Logical Characterizations of Recurrent Graph Neural Networks with Reals and Floats

NEURAL INFORMATION PROCESSING SYSTEMS

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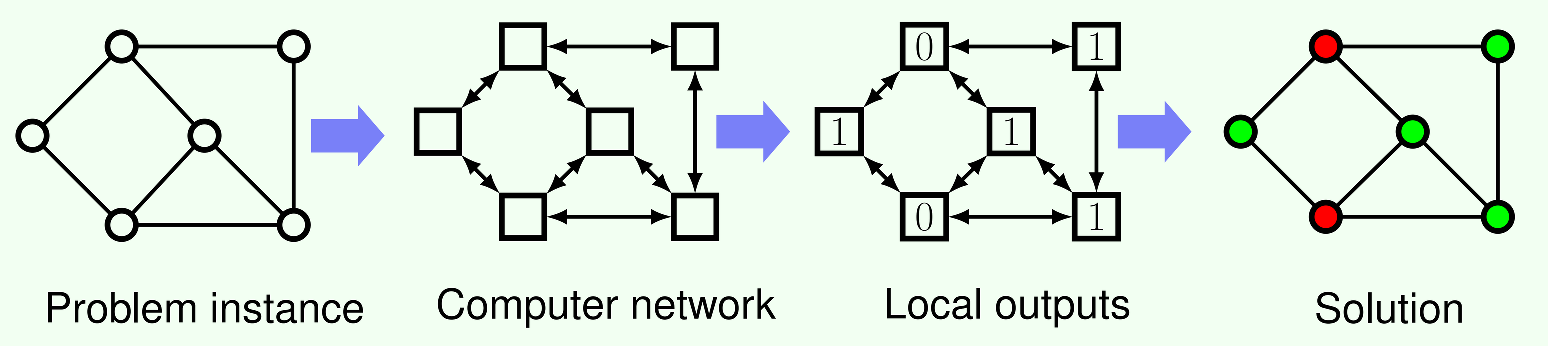
Overview

We give the first logical characterization of recurrent graph neural networks (GNNs) without restriction to a background logic. We cover scenarios with both real numbers and floating-point numbers, and analyze where they coincide.

Related work: Pioneering characterizations of constant-iteration graph neural networks were given in [1] and [2], and a characterization of recurrent graph neural networks was given in [3] w.r.t. a background logic.

Recurrent GNNs with reals and floats

A **recurrent graph neural network** ($\mathrm{GNN}[\mathbb{R}]$) receives a (directed, labeled) graph as input and gives a Boolean classification for each node in the graph.



A $\mathrm{GNN}[\mathbb{R}]$ is a tuple $(\boldsymbol{\pi}, \mathbf{AGG}, \mathbf{COM}, \boldsymbol{F})$, where

- an initialization function $\boldsymbol{\pi}$ maps each set of node label symbols to $\mathbb{R}^d$,
- $\mathbf{AGG}$: multisets$(\mathbb{R}^d) \to \mathbb{R}^d$ is an aggregation function,
- $\mathbf{COM}$: $\mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a combination function,
- $\boldsymbol{F} \subseteq \mathbb{R}^d$ is a set of accepting vectors.

The **feature vector** $\boldsymbol{x}_v^t \in \mathbb{R}^d$ of node v in round $t \in \mathbb{N}$ is computed as follows:

$\boldsymbol{x}_v^0 = \boldsymbol{\pi}(L)$, where L is the set of node labels of v.

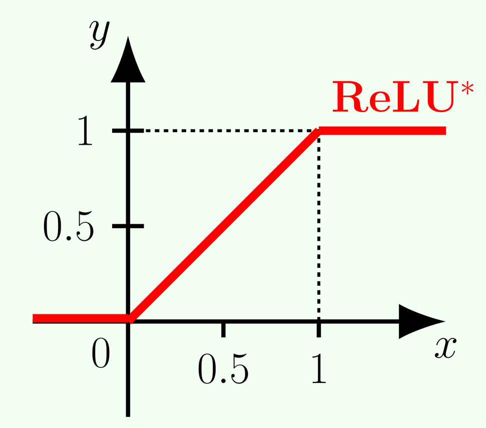
$$\boldsymbol{x}_v^{t+1} = \mathbf{COM}(\boldsymbol{x}_v^t, \mathbf{AGG}(\{\{\, \boldsymbol{x}_u^t \mid u \text{ is a neighbour of } v \,\}\})).$$

The classification for a node is "yes" if during the computation a feature vector of the node is in $\boldsymbol{F}$ and otherwise "no".

A **floating-point GNN** ($\mathrm{GNN}[\mathrm{F}]$) is the same as a $\mathrm{GNN}[\mathbb{R}]$, but it uses floating-point numbers instead of real numbers.

★ A floating-point GNN cannot distinguish arbitrarily large multisets because its calculations are finite!

