Graph Neural Networks: introduction

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Jagiellonian University

Inspirations

Machine Learning with Graphs course from Stanford: webpage

Geometric Deep Learning: The Erlangen Programme of ML: video

Group Equivariant Deep Learning: yt series

Machine Learning in Drug Discovery: UJ lectures and labs

Table of Content

What are graphs?

Definition of a graph

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$$G = (V, E)$$

$$V = \{v_i : i \in \{1,2,\ldots,N\}\}$$

$$E \subseteq \{(v_i, v_j) : \ v_i, v_j \in V\}$$

Many Types of Graphs

Image credit: Medium

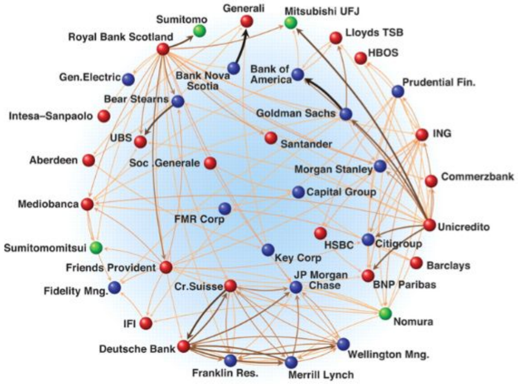


Image credit: Science

Image credit: Lumen Learning

Many Types of Graphs

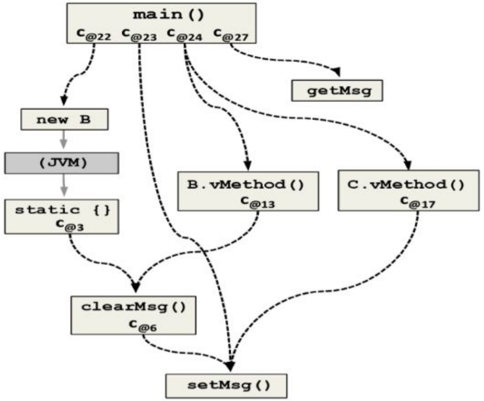


Image credit: ResearchGate

Code Graphs

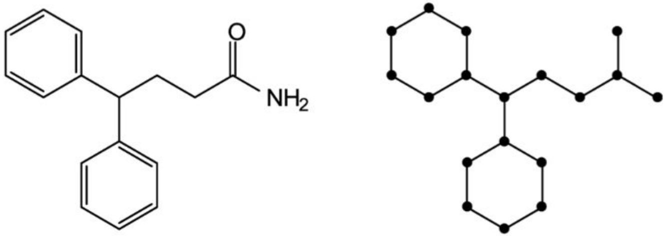


Image credit: MDPI

Molecules

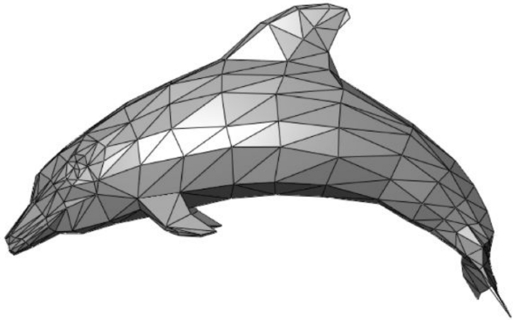
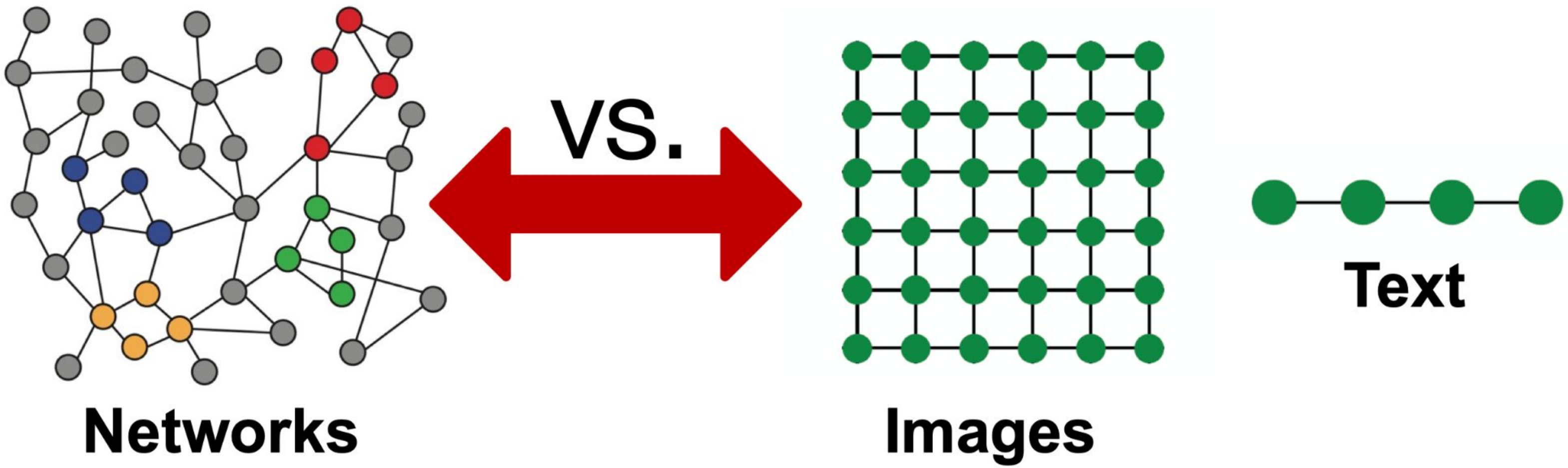


Image credit: Wikipedia

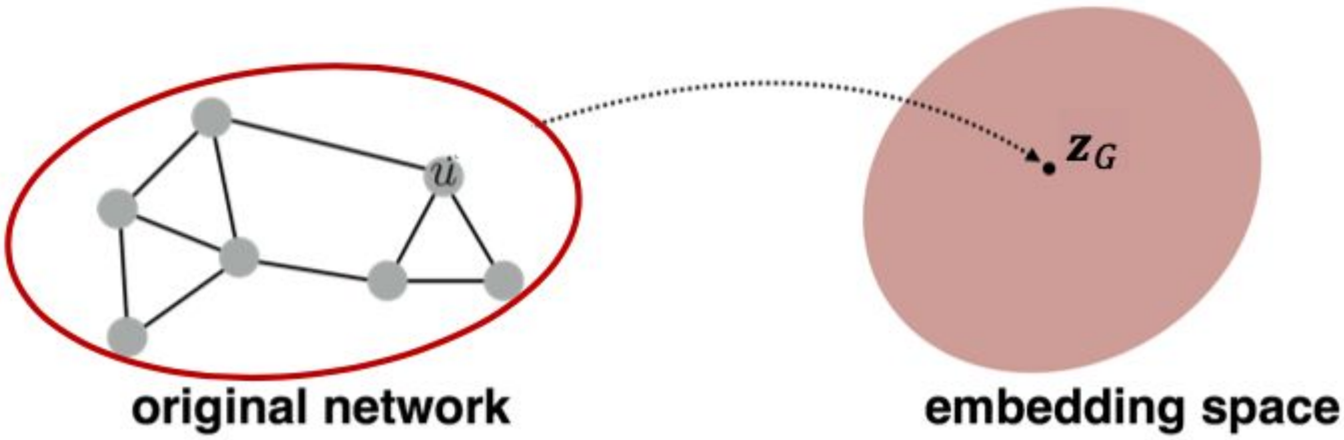
3D Shapes

Graphs are complex!

