Stanford CS224W: How Expressive are Graph Neural Networks?

CS224W: Machine Learning with Graphs

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http://cs224w.stanford.edu

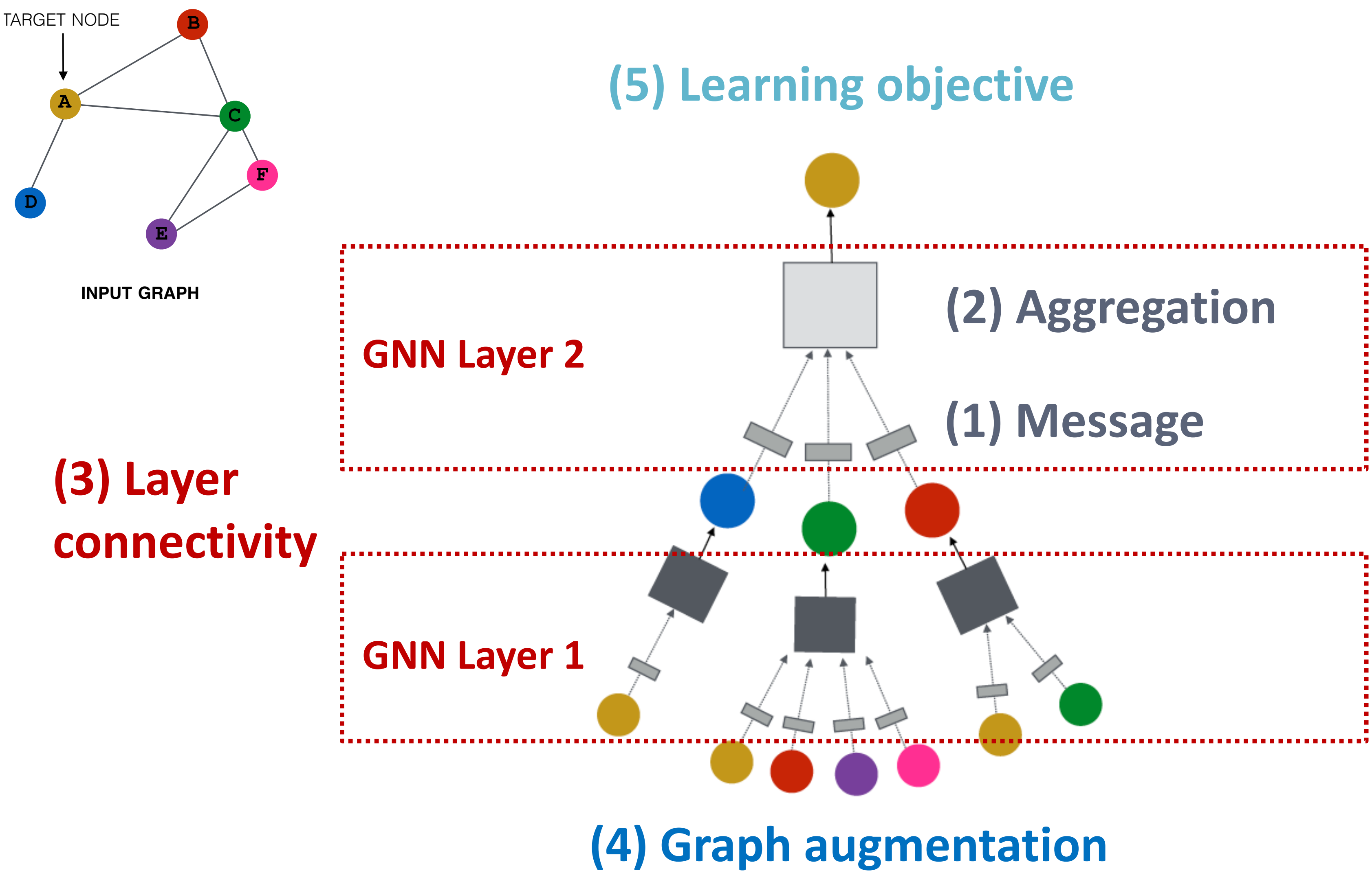
ANNOUNCEMENTS

- My email: joshrob@cs.stanford.edu
- Please reach out with any questions, etc.!

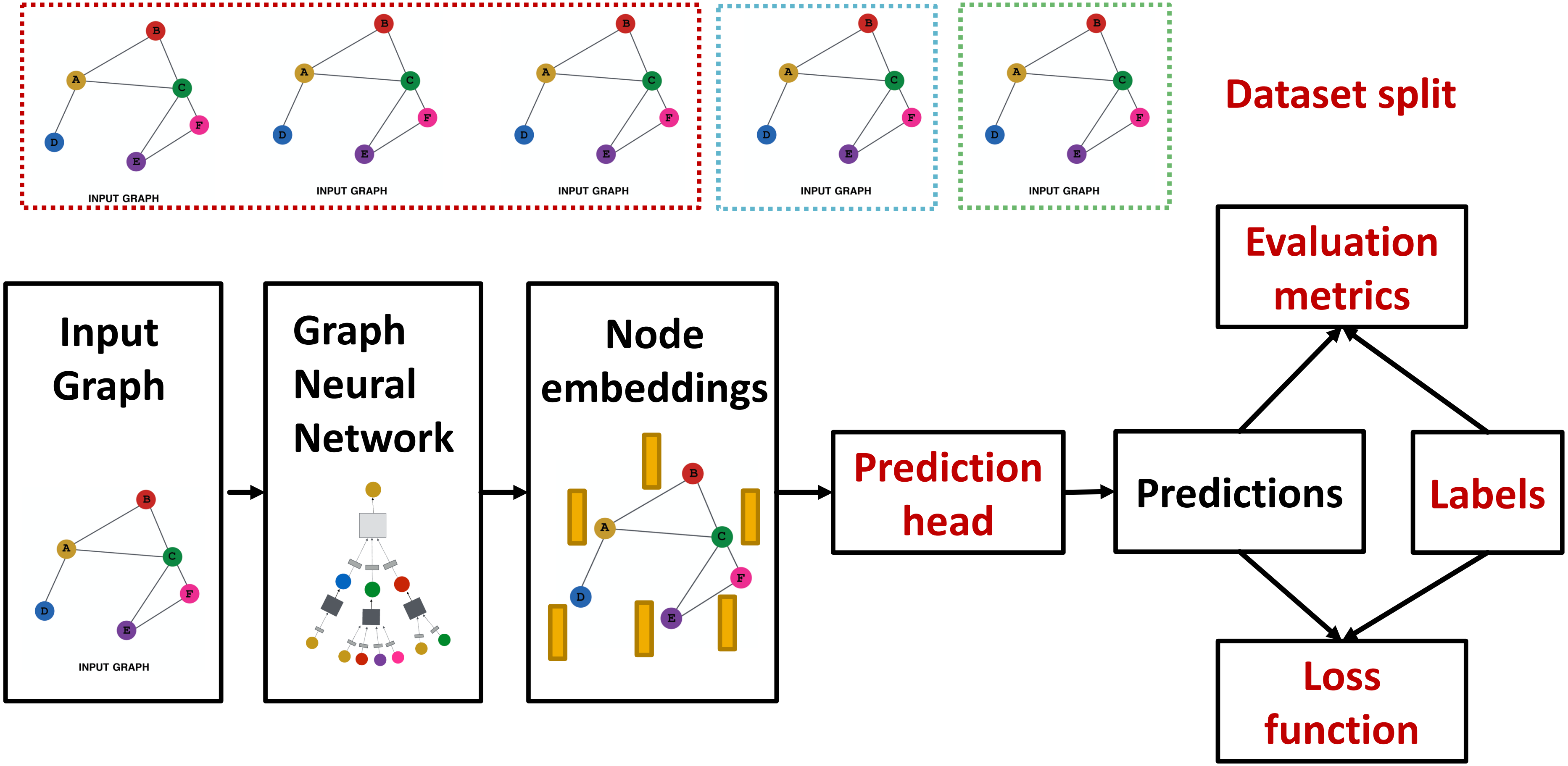
Announcements

- **Homework 1** recitation session 1pm-3pm tomorrow
  - Details on Ed
- **Colab 2** will be released today by 9PM on our course website
  - Due on Thursday, October 26 (2 weeks from now)

Recap: A General GNN Framework



Recap: GNN Training Pipeline



Implementation resources:

PyG provides core modules for this pipeline

GraphGym further implements the full pipeline to facilitate GNN design

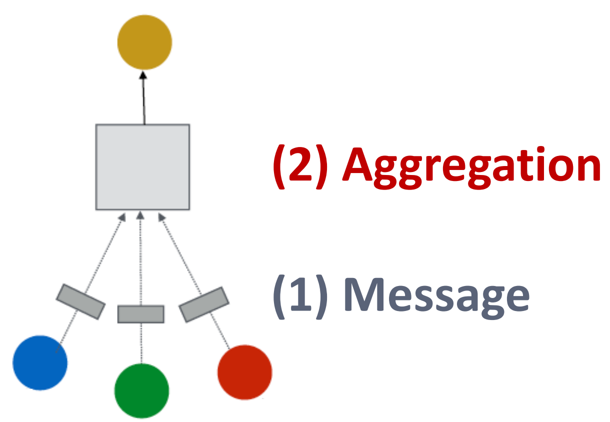
Theory of GNNs

How powerful are GNNs?

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

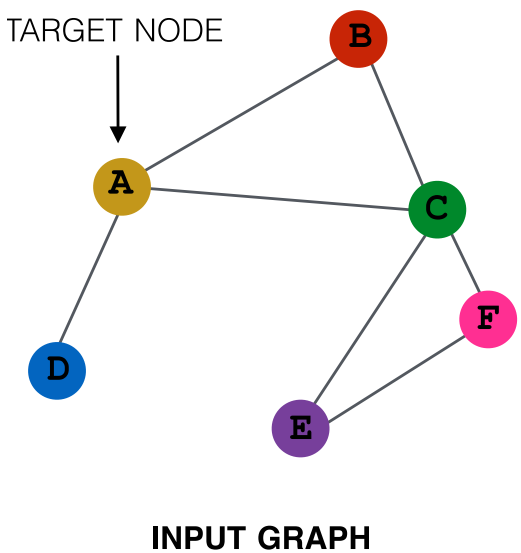
Background: A Single GNN Layer

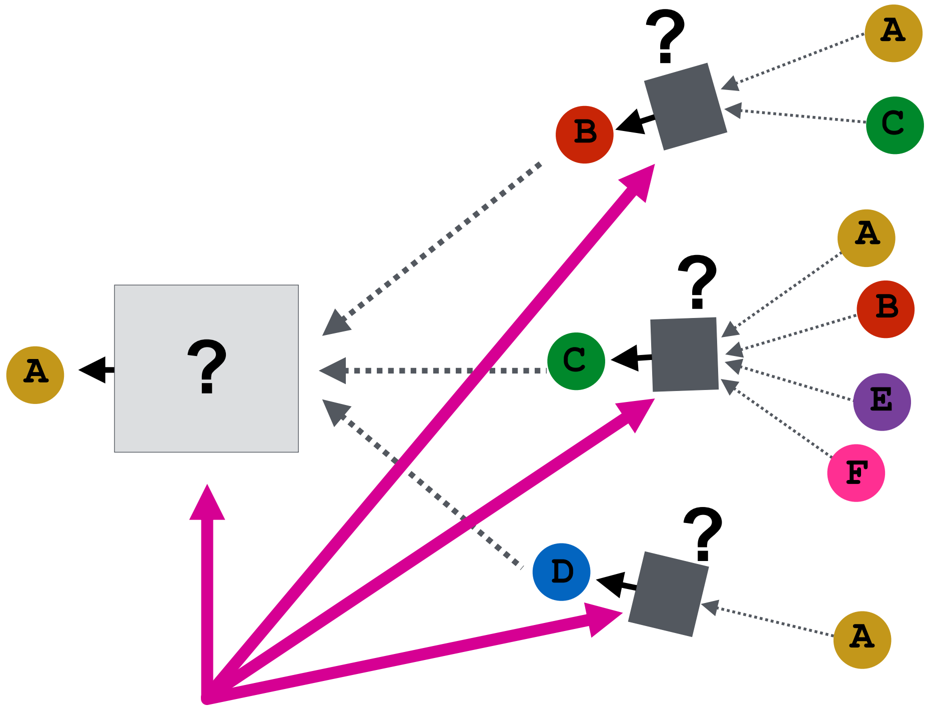
- **We focus on message passing GNNs:**
  - **(1) Message**: each node computes a message
    $$\mathbf{m}_u^{(l)} = \mathrm{MSG}^{(l)}\left(\mathbf{h}_u^{(l-1)}\right), u \in \{N(v) \cup v\}$$
  - **(2) Aggregation**: aggregate messages from neighbors
    $$\mathbf{h}_v^{(l)} = \mathrm{AGG}^{(l)}\left(\left\{\mathbf{m}_u^{(l)},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



