1. COMP5214 Assignment Part 2 Report
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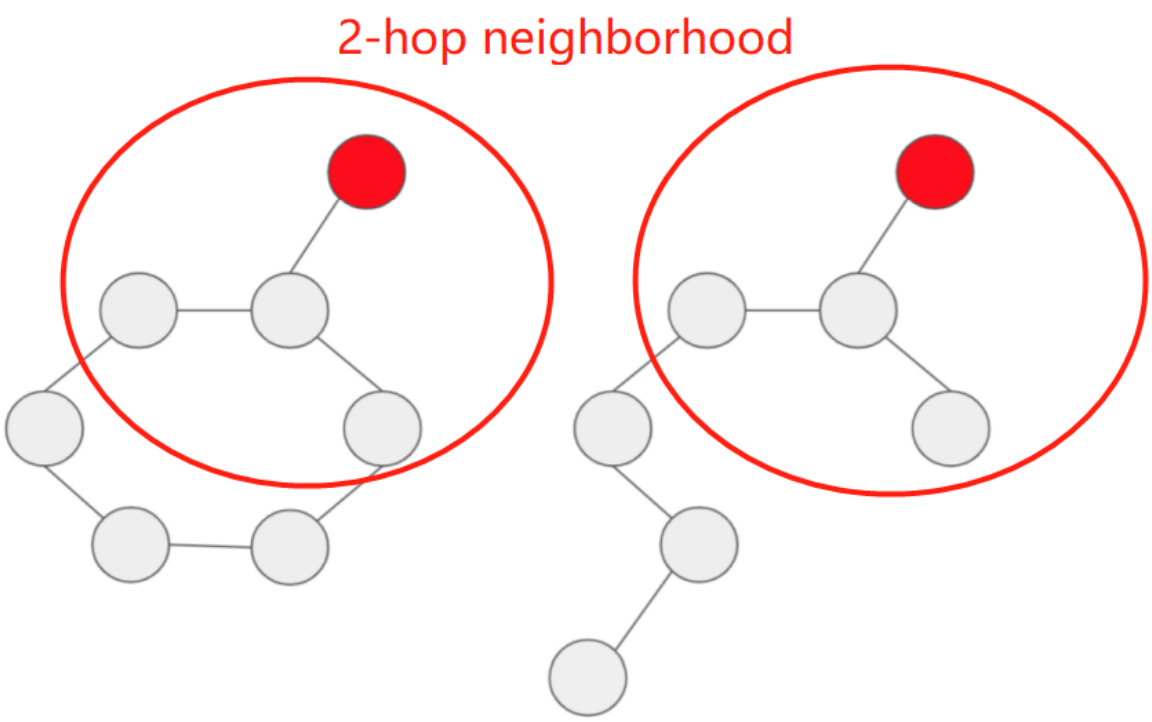
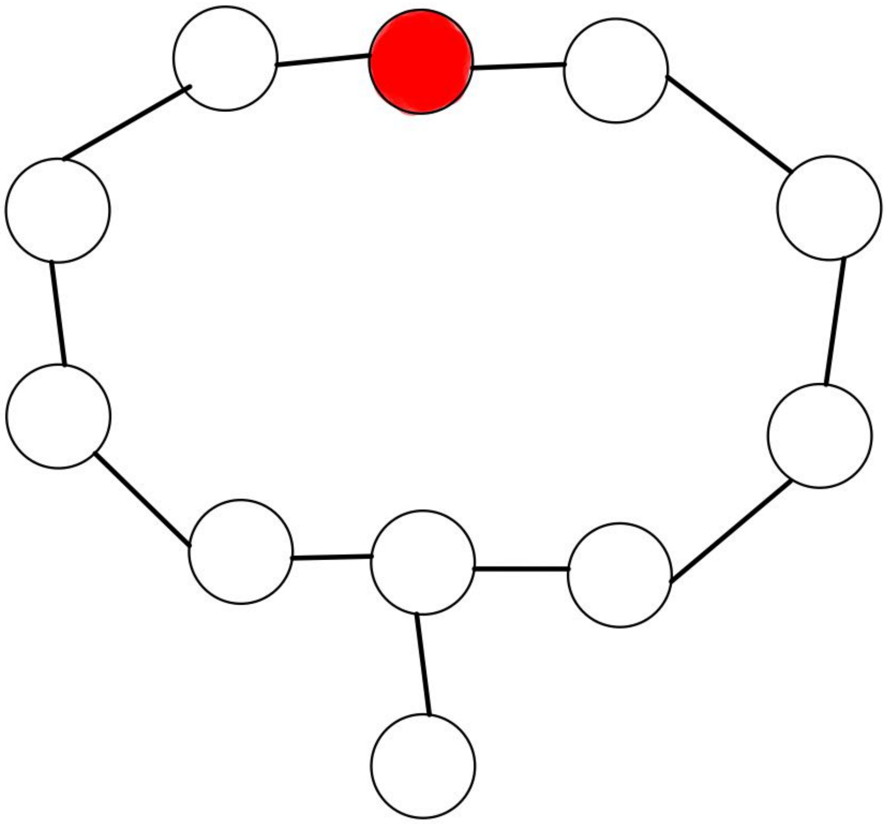
2.1 Effect of Depth on Expressiveness

