Foundations of Graph Neural Networks
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Problem Sheet 1

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Question 1

Consider *basic sum-plus GNNs with trReLU*, which updates the embedding as

$$\mathbf{x}_v^{(\ell)} ::= trReLU\left(\mathbf{A}^{(\ell)}\mathbf{x}_v^{(\ell-1)} + \mathbf{C}^{(\ell)}(\Sigma_{u\in\mathcal{N}_G(v)}\mathbf{x}_u^{(\ell-1)}) + \mathbf{b}^{(\ell)}\right);$$

recall that $trReLU(x) = \{0 \text{ if } x < 0;\ x \text{ if } 0 < x < 1;\ 1 \text{ otherwise}\}$. Write such a GNN with input dimension 2 that realises the function 'there is a node with the first component equal to 1 at distance at most 2 from the given node'. For simplicity, you may assume that all input graphs have only 1-0 labels (i.e., are equivalent to logical structures with two unary predicates).

Question 2

Describe (briefly) a run of the WL algorithm on a linear (undirected) graph of length n, for every $n > 0$, where all nodes are labelled the same. How many iterations does the colouring take to stabilise (in n)? Is it possible to find a graph with n nodes that take more iterations for WL to stabilise?

Question 3

Recall that the update rule of the WL-test is the following 'two nodes v, v' are assigned the same colour iff they have same colour and same multisets of colours of neighbours'. Consider the modification of the WL, call *set-WL*, that does the same, except that they take into account sets rather than multisets (i.e., ignore multiplicites). Describe the sub-class of GNNs with the same distinguishing power as set-WL.

Question 4

Consider the distinguishing power of graph embeddings, which is defined in the same way as the distinguishing power of node embeddings, except that graphs are considered instead of graph-node pairs. Observe that the final multiset of the WL test realises a node embeddings, and the same holds for the 'folklore' WL test. Compare the distinguishability power of these two formalisms.

Question 5

Recall the simplified version of GCNs we considered in the lectures, that updates as

$$\mathbf{x}_v^{(\ell)} ::= ReLU\left(\mathbf{A}^{(\ell)}(\text{avg}_{u \in \mathcal{N}_G(v) \cup \{v\}} \mathbf{x}_u^{(\ell-1)})\right).$$

Show that its distinguishing power is strictly less than the stable colouring of the WL test.

Question 6

Consider the sub-class of AC-GNNs that has all intermediate dimensions equal 1 (i.e., $d_1 = \cdots = d_{L-1} = 1$ in our notation). Demonstrate that this class has the same uniform expressive power as the class of all AC-GNNs.