Graph Neural Network

엔자이너 연구실

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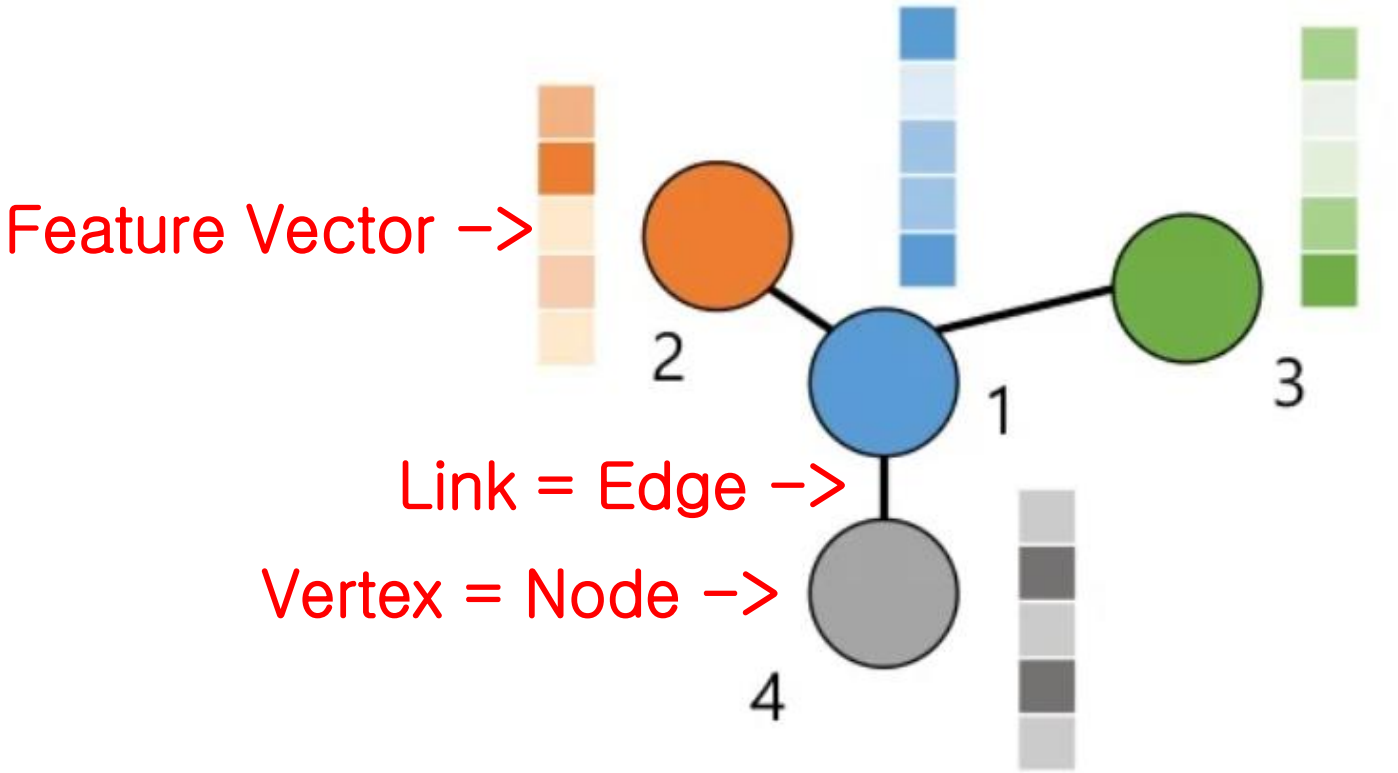
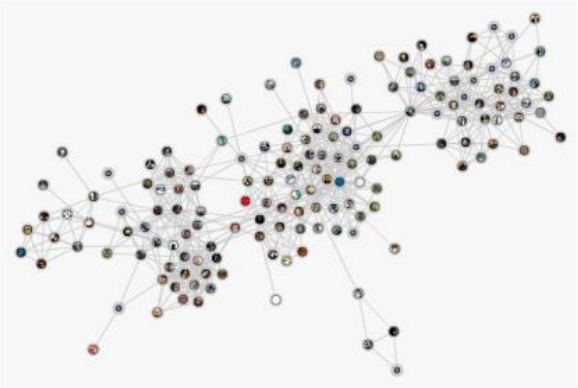
- Graph Neural Network

