



## Baseline GNNs

### 1. GCN (Graph Convolutional Network)

$$\mathbf{h}'_v = \max_{u \in \mathcal{N}(v) \cup \{u\}} \frac{1}{\sqrt{|\mathcal{N}(v)| |\mathcal{N}(u)|}} \mathbf{h}_u^{(l)} W^{(l)} \quad (1)$$

### 2. GIN (Graph Isomorphism Network)

$$\mathbf{h}'_v = \sigma \left( (1 + \epsilon) \cdot \mathbf{h}_v^{(l)} + \max_{u \in \mathcal{N}(v)} \mathbf{h}_u^{(l)} \right) \quad (2)$$

where  $\sigma$  is a linear layer.

### 3. GraphSAGE (Graph Sampling and Aggregation)

$$\mathbf{h}'_v = \mathbf{W}_1 \cdot \mathbf{h}_v^{(l)} + \mathbf{W}_2 \cdot \max_{u \in \mathcal{N}(v)} \mathbf{h}_u^{(l)} \quad (3)$$

### 4. PNA (Principal Neighbourhood Aggregation)

$$\mathbf{h}'_v = \bigoplus_{u \in \mathcal{N}(v)} \mathbf{MLP}_1 \cdot \left( \mathbf{h}_u^{(l)}, \mathbf{h}_v^{(l)} \right) \quad (4)$$

$$\text{where } \bigoplus = \underbrace{\begin{bmatrix} 1 \\ S(\mathbf{D}, \alpha = 1) \\ S(\mathbf{D}, \alpha = -1) \end{bmatrix}}_{\text{scalers}} \otimes \underbrace{\begin{bmatrix} \mu \\ \sigma \\ \max \\ \min \end{bmatrix}}_{\text{aggregators}} \quad (5)$$

- GRU is the default choice for updating the current state in all baseline GNNs.

$$\mathbf{h}_v^{(l+1)} = \mathbf{GRU} \left( \mathbf{h}_v^{(l)}, \mathbf{h}'_v \right) \quad (6)$$