Graph Neural Network:
Paradigm, Limitation and Future

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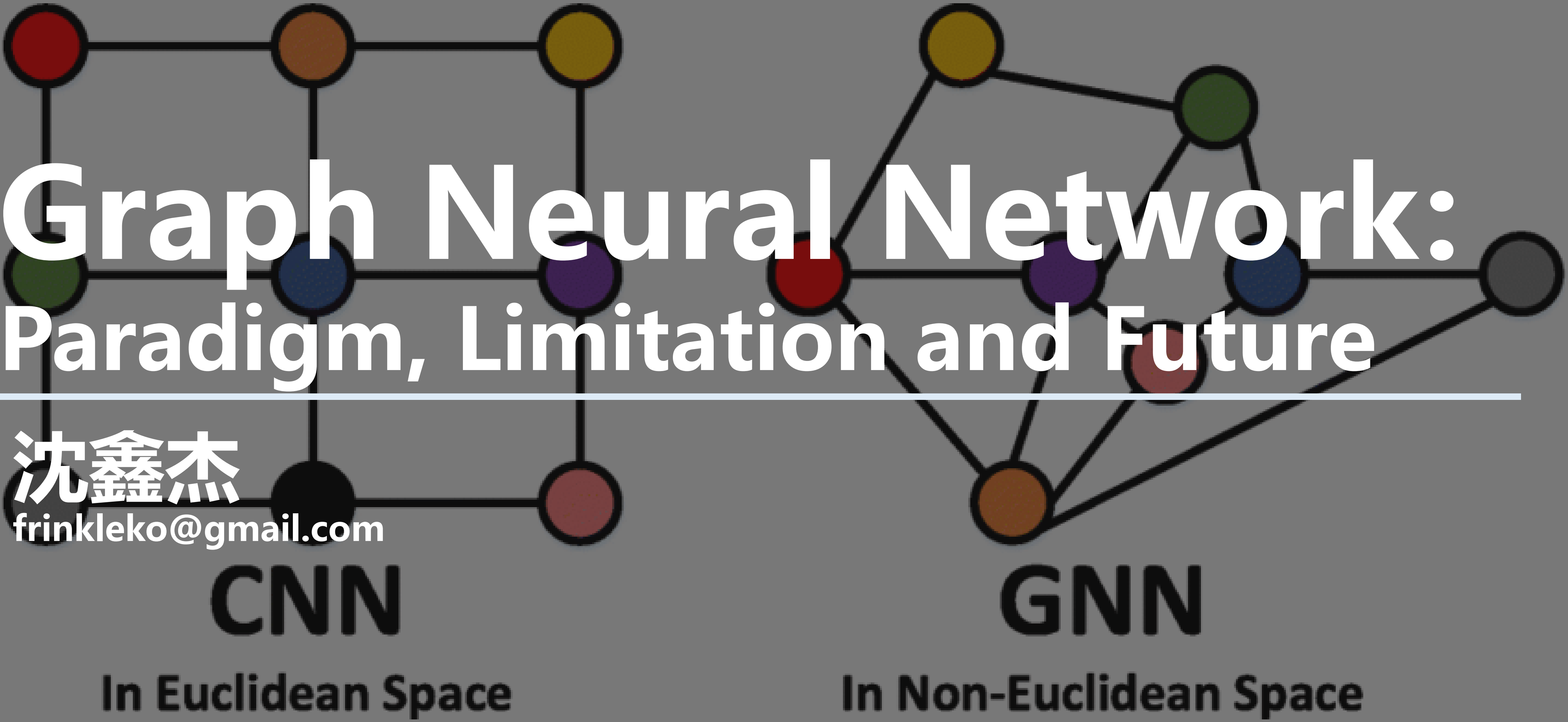
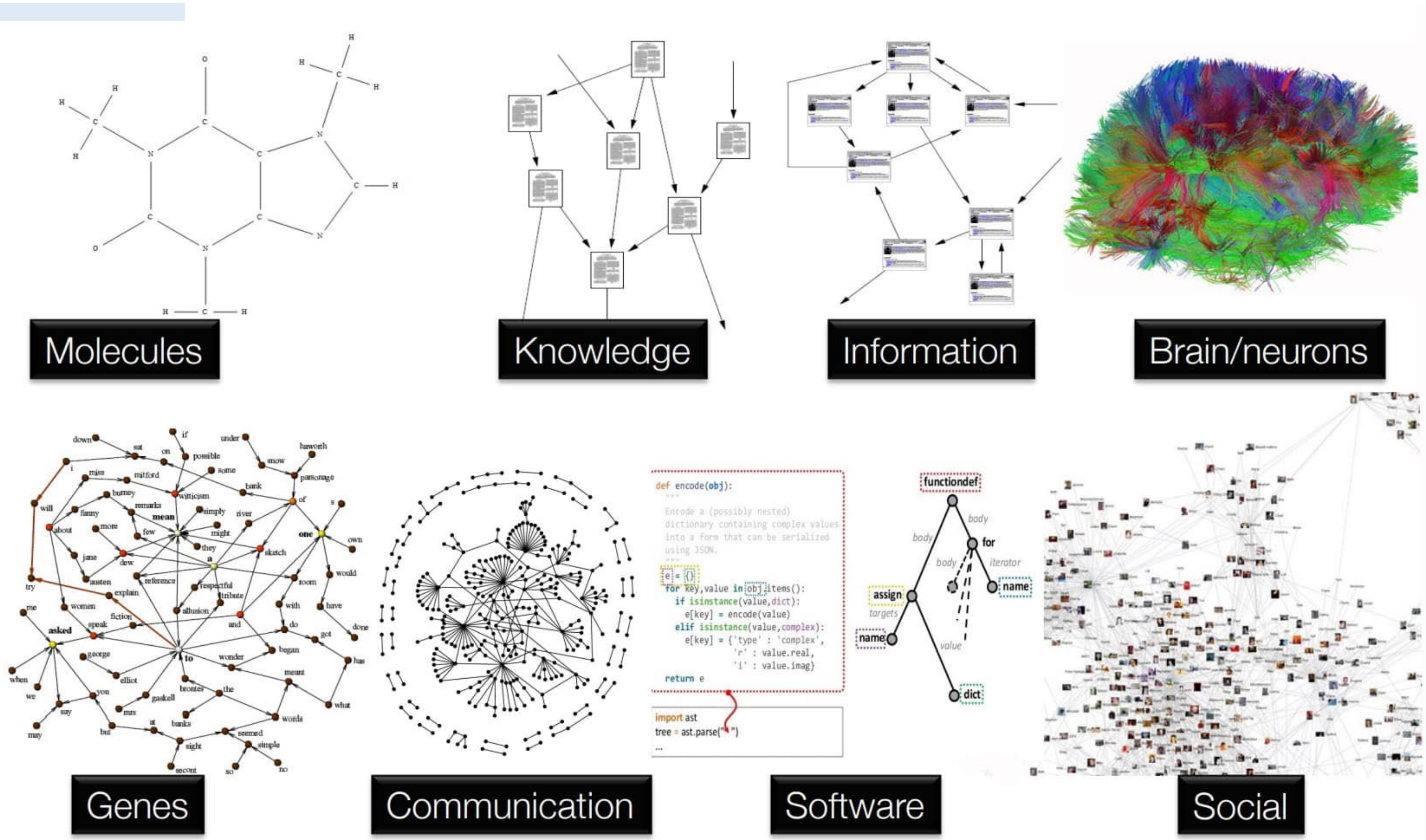