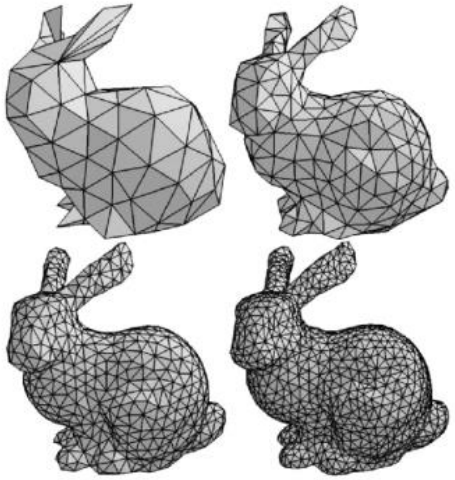
Graph Data Structure



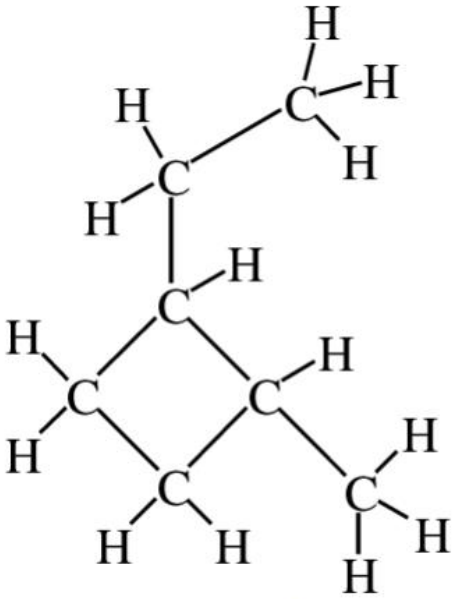
Graph Data Structure



Social Graph



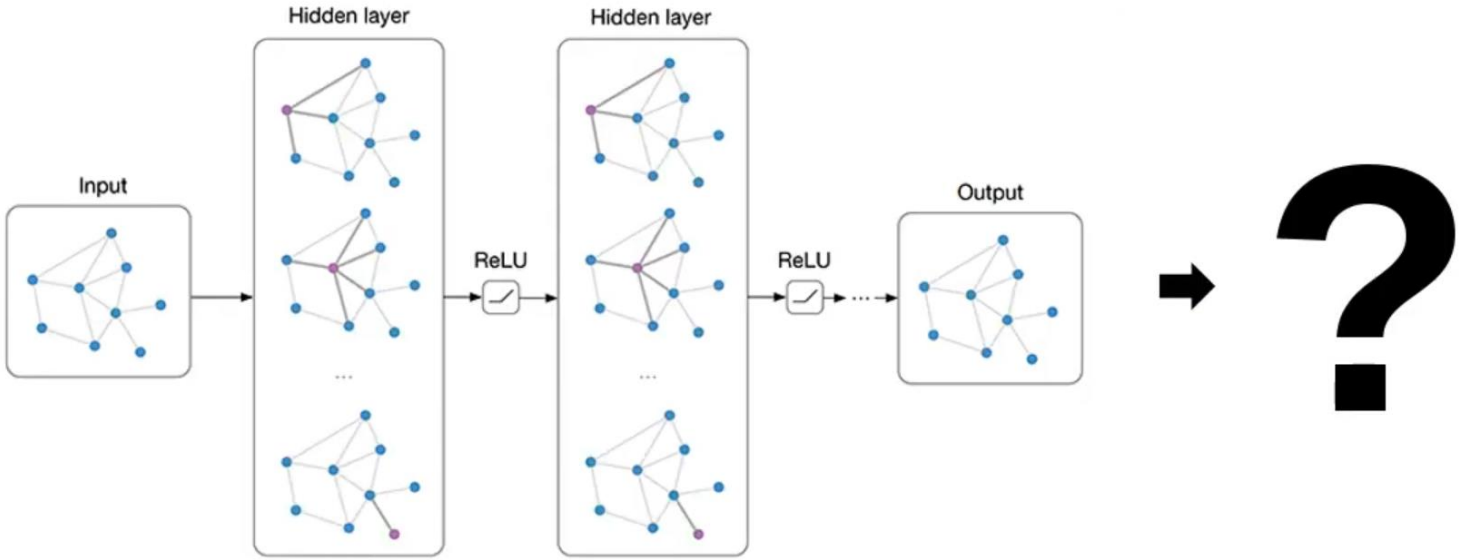
3D Mesh



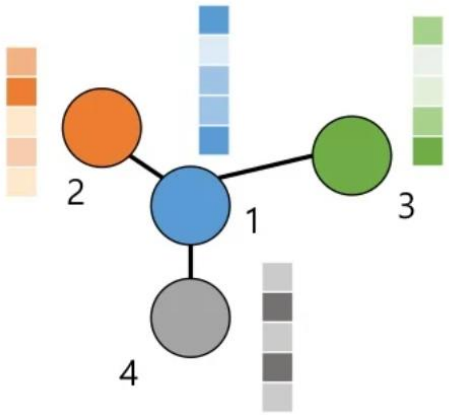
Molecular Graph

Graph Neural Network

- Node focused task
  - Node classification
  - Link prediction
