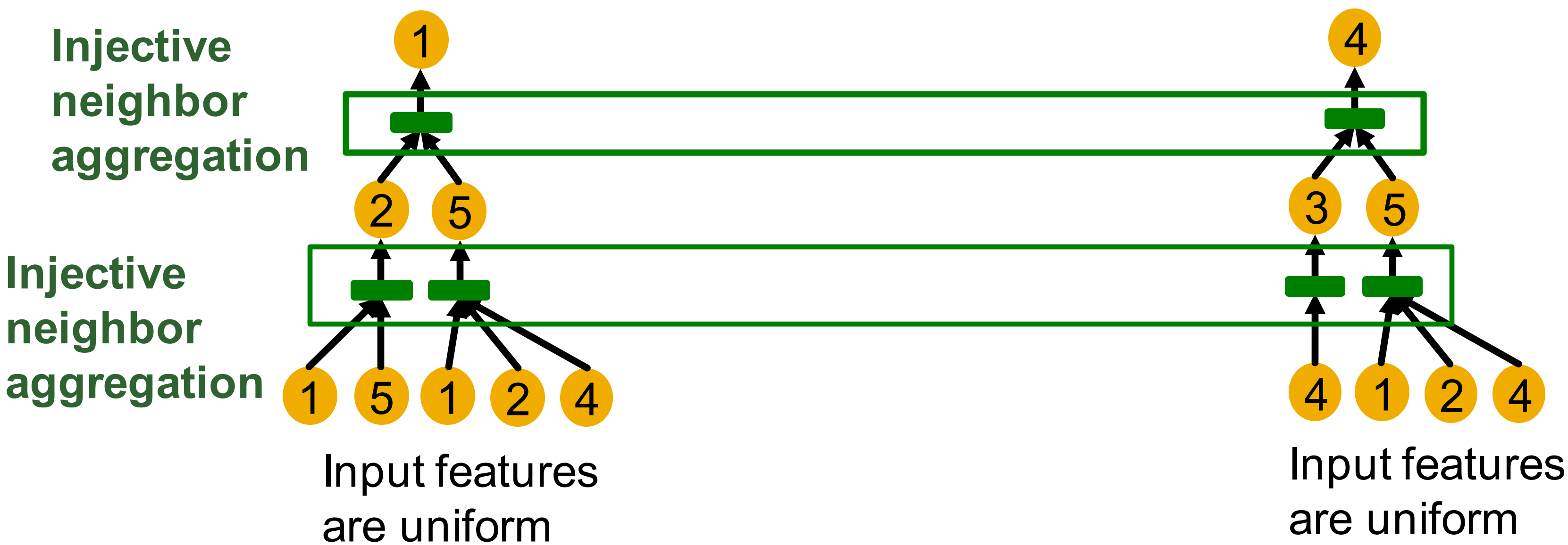
- If each step of GNN's aggregation **can fully retain the neighboring information**, the generated node embeddings can distinguish different rooted subtrees.

理想GNN：不同的计算图根节点，输出不同Embedding



# How Expressive is a GNN?

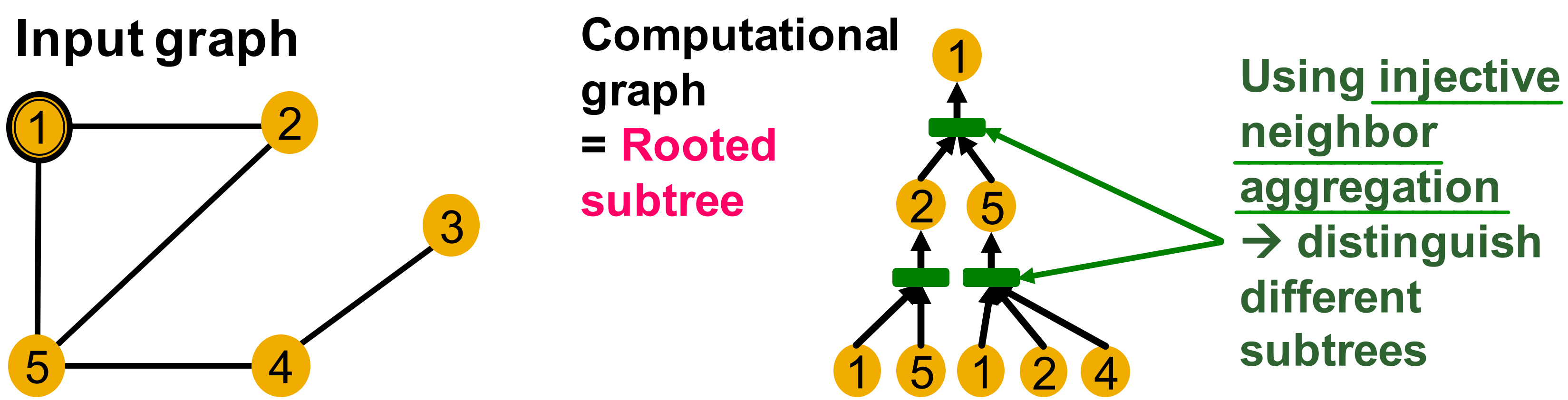
- In other words, most expressive GNN would use an **injective neighbor aggregation** function at each step. 聚合操作应该单射 最完美的单射聚合操作：哈希 Hash
  - Maps different neighbors to different embeddings.



