

Graph Neural Network: Paradigm, Limitation and Future

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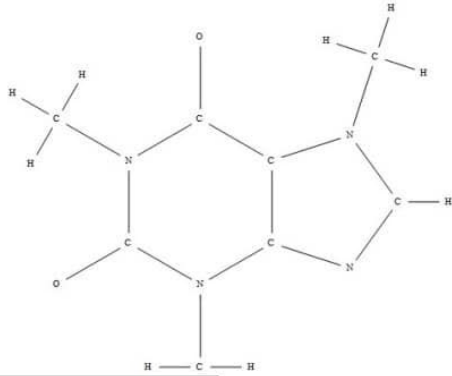
CNN

In Euclidean Space

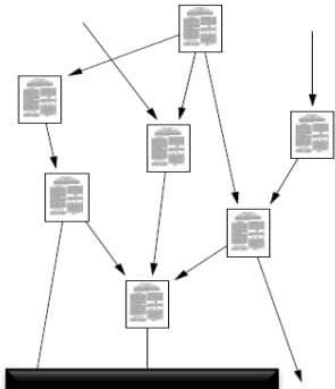
GNN

In Non-Euclidean Space

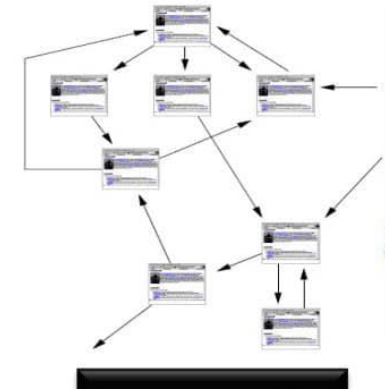
Graph?



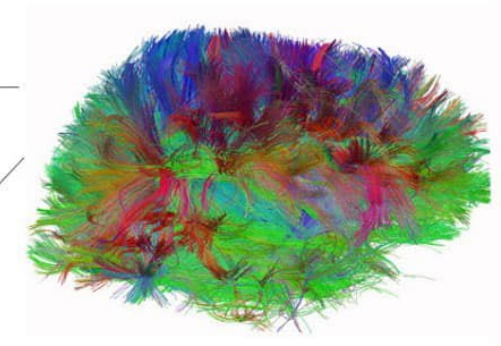
Molecules



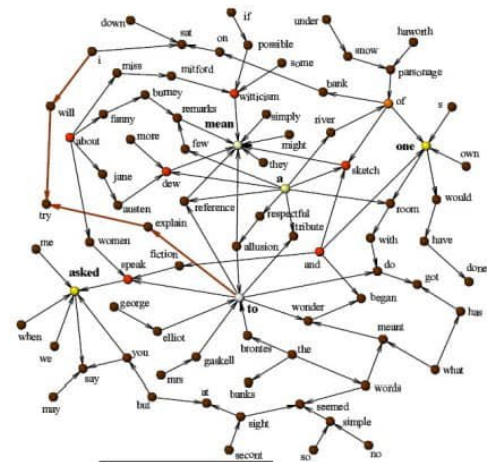
Knowledge



Information



Brain/neurons



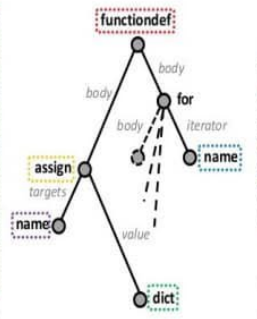
Genes



Communication

```
def encode(obj):  
    """  
    Encode a (possibly nested)  
    dictionary containing complex values  
    into a form that can be serialized  
    using JSON.  
    """  
    e = {}  
    for key, value in obj.items():  
        if isinstance(value, dict):  
            e[key] = encode(value)  
        elif isinstance(value, complex):  
            e[key] = {'type': 'complex',  
                    'r': value.real,  
                    'i': value.imag}  
    return e  
  
import ast  
tree = ast.parse("""  
...  
""")
```