Background: Many GNN Models

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

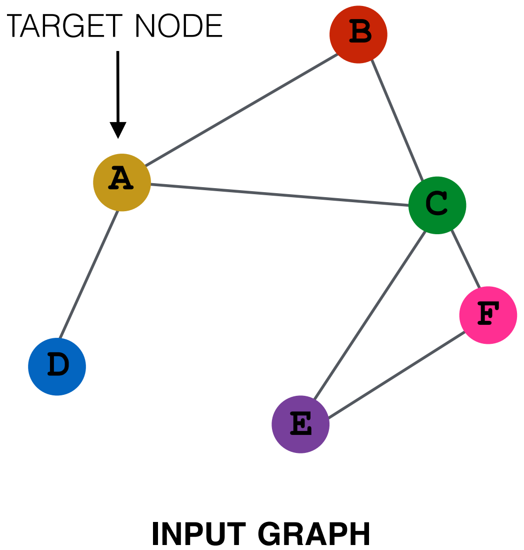


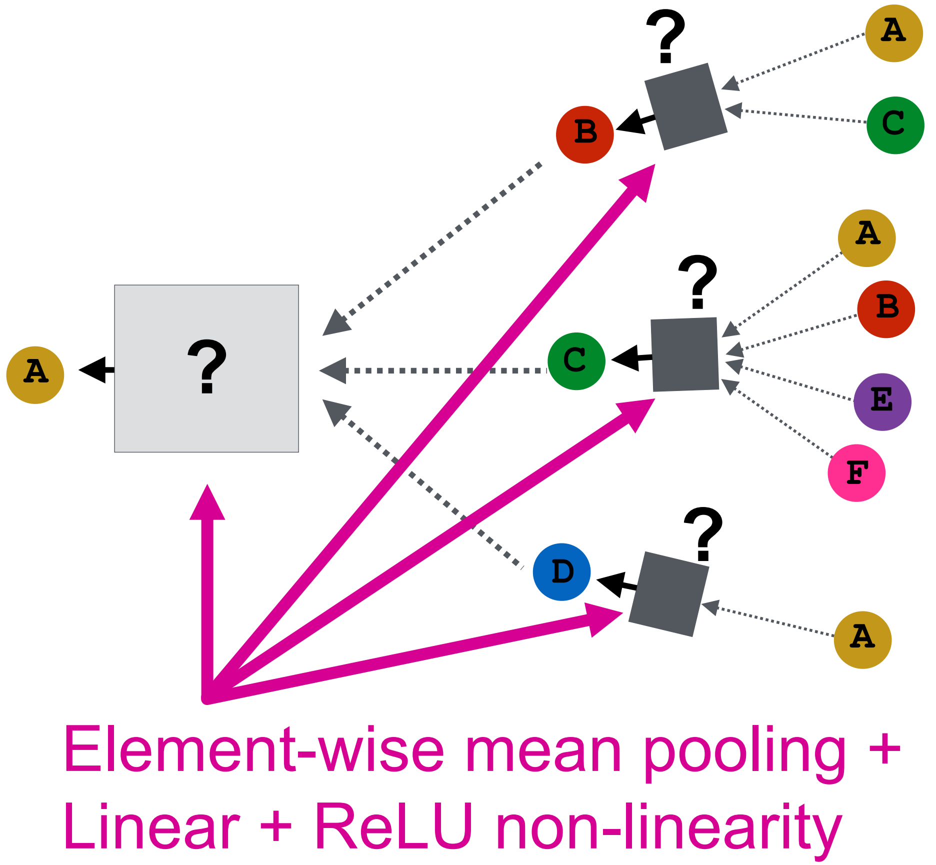


Different GNN models use different neural networks in the box

GNN Model Example (1)

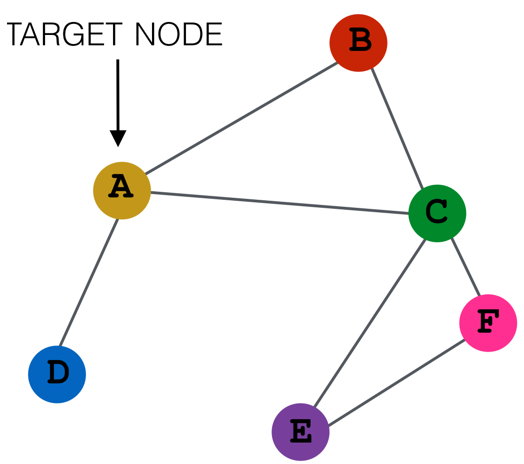
- **GCN (mean-pool)** [Kipf and Welling ICLR 2017]



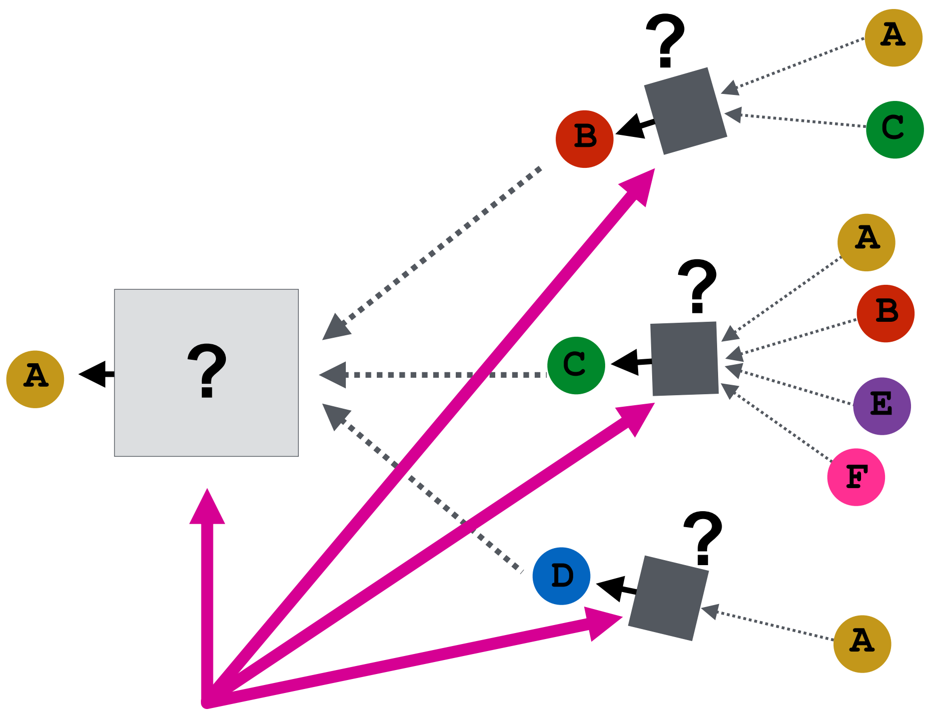


GNN Model Example (2)

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



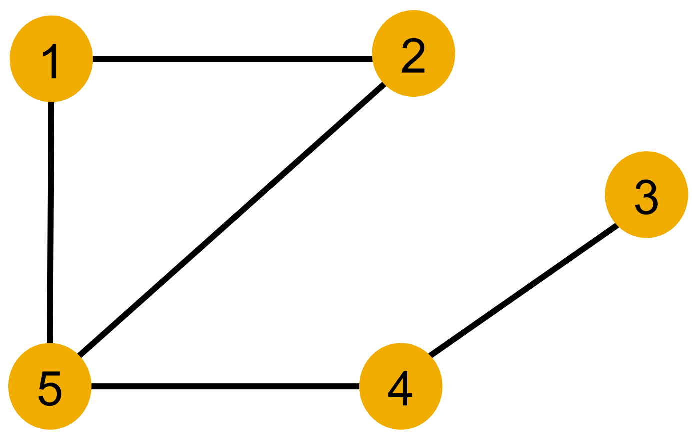
INPUT GRAPH



MLP + element-wise max-pooling

Note: Node Colors

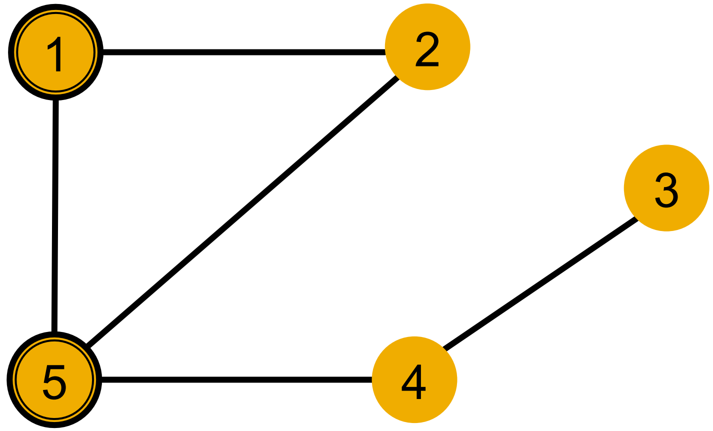
- We use node same/different **colors** to represent nodes with same/different features.
  - For example, the graph below assumes all the nodes share the same feature.