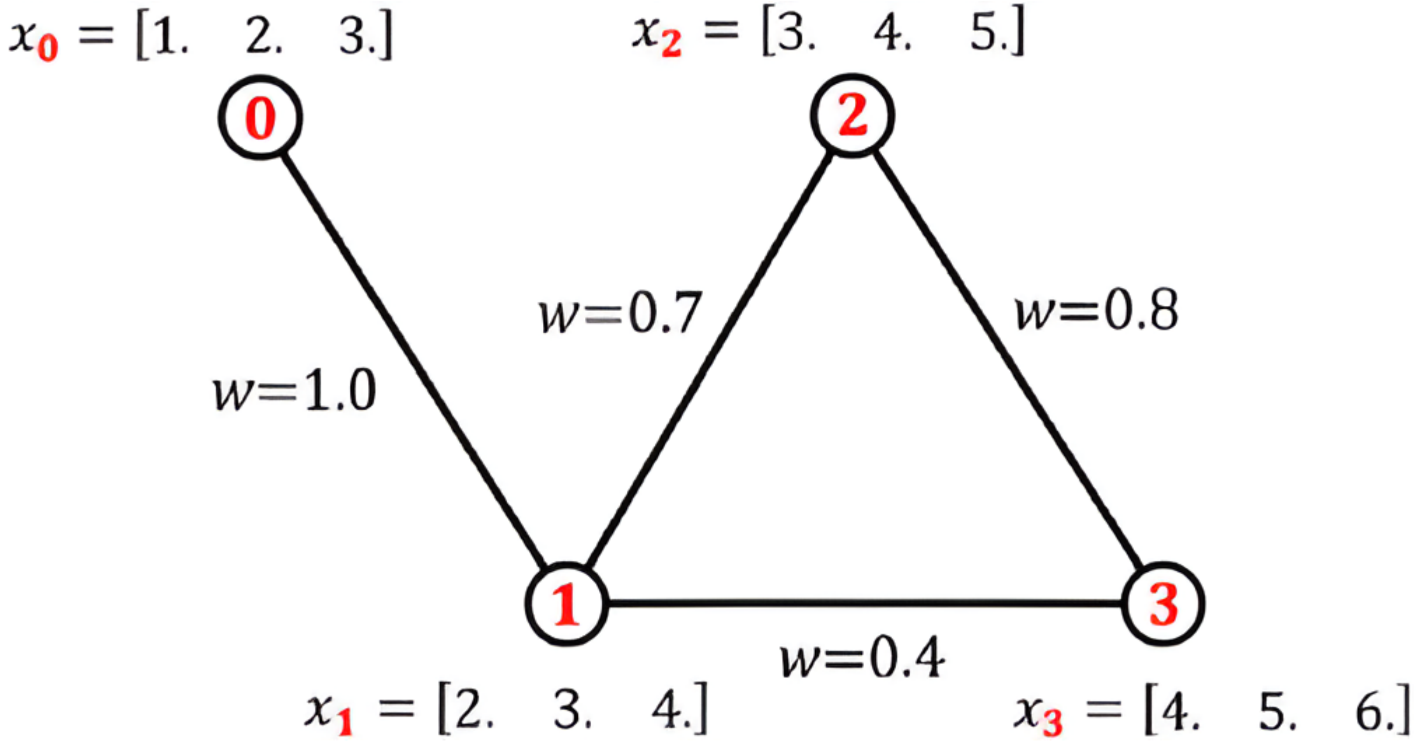
MAGIC&SCUT AI Association

Graph?



={{Entities}, {Relations}}

Represent



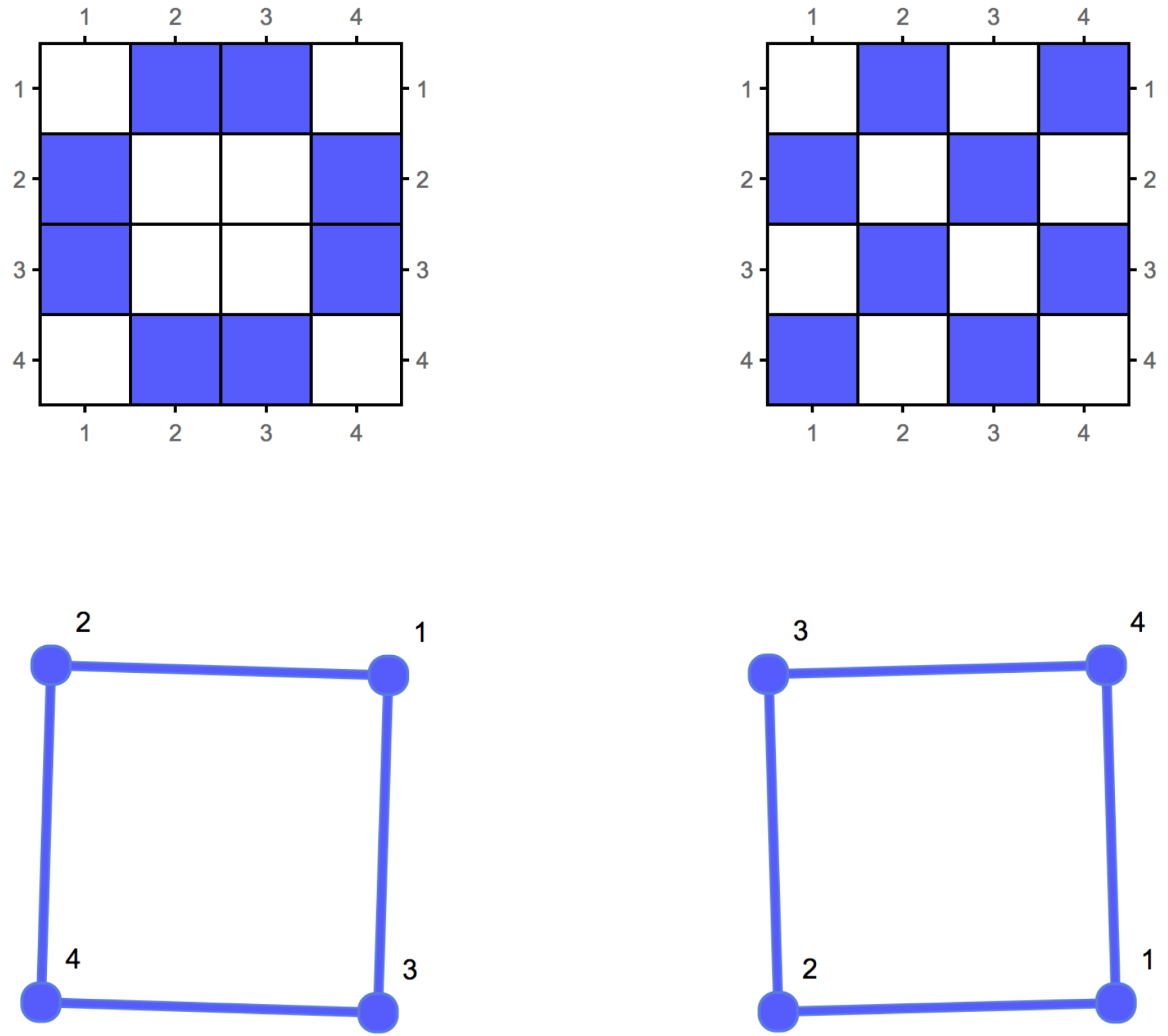
$$\boldsymbol{A} = \begin{bmatrix} 0 & 1.0 & 0 & 0 \\ 1.0 & 0 & 0.7 & 0.4 \\ 0 & 0.7 & 0 & 0.8 \\ 0 & 0.4 & 0.8 & 0 \end{bmatrix}$$

$$\boldsymbol{X} = \begin{bmatrix} 1. & 2. & 3. \\ 2. & 3. & 4. \\ 3. & 4. & 5. \\ 4. & 5. & 6. \end{bmatrix}$$