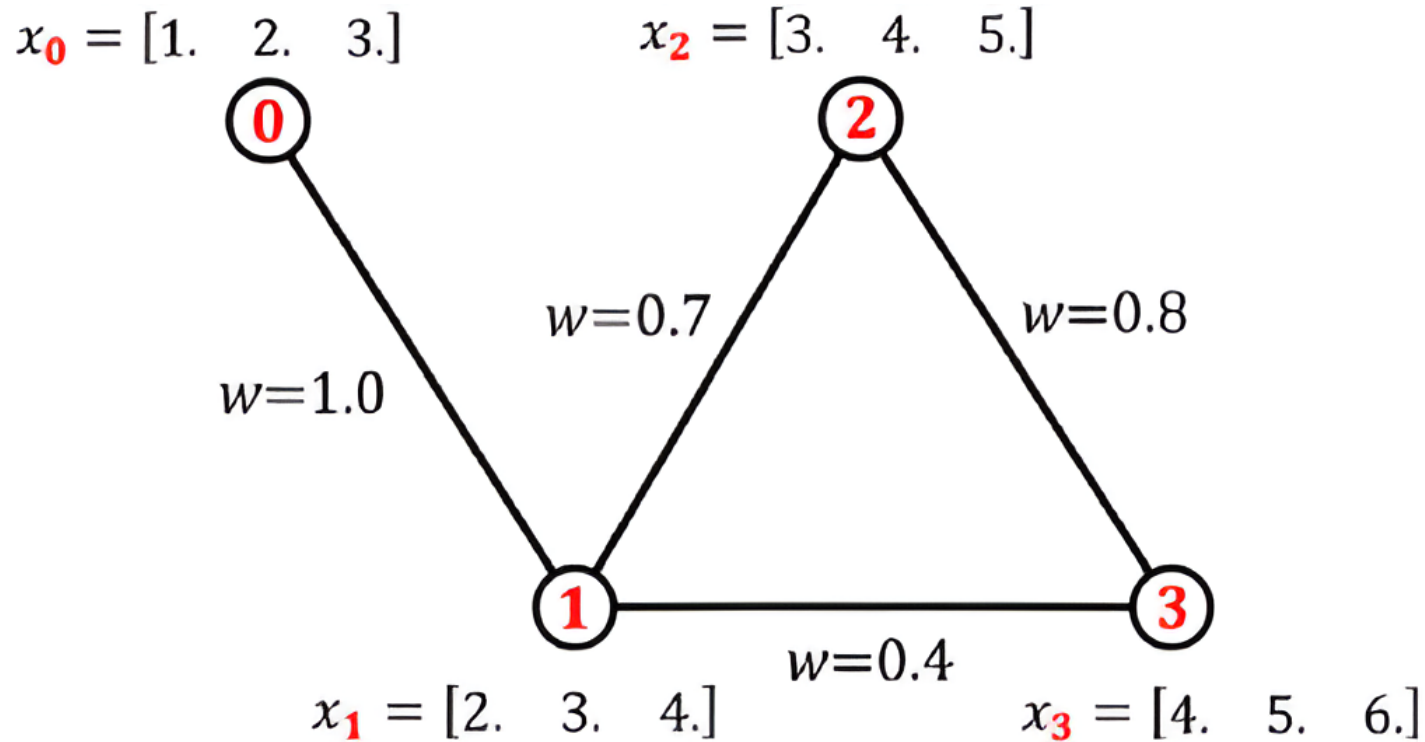
Software



Social

= {{Entities}, {Relations}}

Represent

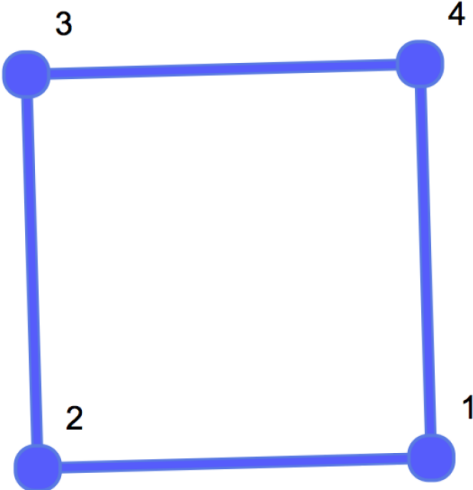
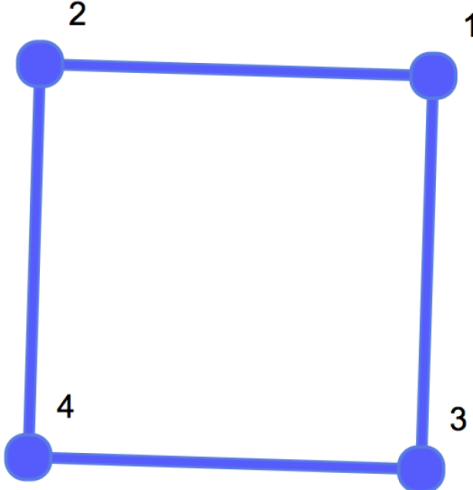
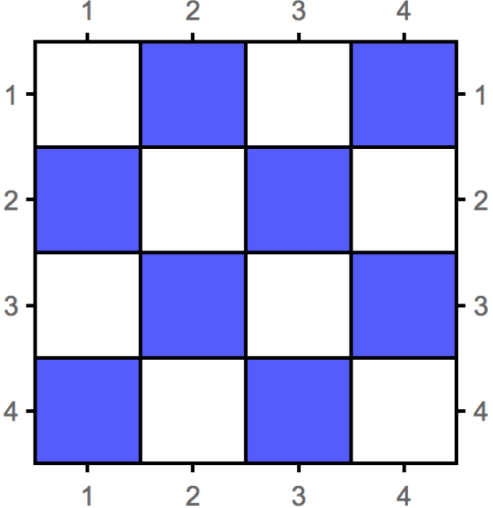
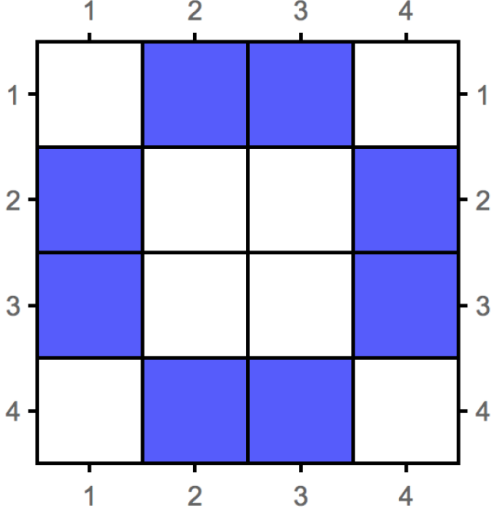


$$A = \begin{bmatrix} 0 & 1.0 & 0 & 0 \\ 1.0 & 0 & 0.7 & 0.4 \\ 0 & 0.7 & 0 & 0.8 \\ 0 & 0.4 & 0.8 & 0 \end{bmatrix}$$
$$X = \begin{bmatrix} 1. & 2. & 3. \\ 2. & 3. & 4. \\ 3. & 4. & 5. \\ 4. & 5. & 6. \end{bmatrix}$$

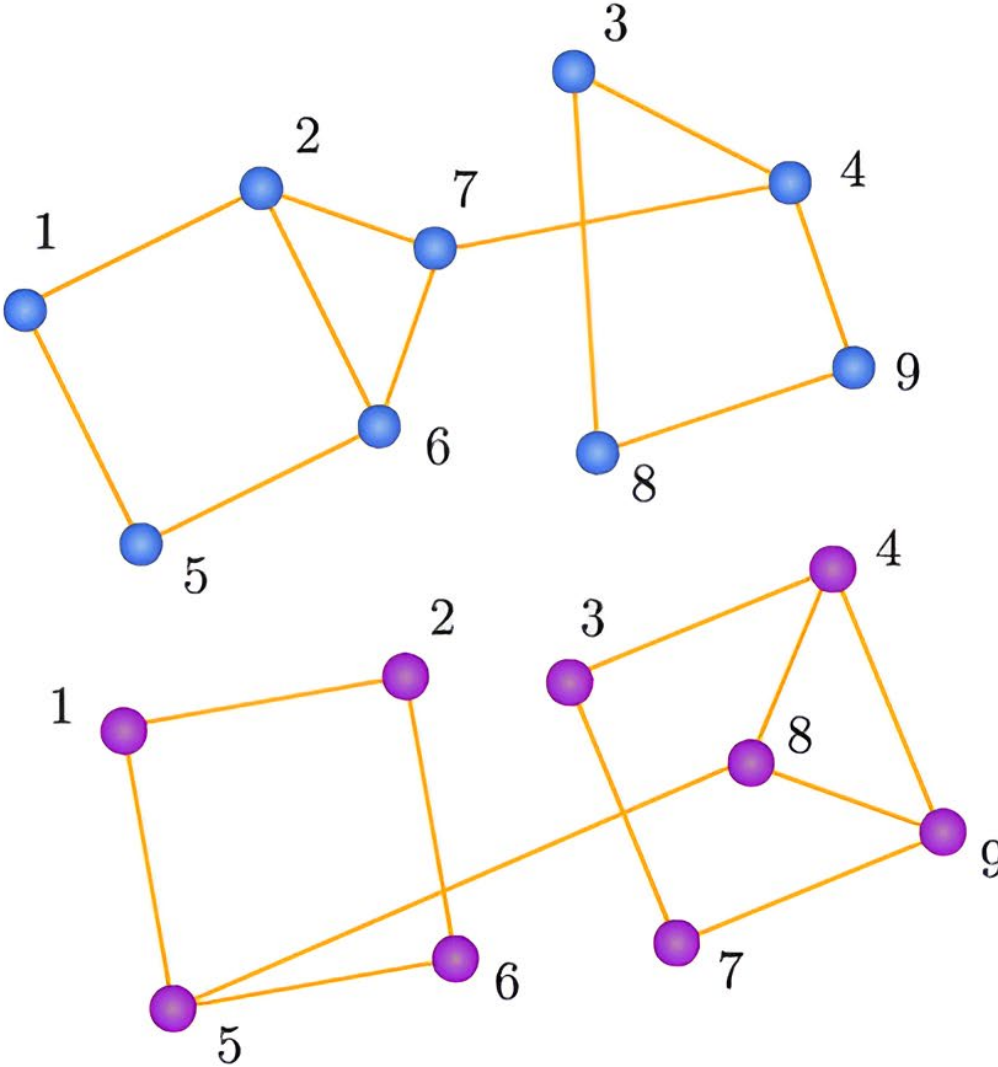
Label could be **node-level**, **graph-level**...

