

# Graph Neural Network

엔자이너 연구실

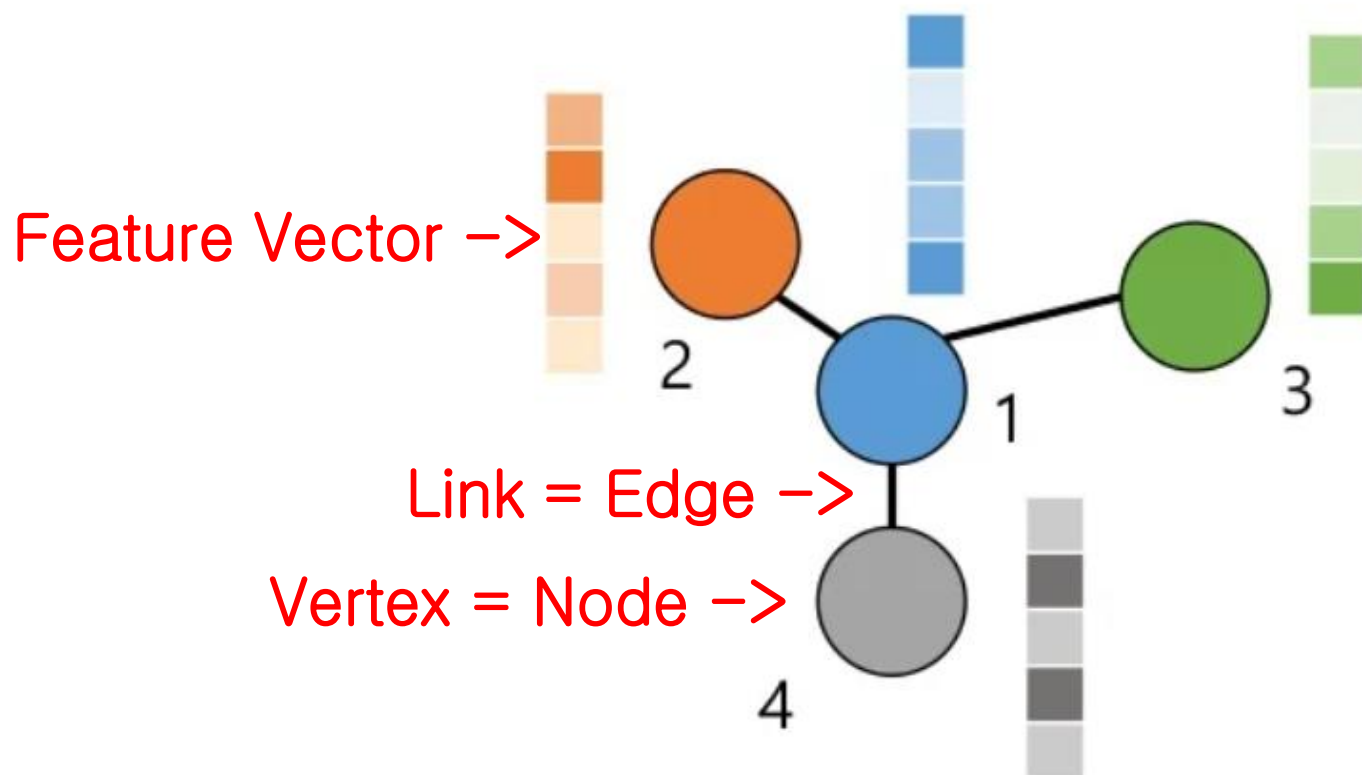
# Contents

---

- ▶ Graph Data Structure
- ▶ Graph Neural Network

# Graph Data Structure

---

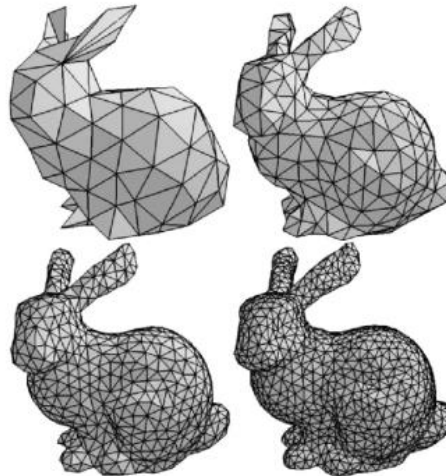


# Graph Data Structure

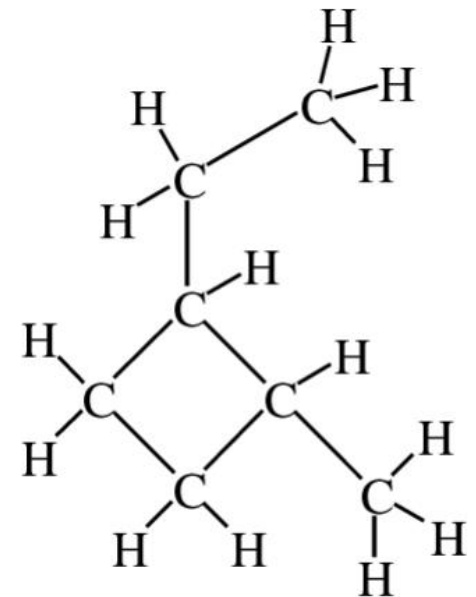
---



Social Graph



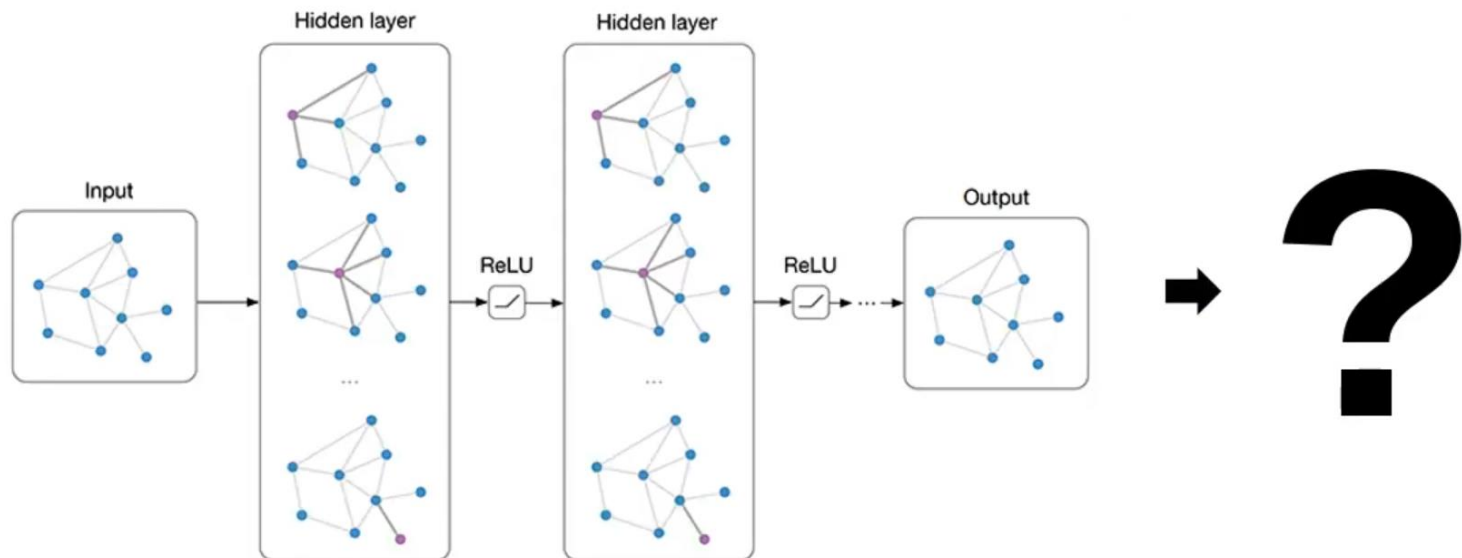
3D Mesh



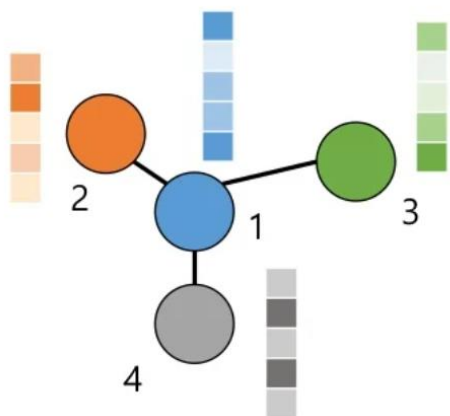
Molecular Graph