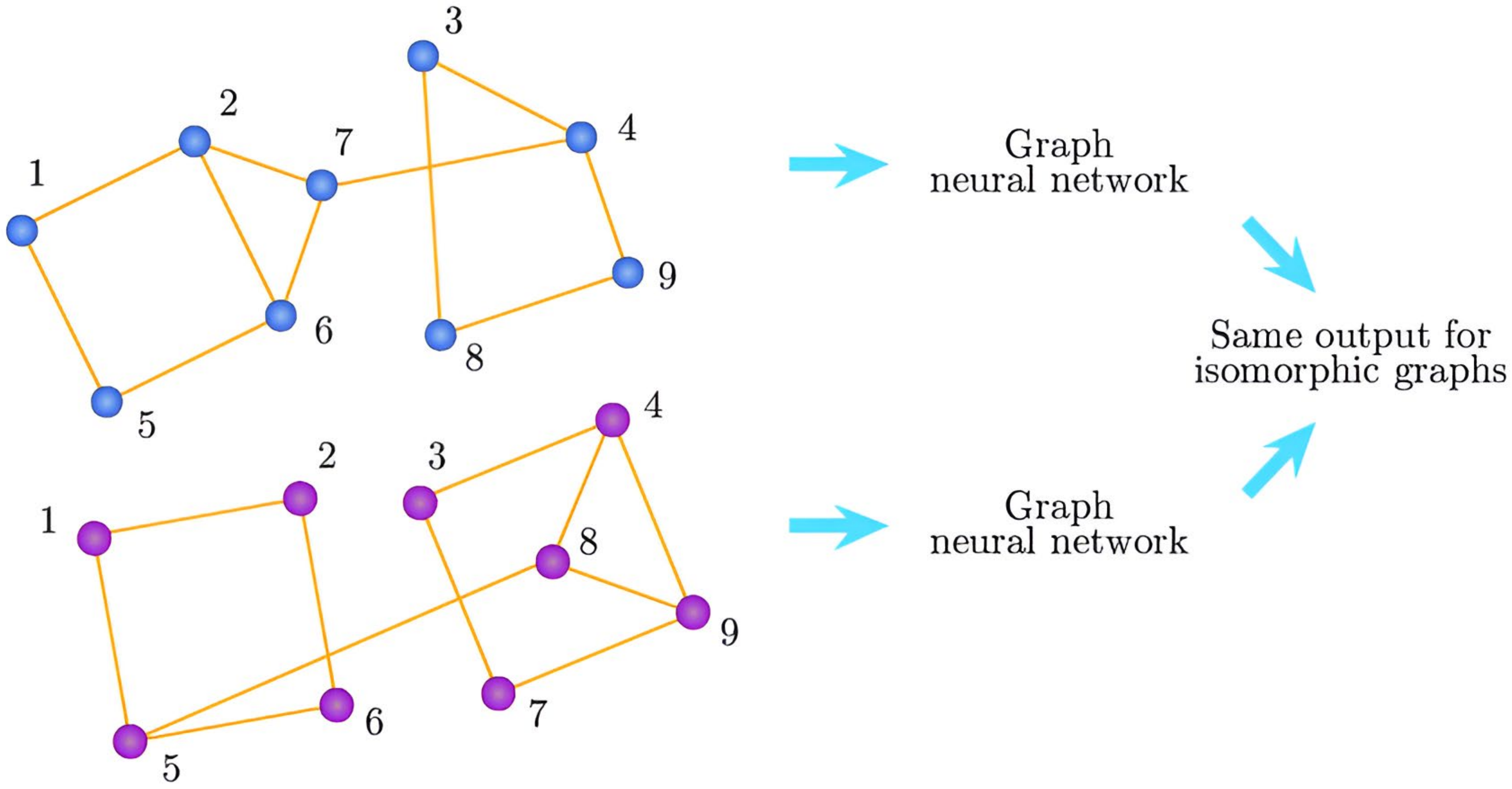
Label could be **node-level, graph-level...**