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

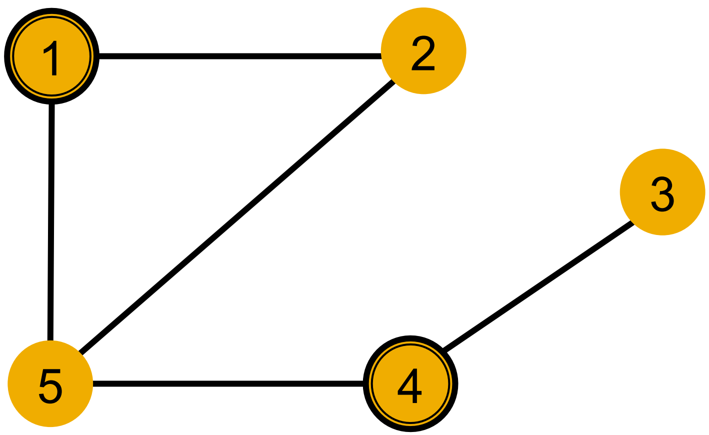
Local Neighborhood Structures

- 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

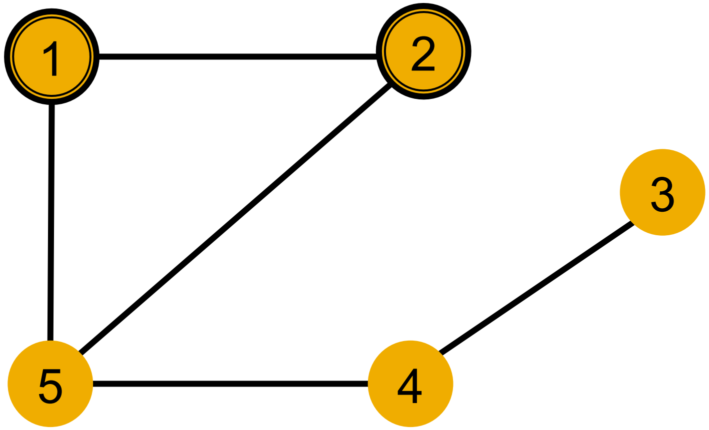
- We specifically consider **local neighborhood structures** around each node in a graph.
  - **Example:** Nodes 1 and 4 both have the same node degree of 2. However, they still have **different** neighborhood structures because **their neighbors have different node degrees.**



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)

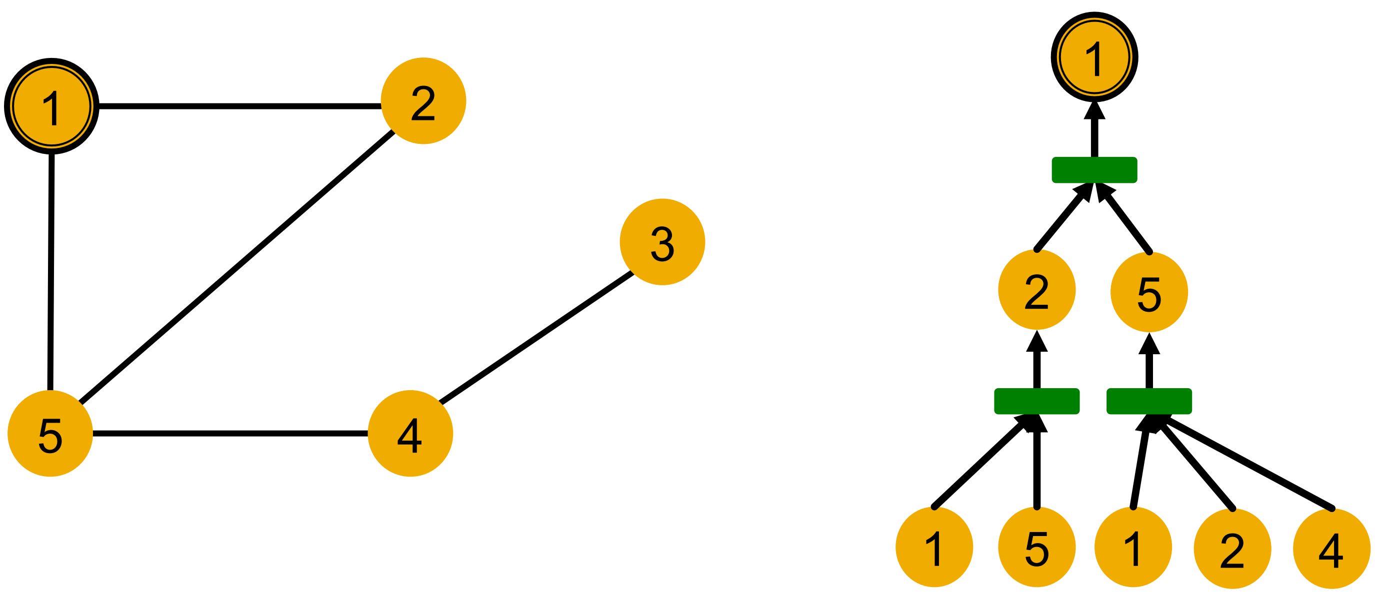
Local Neighborhood Structures

- **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**

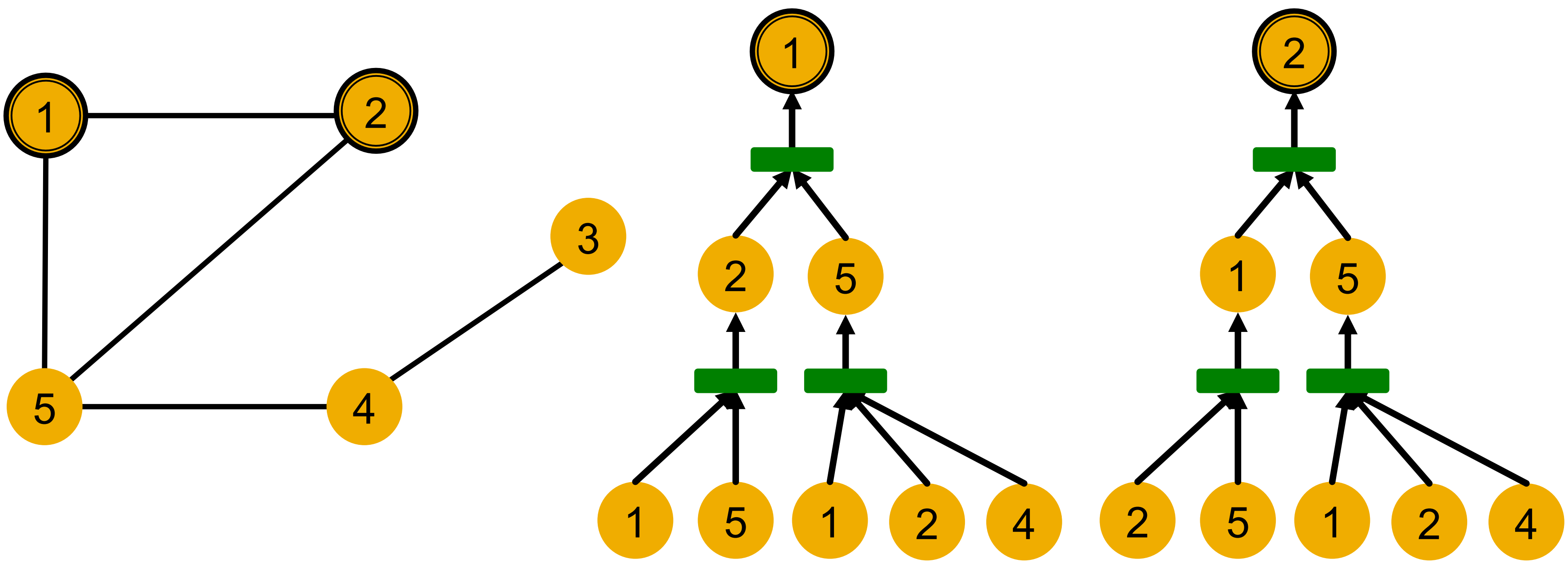
Computational Graph (1)

- **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)



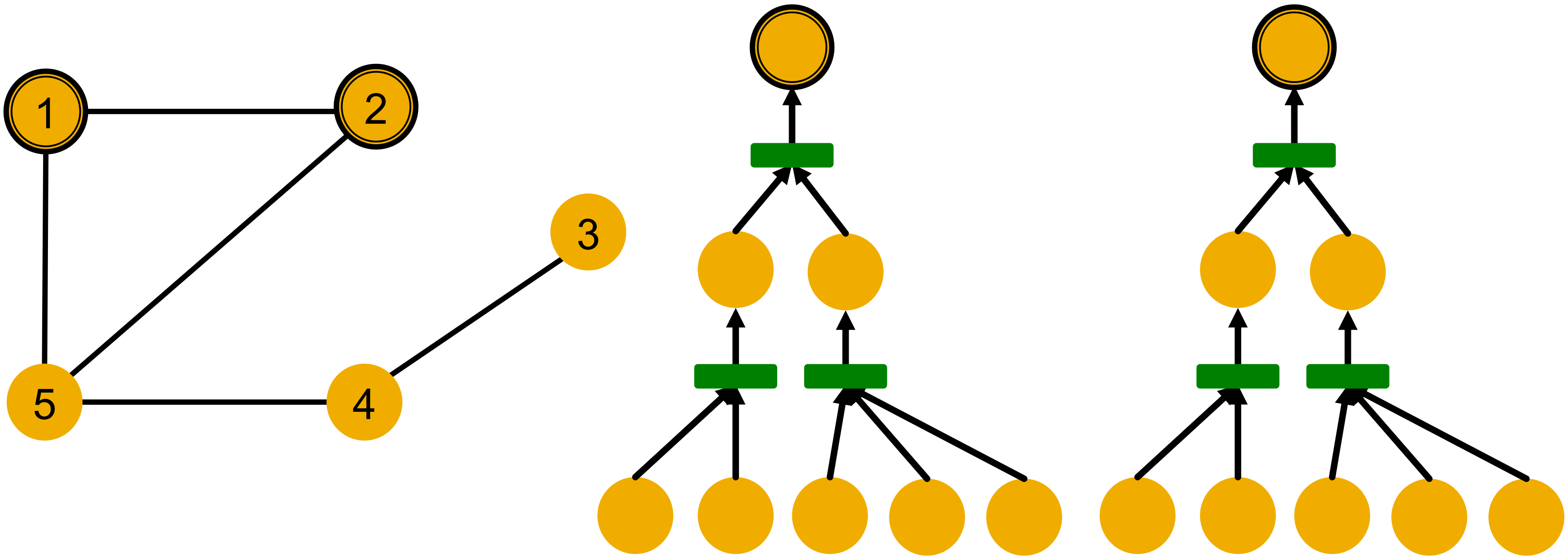
Computational Graph (2)

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



Computational Graph (3)

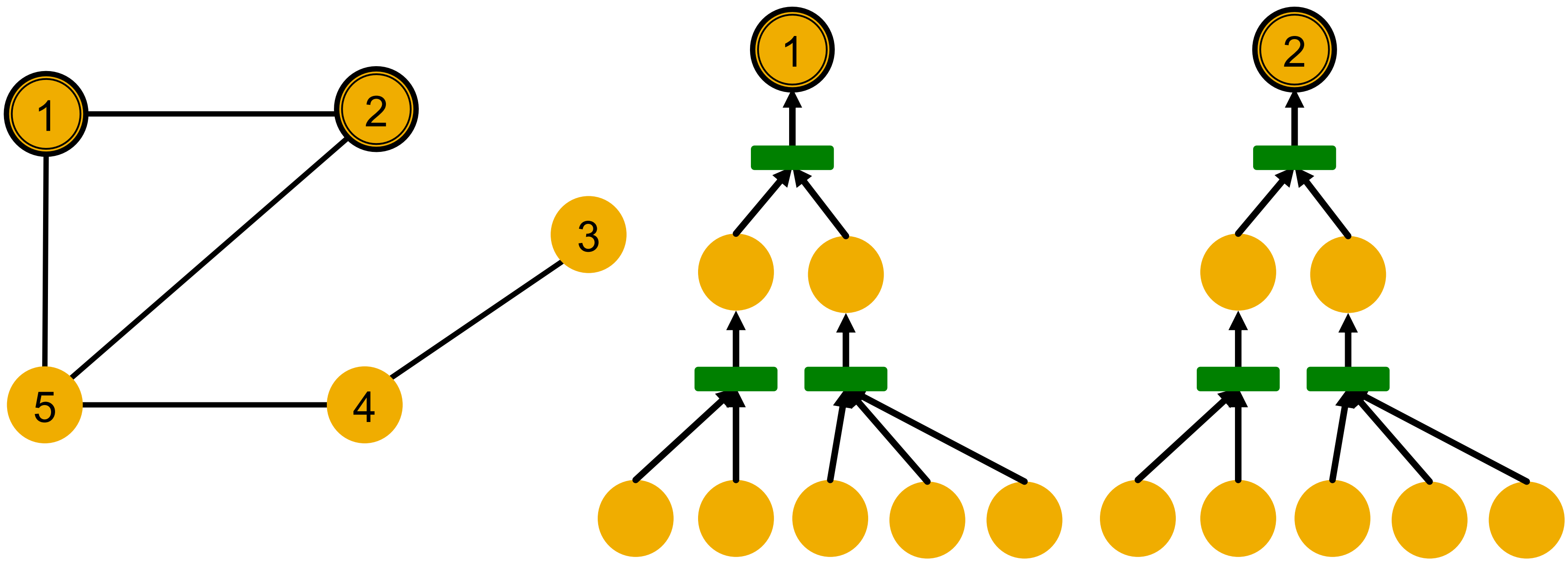
- **Ex:** Nodes 1 and 2's computational graphs.
- **But GNN only sees node features (not IDs):**



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.