# Graph Neural Network

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



# Graph Neural Network



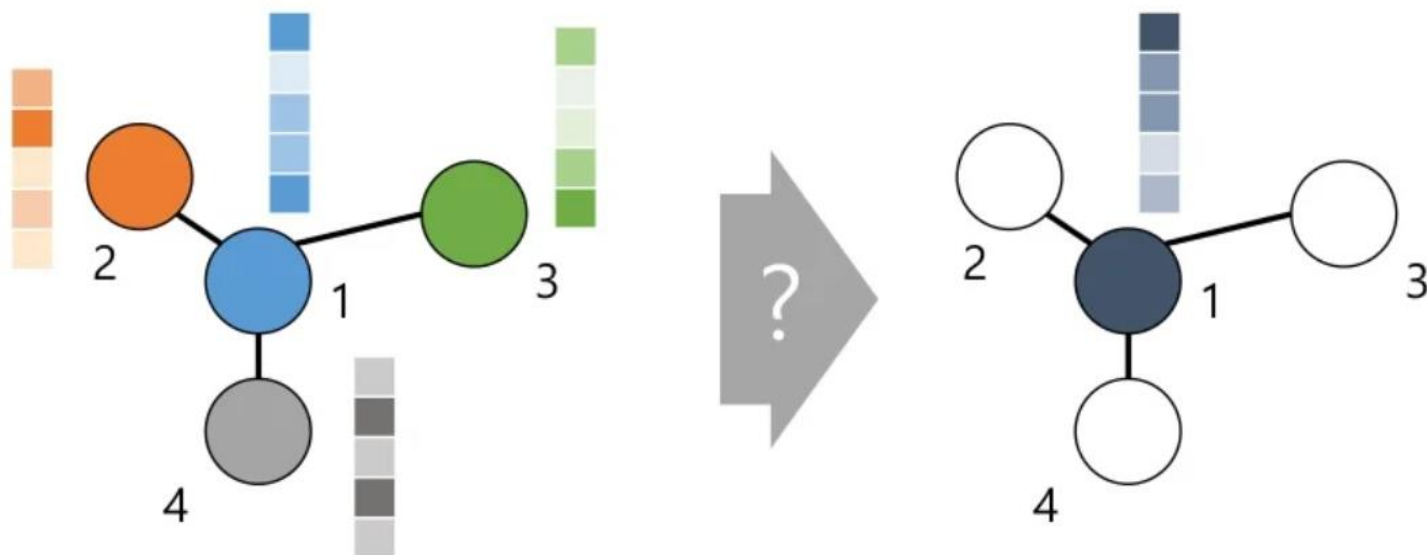
Adjacency Matrix  $\mathbf{A}$  (4 x 4)

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

Feature Matrix  $\mathbf{X}$  (4 x 5)

Blue	Light Blue	Light Blue	Light Blue	Blue
Orange	Dark Orange	Light Orange	Light Orange	Light Orange
Green	Light Green	Light Green	Light Green	Dark Green
Gray	Dark Gray	Light Gray	Dark Gray	Light Gray