Invariant Property

Same Graph
may have
Different
Representation

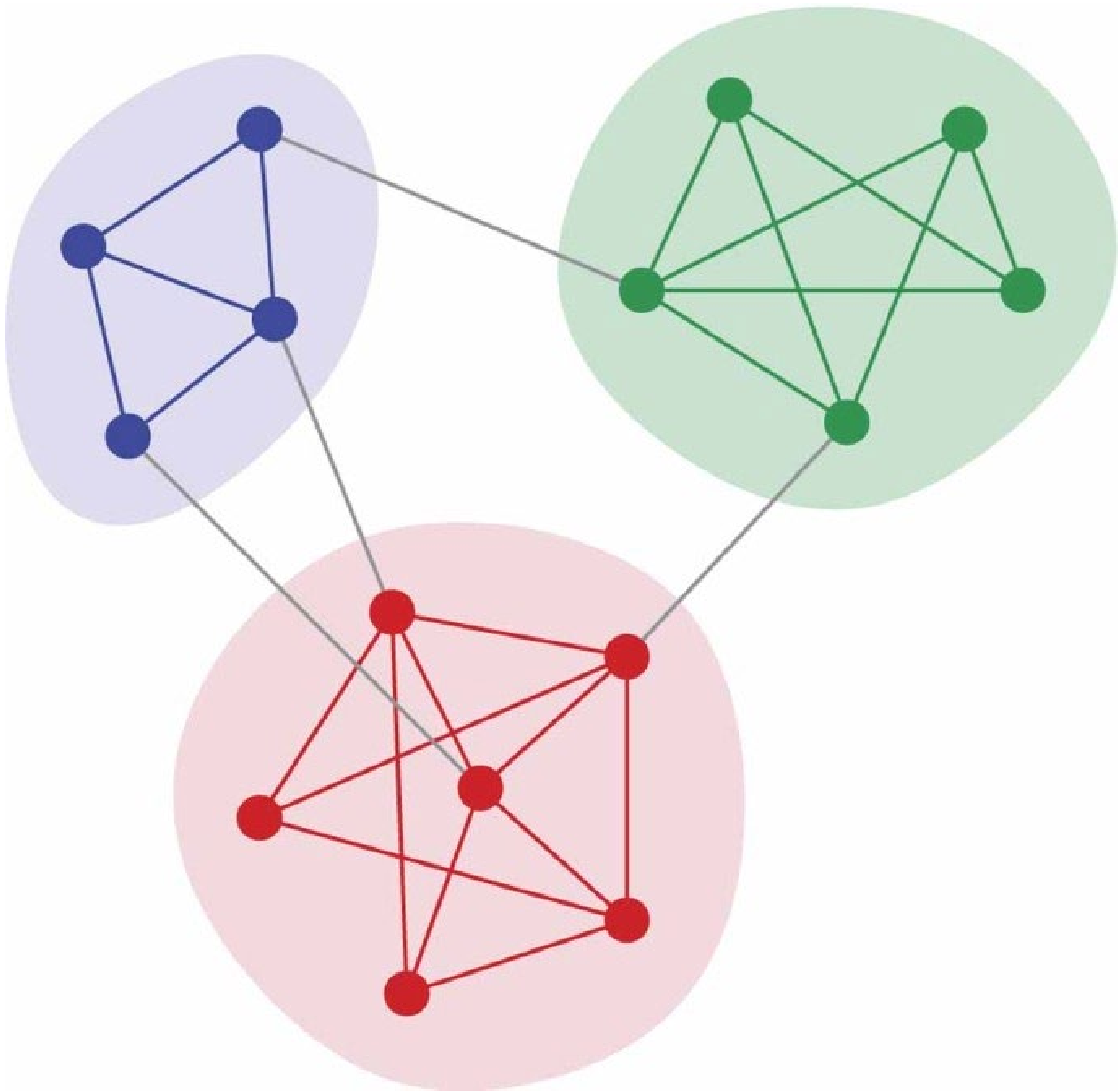


Invariant Property

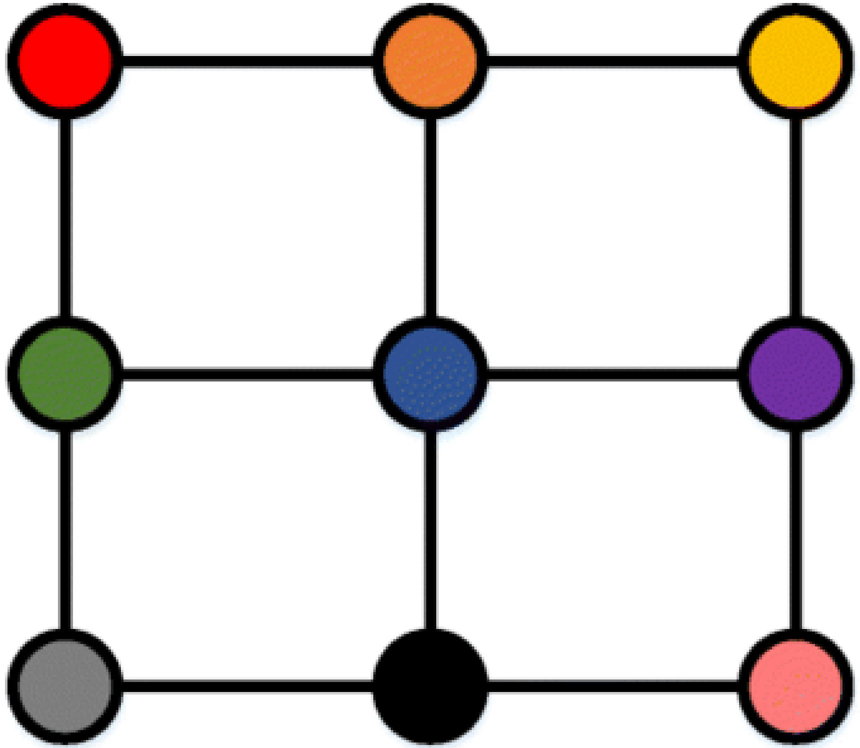


Homogeneity

Edge
represent **similarity**

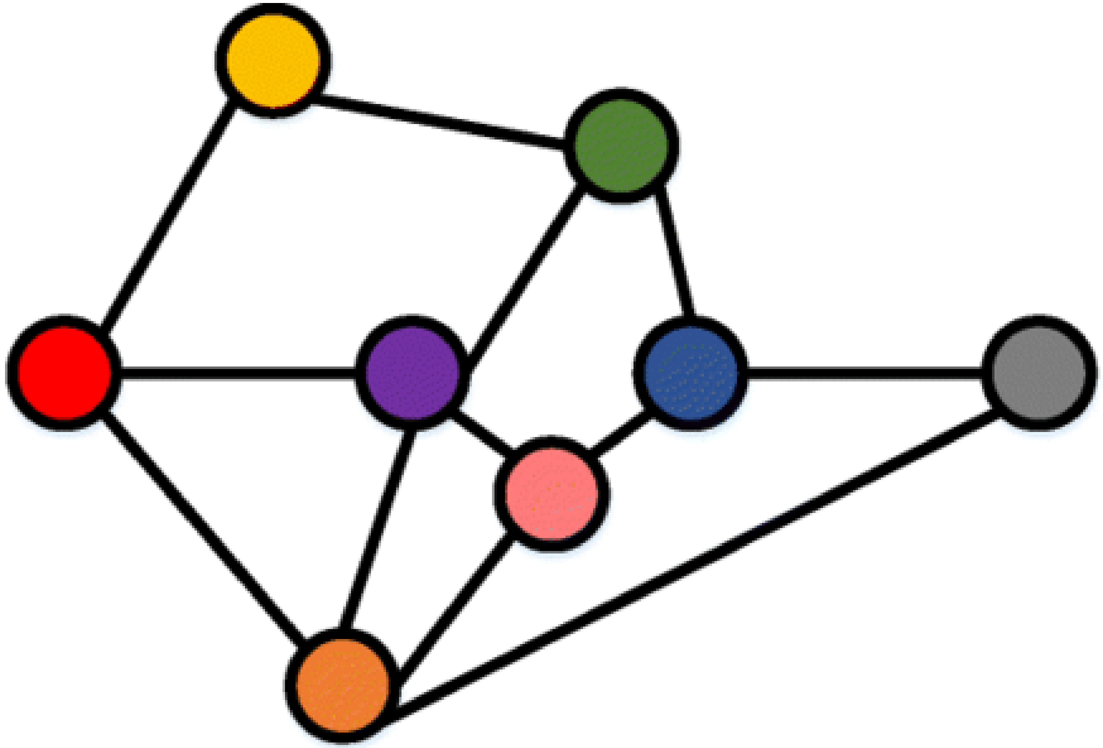


Paradigm



CNN