Invariant Property

Same Graph
may have
Different
Representation



Invariant Property



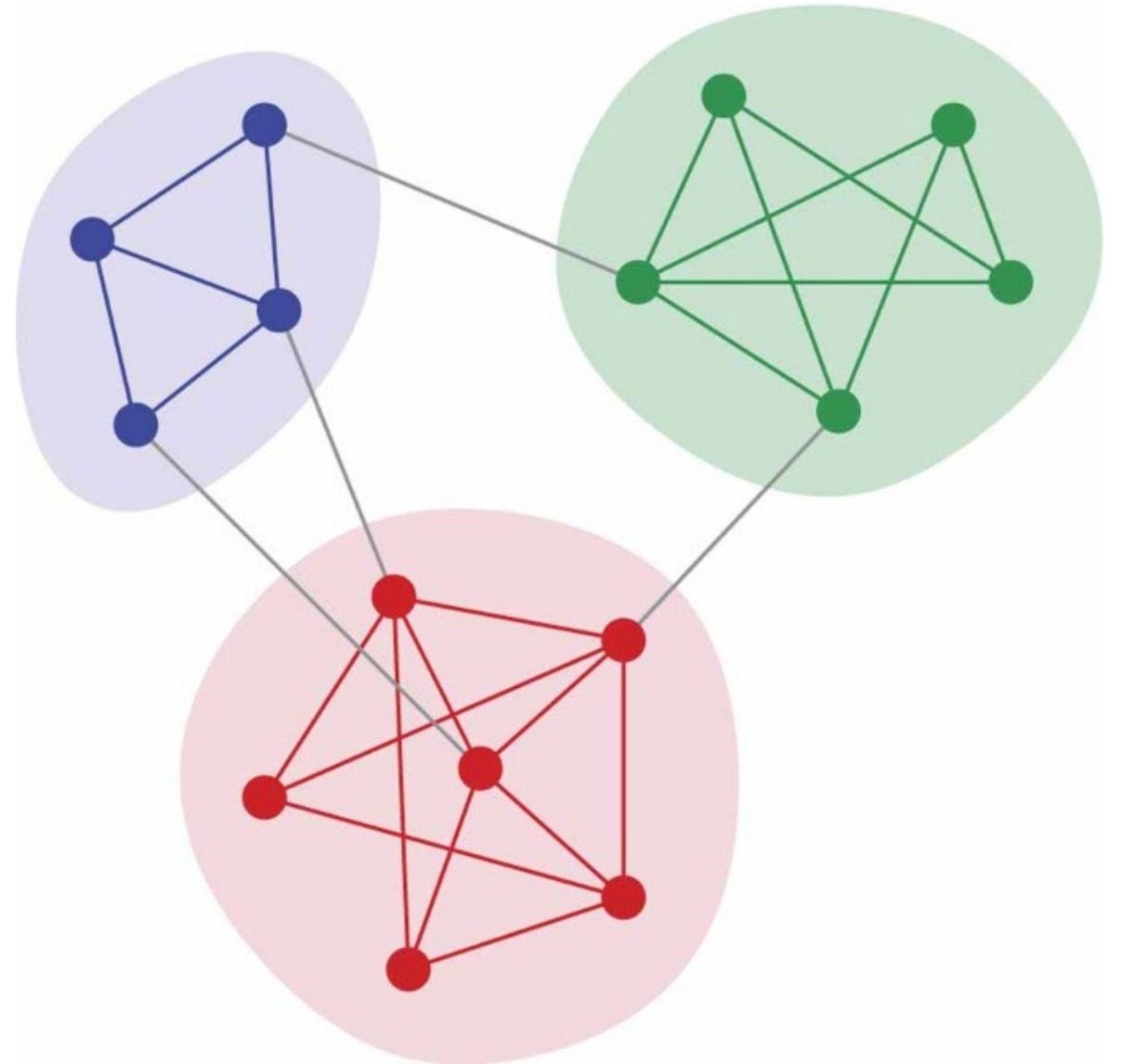
Graph neural network

Graph neural network

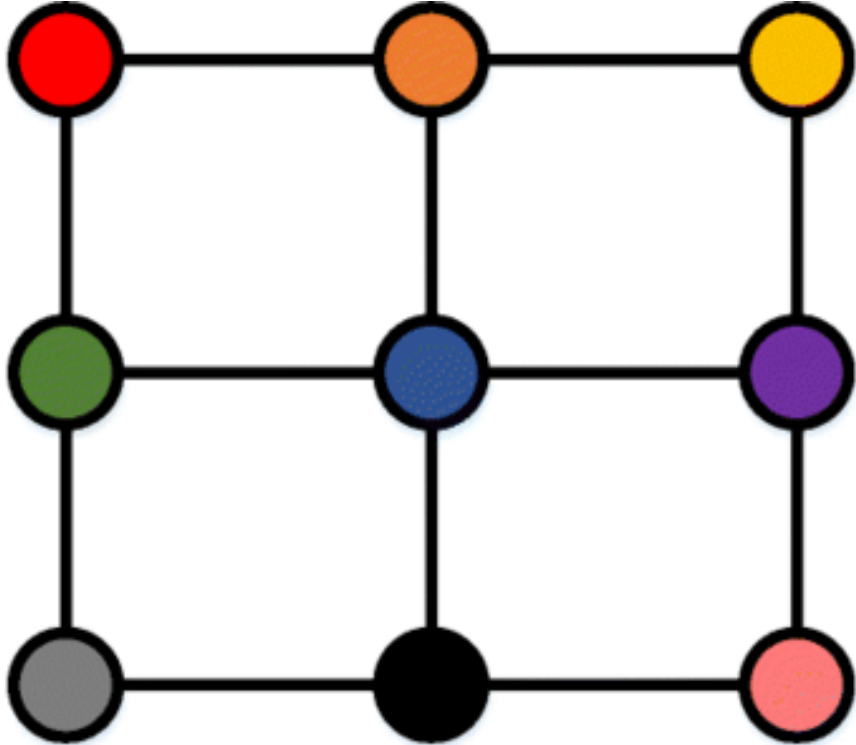
Same output for isomorphic graphs

Homogeneity

Edge
represent **similarity**

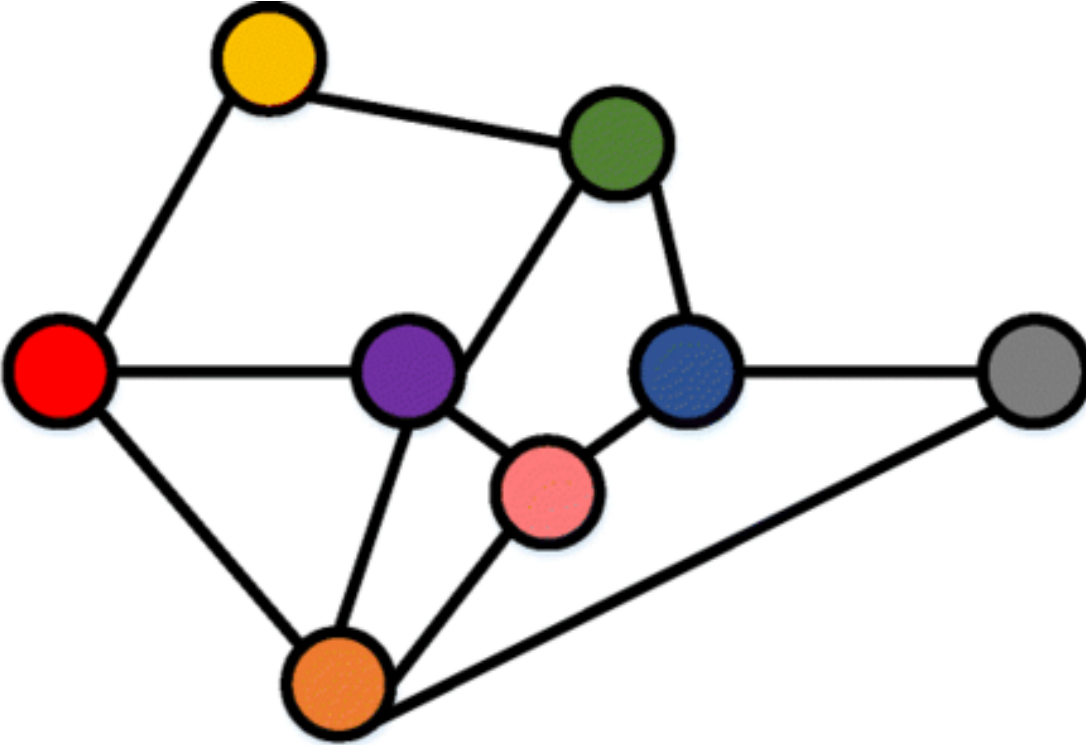


Paradigm



CNN

In Euclidean Space



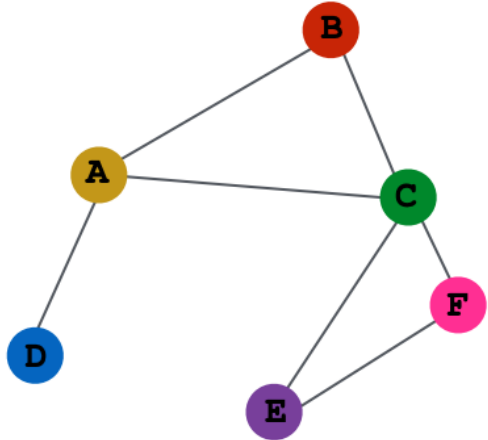