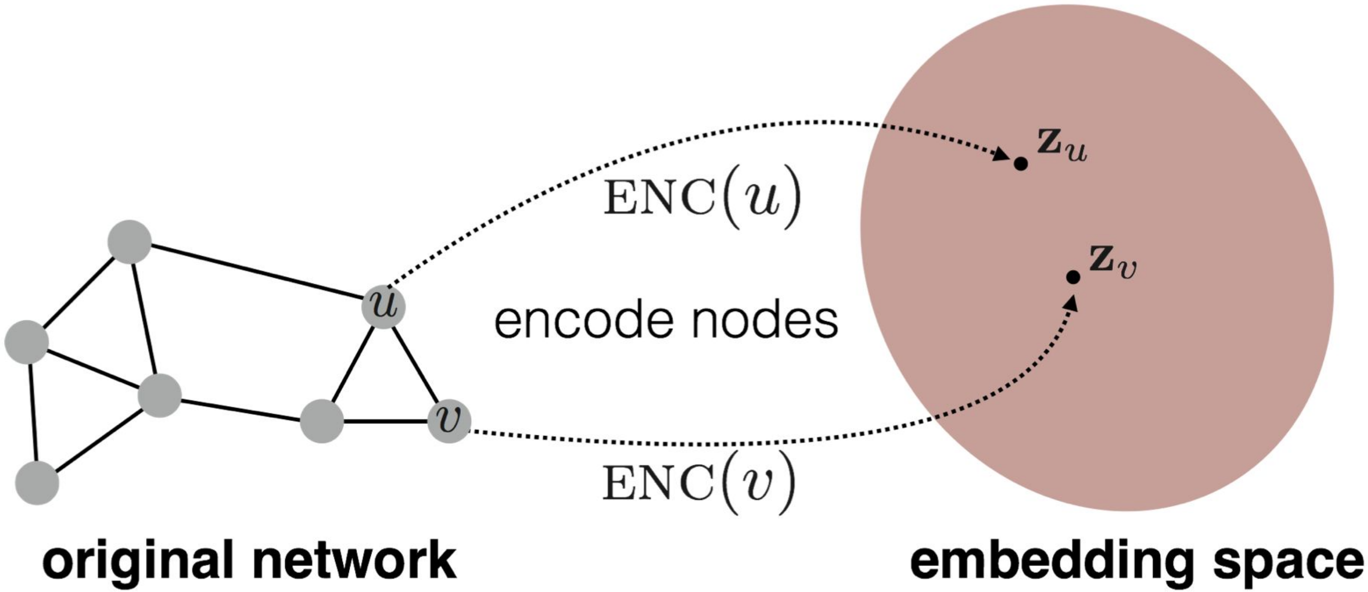


How to embed a graph?

Embedding Space



Embedding Space



Node Encodings

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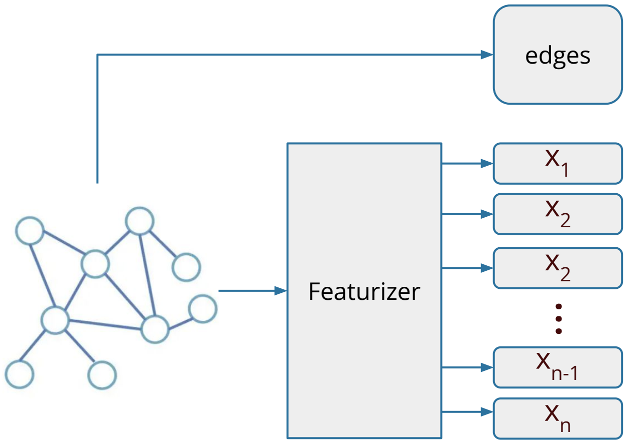

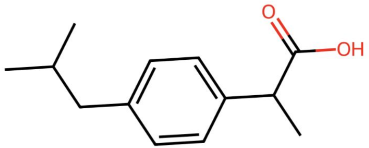

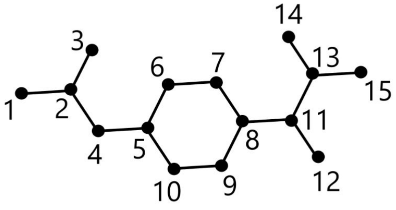

$$X = \begin{array}{cc} & \begin{array}{cccccc} \mathrm{C} & \mathrm{O} & \mathrm{N} & \#\mathrm{H} & \delta & q^* \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ \\ 13 \\ 14 \\ 15 \end{array} & \begin{bmatrix} 1 & 0 & 0 & 3 & 1 & 0 \\ 1 & 0 & 0 & 1 & 3 & 0 \\ 1 & 0 & 0 & 3 & 1 & 0 \\ 1 & 0 & 0 & 2 & 2 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & 3 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \end{bmatrix} \end{array}$$

$$A = \begin{array}{cc} & \begin{array}{cccccccc} 1 & 2 & 3 & 4 & & 13 & 14 & 15 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ \\ 13 \\ 14 \\ 15 \end{array} & \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1 & 0 & 0 \end{bmatrix} \end{array}$$

Graph Neural Network

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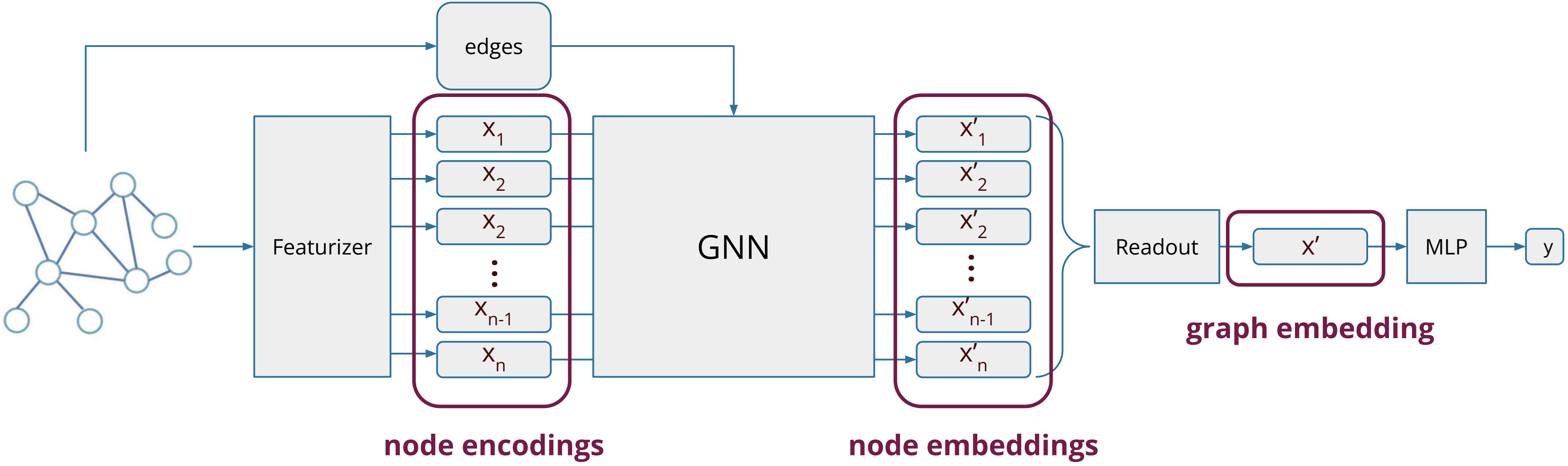
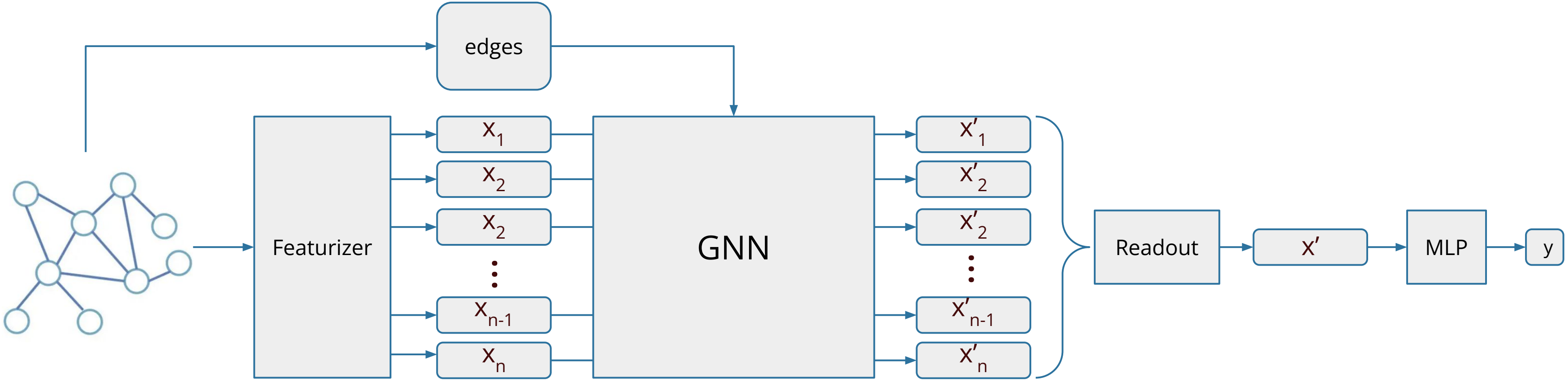


How shouldn’t GNN look like?



How should GNN look like?