In Euclidean Space



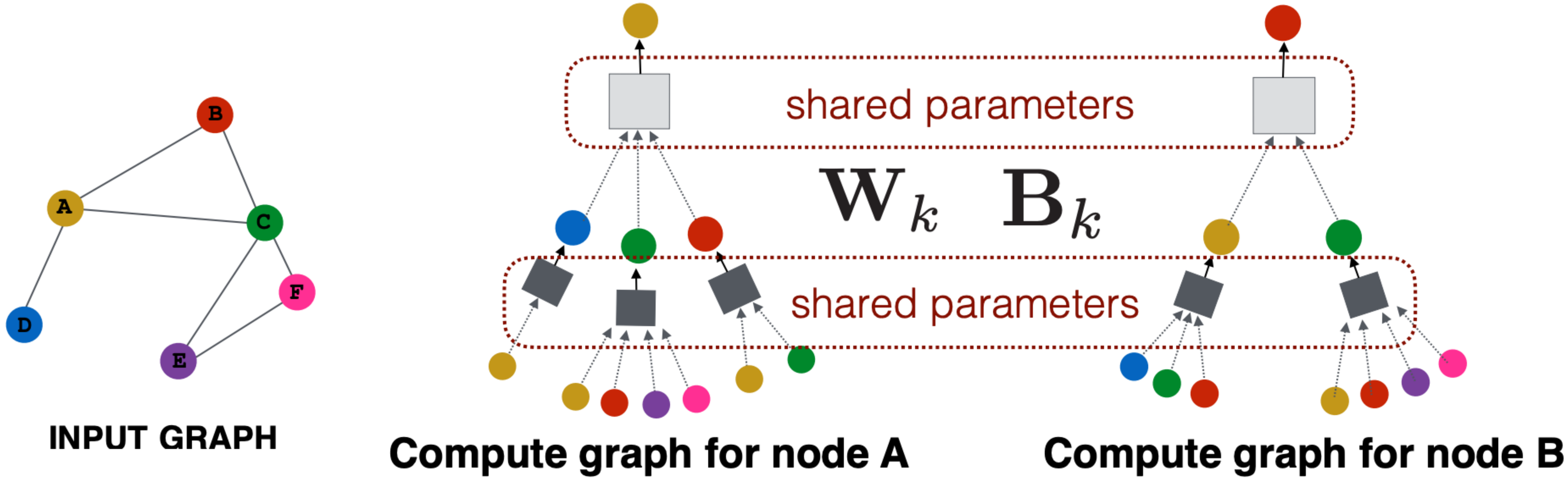
GNN

In Non-Euclidean Space

Message Passing

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

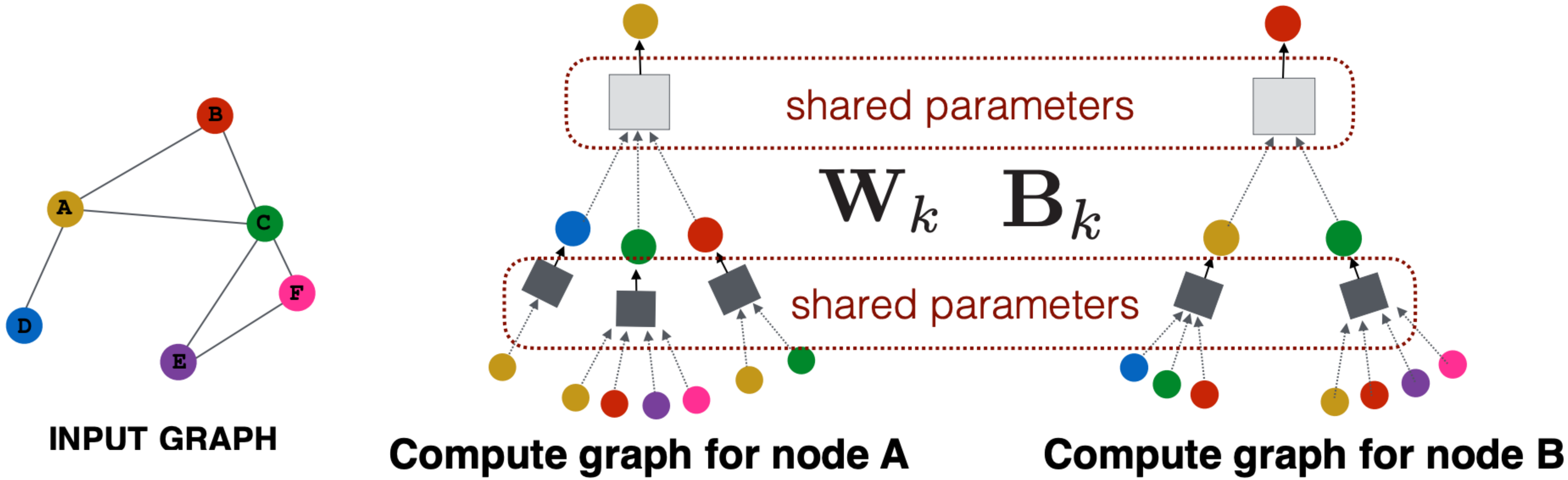
$$h_i^{(l)} = \sigma(\sum_{j \in N(i)} h_j^{(l-1)} W^{(l-1)})$$