GNN

In Non-Euclidean Space

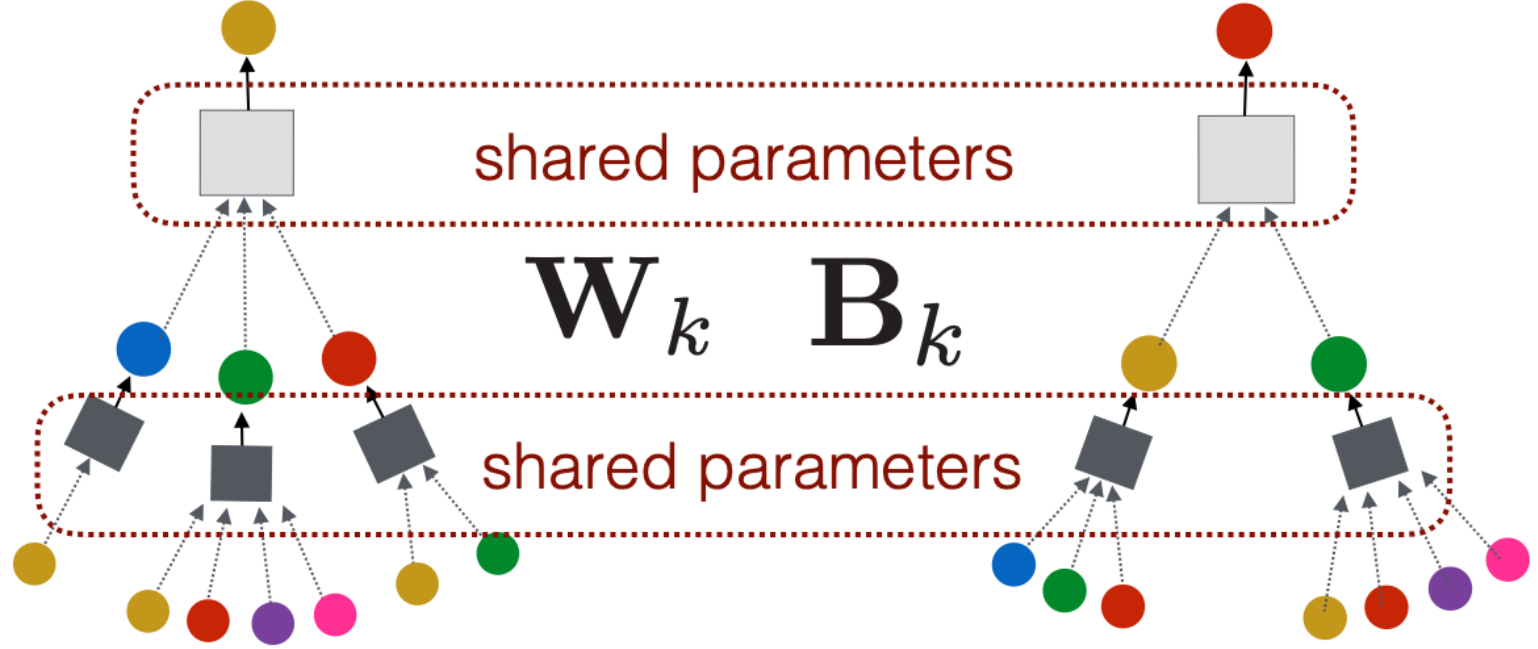
Message Passing

$$h_i^{(1)} = \sigma\left(\sum_{j \in N(i)} x_j W^{(0)}\right)$$

$$h_i^{(l)} = \sigma\left(\sum_{j \in N(i)} h_j^{(l-1)} W^{(l-1)}\right)$$



INPUT GRAPH



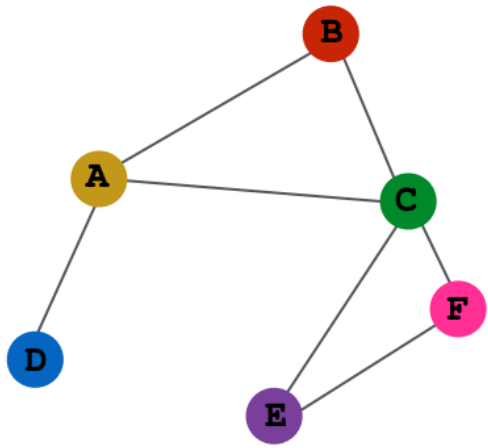
Compute graph for node A

Compute graph for node B

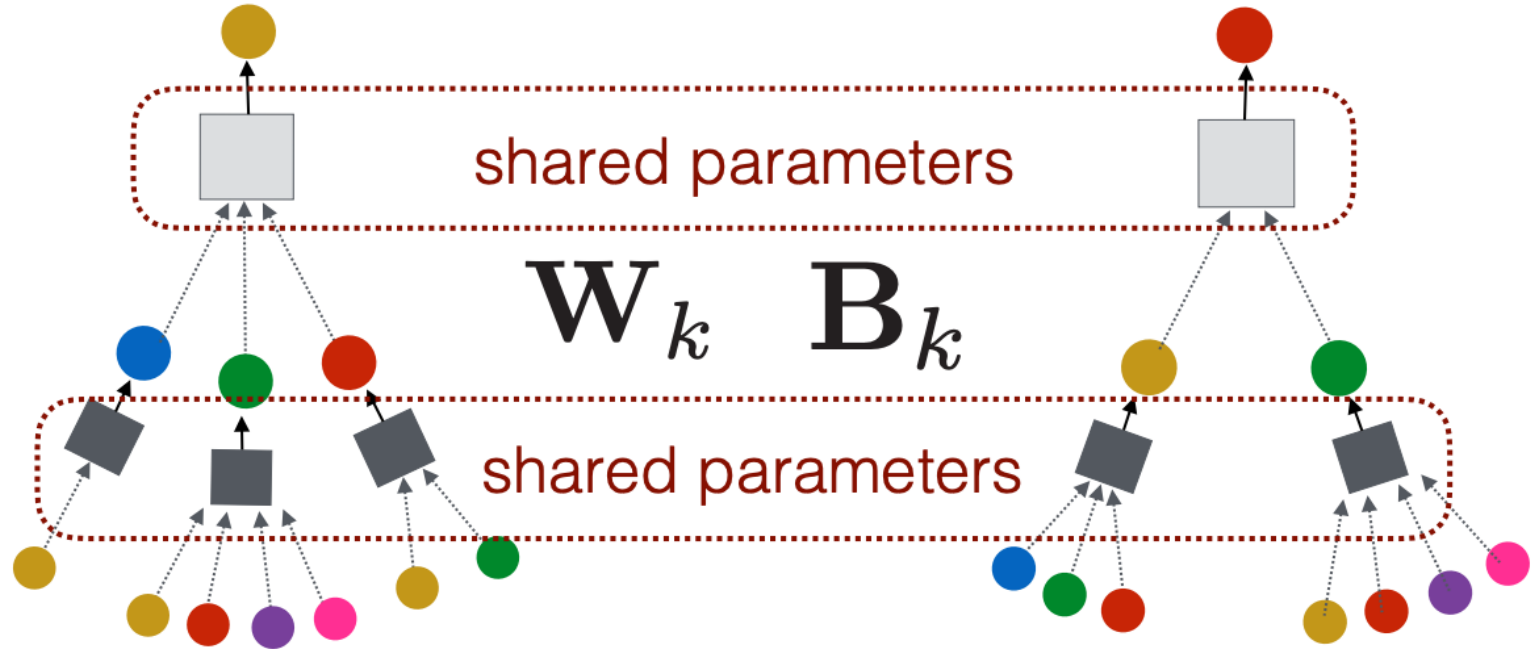