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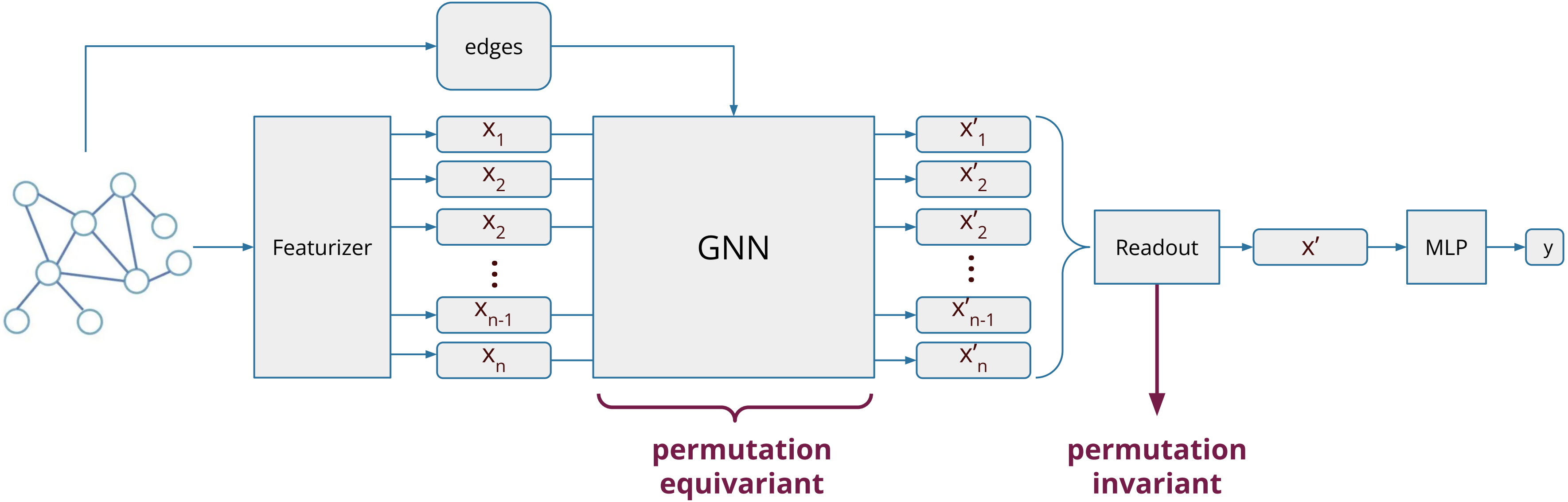
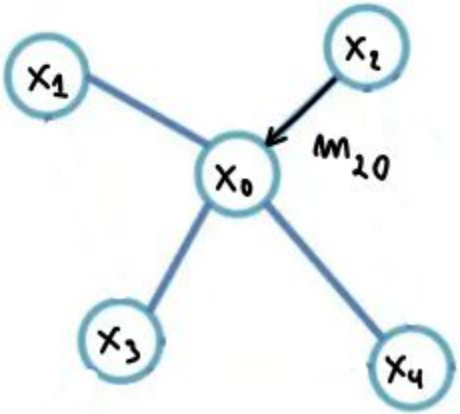


1. GNN should be permutation-equivariant.
2. GNN should deal with the graph structure given by edges.

Message Passing Neural Networks

Message Passing

Message Passing



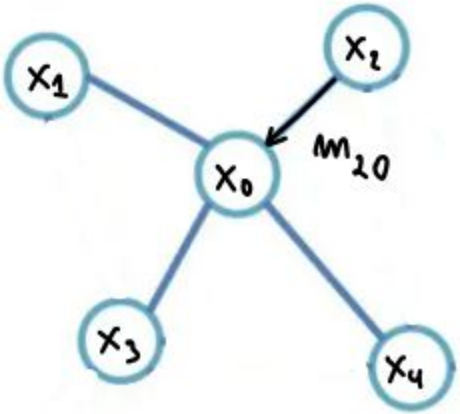
General:

$$m_{ji} = \psi(x_j, x_i)$$

Example:

$$m_{ji} = Wx_j$$

Message Passing



General:

$$m_{ji} = \psi(x_j, x_i)$$

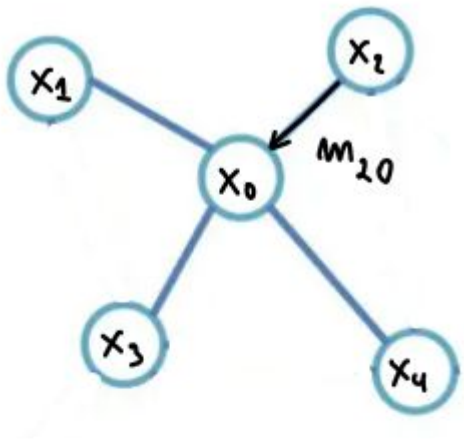
$$m_i = \square_{j \in N(i)} m_{ji}$$

Example:

$$m_{ji} = W x_j$$

$$m_i = \sum_{j \in N(i)} m_{ji}$$

Message Passing



General:

$$m_{ji} = \psi(x_j, x_i)$$

$$m_i = \square_{j \in N(i)} m_{ji}$$

$$x_i' = \rho(x_i, m_i)$$

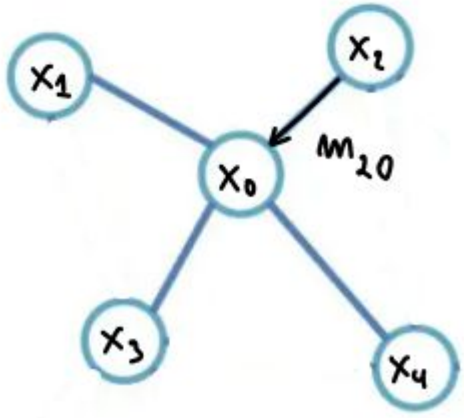
Example:

$$m_{ji} = W x_j$$

$$m_i = \sum_{j \in N(i)} m_{ji}$$

$$x_i' = W_1 x_i + W_2 m_i$$

Message Passing



General:

$$m_{ji} = \psi(x_j, x_i)$$

$$m_i = \square_{j \in N(i)} m_{ji}$$

$$x_i' = \rho(x_i, m_i)$$

$$x_i' = \rho(x_i, \square_{j \in N(i)} \psi(x_j, x_i))$$

Example:

$$m_{ji} = W x_j$$

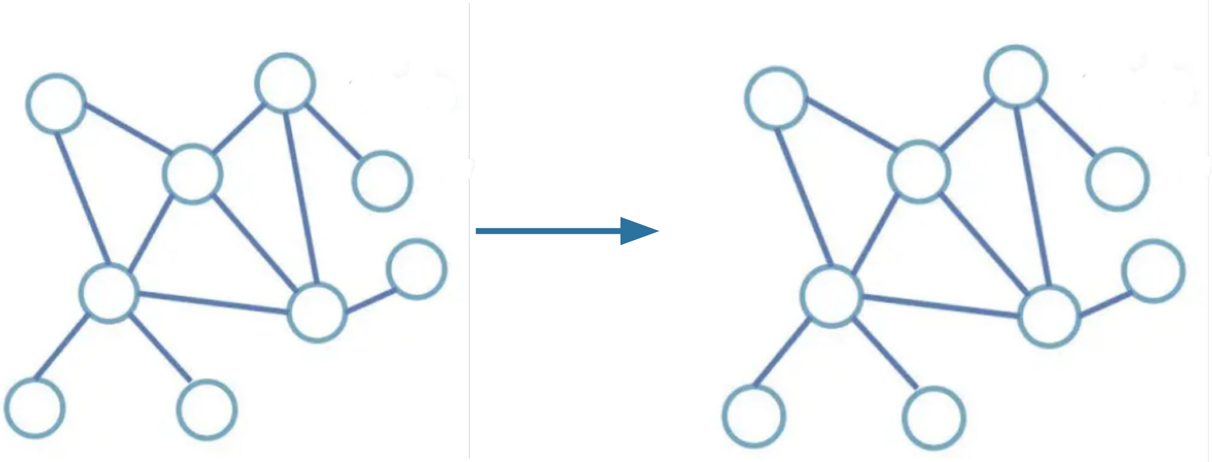
$$m_i = \sum_{j \in N(i)} m_{ji}$$

$$x_i' = W_1 x_i + W_2 m_i$$

$$x_i' = W_1 x_i + W_2 \sum_{j \in N(i)} W_3 x_j$$

Message Passing

Information Propagation

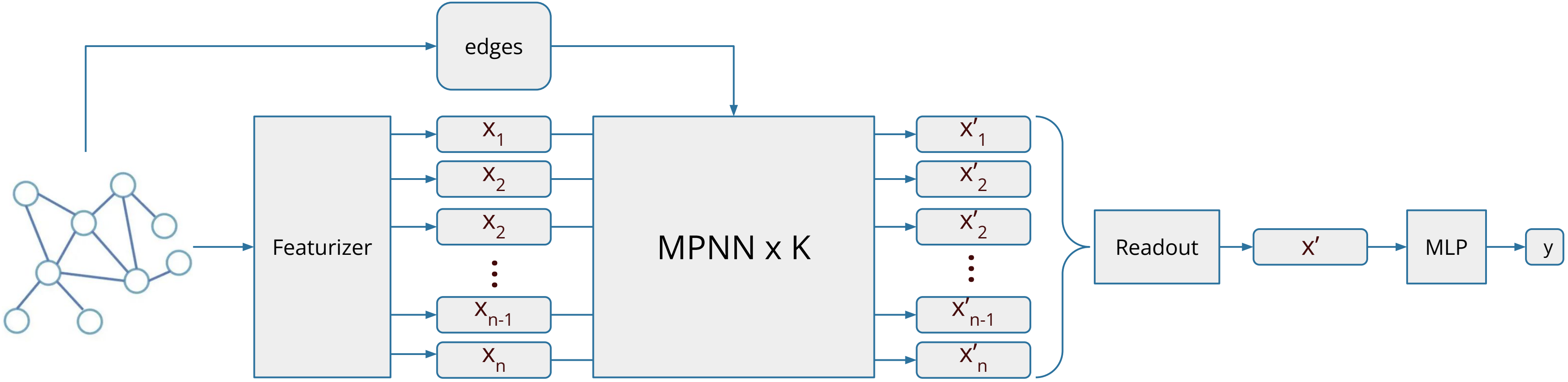


$(x_1^t, x_2^t, \ldots, x_n^t)$ $\quad$ $(x_1^{t+1}, x_2^{t+1}, \ldots, x_n^{t+1})$

$$x_i^{t+1} = \rho(x_i^t, \square_{j \in N(i)} \psi(x_j^t, x_i^t))$$

Message Passing

Is it a proper GNN?



1. MPNN is permutation-equivariant.
2. MPNN deals with the graph structure given by edges.

Message Passing

Examples

GIN:

$$\mathbf{x}'_i = h_{\mathbf{\Theta}}\left((1+\epsilon)\cdot\mathbf{x}_i + \sum_{j\in\mathcal{N}(i)}\mathbf{x}_j\right)$$

GCN:

$$\mathbf{x}'_i = \mathbf{\Theta}^\top \sum_{j\in\mathcal{N}(i)\cup\{i\}} \frac{e_{j,i}}{\sqrt{\hat{d}_j\hat{d}_i}}\mathbf{x}_j$$

GraphSAGE:

$$\mathbf{x}'_i = \mathbf{W}_1\mathbf{x}_i + \mathbf{W}_2\cdot\mathrm{mean}_{j\in\mathcal{N}(i)}\mathbf{x}_j$$

GAT:

$$\mathbf{x}'_i = \alpha_{i,i}\mathbf{\Theta}_s\mathbf{x}_i + \sum_{j\in\mathcal{N}(i)}\alpha_{i,j}\mathbf{\Theta}_t\mathbf{x}_j,$$

Message Passing

Issues

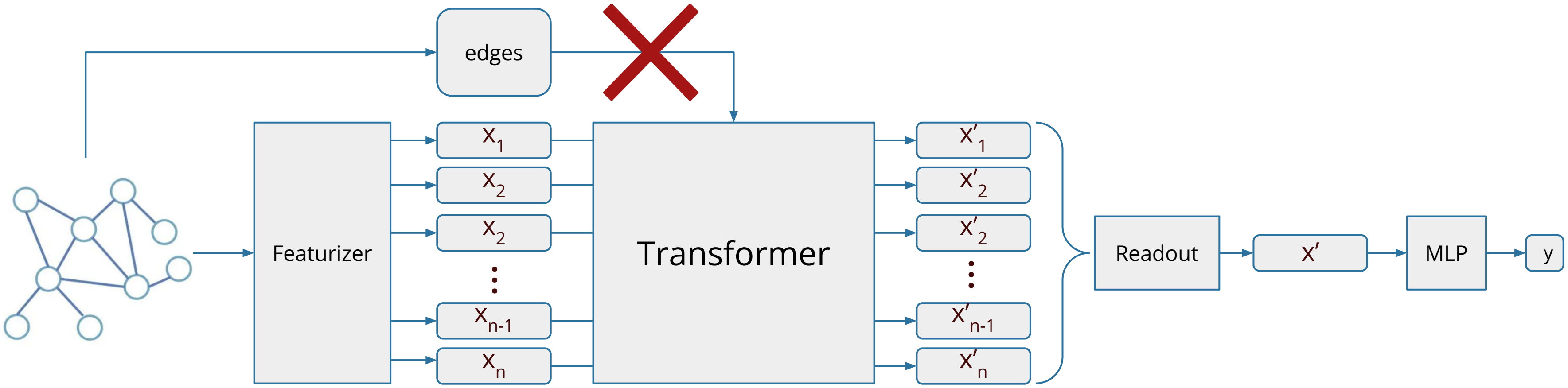
What are the issues?

- Long-range dependencies.
- Oversquashing
- Oversmoothing
- Expressivity: some graphs cannot be differentiated with MPNN!

Transformers as GNNs

Transformers

Is it a proper GNN?

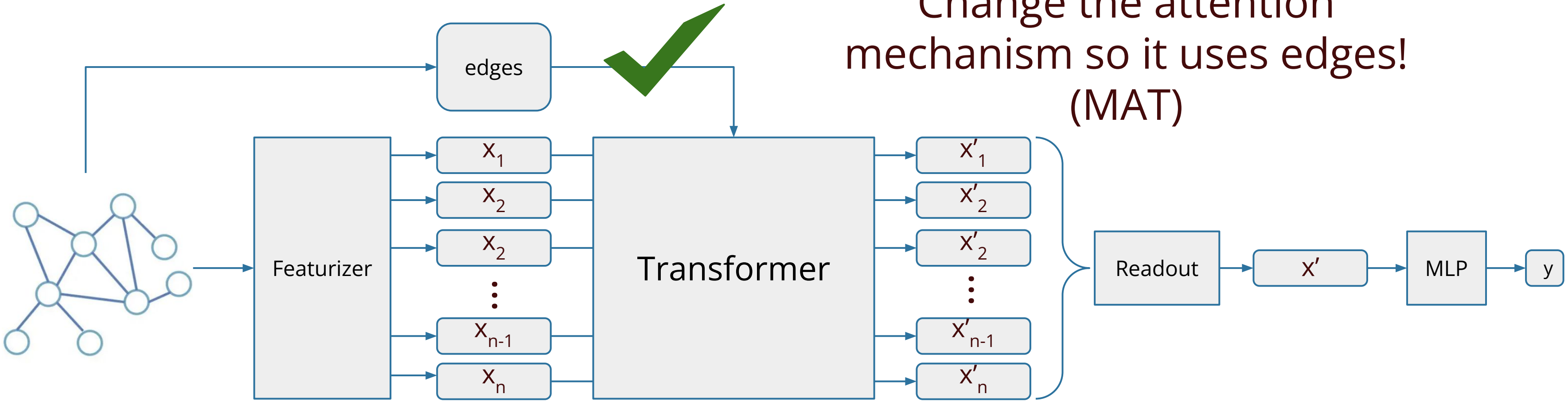


1. Transformer is permutation-equivariant.
2. Transformer cannot deal with the graph structure given by edges by default :<

Transformers

Is it a proper GNN?

