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1 Question 1

$$N(v_1) = \{v_2 ; v_3\} \Rightarrow z_1^{(2)} = \sum_{j \in \mathcal{N}_1} \left(\alpha_{1j}^{(2)}\right)\left(W^{(2)}\right)\left(z_j^{(1)}\right)$$

$$\boxed{z_1^{(2)} = \alpha_{12}^{(2)} W^{(2)} z_2^{(1)} + \alpha_{13}^{(2)} W^{(2)} z_3^{(1)}}$$

$$N(v_4) = \{v_2 ; v_3 ; v_5 ; v_6\} \Rightarrow z_4^{(2)} = \sum_{j \in \mathcal{N}_4} \left(\alpha_{4j}^{(2)}\right)\left(W^{(2)}\right)\left(z_j^{(1)}\right)$$

$$z_4^{(2)} = \alpha_{42}^{(1)} W^{(2)} z_2^{(1)} + \alpha_{43}^{(1)} W^{(2)} z_3^{(1)} + \alpha_{45}^{(1)} W^{(2)} z_5^{(1)} + \alpha_{46}^{(1)} W^{(2)} z_6^{(1)}$$

$$z_4^{(2)} = \left(\alpha_{42}^{(1)} W^{(2)} + \alpha_{46}^{(1)} W^{(2)}\right) z_2^{(1)} + \left(\alpha_{43}^{(1)} W^{(2)} + \alpha_{45}^{(1)} W^{(2)}\right) z_3^{(1)} \qquad \left(z_2^{(1)} = z_6^{(1)} \,//\, z_3^{(1)} = z_5^{(1)}\right)$$

$$z_4^{(2)} = \left(\alpha_{42}^{(1)} + \alpha_{46}^{(1)}\right) W^{(2)} z_2^{(1)} + \left(\alpha_{43}^{(1)} + \alpha_{45}^{(1)}\right) W^{(2)} z_3^{(1)}$$

$$\alpha_{42}^{(1)} = \frac{\exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_2^{(1)}\right]\right)\right)}{\exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_2^{(1)}\right]\right)\right) + \exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_3^{(1)}\right]\right)\right) + \exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_5^{(1)}\right]\right)\right) + \exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_6^{(1)}\right]\right)\right)}$$

$$\alpha_{42}^{(1)} = \frac{\exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_2^{(1)}\right]\right)\right)}{2 \times \exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_2^{(1)}\right]\right)\right) + 2 \times \exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_4^{(1)} \| W^{(1)} z_3^{(1)}\right]\right)\right)} = \alpha_{46}^{(1)} \qquad \left(z_2^{(1)} = z_6^{(1)} \,//\, z_3^{(1)} = z_5^{(1)}\right)$$

$$\alpha_{12}^{(1)} = \frac{\exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_1^{(1)} \| W^{(1)} z_2^{(1)}\right]\right)\right)}{\exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_1^{(1)} \| W^{(1)} z_2^{(1)}\right]\right)\right) + \exp\left(\text{LeakyRelu}\left(a^{(1)T}\left[W^{(1)} z_1^{(1)} \| W^{(1)} z_3^{(1)}\right]\right)\right)} = \frac{1}{2} \alpha_{42}^{(1)} \qquad \left(z_1^{(1)} = z_4^{(1)}\right)$$

So: $\boxed{\alpha_{12}^{(2)} = \alpha_{42}^{(1)} + \alpha_{46}^{(2)}}$ It's same to have: $\boxed{\alpha_{13}^{(2)} = \alpha_{43}^{(1)} + \alpha_{45}^{(1)}}$

<u>CONCLUSION</u> $\boxed{z_1^{(2)} = z_4^{(2)}}$

2 Question 2

If all the nodes in a model have the same characteristics, the model will not be discriminatory and will have poor classification accuracy. This is because all the nodes will have the same representation, which will prevent the model from distinguishing between different classes. This can be seen in question 1, where the representation does not change recursively.

3 Question 3

$$G_1 = \begin{bmatrix} 2.2 & -0.6 & 1.4 \\ 0.2 & 1.8 & 1.5 \\ 0.5 & 1.1 & -1.0 \end{bmatrix}, G_2 = \begin{bmatrix} 0.7 & 0.1 & 1.3 \\ 1.2 & -0.9 & 0.3 \\ 2.2 & 0.9 & 1.2 \\ -0.7 & 1.8 & 1.5 \end{bmatrix}, G_3 = \begin{bmatrix} -0.4 & 1.8 & 0.1 \\ 2.2 & -0.6 & 1.5 \end{bmatrix}$$

For the sum function :

- $Z_{G_1} = \begin{bmatrix} 2.9 & 2.3 & 1.9 \end{bmatrix}$
- $Z_{G_2} = \begin{bmatrix} 3.4 & 1.9 & 4.3 \end{bmatrix}$
- $Z_{G_3} = \begin{bmatrix} 1.8 & 1.2 & 1.6 \end{bmatrix}$

For the mean function :

- $Z_{G_1} \approx \begin{bmatrix} 0.97 & 0.77 & 0.63 \end{bmatrix}$
- $Z_{G_2} \approx \begin{bmatrix} 0.85 & 0.48 & 1.08 \end{bmatrix}$
- $Z_{G_3} \approx \begin{bmatrix} 0.9 & 0.6 & 0.8 \end{bmatrix}$

For the max function :
$Z_{G_1} = Z_{G_2} = Z_{G_3} = \begin{bmatrix} 2.2 & 1.8 & 1.5 \end{bmatrix}$

Sum is the function that is best for having the largest embedding. Indeed, the more disparate the values are, the better the prediction bass will be.

4 Question 4

Let C_n be a cycle graph, $G_1 = C_4$ and $G_2 = C_8$.

$$\tilde{A}_{G_1} = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}, \tilde{A}_{G_2} = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}$$

So,

$$Z_{G_1} = \text{READOUT}(\tilde{A}\ \text{ReLU}(\begin{bmatrix} 3 \\ 3 \\ 3 \\ 3 \end{bmatrix} W^{(1)})W^{(2)}) = \text{READOUT}(\begin{bmatrix} 9 \\ 9 \\ 9 \\ 9 \end{bmatrix} W^{(1)}W^{(2)}) = 36 * W^{(1)}W^{(2)}$$

and

$$Z_{G_2} = \text{READOUT}(\tilde{A}\ \text{ReLU}(\begin{bmatrix} 3 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \\ 3 \end{bmatrix} W^{(1)})W^{(2)}) = \text{READOUT}(\begin{bmatrix} 9 \\ 9 \\ 9 \\ 9 \\ 9 \\ 9 \\ 9 \\ 9 \end{bmatrix} W^{(1)}W^{(2)}) = 72 * W^{(1)}W^{(2)}$$

We conclude that $Z_{G_2} = 2 * Z_{G_1}$