Message Passing

$$\mathbf{x}_i^{(k)} = \gamma^{(k)} \left(\mathbf{x}_i^{(k-1)}, \bigoplus_{j \in \mathcal{N}(i)} \phi^{(k)} \left(\mathbf{x}_i^{(k-1)}, \mathbf{x}_j^{(k-1)}, \mathbf{e}_{j,i} \right) \right),$$

Update, Aggregate



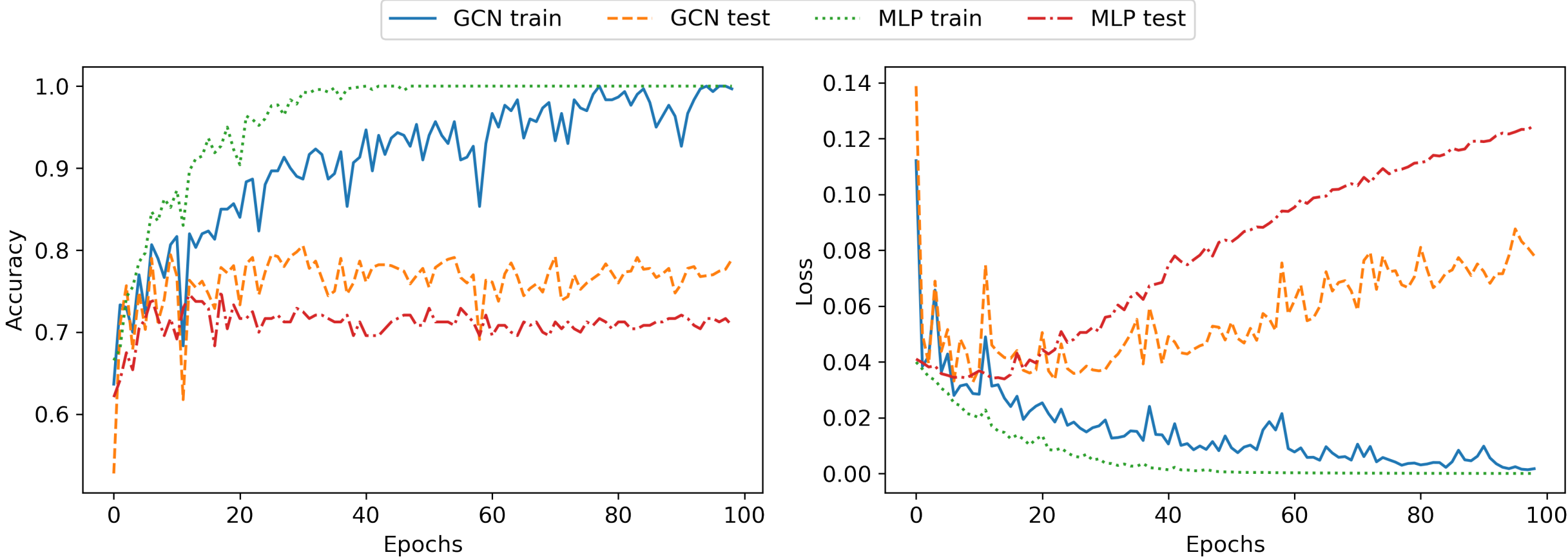
INPUT GRAPH



Compute graph for node A

Compute graph for node B

Failure of MLP

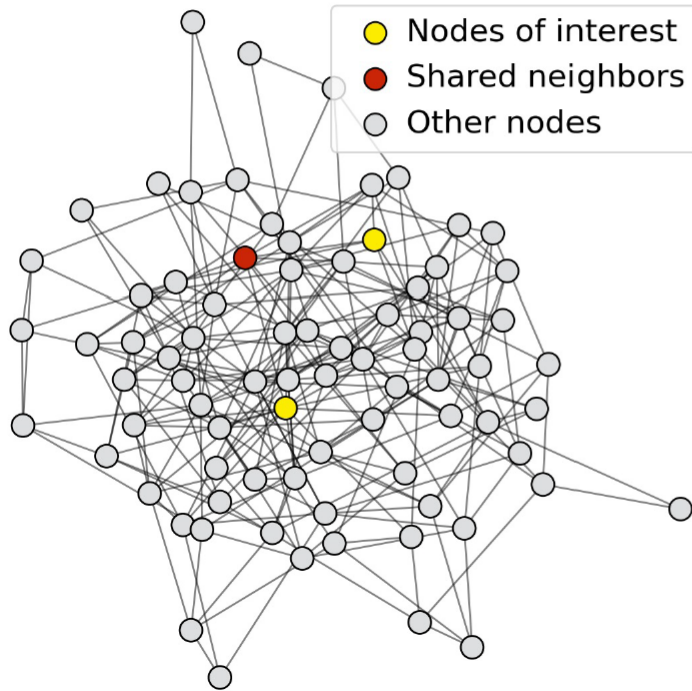


Deep?