  - Feature Prediction
- Graph focused task



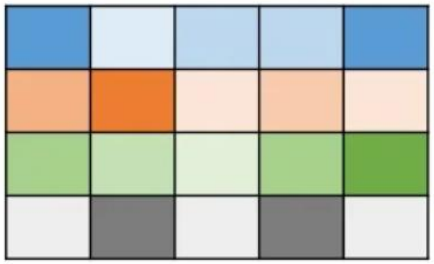
Graph Neural Network



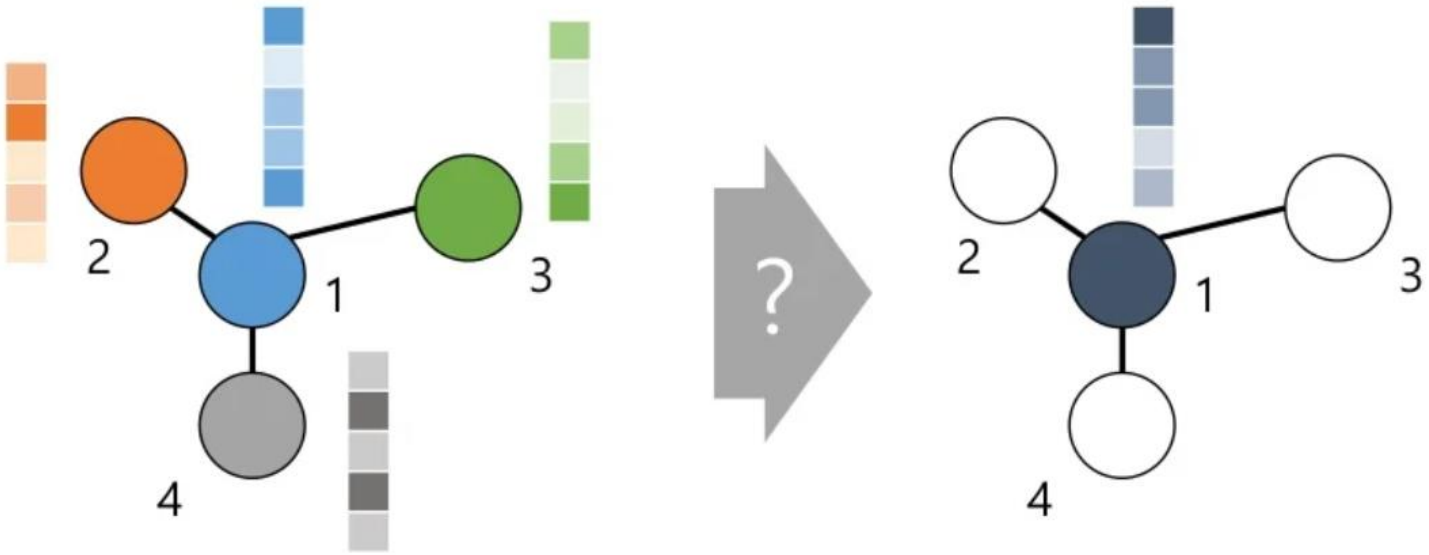
Adjacency Matrix **A** (4 x 4)

1	1	1	1
1	1	0	0
1	0	1	0
1	0	0	1

Feature Matrix **X** (4 x 5)



Graph Neural Network



Graph Neural Network

Adjacency Matrix **A** (4 x 4)