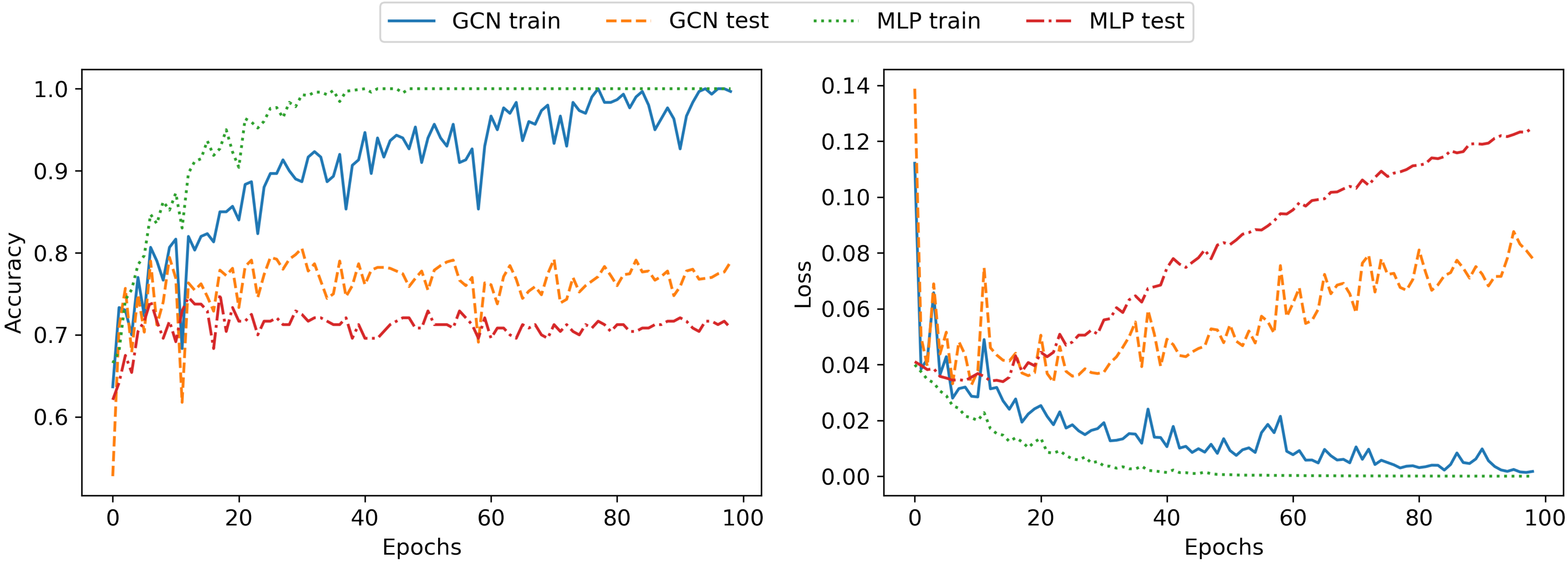
Message Passing

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

Update，Aggregate



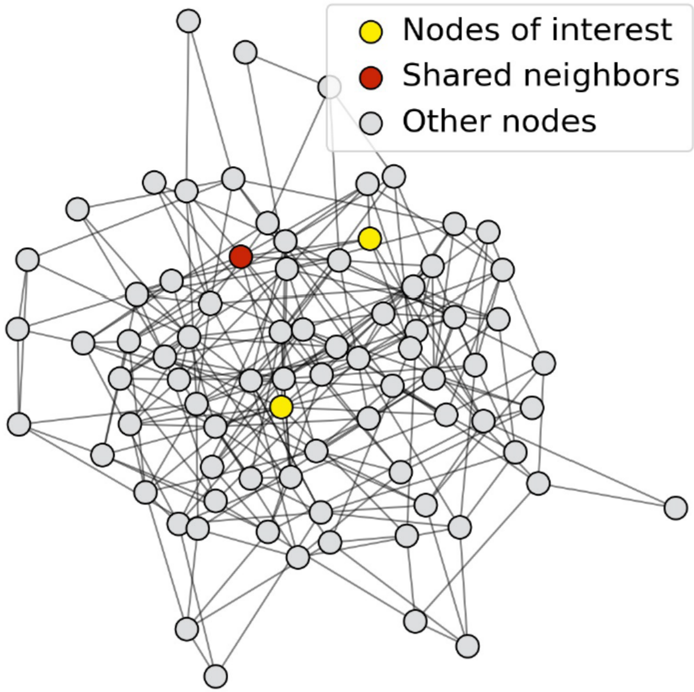
Failure of MLP



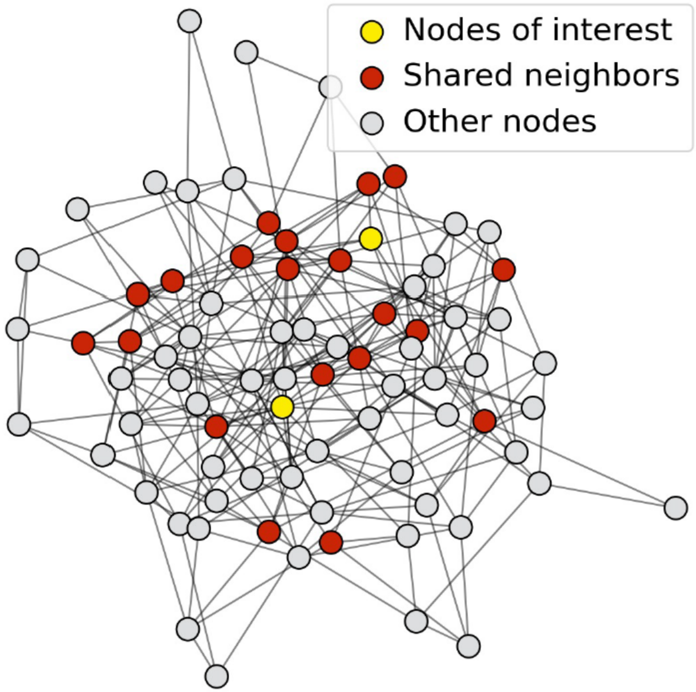
Deep?

Oversmoothing

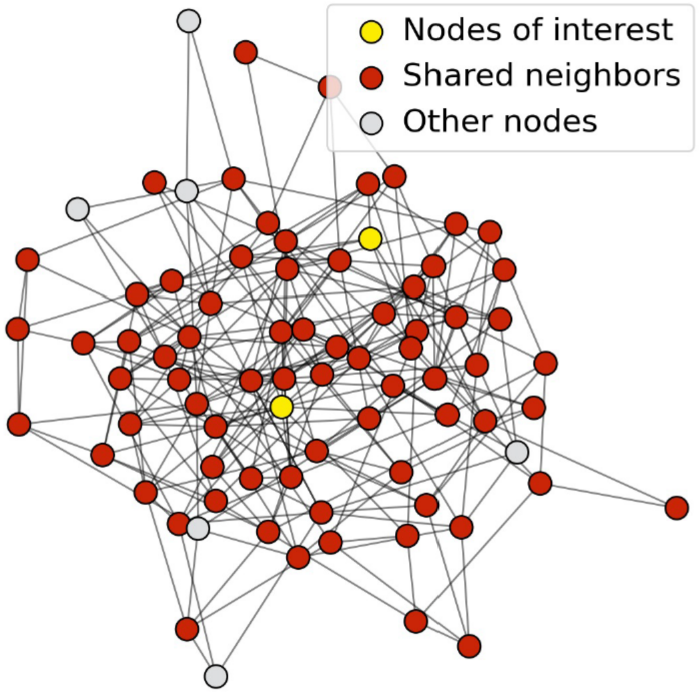
1-hop neighbor overlap
Only 1 node



2-hop neighbor overlap
About 20 nodes



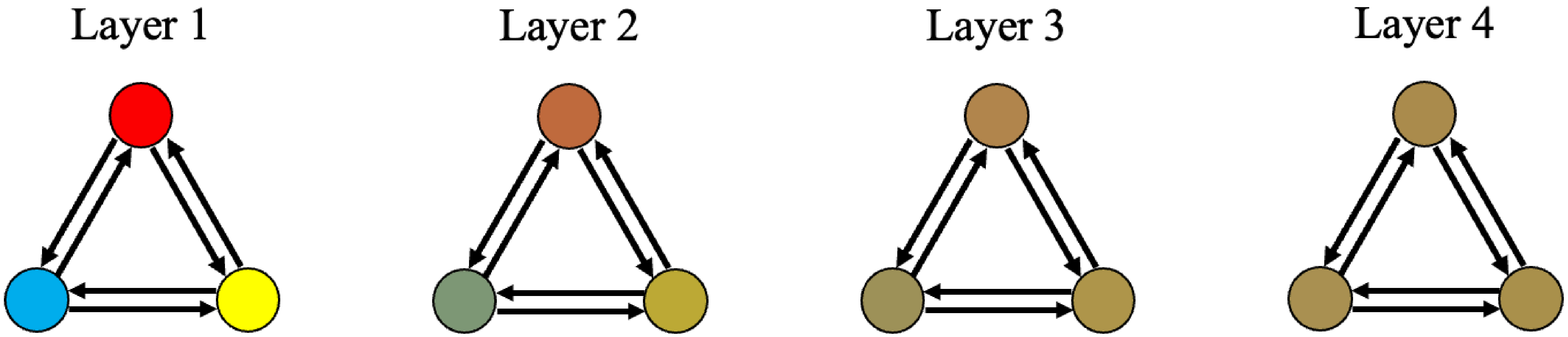
3-hop neighbor overlap
Almost all the nodes!



Deep GNN means Large receptive field

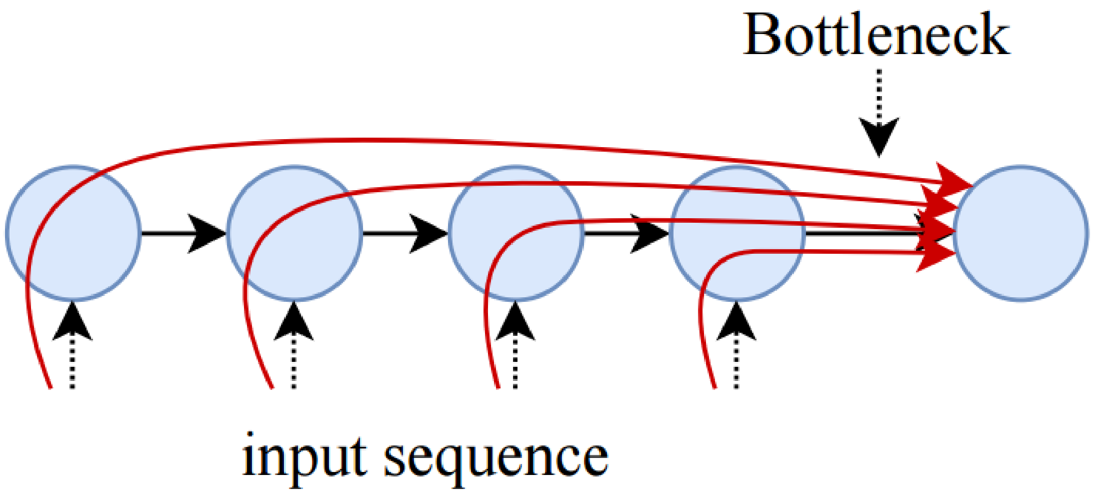
Deep?

