Effect of Depth on Expressiveness

For this sub-question, our update rule is:

$$h_v^{k+1} = h_v^k + \sum_{i \in \mathcal{N}_v} h_i^k$$

where $\mathcal{N}_v$ is the neighbourhood of node v, and k is the layer number. I will just use a recurrence instead of drawing graphs as I think that is much simpler. I will just use the number for the certain node.

Layer $k = 0$:

Does not work, because that means no propagation and these nodes have the same initial feature vector = [1].

Layer $k = 1$:

Also does not work, because these nodes have the same one-hop neighbourhood, which is the node 5.

Layer $k = 2$:

Will also not work, because they have the same 2-hop neighbourhood (nodes 5, 4, and 6), but I will show this case as an example. We need to compute $h_T^{(2)}$ for both graphs, i.e.,

$$h_T^{(2)} = h_T^{(1)} + \sum_{i \in N_T} h_i^{(1)}$$

For the Left Graph:

$$\begin{aligned}
h_T^{(2)} &= h_T^{(1)} + \sum_{i \in N_T} h_i^{(1)} \\
&= (h_T^{(0)} + h_5^{(0)}) + h_5^{(1)} \\
&= [2] + (h_5^{(0)} + h_4^{(0)} + h_T^{(0)} + h_6^{(0)}) \\
&= [6]
\end{aligned}$$

This will be the same for the Right Graph.

Layer $k = 3$:

Will work. We need to compute $h_T^{(3)}$ for both graphs, i.e.,

$$h_T^{(3)} = h_T^{(2)} + h_5^{(2)}$$

For the Left Graph:

$$\begin{aligned}
h_T^{(3)} &= h_T^{(2)} + h_5^{(2)} \\
&= [6] + (h_5^{(1)} + h_4^{(1)} + h_T^{(1)} + h_6^{(1)}) \\
&= [6] + (h_5^{(0)} + h_4^{(0)} + h_T^{(0)} + h_6^{(0)}) \\
&\quad + (h_4^{(0)} + h_5^{(0)} + h_3^{(0)}) + (h_T^{(0)} + h_5^{(0)}) \\
&\quad + (h_5^{(0)} + h_6^{(0)} + h_7^{(0)}) \\
&= [18]
\end{aligned}$$

For the Right Graph:

$$\begin{aligned}
h_T^{(3)} &= h_T^{(2)} + h_5^{(2)} \\
&= [6] + (h_5^{(1)} + h_4^{(1)} + h_T^{(1)} + h_6^{(1)}) \\
&= [6] + (h_5^{(0)} + h_4^{(0)} + h_T^{(0)} + h_6^{(0)}) \\
&\quad + (h_4^{(0)} + h_5^{(0)} + h_3^{(0)}) + (h_T^{(0)} + h_5^{(0)}) \\
&\quad + (h_A^{(0)} + h_6^{(0)} + h_7^0 + h_8^0) \\
&= [19]
\end{aligned}$$

The only difference was Node 6 having vs. not having a connection to Node 8.