# 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.** 聚合操作应该单射

# Stanford CS224W: Designing the Most Powerful Graph Neural Network

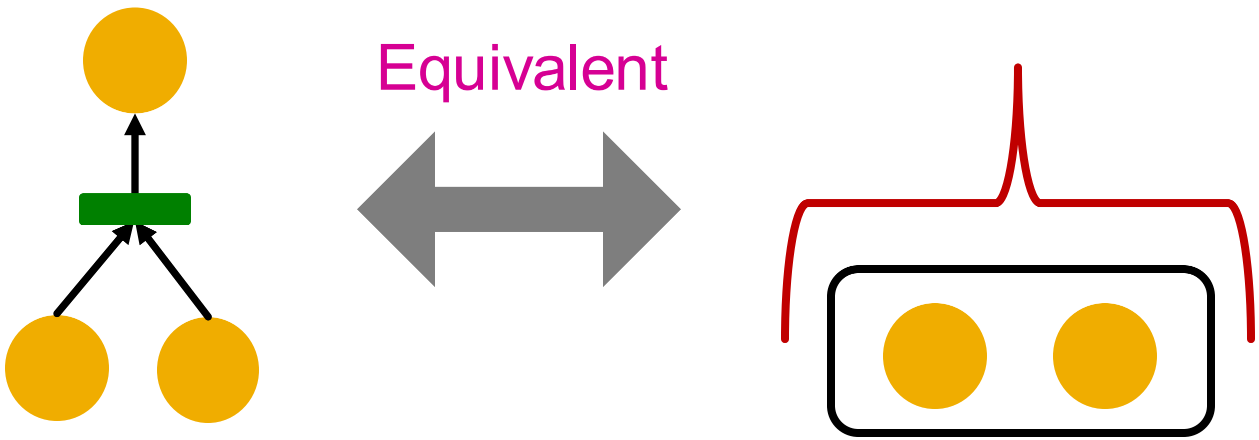
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

# 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 a GNN.
  - Injective aggregation function leads to the most expressive GNN. 单射聚合操作
- **Next:**
  - Theoretically analyze expressive power of aggregation functions.

# Neighbor Aggregation

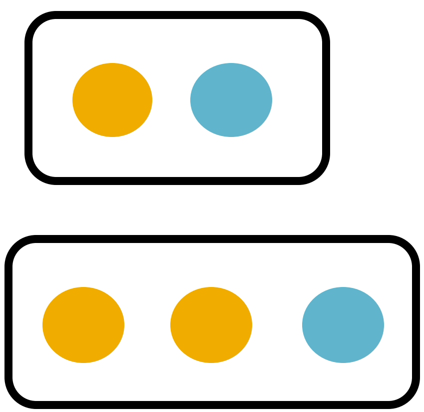
- **Observation**: **Neighbor aggregation** can be abstracted as 超集 **a function over a multi-set** (a set with 重复的元素 repeating elements).