1	1	1	1
1	1	0	0
1	0	1	0
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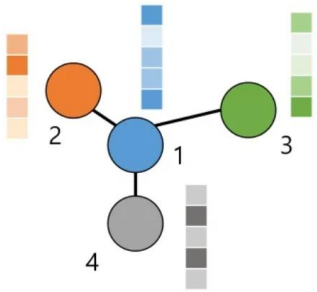
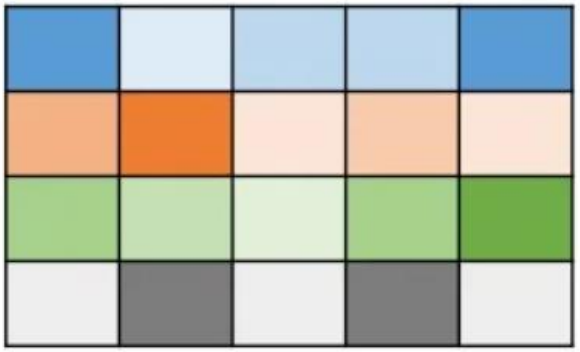
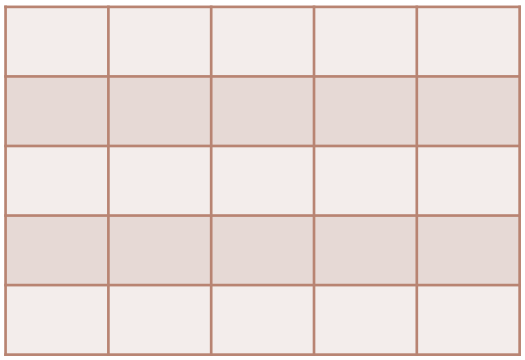
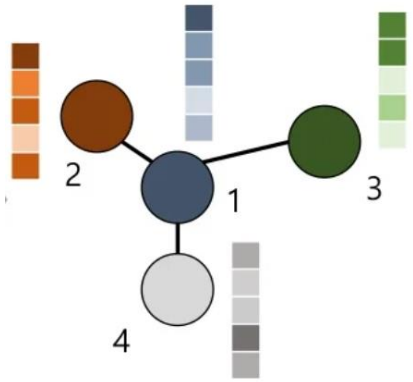


Feature Matrix **X** (4 x 5)



Weight

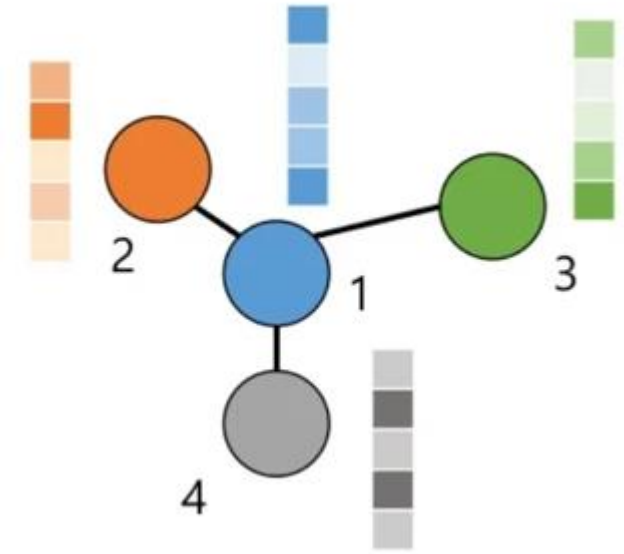




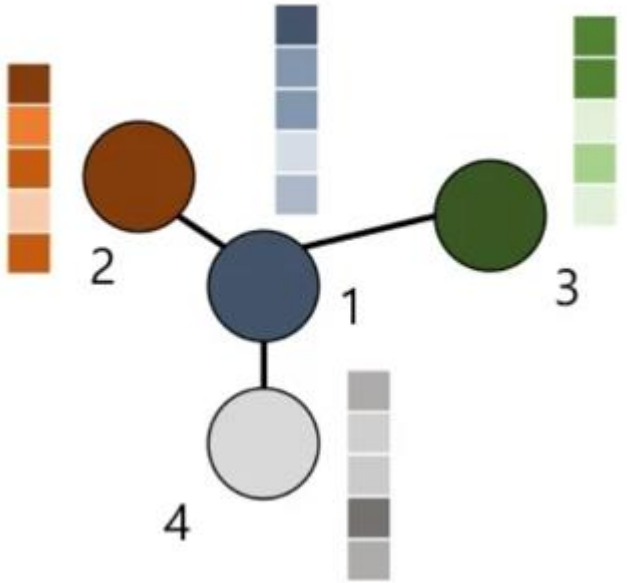
$$H_2^{(l+1)} = \sigma\left(H_1^{(l)}W^{(l)} + H_2^{(l)}W^{(l)} + H_3^{(l)}W^{(l)} + H_4^{(l)}W^{(l)} + b^{(l)}\right)$$