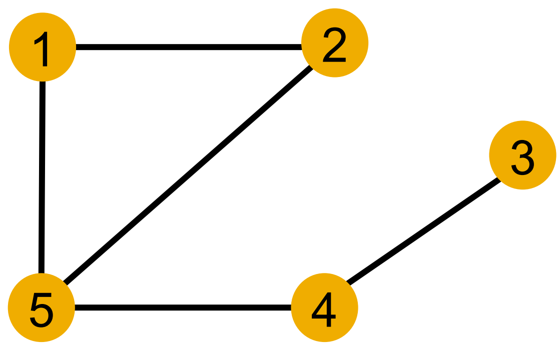
Note: GNN does not care about node ids, it just aggregates features vectors of different nodes.

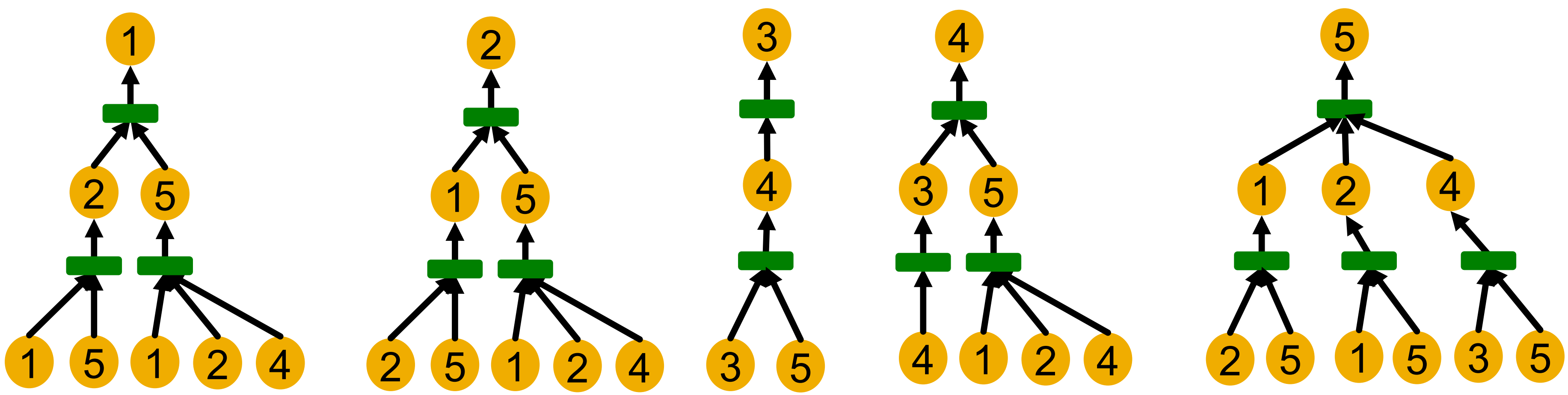


GNN won't be able to distinguish nodes 1 and 2

Computational Graph

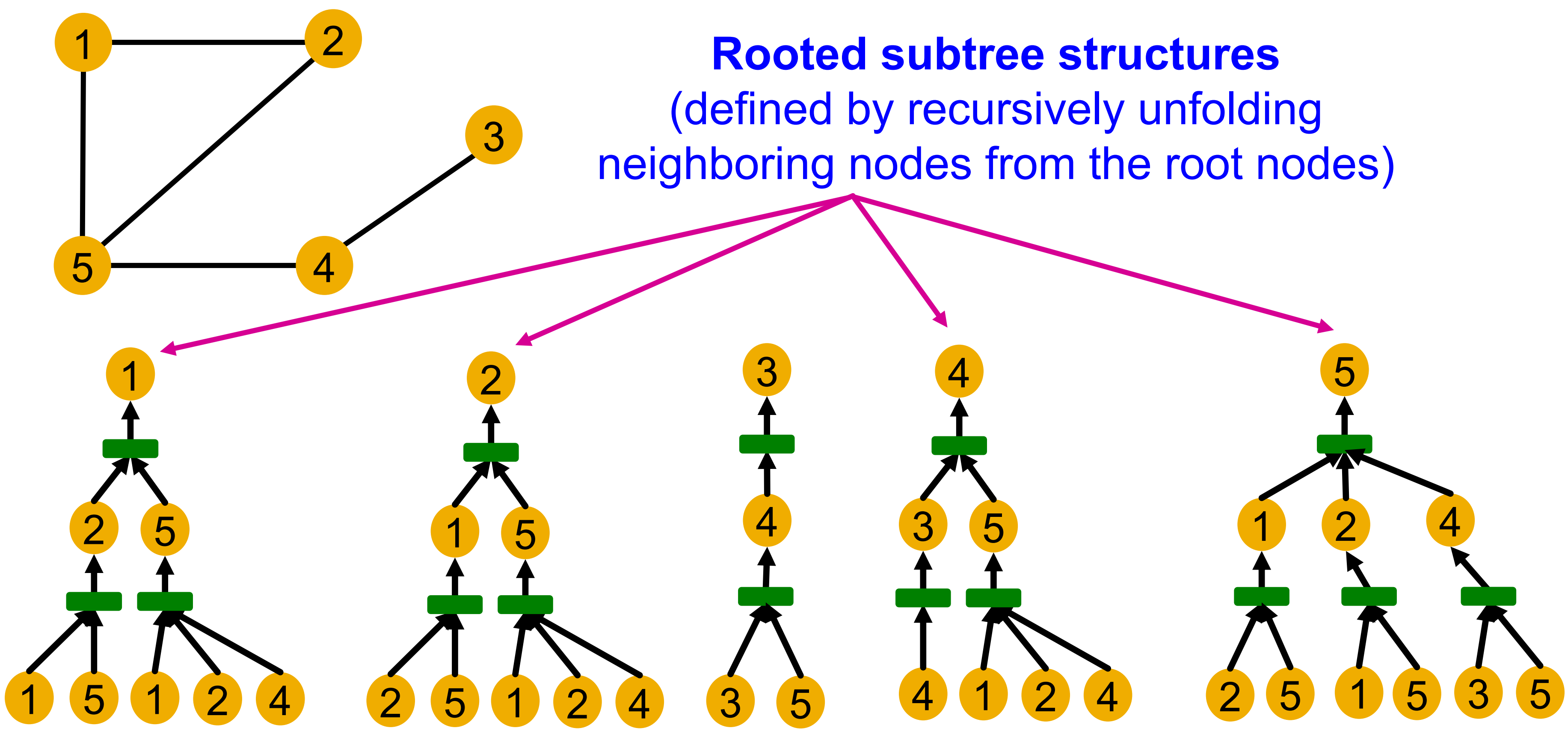
- **In general, different local neighborhoods define different computational graphs**