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

逐元素求平均 $$\mathrm{Mean}(\{x_u\}_{u\in N(v)})$$

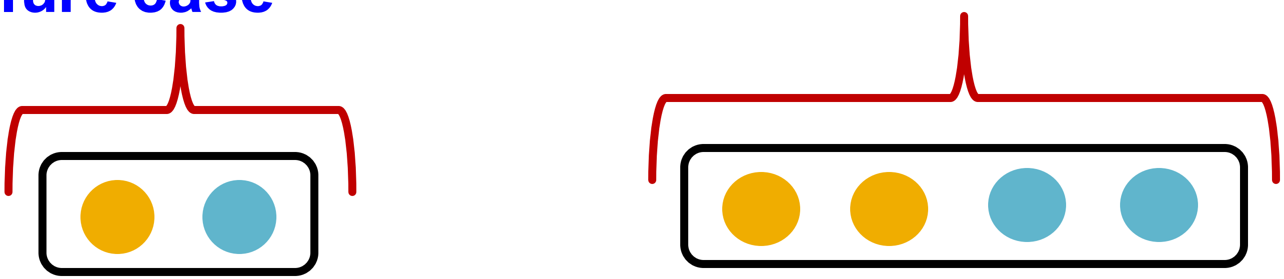
  - **GraphSAGE** (max-pool) [Hamilton et al. NeurIPS 2017]
    - Uses **element-wise** max pooling over neighboring node features

逐元素求最大值 $$\mathrm{Max}(\{x_u\}_{u\in N(v)})$$

# 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.**

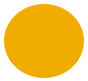
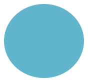
**Failure case**



- **Why?**

# Neighbor Aggregation

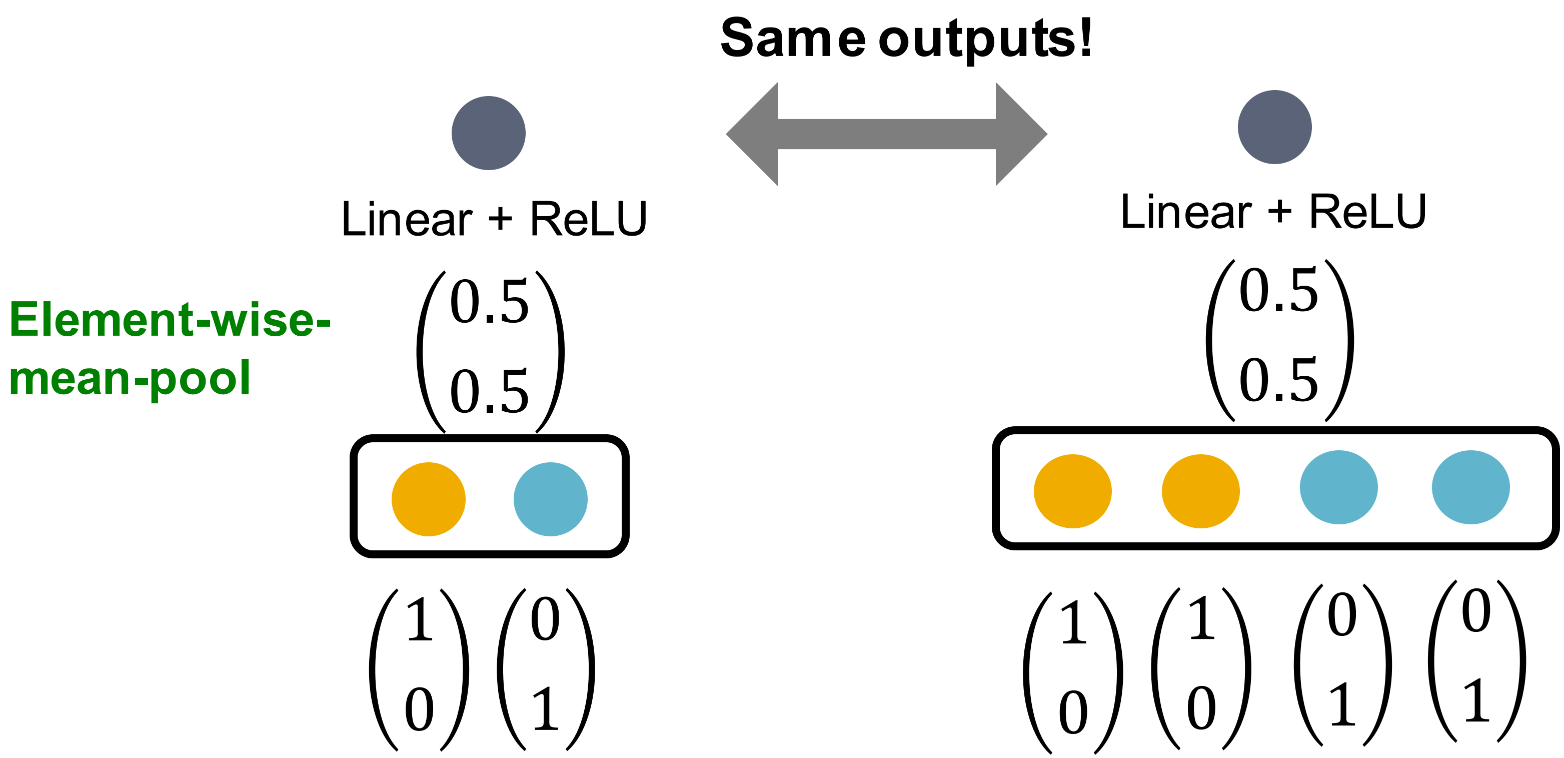
- For simplicity, we assume node features (colors) are represented by **one-hot encoding**.
  - **Example:** If there are two distinct colors:

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

  - This assumption is sufficient to illustrate how GCN fails.

# Neighbor Aggregation: Case Study

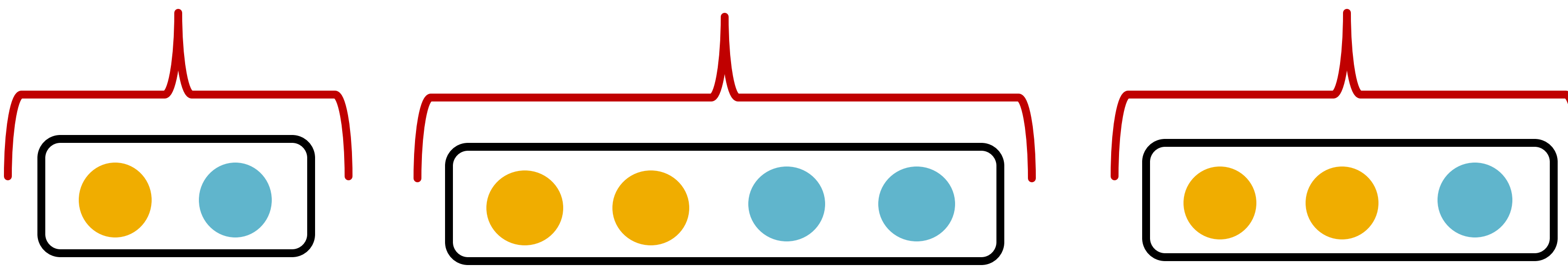
- **GCN (mean-pool)** [Kipf & Welling ICLR 2017]
  - **Failure case illustration**



# 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

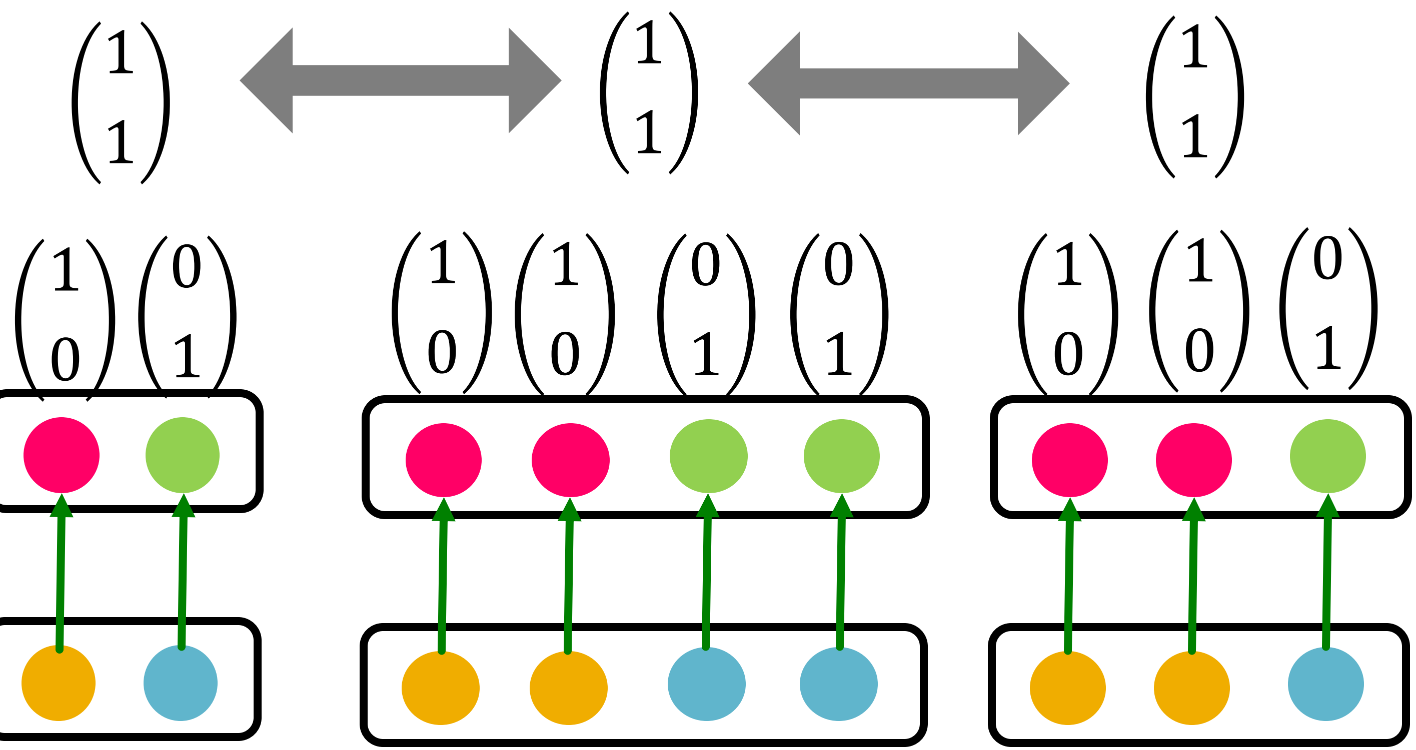
- **GraphSAGE (max-pool)** [Hamilton et al. NeurIPS 2017]
  - **Failure case illustration**

