Foundations of Graph Neural Networks
PhD Open, 21-23 May 2025
Problem Sheet 2

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Question 1

Translate the following GML formula (in FOL syntax) to an AC-GNN:

$$A(x) \wedge \exists^3 y\, E(x, y).$$

(as usual, $\exists^3 y \phi$ quantifier means 'there exists exactly 3 y's such that ϕ').

Question 2

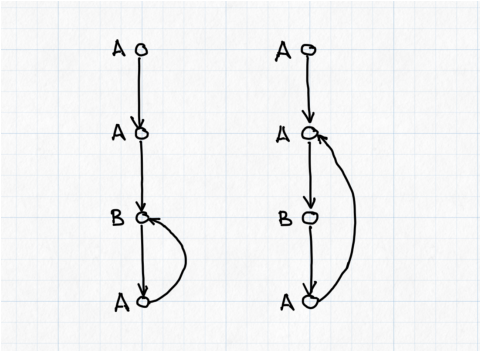
Translate the following unary FOL formula to an AC-GNN:

$$A(x) \wedge \exists^3 y\, B(y).$$

If you think it is not possible, translate it to a more general class of GNNs.

Question 3

We defined bisimulation for undirected graphs, but the definition can be adapted to directed graphs in a direct way: we just consider successors instead of neighbours. Does the following graphs have a bisimulation? If no, explain why, if yes, give an example. Are the two top nodes bisimilar? If yes, demonstrate this, if no, give a Graded Modal Logic formula (in FOL syntax) that separates these nodes.



Question 4

Suggest a generalisation of the WL stable colouring algorithm (i.e., the node-level WL) so that it can distinguish nodes on a triangle from nodes not on a triangle (i.e., for every two nodes in every two graphs such that one is on a triangle and another is not the stable colouring is different).

Question 5

Let uniform approximation power be defined as expected: a class $\mathcal{C}_2$ of node embeddings has as strong uniform approximation power as a class $\mathcal{C}_1$ if for every $\epsilon > 0$ and every $\xi_1 \in \mathcal{C}_1$ there is $\xi_2^\epsilon \in \mathcal{C}_2$ such that the (absolute value of the) difference between ξ_1 and ξ_2^ϵ is less that ϵ for every node in every graph (of any size).

Demonstrate that AC-GNNs with update

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

do not have stronger approximation power than

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

Question 6

Consider the GNN with the update function

$$\mathbf{x}_v^{(1)} ::= ReLU\left(\mathbf{A}^{(1)}\mathbf{x}_v^{(0)} + \mathbf{C}^{(1)}(\max_{u\in\mathcal{N}_G(v)}\mathbf{x}_u^{(0)}) + \mathbf{b}^{(1)}\right)$$

where

$$\mathbf{A}^{(1)} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \qquad \mathbf{C}^{(1)} = \begin{pmatrix} 4 & 3 \\ 2 & 1 \end{pmatrix} \qquad \mathbf{b}^{(1)} = \begin{pmatrix} -5 \\ 1 \end{pmatrix},$$

and with the output function being the 0.5-threshold function of the first element. Write a tree-UCQ that is equivalent to this GNN or explain why it does not exist.