Graph Convolution Network (GCN) Example

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Given the following matrices:

Adjacency Matrix A (with self-loops):

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}, \quad \text{dimension: } 3 \times 3$$

Feature Matrix X:

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \end{bmatrix}, \quad \text{dimension: } 3 \times 2$$

Weight Matrix W:

$$W = \begin{bmatrix} 0.5 & 0.2 & 0.1 \\ 0.1 & 0.4 & 0.3 \end{bmatrix}, \quad \text{dimension: } 2 \times 3$$

Step 1: Normalize the Adjacency Matrix

The degree matrix D is:

$$D = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 3 \end{bmatrix}, \quad \text{dimension: } 3 \times 3$$

The normalized adjacency matrix $\hat{A}_{\text{norm}}$ is computed as:

$$\hat{A}_{\text{norm}} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

The inverse square root of D is:

$$D^{-\frac{1}{2}} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{3}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \approx \begin{bmatrix} 0.707 & 0 & 0 \\ 0 & 0.577 & 0 \\ 0 & 0 & 0.577 \end{bmatrix}$$

Thus, the normalized adjacency matrix is:

$$\hat{A}_{\text{norm}} = \begin{bmatrix} 0.707 & 0.5 & 0 \\ 0.5 & 0.707 & 0.577 \\ 0 & 0.577 & 0.707 \end{bmatrix}, \quad \text{dimension: } 3 \times 3$$

Step 2: Aggregation Step

Next, compute the product of the normalized adjacency matrix and the feature matrix:

$$\hat{A}_{\text{norm}}X = \begin{bmatrix} 0.707 & 0.5 & 0 \\ 0.5 & 0.707 & 0.577 \\ 0 & 0.577 & 0.707 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \end{bmatrix}$$

The multiplication results in:

$$\hat{A}_{\text{norm}}X = \begin{bmatrix} 1.707 & 2.914 \\ 3.622 & 5.364 \\ 3.172 & 4.657 \end{bmatrix}, \quad \text{dimension: } 3 \times 2$$

Step 3: Apply the Weight Matrix

Now apply the weight matrix W to the aggregated result:

$$Z = (\hat{A}_{\text{norm}}X)W = \begin{bmatrix} 1.707 & 2.914 \\ 3.622 & 5.364 \\ 3.172 & 4.657 \end{bmatrix} \begin{bmatrix} 0.5 & 0.2 & 0.1 \\ 0.1 & 0.4 & 0.3 \end{bmatrix}$$

Performing the multiplication row by row, we get:

$$Z = \begin{bmatrix} 1.162 & 1.625 & 1.235 \\ 2.691 & 3.395 & 2.241 \\ 2.166 & 3.058 & 2.026 \end{bmatrix}, \quad \text{dimension: } 3 \times 3$$

Step 4: Apply Activation Function

We apply the ReLU activation function $\sigma(x) = \max(0, x)$ to the result. Since all values are positive, the result remains unchanged:

$$Z = \begin{bmatrix} 1.162 & 1.625 & 1.235 \\ 2.691 & 3.395 & 2.241 \\ 2.166 & 3.058 & 2.026 \end{bmatrix}, \quad \text{dimension: } 3 \times 3$$