**The same outputs!**

**Element-wise-max-pool**

For simplicity, assume the one-hot encoding after **MLP**.

**MLP**



# Summary So Far

- We analyzed the **expressive power of GNNs.**
- **Main takeaways**: 总结
  - 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:

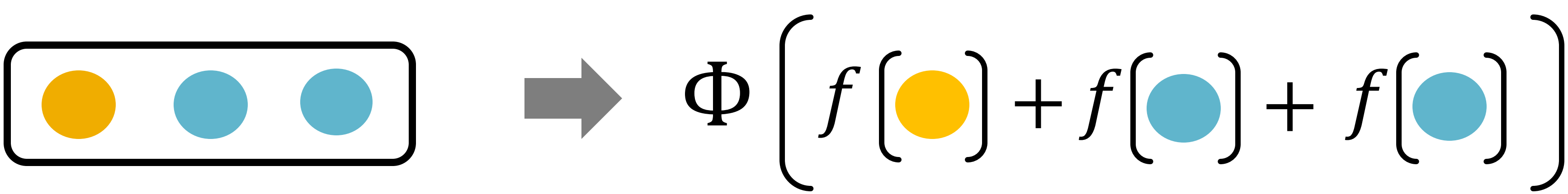
Some non-linear function

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.

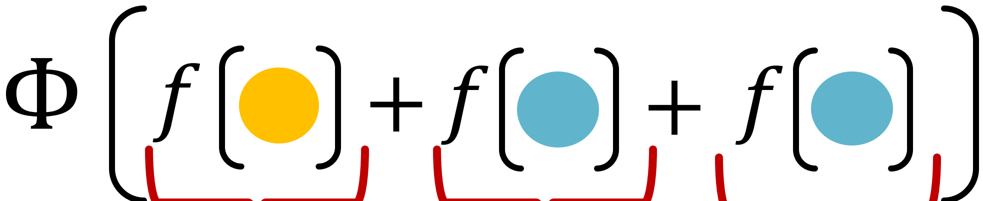
$$\Phi\left(\sum_{x\in S} f(x)\right)$$

f: 产生"颜色"