Oversmoothing

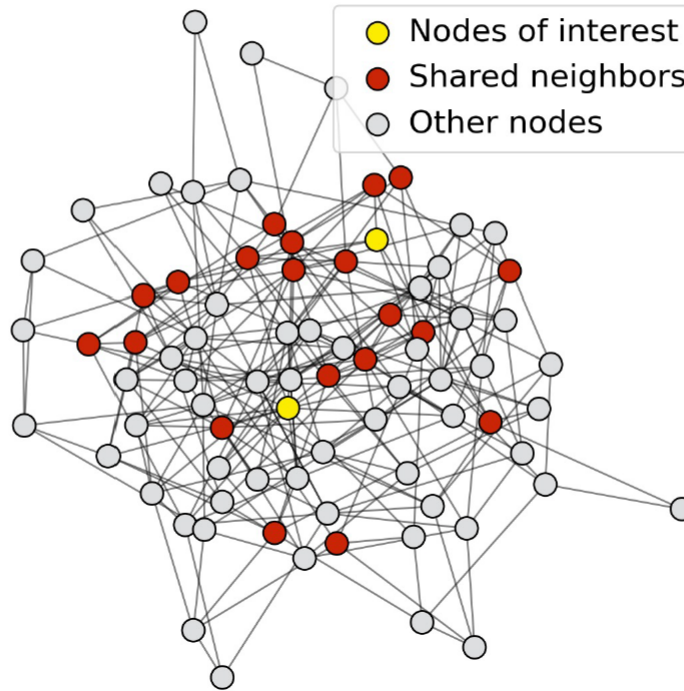
1-hop neighbor overlap

Only 1 node



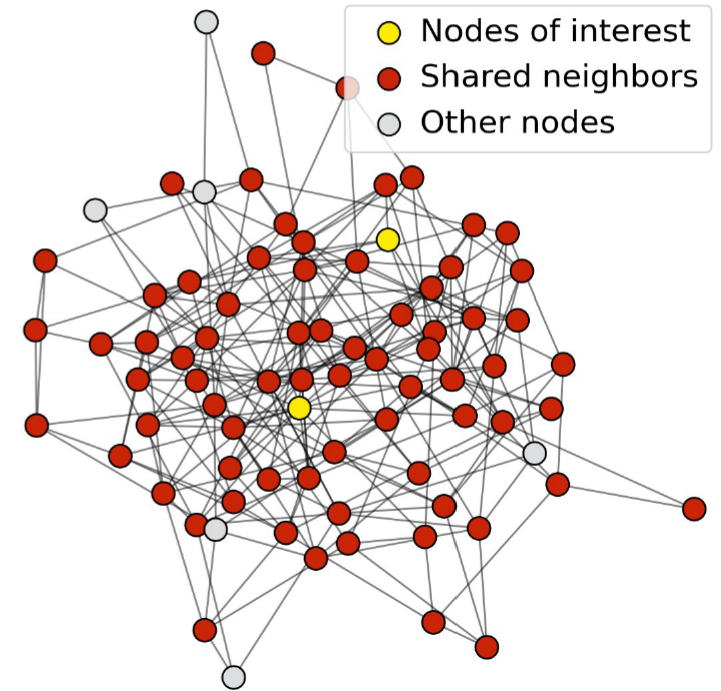
2-hop neighbor overlap

About 20 nodes



3-hop neighbor overlap

Almost all the nodes!

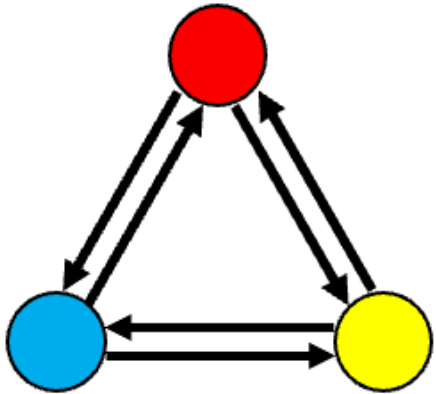


Deep GNN means Large receptive field

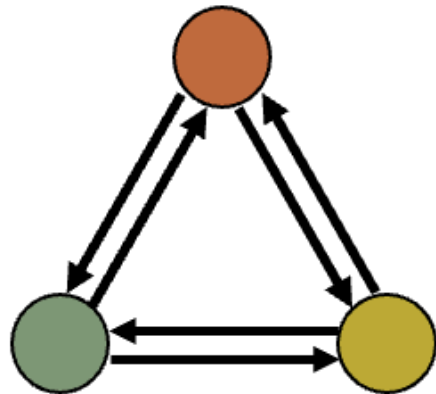
Deep?