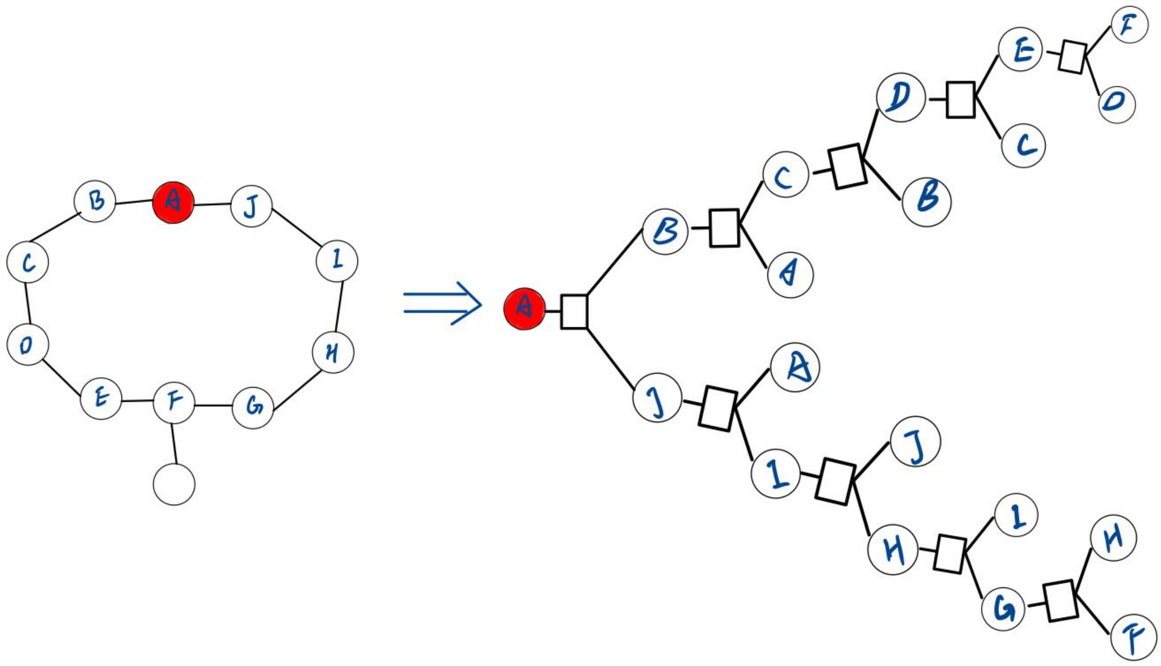
1. From the two graphs we can see that the 1-hop neighborhood of the two red nodes are identical, the 2-hop neighborhood of the red nodes are also identical. Only when we consider up to the 3-hop neighborhood will we obtain a structural difference. **Therefore a minimum of 3 message passing is needed to distinguish the two red nodes.**



2. An example of a graph where the red node should be classified as True is shown as follows:



To perfectly perform this classification task, it's obvious that we need to include the 10 nodes in the induced cyclic subgraph in our network. Therefore, we need at least 5 layers to include all 10 nodes. As shown in the following graph, if we only have the first 4 layers, the graph cannot include the information about node F, and hence it can either represent a length 10 cycle or just simply 9 nodes that do not form a cycle, which means we can't guarantee to classify node A as `True`.



2.2 Relation to Random Walk

1. The transition matrix P can be expressed using the adjacency matrix A and degree matrix D as:

$$P = (AD^{-1})^T = (D^{-1})^T A^T$$

As D is a diagonal matrix and A is a symmetric matrix, so

$$A^T = A, D^T = D, (D^{-1})^T = D^{-1}$$

So P can also be expressed as

$$P = D^{-1}A$$

2. In this case, the transistion matrix P' is:

$$P' = \frac{1}{2}P + \frac{1}{2}I = \frac{1}{2}(I + D^{-1}A)$$

2.3 Learning BFS with GNN

1.

$$h_v^{(t)} = min(1, h_v^{(t-1)} + \sum_{u \epsilon N(v)} h_u)$$

2. Message function can be an identity function:

$$MSG(v) = v$$

Aggregation function can be a clamped sum:

$$AGG(v) = min(1, \sum_{u \epsilon N(v)} u)$$