求和: 记录颜色个数

Φ: 单射函数

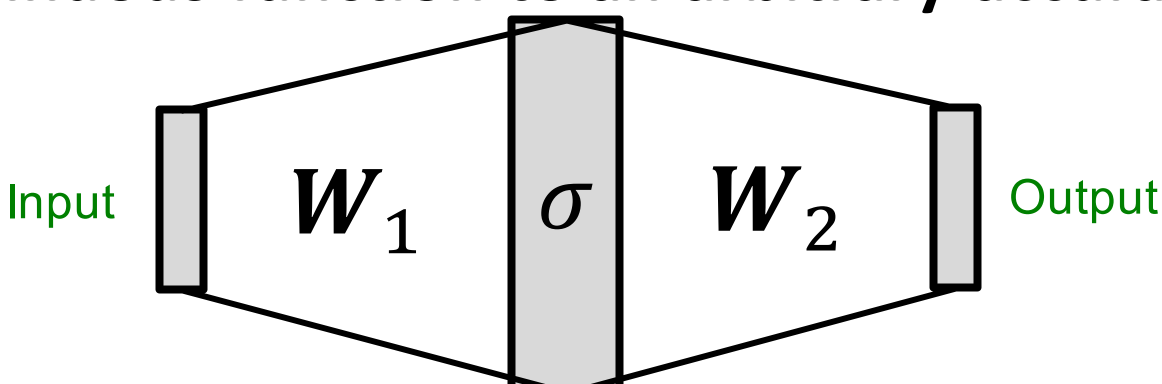
Example:



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] 万能近似定理
  - 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**. 任意



# Injective Multi-Set Function

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

$$\Phi \qquad\qquad f$$

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

  - 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!**
- $\boxed{\text{GIN is THE most expressive GNN}}$ **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.**

Weisfeiler-Lehman Kernel 见"传统图机器学习的特征工程"

- 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.

# 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

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

where HASH maps different inputs to different colors.

