The Correspondence Between Bounded Graph Neural Networks and Fragments of First-Order Logic (Extended Abstract)

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Abstract

Recent years have witnessed a surge of interest in characterising the expressive power of machine learning models with logical languages — the so-called logical expressive power. Notably, in the domain of graph representation learning, prior work has characterised the logical expressiveness of GNNs that is expressible in first order logic (FO). In this paper, we remove the requirement of FO expressibility and propose GNN architectures that correspond precisely to prominent fragments of FO, including various modal logics as well as more expressive two-variable fragments. *Extended version:* https://arxiv.org/abs/2505.08021

1 Introduction

Expressive power is a recurring theme in Knowledge Representation and Reasoning, studied through the lenses of logics, logic programming, query languages, and other symbolic formalisms. Recent years have witnessed a surge of interest in characterising the expressive power of machine learning models with logical languages — the so-called logical expressive power. Notably, in the domain of graph representation learning, the flagship paper by Barceló et al. (2020) started a line of work on the logical expressive power of graph neural networks (GNNs). GNNs are machine learning models that operate natively on graph-structured data, handling variable graph sizes while respecting permutation invariance. They have been applied in recommendation systems, molecular property prediction, traffic navigation, computer vision, and reasoning over knowledge graphs, among others (Zhou et al., 2020). Consequently, these expressive power results shed light on the power and limitations of different GNN architectures and can guide applications and implementations in real-world scenarios.

More specifically, Barceló et al. (2020) has estabilshed the following connections between logic and GNNs. Graded modal logic ($\mathcal{GML}$) formulas, a.k.a. concepts in the description logic $\mathcal{ALCQ}$, can be captured by GNNs without readout functions, just as FO formulas with two variables and counting quantifiers (C^2) can be realised by GNNs with readouts. This relationship is, however, asymmetric: while any $\mathcal{GML}$ classifier can be expressed by an AC GNN, the converse requires an assumption of FO expressibility. The expressiveness of GNNs goes beyond first-order logic (FO) since aggregation can only be captured using extensions such as Presburger quantifiers (Benedikt et al., 2024). The conditions ensuring FO expressibility of a GNN remain largely unexplored. To fill this gap, we study the exact correspondences between special families of GNNs, called bounded GNNs, and standard fragments of FO.

Contributions We introduce bounded GNNs with k-bounded aggregation, where multiplicities greater than k in a multiset are capped at k. If k= 1, the multiplicities do not matter, and we speak of set-based aggregation. As we show, families of bounded GNNs share the exactly same logical expressiveness as modal and two-variable FO fragments as depicted in Figure 1.

We first establish that AC GNNs with set-based aggregation ($\mathrm{GNN}_\mathsf{s}^\mathsf{AC}$) correspond to basic modal logic ($\mathcal{ML}$) and thus to concepts in the description logic $\mathcal{ALC}$. This extends to GNNs using bounded aggregation ($\mathrm{GNN}_\mathsf{b}^\mathsf{AC}$), which correspond to graded modal logic ($\mathcal{GML}$), that is, concepts of $\mathcal{ALCQ}$. Readouts enable global quantification: GNNs with set-based aggregation and readout ($\mathrm{GNN}_\mathsf{s}^\mathsf{ACR}$) capture modal logic with the global modality ($\mathcal{ML}(\mathsf{E})$), which corresponds to $\mathcal{ALC}$ with the universal role, while those with bounded aggregation and readout ($\mathrm{GNN}_\mathsf{b}^\mathsf{ACR}$) match graded modal logic with counting ($\mathcal{GMLC}$), which corresponds to $\mathcal{ALCQ}$ equipped with the universal role. While bounded readouts enable global quantification, they cannot express certain first-order properties like “nodes with exactly k non-neighbours”. To overcome this limitation, we introduce $\mathrm{GNN}_\mathsf{b}^\mathsf{AC+}$: a family of bounded GNNs augmented with an aggregation function over non-neighbours. We prove that $\mathrm{GNN}_\mathsf{b}^\mathsf{AC+}$ captures C^2 (the two-variable fragment of FO with counting), while its set-based variant $\mathrm{GNN}_\mathsf{s}^\mathsf{AC+}$ corresponds to the two-variable FO fragment FO^2.

2 Bounded GNN and FO Fragments

We consider *finite, undirected, simple, and binary-vector-node-labelled graphs*. A *node classifier* is a function mapping pointed graphs (graph-vertex pairs) to true or false. If each classifier in a family $\mathcal{F}$ of classifiers has an equivalent one in a family $\mathcal{F}'$ of classifiers, then we write $\mathcal{F} \leq \mathcal{F}'$. If $\mathcal{F} \leq \mathcal{F}'$ and $\mathcal{F}' \leq \mathcal{F}$, then we write $\mathcal{F} \equiv \mathcal{F}'$.