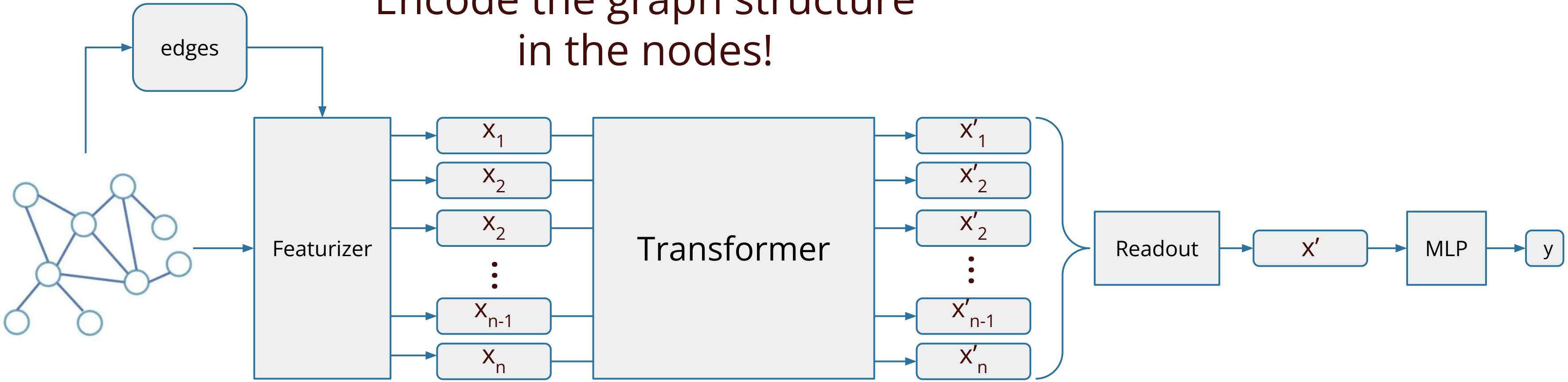
Change the attention
mechanism so it uses edges!
(MAT)



Transformers

Is it a proper GNN?

Encode the graph structure
in the nodes!



1. It can be done with structural/positional encodings (e.g. Random Walk).
2. Or it can be than with MPNN! (GraphGPS)

Transformers

Issues

Transformers deal with long-range dependencies and oversquashing.

Expressivity of Message Passing

Can MPNN distinguish all graphs?

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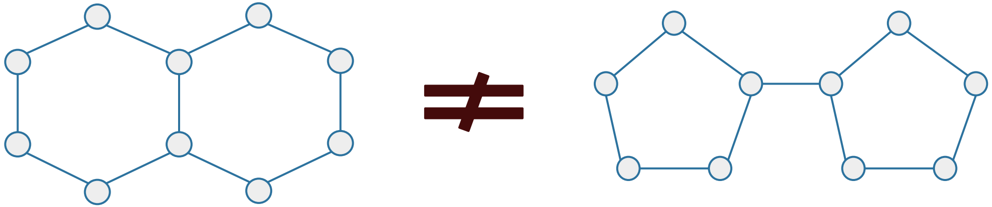
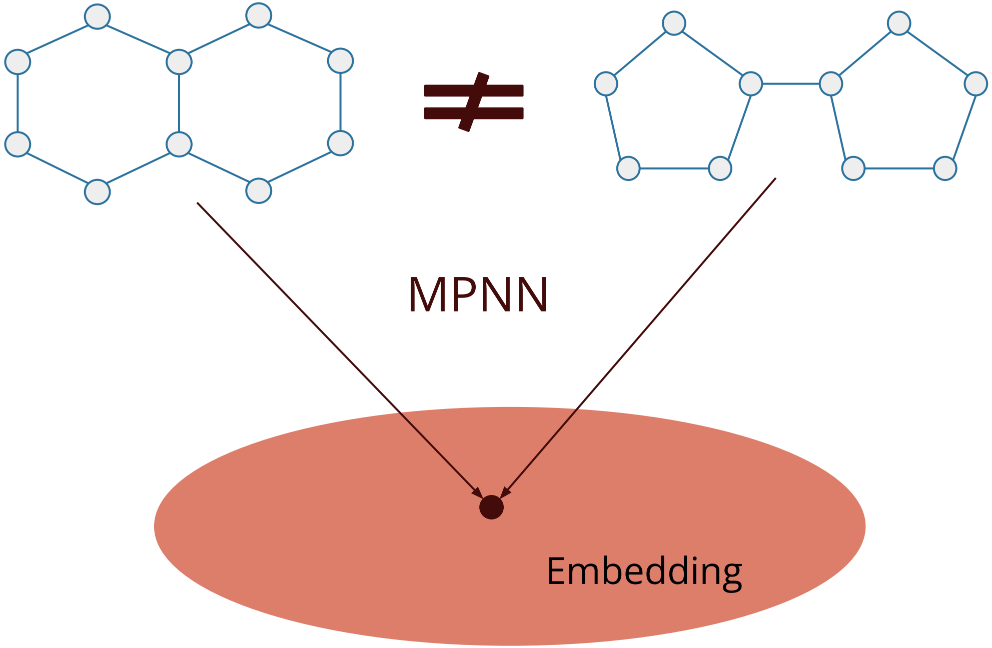


MPNN cannot distinguish all graphs!



The most powerful MPNN

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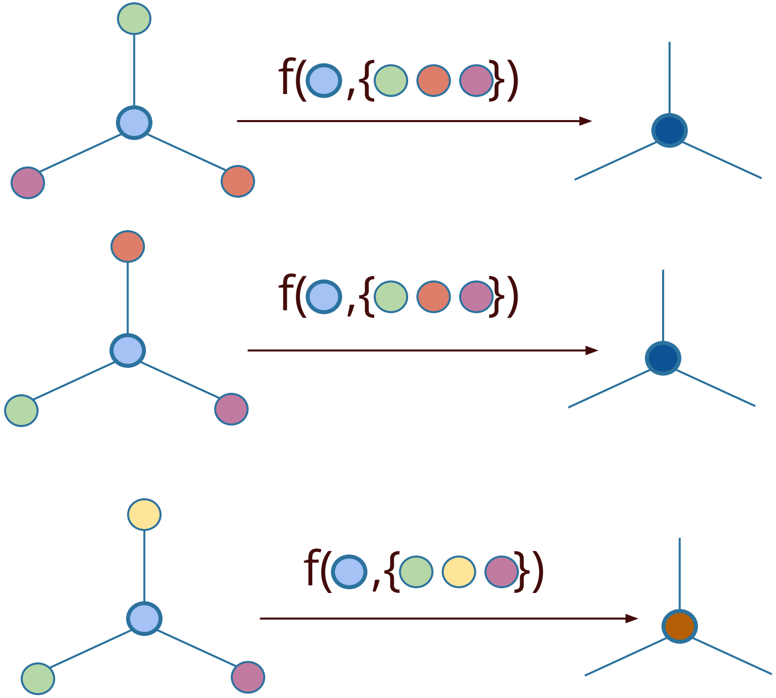
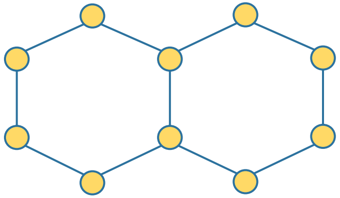
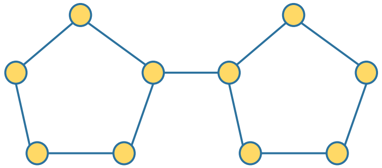
- Let us assume that all nodes in a graph have the same initial encodings.
- Let us denote node embeddings as colors. Different color -> different embedding.
- MPNN can only return different colors for nodes with different neighborhood.
- Our coloring MPNN always returns different color for nodes with different neighbors.