0 0

Graph Neural Network

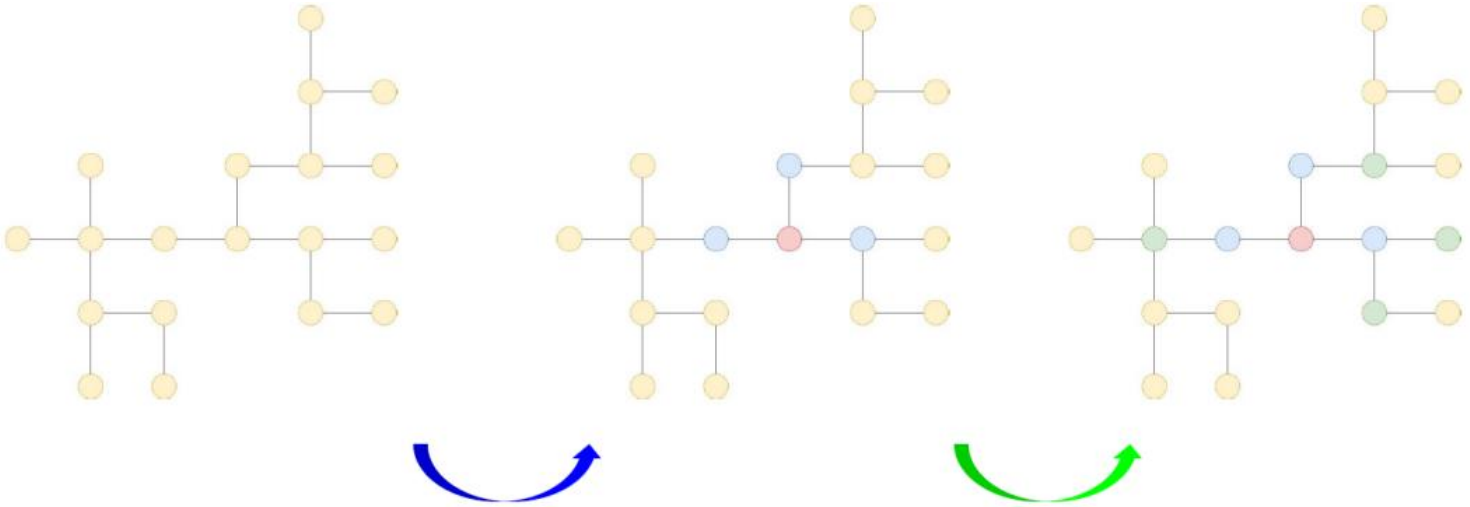


$(l+1)$ 번째 레이어



$$H^{(l+1)} = \sigma\left(AH^{(l)}W^{(l)} + b^{(l)}\right)$$

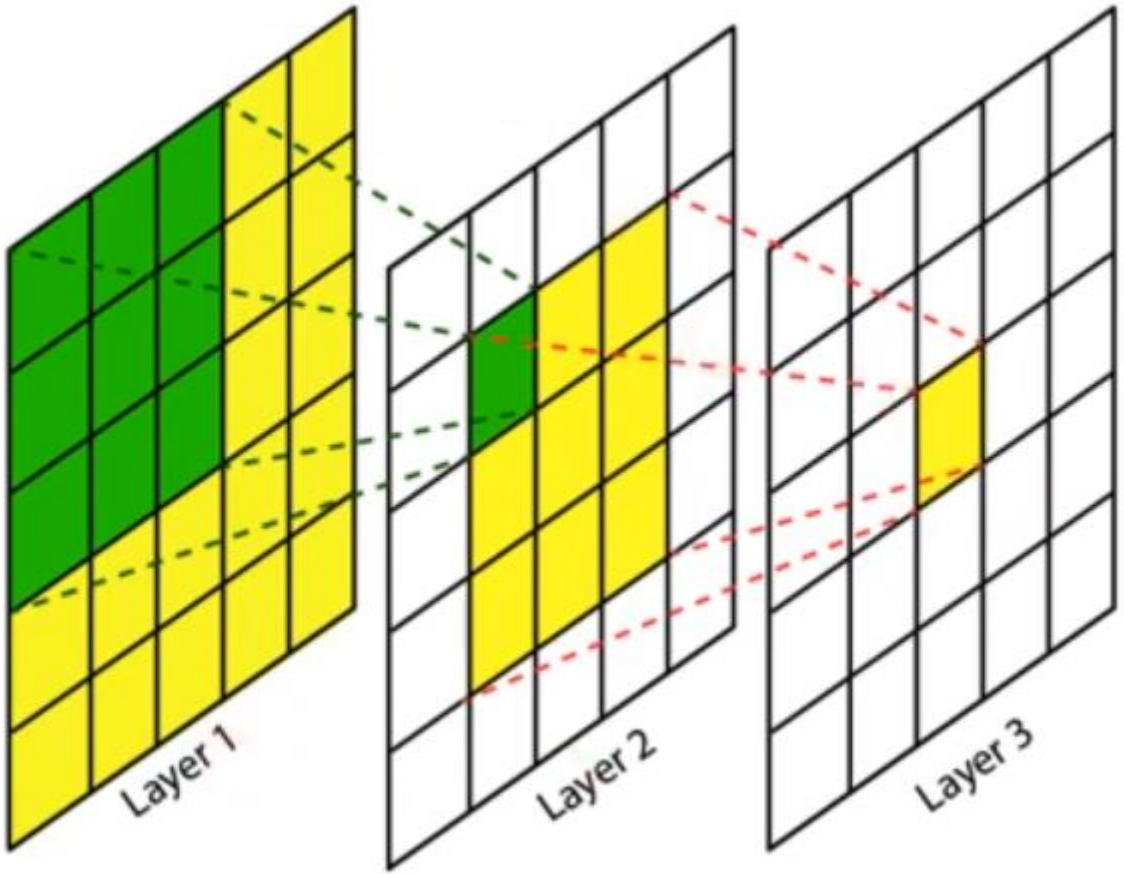