Oversquanshing

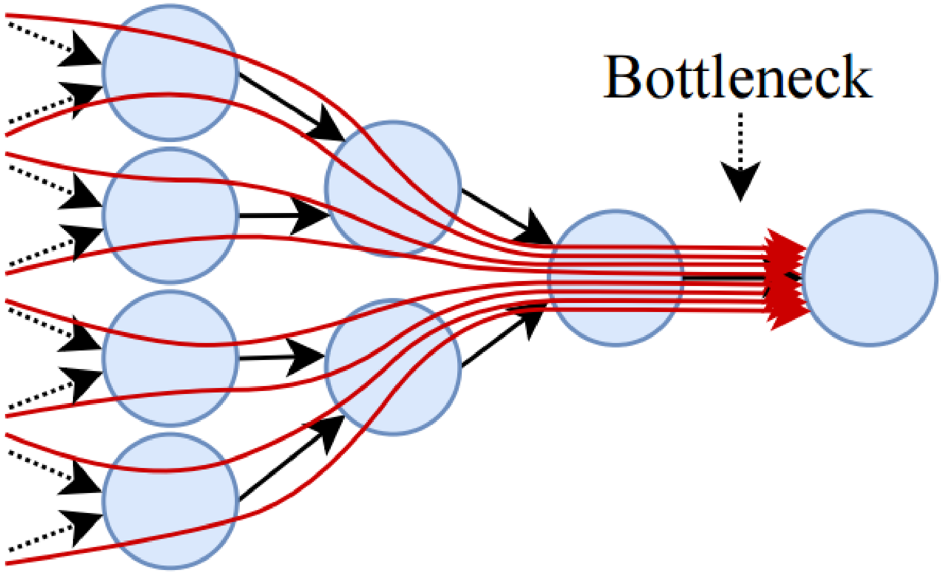


Mean undisguised for target node

Deep?



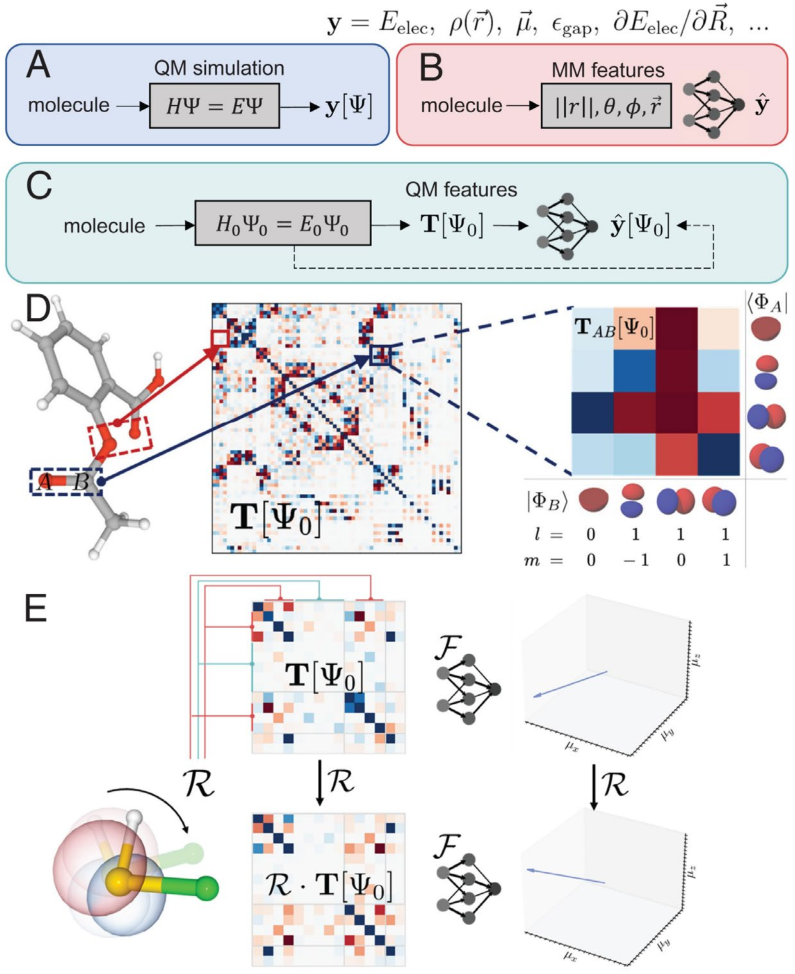
(a) The bottleneck of RNN seq2seq models

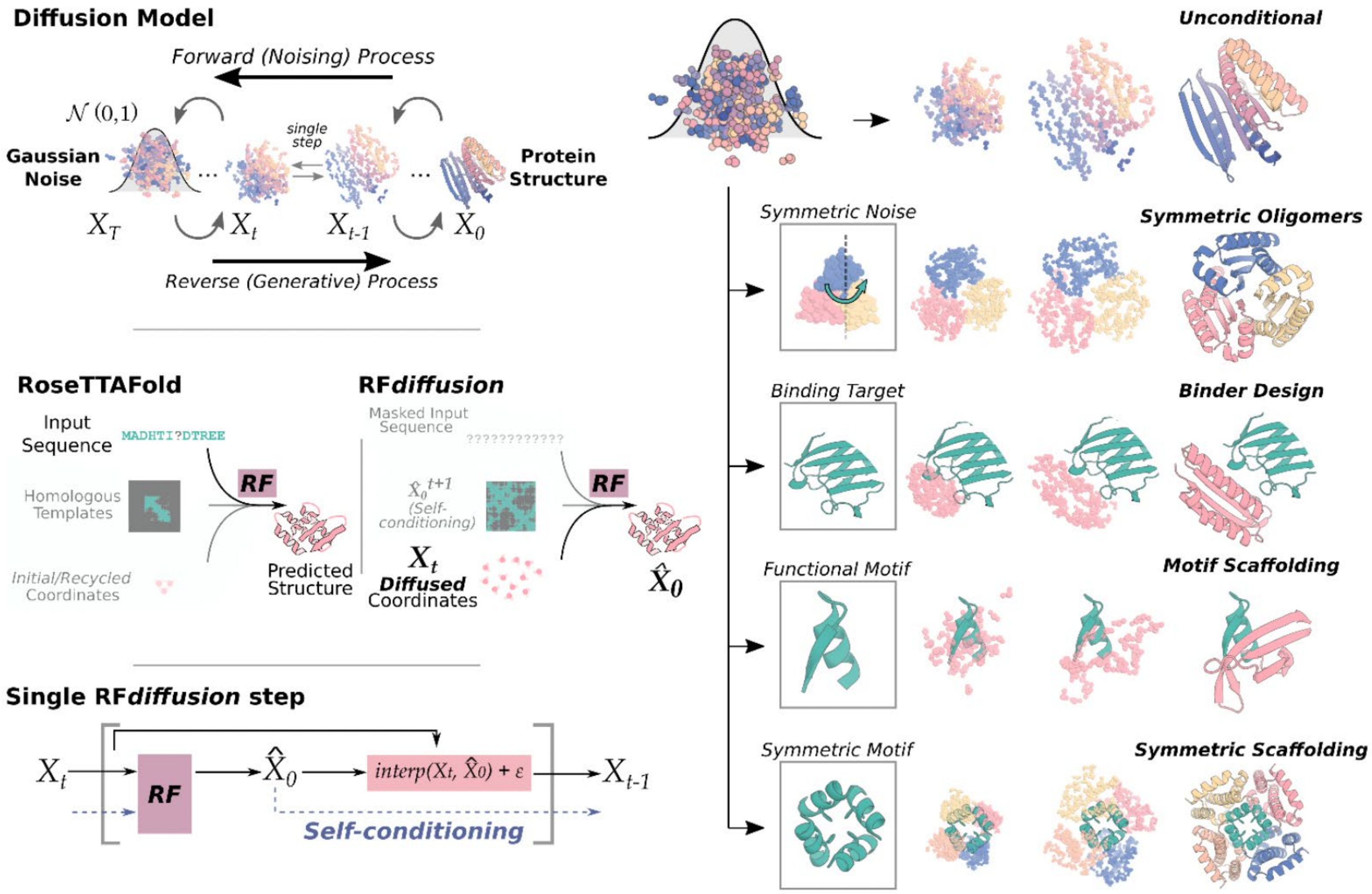


(b) The bottleneck of graph neural networks

Future

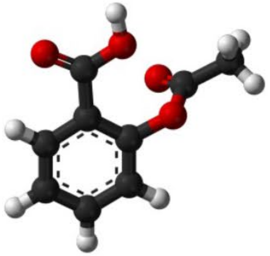
"AI4Science"