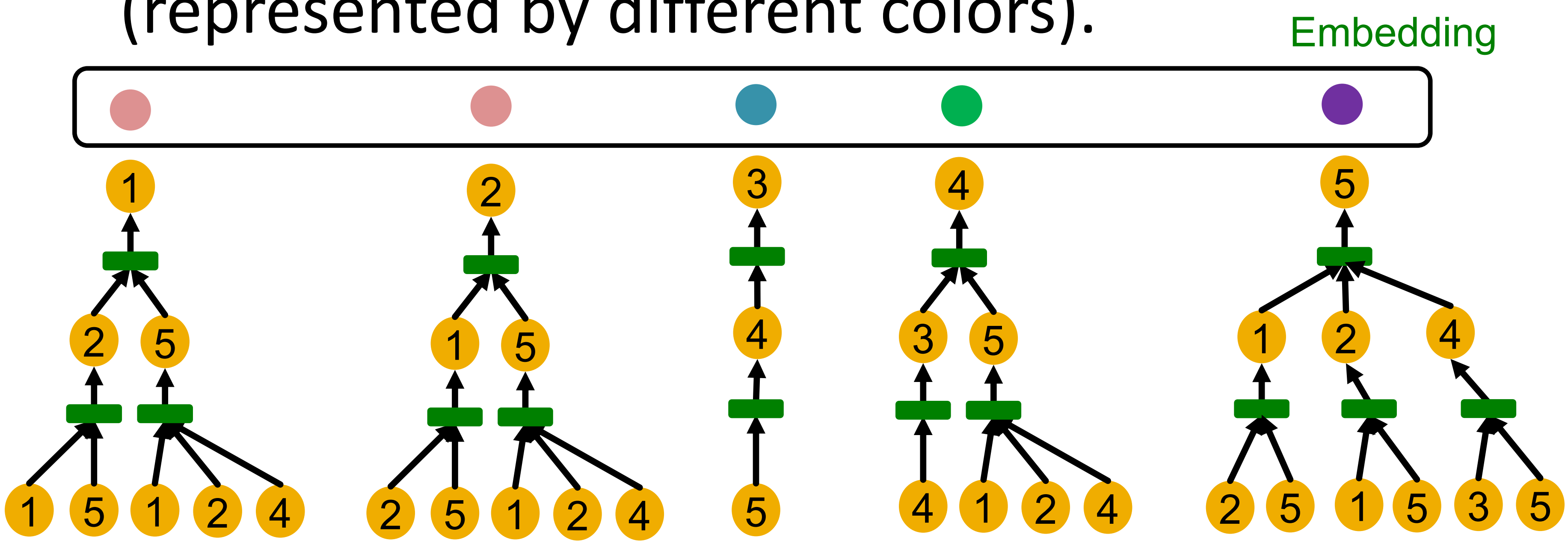
Computational Graph

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



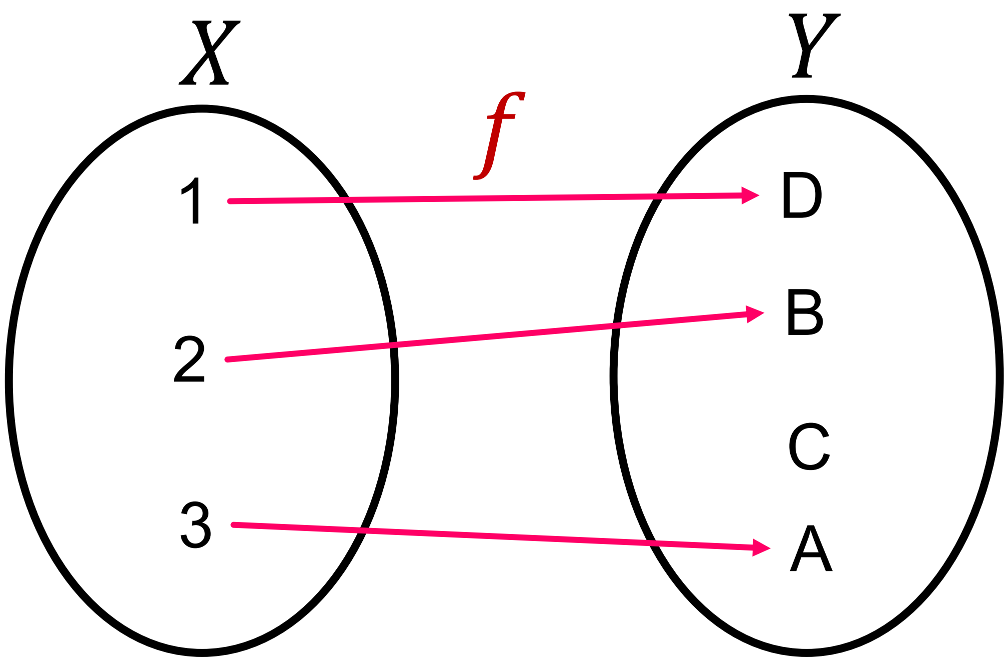
Computational Graph

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



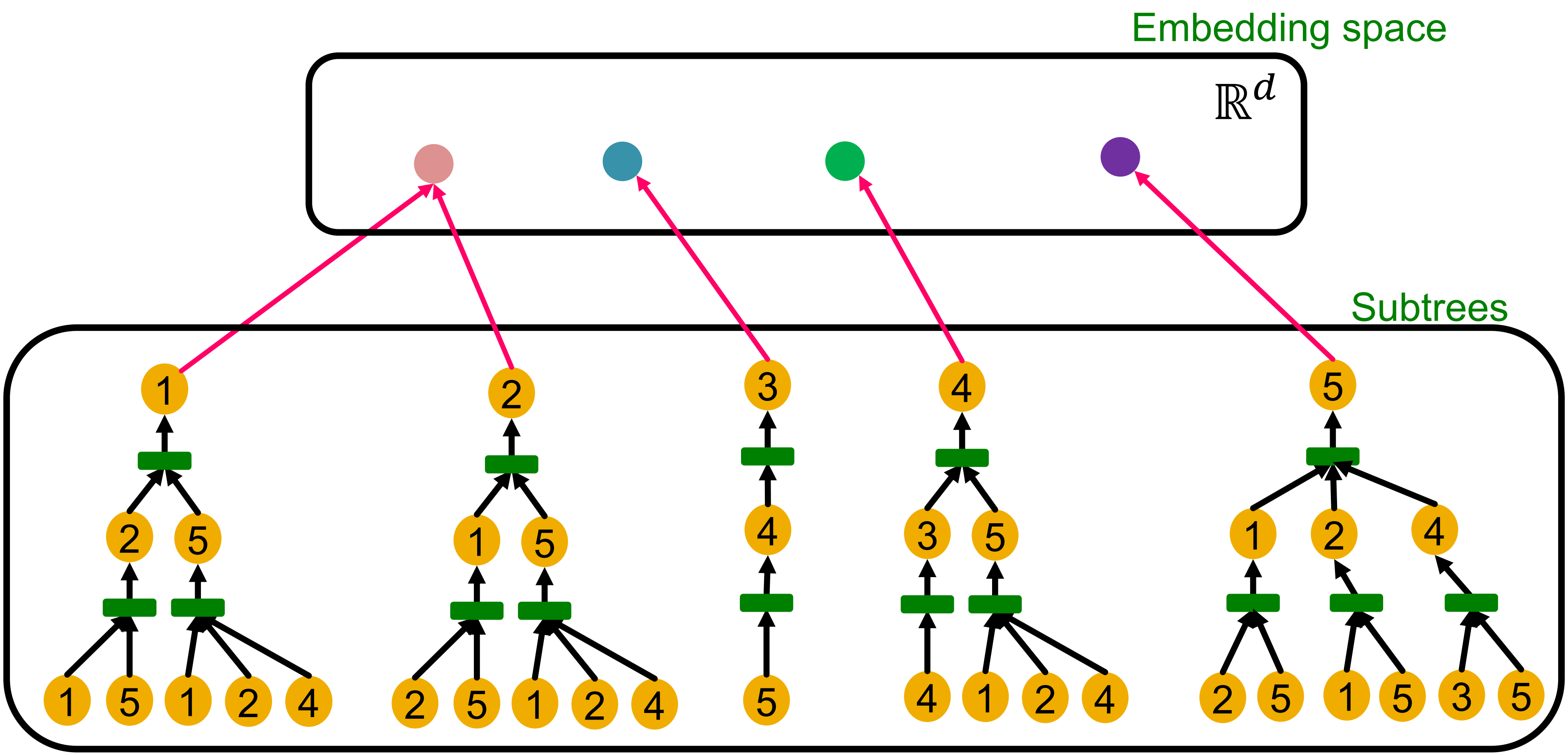
Recall: Injective Function

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



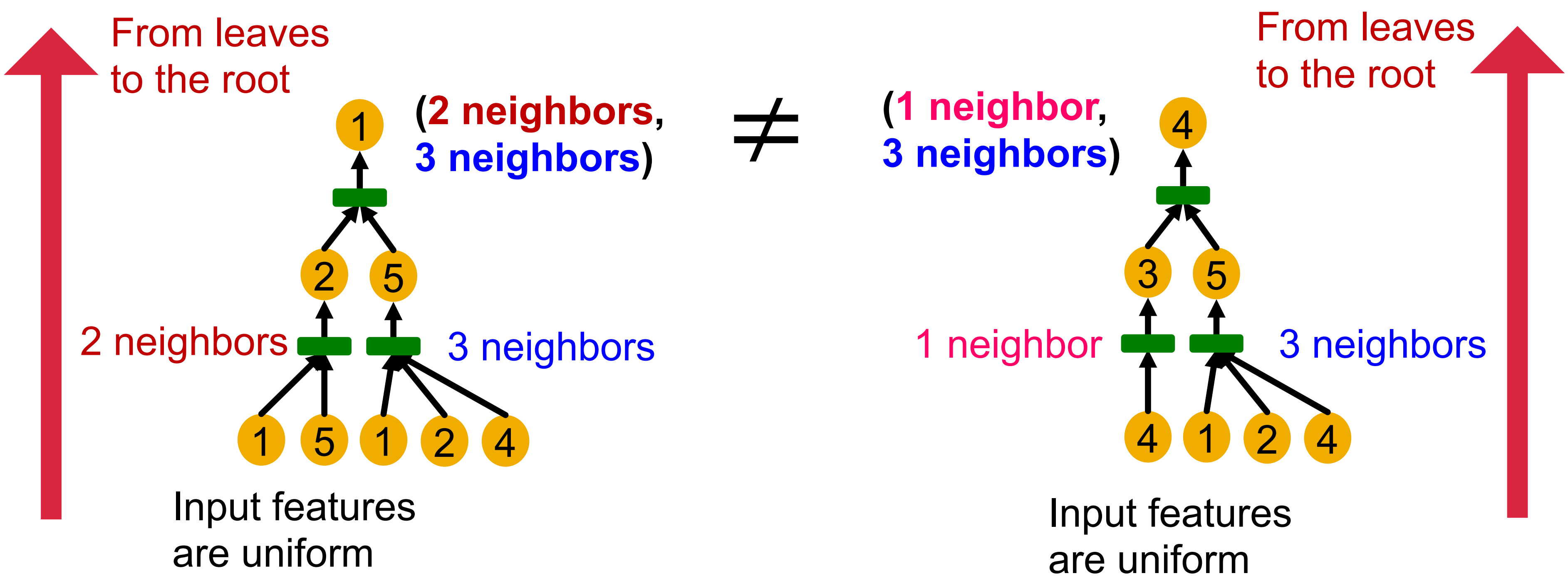
How Expressive is a GNN?

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



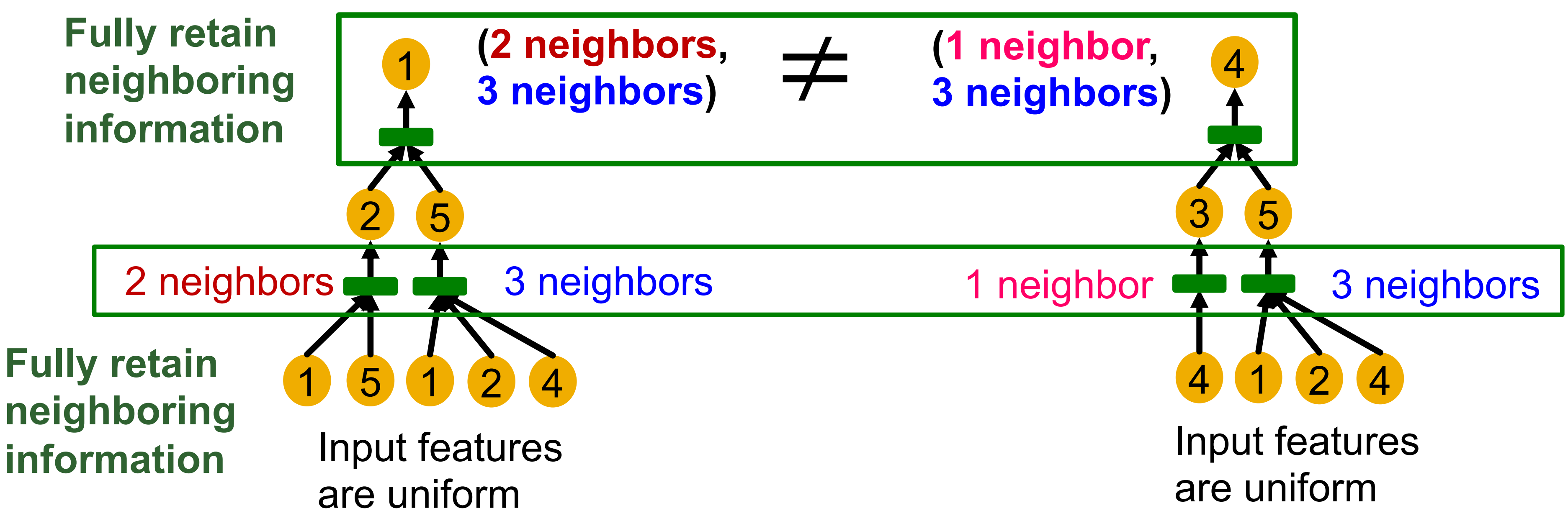
How Expressive is a GNN?

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



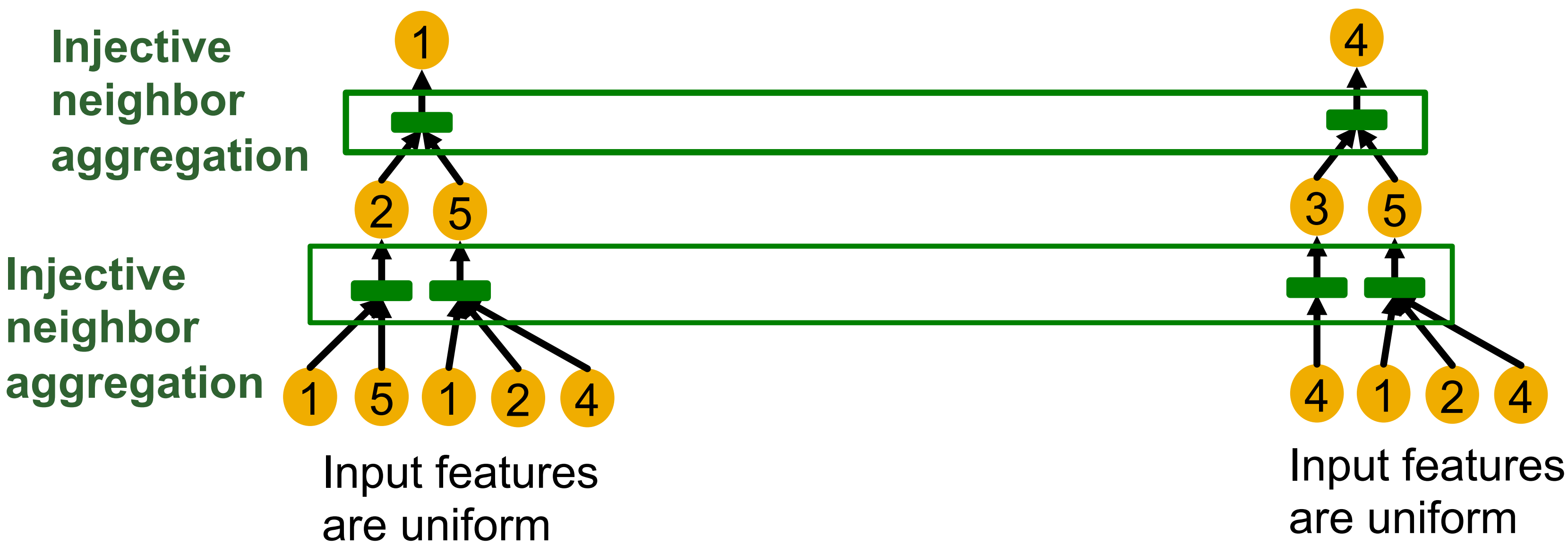
How Expressive is a GNN?