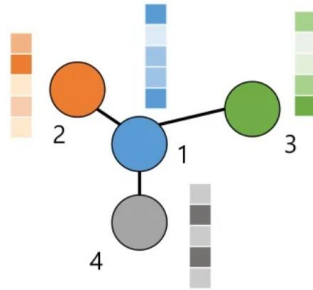
# Graph Neural Network



# Graph Neural Network

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

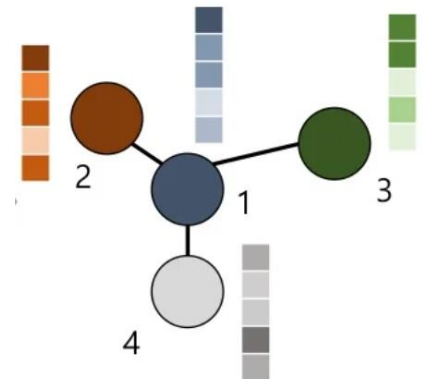
1	1	1	1
1	1	0	0
1	0	1	0
1	0	0	1



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

Blue	Light Blue	Light Blue	Light Blue	Blue
Orange	Orange	Light Orange	Light Orange	Light Orange
Green	Green	Light Green	Light Green	Green
Grey	Dark Grey	Light Grey	Dark Grey	Light Grey