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

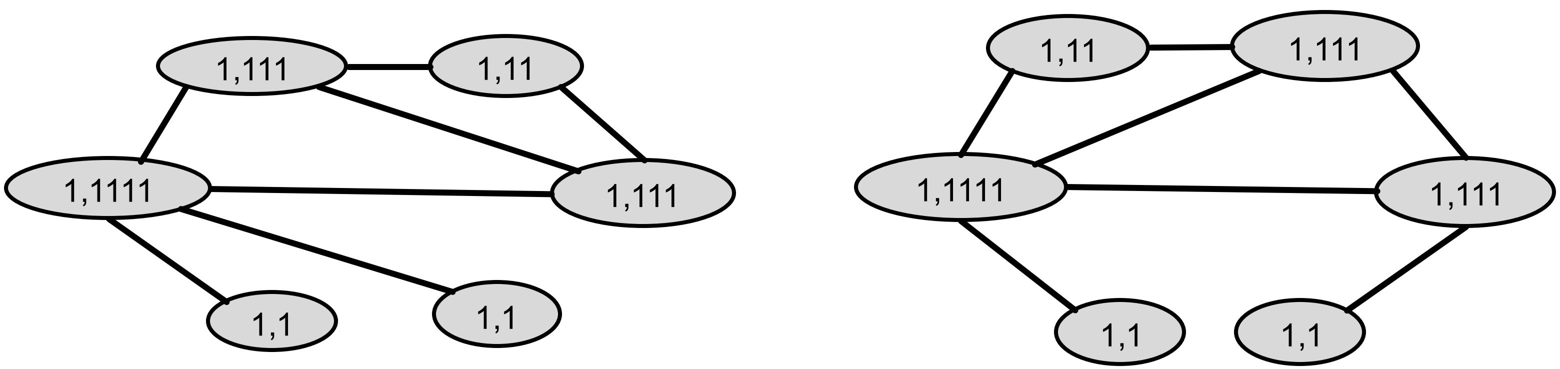
Hash：硬编码的单射函数

# Color Refinement (1)

## Example of color refinement given two graphs

- Assign initial colors

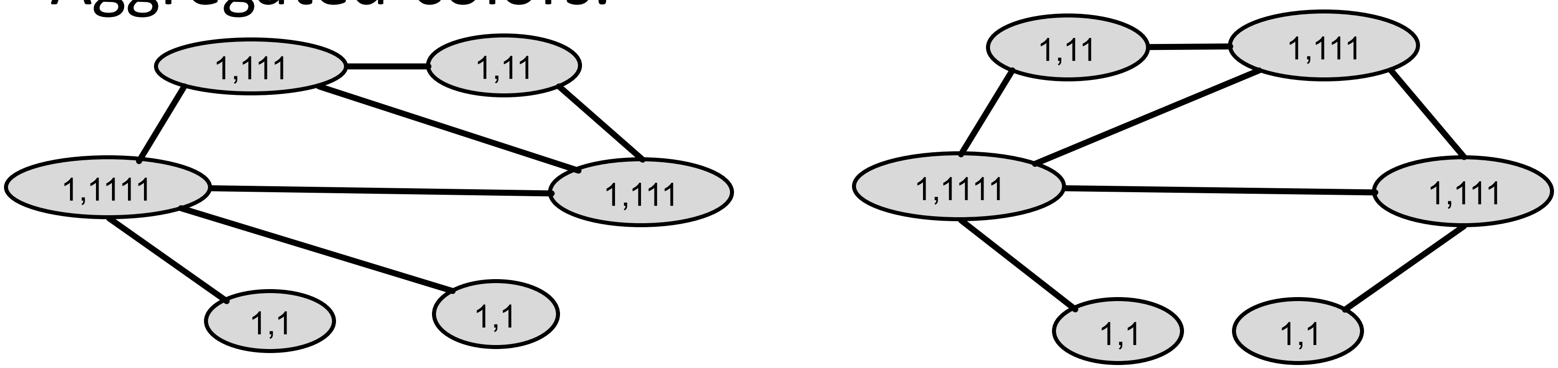

- Aggregate neighboring colors



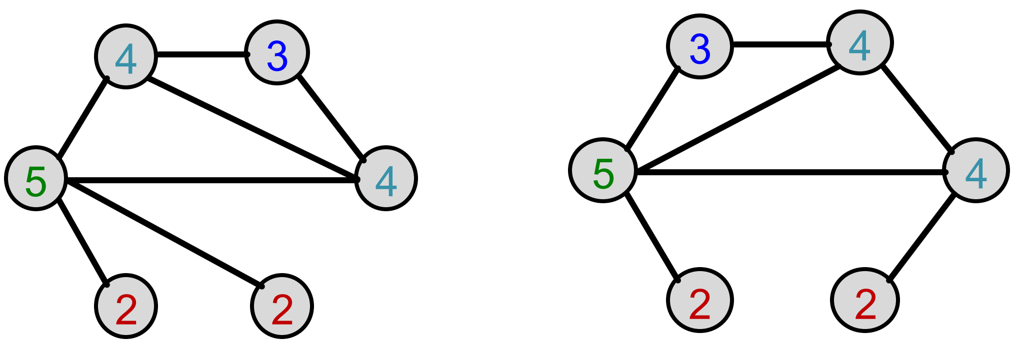
# Color Refinement (2)

## Example of color refinement given two graphs

- Aggregated colors:




- **Injectively** HASH the aggregated colors



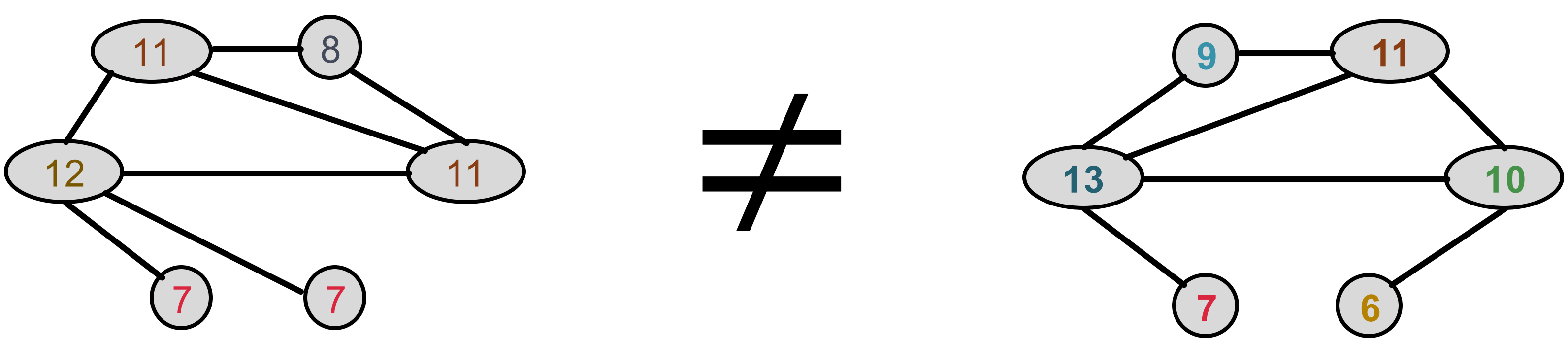

HASH table: **Injective!**

| | | |
|---|---|---|
| 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 同形 **isomorphic** if they have the same set of colors.