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



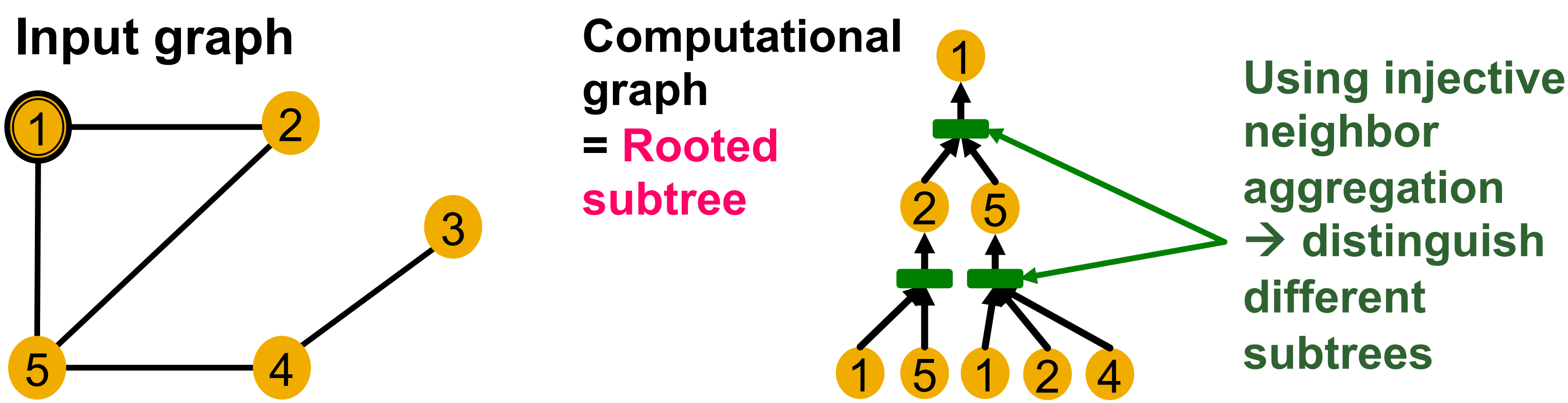
How Expressive is a GNN?

- 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

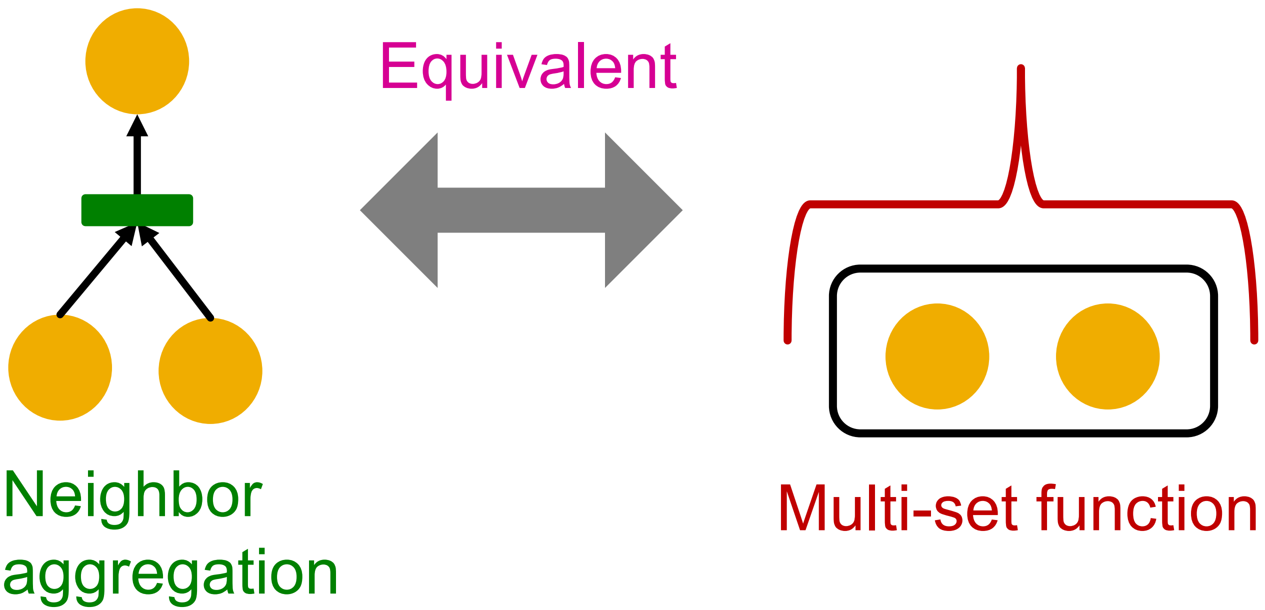
CS224W: Machine Learning with Graphs
Jure Leskovec, Stanford University
http://cs224w.stanford.edu

Expressive Power of GNNs

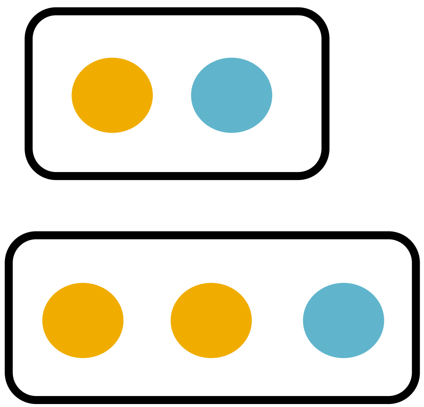
- **Key observation: Expressive power of GNNs can be characterized by that of neighbor aggregation functions they use.**
  - A more expressive aggregation function leads to a more expressive GNN.
  - Injective aggregation function leads to the most expressive GNN.
- **Next:**
  - Theoretically analyze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



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

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

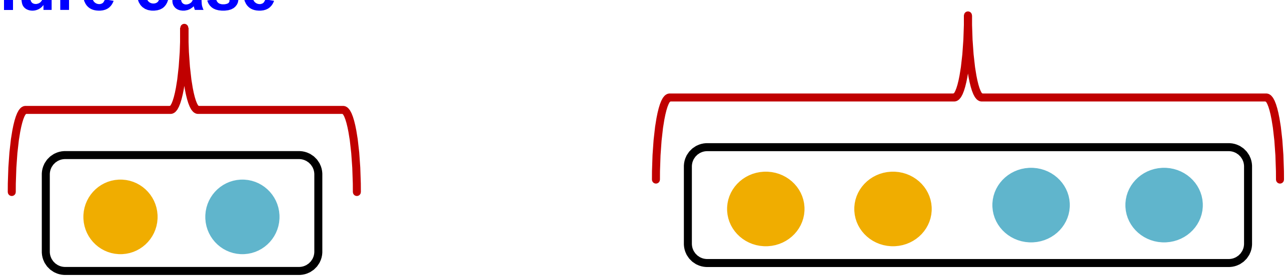
  - **GraphSAGE** (max-pool) [Hamilton et al. NeurIPS 2017]
    - Uses **element-wise** max pooling over neighboring node features

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

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.**

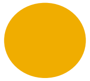
Failure case



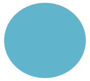
- **Why?**

Neighbor Aggregation

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



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



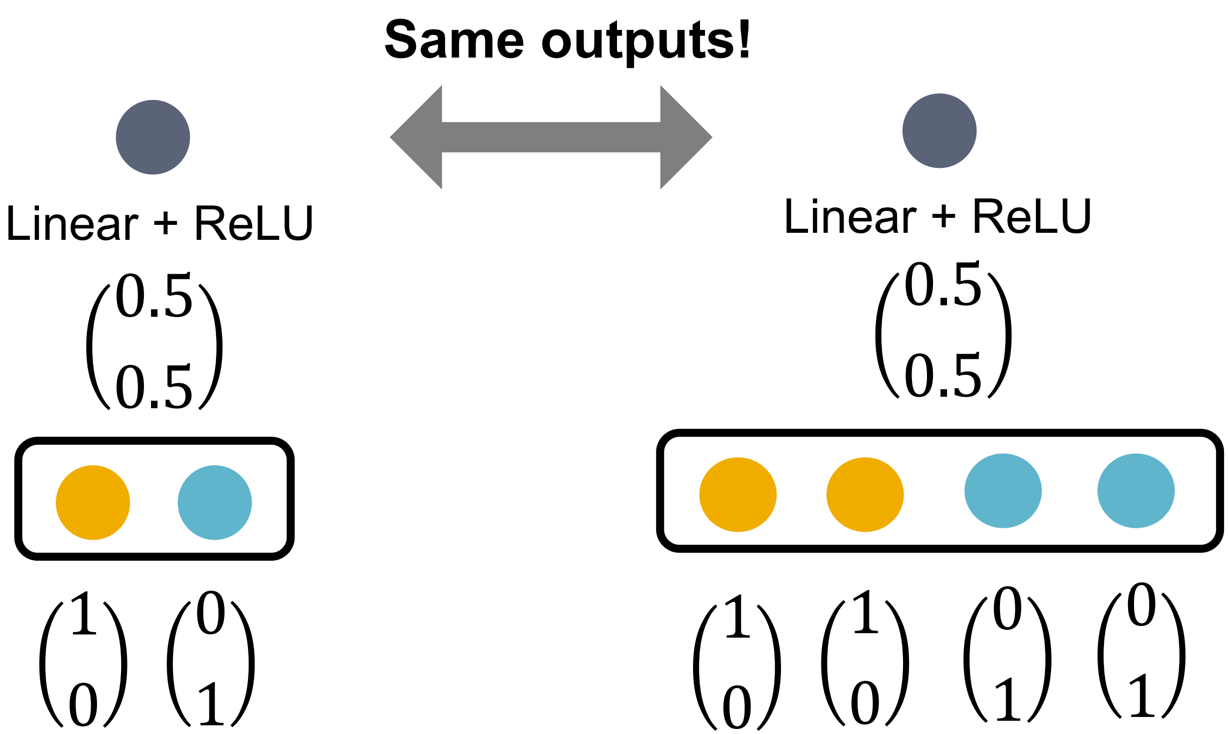
$$= \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

  - This assumption is sufficient to illustrate how GCN fails.