Oversquanshing

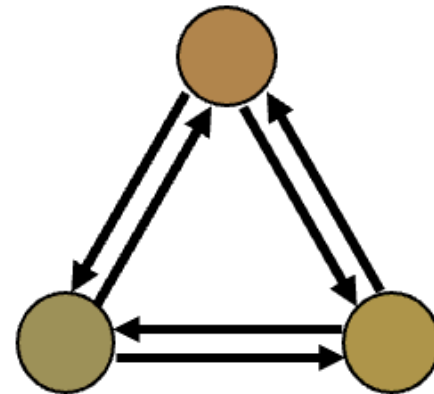
Layer 1



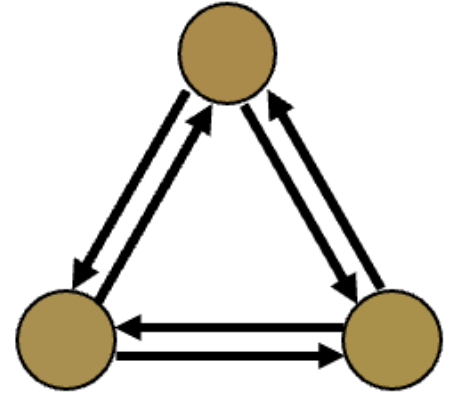
Layer 2



Layer 3

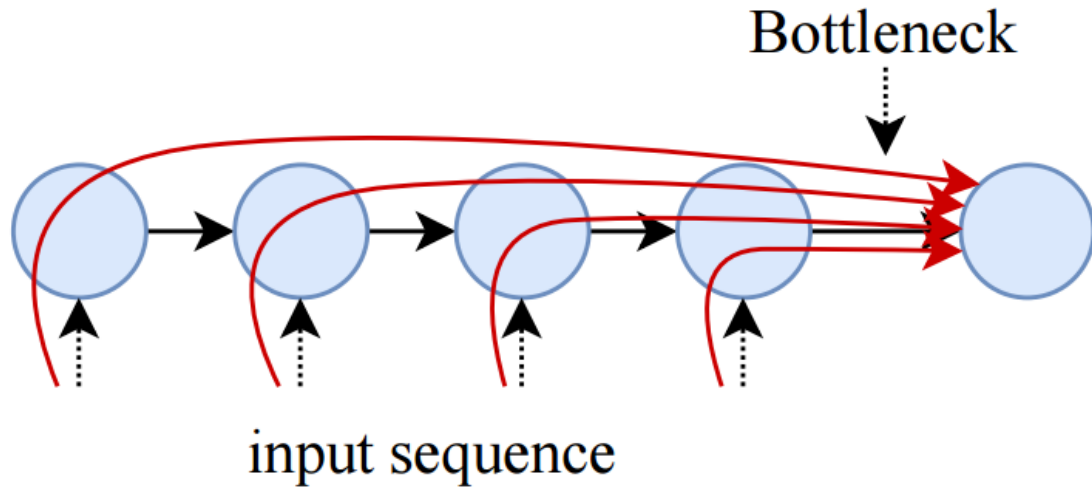


Layer 4

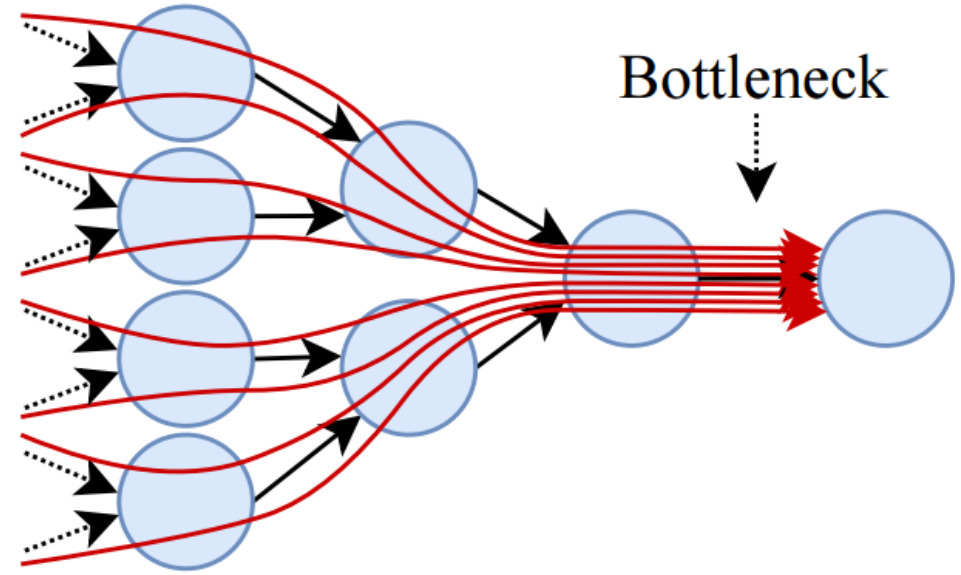


Mean undisguised for target node

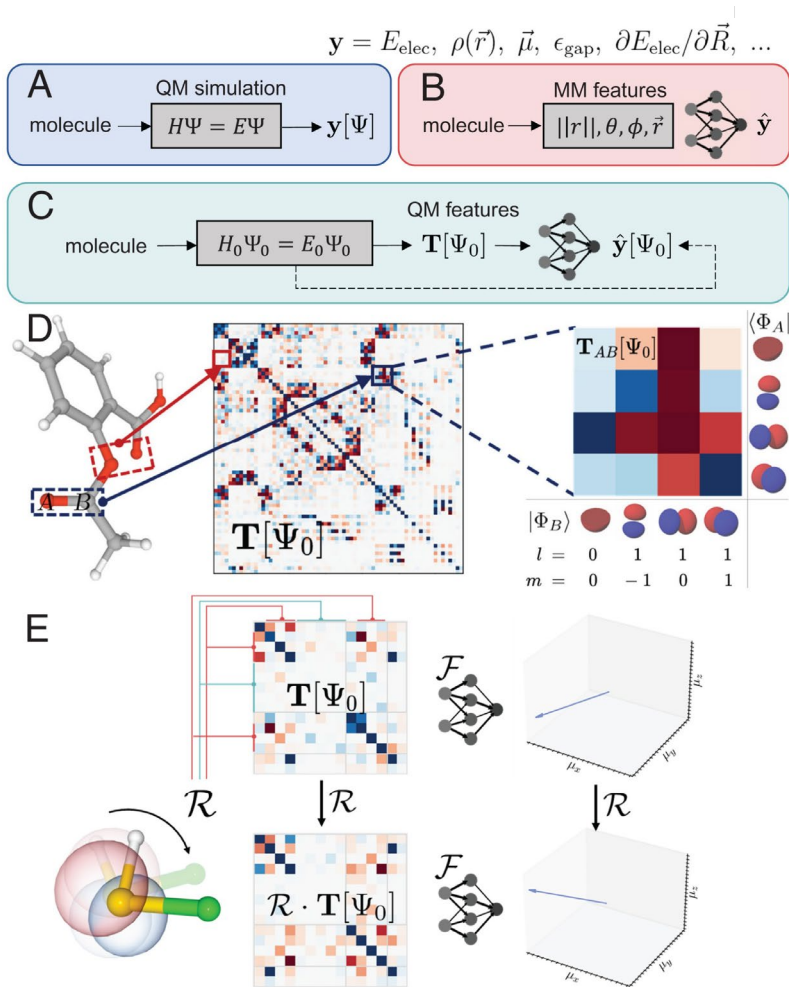
Deep?



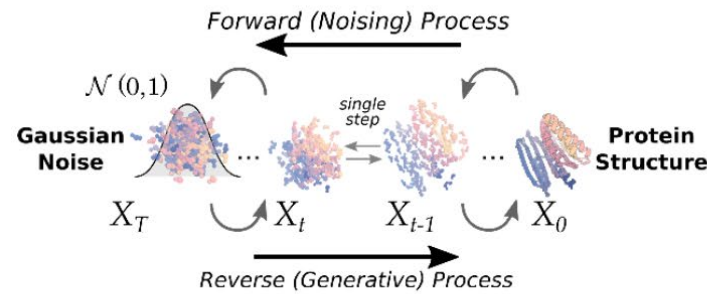
(a) The bottleneck of RNN seq2seq models



(b) The bottleneck of graph neural networks



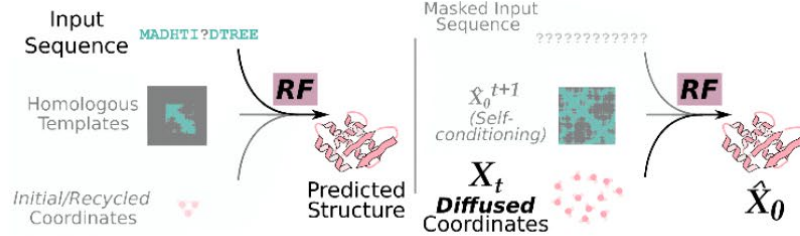
Diffusion Model



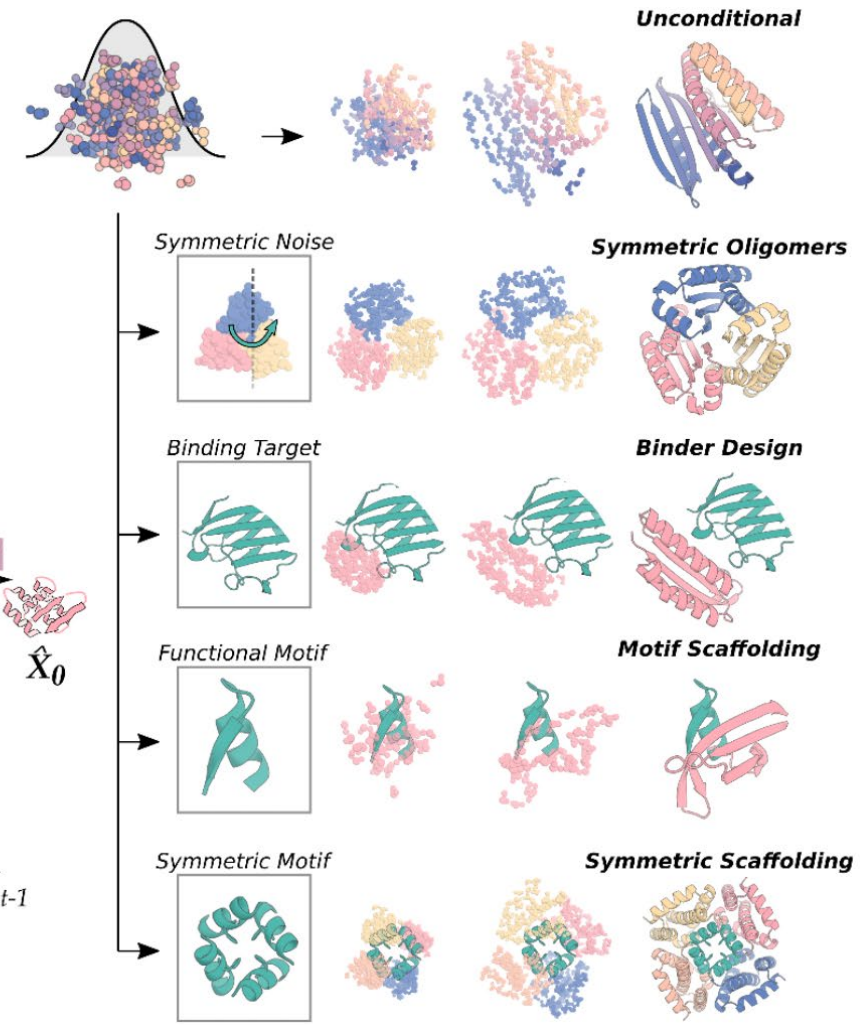
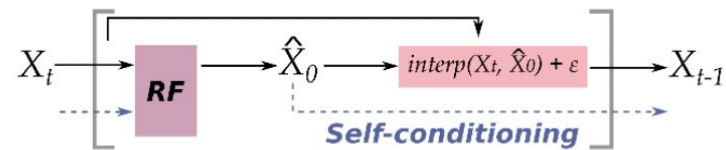
RoseTTAFold