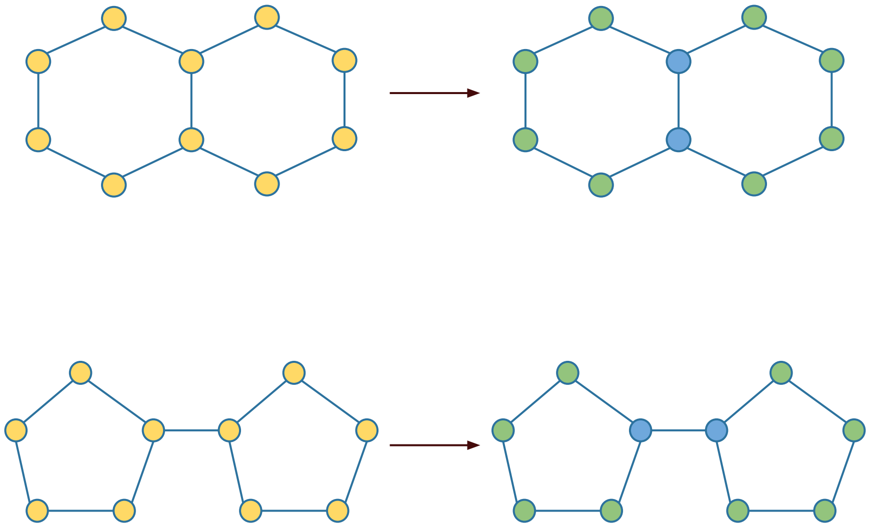


Coloring MPNN

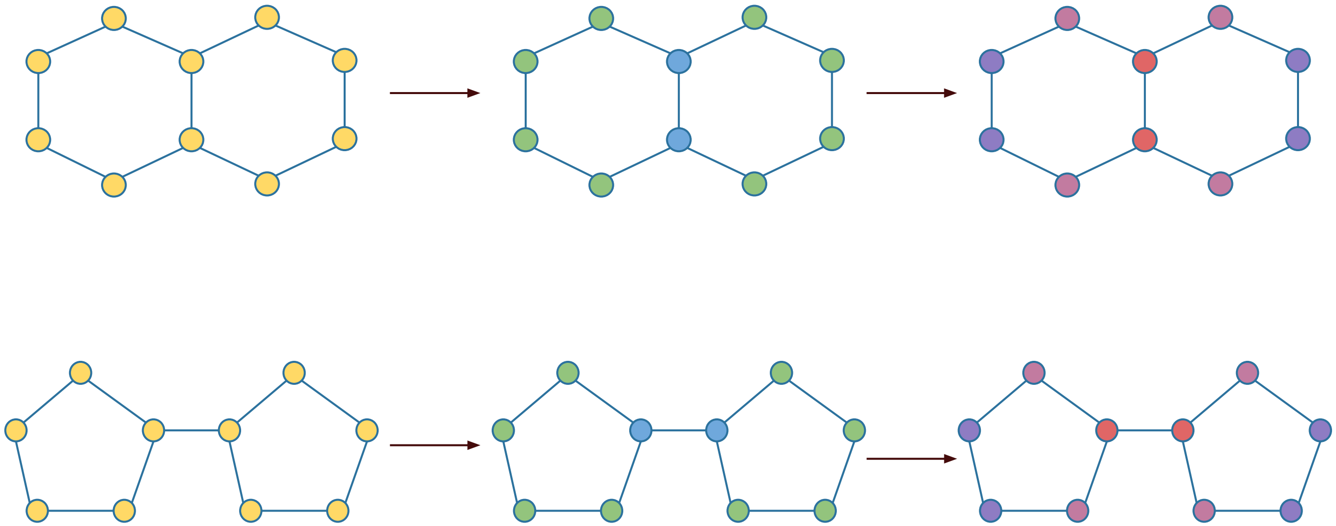




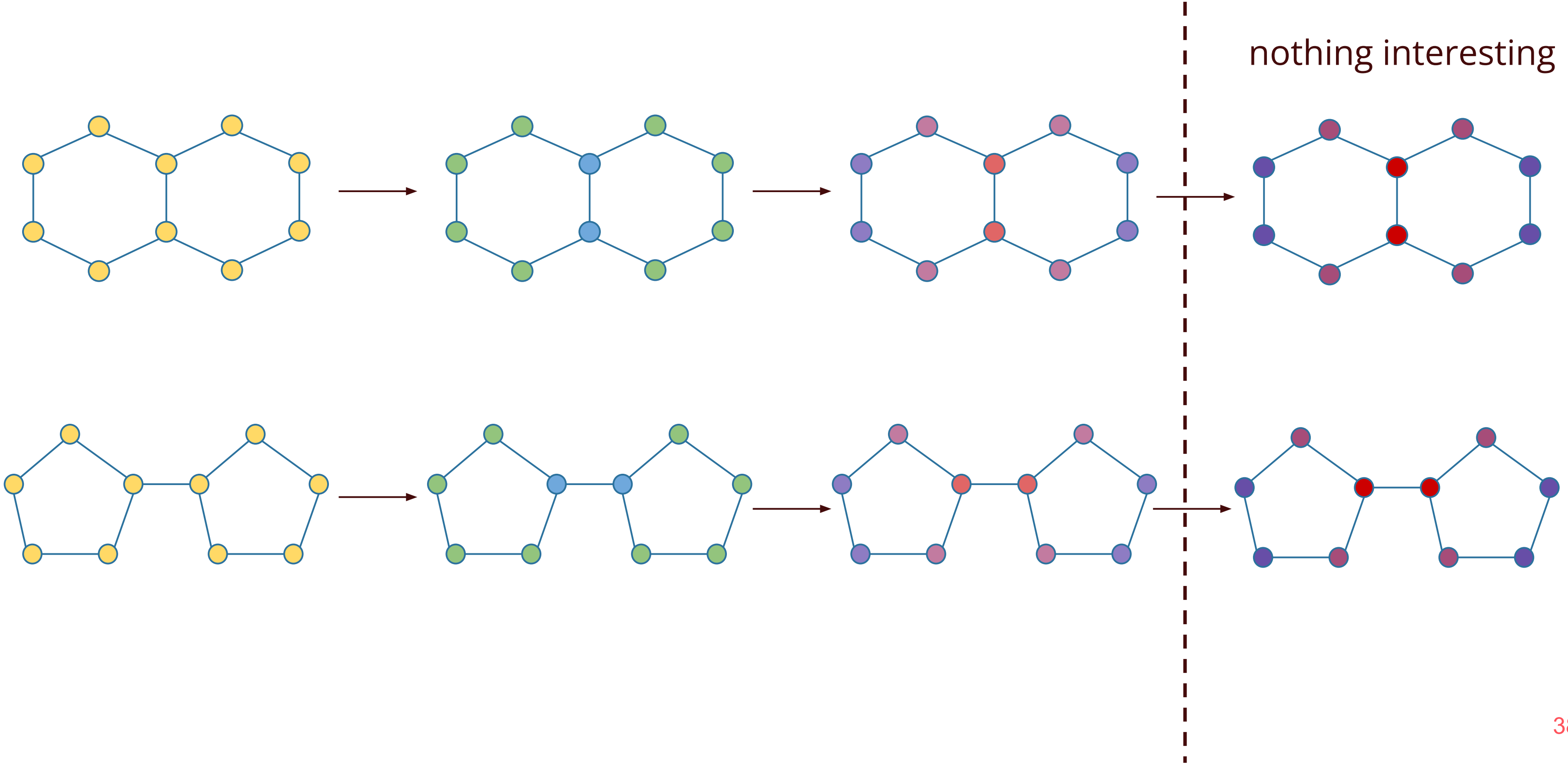
Coloring MPNN



Coloring MPNN

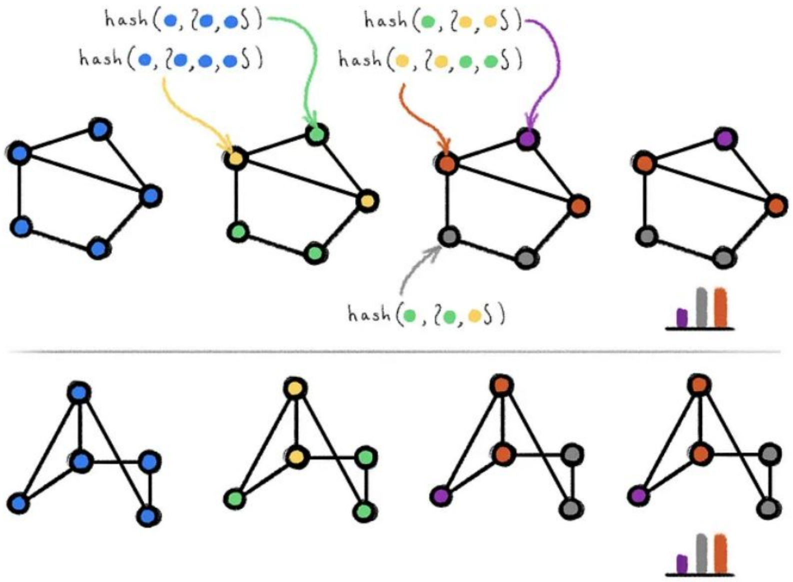


Coloring MPNN



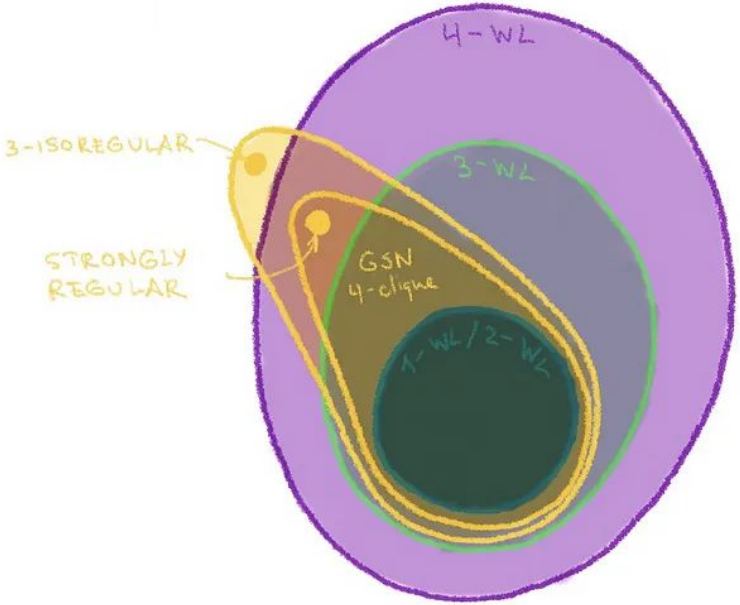
WL test

- Our coloring MPNN works very similar to Weisfeiler-Lehman graph isomorphism test.
- No MPNN is more powerful than WL test.



k-WL test

- We can easily generalize the WL test and obtain k-WL test. (k+1)-WL test is strictly more powerful than k-WL test (for k>1).
- There is k-GNN model which mimics the k-WL test and is O(n^k).
- There is an IGN model as powerful as 3-WL and O(n^2).
- But we can escape the k-WL classification...