Neighbor Aggregation: Case Study

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

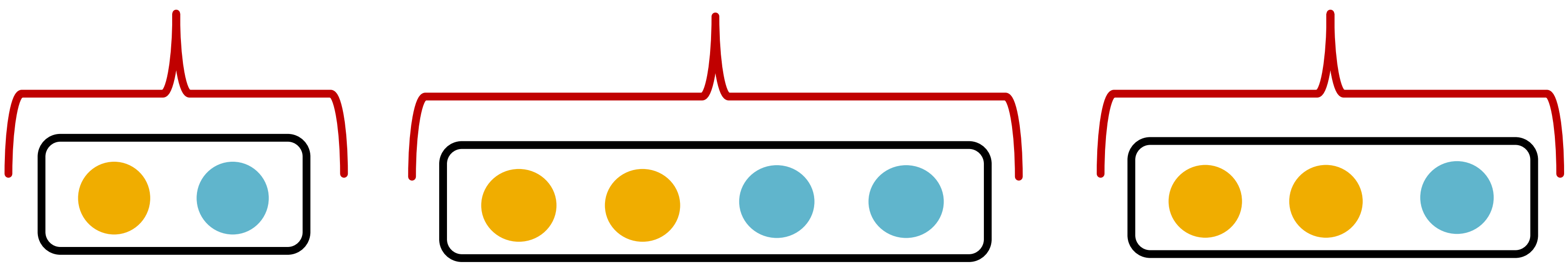
Element-wise-mean-pool



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?**

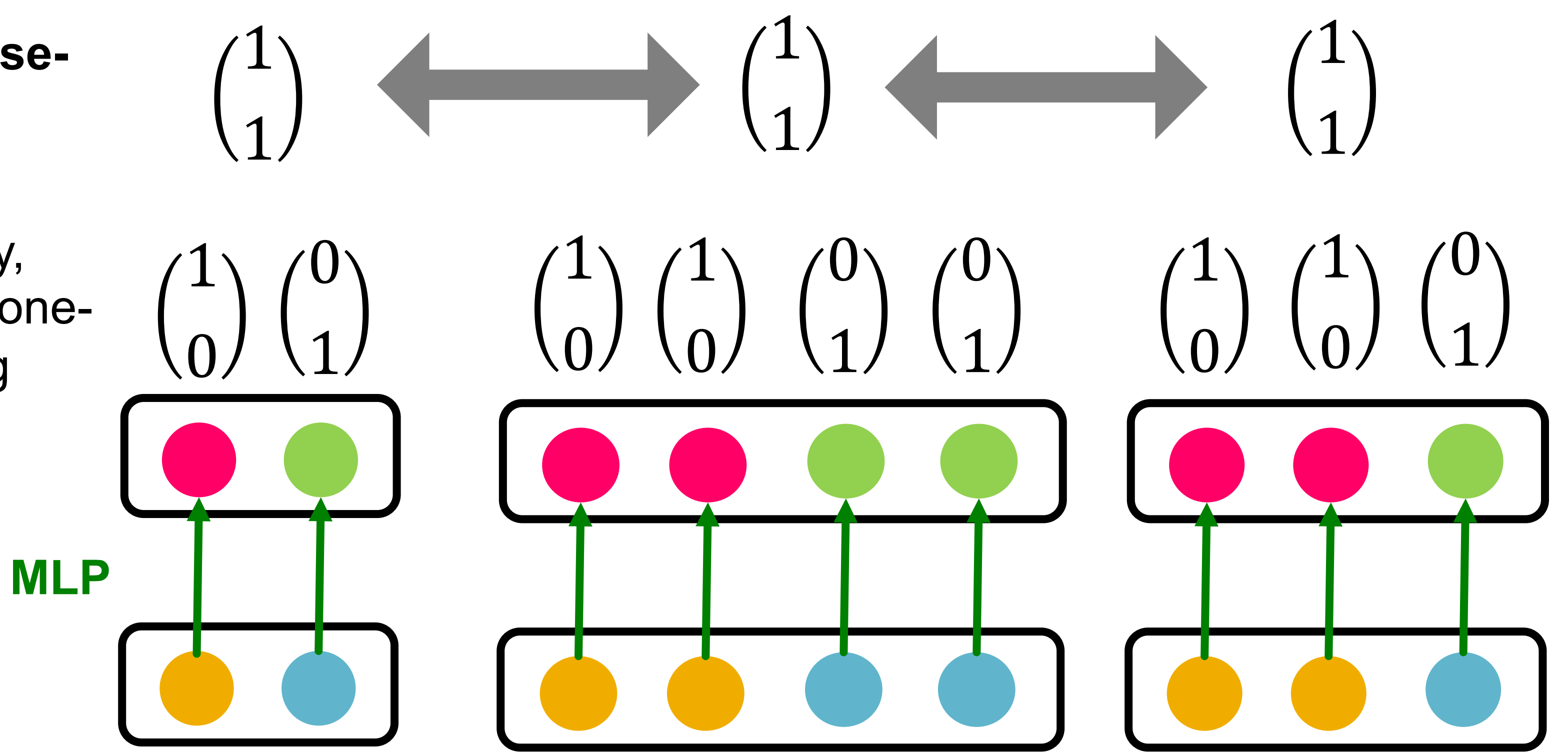
Neighbor Aggregation: Case Study

- **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**.



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:

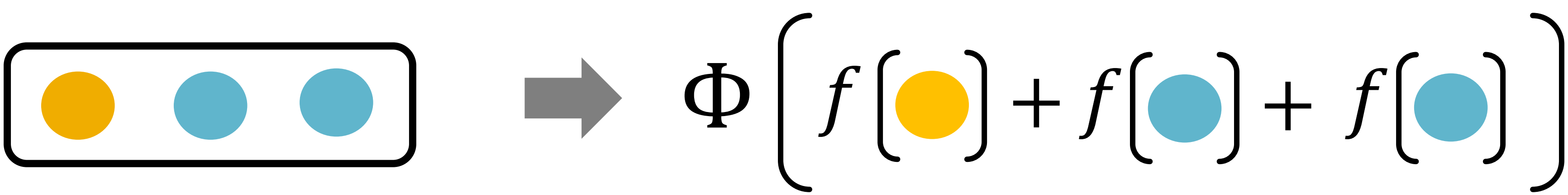
Some non-linear function

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

Some non-linear function

Sum over multi-set

S : multi-set



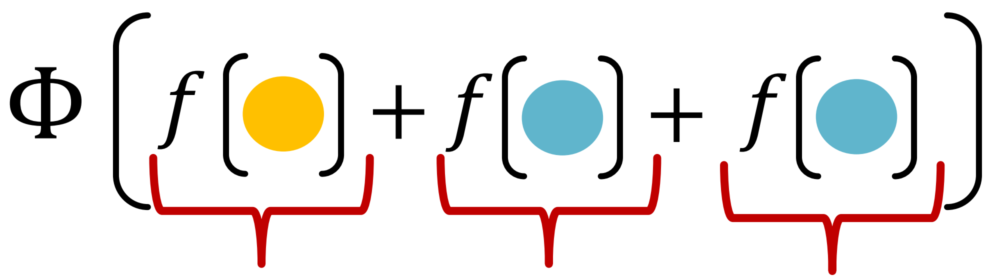
Injective Multi-Set Function

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.

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

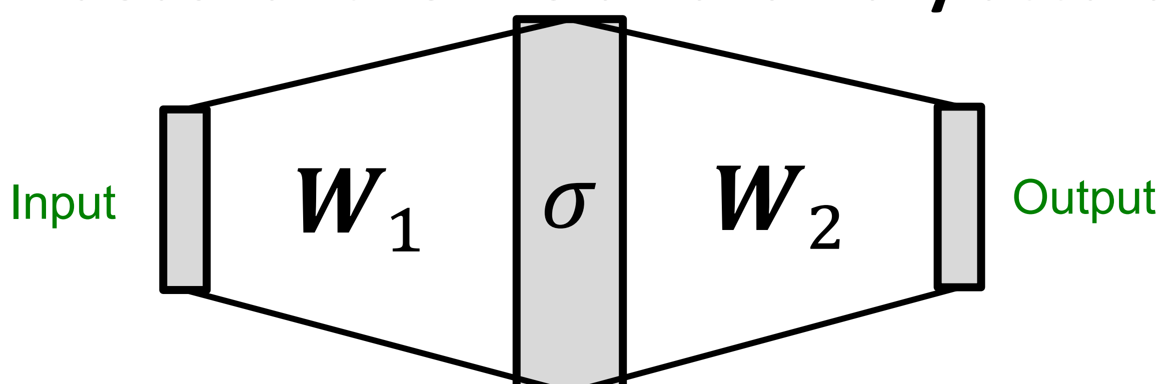
Example:



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 Φ and f in $\Phi\left(\sum_{x \in S} f(x)\right)$?**
- 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!**

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.

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

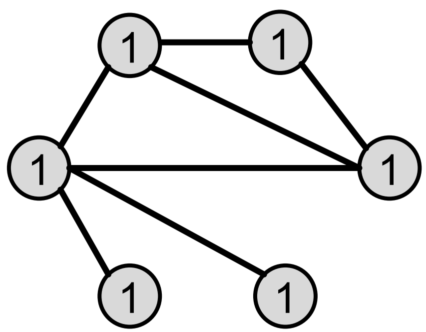
$$\boxed{c^{(k+1)}(v) = \text{HASH}\left(c^{(k)}(v), \left\{c^{(k)}(u)\right\}_{u \in N(v)}\right),}$$

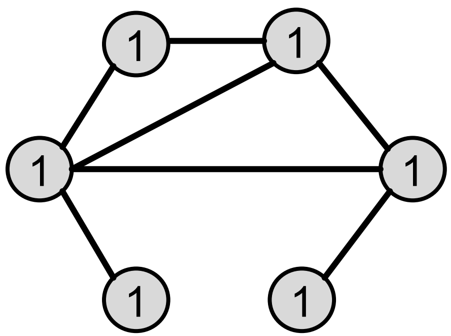
  where HASH maps different inputs to different colors.
  - After K steps of color refinement, $c^{(K)}(v)$ summarizes the structure of K-hop neighborhood

Color Refinement (1)

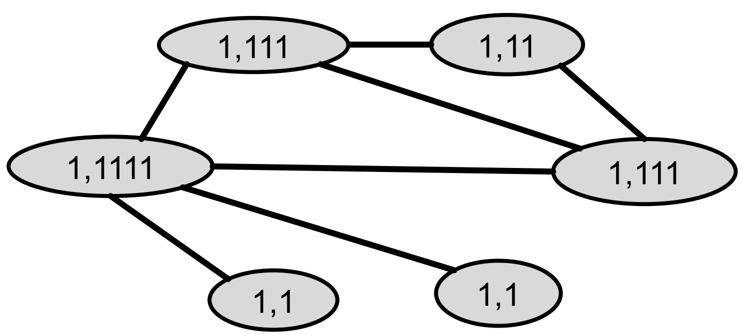
Example of color refinement given two graphs