Bounded GNN Classifiers We consider standard GNNs with *aggregate-combine* (AC) and *aggregate-combine-*

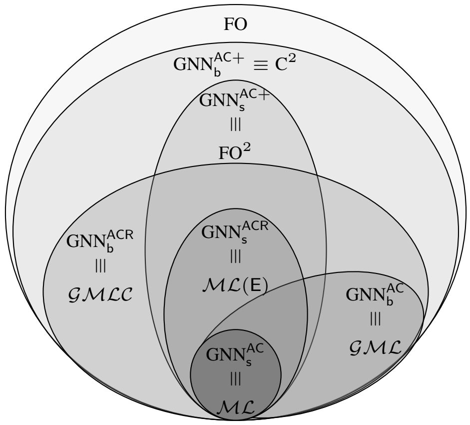

Figure 1: The landscape of our expressive power results

readout (ACR) layers (Barceló et al., 2020), and propose also *extended aggregate-combine* (AC+) layers equipped with one aggregation over neighbours and another over non-neighbours.

Next, we introduce *bounded GNNs*, which generalise max-sum GNNs (Tena Cucala et al., 2023). Bounded GNNs restrict aggregation and readout by requiring the existence of a bound k such that all multiplicities $k' > k$ in an input multiset are replaced by k. Thus, multiplicities greater than k do not affect the output of a k-bounded function. Set-based functions ignore multiplicities altogether.

Logic Classifiers We consider modal logics without global modalities ($\mathcal{ML}$ and $\mathcal{GML}$), modal logics with global modalities ($\mathcal{ML}(\mathsf{E})$ and $\mathcal{GMLC}$), and 2-variable fragments (FO^2 and C^2). Formulas of the *graded modal logic of counting* ($\mathcal{GMLC}$) are defined as follows:

$$\varphi := p \mid \neg\varphi \mid \varphi \land \varphi \mid \Diamond_k \varphi \mid \exists_k \varphi.$$

The formula $\Diamond_k \varphi$ uses a counting modality to express that at least k accessible worlds satisfy φ, while $\exists_k \varphi$ uses a global modality to state that at least k worlds in total satisfy φ. Graded modal logic ($\mathcal{GML}$) is obtained from $\mathcal{GMLC}$ by disallowing counting modalities. Modal logic with the global modality ($\mathcal{ML}(\mathsf{E})$) is obtained from $\mathcal{GMLC}$ by restricting both counting and graded modalities to $k = 1$. Basic modal logic ($\mathcal{ML}$) further restricts $\mathcal{ML}(\mathsf{E})$ by disallowing counting modalities entirely. We also consider the two-variable fragment of first-order logic with counting quantifiers (C^2), where $\exists_k$ denotes counting quantifiers. Note that we use the symbols $\exists_k$ for both counting quantifiers and counting modalities. The classical two-variable fragment (FO^2) is obtained from C^2 by restricting counting quantifiers to $k = 1$.

3 Proof Recipe

The proof of each correspondence of the form $L \equiv \text{GNN}_Y^X$ follows roughly the same 3-step proof recipe:

1. First, we show that $L \leq \text{GNN}_Y^X$. The idea is to simulate truth value derivation inductively by linear combinations, where each component of the vector label keeps track of the truth value of a subformula.
2. Second, we introduce game equivalence $\sim$ over pointed graphs and show that $\sim$-invariant classes of models can be represented as a finite disjunction of the characteristic formulas of $\mathcal{L}$ (Otto, 2019; Libkin, 2004).
3. Finally we show that GNNs in GNN_Y^X are $\sim$-invariant. This in turn shows that $\text{GNN}_Y^X \leq L$, completing the proof.

4 Conclusion

We have introduced families of bounded GNNs, whose expressive power corresponds exactly to well-known modal logics and 2-variable first-order logics. The results are summarised in Figure 1. In particular, we have showed that aggregate-combine GNNs with bounded aggregation have the same expressive power as the graded modal logic, the aggregate-combine-readout GNNs with bounded aggregation have the same expressive power as the graded modal logic with global modalities, and the extended aggregate-combine GNNs with bounded aggregation have the same expressive power as the two-variable fragment of FO with counting quantifiers. The correspondence between FO-expressibility and bounding aggregation (and readout) occurs as an interesting phenomenon to study. In particular, we find it interesting to determine for which classes of GNNs classifiers, FO-expressibility is equivalent to expressibility by bounded GNNs. For future work, we consider establishing tight bounds on the size of logical formulas capturing GNNs and extracting logical formulas from GNNs in practice.

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