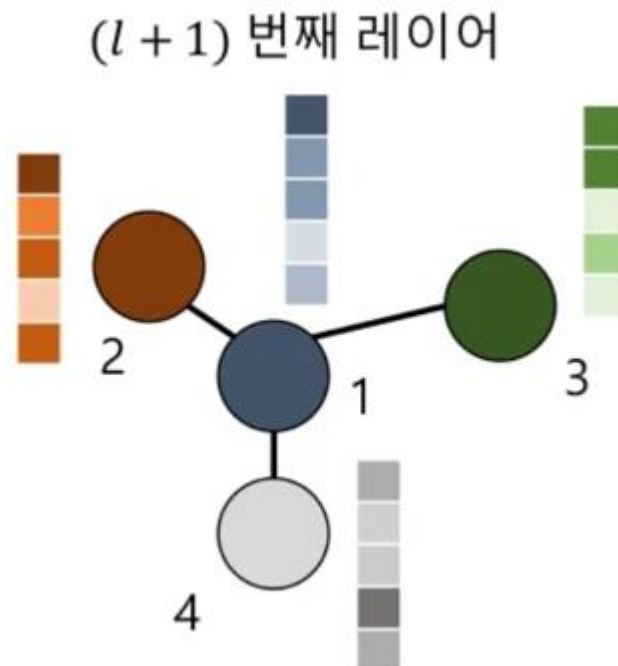
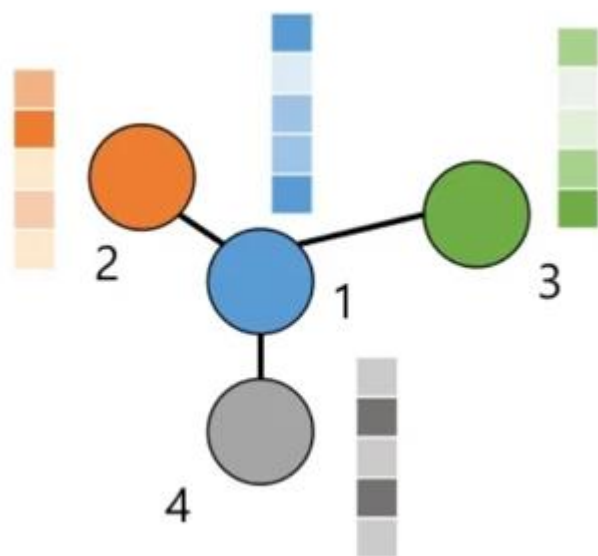
Weight