R-simple GNNs



- Matrices $\boldsymbol{A}, \boldsymbol{C} \in \mathbb{R}^{d \times d}$
- A bias vector $\boldsymbol{b} \in \mathbb{R}^d$
- Truncated ReLU: $\mathbf{ReLU}^*(x) = \min(\max(0, x), 1)$

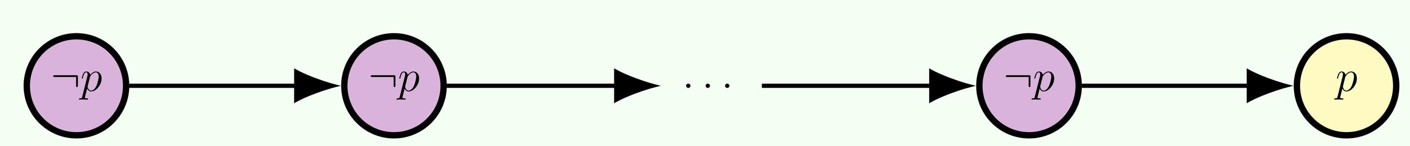
A new feature vector is computed as follows:

$$\boldsymbol{x}_v^{t+1} = \mathbf{ReLU}^*(\boldsymbol{x}_v^t \cdot \boldsymbol{C} + \left(\sum \boldsymbol{x}_u^t\right) \cdot \boldsymbol{A} + \boldsymbol{b}).$$

Example: reachability

A node label symbol p is **reachable** from a node v if there is a path from v to a node where p appears.

★ Reachability can be expressed even with an R-simple recurrent GNN but not with any constant-iteration GNN!



Logics GMSC and ω-GML

Graded modal substitution calculus (GMSC) is a logic consisting of programs. Each program consists of two lists of the below form:

$$\begin{array}{ll} X_1(0) :- p \land q & X_1 :- p \land X_3 \land \Diamond_{\geq 8} X_1 \\ X_2(0) :- q & X_2 :- \neg q \land \neg \Diamond_{\geq 2} X_1 \\ X_3(0) :- p & X_3 :- X_2 \land \Diamond_{\geq 3} \neg X_3 \end{array}$$

Base rules: $\varphi ::= p \mid \neg\varphi \mid \varphi \land \varphi \mid \Diamond_{\geq k}\varphi$

Induction rules: $\varphi ::= p \mid X \mid \neg\varphi \mid \varphi \land \varphi \mid \Diamond_{\geq k}\varphi$

A formula $\Diamond_{\geq k}\varphi$ states that φ is true in at least k neighbours.

We define iteration formulae X^t of variables X as follows.

- X^0 is the base rule of X,
- X^{t+1} is the induction rule of X where each Y is replaced with Y^t.

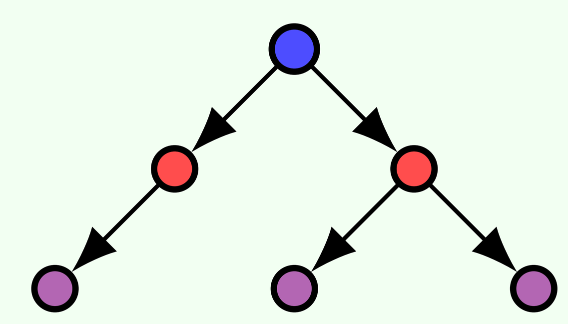
Each program also includes a set $\mathcal{A}$ of accepting variables. A graph node v is accepted if for any $X \in \mathcal{A}$ the iteration formula X^t is true in v for some $t \in \mathbb{N}$.

The **logic** ω-$\mathbf{GML}$ consists of countable disjunctions $\bigvee_{\varphi \in S} \varphi$ where each $\varphi \in S$ is a finite formula using the same grammar as the base rules above.

Example: centre-point property

A node v has the **centre-point property**, if every outgoing path starting from v leads to a dead-end in the *same number of steps*.

★ Expressible in GMSC but not in monadic second-order logic!



Program:

$X(0) :- \Box\bot \quad X :- \Box X \land \Diamond X$

Run of the program:

- $X^0 := \Box\bot$
- $X^1 := \Box X^0 \land \Diamond X^0$
- $X^2 := \Box X^1 \land \Diamond X^1$ (accepting)

...

Logical characterizations

Theorem 1

Same expressive power:

$$\mathrm{GNN}[\mathrm{F}]\text{s} \equiv \text{R-simple } \mathrm{GNN}[\mathrm{F}]\text{s} \equiv \mathrm{GMSC}$$

Theorem 2

Same expressive power:

$$\mathrm{GNN}[\mathbb{R}]\text{s} \equiv \omega\text{-}\mathrm{GML}$$

Theorem 3

In restriction to monadic second-order logic:

$$\mathrm{GMSC} \equiv \mathrm{GNN}[\mathrm{F}]\text{s} \equiv \text{R-simple } \mathrm{GNN}[\mathrm{F}]\text{s} \equiv \mathrm{GNN}[\mathbb{R}]\text{s} \equiv \omega\text{-}\mathrm{GML}$$

★ We also obtain characterizations for models of distributed computing.

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