1 Question 1

After the message passing layer, the representations of the nodes are updated as follows :

$$z_i^{(2)} = \sum_{j \in \mathcal{N}_i} \alpha_{ij}^{(2)} \mathbf{W}^{(2)} z_j^{(1)}$$

Thus, we can see how the formuly apply for $z_1^{(2)}$ and $z_4^{(2)}$:

$$z_1^{(2)} = \alpha_{1,2}^{(2)} \mathbf{W}^{(2)} z_2^{(1)} + \alpha_{1,3}^{(2)} \mathbf{W}^{(2)} z_3^{(1)}$$

$$\begin{aligned} z_4^{(2)} &= \alpha_{4,2}^{(2)} \mathbf{W}^{(2)} z_2^{(1)} + \alpha_{4,3}^{(2)} \mathbf{W}^{(2)} z_3^{(1)} + \alpha_{4,5}^{(2)} \mathbf{W}^{(2)} z_5^{(1)} + \alpha_{4,6}^{(2)} \mathbf{W}^{(2)} z_6^{(1)} \\ &= 2\alpha_{4,2}^{(2)} \mathbf{W}^{(2)} z_2^{(1)} + 2\alpha_{4,3}^{(2)} \mathbf{W}^{(2)} z_3^{(1)} \end{aligned}$$

As well, with the formula of $\alpha_{i,j}^{(t+1)}$ and with $z_1^{(2)} = z_4^{(2)}$, that :

$$2\alpha_{4,2}^{(2)} = \alpha_{1,2}^{(2)}$$
$$2\alpha_{4,3}^{(2)} = \alpha_{1,3}^{(2)}$$

Thus, we can conclude that :

$$z_1^2 = z_4^2$$

2 Question 2

This must comes from the adjacency matrix A. In fact, we are here focusing on the relationship between the members of a karate club, so the edges in the graph will be very important. And that's why we will still get a good accuracy, even without discrimination according to the features matrix X.

3 Question 3

Here are the representations of the three graph for each one of the readout functions.

Sum Readout:

$$z_{G1} = \begin{bmatrix} 2.9 & 2.3 & 1.9 \end{bmatrix}, \quad z_{G2} = \begin{bmatrix} 3.4 & 1.9 & 4.3 \end{bmatrix}, \quad z_{G3} = \begin{bmatrix} 1.8 & 1.2 & 1.6 \end{bmatrix}$$

Mean Readout:

$$z_{G1} = \begin{bmatrix} 0.9667 & 0.7667 & 0.6333 \end{bmatrix}, \quad z_{G2} = \begin{bmatrix} 0.85 & 0.475 & 1.075 \end{bmatrix}, \quad z_{G3} = \begin{bmatrix} 0.9 & 0.6 & 0.8 \end{bmatrix}$$

Max Readout:

$$z_{G1} = \begin{bmatrix} 2.2 & 1.8 & 1.5 \end{bmatrix}, \quad z_{G2} = \begin{bmatrix} 2.2 & 1.8 & 1.5 \end{bmatrix}, \quad z_{G3} = \begin{bmatrix} 2.2 & 1.8 & 1.5 \end{bmatrix}$$

As we can see, the mean readout is the best to distinguish theses graphs. We could also have chose the sum readout, but the max readout gives us the same representation for each graph.

4 Question 4

G_1 and G_2 have the same structure but not the same number of nodes. G_1 got 4 and G_2 got 8. As long as we are working on the Sum Readout, and G_2 has 2 times more nodes than G_1, we can deduce that $2z_{G1} = z_{G2}$

5 Figures

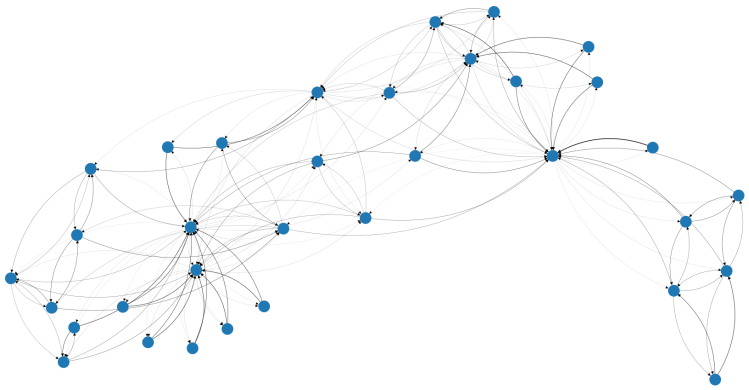

Figure 1: Visualize the karate network