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

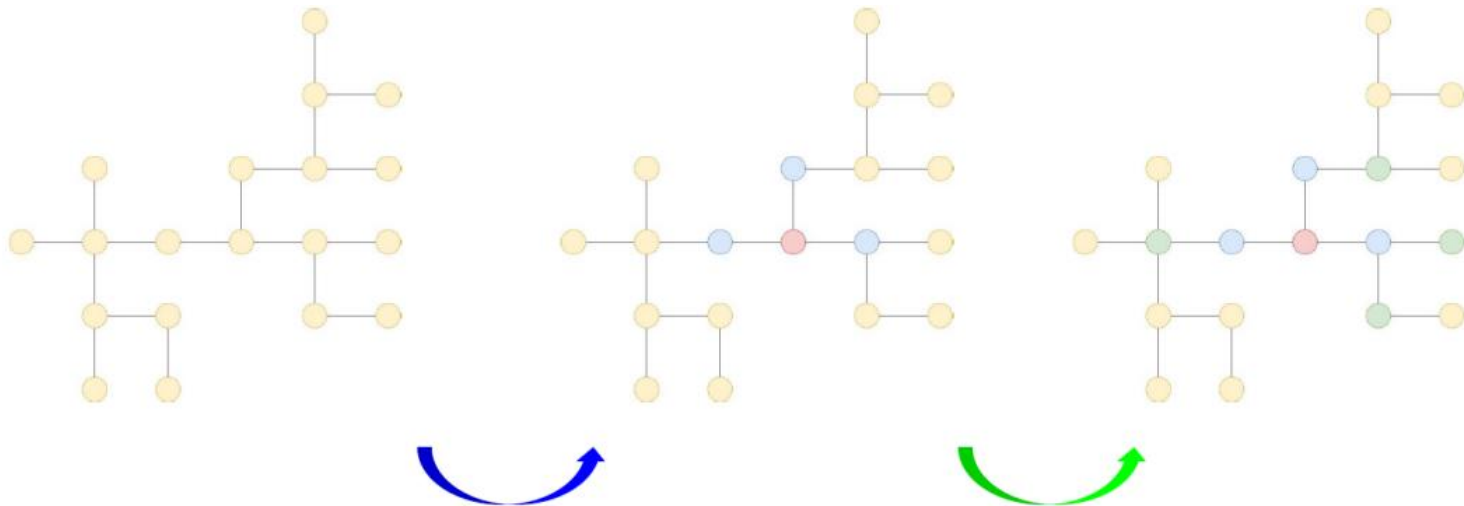


# Graph Neural Network



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

# Graph Neural Network

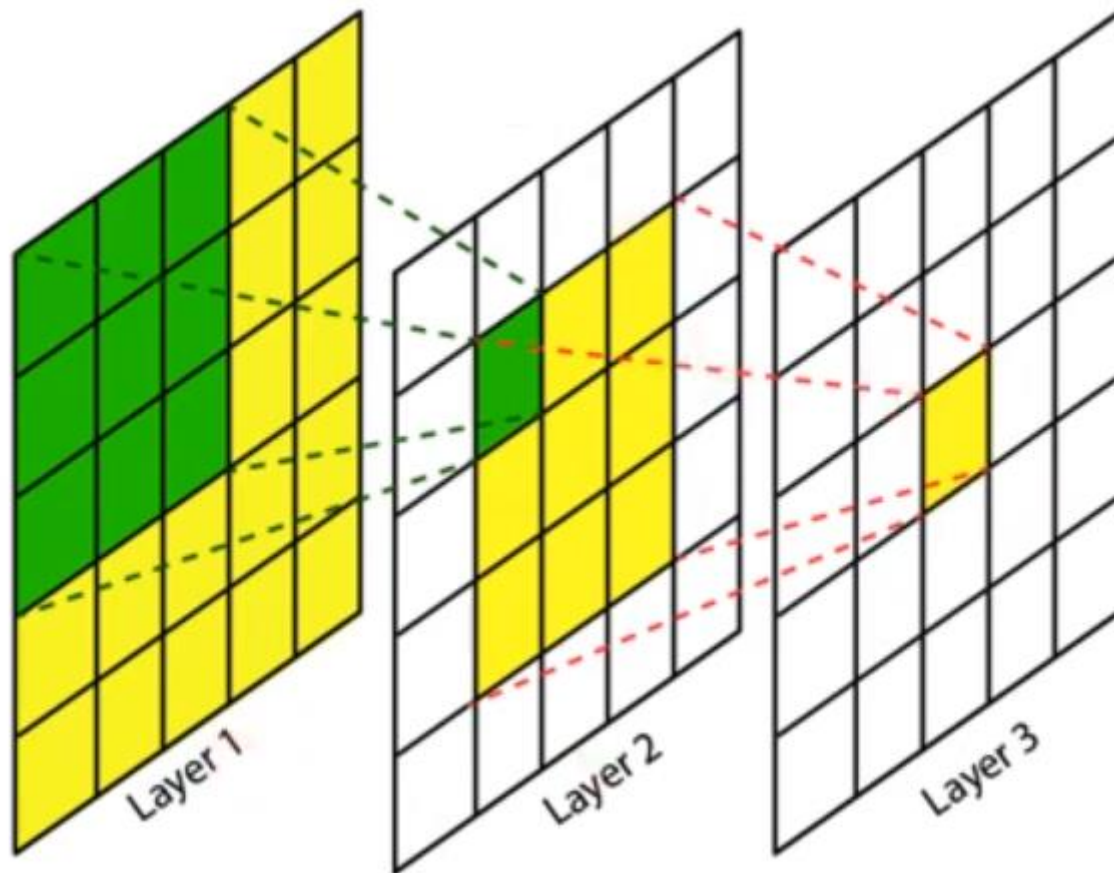


$$H^{(1)} = \sigma(AH^{(0)}W^{(0)})$$

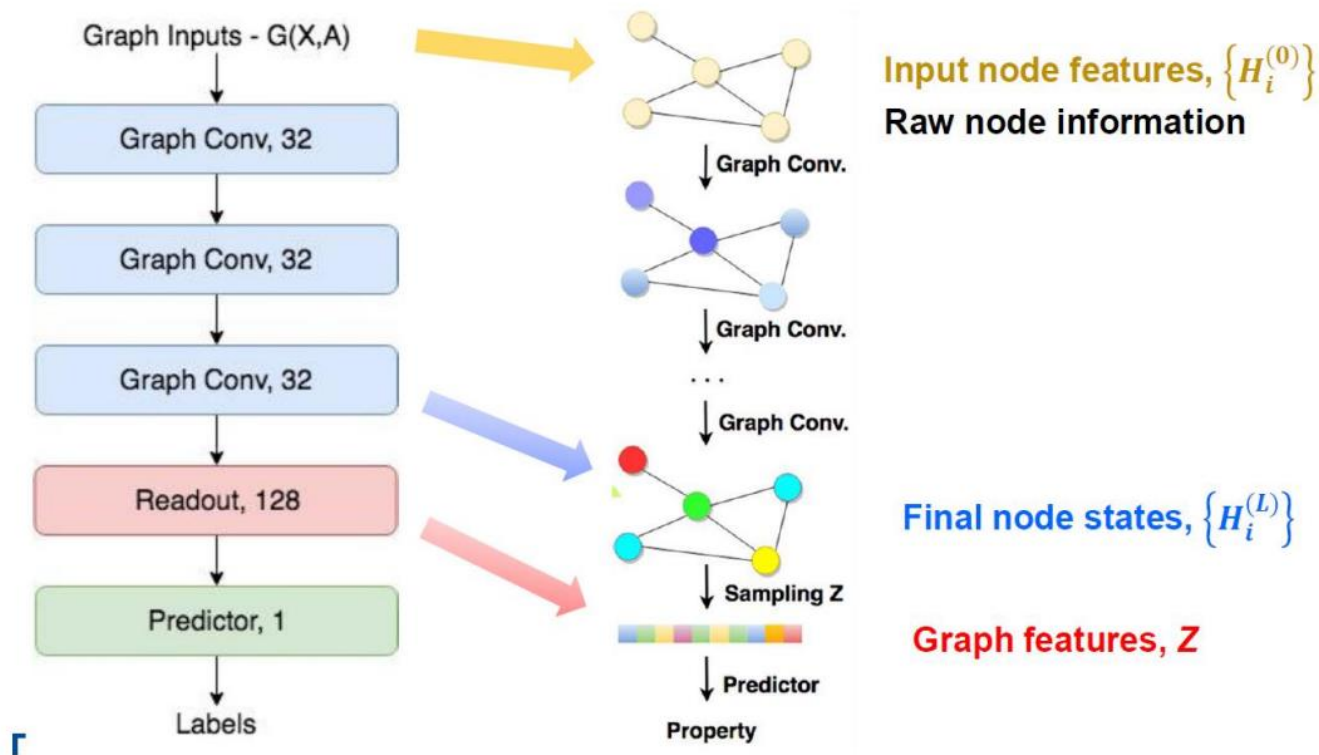
$$H^{(2)} = \sigma(AH^{(1)}W^{(1)})$$

# Graph Neural Network

## ▶ CNN



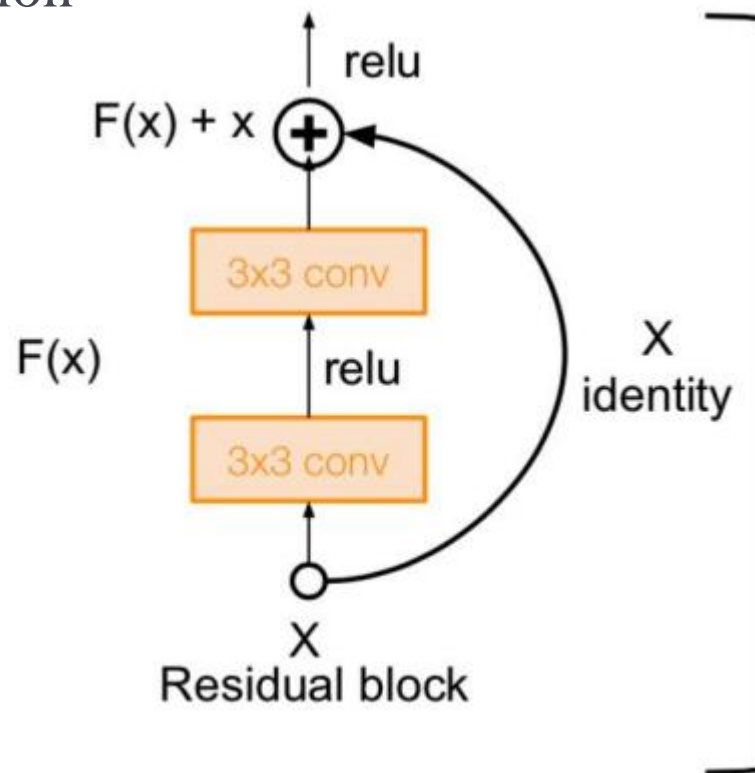
# Graph Neural Network



# Graph Neural Network

## ▶ ResNet

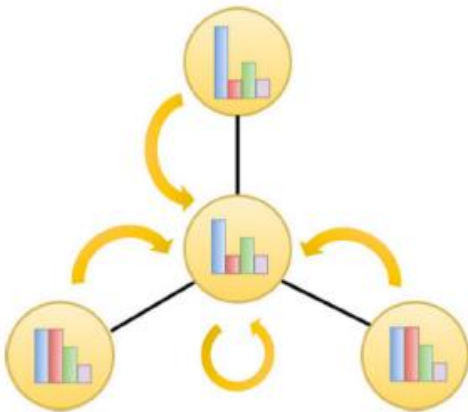