Beyond k-WL classifiation

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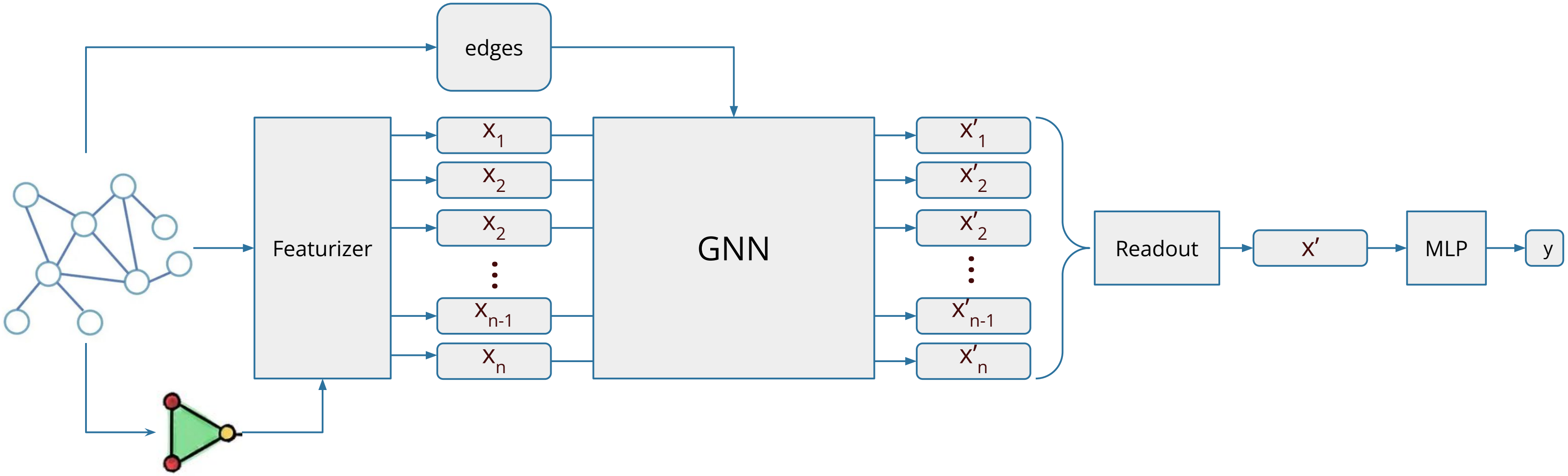
Examples of non-isomorphic graphs that cannot be distinguished by 1-WL but can be distinguished by 3-WL due to its capability of counting triangles.

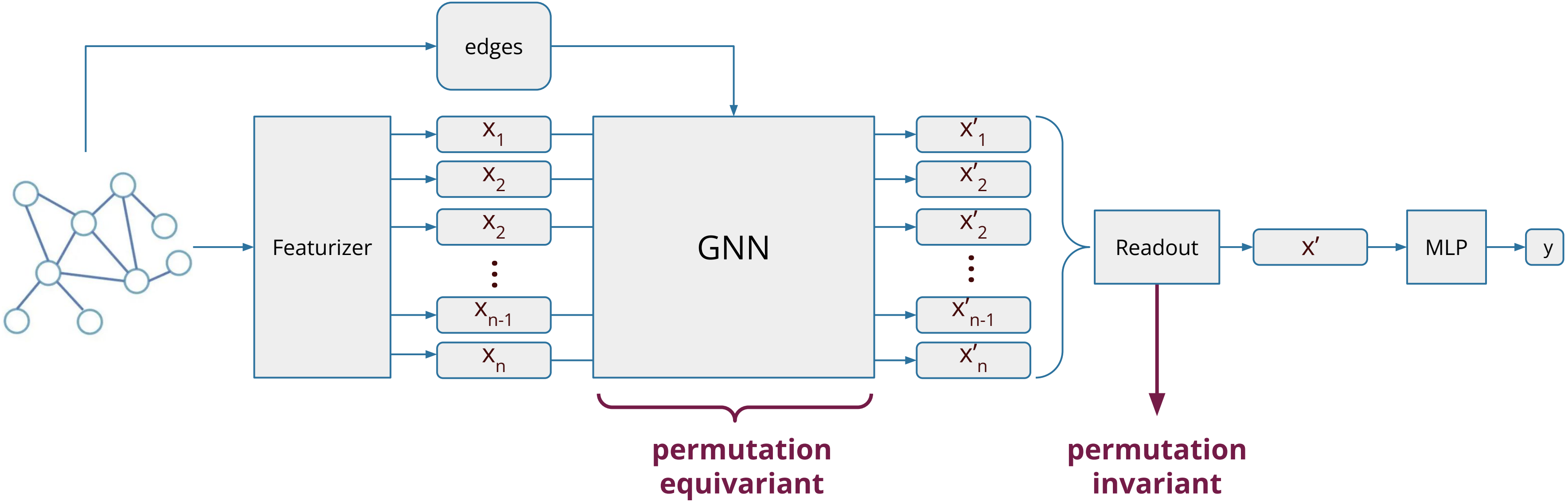
Beyond k-WL classifiation



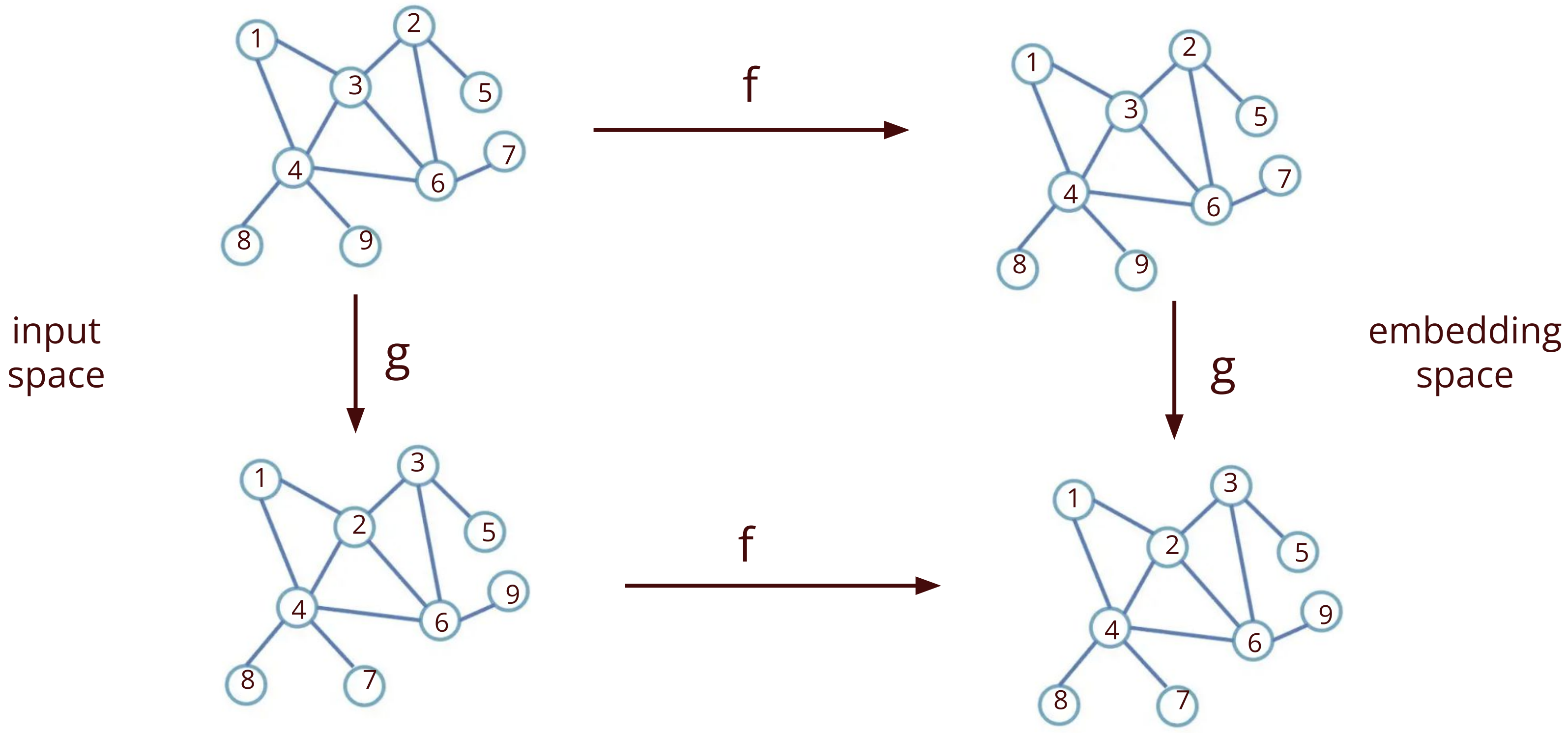
We can simply count triangles and
enrich the node encodings!