RFdiffusion

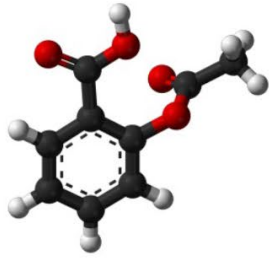


Single RFdiffusion step

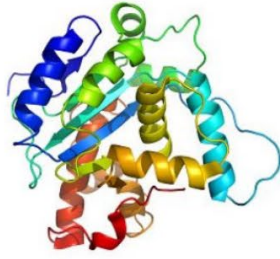


Future

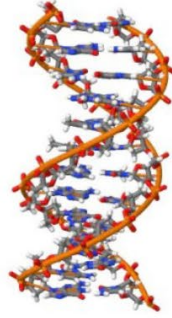
“Geometric Graphs”



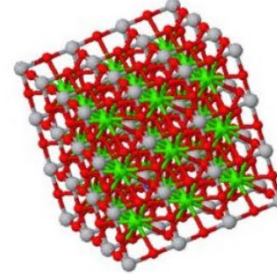
Small
Molecules



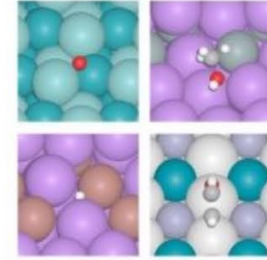
Proteins



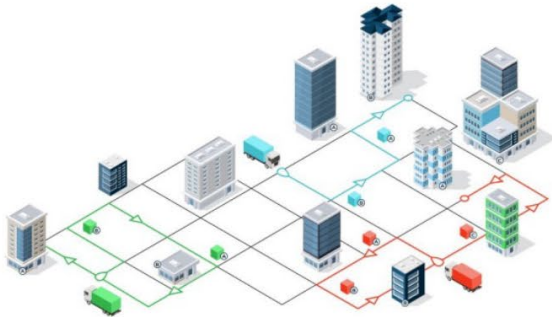
DNA/RNA



Inorganic
Crystals



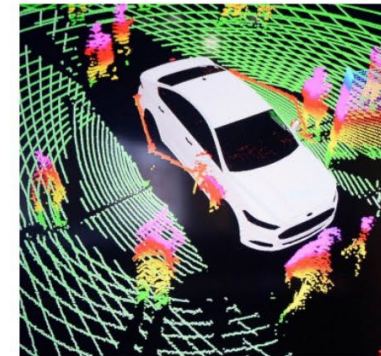
Catalysis
Systems



Transportation &
Logistics



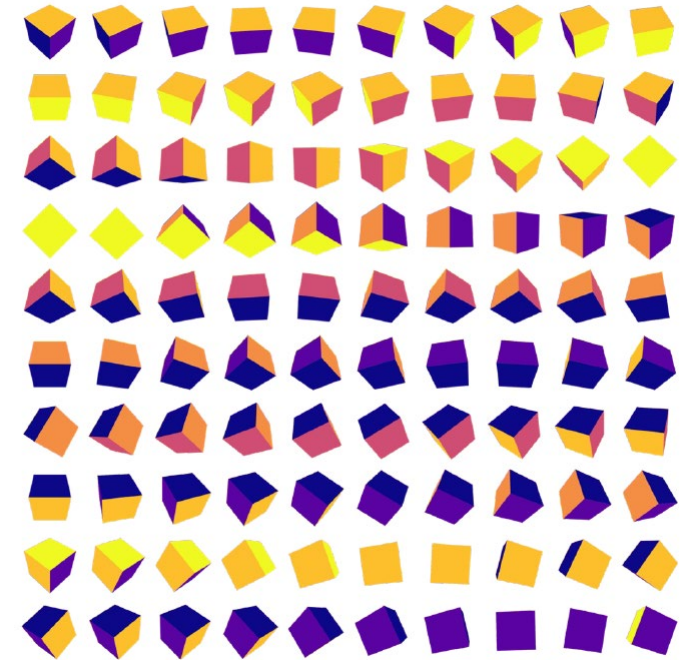
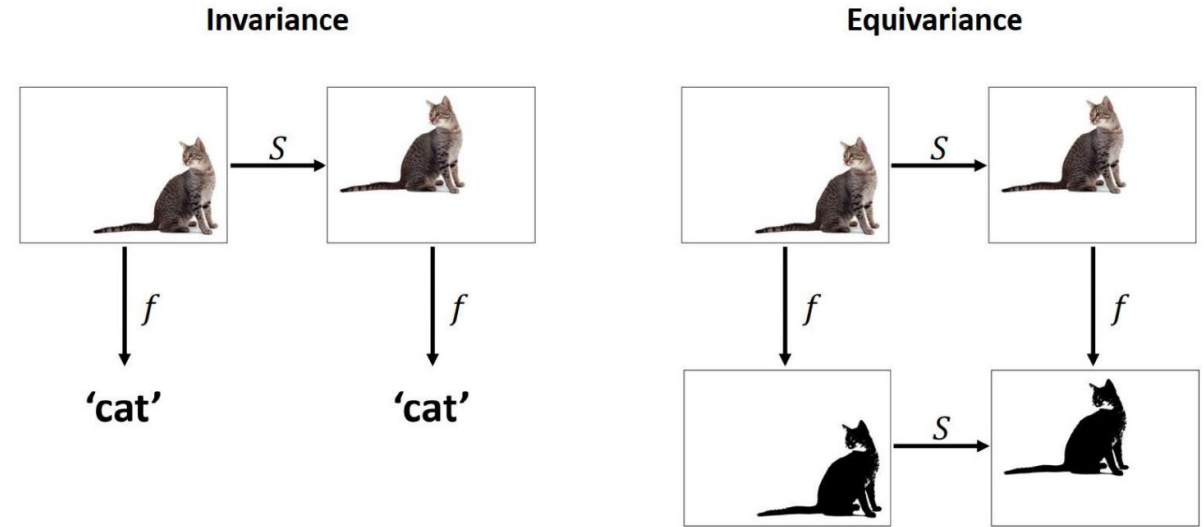
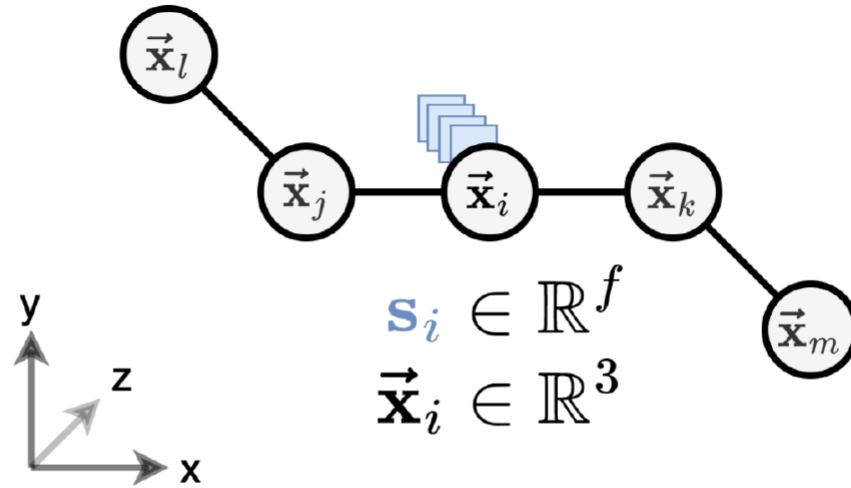
Robotic
Navigation



3D Computer
Vision

Future

“Geometric Graphs”



- A : an $n \times n$ adjacency matrix.
- $S \in \mathbb{R}^{n \times f}$: scalar features.
- $X \in \mathbb{R}^{n \times d}$: tensor features, e.g., coordinates.

Thank you

&More Discussion