# The Complete GIN Model

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

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

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

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

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

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

where $\epsilon$ is a learnable scalar.

# The Complete GIN Model

- If input feature $c^{(0)}(v)$ is represented as one-hot, **direct summation is injective.** 如果feature已经是one-hot 则不需要f

Example: $\Phi\left(\underbrace{\text{●}}_{\begin{pmatrix}1\\0\end{pmatrix}} + \underbrace{\text{●}}_{\begin{pmatrix}0\\1\end{pmatrix}} + \underbrace{\text{●}}_{\begin{pmatrix}0\\1\end{pmatrix}}\right)$

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

- We only need $\Phi$ to ensure the injectivity.

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

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

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

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:**

  低维，连续、稠密、包含语义

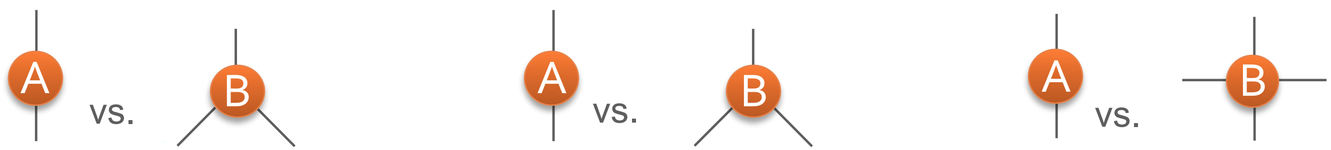
  - Node embeddings are **low-dimensional**; hence, they can capture the fine-grained similarity of different nodes.
  - Parameters of the update function can be **learned for the downstream tasks.** 根据下游任务学习优化

# Expressive Power of GIN

- **Because of the relation between GIN and the WL graph kernel, their expressive is exactly the same.** WL是表达能力的上界
  - 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) Mean and Max both fail (b) Max fails (c) Mean and Max both fail

Colors represent feature values

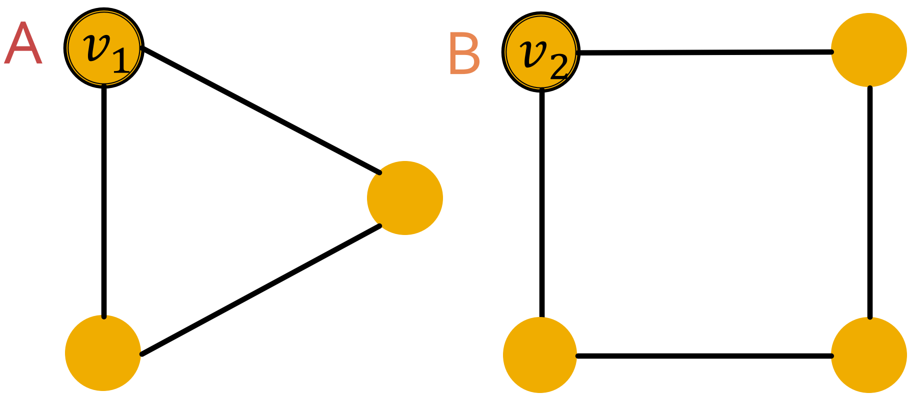
## Ranking by discriminative power:


**Input** sum - multiset mean - distribution max - set

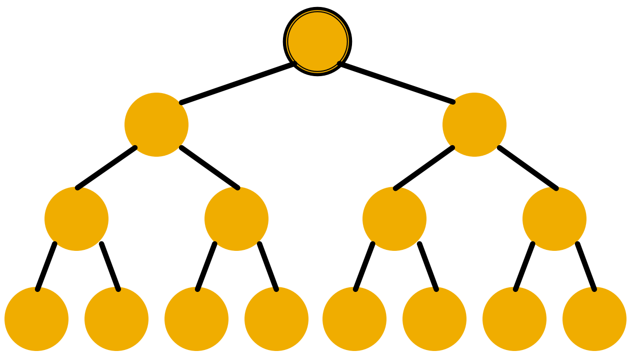
# Improving GNNs' Power

- **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 超出"消息传递GNN范畴" 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
  - 仔细观察
    **Scrutinize loss function!**
- **Important for model development:**
  - **Overfit on (part of) training data:**
    - 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)**

PyG    DGL    GraphNets

**GNN frameworks:**
**Implements a variety of GNN architectures**

PyTorch    TensorFlow

**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)