Symmetries: Equivariant Deep Learning

Permutation Equivariance

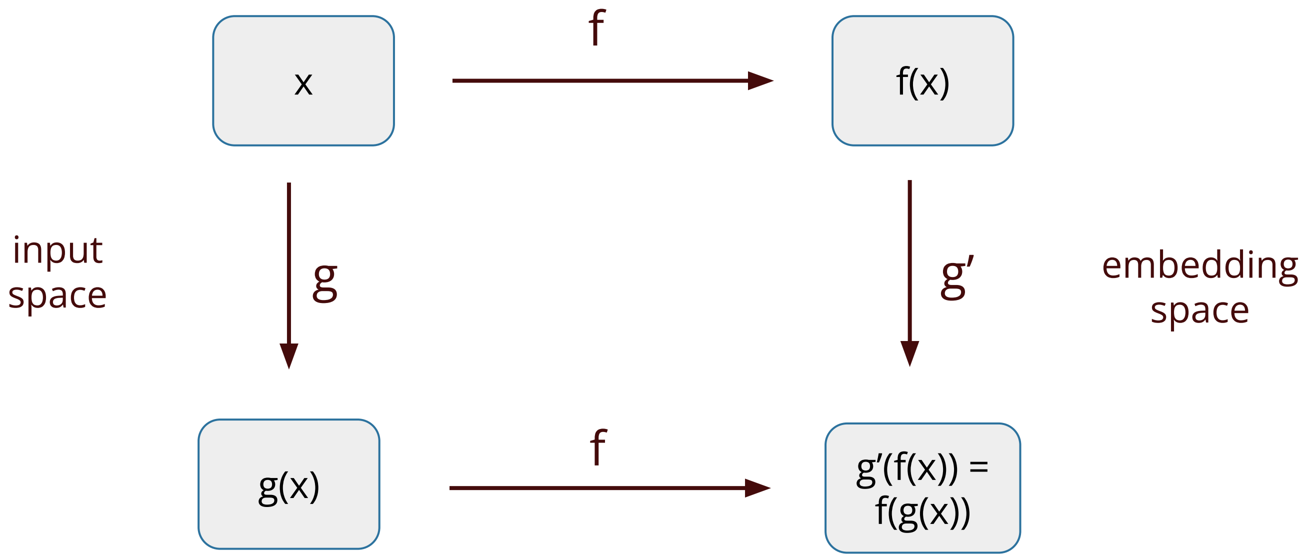


Permutation Equivariance



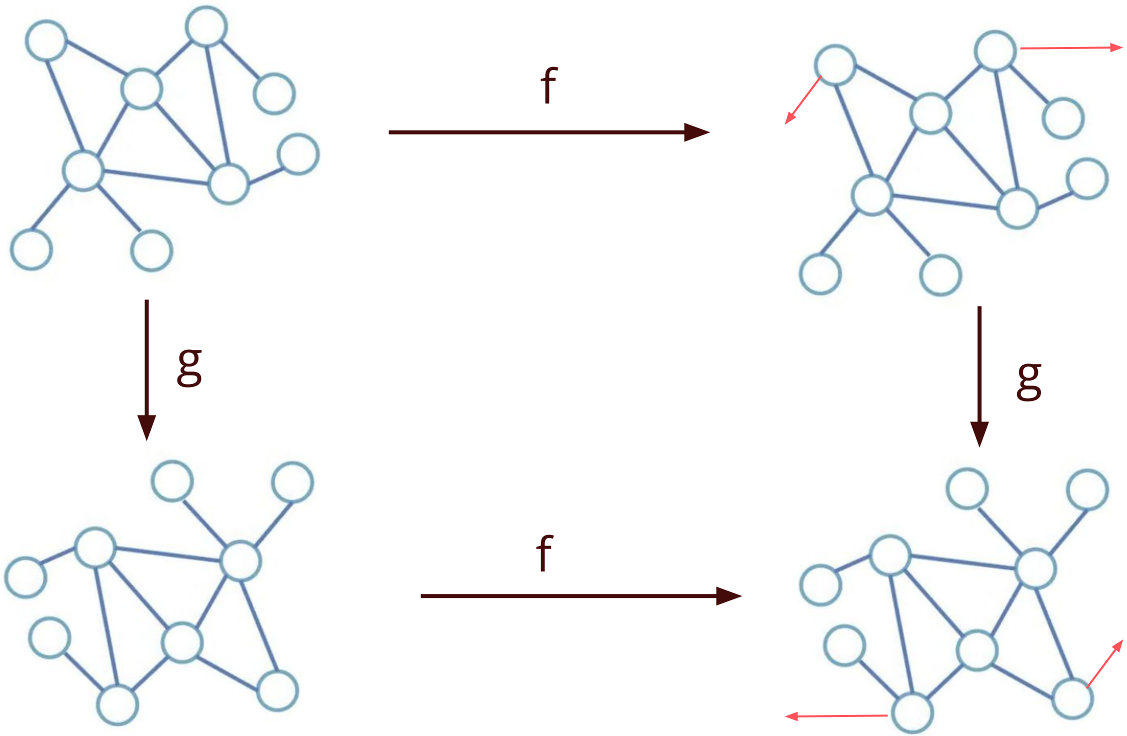
Equivariance

f - G-equivariant function
g - operation from group G defined in input space
g' - operation from group G' defined in embedding space corresponding to G



Rotation Equivariance

input
space



embedding
space

Deep Equivariant Learning

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- Some node-level prediction tasks requires equivariance with respect to e.g. rotations.
- Equivariance can be used to incorporate invariance.
- Deep Equivariant Learning is a fast growing field. It definitely requires its own course.

GNNs are great!

Deep Equivariant Learning

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Machine Learning in Drug Discovery

by Sabina Smusz and Tomasz Danel

Worth reading

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- MPNNs:
  - GAT: Graph Attention Networks
  - GraphSAGE: Inductive Representation Learning on Large Graphs
  - GIN: How Powerful are Graph Neural Networks?
- Transformers:
  - MAT: Molecule Attention Transformer (GMUM)
  - GraphGPS: Recipe for a General, Powerful, Scalable Graph Transformer
  - SAN: Rethinking Graph Transformers with Spectral Attention
- k-WL GNNs:
  - k-GNN: Weisfeiler and Leman go neural: Higher-order graph neural networks

  - IGN: Convergence of Invariant Graph Networks

Worth reading

- Geometric GNNs:
  - SGCN: Spatial Graph Convolutional Networks (GMUM)
  - Geometric Transformer: Geometric Transformer for End-to-End Molecule Properties Prediction
- Equivariant GNNs:
  - EGNN: E(n) Equivariant Graph Neural Networks
  - SE(3)-Transformers: 3D Roto-Translation Equivariant Attention Networks
- Symmetry-breaking GNNs:
  - ChIRo: Learning 3D Representations of Molecular Chirality with Invariance to Bond Rotations
  - ChiENN: Embracing Molecular Chirality with Graph Neural Networks (GMUM)
- Random:
  - Understanding convolution on graphs via energies

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Thanks for your attention!