Graph Neural Network



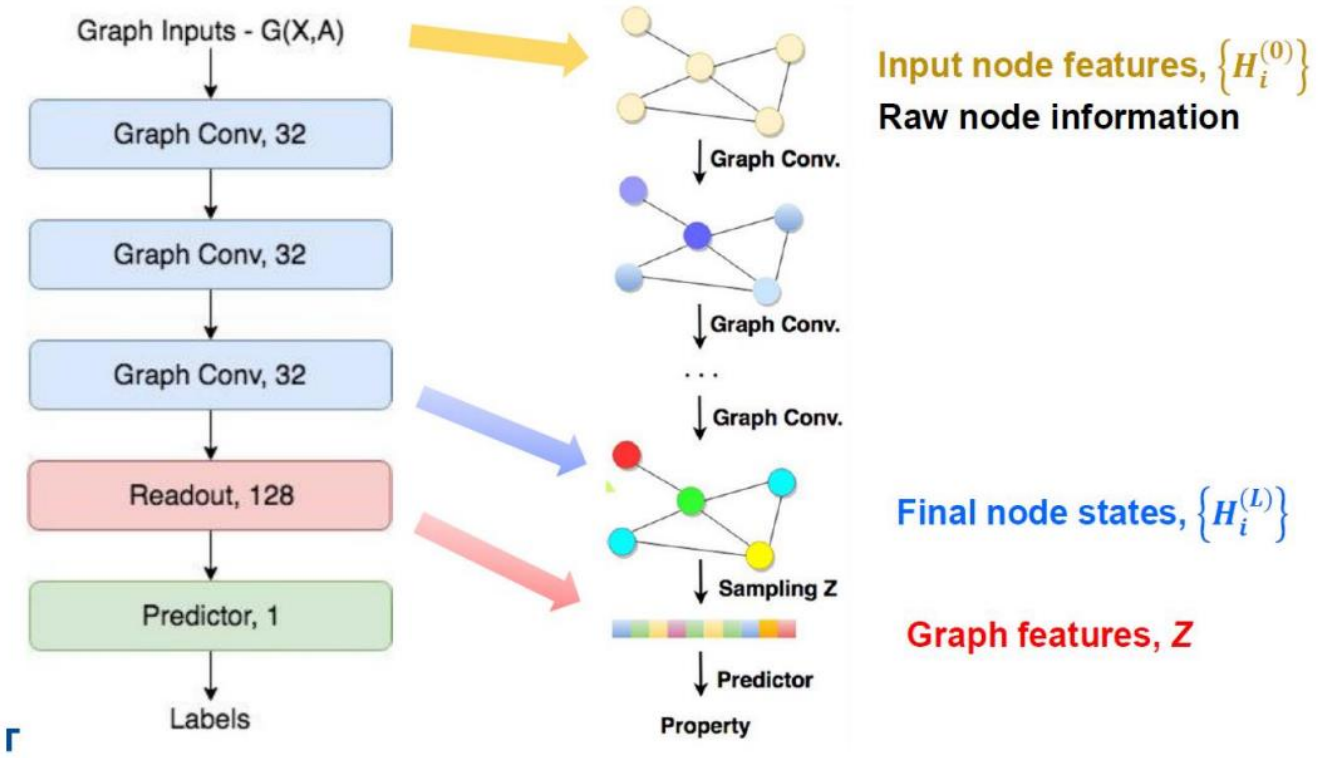
$$H^{(1)} = \sigma\left(AH^{(0)}W^{(0)}\right) \qquad H^{(2)} = \sigma\left(AH^{(1)}W^{(1)}\right)$$