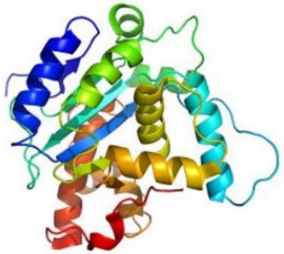


Future

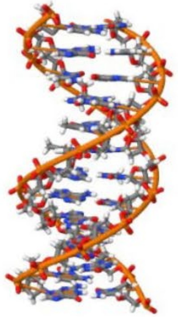
“Geometric Graphs”



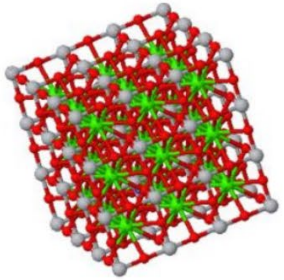
Small Molecules



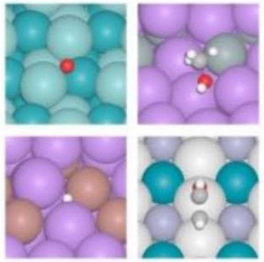
Proteins



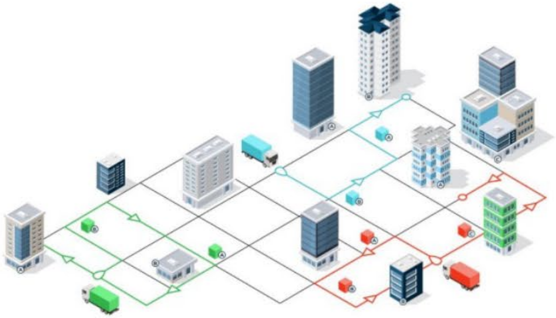
DNA/RNA



Inorganic Crystals

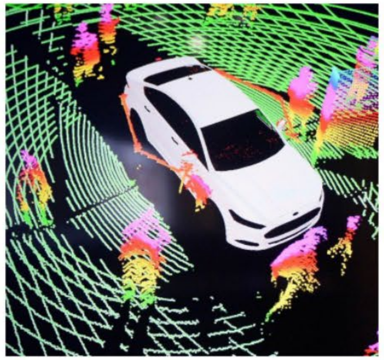


Catalysis Systems



Transportation & Logistics

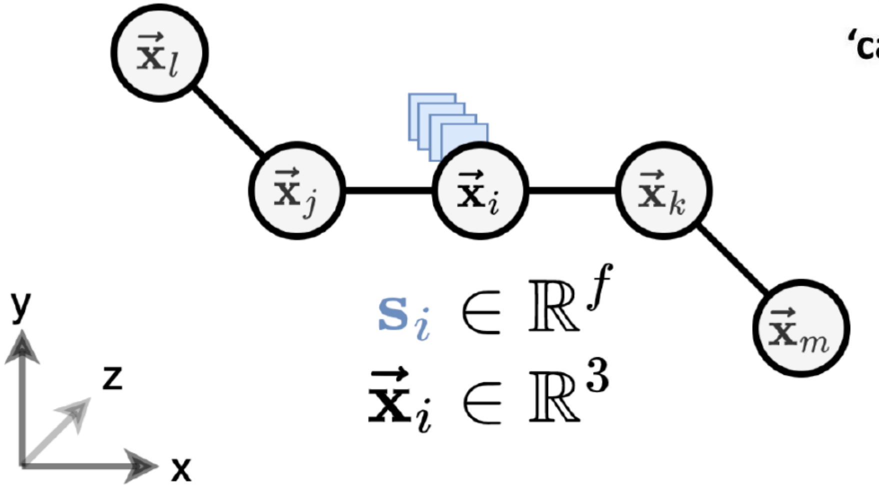
Robotic Navigation

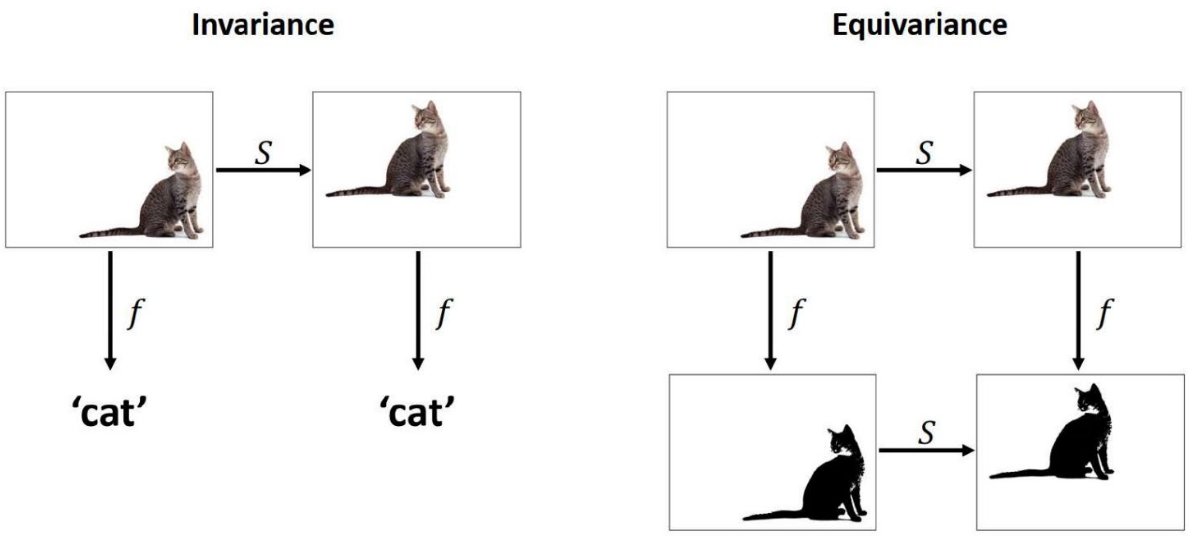


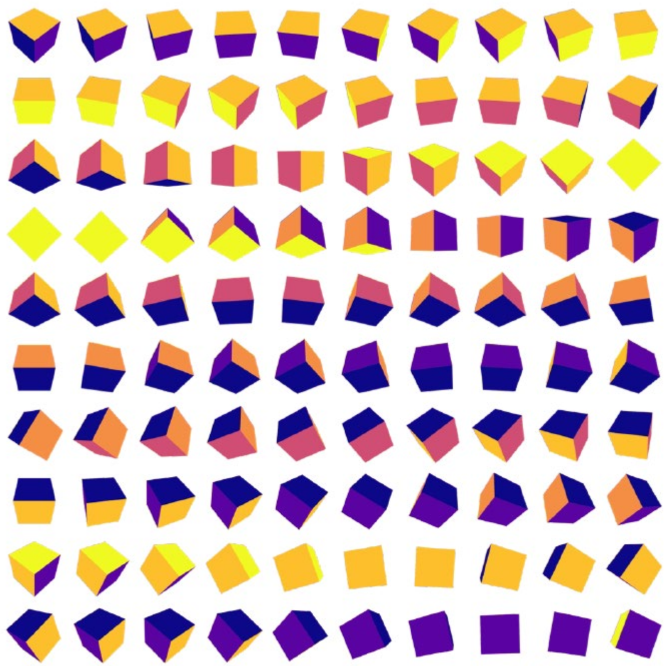
3D Computer Vision

Future

“Geometric Graphs”







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

Thank you

&More Discussion