### ▶ Skip connection



# Graph Neural Network

## ▶ Attention mechanism

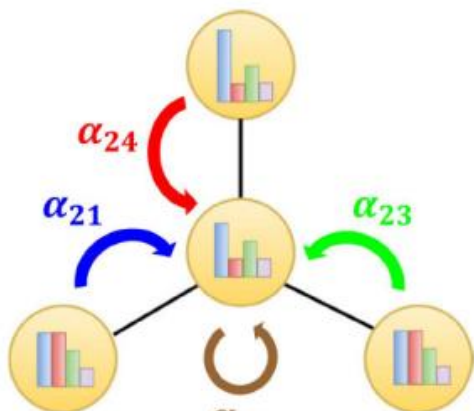
Vanilla GCN updates information of neighbor atoms **with same importance**.



The diagram shows a central node (yellow circle with a bar chart) connected to three other nodes (yellow circles with bar charts). Three yellow curved arrows point from the three neighbor nodes towards the central node, indicating that all neighbors contribute equally to the update.

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

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



The diagram shows a central node (yellow circle with a bar chart) connected to three other nodes (yellow circles with bar charts). Three colored curved arrows point from the neighbor nodes towards the central node, representing different attention weights: a red arrow labeled  $\alpha_{24}$  from the top node, a blue arrow labeled  $\alpha_{21}$  from the bottom-left node, and a green arrow labeled  $\alpha_{23}$  from the bottom-right node. A brown self-loop arrow labeled  $\alpha_{22}$  is also shown on the central node.

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

# How to implement GNNs in my study