Graph Neural Network

- CNN

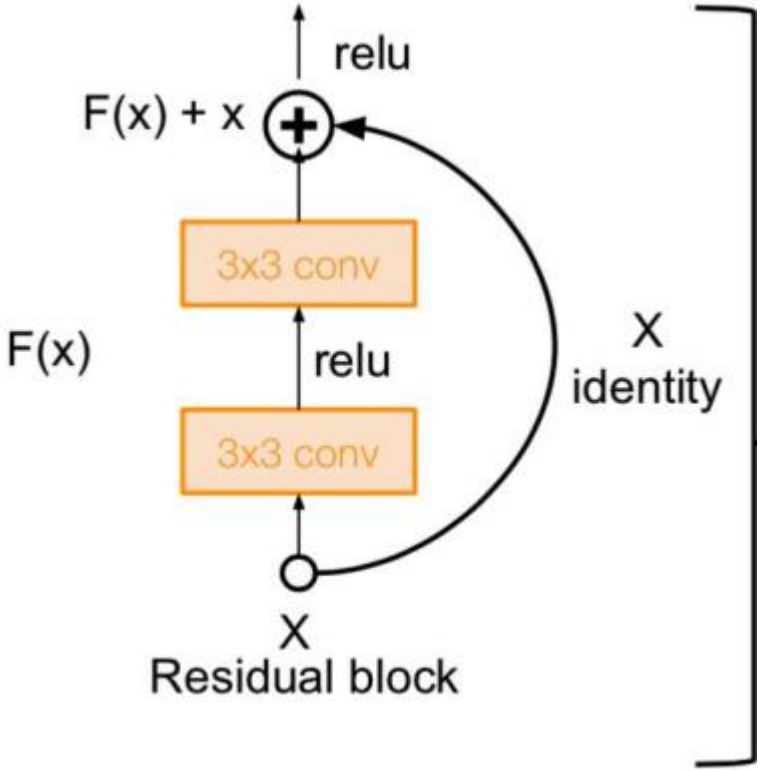


Graph Neural Network



Graph Neural Network

- ResNet
  - Skip connection



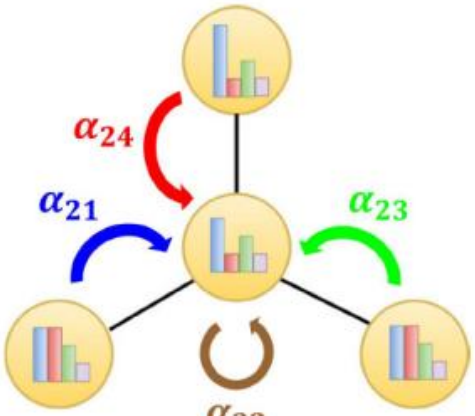
Graph Neural Network

- Attention mechanism

Vanilla GCN updates information of neighbor atoms **with same importance**.

$$H^{(l+1)} = \sigma\left(\sum_{j \in N(i)} H_j^{(l)} W^{(l)}\right)$$

Attention mechanism enables it to update nodes **with different importance**



$$H^{(l+1)} = \sigma\left(\sum_{j \in N(i)} \alpha_{ij} H_j^{(l)} W^{(l)}\right)$$

How to implement GNNs in my study