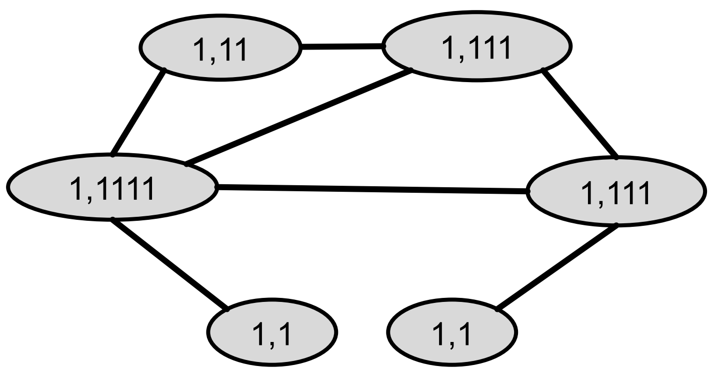
- Assign initial colors





- Aggregate neighboring colors

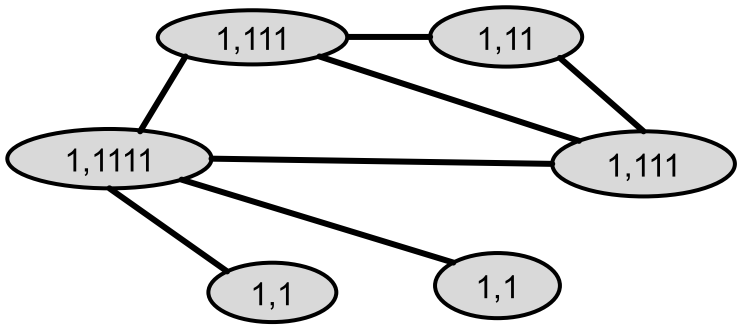


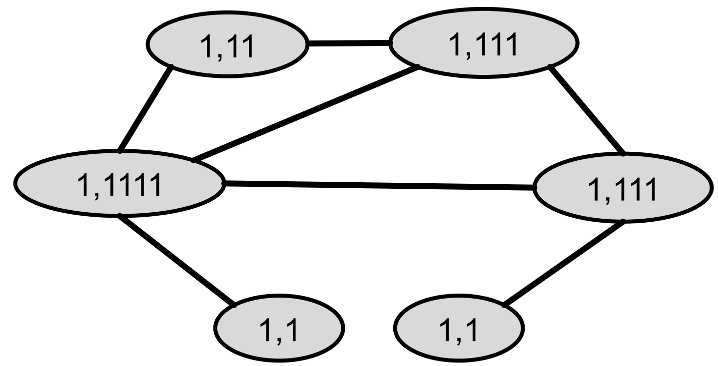


Color Refinement (2)

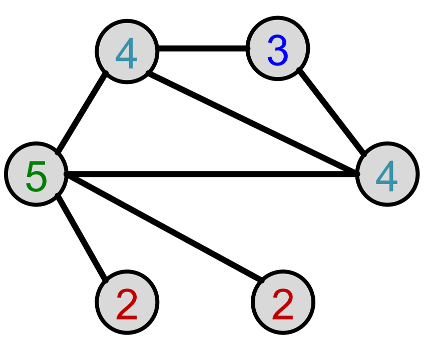
Example of color refinement given two graphs

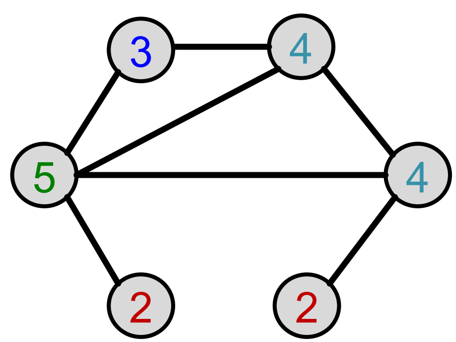
- Aggregated colors:





- **Injectively** HASH the aggregated colors





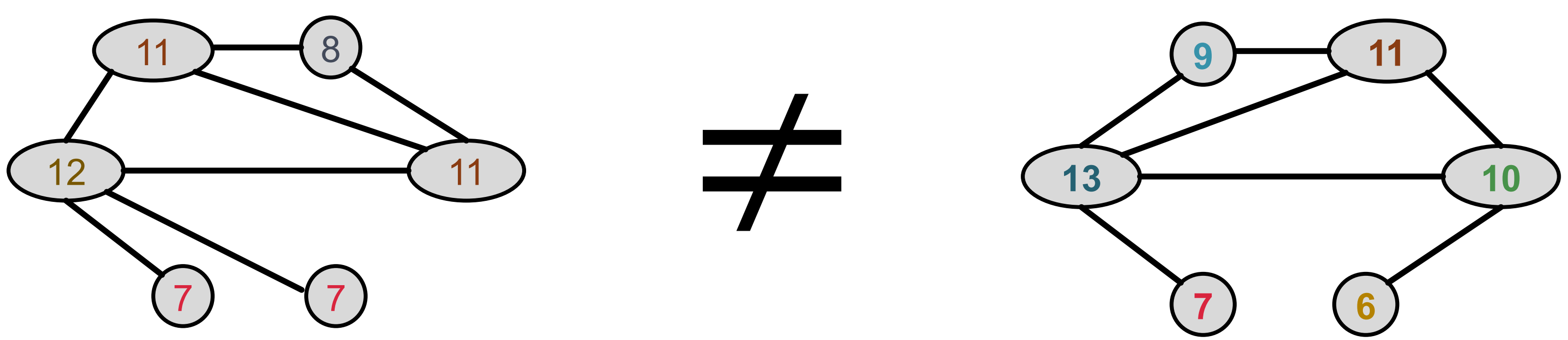
HASH table: **Injective!**

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.**

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

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

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

The Complete GIN Model

Theorem (Xu et al. ICLR 2019)

Any injective function over the tuple

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

can be modeled as

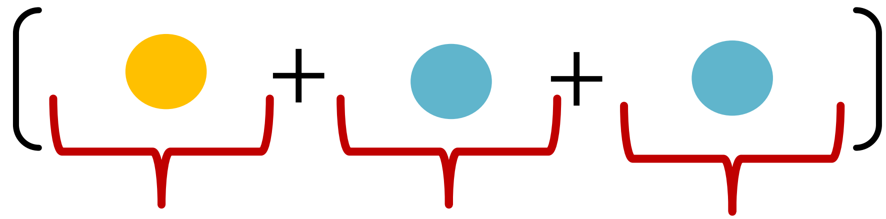
$$\mathrm{MLP}_{\Phi}\left((1+\epsilon) \cdot \mathrm{MLP}_{f}\left(c^{(k)}(v)\right) + \sum_{u \in N(v)} \mathrm{MLP}_{f}\left(c^{(k)}(u)\right)\right)$$

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: Φ



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

- We only need Φ to ensure the injectivity.

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

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

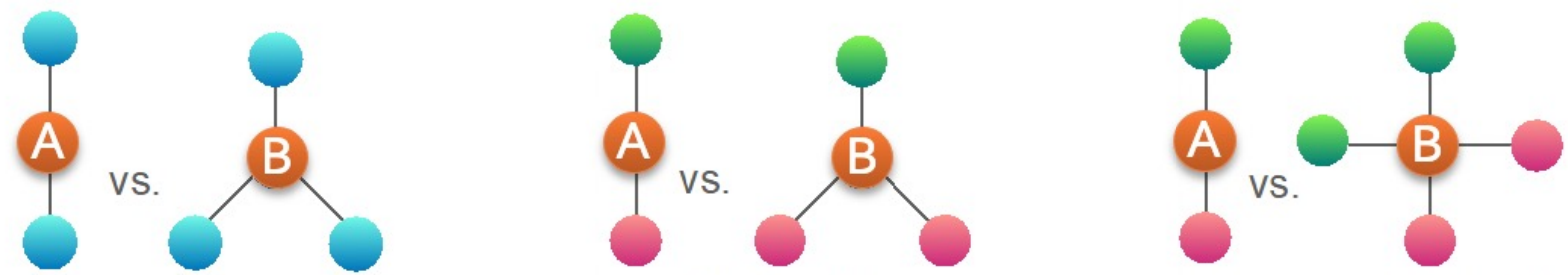
- **Advantages of GIN over the WL graph kernel are:**
  - Node embeddings are **low-dimensional**; hence, they can capture the fine-grained similarity of different nodes.
  - Parameters of the update function can be **learned for the downstream tasks.**

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!

Discussion: The Power of Pooling

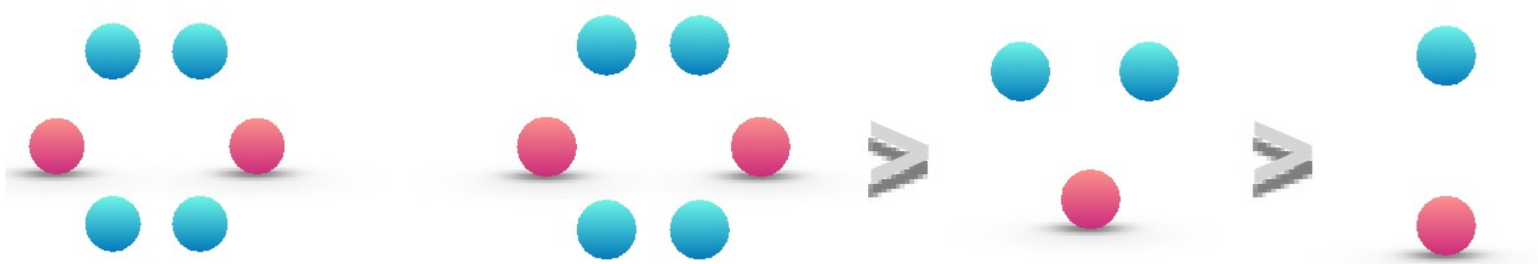
Failure cases for mean and max pooling:



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

Colors represent feature values

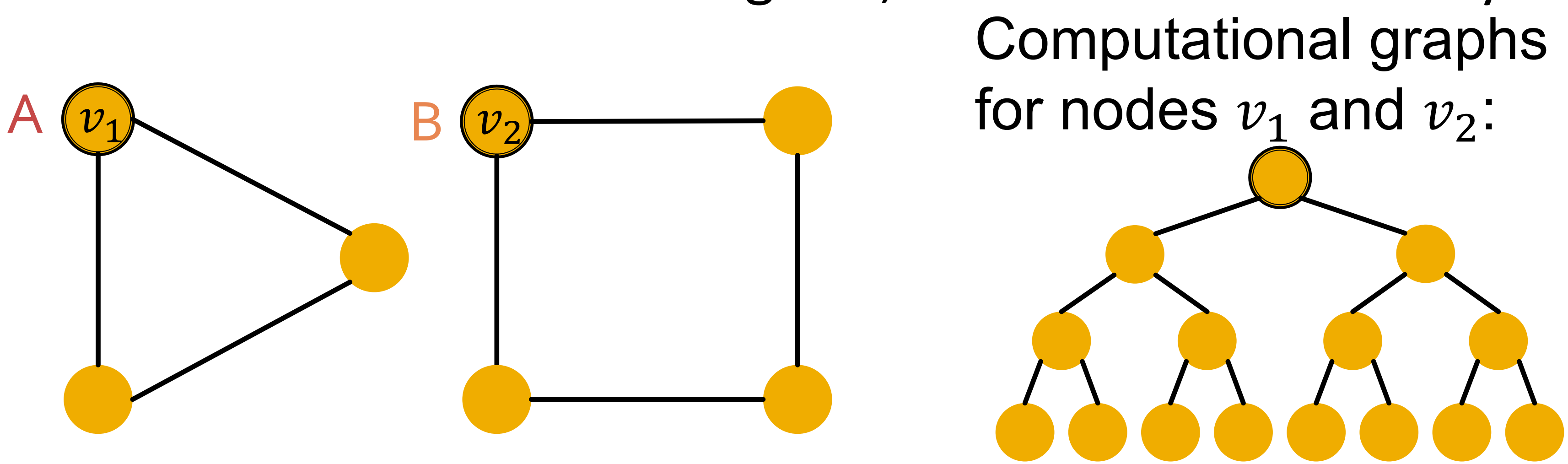
Ranking by discriminative power:



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.



  - GNNs' expressive power **can be improved** to resolve the above problem. [You et al. AAAI 2021, Li et al. NeurIPS 2020]
    - Stay tuned for **Lectures 13 and 14: Advanced Topics in GNNs, Graph Transformers**

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!

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:**
    - 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)